RESEARCH CENTER

FIELD
Applied Mathematics, Computation and Simulation

Activity Report 2012

Section New Results

Edition: 2013-04-24

STOCHASTIC METHODS AND MODELS

BACCHUS Team

6. New Results

6.1. Residual distribution schemes

Participants: Rémi Abgrall [Corresponding member], Mario Ricchiuto, Dante De Santis, Algiane Froehly, Cécile Dobrzynski.

We have understood how to approximate the advection diffusion problem in the context of residual distribution schemes. A third order version for scalar problem has been written. It is uniformly accurate, from pure viscous to pure convection problems. This scheme has been generalised to the laminar Navier Stokes equations. An extension to the turbulent case (with Spalart Allmaras model) has also been written and tested. 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 in [37] and has been the topic of [20].

A. Froehly has submitted her PhD thesis about the extension of the residual distribution scheme using isogeometric analysis. In particular, we have foccussed on mesh adaption, including at the boundary. A paper is being written to summarized the work.

6.2. Curved meshes

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

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 streched, 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 isogeometrical analysis, we have been able to construct a prototype computing curved meshes (in 2D and 3D), while keeping the structure of the mesh.

6.3. Hypoelastic models

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

In collaboration with CEA (P.H. maire), we have developped and tested a new finite volume like algorithm able to simulate hypoelastic-plastics problems on unstructured meshes. This has been published in [47].

6.4. Penalisation methods using unstructured meshes

Participants: Rémi Abgrall, Cécile Dobrzynski, Héloïse Beaugendre [Corresponding member].

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.

6.5. Unsteady problem

Participants: Rémi Abgrall, Mario Ricchiuto [Corresponding member], Luca Arpaia, Jan Klosa.

Using a reinterpretation of the explicit RD scheme we had designed 2 years ago, we have been able to construct a third order accurate RD scheme in one space dimension. The extension to multidimensional problems is pending.

We have studied the extention of second order unsteady RD scheme to the ALE formulation. New version of the explsiict unsteady RD schemes have been studied.

6.6. Lagrangian hydrodynamics

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

F. Vilar has achieved his thesis on the approximation of the Euler equations written in pure Lagrangian coordinates. He has foccussed on third order accuracy in time and space, usning a Discontinuous Galerkin formulation. The solution is approximated localy by quadratic polynomials. The boundary of elements are approximated by Bezier curves. He has managed to achieve an approximation consistant with the geometric Cosnervation Law. Many test cases have been computed, showing both a dramatic improvement of the accuracy and the robustness of the method with respect to its second order counterpart.

6.7. Boundary Layer Enrichment

Participants: Rémi Abgrall [Corresponding member], Arnaud Krust.

Arnaud Krust has finished his PhD thesis on boundary layer enrichment. We developed a numerical framework well suited for advection- diffusion problems when the advection part is dominant. In that case, given Dirichlet type boundary condition, it is well known that a boundary layer develops. In order to resolve correctly this layer, standard methods consist in increasing the mesh resolution and possibly increasing the formal accuracy of the numerical method. In this work, we follow another path: we do not seek to increase the formal accuracy of the scheme but, by a careful choice of finite element, to lower the mesh resolution in the layer. Indeed the finite element representation we choose is locally the sum of a standard one plus an enrichment. This work proposes such a method and with several numerical examples, we show the potential of this approach. In particular we show that the method is not very sensitive to the choice of the enrichment functions. The best choice of enrichment are shown to be obtained by an iterative mechanisms which bears some common features with mesh refinement.

6.8. Uncertainty Quantification

Participants: Rémi Abgrall, Pietro Congedo [Corresponding member], Gianluca Geraci, Mario Ricchiuto.

We developed two research lines: the first one focused on the computation of high-order statistics, the second one is related to the formulation of a global framework in the coupled physical/stochastic space. First, 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. Secondly, 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. 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.

Application of some of these techniques to tsunami simulations have been conducted.

6.9. Robust Design Optimization

Participant: Pietro Congedo [Corresponding member].

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 a realistic problem of robust optimization of a multi-component airfoil. In this work, we present an extension of this method for treating epistemic uncertainty in the context of interval analysis approach. This method consists in a multi-scale strategy based on simplex space representation in order to minimize global cost of mixed epistemic-aleatory uncertainty quantification. This reduction is obtained i) by a coupled stopping criterion, ii) by an adaptive polynomial interpolation that could be used as a response surface in order to accelerate optimization convergence, iii) by a simultaneous min/max optimization sharing the same interpolating polynomials at each iteration [.....].

6.10. Multiphase flows

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

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. 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.

Another topic covered by Bacchus is about the numerical approximation of non conservative systems. One very interetsing 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.

6.11. Parallel remeshing

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

Our studies regarding parallel remeshing use a dedicated software framework called `PaMPA` (for "*Parallel Mesh Partitioning and Adaptation*"; see Section 5.6 for more details about it). This software, whose development started three years ago, allow one to describe distributed meshes in an abstract way.

The work carried out this year concerns the definition of suitable algorithms for performing remeshing in parallel, using a sequential remesher. To do so, areas suitable for remeshing (that is, cells for which a quality measurement routine indicates that remeshing is necessary) are grouped into boules of a size small enough to be handled by a sequential remesher, and big enough so that this remesher can do useful work on each of the boules. The core of the work is therefore to identify and build relevant boules, to send them to as many processors as possible, to remesh them sequentially, and to merge the remeshed boules into what remains of the original mesh. Then, areas that have not already been processed (e.g. areas at the interface of two or more boules) can be considered in turn, until all relevant cells have been considered. The structure and operations of PaMPA have been presented in [29].

Several algorithms have been experimented in order to build the boules. The one which proved the most efficient is based on a partitioning of an induced subgraph of the element graph, using the PT-Scotch tool which is already used for mesh redistribution. PaMPA has been interfaced with MMG3D in order to create a demonstrator for remeshing in parallel tetraedral meshes. A set of tetrahedral cube-shaped test meshes has been created, with a metric that coerces remeshing in the interior of the cubes. PaMPA was able to remesh a 12 million tetrahedral mesh into 18 million tetrahedra on 80 processors, yielding a quality equivalent to the one of the sequential remesher used alone. Scalability experiments on much larger test cases are in progress; yet, their quality will no longer be comparable to a sequential test case. This version of PaMPA will soon be released and made available to the community.

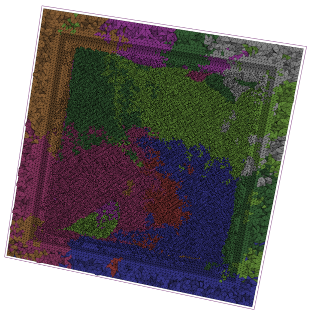


Figure 4. Cut of a 3D cube made of tetrahedra showing the effect of parallel remeshing by PaMPA.

6.12. Parallel graph remapping

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

Last year, a set of new algorithms for sequential remapping and mapping with fixed vertices has been devised. These algorithms had been intergrated in the Charm++ parallel environment, in the context of a collaboration with the Joint Laboratory for Petascale Computing (JLPC) between Inria and UIUC.

These algorithms have been integrated in version 6.0 of Scotch, which has been released in the beginning of December. This release also comprises new threaded formulations of the critical and most time-consuming algorithms used in graph partitioning, namely: graph coarsening and our diffusion-based method.

All the remapping algorithms that have been designed last year were meant to be easily parallelizable. The work of this year has been to derive and implement their parallel formulation. This is now the case, which completes this five year long work. These algorithms, which offer a quality similar to the one of the sequential algorithms, will be released in version 6.1 of Scotch.

6.13. Sparse matrix reordering for ILU solvers

Participants: Astrid Casadei, 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.

This year, we have set-up a software testbed for experimenting such methods. It comprises 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 are provided by the industrial partners of the PETALh project.

Our first experiments show that injecting information regarding off-diagonal terms can indeed improve convergence. However, many parameters have to be evaluated in a thorough experimentation plan. Since Scotch uses integer terms only, some scaling has to be performed, which imposes to determine how to scale the coefficients (type of scaling and range), whether to filter small values, etc. This work is in progress.

6.14. Subdomain decomposition

Participants: Astrid Casadei, François Pellegrini, Pierre Ramet [Corresponding member].

This work aims at finding subdomain decompositions that balance the sizes of off-diagonal contribution blocks.

In terms of graph partitioning, we have expressed this problem as a multi-constraint partitioning problem. In addition to bearing a weight that expresses the workload associated with its degrees of freedom, every graph vertex bears a second weight that holds the number of unknowns to which it is linked outside of its subdomain. Hence, in the nested dissection process, every time a separator is computed, this second weight is updated for each frontier vertex of the separated parts, before they are also recursively separated.

This year, we have set-up a software testbed for experimenting this approach. The Scotch sparse matrix ordering library has been modified so that graph vertices can bear multiple vertex weights. This required a slight change in the interfaces, but also modifications of the internal handling of graphs in many modules (nested dissection, graph coarsening, etc).

6.15. Development of a simulation code for rarefied gas flows

Participants: Luc Mieussens [Corresponding member], Florent Pruvost [IMB, engineer].

The simulation code CORBIS (rarefied gases in 2 space dimensions on structured meshes) has been entirely modified: 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.

6.16. Numerical methods for high altitude aerodynamics

Participants: Luc Mieussens [Corresponding member], N. Hérouard [CEA-CESTA, PhD].

In collaboration with CEA-CESTA, we have worked on the following subjects.

- A new method to generate locally refined velocity grids has been proposed. Very high performance improvement have been obtained (acceleration of the CPU time by a ratio around 30 for 3D computations). This work has been published in the proceedings of the 28th Symposium on rarefied Gas Dynamics, and is the subject of a paper submitted for publication.
- The second order Discontinuous Galerkin method has been studied for a one-dimensional problem of rarefied gases: we have shown that this method is clearly more accurate and faster than our finite volume method (which was used up to fourth order). This study will be developed in 2013 (numerical analysis and application to 2D problems).

6.17. Numerical methods for rarefied gas flows around moving obstacles

Participants: Luc Mieussens [Corresponding member], G. Dechristé [IMB, PhD].

We have presented one of the first numerical simulation of the Crookes radiometer. This phenomenon, due to the thermal creep flow, has been simulated with a Cartesian grid approach, with a cut-cell techniques that allow for an accurate treatment of solid boundaries. This work has been published in the proceedings of the 28th Symposium on rarefied Gas Dynamics.

6.18. Fast numerical methods for rarefied gases

Participants: Luc Mieussens [Corresponding member], Stéphane Brull [IMB], L. Forestier-Coste [IMB, Post Doc].

We have proposed a new method to discretize kinetic equations. It is basedd 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 rpesented in a paper submitted for publication). Two-dimensional extensions are under development.

6.19. Asymptotic Preserving schemes for the linear transport

Participant: Luc Mieussens [Corresponding member].

We have shown that the recent method “Unified Gas Kinetic Scheme”, proposed by K. Xu to simulated multiscale 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 presented in a paper submitted for publication.

CAD Team

6. New Results

6.1. Geometry Modeling and Processing

6.1.1. Relaxed lightweight assembly retrieval using vector space model

Participants: Kai-Mo Hu, Bin Wang, Jun-Hai Yong, Jean-Claude Paul.

Assembly searching technologies are important for the improvement of design reusability. However, existing methods require that assemblies possess high-level information, and thus cannot be applied in lightweight assemblies. In this paper, we propose a novel relaxed lightweight assembly retrieval approach based on a vector space model (VSM). By decomposing the assemblies represented in a watertight polygon mesh into bags of parts, and considering the queries as a vague specification of a set of parts, the resilient ranking strategy in VSM is successfully applied in the assembly retrieval. Furthermore, we take the scale-sensitive similarities between parts into the evaluation of matching values, and extend the original VSM to a relaxed matching framework. This framework allows users to input any fuzzy queries, is capable of measuring the results quantitatively, and performs well in retrieving assemblies with specified characteristics. To accelerate the online matching procedure, a typical parts based matching process, as well as a greedy strategy based matching algorithm is presented and integrated in the framework, which makes our system achieve interactive performance. We demonstrate the efficiency and effectiveness of our approach through various experiments on the prototype system. [19]

6.1.2. Calculating Jacobian coefficients of primitive constraints with respect to Euler parameters

Participants: Hai-Chuan Song, Jun-Hai Yong.

It is a fundamental problem to calculate Jacobian coefficients of constraint equations in assembly constraint solving because most approaches to solving an assembly constraint system will finally resort to a numerical iterative method that requires the first-order derivatives of the constraint equations. The most-used method of deriving the Jacobian coefficients is to use virtual rotation which is originally presented to derive the equations of motion of constrained mechanical systems. However, when Euler parameters are adopted as the state variables to represent the transformation matrix, using the virtual rotation will yield erroneous formulae of Jacobian coefficients. The reason is that Euler parameters are incompatible with virtual rotation. In this paper, correct formulae of Jacobian coefficients of geometric constraints with respect to Euler parameters are presented in both Cartesian coordinates and relative generalized coordinates. Experimental results show that our proposed formulae make Newton-Raphson iterative method converge faster and more stable. [22]

6.1.3. An extended schema and its production rule-based algorithms for assembly data exchange using IGES

Participants: Kai-Mo Hu, Bin Wang, Jun-Hai Yong.

Assembly data exchange and reuse play an important role in CAD and CAM in shortening the product development cycle. However, current CAD systems cannot transfer mating conditions via neutral file format, and their exported IGES files are heterogeneous. In this paper, a schema for the full data exchange of assemblies is presented based on IGES. We first design algorithms for the pre-and-post processors of parts based on solid model, in which the topologies are explicitly specified and will be referred by mating conditions, and then extend the IGES schema by introducing the Associativity Definition Entity and Associativity Instance Entity defined in IGES standard, so as to represent mating conditions. Finally, a production rule-based method is proposed to analyze and design the data exchange algorithms for assemblies. Within this schema, the heterogeneous representations of assemblies exported from different CAD systems can be processed appropriately, and the mating conditions can be properly exchanged. Experiments on the prototype system verify the robustness, correctness, and flexibility of our schema. [18]

6.1.4. Robust shape normalization of 3D articulated volumetric models

Participants: Yu-Shen Liu, Jun-Hai Yong, Jean-Claude Paul.

3D shape normalization is a common task in various computer graphics and pattern recognition applications. It aims to normalize different objects into a canonical coordinate frame with respect to rigid transformations containing translation, rotation and scaling in order to guarantee a unique representation. However, the conventional normalization approaches do not perform well when dealing with 3D articulated objects.

To address this issue, we introduce a new method for normalizing a 3D articulated object in the volumetric form. We use techniques from robust statistics to guide the classical normalization computation. The key idea is to estimate the initial normalization by using implicit shape representation, which produces a novel articulation insensitive weight function to reduce the influence of articulated deformation. We also propose and prove the articulation insensitivity of implicit shape representation. The final solution is found by means of iteratively reweighted least squares. Our method is robust to articulated deformation without any explicit shape decomposition. The experimental results and some applications are presented for demonstrating the effectiveness of our method. [24]

6.1.5. G^1 continuous approximate curves on NURBS surfaces

Participant: Jun-Hai Yong.

Curves on surfaces play an important role in computer aided geometric design. In this paper, we present a parabola approximation method based on the cubic reparameterization of rational Bézier surfaces, which generates G^1 continuous approximate curves lying completely on the surfaces by using iso-parameter curves of the reparameterized surfaces. The Hausdorff distance between the approximate curve and the exact curve is controlled under the user-specified tolerance. Examples are given to show the performance of our algorithm. [28]

6.1.6. The IFC-based path planning for 3D indoor spaces

Participant: Yu-Shen Liu.

Path planning is a fundamental problem, especially for various AEC applications, such as architectural design, indoor and outdoor navigation, and emergency evacuation. However, the conventional approaches mainly operate path planning on 2D drawings or building layouts by simply considering geometric information, while losing abundant semantic information of building components. To address this issue, this paper introduces a new method to cope with path planning for 3D indoor space through an IFC (Industry Foundation Classes) file as input. As a major data exchange standard for Building Information Modeling (BIM), the IFC standard is capable of restoring both geometric information and rich semantic information of building components to support lifecycle data sharing. The method consists of three main steps: (1) extracting both geometric and semantic information of building components defined within the IFC file, (2) discretizing and mapping the extracted information into a planar grid, (3) and finally finding the shortest path based on the mapping for path planning using Fast Marching Method. The paper aims to process different kinds of building components and their corresponding properties to obtain rich semantic information that can enhance applications of path planning. In addition, the IFC-based distributed data sharing and management is implemented for path planning. The paper also presents some experiments to demonstrate the accuracy, efficiency and adaptability of the method. Video demonstration is available from http://cgcad.thss.tsinghua.edu.cn/liuyushen/ifcpath/. [20]

6.1.7. Recovering Geometric Detail by Octree Normal Maps

Participants: Bin Wang, Jean-Claude Paul.

This paper presents a new approach for constructing normal maps that capture high-frequency geometric detail from dense models of arbitrary topology and are applied to the simplified version of the same models generated by any simplification method to mimic the same level of detail. A variant of loose octree scheme is used to optimally calculate the mesh normals. A B-spline surface fitting based method is employed to solve the issue of thin plate. A memory saving Breadth-First Search (BFS) order construction is designed. Furthermore, a speedup scheme that exploits access coherence is used to accelerate filtering operation. The proposed method can synthesize good quality images of models with extremely high number of polygons while using much less memory and render at much higher frame rate. [31]

6.1.8. An improved example-driven symbol recognition approach in engineering drawings

Participants: Hui Zhang, Ya-Mei Wen.

In this paper, an improved example-driven symbol recognition algorithm is proposed for CAD engineering drawings. First, in order to represent the structure of symbols more clearly and simply, we involve the text entity as one of the basic elements and redefine the relation representation mechanism, which is the foundation for the following algorithms. Then, the structure graph and a constrained tree can be established automatically for the target symbol, using the knowledge acquisition algorithm. In this process, the highest priority element is considered as the key feature, which will be regarded as the root node of the tree. The sequence of breadth first traveling will be recorded to be the recognition rule and saved in the symbol library. In the recognition process, the nodes with the same type as the key features can be located first in the drawing. Unnecessary matching calculations would be greatly reduced because of the accurate location. The other elements around, which satisfy the topology structure of the constrained tree, will be found next. The target symbol is recognized if all of the elements and constraints in the tree are found. Moreover, an extra preprocessing analysis approach is proposed to address repeat modes in a symbol. Thus, similar symbols can be recognized by one rule. We evaluate the proposed approach on the GREC databases and the real engineering drawings. The experimental results validate its effectiveness and efficiency. [17]

6.1.9. 3DMolNavi: A web-based retrieval and navigation tool for flexible molecular shape comparison

Participants: Yu-Shen Liu, Jean-Claude Paul.

Many molecules of interest are flexible and undergo significant shape deformation as part of their function, but most existing methods of molecular shape comparison treat them as rigid shapes, which may lead to incorrect measure of the shape similarity of flexible molecules. Currently, there still is a limited effort in retrieval and navigation for flexible molecular shape comparison, which would improve data retrieval by helping users locate the desirable molecule in a convenient way. To address this issue, we develop a web-based retrieval and navigation tool, named 3DMolNavi, for flexible molecular shape comparison. This tool is based on the histogram of Inner Distance Shape Signature (IDSS) for fast retrieving molecules that are similar to a query molecule, and uses dimensionality reduction to navigate the retrieved results in 2D and 3D spaces. We tested 3DMolNavi in the Database of Macromolecular Movements (MolMovDB) and CATH. Compared to other shape descriptors, it achieves good performance and retrieval results for different classes of flexible molecules. The advantages of 3DMolNavi, over other existing softwares, are to integrate retrieval for flexible molecular shape comparison and enhance navigation for user's interaction. [23]

6.1.10. Manifold-ranking based retrieval using k-regular nearest neighbor graph

Participants: Bin Wang, Kai-Mo Hu, Jean-Claude Paul.

Manifold-ranking is a powerful method in semi-supervised learning, and its performance heavily depends on the quality of the constructed graph. In this paper, we propose a novel graph structure named k-regular nearest neighbor (k-RNN) graph as well as its constructing algorithm, and apply the new graph structure in the framework of manifold-ranking based retrieval. We show that the manifold-ranking algorithm based on our proposed graph structure performs better than that of the existing graph structures such as k-nearest neighbor (k-NN) graph and connected graph in image retrieval, 2D data clustering as well as 3D model retrieval. In addition, the automatic sample reweighting and graph updating algorithms are presented for the relevance feedback of our algorithm. Experiments demonstrate that the proposed algorithm outperforms the state-of-the-art algorithms. [25]

6.2. Computer Graphics

6.2.1. Content-Based Color Transfer

Participants: Fuzhang Wu, Weiming Dong, Yan Kong, Xing Mei, Jean-Claude Paul, Xiaopeng Zhang.

This paper presents a novel content-based method for transferring the colour patterns between images. Unlike previous methods that rely on image colour statistics, our method puts an emphasis on high-level scene content analysis. We first automatically extract the foreground subject areas and background scene layout from the scene. The semantic correspondences of the regions between source and target images are established. In the second step, the source image is re-coloured in a novel optimization framework, which incorporates the extracted content information and the spatial distributions of the target colour styles. A new progressive transfer scheme is proposed to integrate the advantages of both global and local transfer algorithms, as well as avoid the over-segmentation artefact in the result. Experiments show that with a better understanding of the scene contents, our method well preserves the spatial layout, the colour distribution and the visual coherence in the transfer process. As an interesting extension, our method can also be used to re-colour video clips with spatially-varied colour effects. [26]

6.2.2. Large-scale forest rendering: Real-time, realistic, and progressive

Participants: Xiaopeng Zhang, Weiming Dong.

Real-time rendering of large-scale forest landscape scenes is important in many applications, such as video games, Internet graphics, and landscape and cityscape scene design and visualization. One challenge in the field of virtual reality is transferring a large-scale forest environment containing plant models with rich geometric detail through the network and rendering them in real time. We present a new framework for rendering large-scale forest scenes realistically and quickly that integrates extracting level of detail (LOD) tree models, rendering real-time shadows for large-scale forests, and transmitting forest data for network applications. We construct a series of LOD tree models to compress the overall complexity of the forest in view-dependent forest navigation. A new leaf phyllotaxy LOD modeling method is presented to match leaf models with textures, balancing the visual effect and model complexity. To progressively render the scene from coarse to fine, sequences of LOD models are transferred from simple to complex. The forest can be rendered after obtaining a simple model of each tree, allowing users to quickly see a sketch of the scene. To improve client performance, we also adopt a LOD strategy for shadow maps. Smoothing filters are implemented entirely on the graphics processing unit (GPU) to reduce the shadows' aliasing artifacts, which creates a soft shadowing effect. We also present a hardware instancing method to render more levels of LOD models, which overcomes the limitation of the latest GPU that emits primitives into only a limited number of separate vertex streams. Experiments show that large-scale forest scenes can be rendered with smooth shadows and in real time. [14]

6.2.3. Fast Multi-Operator Image Resizing and Evaluation

Participants: Weiming Dong, Xiaopeng Zhang, Jean-Claude Paul.

Current multi-operator image resizing methods succeed in generating impressive results by using image similarity measure to guide the resizing process. An optimal operation path is found in the resizing space. However, their slow resizing speed caused by inefficient computation strategy of the bidirectional patch matching becomes a drawback in practical use. In this paper, we present a novel method to address this problem. By combining seam carving with scaling and cropping, our method can realize content-aware image resizing very fast. We define cost functions combing image energy and dominant color descriptor for all the operators to evaluate the damage to both local image content and global visual effect. Therefore our algorithm can automatically find an optimal sequence of operations to resize the image by using dynamic programming or greedy algorithm. We also extend our algorithm to indirect image resizing which can protect the aspect ratio of the dominant object in an image. [16]

6.2.4. Easy modeling of realistic trees from freehand sketches

Participant: Xiaopeng Zhang.

Creating realistic 3D tree models in a convenient way is a challenge in game design and movie making due to diversification and occlusion of tree structures. Current sketch-based and image-based approaches for fast tree modeling have limitations in effect and speed, and they generally include complex parameter adjustment, which brings difficulties to novices. In this paper, we present a simple method for quickly generating various 3D tree models from freehand sketches without parameter adjustment. On two input images, the user draws strokes representing the main branches and crown silhouettes of a tree. The system automatically produces a 3D tree at high speed. First, two 2D skeletons are built from strokes, and a 3D tree structure resembling the input sketches is built by branch retrieval from the 2D skeletons. Small branches are generated within the sketched 2D crown silhouettes based on self-similarity and angle restriction. This system is demonstrated on a variety of examples. It maintains the main features of a tree: the main branch structure and crown shape, and can be used as a convenient tool for tree simulation and design. [21]

6.2.5. Real-time ink simulation using a grid-particle method

Participants: Shibiao Xu, Xing Mei, Weiming Dong, Xiaopeng Zhang.

This paper presents an effective method to simulate the ink diffusion process in real time that yields realistic visual effects. Our algorithm updates the dynamic ink volume using a hybrid grid-particle method: the fluid velocity field is calculated with a low-resolution grid structure, whereas the highly detailed ink effects are controlled and visualized with the particles. To facilitate user interaction and extend this method, we propose a particle-guided method that allows artists to design the overall states using the coarse-resolution particles and to preview the motion quickly. To treat coupling with solids and other fluids, we update the grid-particle representation with no-penetration boundary conditions and implicit interaction conditions. To treat moving "ink-emitting" objects, we introduce an extra drag-force model to enhance the particle motion effects; this force might not be physically accurate, but it proves effective for producing animations. We also propose an improved ink rendering method that uses particle sprites and motion blurring techniques. The simulation and the rendering processes are efficiently implemented on graphics hardware at interactive frame rates. Compared to traditional fluid simulation methods that treat water and ink as two mixable fluids, our method is simple but effective: it captures various ink effects, such as pinned boundaries and filament patterns, while still running in real time, it allows easy control of the animation, it includes basic solid-fluid interactions, and it can address multiple ink sources without complex interface tracking. Our method is attractive for animation production and art design.

6.2.6. Image zooming using directional cubic convolution interpolation

Participant: Weiming Dong.

Image-zooming is a technique of producing a high-resolution image from its low-resolution counterpart. It is also called image interpolation because it is usually implemented by interpolation. Keys' cubic convolution (CC) interpolation method has become a standard in the image interpolation field, but CC interpolates indiscriminately the missing pixels in the horizontal or vertical direction and typically incurs blurring, blocking, ringing or other artefacts. In this study, the authors propose a novel edge-directed CC interpolation scheme which can adapt to the varying edge structures of images. The authors also give an estimation method of the strong edge for a missing pixel location, which guides the interpolation for the missing pixel. The authors' method can preserve the sharp edges and details of images with notable suppression of the artefacts that usually occur with CC interpolation. The experiment results demonstrate that the authors' method outperforms significantly CC interpolation in terms of both subjective and objective measures. [30]

CAGIRE Team

6. New Results

6.1. Low Mach number flows simulations issue

The time-step dependency and the scaling of the pressure-velocity coupling suitable for unsteady calculations of low Mach number flows including acoustic features has been identified in the Momentum Interpolation approach. It has been shown that the proper form of the inertia term in the transporting velocity definition is related to the time-step independency of the steady state. The suitable scaling of the pressure gradient dissipation has been used to suggest a modification of AUSM+-up that allows acoustic simulations of low Mach number flows. The accuracy improvement when the solution is compared to the one of the original AUSM+-up scheme indicates that the scaling identified in the Momentum Interpolation approach can be applied with advantage to Godunov-type schemes [3].

6.2. Experimental results

The MAVERIC test facility has been significantly upgraded with the acquisition of a complete GPU-based system (hardware+software) that speeds up by a factor of 10 the processing of the PIV data. The strong sensitivity of the flow topology to the presence of an acoustic standing wave in the cross-flow has been clearly evidenced. The presently available measurements give already the possibility of extracting numerous velocity profiles for a future fruitful LES assessment. The dedicated 1-jet experiment for DNS assessment will start at the beginning of 2013 [8].

CALVI Project-Team

6. New Results

6.1. Mathematical analysis of kinetic models

6.1.1. Gyrokinetic and Finite Larmor radius approximations

Participants: Mihai Bostan, Céline Caldini, Emmanuel Frénod, Mathieu Lutz.

In a work in progress by E. Frénod and M. Lutz, the deduction of the Geometrical Gyro-Kinetic Approximation, which was originally obtained by Littlejohn in [75], [76], [77] using a physical approach which was mathematically formal, is done. The rigorous mathematical theory is built and explained in a form for providing it, especially, for analysts, applied mathematicians and computer scientists.

In the Note [16], we present the derivation of the finite Larmor radius approximation, when collisions are taken into account. We concentrate on the Boltzmann relaxation operator whose study reduces to the gyroaverage computation of velocity convolutions, which are detailed here. We emphasize that the resulting gyroaverage collision kernel is not local in space anymore and that the standard physical properties (i.e., mass balance, entropy inequality) hold true only globally in space and velocity. This work is a first step in this direction and it will allow us to handle more realistic collisional mechanisms, like the Fokker-Planck or Fokker-Planck-Landau kernels.

The subject matter of the paper [34] concerns the derivation of the finite Larmor radius approximation, when collisions are taken into account. Several studies are performed, corresponding to different collision kernels. The main motivation consists in computing the gyroaverage of the Fokker-Planck-Landau operator, which plays a major role in plasma physics. We show that the new collision operator enjoys the usual physical properties ; the averaged kernel balances the mass, momentum, kinetic energy and dissipates the entropy.

6.1.2. Singularities of the stationary Vlasov–Poisson system in a polygon

Participant: Simon Labrunie.

In collaboration with Fahd Karami (Université Cadi Ayyad, Morocco) and Bruno Pinçon (Université de Lorraine and project-team CORIDA), we conducted in [43] a theoretical and numerical study of the so-called “point effect” in plasma physics. The model (stationary Vlasov–Poisson system with external potential) corresponds a fully ionised plasma considered on a time scale much smaller than that of ions, but much larger than that of electrons. It appears as the relevant non-linear generalisation of the electrostatic Poisson equation. This may be a first step toward a quasi-equilibrium model valid on a larger time scale, where the equilibrium description of the electrons would be coupled to a kinetic or fluid model for the ions. This approximation is classical in plasma physics. We proved a general existence result for our model in a bounded domain $\Omega \subset \mathbb{R}^N$, which is not assumed to be smooth. When Ω is a polygonal domain of $\mathbb{R}^2$, we described the singular behavior of the solution near a reentrant corner. In the important case of the Maxwell–Boltzmann distribution, we established a link between various asymptotics of the problem and the (suitably extended) theory of large solutions to nonlinear elliptic problems (for a review of this theory, see e.g. [50]). This allowed us to determine the the dependence of the singularity coefficients on the parameters of the problem, such as the total mass of the distribution, or the boundary conditions of the potential. Numerical tests confirmed the theory.

6.2. Two-Scale Asymptotic-Preserving schemes

Participants: Nicolas Crouseilles, Emmanuel Frénod, Michaël Gutnic, Sever Hirstoaga.

In paper [20], 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 circumscribed 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.

During CEMRACS 2011, we have started the project to test on a simplified model the Two-Scale Asymptotic-Preserving Schemes. The model, a two dimensional in phase space Vlasov-Poisson equation with small parameter, is used for a long time simulation of a beam in a focusing channel. This work was already done in [68] in the case where the solution is approximated by the two scale limit. The first goal is to improve this approximation, by going further, to the first order one; this was done in [41]. The second goal is to replace this approximation by an exact decomposition, using the macro-micro framework. This last approach will permit to treat the case of a not necessary small parameter. In order to accomplish the first task we have writen a Particle-In-Cell code in SeLaLib.

6.3. Development of numerical methods

Participants: Morgane Bergot, Anaïs Crestetto, Nicolas Crouseilles, Pierre Glanc, Michel Mehrenberger, Hocine Sellama, Eric Sonnendrücker, Christophe Steiner.

The work [19] is devoted to the numerical simulation of the Vlasov equation in the fluid limit using particles. To that purpose, we first perform a micro-macro decomposition as in [53] where asymptotic preserving schemes have been derived in the fluid limit. In [53], a uniform grid was used to approximate both the micro and the macro part of the full distribution function. Here, we modify this approach by using a particle approximation for the kinetic (micro) part, the fluid (macro) part being always discretized by standard finite volume schemes. There are many advantages in doing so: (i) the so-obtained scheme presents a much less level of noise compared to the standard particle method; (ii) the computational cost of the micro-macro model is reduced in the fluid regime since a small number of particles is needed for the micro part; (iii) the scheme is asymptotic preserving in the sense that it is consistent with the kinetic equation in the rarefied regime and it degenerates into a uniformly (with respect to the Knudsen number) consistent (and deterministic) approximation of the limiting equation in the fluid regime.

In [39] we present finite volumes schemes for the numerical approximation of the one-dimensional Vlasov-Poisson equation (FOV CEMRACS 2011 project). Stability analysis is performed for the linear advection and links with semi-Lagrangian schemes are made. Finally, numerical results enable to compare the different methods using classical plasma test cases.

In [40], we test an innovative numerical scheme for the simulation of the guiding-center model, of interest in the domain of plasma physics, namely for fusion devices. We propose a 1D Discontinuous Galerkin (DG) discretization, whose basis are the Lagrange polynomials interpolating the Gauss points inside each cell, coupled to a conservative semi-Lagrangian (SL) strategy. Then, we pass to the 2D setting by means of a second-order Strang splitting strategy. In order to solve the 2D Poisson equation on the DG discretization, we adapt the spectral strategy used for equally-spaced meshes to our Gauss-point-based basis. The 1D solver is validated on a standard benchmark for the nonlinear advection; then, the 2D solver is tested against the swirling deformation ow test case; finally, we pass to the simulation of the guiding-center model, and compare our numerical results to those given by the Backward Semi-Lagrangian method.

In [44] we have developed the guiding-center model in polar coordinates; numerical issues/difficulties can be tackled in such a test case which thus may be viewed as a first intermediate step between a classical center guide simulation in a 2D cartesian mesh and a 4D drift kinetic simulation.

In [25] and [28], we are interested in the numerical solution of the collisionless kinetic or gyrokinetic equations of Vlasov type needed for example for many problems in plasma physics. Different numerical methods are classically used, the most used is the Particle In Cell method, but Eulerian and Semi-Lagrangian (SL) methods that use a grid of phase space are also very interesting for some applications. Rather than using a uniform mesh of phase space which is mostly done, the structure of the solution, as a large variation of the gradients on different parts of phase space or a strong anisotropy of the solution, can sometimes be such that it is more interesting to use a more complex mesh. This is the case in particular for gyrokinetic simulations for magnetic fusion applications. We develop here a generalization of the Semi-Lagrangian method on mapped meshes. Classical Backward Semi-Lagrangian methods (BSL), Conservative Semi-Lagrangian methods based on one-dimensional splitting or Forward Semi-Lagrangian methods (FSL) have to be revisited in this case of mapped meshes. We consider here the problematic of conserving exactly some equilibrium of the distribution function, by using an adapted mapped mesh, which fits on the isolines of the Hamiltonian. This could be useful in particular for Tokamak simulations where instabilities around some equilibrium are investigated. We also consider the problem of mass conservation. In the cartesian framework, the FSL method automatically conserves the mass, as the advective and conservative form are shown to be equivalent. This does not remain true in the general curvilinear case. Numerical results are given on some gyrokinetic simulations performed with the GYSELA code and show the benefit of using a mass conservative scheme like the conservative version of the FSL scheme. Inaccurate description of the equilibrium can yield to spurious effects in gyrokinetic turbulence simulations. Also, the Vlasov solver and time integration schemes impact the conservation of physical quantities, especially in long-term simulations. Equilibrium and Vlasov solver have to be tuned in order to preserve constant states (equilibrium) and to provide good conservation property along time (mass to begin with). Several illustrative simple test cases are given to show typical spurious effects that one can observes for poor settings. We explain why Forward Semi-Lagrangian scheme bring us some benefits. Some toroidal and cylindrical GYSELA runs are shown that use FSL.

In [12] we present the Semi-Lagrangian method which is composed by essentially two ingredients : the computation of the characteristics along which the distribution function is constant and the interpolation step. We analyse high order schemes in time based on directional splitting, which are a succession of linear transport steps. We then study the Semi-Lagrangian methods in this particular case and we make the link between different formulations. We also obtain a convergence theorem for the Vlasov-Poisson system in this framework, which remains valid in the case of small displacements. We then develop this type of methods in a more general framework, by using one dimensionnal conservative splitting. We also consider a discontinuous Galerkin variant of such schemes. In a last part, we study the gyroaverage operator which appears in plasma physics by taking care of finite Larmor radius corrections. Finally, we discuss the problematic of zero discrete divergence which gives a compatibility between field computations and the numerical method of transport.

6.4. Finite Element Methods

6.4.1. Gyrokinetic quasi-neutrality equation

Participants: Nicolas Crouseilles, Eric Sonnendrücker.

In [21], a new discretization scheme of the gyrokinetic quasi-neutrality equation is proposed. We discretised the gyrokinetic Poisson equation using arbitrary order spline finite elements which enables to accommodate more complex domains. Moreover in standard polar coordinates we developed a fast solver which is comparable in computational time to the original FFT-second order finite differences, but can become more efficient for higher order as fewer grid points are needed for the same accuracy.

6.4.2. Dissipative boundary conditions for finite element codes

Participants: Philippe Helluy, Laurent Navoret, Eric Sonnendrücker.

We are developing finite-element codes for the Vlasov-Poisson system that would be able to capture the filamentation phenomenon. The filamentation is a mechanism that transfers the space fluctuations of the distribution function to high frequency oscillations in the velocity direction. For stability purpose, most numerical schemes contain dissipation that may affect the precision of the finest oscillations that could be resolved. In [60], [61], [62] Eliasson constructs a non reflecting and dissipative condition for the Fourier-transformed Vlasov-Poisson system. The condition enables the high velocity-frequency oscillations to leave the computational domain in a clean way.

We are currently developing a finite-element code based on this dissipative boundary condition. The code is part of the Selalib library. We also propose an approximation of the Eliasson method, based on the Béranger's PML formalism. Contrary to the original boudary conditions that requires a space Fourier transformation, this method is local and thus could be extended to higher dimensionnal problems and more complex geometries.

6.4.3. High order finite element methods for Maxwell

Participants: Stéphanie Salmon, Eric Sonnendrücker.

In paper [23], we study high order discretization methods for solving the Maxwell equations on hybrid triangle-quad meshes. We have developed high order finite edge element methods coupled with different high order time schemes and we compare results and efficiency for several schemes. We introduce in particular a class of simple high order low dissipation time schemes based on a modified Taylor expansion.

6.5. Waterbag models: analysis and simulations

Participant: Nicolas Besse.

In paper [33], we revisit the linear theory of kinetic flute-like modes such as ionic instabilities by using the exact geometric reduction of Vlasov equation yielded by waterbag invariants which are reminiscent to the geometric Liouville invariants. The waterbag representation of the statistical distribution function of particles can be viewed as a special class of exact weak solution of the Vlasov equation, allowing to reduce this latter into a set of hydrodynamic equations (with the complexity of a multi-fluid model) while keeping its kinetic features (Landau damping and resonant wave-particle interaction). For high toroidal-number-mode, from ballooning transformation and multi-scale WKB-type analysis, we demonstrate that one can construct eigenmode solutions of the two-dimensional integro-differential gyrowaterbag operator by solving a nested one-dimensional Fredholm-type integral equation. Qualitatively, the solution of the nested one-dimensional Fredholm-type equation is equivalent to first solving for the mode structure along the field lines locally in radius, and then constructing the two-dimensional global mode structure through a radially weighted superposition of local solutions. The radial weighted function is solution of a Schrödinger equation or a Riccati equation in the dual space. Solving the linear turning points problem and using connection formulas, the global dispersion relation arises from the WKB-type phase integral quantization condition which involves the local eigenfrequency. Finally we perform the spectral analysis of the nested one-dimensional Fredholm-type operator which constitutes a meromorphic family of compact operators and extend all the results proved for unstable eigenmodes to stable and damped ones by analytic continuation.

In paper [36], 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 [55]. 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 quasi-linear 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.

In paper [32], we first present the derivation of the anisotropic Lagrangian averaged gyrowaterbag continuum (LAGWBC) equations. The gyrowaterbag continuum can be viewed as a special class of exact weak solution of the Vlasov-gyrokinetic equation, allowing to reduce this latter into an infinite dimensional set of hydrodynamic equations (i.e. an infinite dimensional hyperbolic system of first-order conservation laws in several space dimensions with non-local fluxes) while keeping its kinetic features (Landau damping and nonlinear resonant wave-particle interaction). These models are very promising because they reveal to be very useful for analytical theory (such as the resolution of the eigenvalue problem for analytical description of various instabilities) and numerical simulations (when the continuum is converted into a small finite set of "fluid" or waterbag, the problem has the complexity of a multifluid model instead of a kinetic one) of laser-plasma and gyrokinetic physics (electrostatic turbulence problem). The gyrowaterbag waterbag continuum is derived from two phase-space variable reductions of the Vlasov equation through the existence of two underlying invariants. The first one, coming from physic properties of the dynamics (the fast gyromotion of particles around magnetic field lines) is adiabatic and called the magnetic moment. The second one, named "waterbag" and coming from geometric invariance property of the phase-space, is just the direct consequence of the Liouville Theorem and is reminiscent to the geometric Liouville invariant. In order to obtain the LAGWBC equations from the gyrowaterbag continuum we use an Eulerian variational principle and Lagrangian averaging techniques. Regarding to the original gyrowaterbag continuum, the LAGWBC equations show some additional properties and several advantages from the mathematical and physical viewpoints, which make this model a good candidate for describing accurately gyrokinetic turbulence in magnetically confined plasma. In the second part of this paper we prove local in time well-posedness of an approximated version of the anisotropic LAGWBC equations, that we call the “isotropic” LAGWBC equations, by using quasilinear PDE type methods and elliptic regularity estimates for several operators.

6.6. Simulations for Vlasov-Maxwell model

Participants: Anaïs Crestetto, Philippe Helluy.

In [37] (see also [11]), we present an implementation of a Vlasov-Maxwell solver for multicore processors. The Vlasov equation describes the evolution of charged particles in an electromagnetic field, solution of the Maxwell equations. We propose to solve the Vlasov equation by a Particle-In-Cell method (PIC), while the Maxwell system is computed by a Discontinuous Galerkin method. These methods are detailed, as well as the emission law for the particles and the implementation of the boundary conditions. We use the OpenCL framework, which allows our code to run on multicore processors or recent Graphic Processing Units (GPU). The key points of the implementation on this architecture are presented. We then study several numerical applications to two-dimensional test cases in cartesian geometry. The acceleration between the computation on a CPU and on a graphic card is very high, especially for the Maxwell part.

We have started a new software project called CLAC (for “Conservation Laws Approximation on many Cores”). This a 3D Discontinuous Galerkin solver, which runs on cluster of GPU’s, thanks to the OpenCL environment and the MPI library. CLAC is open source and developed in collaboration with the AxesSim company, a SME near Strasbourg. For the moment, it is applied to the Maxwell equations. But we plan to apply it to the MHD equations or mixed kinetic/fluid plasma models.

6.7. Free-streaming ELM formulae vs. Vlasov simulations

Participants: Sever Hirstoaga, Giovanni Manfredi.

One of the main challenges for future tokamak operation, such as ITER, is constituted by the large heat load on the divertor plates. The divertor surfaces are constantly bombarded with high-energy particles and may see their lifetime considerably reduced. The intensity of the particles and energy fluxes is particularly high during transient events known as edge-localised modes (ELMs). Our purpose here is to propose and investigate a kinetic model for ELMs.

The free-streaming model [69] is a simple analytical model for ELM transport in the scrape-off layer (SOL) of a tokamak. It is a force-free Vlasov equation with a source term for the ions distribution function (the Coulomb forces are ignored). Even though this model reproduces with good accuracy some of the main features of an ELM signal, it has two main drawbacks: (i) the self-consistent electric potential is not accounted for and (ii) only solutions for the ion distribution are considered.

In this contribution [24] we propose a set of modified free-streaming equations in order to overcome the above drawbacks. More precisely, some hypotheses on the Maxwellian initial condition lead to a model that includes the self-consistent electric potential. Assuming quasinetrality and using energy conservation we could derive analytical formulae for the electron quantities. This augmented free-streaming model was benchmarked to the Vlasov-Poisson simulations reported in [78]. The match is encouragingly good, thus justifying the applicability of the free-streaming approach.

Finally, from a computational point of view, transport in the SOL was studied by means of three different approaches – fluid, Vlasov and particle-in-cell (PIC). In spite of kinetic effects due to fast electrons which are not captured in the fluid code, the overall agreement between the codes was found to be quite satisfactory [22].

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

Participants: Pierre Bertrand, Takashi Hattori, Simon Labrunie, Jean Rodolphe 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 $\lambda << \phi_B << R$, where ϕ_B is the size of the beam transverse to the rf power flow direction, may be overcome. Since conditions are corresponding to $\lambda << \phi_B \sim R$, 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 filled 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.

During 2012 we have developed a domain decomposition method and a new behavior of the plasma density was considered in the code "FullWaveFEM". A 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.

6.9. Nearby fields to plasma physics

6.9.1. Neutrino transport in supernova

Participant: Emmanuel Frénod.

In [31] we give an introduction to the Boltzmann equation for neutrino transport used in core collapse supernova models as well as a detailed mathematical description of the Isotropic Diusion Source Approximation (IDSA). Furthermore, we present a numerical treatment of a reduced Boltzmann model problem based on time splitting and finite volumes and revise the discretization of the IDSA for this problem. Discretization error studies carried out on the reduced Boltzmann model problem and on the IDSA show that the errors are of order one in both cases. By a numerical example, a detailed comparison of the reduced model and the IDSA is carried out and interpreted. For this example the IDSA modeling error with respect to the reduced Boltzmann model is numerically determined and localized.

In [30] 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.

6.9.2. Inverse problem governed by Maxwell equations

Participant: Jean Rodolphe 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, ...), 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 [18]. In this year we aim to overcome this constraint, and look for configurations of inductors considering different topologies with the purpose of obtaining better results. In order to manage this new situation 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 [35] and [29].

CASTOR Team

5. New Results

5.1. Simulations in plasma Physics

5.1.1. Fourier-spectral element approximation of a two fluid model of edge plasma

Participants: Richard Pasquetti, Sebastian Minjeaud.

We especially work on a two fluid physical model developed in close connection with Ph. Ghendrih (IRFM). It is based on the electrostatic assumption, i.e. the magnetic field is given (the magnetic field induced by the plasma itself is negligible), and on the hypothesis of electroneutrality (the density of ions and electrons are proportional). On the basis of the conservation equations of density, electron and ion velocities, electron and ion temperatures and electrical charges, a set of 10 non-linear coupled partial differential equations (PDE) can be set up. A high order Fourier-SEM (Spectral Element Method) code is currently developed. This Fourier-SEM code is now operational for the full set of PDEs in a 3D toroidal geometry. The torus section is discretized with quadrangular elements, within which the polynomial approximation degree is an input to the code. In time one uses an RK3 (third order Runge-Kutta) IMEX (Implicit-Explicit), so that the Lorentz terms are handled implicitly. The capability of this code to handle a strongly anisropic diffusion in a 3D toroidal geometry has already been tested. The Braginskii closure has been implemented. The Bohm boundary conditions at the plates are also considered. A parallel version of this code is currently developed. It remains to improve the robustness of our algorithms, i.e. to implement an efficient stabilization strategy. This could be based on the so-called spectral vanishing viscosity or entropy viscosity techniques. Up to our knowledge, this will be the first code that fully implements a two fluid ion-electron approximation (i.e. without using the drift velocity approximation), and the Braginskii closure of the governing equations.

5.1.2. Hydrodynamic model with strong Lorentz force

Participants: Audrey Bonnement, Hervé Guillard, Boniface Nkonga, Richard Pasquetti.

The thesis of A. Bonnement [1] was devoted to the development of a code based on the FluidBox/plaTo software of B. Nkonga and co-workers. It is based on a Finite volume / Finite element approach. This code is now operational in an axisymmetric geometry for a simplified PDE system in which the Lorentz force is approximated by a constant forcing field. Thus, the FluidBox/PlaTo code essentially solves the 3D axisymmetric Euler, Navier-Stokes or Braginskii PDEs to compute the ion density, momentum and energy. In the Braginskii system, the thermal diffusion and the kinematic viscosity are both non-linear and strongly anisotropic. A. Bonnement, who was co-directed by H. Guillard and R. Pasquetti, defended her thesis "Modélisation numérique bi-fluide du plasma de bord des tokamaks: application à ITER" in July 2012. A. Bonnement has provided a detailed description of the works carried out with the FluidBox/PlaTo code in her thesis manuscript. She has specially addressed one of the main difficulties related to simulations of tokamak plasmas, which is that the dynamic of the flows occurs in the vicinity of an equilibrium where the plasma pressure balances the Lorentz force. There are two ways to deal with this difficulty. The most common one in tokamak studies is to work with a set of governing equations such that this equilibrium is already contained in the formulation. This can be done by using formulations where the variables are indeed fluctuating departures from the equilibrium or by using special approximations as done in reduced MHD. The other way is purely numerical and consists to design a numerical method such that the equilibrium is an exact solution of the discrete equations. This has been the subject of the thesis of Audrey Bonnement in the framework of a finite volume method on non-structured meshes and where special Riemann solvers have been designed incorporating plasma equilibrium in the definition of the numerical fluxes. Combined with mesh refinement, this approach has been applied to some preliminary numerical experiments studying the effect of density perturbations (as a crude model of pellet injections) on the dynamics of the flow. At present, this approach is under evaluation to qualify its interest with respect to reduced MHD or formulations using a potential representation of the velocity field.

5.1.3. Finite volume methods in curvilinear system of coordinates

Participants: Hervé Guillard, Boniface Nkonga, Afeintou Sangam, Marco Bilanceri.

Finite volume methods are specialized techniques to approximate systems of conservation laws. The application of these methods to curvilinear systems of coordinate is however problematic because the space variation of the metric coefficients introduces artificial source terms. However it can be shown that whatever the curvilinear system used, a strong conservation form of the equations exists at the level of vector variables (but not at the level of the scalar components of the vectors in the curvilinear system due to the aforementioned space dependence of the metric coefficients). Based on this result, we have developed an original technique that uses an approximation of the vector form of the equation followed by local projection on the curvilinear system (here parallel to the poloidal magnetic field).

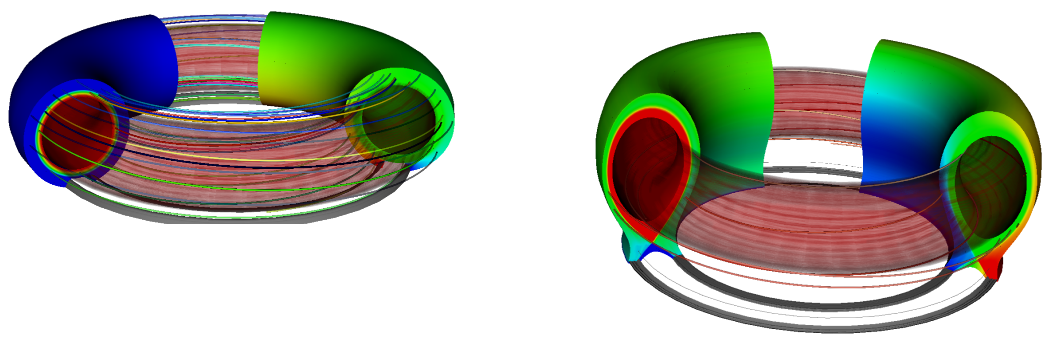


Figure 1. Density (left side) and parallel velocity (right side) color plots of the edge region of a tokamak with limiter (left plot) and tokamak with X point and divertor(right plot). Due to Bohm's boundary conditions, the parallel flux of out-flowing ions is supersonic on the limiter and divertor plates

This method has been applied to the approximation of a reduced MHD model using a decomposition of the velocity field into a parallel component and a perpendicular one given by the electric drift. The method is general and can be applied to any type of geometry. Figure 2 shows for instance the steady state density and parallel velocity fields in the edge region of a limiter tokamak (left) and of a divertor tokamak (right). Bohm's boundary conditions have been applied to the limiter and divertor plates producing a supersonic outflow velocity field.

5.1.4. Mesh singularities and triangular elements

Participants: Boniface Nkonga, Marie Martin, José Costa.

C1-finite elements as used for instance in the Jorek code are associated to isoparametric cubic-Bezier representation over quadrangles in the poloidal plane and sine-cosine Fourier expansion in the toroidal direction. Mesh singularities are associated to the structure imposed by the cubic-Bezier representation over quadrangles. In the context of the ANR-ANEMOS and in collaborations with IRFM and the Galaad team (Inria Sophia Antipolis), a geometrical toolbox is under development to manage these singularities and improve the alignment with equilibrium flux surfaces. As an alternative, we are also developing a more flexible C1-element over triangles using either Reduced-quintic (Bell) or quadratic Powell-Sabin polynomials. Optimal order of accuracy is achieved with simple boundary conditions. Many cycles of the "current hole" instability has been accurately reproduced. Additional improvement, with isoparametric formulation, will hopefully achieve this optimality for curved boundaries and improve mesh alignment to flux surfaces. We have investigated the possibility to use cubic splines representation in the toroidal direction. Indeed, for pellet injection the local resolution needed in the toroidal direction requires a large number of Fourier modes. This resolution need is very local, adapted splines representation can be more efficient. This solution is under analysis and structuration. First application is expected at end of 2013 with a possible update of Jorek in 2014.

5.1.5. Mesh adaptation Methods

Participants: Hubert Alcin [Projet Tropics], Alain Dervieux, Frédéric Alauzet [Projet Gamma, Inria-Rocquencourt].

This activity results from a cooperation between Gamma, Tropics, Castor, and Lemma company. See details in Tropics and Gamma activity reports. Its concerns Castor's subject through the current applications of mesh adaptation to flows with interfaces and to Large Eddy Simulation. It is also planned to use mesh adaptation for simplified plasma models in the context of ANEMOS ANR project.

5.1.6. Stabilization for finite / spectral element

Participants: Boniface Nkonga, Marie Martin, Richard Pasquetti, Sebastian Minjeaud.

Formulation of Reduced MHD eliminates fast acoustic waves but material, slow acoustic and Alfven waves are included in this model. On the other hand, finite element approximation, when applied to hyperbolic systems (with finite speed waves) needs additional control of the effect of unresolved scales. We have developed and validated a Taylor Galerkin Stabilizations of order 2 and 3 (TG2-TG3) for reduced MHD. This global approach has been implemented in a simplified form, validated and updated in the latest versions of the Jorek code. Even if significant improvements have been observed with this stabilization where only material and Alfven waves subscales are stabilized, more robustness is expected by taking into account slow acoustic waves. Stabilization techniques well adapted to high order approximations, like the spectral vanishing viscosity method or the entropy viscosity technique, remain to be implemented in the Fourier-SEM code.

5.1.7. Validity of the Reduced MHD and extensions

Participants: Hervé Guillard, Boniface Nkonga, Afeintou Sangam.

The available reduced MHD model in Jorek uses a set of assumption that can be reasonable close to the equilibrium and during the linear grow of instabilities. In order to obtain accurate and robust simulations of the nonlinear instabilities saturations, careful analysis and derivation of the reduced MHD has been performed, more mathematical derivations are under progress under the asymptotic analysis framework. It turns out that some of the neglected terms can be of relative importance for the saturation process when MHD instabilities move the plasma far from equilibrium.

5.1.8. High performance parallel computing

Participants: Hervé Guillard, Boniface Nkonga, Sebastian Minjeaud.

Applications under concern in this project needs to manage large meshes (10^7 to 10^9 nodes) and solve many huge sparse nonlinear systems. This makes the use of domain partitioning techniques unavoidable. In addition, since different numerical methodologies are under studies and evaluations in this project, we need to develop a quite general setting allowing the use of different data structures (element-oriented for FE vs edge-oriented for FV) and the possibility to consider different domain overlapping to efficiently communicate between processors. For this we develop the PaMPA (Parallel Mesh Partitioning and Adaptation) software in collaboration with the Bacchus team (Inria, Bordeaux). PaMPA is based on the PT-Scotch graph partitioning tool and allows on the fly mesh redistribution. Up to now, PaMPA has been tested on 10000 processors with a mesh of 20M tetrahedrons. Integration of PaMPA as an external library to the codes developed in this project is under progress and early results are promising. Similarly, the Fourier-SEM code is currently parallelized.

5.2. Optimisation and control for magnetic fusion plasmas

5.2.1. Evolutive equilibrium and transport coupling and optimization of scenarii

Participants: Jacques Blum, Cédric Boulbe, Afeintou Sangam, Gael Selig, Blaise Faugeras, Holger Heumann.

5.2.1.1. Research of optimal trajectories for the monitoring of Tokamak discharges

The direct equilibrium code CEDRES++ in its static version (resp.dynamic) computes for externally applied PF currents (resp. voltages) and given plasma current density profile the (resp. evolution of the) poloidal flux and the plasma free boundary. The research of optimal trajectories is the corresponding inverse problem : find externally applied currents (resp. voltages), such that the plasma reaches a certain desired state. This desired state is mainly (resp. the evolution of) a prescribed plasma boundary. We formulate these inverse problems as so-called optimal control problems, where the PF currents (voltages) are the so-called control variables and the poloidal flux the so-called state variable. Optimal control problems are optimization problems with PDE (partial differential equations) constraints. In our case, the Grad-Shafranov equation is the constraint and the functional to be minimized is a cost-function that measures the mismatch between the computed plasma boundary and the desired plasma boundary. The Sequential Quadratic Programming (SQP) method is known to be a very efficient algorithm for solving non-linear constrained optimization problems. We implemented in CEDRES++ the SQP method for the two cases of finding either currents or voltages that corresponds to a desired boundary or a desired evolution of the boundary. These implementations are built on the orignal Newton methods for the direct non-linear problems. For optimization problems it is of great importance that the Newton methods are 'real' Newton methods in the sense that the Newton matrices are real derivatives. In the original implementation of CEDRES++ these matrices were the discretization of analytic derivatives of the non-linear operators, hence not derivatives of the discrete problem. We had to rewrite large parts of the code to eliminate this problem. Further, we added an interface to the linear solver library UMFPACK. For the current mesh resolution level, the performance of this linear solver for the stationary problems, both in the direct and in the inverse versions, is superior to iterative linear solvers. In the case of the inverse non-stationary problem, the problem of finding voltages that correspond to a desired evolution, the memory requirements forbid the use of UMFPACK. There, we used Conjugate Gradient-type iterations. In the future, we will have to investigate if other types of iterative solvers are suitable and allow a certain parallelism that will speed up the simulation time.

5.2.1.2. A new method of coupling equilibrium and resistive diffusion equations

In the framework of Gael Selig's PhD thesis, the resistive diffusion equation has been incorporated in the evolutive equilibrium system of CEDRES++. This equation has as unknown variable the derivative of the poloidal flux with respect to the averaged minor radius of the magnetic surface. This choice was made instead of the poloidal flux itself because this is the quantity directly involved in the averaged Grad-Shafranov equation used to compute the FF' term and thus this allows us not to perform a supplementary numerical differentiation which might introduce some numerical instability. An algorithm based on a successive prediction and correction method is proposed in order to ensure the consistency between the evolution of the 2D poloidal flux in the equilibrium equation and the evolution of the poloidal flux in the 1D resistive diffusion equation. The algorithm guarantees that at the end of each time step the total plasma current Ip and the mean radius of the plasma have the same values in both systems (see fig.2). The convergence of this new code (called CEDRES-DIF) has been numerically validated and the method has been successfully compared by G. Selig to the CEDRES-CRONOS coupled code which uses another coupling algorithm.

5.2.1.3. Introduction of halo currents in the equilibrium resolution

When VDE (Vertical Displacement events) instabilities occur in a Tokamak, currents flow from the plasma to the machine vessel structures, and then return to the plasma. These currents are called halo currents . In turn, these currents induce forces on the wall when crossing with Tokamak poloidal and toroidal magnetic fields. Moreover, when VDE instabilities take place, the plasma hits the wall with all its energy. Therefore, it is worth understanding the contribution of halo currents to total plasma current and other related plasma parameters, particularly the distribution, magnitude, and temporal evolution of halo currents for large scale machine such as ITER. Even if halo currents are actually 3D phenomena, it is important to take into account their effects in 2D free boundary equilibrium codes. In halo region, the pressure can be considered as negligeable so that the current follows the magnetic field lines. The magnetic field satisfies the force free equation $jxB = 0, \nabla .B = 0$ which can be rewritten

$$-\Delta^*\Psi = \frac{1}{\mu_0 R}\frac{\partial}{\partial\Psi}f_H^2(\Psi)$$

in an axisymmetric configuration. The function $f_H(\Psi)$ is supposed to be known. This simple model has been implemented in CEDRES++ and first tests have been done. This first simplified model has to be improved to get more realistic simulations and to be validated. The choice of the function f_H, the value of the total halo current, the geometry and the size of the halo region need to be enhanced with respect to experimental data.

5.2.2. Equilibrium reconstruction and current density profile identification

Participants: Jacques Blum, Cédric Boulbe, Blaise Faugeras.

EQUINOX is a real-time equilibrium reconstruction code. It solves the equation satisfied by the poloidal flux in a computation domain, which can be the vacuum vessel for example, using a P1 finite element method and solves the inverse problem of the identification of the current density profile by minimizing a least square cost-function. It uses as minimal input the knowledge of the flux and its normal derivative on the boundary of the computation domain. It can also use supplementary constraints to solve the inverse problem: interferometric, polarimetric and MSE measurements. Part of the work reported here has been done in the frame of a RTM-JET contract.

5.2.2.1. Direct use of the magnetic measurements

Equinox was not originally designed to take as magnetic inputs directly the magnetic measurements, as it should be the case in the ITM, but some outputs from the real-time codes Apolo at ToreSupra and Xloc at JET. These codes provide Equinox with the values of the flux and its normal derivative on a closed contour defining the boundary of the computation domain (this contour can be the limiter for example). As a consequence the main difficulty arising in the objective of integrating the code Equinox in the ITM structure was to interpolate between the magnetic measurements (flux loops and poloidal B-probes) with a machine independent method. This has already been achieved by using toroidal harmonic functions, as a basis for the decomposition of the poloidal flux in the vacuum region, in complement to the contribution of the PF coils. This method can provide an alternative tool, comparable to APOLO (for Tore Supra) and FELIX (for JET), to compute the plasma boundary in real time from the magnetic measurements. Some twin experiments for WEST (Tore Supra upgrade) have been successfully conducted. In a first step the equivalents of magnetic measurements were generated using the FBE code CEDRES++. In a second step these measurements were used by the toroidal harmonics algorithm to reconstruct the plasma boundary. The results are very promising and the work on this subject is ongoing for JET.

5.2.2.2. Boundary conditions for EQUINOX

In the present version of EQUINOX the boundary condition is a flux condition (Dirichlet boundary condition) and the tangential component of the poloidal field is incorporated in the cost-function to be minimized. This is a constant criticism which is made on EQUINOX. The idea was to inverse these two boundary conditions in order to determine if this choice is determinant in the results. We tried to use the tangential poloidal field (Neumann boundary condition for the flux) as boundary condition for the boundary value problem, and to put the flux (or its tangential derivative linked to the normal component of the poloidal field) in the cost function. However no convincing results could be obtained because the numerical resolution of the boundary value problem associated with Neumann boundary conditions proved to be unstable. This might be explained by the fact that a compatibility condition has to be satisfied between the Neumann conditions and the current density in the plasma which evolves during the mixed fixed-point and optimization iterations.

5.2.2.3. Induced currents in EQUINOX

In a disruption when the total plasma current disappears, there are very important induced currents, for example in the toroidal pumped limiter. These currents are in the domain of resolution of EQUINOX. Therefore it is necessary to take them into account in the resolution of the equilibrium reconstruction problem. This has been tested on a Tore Supra disruption case. The mesh generation has been modified in order to incorporate the real structure of the limiter. The structure of the equations being solved in the code also had to be modified in order to take into account the measured induced currents.

5.3. Turbulence models

5.3.1. Hybrid RANS/LES models

Participants: Hubert Alcin [Tropics], Alain Dervieux, Bruno Koobus [University of Montpellier 2], Carine Moussaed [University of Montpellier 2], Maria-Vittoria Salvetti [University of Pisa], Stephen Wornom [Lemma].

The purpose of our works in hybrid RANS/LES is to develop new approaches for industrial applications of LES-based analyses. In the foreseen applications (aeronautics, hydraulics), the Reynolds number can be as high as several tenth millions, a far too large number for pure LES models. However, certain regions in the flow can be much better predicted with LES than with usual statistical RANS (Reynolds averaged Navier-Stokes) models. These are mainly vortical separated regions as assumed in one of the most popular hybrid model, the hybrid Detached Eddy Simulation model. Here, “hybrid” means that a blending is applied between LES and RANS. The french-italian team has designed a novel type of hybrid model. This year, a novel dynamic formulation has been introduced in our models and tested. the new model has been adapted to very high Reynolds number. Carine Moussaed has presented her results in ECCOMAS (Vienna). In our set of benchmark test cases which are also ECINADS test cases, the flow past a circular cylinder at Reynolds number from 3900 to 1 Million could be passed with improved predictions of main properties like mean drag, root mean square of lift fluctuation, and base pressure.

5.3.2. Acoustics

Participants: ILya Abalakin [IMM-Moscou], Alain Dervieux [Tropics], Alexandre Carabias [Tropics], Tatyana Kozubskaya [IMM-Moscow], Bruno Koobus [University of Montpellier 2].

A method for the simulation of aeroacoustics on the basis of hybrid RANS/LES models has been designed and developed by a cooperation between the Computational Aeroacoustics Laboratory (CAL) of Intitute for Mathematical Modeling at Moscow and Inria. Further applications has been developed by the Russian team from the two common numerical scheme, the Mixed-Element-Volume at sixth-order, and the quadratic reconstruction scheme. This year the cooperation is concentrated on the study by Alexandre Carabias of a new quadratic reconstruction scheme, which extends the one developed by Hilde Ouvrard and Ilya Abalakin. This year, this scheme is also introduced in the Gamma-Sciport mesh adaptation loop.

5.4. Environmental flows

Participants: Hervé Guillard, Boniface Nkonga, Marco Bilanceri, Maria-Vittoria Salvetti [University of Pisa, Italy], Imad Elmahi [University of Oudja, Morocco].

Mobile bed and sediment transport

The numerical approximation of a model coupling the shallow-water equations with a sediment transport equation for the morphodynamics have been studied. In shallow-water problems, time advancing can be carried out by explicit schemes. However, if the interaction with the mobile bed is weak, the characteristic time scales of the flow and of the sediment transport can be very different introducing time stiffness in the global problem. For this case, it is of great interest to use implicit schemes. The time integration stategy that we have devised is based on a defect-correction approach and on a time linearization, in which the flux Jacobians are computed through automatic differentiation. The aim of the present work is to investigate the behaviour of this time scheme in different situations related to environmental flows. This work has been published in [14] and is now applied to the study of the Nador Lagoon in Morocco.

COFFEE Project-Team (section vide)

CONCHA Project-Team

6. New Results

6.1. Convergence of adaptive finite element algorithms

Participants: Roland Becker, Shipeng Mao, David Trujillo.

The theoretical analysis of mesh-adaptive methods is a very active field of research. We have generalized our previous results concerning optimality of adaptive methods to nonconforming finite elements [53]. Our results include the error due to iterative solution of the system matrices by means of a simple stopping criterion related to the error estimator. The main difficulty was the treatment of the nonconformity which leads to a perturbation of the orthogonality relation at the heart of the proofs for conforming finite elements. We have been able to extend this result to the Stokes equations, considering different lowest-order nonconforming finite elements on triangular and quadrilateral meshes [16].

In [19] we have shown that the smallness assumption required in all former proofs of optimality of adaptive finite element methods can be overcome, at least in some situations.

Finally, we have shown optimality of a new goal-oriented method in [21].

Our theoretical studies, which are motivated by the aim to develop better adaptive algorithms, have been accompanied by software implementation with the Concha library, see Section 5.1 . It hopefully opens the door to further theoretical and experimental studies.

6.2. Finite element methods for interface problems

Participants: Nelly Barrau, Roland Becker, Robert Luce.

The original formulation of NXFEM [63] is based on the doubling of elements. In some situations, as the case of a moving interface, it is computationally more convenient to have a method with local enrichment, as for the standard XFEM. In [47] we have developed such an approach based on NXFEM. We have developed an hierarchical formulation for a fictitious domain formulation in [7].

One of the technical difficulties is the simultaneous robustness of the method with respect to the size of the intersection of a mesh cell with the interface and with respect to the discontinuous diffusion parameters. In [ ] (note CRAS 2012) we proposed a modified formulation of the NXFEM which allows us to obtain this robustness to solve the Darcy equation.

In connection with the thesis of Nelly Barrau, supervised by Robert Luce and Eric Dubach (LMAP) we have:

- implemented lots of geometrical tools in 2D and 3D necessary to use the NXFEM methods,
- extended the method to P_k and Q_k finite elements ([42],
- generalized the residual estimator and developed an adaptative process with hanging node (8),
- adapted the method to the transport equation.

6.3. A posteriori error estimators based on $H(\mathrm{div})$-reconstructed fluxes

Participants: Roland Becker, Daniela Capatina, Robert Luce.

Mesh adaptivity is nowadays an essential tool in numerical simulations; in order to achieve it, reliable and efficient, easily computable *a posteriori* error estimators are needed. Such estimators obtained by reconstructing locally conservative fluxes in the Raviart-Thomas finite element space have been largely employed in the past years.

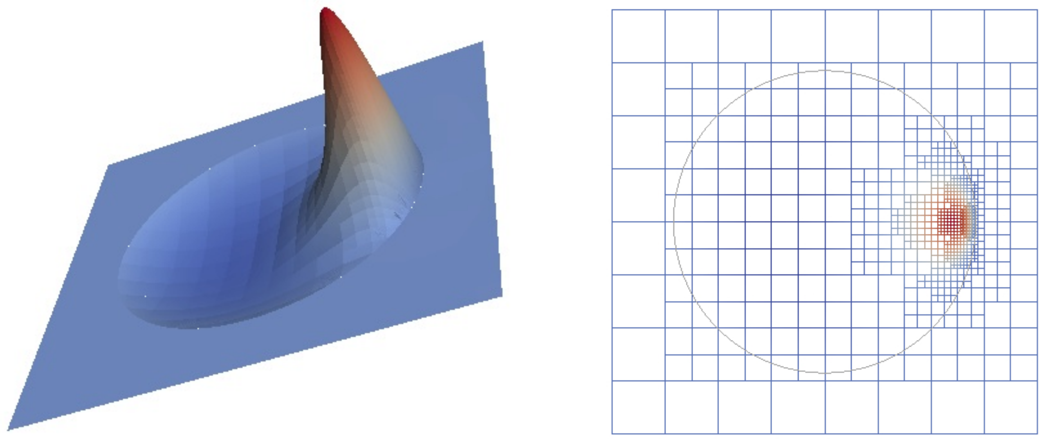


Figure 8. Result of an adaptative process with hanging node

We have so far considered the convection-diffusion equation and proposed a unified framework for several finite element approximations (conforming, nonconforming and discontinuous Galerkin). The main advantage of our approach is to use, contrarily to the existing references, only the primal mesh for the flux reconstruction, which presents certain facilities from a computational point of view.

For this purpose, the construction of the $H(\text{div})$-vector involved in the error estimator is inspired by the hypercircle method cf. [56] and is achieved on patches, which may overlap. A patch depends on the type of the employed finite elements and is defined as the support of a basis function.

Our first results were presented in [12]. We are working on the extension to higher-order approximations, to quadrilateral meshes and to other model problems.

6.4. Discretization of Euler's equations

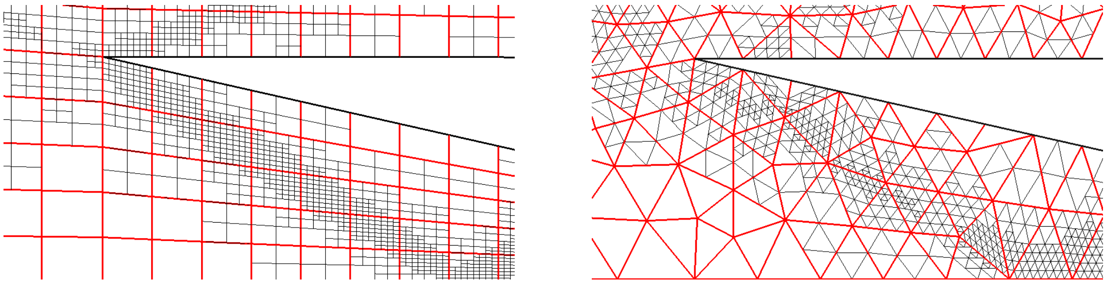
Participants: Roland Becker, Kossivi Gopki, Eric Schall, David Trujillo.

Over the past years, significant advances have been made in developing discontinuous Galerkin finite element methods (DGFEM) for applications in fluid flow and heat transfer. Certain features of the method have made it attractive as an alternative to other popular methods such as finite volume and more convenient finite element methods in thermal fluid engineering analyses. The DGFEM has been used successfully to solve hyperbolic systems of conservation laws. It makes use of the same local function space as the continuous method, but with relaxed continuity at inter-element boundaries. Since it uses discontinuous piecewise polynomial bases, the discretization is locally conservative and in the considered lowest-order case, the method preserves the maximum principle for scalar equations.

One of the challenges in Computational Fluid Dynamic (CFD) is to obtain as accurate as possible the solution of the problem under consideration at very low cost in terms of computational time. So our principal work is to find some relevant and robust strategies and technics of meshes adaptation in order to concentrate just the calculation where there are physical phenomena to capture. From Industrial point of view, the aim is to get the stationary solution as quick as possible with as much accuracy as possible. The main limitation of these results in CFD concern the underlying models: for example, nearly nothing seems to be known for (even linear) first-order systems or for realistic nonlinear equations. We therefore have developed different modern techniques, especially adaptive methods, to tackle this kind of problems in compressible CFD. The strategy is to iteratively improve the quality of the approximate solutions based on computed information (a posteriori error analysis).

In this way, a sequence of locally refined meshes is constructed, which allows for better efficiency as compared to more classical approaches in the presence of different kind of singularities. The main goal is to improve the aerodynamical design process for complex configurations by significantly reducing the time from geometry to solution at engineering-required accuracy using high-order adaptive methods.

One of our strategies of refinement is based on the creation of hanging nodes commonly called non-conforming refinement. The figures 9 show superposition of two kinds of meshes. One is a non-conforming refined mesh (black color) and the other one is the initial grid (red color) on which the refinement has been performed. It shows the technic of cutting the cells where singularities occur in the scramjet inlet.



(a) (b)

Figure 9. Superposition of non-conforming adapted black color) grid and initial grid (red color) – (a) quadrangles and (b) triangles.

The mesh adaptation is designed using some criteria as a posteriori error estimates. We have designed criteria based on the calculation of the jump of physical quantities like density, pressure, entropy, temperature and mach number at the inter-element. This criteria seems to be a very good indicator for the mesh adaptation. Figure 10 is the comparison of isoline of the density in scramjet internal flow at mach 3 of the initial mesh, the third and the sixth mesh after refinement.The indicator used is the density jump. It shows the impact and the accuracy of the solution obtained after the sixth iteration of the refinement.

The figure 11 shows the streamlines of the density in the scramjet inlet after the seventh iteration. This shows how the adaptation depicts almost clearly and accurately the shock waves and the expansion waves and their interactions in the domain.

Figure 12 represent the density isolines of a flow past cylinder test case using the non-conforming mesh adaptation with quadrangular an triangular girds.

We have also settled another indication which is hierarchical. It measures the difference of g_h with the physical quantity $g_{h/2}$ obtained by computation on a globally refined mesh $h/2$. This allows us the make comparison with the previous indicator. The case test considered for this comparison is an external flows past a cylinder airfoil at fixed free stream conditions : $M_\infty = 3$. The result is quite surprising the way one type of indicator can capture phenomenon that are not capture by the another one. In fact the hierarchical indicator seems to capture recirculation downstream to the obstacle which was not capture by the jump indicator (see figure 13)

We compare the computational time between a non-conforming mesh refinement and a globally mesh refined with nearly the same amount of cells. The meshes contain quadrangles or triangles. We can observe trough the following tables that the adapted meshes wether triangular or quadrangular meshes allow to save 20 to 90 times the computational time than the normal globally refined mesh. (see tables 1 and 2)

In table 1, the gain in time is 35 times in quadrangular grid case and 90 times triangular ones and in table 2, the gain in time: 18 times in quadrangular grid case and 58 times triangular ones. So one can say that the

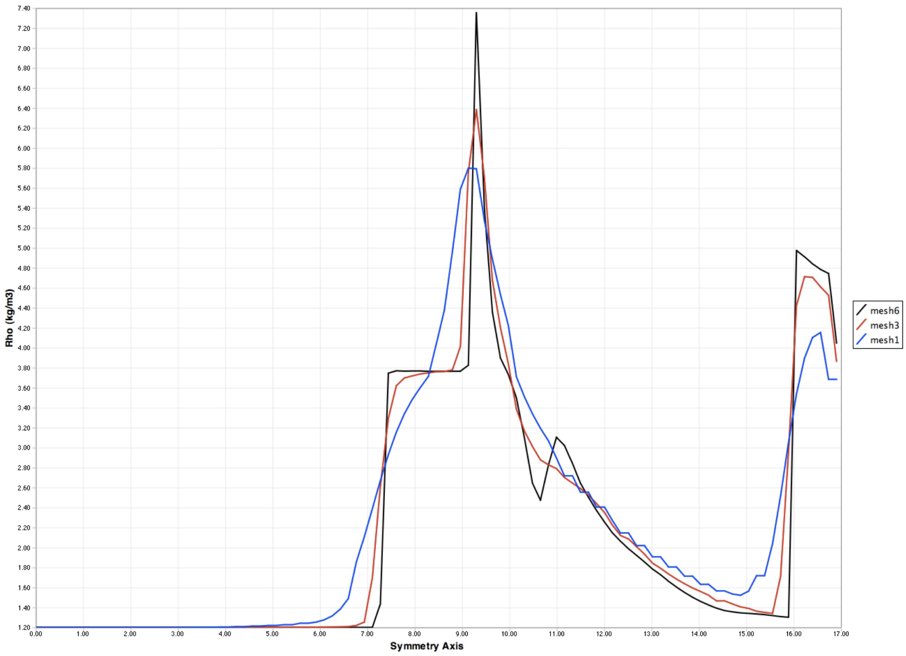


Figure 10. Cutlines along the symmetry axis of various meshes for the scramjet test case

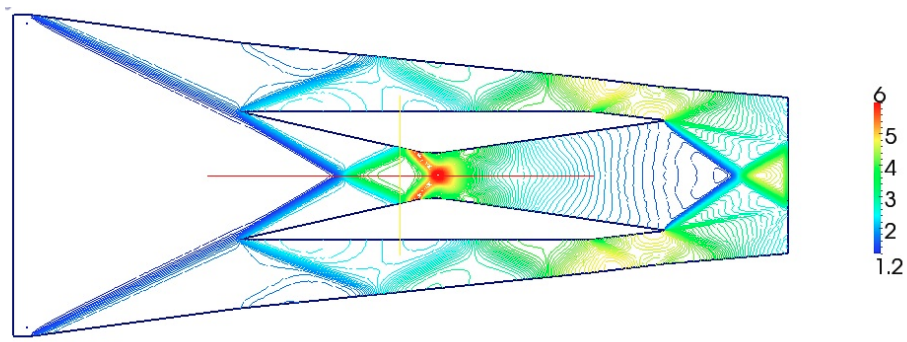
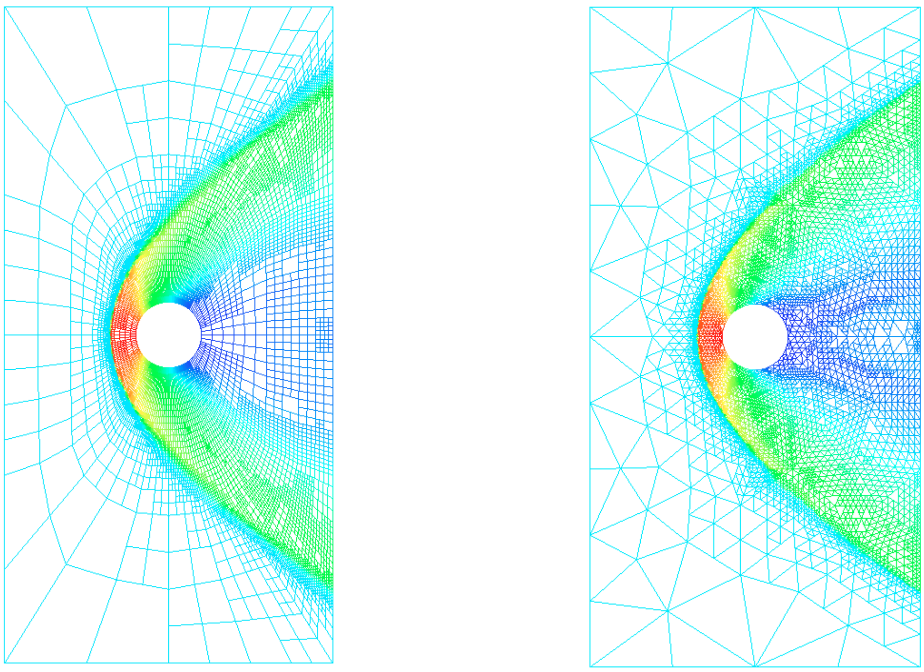
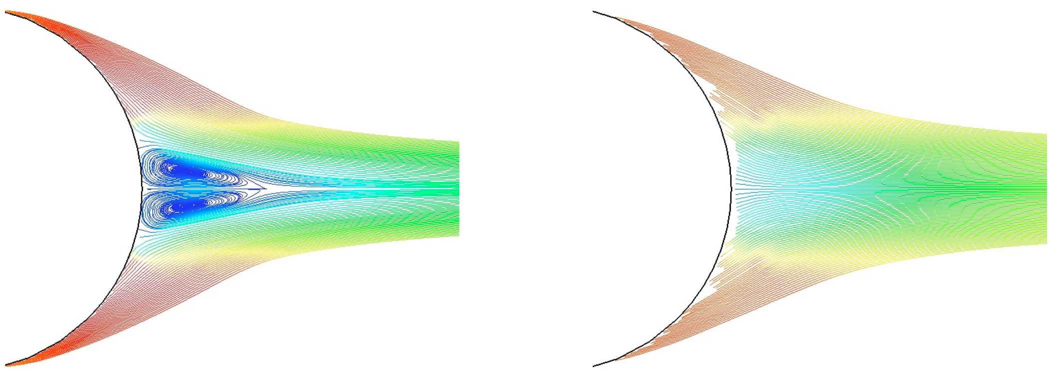


Figure 11. Density streamlines on grid obtained after the seveneth iteration of adaptive refinement procedure with density jump as indicator



(a) (b)

Figure 12. Locally adapted mesh on quadrilaterals (a) and triangles (b)



(a) (b)

Figure 13. Streamlines coloured by the density on meshes generated with hierarchical indicator (a) and with jump indicator (b)

Scramjet test case at mach=3

	Nodes	Cells	Segments	Compt. Time(s)
Scram_Quad_4	17043	15485	34308	25.0236
Scram_Quad_Uniform	17183	16640	33824	865.0177
Scram_Tri_4	9951	17005	29138	22.3141
Scram_Tri_Uniform	13295	25504	38800	2000.4269

Table 1

Flow past cylinder test case at mach=3

	Nodes	Cells	Segments	Compt. Time(s)
Cyl_Quad_5	11203	10174	23105	47.2187
Cyl_Quad_Uniform	10496	10240	20736	814.6168
Cyl_Tri_6	6480	10867	19264	79.7836
Cyl_Tri_Uniform	6032	11776	17808	4258.6618

Table 2

Figure 14. Comparison of computational times

adaptive mesh with the strategies and technics we have settled are efficient and robust in capturing physical phenomenon at a very reasonable low cost.

In concluding, the procedure of refinement permit to save computational time and have good accuracy of the approximated solution computed. Our focus is to continue the improve our methods and strategies in order to meet the requirement of accuracy, robustness and efficiency. Many other works are in hand such as slope limiters for high-order Discontinous Galerkin, low mach number computation with some remarkable approaches.

DEFI Project-Team

6. New Results

6.1. Qualitative methods for inverse scattering problems

6.1.1. Sampling methods with time dependent data

Participant: Houssem Haddar.

Together with A. Lechleiter and S. Marmorat we proposed and analyzed a time domain linear sampling method as an algorithm to solve the inverse scattering problem of reconstructing an obstacle with Robin or Neumann boundary condition from time-dependent near-field measurements of scattered waves. Our algorithm is based on our earlier work to solve a similar inverse scattering problem for obstacles with Dirichlet boundary conditions. In addition to the analysis of a different scattering problem, we provided a substantial improvement of the method on both theoretical and numerical levels. More specifically, we analyzed the method for incident waves generated by pulses with bounded spectrum. Moreover, adapting the function space setting to this type of data allowed us to provide a simpler analysis. On the numerical side, we presented a fast implementation of the inversion algorithm that relies on a FFT-based evaluation of the near-field operator [34].

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 [24], [25], [23], 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 [4], [44], [43], [48].

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-direction.inria.fr/international/PHP/Networks/LiEA.php 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 [32]. We are also in the process of editing a spacial issue of the journal Inverse Problems dedicated to the use of these transmission eigenvalues in inverse problems. Our recent contributions are the following:

- In collaboration with M. Fares and F. Collino from CERFACS and A. Cossonnière from ENSIEETA we finalized our work on the use of a surface integral equation approach to numerically compute transmission eigenvalues for inclusions with piecewise constant index. The main difficulty behind this procedure is the compactness of the obtained integral operator in usual Sobolev spaces associated with the forward scattering problem. We solved this difficulty by introducing a preconditioning operator associated with a “coercive” transmission problem. On the theoretical side, together with A; Cossonnière we also finalyzed the analysis of the Fredholm properties of the interior transmission problem for the cases where the index contrast changes sign outside the boundary by using the surface integral equation approach [16].

- With G. Giorgi, we developed a method that give estimates on the material properties using the first transmission eigenvalue. This method is based on reformulating the interior transmission eigenvalue problem into an eigenvalue problem for the material coefficients. We validated our methodology for homogeneous and inhomogeneous inclusions and backgrounds. We also treated the case of a background with absorption and the case of scatterers with multiple connected components of different refractive indexes [21].
- With F. Cakoni and D. Colton we initiated the study of transmission eigenvalues for absorbing media. In particular, we showed that, in the case of absorbing media, transmission eigenvalues form a discrete set, exist for sufficiently small absorption and for spherically stratified media exist without this assumption. For constant index of refraction, we also obtained regions in the complex plane where the transmission eigenvalues cannot exist and obtain a priori estimates for real transmission eigenvalues [14].
- With F. Cakoni and A. Cossonnière we considered the interior transmission problem corresponding to the inverse scattering by an inhomogeneous (possibly anisotropic) media in which an impenetrable obstacle with Dirichlet boundary conditions is embedded. Our main focus is to understand the associated eigenvalue problem, more specifically to prove that the transmission eigenvalues form a discrete set and show that they exist. The presence of Dirichlet obstacle brings new difficulties to already complicated situation dealing with a non-selfadjoint eigenvalue problem. In this work we employed a variety of variational techniques under various assumptions on the index of refraction as well as the size of the Dirichlet obstacle [15].

6.1.4. The factorization method for inverse scattering problems

6.1.4.1. The factorization method for cracks with impedance boundary conditions

Participants: Yosra Boukari, Houssem Haddar.

We use 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 [38].

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 real-izations 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 [42].

6.1.4.3. The factorization method for GIBC

Participants: Mathieu Chamaillard, Nicolas Chaulet, Houssem Haddar.

We are concerned with 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 are finalizing our 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 finalizing 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 are currently investigating two research directions:

- The development of 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.
- The extension of this work to 3D configurations with axisymmetric configuration at infinity, which has been started with the PostDoc of K. Riahi.

6.2.2. A min-max formulation for inverse scattering problems

Participants: Grégoire Allaire, Houssem Haddar, Dimitri Nicolas.

After having developed an inverse solver combining the use of Level-Set method and topological garadient method for multistatic inverse scattering problem and numerically showed how convergence can be achieved with intial guess provided by the Linear Sampling Method, we explored the use of an objective function that would lead to quicker and more stable reconstructions. This has been achieved through maximizing the least-square difference with respect to the Herglotz kernel of used incident wave while minimizing with respect to the geometrical parameters. Premliminary numerical experimentations showed that this procedure is viable and lead to quicker inversion algorithms [5].

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

Participant: Houssem Haddar.

Together with R. Kress we have 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 [41] 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.

6.2.4. A steepest descent method for inverse electromagnetic scattering problems

Participants: Houssem Haddar, Nicolas Chaulet.

In a continuation of our earlier work jointly with L. Bourgeois [13], we studied the application of 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 constraints in shape and topology optimization

Participant: Grégoire Allaire.

With François Jouve (LJLL) and Georgios Michailidis (Renault and CMAP), we propose a method to handle geometric constraints in shape and topology optimization. In the framework of the level-set method we rely on a notion of local thickness which is computed using the signed-distance function to the boundary of the shape. We implement this method in two and three space dimensions for a model of linear elasticity. We consider various formulations of the constrained optimization problem and compute a shape derivative to advect the shape. We discuss different ways to handle the constraints. The resulting optimized shape is strongly dependent on the initial guess and on the way the constraints are being treated.

6.3.2. A hybrid optimization method

Participant: Grégoire Allaire.

With Charles Dapogny (Renault and LJLL) and Pascal Frey (LJLL) we propose a method for structural optimization that relies on two alternative descriptions of shapes : on the one hand, they are exactly meshed so that mechanical evaluations by finite elements are accurate ; on the other hand, we resort to a level-set characterization to describe their deformation along the shape gradient. The key ingredient is a meshing algorithm for building a mesh, suitable for numerical computations, out of a piecewise linear level-set function on an unstructured mesh. Therefore, our approach is at the same time a geometric optimization method (since shapes are exactly meshed) and a topology optimization method (since the topology of successive shapes can change thanks to the power of the level-set method).

6.3.3. DeHomogenization

Participant: Olivier Pantz.

In most shape optimization problems, the optimal solution does not belong to the set of genuine shapes but is a composite structure. The homogenization method consists in relaxing the original problem thereby extending the set of admissible structures to composite shapes. From the numerical viewpoint, an important asset of the homogenization method with respect to traditional geometrical optimization is that the computed optimal shape is quite independent from the initial guess (even if only a partial relaxation is performed). Nevertheless, the optimal shape being a composite, a post-treatment is needed in order to produce an almost optimal non-composite (i.e. workable) shape. The classical approach consists in penalizing the intermediate densities of material, but the obtained result deeply depends on the underlying mesh used and the details level is not controllable. We proposed in [51] a new post-treatment method for the compliance minimization problem of an elastic structure. The main idea is to approximate the optimal composite shape with a locally periodic composite and to build a sequence of genuine shapes converging toward this composite structure. This method allows us to balance the level of details of the final shape and its optimality. Nevertheless, it was restricted to particular optimal shapes, depending on the topological structure of the lattice describing the arrangement of the holes of the composite. We lifted this restriction in order to extend our method to any optimal composite structure for the compliance minimization problem in [50]. Since, the method has been improved and a new article presenting the last results is in preparation. Moreover, we intend to extend this approach to other kinds of cost functions. A first attempt, based on a gradient method, has been made. Unfortunately, it was leading to local minima. Thus a new strategy has to be worked out. It will be mainly based on the same ideas than the one developed for the compliance minimization problem, but some difficulties are still to be overcome.

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. Robust Optimization

Participant: Olivier Pantz.

One of the main problem in shape optimization problems is due to the fact that the gradient is never computed exactly. When the current solution is far from a local optimum, this is not a problem: even a rough approximation of the gradient enable us to exhibit a descent direction. On the contrary, when close to a local optimal, a very precise computation of the gradient is needed. We intend, with G. Delgado, to use a-posteriori error estimates evaluate the errors made on the computation of the gradient and to ensure that at each step, a genuine descent direction is used in the gradient method.

6.3.6. Level-set method applied to structural optimization with contact

Participants: Houssem Haddar, Olivier Pantz.

The current study covers the design and implementation of a method for topological shape optimization in order to optimize multi-connected structures taking into account the contact that may arise between the different components. This project is motivated by the optimization of leaf springs, issue proposed by the company CORTEL and is conducted in the framework of the Master internship of M. Mahjoub. We proposed a method that relies on the use of a Level Set Method coupled with a penalty method to handle contact with different components. The level set function is used for instance to construct the penalization functional. Preliminary results showed that the method efficiently handle optimal design with a targeted non linear deformation behavior prescribed by the manufacturer.

6.3.7. 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. Asymptotic analysis of the interior transmission eigenvalues related to coated obstacles

Participants: Nicolas Chaulet, Houssem Haddar.

This work is a collaboration with Fioralba Cakoni from the University of Delaware (USA). The interior transmission eigenvalues play an important role in the area of inverse scattering problems. These eigenvalues can actually be determined by multi-static far field data. Thus, they could be used for non destructive testing. We focused on the case where the obstacle is a perfectly conducting body coated by some thin dielectric material. We derived and justified the asymptotic expansion of the first interior transmission eigenvalue with respect to the thickness of the coating for the TM electromagnetic polarization. This expansion provided interesting qualitative information about the behavior of these eigenvalues and also gave an explicit formula to compute the thickness of the coating.

6.4.2. 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 [18], [17]. 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.

6.4.3. Homogenization of thermal radiative transfer models in heterogeneous domains

Participant: Grégoire Allaire.

With my former PhD student, Zakaria Habibi, we studied the homogenization of heat transfer in periodic porous media where the fluid part is made of long thin parallel cylinders, the diameter of which is of the same order than the period. The heat is transported by conduction in the solid part of the domain and by conduction, convection and radiative transfer in the fluid part (the cylinders). A non-local boundary condition models the radiative heat transfer on the cylinder walls. To obtain the homogenized problem we first use a formal two-scale asymptotic expansion method. The resulting effective model is a convection-diffusion equation posed in a homogeneous domain with homogenized coefficients evaluated by solving so-called cell problems where radiative transfer is taken into account. In a second step we rigorously justify the homogenization process by using the notion of two-scale convergence. One feature of this work is that it combines homogenization with a 3D to 2D asymptotic analysis since the radiative transfer in the limit cell problem is purely two-dimensional. Eventually, we provide some 3D numerical results in order to show the convergence and the computational advantages of our homogenization method. We also focused on the contribution of the so-called second order corrector. If the source term is a periodically oscillating function (which is the case in our application to nuclear reactor physics), a strong gradient of the temperature takes place in each periodicity cell, corresponding to a large heat flux between the sources and the perforations. This effect cannot be taken into account by the homogenized model, neither by the first order corrector. We show that this local gradient effect can be reproduced if the second order corrector is added to the reconstructed solution. Z. Habibi received the 2012 Paul Caseau PhD prize in the field "modélisation et simulation numérique", prize created by the Académie des technologies and EDF.

6.4.4. Homogenization of complex flows in porous media

Participant: Grégoire Allaire.

With Robert Brizzi (CMAP), Jean-François Dufrêche (Marcoule and Montpellier), Andro Mikelic (Lyon 1) and Andrey Piatnitski (Narvik) we studied 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. Non-ideal effects are taken into account by the mean spherical approximation (MSA) model. We first study the existence of equilibrium solutions in the absence of external forces. When the motion is governed by a small static electric field and a small hydrodynamic force, we generalize O'Brien's argument to deduce a linearized model. We then proceed to the homogenization of these linearized equations and prove that the effective tensor satisfies Onsager properties, namely is symmetric positive definite. We eventually make numerical comparisons with the ideal case.

With my PhD student Harsha Hutridurga we study the convection and diffusion of a solute in a porous medium in the presence of a linear chemical reaction of adsorption/desorption on the pore surfaces. The mathematical model is a system of two coupled convection-diffusion equations, one in the bulk of the saturated fluid flowing in the porous medium, the other on the pore surface, at the interface with the solid part of the porous medium. The coupling takes place through a linear reaction term expressing the exchange of mass between the bulk concentration and the surface concentration. By a method of two-scale asymptotic expansion with drift we obtain the homogenized problem in a moving frame. We rigorously justify our upscaling approach by using the notion of two-scale convergence with drift. Some 2-d numerical tests are performed in order to study the effect of variations of the adsorption rate constant and surface molecular diffusion on the effective dispersion tensor.

With Irina Pankratova (Narvik) and Andrey Piatnitski (Narvik) we consider the homogenization of a non-stationary convection-diffusion equation posed in a bounded domain with periodically oscillating coefficients and homogeneous Dirichlet boundary conditions. Assuming that the convection term is large, we give the asymptotic profile of the solution and determine its rate of decay. In particular, it allows us to characterize the “hot spot”, i.e., the precise asymptotic location of the solution maximum which lies close to the domain boundary and is also the point of concentration. Due to the competition between convection and diffusion, the position of the “hot spot” is not always intuitive as exemplified in some numerical tests.

6.4.5. Multiscale finite elements

Participant: Grégoire Allaire.

With my PhD student Franck Ouaki we introduced a new multiscale finite element method to solve convection-diffusion problems where both velocity and diffusion coefficient exhibit strong variations at a much smaller scale than the domain of resolution. In that case, classical discretization methods, used at the scale of the heterogeneities, turn out to be too costly or useless. Our method aims at solving this kind of problems on coarser grids with respect to the size of the heterogeneities by means of particular basis functions. These basis functions are solutions to cell problems and are designed to reproduce the variations of the solution on an underlying fine grid. Since all cell problems are independent from each other, these problems can be solved in parallel, which makes the method very efficient when used on parallel architectures. The convergence proof of our method is still in progress. But, on the basis of results of periodic homogenization, an a priori error estimate, that represents a first step in the proof, has already been proved. A 2-d numerical implementation in FreeFem++ has also been performed.

6.4.6. 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.

6.4.7. 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. An article on this subject is currently in preparation.

6.4.8. Lattices

Participant: Olivier Pantz.

With A. Raoult and N. Meunier (Université Paris Descartes), we have compute the asymptotic limit of a square lattice with three-points interactions. Considering such interaction is important in the case of square lattices, because such lattices, if only endowed with two-points closest neighbor interactions, show no resistance to compression, what is quit restrictive. We prove in particular that under some symmetry assumptions on the type of elementary interactions, no micro-relaxation do occur and that the limit can be obtained by a mere quasiconvexication. Without those assumptions, the computation of the limit requires the resolution of a homogenization problem on an infinite number of cells, what is usually out of reach. Our work has been published in M3AS [26].

6.5. Diffusion MRI

Participants: Jing-Rebecca Li, Houssem Haddar, Julien Coatléven, 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.

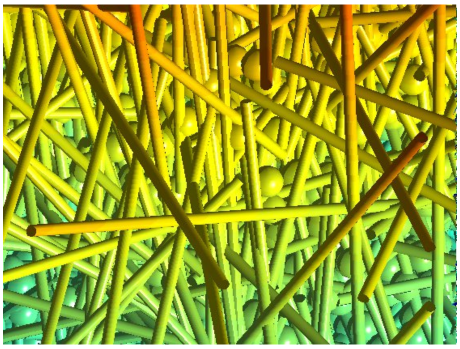


Figure 1. Computational domain for simulating diffusion in cerebral gray matter.

  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.

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.

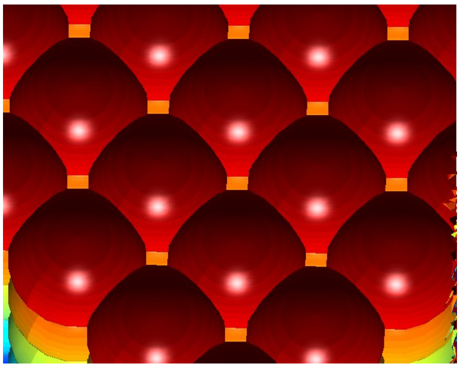


Figure 2. Computational domain for simulating tumor cells.

- We developed a homogenized model for the apparent diffusion coefficient (the slope of the log of the DMRI signal) of heterogenous cellular domains. An article on this topic has been submitted.
- We developed a reduce model of the complete DMRI signal (not just the slope as in the above) using more sophisticated homogenization methods. An article on this topic is under preparation.

GAMMA3 Project-Team

3. New Results

3.1. Validité des éléments finis usuels

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

éléments finis-éléments finis généralisés-P1-P2-Q1-Q2-Bézier

On continue l'étude sur les conditions assurant la validité géométrique des éléments finis usuels de degré 1 et 2. La formulation éléments finis ne conduisant pas toujours à une conclusion simple, on formule les éléments finis sous leur forme de Bézier. Ceci conduit à exhiber des conditions suffisantes (parfois nécessaires et suffisantes) de validité des éléments, c'est-à-dire des conditions garantissant la positiivité de leur jacobien. Pour les éléments de degré 2, on donne l'interprétion géométrique de ces conditions. Les éléments étudiés sont le triangle à 3 nœuds, le triangle à 6 nœuds, le quadrilatère à 4 nœuds et les quadrilatère à 8 et 9 nœuds, le tétraèdre à 4 nœuds et le tétraèdre à 10 nœuds puis les pentaèdres à 6, 15 et 18 nœuds et les hexaèdres à 8, 27 et 20 nœuds.

On regarde ensuite les éléments finis généralisés déduits d'une formulation en Bézier rationnels puis basés sur des fonctions B-splines et Nurbs.

3.2. Maillages tétraédriques de grande taille

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

Triangulation-tétraèdre p1-Hilbert- Maillage de grande taille

Le comportement en complexité des algorithmes de triangulation sur les "gros" maillage nous amène à utiliser les algorithmes de renumérotation de type Hilbert qui minimisent les défauts de cache. Cette technique est également utilisée comme aide à l'optimisation des "gros" maillages avec des gains en temps important. L'algorithme de renumérotation est multi-cœurs.

Des triangulations de plusieurs dizaines de millions de sommets sont construites en utilisant un "simple" ordinateur. La vitesse d'insertion frole le million de tétraèdres à la seconde.

Par coquetterie (et pour améliorer la robustesse dans l'absolu), on regarde ce que donne nos méthodes quand on construit des maillages de plus de un milliard de tétraèdres en séquentiel (une machine de un Tera de mémoire est utilisée). On vérifie que la taille des cavités peut être arbitrairement grande ce qui nécessite une programmation plus délicate permettant de traiter ces cas peu courants dans les situations habituelles.

3.3. Surface meshing with metric gradation control

Participants: Patrick Laug [correspondant], Houman Borouchaki.

Scientific computing requires the automatic generation of high quality meshes, in particular isotropic or anisotropic meshes of surfaces defined by a CAD modeler. For this purpose, two major approaches are called direct and indirect. Direct methods (octree, advancing-front or paving) work directly in the tridimensional space, while indirect methods consist in meshing each parametric domain and mapping the resulting mesh onto the composite surface. Using the latter approach, we propose a general scheme for generating “geometric” (or geometry-preserving) meshes by means of metrics. In addition, we introduce a new methodology for controlling the metric gradation in order to improve the shape quality. Application examples have shown the capabilities of this approach.

3.4. Metric field interpolation

Participants: Patrick Laug [correspondant], Houman Borouchaki.

To solve a physical problem formulated in terms of partial differential equations, the finite element method is generally used, based on a spatial discretization, or *mesh*, of the domain studied. Local adaptations of meshes to the behavior of the physical phenomena can improve the accuracy to the computed solutions, and in particular it is possible to capture high variations of the solution in specific areas while maintaining a reasonable number of degrees of freedom. In an initial phase, a mesh of the domain is built by using any particular method, then a first calculation of the solution of the problem is made. After choosing an appropriate criterion (Hessian and/or gradient of the solution, error estimate in general), areas that must be adapted by refinement or coarsening are detected in the initial mesh, and a new mesh is generated which is better adapted to the problem. This process is iterated until obtaining a mesh which satisfies the specified criterion (for which the finite element error is bounded by a specified threshold).

In practice, via an *a posteriori* analysis of the finite element error, a discrete map of sizes or metrics is set to the mesh vertices. This discrete size or metric field is made continuous by interpolating on the mesh, and the new mesh is generated according to this new field. In general, for a given point of the domain, a mesh element containing this point is found, and the interpolation of the size or metric field at this point is made from the sizes or metrics associated with the vertices of the containing element. For a scalar size field, the interpolation is straightforward by considering any interpolation scheme (for instance linear or geometric). On the other hand, the same scheme cannot be applied in the case of metrics representing a tensor field. However, several approaches have been proposed based on the link between a size and the corresponding metric and, in most cases, the interpolation scheme for sizes is applied to a power or the logarithm of the metrics. In particular, as a size h is represented by the isotropic metric $\mathcal{M} = \frac{1}{h^2}\,\mathcal{I}$, where $\mathcal{I}$ is the identity matrix, a possible link consists in approximating the size by $\mathcal{M}^{-\frac{1}{2}}$, then applying the size interpolation scheme to this new metric and finally recovering the interpolated metric. These schemes are still an approximation and require the calculation of the eigenvalues of $\mathcal{M}$ which is generally costly.

In this work, a new method for interpolating discrete metric fields is proposed. It is based on the "natural decomposition" of metrics using the LU factorization. With this decomposition, for each metric, the natural sizes along particular (or natural) directions can be retrieved, thus the size interpolation scheme can be applied to both natural directions and sizes, and the interpolation on the metrics is obtained. The proposed method is faster than those mentioned above and provides a continuous metric field with low variations. Some numerical examples illustrate our methodology.

3.5. Large deformation simulation using adaptive remeshing

Participants: Patrick Laug [correspondant], Houman Borouchaki.

The object of non-linear solid and structural mechanics is the modeling and the computation of structures with strong non-linearities, both geometrical and physical. The aim is to simulate the behavior of a mechanical part submitted to various mechanical stresses, in order to improve its mechanical strength, or even to optimize its manufacturing process with respect to damage occurrence. Among various theoretical, numerical and geometric tools involved in such a simulation, the interest in adaptive remeshing is really high nowadays. It is generally based on local refinement (governed by error estimation) and vertex smoothing strategies. Let us mention that the main difficulty lies in the fact that, in large strains, the domain geometry is variable and cannot be defined in an explicit way.

New contributions to the strategy using adaptive meshing and *a posteriori* error estimation in large elasto-plasticity have been developed. We are interested in the problem of remeshing a mechanical structure composed of several parts (which are in contact) subjected to large plastic deformations. A general scheme, constituted by several steps necessary to an almost optimal representation of the evolving domain, is proposed. These steps are divided into two main categories: the definition of the boundary of the deformed parts and the whole remeshing of the parts. The remeshing is governed by a mesh size map representing the conformity with the underlying geometry of the deformed parts, the improvement of the accuracy of the desired mechanical fields, and the convergence of the mechanical process as well. This size map results from an *a posteriori* estimation of the "interpolation error" independently from the considered mechanical fields. The final deformation after the whole simulation is assumed to be obtained iteratively by "small" deformations (which is the case in the framework of an explicit integration scheme to solve the problem). After such a small deformation, rigid parts are moved and deformable parts are slightly distorted (assuming that each mesh element is still valid). The remeshing is applied to deformable parts after each deformation increment. The proposed technique is used to simulate the impact of a projectile on a confined explosive. We show in particular that the ignition of the explosive appears in two different areas.

3.6. Maillage d'un milieu géologique et d'ouvrages de stockage

Participants: Patrick Laug [correspondant], Houman Borouchaki.

Cette étude a été menée dans le cadre du partenariat stratégique ANDRA/Inria. L'objectif est la construction d'un maillage statique 3D prenant en compte la géométrie des couches d'un milieu géologique et celle d'ouvrages de stockage afin de réaliser un calcul d'hydraulique et de transfert de solutés. En particulier, ce maillage sera exploité pour mener des calculs préparatoires aux calculs de sûreté. Il permettra de mieux représenter à l'échelle du milieu géologique les différentes voies de transfert (ouvrages et géologie multi-couches) des radionucléides, en considérant les évolutions géodynamiques, et de contribuer à identifier les simplifications éventuelles qui seront définies pour établir le modèle conceptuel de calcul de performances et de sûreté.

Les données d'entrée représentent la description géométrique du milieu géologique incluant les ouvrages de stockage. Le schéma de construction comprend quatre étapes :

1. Prétraitement des données d'entrée. Les sommets multiples du maillage volumique sont fusionnés afin de pouvoir extraire une topologie conforme. Grâce à cette topologie, les surfaces interfaces entre deux couches consécutives sont identifiées. Ces surfaces représentent des contraintes surfaciques que le mailleur volumique doit respecter. En outre, les lignes intersections entre ces surfaces contraintes, appelées lignes d'affleurement, sont identifiées. De même, ces lignes représentent des contraintes linéiques pour le mailleur volumique. Afin de définir la ligne polygonale associée à chaque rivière, les arêtes de l'enveloppe supérieure du maillage volumique de référence (surface topographique) dont les deux extrémités ont le même code de rivière sont identifiées.

2. Définition de la géométrie du domaine 2D de référence. On définit le plan de référence comme étant le plan d'équation $z = 0$, et le domaine 2D de référence comme la trace du polygone de l'extension horizontale dans ce plan. Toutes les contraintes linéiques (lignes d'affleurement, rivières et contours des ouvrages) sont projetées verticalement sur le plan de référence et leurs traces dans le domaine de référence sont retenues. En outre, des nouvelles lignes contraintes parallèles aux contours des ouvrages sont insérées afin de mieux contrôler la génération du maillage du domaine de référence. L'ensemble de toutes les lignes du domaine de référence est rendu conforme par ajout des points aux intersections éventuelles de ces lignes, et aussi par fusion des points et des lignes coïncidents.

3. Construction du maillage quad-dominant du domaine 2D de référence. Le maillage du domaine de référence est généré en utilisant un schéma adaptatif de construction de maillages quad-dominants. Dans un premier temps, un maillage quad-dominant initial du domaine est construit en spécifiant une taille fixe sur les lignes d'affleurement et les rivières et une taille dépendant de la grandeur des ouvrages sur ces derniers. Afin de contrôler la gradation du maillage (rapport maximal entre les longueurs d'arêtes issues d'un même sommet), deux maillages quad-dominants adaptés sont générés. Ici, l'adaptation consiste à modifier la carte de taille courante pour respecter le seuil de gradation spécifié.

4. Construction du maillage hex-dominant 3D du milieu. Le maillage volumique du milieu géologique est généré par extrusion verticale du maillage quad-dominant du domaine de référence. Deux types de configuration sont considérés : extrusion d'un quadrilatère (dit de base) du maillage du domaine de référence et extrusion d'un triangle (dit de base) du maillage du domaine de référence. Dans le premier cas, selon la configuration des surfaces (surfaces interfaces entre deux couches ou faces supérieures ou inférieures d'ouvrages) rencontrées, des hexaèdres et des prismes sont générés. Plus précisément, dans ce cas, l'extrusion résulte en un ensemble de quadrilatères ordonnés verticalement avec quatre arêtes appartenant à la même surface ou deux arêtes opposées appartenant chacune à une surface. Les quadrilatères consécutifs sont connectés et, en fonction du nombre de sommets communs entre deux quadrilatères consécutifs, des hexaèdres ou des prismes sont générés. Par ailleurs, une configuration de quadrilatère est validée si d'une part chaque élément résultant est géométriquement valide (hexaèdre, prisme ou pyramide) et si, d'autre part, il contient son barycentre et ses faces sont quasi-planes. Dans le cas contraire, le quadrilatère de base est subdivisé en deux triangles et généralement selon la diagonale donnant une configuration de deux triangles de Delaunay.

3.7. Advanced meshing and remeshing procedure for mechanical and numerical simulations

Participants: Abel Cherouat [correspondant], Houman Borouchaki, Paul-Louis George, Patrick Laug, Zhu Aichun, Jie Zhang, Faouzi Slimani, Guillaume Dufaye.

Most metal forming parts involve complex geometry and flow characteristics as large (visco)-plasticity flow, heat exchange, ductile damage, evolving contact with friction. An intrinsic difficulty in metal forming process is the constantly changing configuration of the deforming part (finite transformation, thermo-plastic flow). In metal forming, the mesh size should be adapted to the curvature of complex tools in order to optimize the contact boundaries and the damaged zones. These problems can be resolved if an adaptive remeshing scheme is incorporated automatically in the finite element analysis. It is necessary to adapt the mesh in order to improve the geometry of the deformed part and the damage localization. To mesh the 3D computational domain, we apply a new optimization approach which uses a combined Delaunay-frontal method to define field points and to construct the connection between these points or with a given prescribed size map (error estimate). The first objective of this project is to develop a 3D advanced remeshing procedure (error estimation, field transfer, optimisation meshing) for metal forming. The second objective is to integrate in a computational environment the mechanical model, 3D reconstruction from images, reliability-optimisation and the remeshing procedure using the ABAQUS/Explicit solver and the adaptive mesher. Application is dedicated to some examples (side pressing, blanking and orthogonal cutting, 3D guillotining, thermo-hydroforming and forging) for metal forming and breast and porous metal foam material reconstitution.

3.8. Effect of fibre geometrical morphology on the mechanical properties of PolyPropylene Hemp fibre composite material

Participants: Abel Cherouat [correspondant], Florent Ilczyszyn.

These last years, hemp fibres have been used as reinforcement for compound based on polymer in different industrial manufacturing for their interesting mechanical and ecological properties. Hemp fibres present a non-homogeneous cross section and complex geometry that can have a high effect on their mechanical properties. The mechanical properties of hemp fibres are rather difficult to determine and request a specific characterization method. In this project, micro-tensile tests coupled with numerical imaging treatments, meshing reconstitution and finite elements computations are investigated. The numerical imaging allows to define finely the hemp cross section along the fibre and aims to reconstruct a 3D hemp fibre CAD using adaptive mesh.

3.9. Mise au point de méthodes de remaillage adaptatif 3D dans le cadre de simulations numériques de mise en forme de structure minces

Participants: Houman Borouchaki, Abel Cherouat, Laurence Moreau [correspondant].

Au cours des simulations numériques de mise en forme en 3D, les grandes déformations mises en jeu font que le maillage subit de fortes distorsions. Il est alors nécessaire de remailler continuellement la pièce afin de pouvoir capturer les détails géométriques des surface en contact, adapter la taille du maillage à la solution physique et surtout pouvoir effectuer la simulation jusqu'à la fin du procédé de mise en forme. Lorsque la pièce est comprise entre des outils rigides (cas de l'emboutissage), aux problèmes de remaillage s'ajoutent aussi des difficultés sur la gestion du contact entre les pièce. Une méthode couplant une stratégie de remaillage adaptatif et une technique de projection a été développée. La méthode de remaillage adaptatif, basée sur des techniques de raffinement et déraffinement est contrôlée par des cartes de taille géométrique et physique. La projection des nouveaux nœuds sur l'outil permet de conserver le contact entre la pièce et l'outil. Afin de pouvoir réaliser des simulations numériques de composites tissés, une procédure spécifique a été ajoutée au remailleur afin de pouvoir raffiner les éléments finis bi-composants (association d'éléments finis de barre et de membrane orientés matérialisant le comportement de fibres chaîne et trame). Le formage incrémental est un procédé de mise en forme de tôle récent sans poinçon ni matrice, basé sur la déformation progressive du flan à l'aide d'un simple outil de forme hémisphérique commandé par une machine à commande numérique. L'inconvénient de ce nouveau procédé étant le temps de calcul, nous avons proposé une méthode de remaillage adaptatif permettant de raffiner le maillage uniquement au voisinage de l'outil rigide, là où les déformations ont lieux et permettant de déraffiner le maillage après le passage de l'outil rigide.

3.10. Mise au point de méthodes de remaillage adaptatif 3D dans le cadre de simulations numériques de mise en forme de structure minces

Participants: Houman Borouchaki, Abel Cherouat, Laurence Moreau [correspondant].

L'objectif est de reconstruire un maillage de la surface 3D d'un buste féminin à partir d'images 2D issues des prises de vue simultanées de plusieurs appareils photos numériques (photos prises sous des angles différents). Une cabine de mesure, équipée de 24 appareils photos numériques, 6 vidéoprojecteurs, pilotée par un ordinateur extérieur à la cabine a été développée et permet d'acquérir de manière simultanée 24 photos numériques du buste sous des angles différents. Un algorithme original basé sur l'utilisation d'un motif projeté sur le buste a été développé et programmé pour la corrélation entre les images 2D. Une méthode de triangulation 3D associée à une technique d'optimisation a été développée et permet de déterminer les positions 3D des points à partir des pixels de vues différentes.

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

Participants: Dominique Barchiesi [correspondant], Thomas Grosges, Michael François.

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.

3.12. Développement de méthodes avancées et maillages appliqués àa l’étude de la nanomorphologie des nanotubes/fils en suspension liquide

Participants: Dominique Barchiesi, Houman Borouchaki, Abel Cherouat, Anis Chaari, Thomas Grosges [correspondant], Laurence Moreau.

Ce projet de recherche (NANOMORPH) a pour objet principal le de´veloppement et la mise au point d’une instrumentation optique pour de´terminer la distribution en tailles et le coefficient de forme de nanofils (NF) ou de nanotubes (NT) en suspension dans un e´coulement. Au cours de ce projet, deux types de techniques optiques comple´mentaires sont de´veloppe´es. La premie`re, base´e sur la diffusion statique de la lumie`re, ne´cessite d’e´tudier au pre´alable la physico-chimie de la dispersion, la stabilisation et l’orientation des nanofils dans les milieux d’e´tude. La seconde me´thode, base´e sur une me´thode opto-photothermique pulse´e, ne´cessite en sus, la mode´lisation de l’interaction laser/nanofils, ainsi que l’e´tude des phe´nome`nes multiphysiques induits par ce pro-cessus. L’implication de l’e´quipe-projet GAMMA3 concerne principalement la simulation mul- tiphysique de l’interaction laser-nanofils et l’e´volution temporelle des bulles et leurs formations. L’une des principales difficulte´s de ces proble´matiques est que la ge´ome´trie du domaine est variable (a` la fois au sens ge´ome´trique et topologique). Ces simulations ne peuvent donc eˆtre re´alise´es que dans un sche´ma adaptatif de calcul ne´cessitant le remaillage tridimensionnel mobile, de´formable avec topologie variable du domaine (formation et e´volution des bulles au cours du temps et de l’espace).

3.13. 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], Thomas Grosges, Abel Cherouat, Thomas Grosges, Houman Borouchaki, Laurence Giraud-Moreau, Sameh Kessentini, Anis Chaari, Fadhil Mezghani.

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 une 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 2012 a constitué en une 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.

3.14. Mesh adaptation for very high-order numerical scheme

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

In the past, we have demonstrate that multi-scale anisotropic mesh adaptation is a powerful tool to accurately simulate compressible flow problem 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.

3.15. Visualisation et modification des maillages courbes d'ordre élevé

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

Dans le cadre du projet ILab, des nouveaux algorithmes de visualisation et de modifications interactives des maillages courbes et hybrides ont été développés. En effet, une des principales difficultés dans la génération de maillages courbes reste la visualisation. Il est également nécessaire de disposer d'algorithmes de corrections interactifs car les maillages de surfaces initiaux (de degré 2) sont pour la plupart faux.

3.16. A changing-topology ALE numerical scheme

Participants: Frédéric Alauzet [correspondant], Nicolas Baral.

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.

3.17. 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.

3.18. Maillages hexaédriques et calcul parallèle

Participant: Loïc Maréchal [correspondant].

Développement d'un remailleur de surfaces par la méthode octree. Celui-ci permet de passer d'une surface triangulée à problèmes (intersections de triangles, non-conformités, trous, etc.) à un maillage valide au sens des éléments finis.

Nouvelle version de la librairie d'aide au calcul sur GPU, GMLIB2, permettant de porter des codes travaillant sur des maillages de manière bien plus simple et efficace que la précédente. Des accélérations de l'ordre de 30, par rapport à un CPU en séquentiel, ont été obtenus avec le solveur Wolf et le mailleur Hexotic sur une carte Quadro 6000.

De nombreux développements sur le mailleur hexaédrique Hexotic ont été réalisés suite aux demandes de nombreux acheteurs industriels potentiels.

IPSO Project-Team

5. New Results

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

In [37], 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.

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

In [38], 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. Röß ler, Appl. Num. Math., 59, 2009].

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

In [39], 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.

5.4. High weak order methods for stochastic differential equations based on modified equations

Inspired by recent advances in the theory of modified differential equations, we propose in [11], a new methodology for constructing numerical integrators with high weak order for the time integration of stochastic differential equations. This approach is illustrated with the constructions of new methods of weak order two, in particular, semi-implicit integrators well suited for stiff (mean-square stable) stochastic problems, and implicit integrators that exactly conserve all quadratic first integrals of a stochastic dynamical system. Numerical examples confirm the theoretical results and show the versatility of our methodology.

5.5. Analysis of the finite element heterogeneous multiscale method for nonmonotone elliptic homogenization problems

In [13], an analysis of the finite element heterogeneous multiscale method for a class of quasilinear elliptic homogenization problems of nonmonotone type is proposed. We obtain optimal convergence results for dimension $d \leq 3$. Our results, which also take into account the microscale discretization, are valid for both simplicial and quadrilateral finite elements. Optimal a-priori error estimates are obtained for the H^1 and L^2 norms, error bounds similar as for linear elliptic problems are derived for the resonance error. Uniqueness of a numerical solution is proved. Moreover, the Newton method used to compute the solution is shown to converge. Numerical experiments confirm the theoretical convergence rates and illustrate the behavior of the numerical method for various nonlinear problems.

5.6. Coupling heterogeneous multiscale FEM with Runge-Kutta methods for parabolic homogenization problems: a fully discrete space-time analysis

Numerical methods for parabolic homogenization problems combining finite element methods (FEMs) in space with Runge-Kutta methods in time are proposed in [14]. The space discretization is based on the coupling of macro and micro finite element methods following the framework of the Heterogeneous Multiscale Method (HMM). We present a fully-discrete analysis in both space and time. Our analysis relies on new (optimal) error bounds in the norms $L^2(H^1)$, $C^0(L^2)$, and $C^0(H^1)$ for the fully discrete analysis in space. These bounds can then be used to derive fully discrete space-time error estimates for a variety of Runge-Kutta methods, including implicit methods (e.g., Radau methods) and explicit stabilized method (e.g., Chebyshev methods). Numerical experiments confirm our theoretical convergence rates and illustrate the performance of the methods.

5.7. A priori error estimates for finite element methods with numerical quadrature for nonmonotone nonlinear elliptic problems

The effect of numerical quadrature in finite element methods for solving quasilinear elliptic problems of nonmonotone type is studied in [12]. Under similar assumption on the quadrature formula as for linear problems, optimal error estimates in the L^2 and the H^1 norms are proved. The numerical solution obtained from the finite element method with quadrature formula is shown to be unique for a sufficiently fine mesh. The analysis is valid for both simplicial and rectangular finite elements of arbitrary order. Numerical experiments corroborate the theoretical convergence rates.

5.8. An Isogeometric Analysis Approach for the study of the gyrokinetic quasi-neutrality equation

In [25], a new discretization scheme of the gyrokinetic quasi-neutrality equation is proposed. It is based on Isogeometric Analysis; the IGA which relies on NURBS functions, seems to accommodate arbitrary coordinates and the use of complicated computation domains. Moreover, arbitrary high order degree of basis functions can be used. Here, this approach is successfully tested on elliptic problems like the quasi-neutrality equation.

5.9. Guiding-center simulations on curvilinear meshes using semi-Lagrangian conservative methods

The purpose of this work [32] is to design simulation tools for magnetised plasmas in the ITER project framework. The specic issue we consider is the simulation of turbulent transport in the core of a Tokamak plasma, for which a 5D gyrokinetic model is generally used, where the fast gyromotion of the particles in the strong magnetic field is averaged in order to remove the associated fast time-scale and to reduce the dimension of 6D phase space involved in the full Vlasov model. Very accurate schemes and efficient parallel algorithms are required to cope with these still very costly simulations. The presence of a strong magnetic field constrains the time scales of the particle motion along and accross the magnetic field line, the latter being at least an order of magnitude slower. This also has an impact on the spatial variations of the observables. Therefore, the efficiency of the algorithm can be improved considerably by aligning the mesh with the magnetic field lines. For this reason, we study the behavior of semi-Lagrangian solvers in curvilinear coordinates. Before tackling the full gyrokinetic model in a future work, we consider here the reduced 2D Guiding-Center model. We introduce our numerical algorithm and provide some numerical results showing its good properties.

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

In [45], 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.

5.11. Kinetic/fluid micro-macro numerical schemes for Vlasov-Poisson-BGK equation using particles

This work [24] is devoted to the numerical simulation of the Vlasov equation in the fluid limit using particles. To that purpose, we first perform a micro-macro decomposition as in [Benoune, Lemou, Mieussens, JCP 08] where asymptotic preserving schemes have been derived in the fluid limit. In [Benoune, Lemou, Mieussens, JCP 08] , a uniform grid was used to approximate both the micro and the macro part of the full distribution function. Here, we modify this approach by using a particle approximation for the kinetic (micro) part, the fluid (macro) part being always discretized by standard finite volume schemes. There are many advantages in doing so: (i) the so-obtained scheme presents a much less level of noise compared to the standard particle method; (ii) the computational cost of the micro-macro model is reduced in the fluid regime since a small number of particles is needed for the micro part; (iii) the scheme is asymptotic preserving in the sense that it is consistent with the kinetic equation in the rarefied regime and it degenerates into a uniformly (with respect to the Knudsen number) consistent (and deterministic) approximation of the limiting equation in the fluid regime.

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

In this paper [26], 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.

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

In [55], 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, Jin, SIAM J. Num. Anal. 05], where a coupled system of two equations, one at the mesoscopic and the other at the macroscopic scale, is solved. 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.

5.14. Accuracy of unperturbed motion of particles in a gyrokinetic semi-Lagrangian code

Inaccurate description of the equilibrium can yield to spurious effects in gyrokinetic turbulence simulations. Also, the Vlasov solver and time integration schemes impact the conservation of physical quantities, especially in long-term simulations. Equilibrium and Vlasov solver have to be tuned in order to preserve constant states (equilibrium) and to provide good conservation property along time (mass to begin with). Several illustrative simple test cases are given in [36] to show typical spurious effects that one can observes for poor settings. We explain why Forward Semi-Lagrangian scheme bring us some benefits. Some toroidal and cylindrical GYSELA runs are shown that use FSL.

5.15. High order Runge-Kutta-Nyström splitting methods for the Vlasov-Poisson equation

In this work [46], we derive the order conditions for fourth order time splitting schemes in the case of the $1D$ Vlasov-Poisson system. Computations to obtain such conditions are motivated by the specific Poisson structure of the Vlasov-Poisson system : this structure is similar to Runge-Kutta-Nyström systems. The obtained conditions are proved to be the same as RKN conditions derived for ODE up to the fourth order. Numerical results are performed and show the benefit of using high order splitting schemes in that context.

5.16. A Discontinuous Galerkin semi-Lagrangian solver for the guiding-center problem

In this paper [49], we test an innovative numerical scheme for the simulation of the guiding-center model, of interest in the domain of plasma physics, namely for fusion devices. We propose a 1D Discontinuous Galerkin (DG) discretization, whose basis are the Lagrange polynomials interpolating the Gauss points inside each cell, coupled to a conservative semi-Lagrangian (SL) strategy. Then, we pass to the 2D setting by means of a second-order Strangsplitting strategy. In order to solve the 2D Poisson equation on the DG discretization, we adapt the spectral strategy used for equally-spaced meshes to our Gauss-point-based basis. The 1D solver is validated on a standard benchmark for the nonlinear advection; then, the 2D solver is tested against the swirling deformation ow test case; nally, we pass to the simulation of the guiding-center model, and compare our numerical results to those given by the Backward Semi-Lagrangian method.

5.17. Asymptotic preserving schemes for highly oscillatory kinetic equation

This work [48] is devoted to the numerical simulation of a Vlasov-Poisson model describing a charged particle beam under the action of a rapidly oscillating external electric 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 "double-scale" reformulation of the initial equation, with the introduction of an additional periodic variable.

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

This work [47] focusses 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.

5.19. Orbital stability of spherical galactic models

In [31], we consider the three dimensional gravitational Vlasov Poisson system which is a canonical model in astrophysics to describe the dynamics of galactic clusters. A well known conjecture (Binney, Tremaine in Galactic Dynamics, Princeton University Press, Princeton, 1987) is the stability of spherical models which are nonincreasing radially symmetric steady states solutions. This conjecture was proved at the linear level by several authors in the continuation of the breakthrough work by Antonov (Sov. Astron. 4:859-867, 1961). In the previous work (Lemou et al. in A new variational approach to the stability of gravitational systems, submitted, 2011), we derived the stability of anisotropic models under spherically symmetric perturbations using fundamental monotonicity properties of the Hamiltonian under suitable generalized symmetric rearrangements first observed in the physics literature (Lynden-Bell in Mon. Not. R. Astron. Soc. 144:189-217, 1969; Gardner in Phys. Fluids 6:839-840, 1963; Wiechen et al. in Mon. Not. R. Astron. Soc. 223:623-646, 1988; Aly in Mon. Not. R. Astron. Soc. 241:15, 1989). In this work, we show how this approach combined with a new generalized Antonov type coercivity property implies the orbital stability of spherical models under general perturbations.

5.20. Stable ground states and self-similar blow-up solutions for the gravitational Vlasov-Manev system

In this work [54], we study the orbital stability of steady states and the existence of blow-up self-similar solutions to the so-called Vlasov-Manev (VM) system. This system is a kinetic model which has a similar Vlasov structure as the classical Vlasov-Poisson system, but is coupled to a potential in $-1/r - 1/r^2$ (Manev potential) instead of the usual gravitational potential in -1/r, and in particular the potential field does not satisfy a Poisson equation but a fractional- Laplacian equation. We first prove the orbital stability of the ground states type solutions which are constructed as minimizers of the Hamiltonian, following the classical strategy: compactness of the minimizing sequences and the rigidity of the flow. However, in driving this analysis, there are two mathematical obstacles: the first one is related to the possible blow-up of solutions to the VM system, which we overcome by imposing a sub-critical condition on the constraints of the variational problem. The second difficulty (and the most important) is related to the nature of the Euleri-Lagrange equations (fractional-Laplacian equations) to which classical results for the Poisson equation do not extend. We overcome this difficulty by proving the uniqueness of the minimizer under equimeasurabilty constraints, using only the regularity of the potential and not the fractional- Laplacian Euler-Lagrange equations itself. In the second part of this work, we prove the existence of exact self-similar blow-up solutions to the Vlasov-Manev equation, with initial data arbitrarily close to ground states. This construction is based on a suitable variational problem with equimeasurability constraint.

5.21. Micro-macro schemes for kinetic equations including boundary layers

In this paper [53], we introduce a new micro-macro decomposition of collisional kinetic equations in the specific case of the diffusion limit, which naturally incorporates the incoming boundary conditions. The idea is to write the distribution function f in all its domain as the sum of an equilibrium adapted to the boundary (which is not the usual equilibrium associated with f) and a remaining kinetic part. This equilibrium is defined such that its incoming velocity moments coincide with the incoming velocity moments of the distribution function. A consequence of this strategy is that no artificial boundary condition is needed in the micromacro models and the exact boundary condition on f is naturally transposed to the macro part of the model. This method provides an “Asymptotic preserving" numerical scheme which generates a very good approximation of the space boundary values at the diffusive limit, without any mesh refinement in the boundary layers. Our numerical results are in very good agreement with the exact so-called Chandrasekhar value, which is explicitely known in some simple cases.

5.22. Stroboscopic averaging for the nonlinear Schrödinger equation

In this paper [35], we are concerned with an averaging procedure, -namely Stroboscopic averaging-, for highly-oscillatory evolution equations posed in a (possibly infinite dimensional) Banach space, typically partial differential equations (PDEs) in a high-frequency regime where only one frequency is present. We construct a high order averaged system whose solution remains exponentially close to the exact one over long time intervals, possesses the same geometric properties (structure, invariants, . . .) as compared to the original system, and is non-oscillatory. We then apply our results to the nonlinear Schrödinger equation on the d-dimensional torus T^d, or in R^d with a harmonic oscillator, for which we obtain a hierarchy of Hamiltonian averaged models. Our results are illustrated numerically on several examples borrowed from the recent literature.

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

In [41], we consider the semiclassical limit for the nonlinear Schrödinger 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 Schrödinger equation.

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

In [17], we consider the behaviour 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 analyse the first time at which one of the Markov chains reaches its absorbing state. When the number of Markov chains goes to infinity, we analyse the asymptotic behaviour of the system for an arbitrary probability mass function governing the competition. We give conditions that ensure the existence of the asymptotic distribution and we show how these results apply to cluster-based distributed storage when the competition is handled using a geometric distribution.

5.25. High frequency behavior of the Maxwell-Bloch mdel with relaxations: convergence to the Schrödinger-rate system

We study in [20] the Maxwell-Bloch model, which describes the propagation of a laser through a material and the associated interaction between laser and matter (polarization of the atoms through light propagation, photon emission and absorption, etc.). The laser field is described through Maxwell's equations, a classical equation, while matter is represented at a quantum level and satisfies a quantum Liouville equation known as the Bloch model. Coupling between laser and matter is described through a quadratic source term in both equations. The model also takes into account partial relaxation effects, namely the trend of matter to return to its natural thermodynamic equilibrium. The whole system involves 6+$N(N+1)/2$ unknowns, the six-dimensional electromagnetic field plus the $N(N+1)/2$ unknowns describing the state of matter, where N is the number of atomic energy levels of the considered material. We consider at once a high-frequency and weak coupling situation, in the general case of anisotropic electromagnetic fields that are subject to diffraction. Degenerate energy levels are allowed. The whole system is stiff and involves strong nonlinearities. We show the convergence to a nonstiff, nonlinear, coupled Schrödinger-Boltzmann model, involving 3+N unknowns. The electromagnetic field is eventually described through its envelope, one unknown vector in C^3. It satisfies a Schrödinger equation that takes into account propagation and diffraction of light inside the material. Matter on the other hand is described through a N-dimensional vector describing the occupation numbers of each atomic level. It satisfies a Boltzmann equation that describes the jumps of the electrons between the various atomic energy levels, as induced by the interaction with light. The rate of exchange between the atomic levels is proportional to the intensity of the laser field. The whole system is the physically natural nonlinear model. In order to provide an important and explicit example, we completely analyze the specific (two dimensional) Transverse Magnetic case, for which formulae turn out to be simpler. Technically speaking, our analysis does not enter the usual mathematical framework of geometric optics: it is more singular, and requires an *ad hoc* Ansatz.

5.26. Radiation condition at infinity for the high-frequency Helmholtz equation: optimality of a non-refocusing criterion

In [43], we consider the high frequency Helmholtz equation with a variable refraction index $n^2(x)$ ($x \in \mathbb{R}^d$), supplemented with a given high frequency source term supported near the origin $x = 0$. A small absorption parameter $\alpha_\varepsilon > 0$ is added, which prescribes a radiation condition at infinity for the considered Helmholtz equation. The semi-classical parameter is $\varepsilon > 0$. We let ε and α_ε go to zero *simultaneously*. We study the question whether the prescribed radiation condition at infinity is satisfied *uniformly* along the asymptotic process $\varepsilon \to 0$. This question has been previously studied by the first author, who has proved that the radiation condition is indeed satisfied uniformly in ε, provided the refraction index satisfies a specific *non-refocusing condition*. The non-refocusing condition requires, in essence, that the rays of geometric optics naturally associated with the high-frequency Helmholtz operator, and that are sent from the origin $x = 0$ at time $t = 0$, should not refocus at some later time $t > 0$ near the origin again. In the present text we show the *optimality* of the above mentioned non-refocusing condition. We exhibit a refraction index which *does* refocus the rays of geometric optics sent from the origin near the origin again, and we show that the limiting solution *does not* satisfy the natural radiation condition at infinity in that case.

5.27. Coexistence phenomena and global bifurcation structure in a chemostat-like model with species-dependent diffusion rates

We study in [44] the competition of two species for a single resource in a chemostat. In the simplest space-homogeneous situation, it is known that only one species survives, namely the best competitor. In order to exhibit *coexistence* phenomena, where the two competitors are able to survive, we consider a space dependent situation: we assume that the two species and the resource follow a diffusion process in space, on top of the competition process. Besides, and in order to consider the most general case, we assume each population is associated with a *distinct* diffusion constant. This is a key difficulty in our analysis: the specific (and classical) case where all diffusion constants are equal, leads to a particular conservation law, which in turn allows to eliminate the resource in the equations, a fact that considerably simplifies the analysis and the qualitative phenomena. Using the global bifurcation theory, we prove that the underlying 2-species, stationary, diffusive, chemostat-like model, does possess *coexistence solutions*, where both species survive. On top of that, we identify the domain, in the space of the identified bifurcation parameters, for which the system does have coexistence solutions.

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

In [16], we consider the behaviour 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 analyse the first time at which one of the Markov chains reaches its absorbing state. When the number of Markov chains goes to infinity, we analyse the asymptotic behaviour of the system for an arbitrary probability mass function governing the competition. We give conditions that ensure the existence of the asymptotic distribution and we show how these results apply to cluster-based distributed storage when the competition is handled using a geometric distribution.

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

In this paper [21], we are concernedwith 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.

5.30. A formal series approach to averaging: exponentially small error estimates

The techniques, based on formal series and combinatorics, used nowadays to analyze numerical integrators may be applied to perform high-order averaging in oscillatory periodic or quasi-periodic dynamical systems. When this approach is employed, the averaged system may be written in terms of (i) scalar coefficients that are universal, i.e. independent of the system under consideration and (ii) basis functions that may be written in an explicit, systematic way in terms of the derivatives of the Fourier coefficients of the vector field being averaged. The coefficients may be recursively computed in a simple fashion. We show in [22] that this approach may be used to obtain exponentially small error estimates, as those first derived by Neishtadt. All the constants that feature in the estimates have a simple explicit expression.

5.31. Higher-order averaging, formal series and numerical integration II: the quasi-periodic case

The paper [23] considers non-autonomous oscillatory systems of ordinary differential equations with d>1 non-resonant constant frequencies. Formal series like those used nowadays to analyze the properties of numerical integrators are employed to construct higher-order averaged systems and the required changes of variables. With the new approach, the averaged system and the change of variables consist of vector-valued functions that may be written down immediately and scalar coefficients that are universal in the sense that they do not depend on the specific system being averaged and may therefore be computed once and for all. The new method may be applied to obtain a variety of averaged systems. In particular we study the quasi-stroboscopic averaged system characterized by the property that the true oscillatory solution and the averaged solution coincide at the initial time. We show that quasi- stroboscopic averaging is a geometric procedure because it is independent of the particular choice of co-ordinates used to write the given system. As a consequence, quasi-stroboscopic averaging of a canonical Hamiltonian (resp. of a divergence-free) system results in a canonical (resp. in a divergence-free) averaged system. We also study the averaging of a family of near-integrable systems where our approach may be used to construct explicitly d formal first integrals for both the given system and its quasi-stroboscopic averaged version. As an application we construct three first integrals of a system that arises as a nonlinear perturbation of five coupled harmonic oscillators with one slow frequency and four resonant fast frequencies.

5.32. Existence of densities for the 3D Navier-Stokes equations driven by Gaussian noise

We prove in [50] 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 densities 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 in Fournier and Printems (2010).

5.33. Diffusion limit for a stochastic kinetic problem

We study in [30] the limit of a kinetic evolution equation involving a small parameter and perturbed by a smooth random term which also involves the small parameter. Generalizing the classical method of perturbed test functions, we show the convergence to the solution of a stochastic diffusion equation.

5.34. Global Existence and Regularity for the 3D Stochastic Primitive Equations of the Ocean and Atmosphere with Multiplicative White Noise

The Primitive Equations are a basic model in the study of large scale Oceanic and Atmospheric dynamics. These systems form the analytical core of the most advanced General Circulation Models. For this reason and due to their challenging nonlinear and anisotropic structure the Primitive Equations have recently received considerable attention from the mathematical community. In view of the complex multi-scale nature of the earth's climate system, many uncertainties appear that should be accounted for in the basic dynamical models of atmospheric and oceanic processes. In the climate community stochastic methods have come into extensive use in this connection. For this reason there has appeared a need to further develop the foundations of nonlinear stochastic partial differential equations in connection with the Primitive Equations and more generally. In this work [29] we study a stochastic version of the Primitive Equations. We establish the global existence of strong, pathwise solutions for these equations in dimension 3 for the case of a nonlinear multiplicative noise. The proof makes use of anisotropic estimates, $L^p\_tL^q\_x$ estimates on the pressure and stopping time arguments.

5.35. Weak backward error analysis for SDEs

We consider in [28] numerical approximations of stochastic differential equations by the Euler method. In the case where the SDE is elliptic or hypoelliptic, 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 invariant 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 Euler scheme is exponentially mixing.

5.36. Convergence of stochastic gene networks to hybrid piecewise deterministic processes

In [27], we study the asymptotic behavior of multiscale stochastic gene networks using weak limits of Markov jump processes. Depending on the time and concentration scales of the system we distinguish four types of limits: continuous piecewise deterministic processes (PDP) with switching, PDP with jumps in the continuous variables, averaged PDP, and PDP with singular switching. We justify rigorously the convergence for the four types of limits. The convergence results can be used to simplify the stochastic dynamics of gene network models arising in molecular biology.

5.37. Exponential mixing of the 3D stochastic Navier-Stokes equations driven by mildly degenerate noises

In [15], we prove the strong Feller property and exponential mixing for 3D stochastic Navier-Stokes equation driven by mildly degenerate noises (i.e. all but finitely many Fourier modes are forced) via Kolmogorov equation approach.

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

In [40] 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.

5.39. Fast Weak-Kam Integrators

We consider in [42] a numerical scheme for Hamilton-Jacobi equations based on a direct discretization of the Lax-Oleinik semi-group. We prove that this method is convergent with respect to the time and space stepsizes provided the solution is Lipschitz, and give an error estimate. Moreover, we prove that the numerical scheme is a *geometric integrator* satisfying a discrete weak-KAM theorem which allows to control its long time behavior. Taking advantage of a fast algorithm for computing min-plus convolutions based on the decomposition of the function into concave and convex parts, we show that the numerical scheme can be implemented in a very efficient way.

5.40. Sparse spectral approximations for computing polynomial functionals

In [51], we give a new fast method for evaluating spectral approximations of nonlinear polynomial functionals. We prove that the new algorithm is convergent if the functions considered are smooth enough, under a general assumption on the spectral eigenfunctions that turns out to be satisfied in many cases, including the Fourier and Hermite basis.

MC2 Project-Team

6. New Results

6.1. Multi-fluid flows

- Microfluidics : Participants: Charles-Henri Bruneau, Johana Pinilla (PhD), Sandra Tancogne (MCF Reims).
  To handle oil recovery by chemical processes it is useful to better understand the behaviour of multifluids flows in a saturated soil. The porous medium is mimiced by a network of micro channels. The simulation of immiscible multi-fluids flows is then performed by means of the level-sets and the penalization methods to track the interfaces between the fluids and to get rid of the geometry difficulties. In addition the Cox law is added in the model to better move the interfaces during the simulations.
  Concerning visco-elastic fluids in micro-channel, one has often to compute solutions of system for which the viscosity in the stokes part is much smaller than that involved in the extra-stress. In his thesis, V. Huber has constructed a second order scheme solving Stokes equations for a bifluid flow with surface tension on a cartesian grid using a mixte finite volume-finite element approach.

6.2. 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. In 2011, various improvements to the calibration algorithms were made. The initial seeding of the algorithms was a weak point of the procedure. This has been much improved using a genetic algorithm. 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.
- Metastasis to the liver of a GIST
  Gastro-Intestinal Stromal Tumors often create metastasis to the liver. We have modeled the response to the treatment of such lesion starting from CT-scans.
- 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 SwansonÕs 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). In particular, two models were built. The first one allows to study the efficacy 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. The second model has been validated and we are trying to recover its parameters for a patient in 3D (which is a rather unique initiative to our knowledge).
- Modelling of electrochemotherapy :

Two articles related to the electrical cell modelling have been done ([64], [61]) . 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 accepted in Journal of Math Biology [27]. 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.

- 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 februray by Prof. Suzuki and T.Colin and C.Poignard have been at Osaka in september. 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.

6.3. 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.
- Turbulence flow on an hemisphere : Participants: Charles-Henri Bruneau, Patrick Fischer (MCF Bordeaux 1), Yong Liang Xiong (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 [77]. 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.

6.4. 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.

6.5. Calculation of Ice Chunk Trajectory

- Participants: Héloise Beaugendre, Ramesh Yapalparvi.
  In this work, calculation of trajectories of ice chunk are carried out at varying values of ratio of density of ice piece to that of the ambient fluid. Proper Orthogonal Decomposition with Interpolation (PODI) method is then applied on snapshots of trajectories simulated by computational fluid dynamics. Snapshots of trajectories are obtained based on cartesian grids, penalization, and level sets. The extracted POD modes from snapshots are then used to reconstruct solutions and capabilities of POD with interpolation are demonstrated on ice trajectory calculations for flow around iced airfoil and cylinder for density ratio's that are not part of the snapshot set.

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, V. Ehrlacher, S. Lahbabi and G. Stoltz 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 [24], E. Cancès and G. Stoltz have studied the time evolution of defects within this model, in the context of linear response, which allowed them to give a rigorous meaning to the Adler-Wiser formula for the frequency-dependent dielectric permittivity of crystals. In collaboration with M. Lewin, E. Cancès and S. Lahbabi have introduced in [54] 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.

On the numerical side, E. Cancès has worked with Y. Maday and R. Chakir (University Paris 6) on the numerical analysis of the electronic structure models. In [22], they have obtained optimal *a priori* error bounds for the the planewave approximation of the Thomas-Fermi-von Weizsäcker and the Kohn-Sham LDA models. Together with Y. Maday, E. Cancès and V. Ehrlacher have analyzed the computation of eigenvalues in spectral gaps of locally perturbed periodic Schrödinger operators [23]. In [53], they have introduced a general theoretical framework to analyze non-consistent approximations of the discrete eigenmodes of a self-adjoint operator, focusing in particular on the discrete eigenvalues laying in spectral gaps. Applying this analysis to the supercell method for perturbed periodic Schrödinger operators, they derive optimal convergence rates for the planewave discretization method, taking numerical integration errors into account. These results, along with earlier work on greedy algorithms for nonlinear convex problems and the study of local defects in the Thomas-Fermi-von Weiszacker theory, are collected in [7].

In the work [38], Claude Le Bris, in collaboration with Pierre Rouchon (Ecole des Mines de Paris), has introduced 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: Matthew Dobson, Claude Le Bris, Frédéric Legoll, Tony Lelièvre, Francis Nier, Grigorios Pavliotis, Mathias Rousset, Gabriel Stoltz.

The extremely broad field of molecular dynamics is a domain where the MICMAC project-team, originally more involved in the quantum chemistry side, has invested a lot of efforts in the recent years. Molecular dynamics may also be termed computational statistical physics since the main aim is to numerically estimate average properties of materials as given by the laws of statistical physics. The project-team studies both deterministic and probabilistic techniques used in the field. One of the main difficulty is related to the metastable features of the generated trajectories: the system remains trapped over very long times in metastable states, which means that very long trajectories need to be generated in order to obtain macroscopically relevant quantities. This is related to the fact that the timescale at the microscopic level is much smaller than the timescale at the macroscopic level. In [66], we propose a summary of the mathematical approaches to quantify metastability, and which appear to be useful to analyze the numerical methods used in molecular dynamics.

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 the article [42], Tony Lelièvre, Mathias Rousset and Gabriel Stoltz study the application of constrained Langevin dynamics to the computation of free energy differences, by thermodynamic integration techniques and fluctuation relation (à la Jarzynski).

One interest of free energy computation techniques is that they appear to be useful in other fields, like in computational statistics where multimodal measures are also frequently encountered, so that standard Markov Chain Monte Carlo appraoches also suffer from metastability.

For example, in [25], Nicolas Chopin (CREST, ENSAE), T. Lelièvre and G. Stoltz explore the application of the Adaptive Biasing Force method to Bayesian inference. This sampling method belongs to the general class of adaptive importance sampling strategies which use the free energy along a chosen reaction coordinate as a bias. Such algorithms are very helpful to enhance the sampling properties of Markov Chain Monte Carlo algorithms, when the dynamic is metastable.

In [58], G. Fort (Telecom Paris), B. Jourdain (CERMICS), E. Kuhn (INRA), T. Lelièvre and G. Stoltz have considered the Wang-Landau algorithm. The authorshave proved that the Wang-Landau algorithm converges with an associated central limit theorem, and have provided an analysis of the efficiency of the algorithm in a metastable situation.

5.2.2. Convergence to equilibrium

An important question for the analysis of sampling techniques is the rate of convergence to equilibrium for stochastic trajectories.

In [65], F. Nier, T. Lelièvre and G. Pavliotis study the interest of using non-reversible stochastic dynamics to enhance the rate of convergence to equilibrium, compared to reversible dynamics. A well posed optimization problem is obtained and solved in the case of a linear drift for the overdamped Langevin dynamics.

5.2.3. Metropolis Hastings algorithms

A classical sampling tool used in molecular dynamics and in computational statistics is the Metropolis-Hastings algorithm. There has been a lot of work (see G. Roberts et al.) to study how the variance of the proposal should scale with the dimension of the problem, in order to optimize the sampling procedure. Most of these works assume that (i) the target probability is the product of n one dimensional laws and that (ii) the Markov chain starts at equilibrium.

In the two works [60], [59], T. Lelièvre and his co-authors have generalized these results when the initial distribution is not the target probability. The diffusive limit in the latte case is solution to a stochastic differential equation nonlinear in the sense of McKean. They have discussed practical counterparts in order to optimize the variance of the proposal distribution to accelerate convergence to equilibrium. The analysis confirms the interest of the constant acceptance rate strategy (with acceptance rate between $1/4$ and $1/3$) first suggested in the works of G. Roberts et al., at least for the Random Walk Metropolis algorithm.

5.2.4. 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. In the one-dimensional setting, an efficient strategy that bypasses the simulation of the whole system had been proposed in 2010. We refer to [47] for a recent review. In collaboration with X. Blanc (Université Pierre et Marie Curie), F. Legoll has extended this strategy to the so-called membrane setting in [16].

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. In collaboration with E. Tadmor, W. K. Kim, L. Dupuy and R. Miller, F. Legoll has analyzed such an approach in [46]. The numerical tests reported there show the efficiency of the approach, as long as the temperature is indeed small.

5.2.5. 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.

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 [56] the distribution of the lengths of these trajectories, using large deviation techniques.

In [37], C. Le Bris and T. Lelièvre together with M. Luskin and D. Perez from Los Alamos National Laboratoy provide a mathematical analysis of the parallel replica algorithm, which has been proposed by A. Voter in 1997 to simulate very efficiently metastable trajectories. This work opens a lot of perspectives, by using a generic tool (the quasi stationary distribution) to make a link between a continuous state space dynamics (Langevin dynamics) and a discrete state space dynamics (kinetic Monte Carlo models).

In a work in progress, T. Lelièvre and F. Nier have studied the quasi-stationnary distribution in relation 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 compute accurately the spatial exit law along the boundary and non perturbative accurate formulas when the potential is changed inside the domain.

5.2.6. 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.

F. Legoll and T. Lelièvre have introduced and analyzed some years ago a strategy to define a coarse-grained dynamics that approximates $\xi(X_t)$, when the state of the system X_t evolves according to the overdamped Langevin equation (which is ergodic for the Gibbs measure). We refer to [47] for a recent review. The aim was to get a coarse-grained description giving access to some *dynamical* quantities (and not only *equilibrium* quantities). Together with G. Samaey (KU Leuven), they have recently studied how to use this coarse-grained description, accurate when the time scale separation is asymptotically large, to somewhat precondition the dynamics of the actual system in cases when the time scale separation is not large. For that purpose, they have used the parareal framework, to iteratively correct the sequential coarse-grained trajectory by fine scale trajectories performed in parallel. The main difficulty is that the two models (the reference one and the coarse-grained one) do not act on the same variable: the reference model evolves all the variables, whereas the coarse-grained model only evolves the slow variables. As shown in [63] in a simplified context (that of singularly perturbed ODEs), the precise coupling between both models should be done carefully.

The above study is concerned with models with continuous state spaces. S. Lahbabi and F. Legoll have studied in [61] a related question in the framework of kinetic Monte Carlo models, where the state space is discrete. For some models involving some slow and some fast variables, the effective dynamics of the slow component has been identified, and a complete proof of convergence proposed.

5.2.7. 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. Consequently, there is a need for time integration algorithms that take into account these fast phenomena only in an averaged way, and for which the time step is not restricted by the highest frequencies. In [29], M. Dobson, C. Le Bris, and F. Legoll have developed integrators for Hamiltonian systems with high frequencies. The integrators were derived using homogenization techniques applied to the Hamilton-Jacobi PDE associated to the Hamiltonian ODE. This work extends previous works of the team. The proposed algorithms can now handle the case when the (unique) fast frequency depends on the slow degrees of freedom, or when there are several fast constant frequencies.

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. It is based on a decomposition of the time interval into subintervals, and on a predictor-corrector strategy, where the propagations over each subinterval for the corrector stage are concurrently performed on the processors. Using a symmetrization procedure and/or a (possibly also symmetric) projection step, C. Le Bris and F. Legoll, in collaboration with X. Dai and Y. Maday, have introduced several variants of the original plain parareal in time algorithm [28]. These variants, compatible with the geometric structure of the exact dynamics, are better adapted to the Hamiltonian context.

5.2.8. Nonequilibrium systems

The efficient simulation of molecular systems is known to be a much more complicated problem when the system is subjected to a non-conservative external forcing than when the system experiences conservative forces. Together with the sampling of metastable dynamics mentioned above, these are the two major research focus in molecular dynamics of the project-team.

Nonequilibrium molecular dynamics simulations can be used to compute the constitutive relation between the strain rate and stress tensor in complex fluids. This is fulfilled simulating molecular systems subject to a steady, non-zero macroscopic flow at a given temperature. Starting from a bath model, M. Dobson, F. Legoll, T. Lelièvre, and G. Stoltz have derived a Langevin-type dynamics for a heavy particle in a non-zero background flow [57]. The resulting dynamics, which is theoretically obtained when a *unique* large particle is considered, is numerically observed to also perform well when a *system* of many interacting particles within shear flow is considered.

Let us also mention that the article on the computation of the viscosity of fluids using steady state nonequilibrium dynamics with an external nongradient bulk forcing, in the framework of the PhD of Rémi Joubaud, has also been published [34]. In addition, the study by G. Stoltz and C. Bernardin on thermal transport in one-dimensional chains of oscillators whose kinetic and potential energy functions are the same, has been accepted and is now published [13].

5.3. Complex fluids

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

In [41], Claude Le Bris and Tony Lelièvre review the state-of-the-art of numerical and mathematical results on micro-macro models for viscoelastic fluids.

Following previous works, in [32], Claude Le Bris and Tony Lelièvre together with Lingbing He analyze the longtime behaviour of nematic polymeric fluids (liquid crystals). The longtime asymptotic for such models is much richer than for flexible polymers, that were considered in a previous analysis. Indeed, for these models, periodic in time behaviours are observed.

In his PhD under the supervision of Claude Le Bris and Tony Lelièvre, David Benoît 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 [51] 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.

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, and possibly discontinuous solutions were numerically simulated with a new finite-volume scheme of relaxation type that satisfies a discrete counterpart of the natural dissipation [20]. This work is being pursued for other models.

Finally, in [31], Alexandre Ern (CERMICS), Rémi Joubaud (CERMICS) and Tony Lelièvre analyze a model describing equilibrium binary electrolytes surrounded by charged solid walls. This work is done in collaboration with physicists from the group PECSA at Université Pierre et Marie Curie. Applications include the modelization of clays for the burying of nuclear waste.

5.4. Application of greedy algorithms

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

Greedy algorithms are used in many contexts for the approximation of high-dimensional functions: Proper Generalized Decomposition, Reduced Basis techniques, etc.

Various greedy algorithms for high-dimensional non-symmetric problems, and inherent theoretical and practical difficulties have been analyzed in [52]. Current research now aims at extending these techniques to the approximation of high-dimensional spectral problems. Prototypical applications include electronic structure calculations or the computation of buckling modes in mechanics.

In probabilistic methods for uncertainty quantification in mechanics, S. Boyaval has used a greedy algorithm to construct control variates for accelerating Monte-Carlo simuation in the cases where an expectation has to be computed many times [21]. The work is being applied to the uncertainty quantification in numerical models for hydraulic engineering.

Finally, in [55], Fabien Casenave (CERMICS), Alexandre Ern (CERMICS) and Tony Lelièvre study the influence of round-off errors on the evaluation of the a posteriori estimators in the reduced basis approach. In practice, the evaluation of the error estimator can become very sensitive to round-off errors. An explanation of this fact is proposed, as well as efficient remedies.

5.5. Mathematical Physics

Participant: Francis Nier.

In [10], A. Aftalion and F. Nier answer questions asked by J. Dalibard about the feasibility of artificial gauge potentials. This analysis provides the range of small parameters within which the linear adiabatic argument used by the physicists is certainly not destroyed by the non linear effects.

In [43], D. Le Peutrec, F. Nier and C. Viterbo give an accurate Arrhenius law for Witten Laplacian acting on p-forms. In the case of functions the exponentially small eigenvalues are given by exponentiated differences of enegy levels between local minima and saddle points (Arrhenius law). In the case of p-forms the association of critical points with index p and critical points with index p+1 or p-1, is more subtle and is provided by Barannikov's presentation of Morse theory.

In [11], Z. Ammari and F. Nier have proved the mean field dynamics of general bosonic systems in the presence of singular pair interaction potentials, including the important 3 dimensional Coulombic case. As compared with their previous works, they developed a slightly new strategy relying on measure transportation techniques and results presented by Ambrosio-Gigli-Savaré in their book "Gradient Flows: In Metric Spaces And In The Space Of Probability Measures" (2005).

5.6. Homogenization and related topics

Participants: Ronan Costaouec, Claude Le Bris, Frédéric Legoll, William Minvielle, Mathias Rousset, Florian Thomines.

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 in [17] 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.

A theme closely related to homogenization theory and on which several members of the project team have worked a lot in the past few years is the passage from discrete (atomistic) mechanics to continuum mechanics. In this direction, C. Le Bris, in collaboration with X. Blanc and P.-L. Lions, has established in [18] the rigorous continuum limit of the Newton equations of motion for some simple cases of one-dimensional atomistic system.

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.

An interesting case in that context is when the randomness comes as a *small* perturbation of the deterministic case. As previously shown by earlier works of the project-team, this situation can indeed be handled with a dedicated approach, which turns out to be far more efficient than the standard approach of stochastic homogenization. A final component of the work completed by Florian Thomines during his PhD thesis has concerned the application of Reduced Basis techniques to that specific context of weakly stochastic homogenization problems. In particular, the approach has been adapted in [39] to efficiently compute the terms of the expansion previously developed by A. Anantharaman and C. Le Bris to approximate a certain category of weakly random homogenization problems. It has been demonstrated that the reduced basis technique is very helpful in this particular context and indeed allows for a speed up of the computation. Another application of the same technique, for a slightly different category of models (still in the framework of weakly random homogenization problems) originally derived by X. Blanc, P.-L. Lions and C. Le Bris, has also been explored. The difficulty, there, is to compute the various corrector equations that parametrically depend on the macroscopic location of the microstructure and the particular realization of that microstructure. The problem is definitely amenable to reduced basis techniques, as demonstrated by some preliminary tests, but definite conclusions on the general validity of the approach are yet to be obtained.

The team has also proceeded to address, from a numerical viewpoint, the case when the randomness is not small. In that case, 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 shown in [14] that the variance of this matrix can be reduced using the technique of antithetic variables. F. Legoll and W. Minvielle are currently extending this technique to nonlinear, convex homogenization problems.

In addition, C. Le Bris, F. Legoll, W. Minvielle and M. Rousset are currently investigating 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.

Another contribution in stochastic homogenization is the following. C. Le Bris, in collaboration with X. Blanc and P.-L. Lions, has recently introduced a variant of the classical random homogenization. For that variant, as often in random homogenization, the homogenized matrix is again defined from a so-called corrector function, which is the solution to a problem set on the entire space. F. Legoll and F. Thomines have described and proved the almost sure convergence of an approximation strategy based on truncated versions of the corrector problem in [64]. F. Legoll and F. Thomines have also established, in the one-dimensional case, a convergence result on the residual process, defined as the difference between the solution to the highly oscillatory problem and the solution to the homogenized problem.

From a numerical perspective, the Multiscale Finite Element Method 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 extension of this strategy to the stochastic case, when the tensor describing the properties of the material is the sum of a periodic term and a small random term, has been studied by C. Le Bris, F. Legoll and F. Thomines [36]. A method with a much smaller computational cost than the original MsFEM in the stochastic setting has been proposed. Provided the stochastic perturbation is indeed small, the proposed method is as accurate as the original one. The work [36] also provides a complete analysis of the approach, extending that available for the deterministic setting. Such analysis often rely on the rate of convergence of the two scale expansion (in the sense of homogenization theory) of the solution to the highly oscillatory elliptic partial differential equation. Such a result is classic for periodic homogenization. In generic stochastic homogenization, the rate can be arbitrary small, depending on the rate with which the correlations of the random coefficient vanish. C. Le Bris, F. Legoll and F. Thomines have established in [40] such a result for *weakly stochastic homogenization*, using asymptotic properties of the Green function of the elliptic operator $Lu = -\text{div}\ (A\nabla u)$ (where A is a periodic, coercive and bounded matrix), established by F. Legoll in collaboration with X. Blanc and A. Anantharaman [15].

Still in the framework of the Multiscale Finite Element approach, F. Thomines has further investigated, in collaboration with Y. Efendiev and J. Galvis (Texas A&M University), the use of Reduced Basis methods. They have considered an extension of the MsFEM approach, well suited to the high contrast case, i.e. the case when the ratio between the maximum and the minimum values of the heterogeneous coefficient is large. The main idea of this extension is to complement the standard MsFEM basis functions with the eigenfunctions (associated to the first small eigenvalues) of a local eigenvalue problem. In [30], Y. Efendiev, J. Galvis and F. Thomines have considered the case when the problem depends on an additional parameter, and have shown how to use the Reduced Basis approach to more efficiently compute the eigenfunctions mentioned above.

Even in simple deterministic cases, there is actually still room for improvement in many different directions for the MsFEM approach. In collaboration with A. Lozinski (University of Toulouse and now at the University of Besançon) who visited the team-project repeatedly during the year, 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 [35]. In particular, an elliptic problem set on a domain with a huge number of perforations has been considered in [62]. 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, two-week visitor in the project-team in the Spring of 2012), 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.

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? How is this matrix related to the homogenized matrix, in the limit of infinitely rapidly oscillatory coefficients? Current work is directed towards solving such issues.

5.7. Asymptotic 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 [44], the pobabilistic derivation of the chemotaxis equation from the individual motion of bacteriae have been carried out in a rigorous way. In [45], a numerical method simulating the individual evolution of bacteriae with "asymptotic" variance reduction have been proposed.

5.8. Computational materials spectroscopy in electrochemistry and optoelectronics

Participant: Ismaila Dabo.

Many advances in the understanding and design of nanomaterials have been enabled by spectroscopic techniques of increasing spatial and temporal resolution. In electrochemistry and optoelectronics, spectroscopy provides insight into the chain of processes involved in harnessing, storing, and delivering energy.

In support to experimental techniques, much progress has been achieved in simulating spectroscopic phenomena to shed light into energy conversion at the molecular scale. Such understanding is critical to the molecular design of a range of electrical devices, including but not limited to fuel cells, batteries, dye-sensitized solar cells, and optoelectronic devices.

The work of I. Dabo is dedicated to the development of quantum and semiclassical methods to simulate spectroscopies of electrochemical and optoelectronic materials. The achieved level of efficiency and accuracy fosters dialogue between experiment and theory for interpreting complex spectroscopic data. This year, these novel methods have been applied to simulate spectroscopic phenomena spanning the infrared to the visible and ultraviolet ranges.

The first application pertains to the infrared sum-frequency-generation (SFG) spectroscopy of adsorption mechanisms at the origin of the tolerance of fuel-cell catalytic electrodes to chemical poisoning. The study explains the critical influence of the electrode voltage in analyzing surface spectroscopy experiments (work done in collaboration with EPFL). [12], [26], [19]

The second application aims at understanding the sensitizing properties of organometallic dyes in dye-sensitized solar cells by simulating optical photoluminescence (PL) spectra, thereby elucidating the role of electron localization and ligand functionalization on the phosphorescence of organometallic complexes (work done in collaboration with the University of Minnesota). [33]

The third application is focused on the ultraviolet photoelectron spectroscopy (UPS) of photoactive nanomaterials of relevance to the design of organic photovoltaic junctions and photoelectrodes (work done in collaboration with the Italian Institute of Nanoscience, Seoul National University, and Xiamen University). [27]

Future challenges and opportunities are related to the time-dependent simulation of transient and cyclic spectra. These developments, which will be part of the widely used Quantum-ESPRESSO distribution (http://www.quantum-espresso.org), would pave the way for comprehensive studies of kinetic processes in tandem with time-resolved spectroscopic experiments.

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 [14] 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. [52]) and have thus been designed with global conformity requirements (i.e. H_1, $H(\text{rot})$ 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.

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.

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 [14] 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 recently studied [25], and its application to the simulation of the propagation in realistic geometrical models of head tissues is underway.

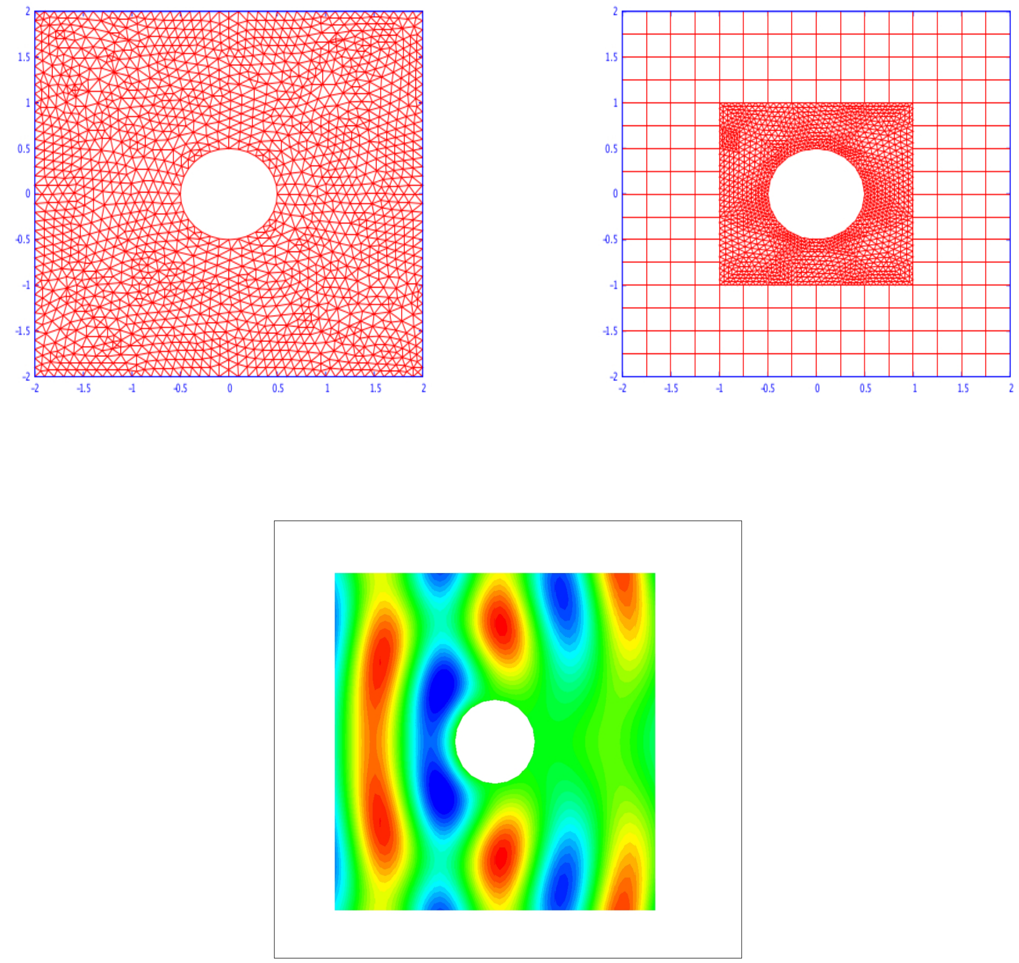


Figure 2. Scattering of a plane wave by an disk. Conforming triangular mesh (top left) and non-conforming quadrangular/triangular mesh (top right). Contour lines of electrical field component E_z from a simulation with a DGTD-$\mathbb{P}_2\mathbb{Q}_4$ method (bottom).

6.1.4. DGTD-$\mathbb{P}_p$ method for Drude media and applications to nanophotonics

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

Nanostructuring of materials has opened up a number of new possibilities for manipulating and enhancing light-matter interactions, thereby improving fundamental device properties. Low-dimensional semiconductors, like quantum dots, enable one to catch the electrons and control the electronic properties of a material, while photonic crystal structures allow to synthesize the electromagnetic properties. These technologies may, e.g., be employed to make smaller and better lasers, sources that generate only one photon at a time, for applications in quantum information technology, or miniature sensors with high sensitivity. The incorporation of metallic structures into the medium allows one to exploit plasmonic effects and adds further possibilities for manipulating the propagation of electromagnetic waves. In particular, this allows subwavelength localisation of the electromagnetic field and, by subwavelength structuring of the material, novel effects like negative refraction, e.g. enabling super lenses, may be realized. Nanophotonics is the recently emerged, but already well defined, field of science and technology aimed at establishing and using the peculiar properties of light and light-matter interaction in various nanostructures. Because of its numerous scientific and technological applications (e.g. in relation to telecommunication, energy production and biomedicine), nanophotonics represents an active field of research increasingly relying on numerical modeling beside experimental studies. We have started this year a new research direction aiming at the numerical modeling of electromagnetic wave interaction with nanoscale metallic structures. In this context, one has to take into account the dispersive characteristics of cartain 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 dispersion model in the framework of a DGFD-$\mathbb{P}_p$ method.

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.* [47] 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. In particular, we have recently designed a HDGFD-$\mathbb{P}_p$ method for the solution of the 2D frequency domain Maxwell equations [22] and, based on the very promising results obtained in this study, the extension to the more challenging 3D case has been initiated.

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 [26].

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) [40]-[35].

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 [38].

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 [39].

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.

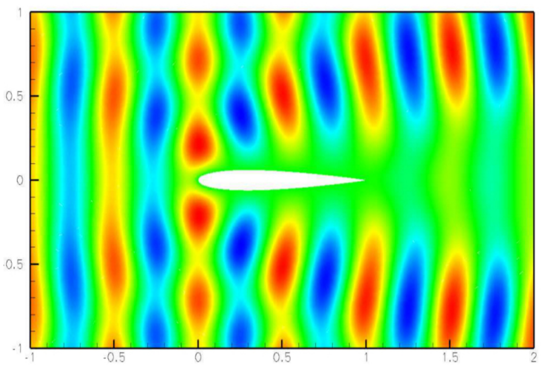
We have started this year a research direction aiming at the development of high order discontinuous Galerkin methods on unstructured meshes for the simulation of frequency domain elastodynamic and viscelastic wave propagation. This study is part of the Depth Imaging Partnership (DIP) between Inria and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

6.3. Time integration strategies and resolution algorithms

6.3.1. 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 [14], we have proposed the use of Crank-Nicolson scheme in place of the explicit leap-frog scheme adopted in this method [4]. 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 [6], 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) [24] and numerically in the 2D case [23]. 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 [33] by applying Richardson extrapolation and composition methods.



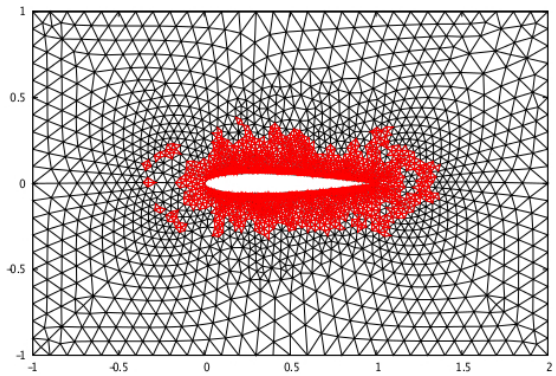


Figure 3. Scattering of a plane wave by an airfoil profile. Contour lines of electrical field component E_z (left) and locally refined triangular mesh with partitioning in explicit/implicit zones (right).

6.3.2. Optimized Schwarz algorithms for the frequency domain Maxwell equations

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

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 [8]. The optimized interface conditions proposed in [8] were devised for the case of non-conducting propagation media. We have recently studied the formulation of such conditions for conducting media [17]. 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 [28].

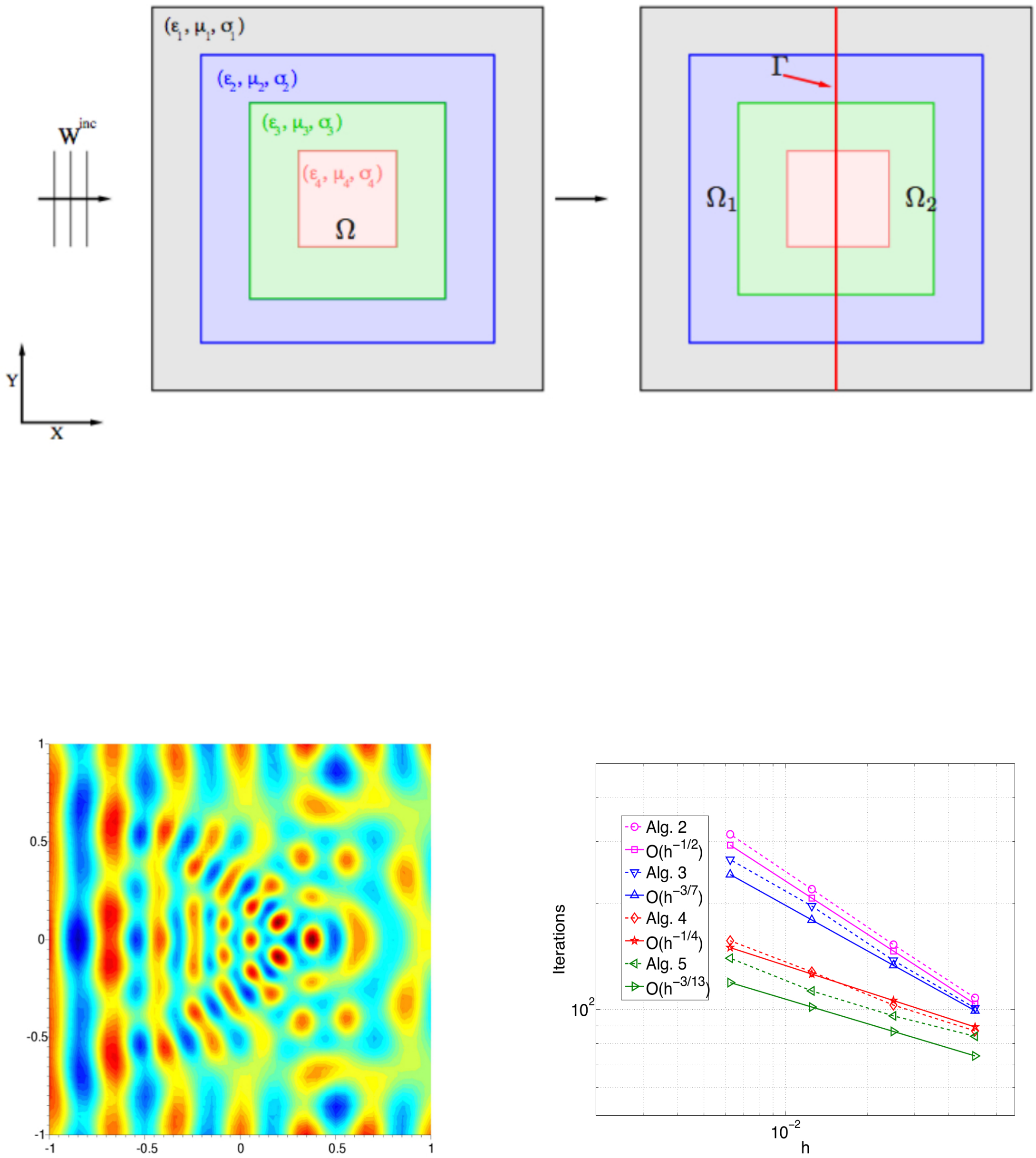


Figure 4. Propagation of a plane wave in a multilayered heterogeneous medium. Problem setting and two-subdomain decompositin (top). Contour lines of the real part of the E_z component of the electrical field (bottom left) and asymptotic convergence of the optimized Schwarz algorithms (bottom right).

NANO-D Team

6. New Results

6.1. Adaptively Restrained Particle Simulations

Participants: Svetlana Artemova, Stephane Redon.

Last year, we have introduced a novel, general approach to speed up particle simulations that we call Adaptively Restrained Particle Simulations (ARPS). This year we continued working on this approach. The obtained results have been published in Physical Review Letters [3], and the patent describing the theoretical basis and the algorithms for the numerical realization of ARPS has been deposited.

Particle simulations are widely used in physics, chemistry, biology [13], [14], and even computer graphics [9], and faster simulations (in particular ARPS) may result in progress on many challenging problems, e.g., protein folding, diffusion across bio-membranes, fracture in metals, ion implantation, etc.

ARPS rely on an adaptively restrained (AR) Hamiltonian used to describe a system of N particles:

$$H_{AR}(\mathbf{q},\mathbf{p}) = \frac{1}{2}\mathbf{p}^T\Phi(\mathbf{q},\mathbf{p})\mathbf{p} + V(\mathbf{q}).$$

This Hamiltonian has an unusual inverse inertia matrix $\Phi(\mathbf{q},\mathbf{p})$, which is made a general function of phase-space coordinates. The precise form of this matrix can be chosen according to the system under study and the problem stated.

We have proposed a particular (diagonal) form of the inverse inertia matrix for the simulations in Cartesian coordinates. In this case, Φ adaptively switches on and off positional degrees of freedom of individual particles while letting particle momenta evolve. The decision whether the particle is restrained or not depends on the particle's momentum, and, precisely, on it's kinetic energy. Two user-defined thresholds regulate the amount of simplification of the particle's motion. When a module of a particle's momentum becomes small enough (without necessarily becoming zero), the particle completelystops moving. Even when a particle is fully restrained, though, its momentum may continue to change, and its kinetic energy might become large enough again for the particle to resume moving. In general, ARPS restrain and release particles repeatedly over time.

This approach has numerous advantages: (a) it is mathematically grounded and is able to produce long, stable simulations; (b) it does not require modifications to the simulated interaction potential, so that any suitable existing force-field can be directly used with ARPS; (c) under frequently-used assumptions on the interaction potential, ARPS make it possible to reduce the number of forces that have to be updated at each time step, which may significantly speed up simulations; (d) when performing constant-energy simulations, ARPS allow users to finely and continuously trade between precision and computational cost, andrapidly obtain approximate trajectories; (e) the trade-off between precision and cost may be chosen for each particle independently, so that users may arbitrarily focus ARPS on specific regions of the simulated system (e.g., a polymer in a solvent); (f) most important, when performing Adaptively Restrained Molecular Dynamics (ARMD) in the canonical (NVT) ensemble, correct static equilibrium properties can be computed.

We have demonstrated the advantages of ARPS on several numerical experiments. For example, a planar collision cascade study in Fig. 7 shows how ARPS make it possible to smoothly trade between precision and speed of the simulation. Reference simulations were derived from the usual Hamiltonian $H(\mathbf{q},\mathbf{p}) = \frac{1}{2}\,\mathbf{p}^T\mathbf{M}^{-1}\mathbf{p} + V(\mathbf{q})$.

6.2. Hierarchical Adaptively Restrained Particle Simulations

Participants: Svetlana Artemova, Stephane Redon.

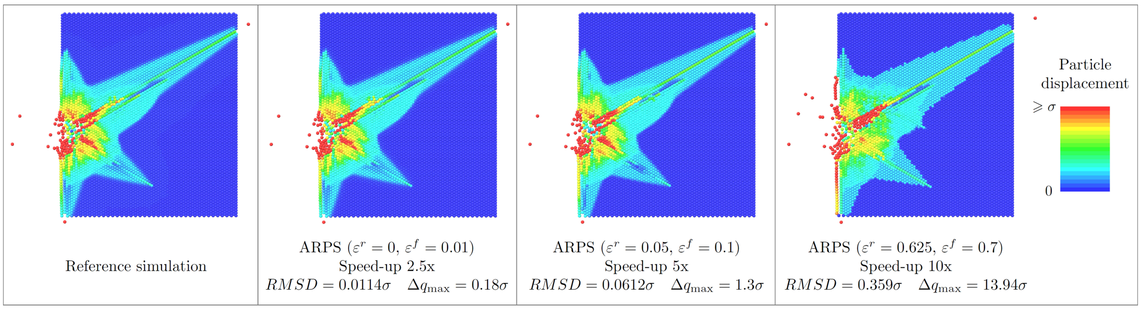


Figure 7. Simulating a collision cascade with controlled precision. Adaptively restrained simulations allow us to smoothly trade between precision and speed. Even for large speed-ups (up to 10x) the features of the shock are extremely well preserved.

It has been shown that algorithms relying on hierarchical representations of molecular systems may accelerate molecular simulations: for example, divide-and-conquer approach for simulations in internal coordinates [10], [11], adaptive algorithms for dynamics of articulated bodies [15], algorithms for neighbor search for system with symmetries [12] or for large rigid molecules [8].

Therefore, we were interested in combining hierarchically-based algorithms with Adaptively Restrained Particle Simulations (ARPS). Precisely, as with classical ARPS, we have considered the adaptively restrained (AR) Hamiltonian:

$$H_{AR}(\mathbf{q},\mathbf{p}) = \frac{1}{2}\mathbf{p}^T\Phi(\mathbf{q},\mathbf{p})\mathbf{p} + V(\mathbf{q}),$$

but we have introduced a different form of the inverse inertia matrix $\Phi(\mathbf{q},\mathbf{p})$. In this case, again, positional degrees of freedom are adaptively switched on and off during the simulation, but, these are *relative* positional degrees of freedom in the system, and not the positional degrees of freedom of individual particles. Precisely, particles are grouped together into rigid bodies according to the tree representation and released repeatedly during the simulation. We call this approach hierarchical Adaptively Restrained Particle Simulations (hierarchical ARPS).

We have performed several numerical experiments to illustrate this new approach. For example, in Fig. 8 we present the planar collision cascade study.

For hierarchical AR simulations, obtained results depend on the tree representation of the system: for the results demonstrated in Fig. 8 the tree was constructed in a top-down manner by recursive dividing of the system in halves and, therefore, the squares of different levels are being activated by the shock.

To clearly demonstrate the effect of the tree, we provide the results for the same four simulations with another tree built in a bottom-up manner by grouping the particles pairwise according to their sequence number (they were enumerated, first, along the y-axis, vertically, and then, along the x-axis, horizontally). These results are shown in Fig. 9 , and are rather different from those in Fig. 8 : vertical lines are being activated when the central part of the plane is reached by the shock.

The patent reporting the principles and the algorithms used to implement hierarchical ARPS has been deposited.

6.3. Interactive quantum chemistry

Participants: Mael Bosson, Caroline Richard, Antoine Plet, Sergei Grudinin, Stephane Redon.

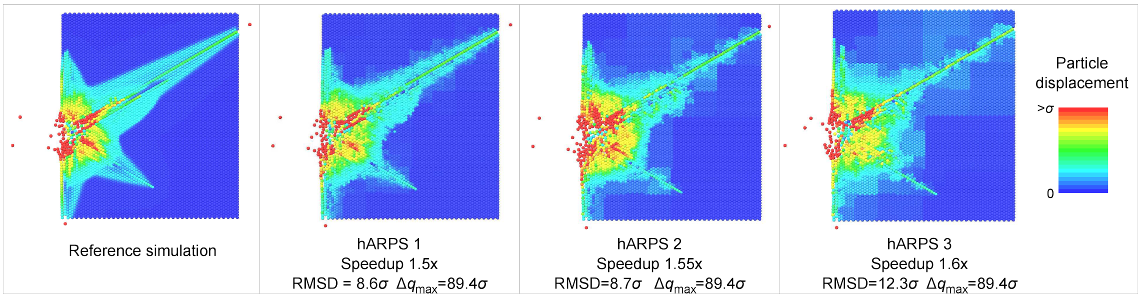


Figure 8. Simulating a collision cascade with controlled precision. Hierarchical adaptively restrained simulations allow us to smoothly trade between precision and speed. The main features of the shock are preserved. The binary tree representation was constructed top-down.

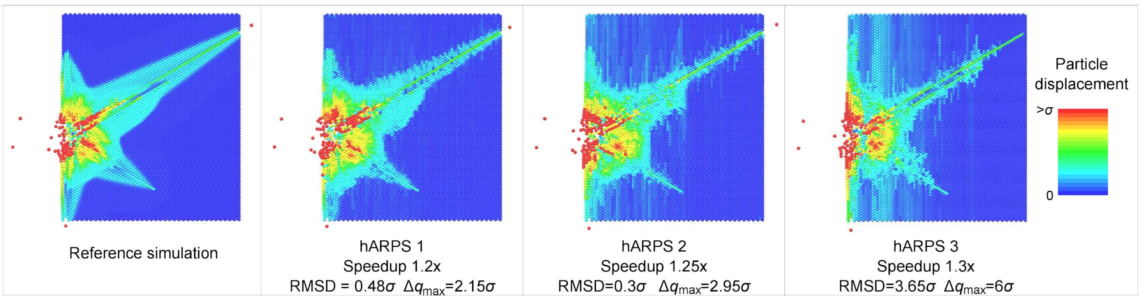


Figure 9. Simulating a collision cascade with controlled precision. Hierarchical adaptively restrained simulations allow us to smoothly trade between precision and speed. The main features of the shock are preserved. The binary tree representation was constructed bottom-up.

Interactive simulation tools allow users to take advantage of their knowledge and intuition to understand physical properties and prototype new devices. To accurately describe bond breaking, bond formation, charge transfer or other electronic phenomena, interactive simulation should ideally be based on quantum mechanics. However, solving quantum chemistry models at interactive rates is a challenging task. Thanks to the algorithms developed in the group, SAMSON is the first software to propose interactive quantum chemistry.

A first contribution allows for interactive quantum chemistry with systems up to a few hundred atoms [6]. The method is based on a divide-and-conquer (D&C) approach. The D&C technique subdivides the system into many subsystems (a–h on the Figure 10). Each of them involves a diagonalisation at each time step. To treat larger systems, we introduce a new algorithm: Block-Adaptive Quantum Mechanics (BAQM) [5] from the combination of two new components.

- **Block-adaptive Cartesian mechanics**

  By freezing atomic positions in some subsystems (d–h on the Figure 10) (with atoms in blue), we may avoid updating some eigenproblems. The Block-adaptive Cartesian mechanics component takes advantage of this to control the simulation cost by adaptively adjusting the number of diagonalisations, based on the forces applied to the atoms. Only the subsystems with the largest applied forces are allowed to have mobile atoms.

- **Adaptive reduced-basis quantum mechanics**

  Solving even just one of the subsystem's eigenproblem may be too costly to achieve interactive rates. The Adaptive reduced-basis quantum mechanics component projects the equation in an adaptive reduced basis composed of low-energy eigenvectors that have been computed at a previous time step, to benefit from temporal coherence between successive eigenproblems (subsystems (b) and (c) with atoms in black and white on the Figure 10). We use a simple distance to decide on the fly when to automatically update the reduced basis during the simulation (subsystem (a) with atoms in red on the Figure 10).

We demonstrated that BAQM may accelerate geometry optimization for several atomic systems. Indeed, each step is solved significantly faster by constraining some nuclei and electrons, and, by focusing computational resources on the most active parts of the system, we obtain a faster potential energy descent. The proposed BAQM approach also allows for interactive rates with many atomic systems.

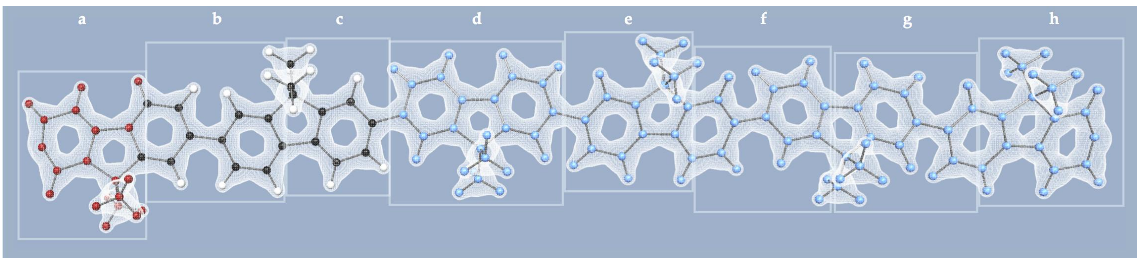


Figure 10. ***Interactive editing of a polyflurorene molecule with the BAQM algorithm***

6.4. Molecular Docking

6.4.1. Development of a new Knowledge-Based Potential for Protein-Ligand Interactions

Participants: Sergei Grudinin, Georgy Cheremovskiy.

Macromolecular complexes formed by proteins with small molecules (ligands) play an important role in many biological processes such as signal transduction, cell regulation, etc. Experimental methods for determining the structures of molecular complexes have a very high cost and still involve many difficulties. Therefore, computational methods, such as molecular docking, are typically used for predicting binding modes and affinities, which are essential to understand molecular interaction mechanisms and design new drugs.

Databases containing three-dimensional protein-ligand structures determined by experimental techniques grow very rapidly. In 2011, the PDB (Protein Data Bank) contained about 70,000 of protein structures, with almost 8,000 structures of protein-ligand complexes having refined binding affinity data. The CSD (Cambridge Structural Database), a database for small molecules, contained about 500,000 entries at the beginning of 2012. Thus, we believe that computational tools based on statistical information extracted from three-dimensional structures of protein-ligand complexes will play an ever more increasing role in the functional study of proteins as well as in structure-based drug design and other fields.

We proposed and validated a new statistical method that predicts binding modes and affinities of protein-ligand complexes. To do so, we have developed a novel machine-learning-based approach. Precisely, we have formulated a new optimization problem with 30,000 unknowns, whose solution is a scoring function. We trained the scoring function on 6,000 structures of protein-ligand complexes of high accuracy from the PDB database. Despite the very high dimensionality of the optimization problem, we manage to solve it on a desktop computer in just a few hours.

Our scoring function has three major applications in drug-design:

- Docking: determination of the binding site of a ligand bound to a protein.
- Ranking: identifying a set of ligands with the highest binding affinity for the given protein target by screening a large ligand database.
- Binding constants prediction: prediction of the absolute value of the binding constant of a protein-ligand complex.

The success rates of our method rank it among the top three methods currently available. Thus, we believe that our scoring function is the first one that performs well in all three major applications in drug-design.

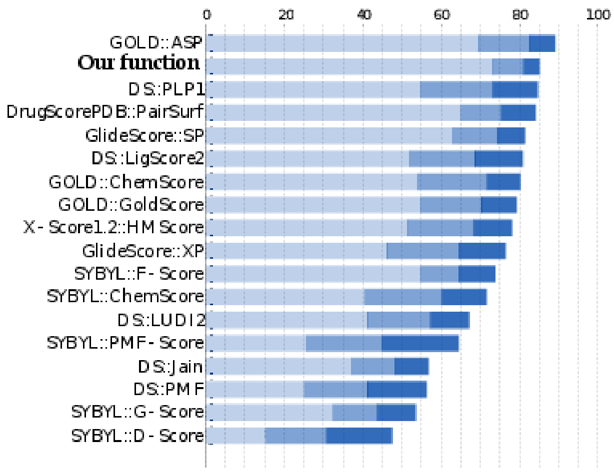


Figure 11. Comparison of the success rates of scoring functions when the best-scored binding pose differs from the true one by RMSD < 1.0 Å (light bars), < 2.0 Å (darker bars) or < 3.0 Å (the darkest bars), respectively. Scoring functions are ranked by success rates when the ligand binding pose is found within RMSD < 3.0 Å.

6.4.2. DockTrina

Participants: Sergei Grudinin, Petr Popov.

We derived analytical formulas for fast evaluation of the Root-Mean-Square-Deviation (RMSD) between rigid protein structures. This work resulted in a RMSD library containing algorithms to calculate the RMSD between two proteins in constant time. Based on this library we introduced an efficient algorithm to predict triangular protein structures and implemented it into the DockTrina software. We collected bound benchmarks of 220 protein trimers with and without symmetry properties from the Protein Data Bank and demonstrated the superiority of DockTrina over standard combinatorial algorithms aimed at predicting nonsymmetrical protein trimers.

6.4.3. Machine Learning for Structural Biology

Participants: Sergei Grudinin, Petr Popov, Mathias Louboutin.

We developed a new formulation of the machine learning optimization problem to predict protein–protein interactions. We implemented several optimization strategies, both in *d*ual and *p*rimal. We studied the effect of different types of loss-functions on the quality of the prediction. We also tested the efficiency of three descent algorithms, Nesterov descent, gradient descent, and stochastic descent. We demonstrated that generally, primal optimization is faster compared to dual optimization. In the primal, Nesterov descent has a better convergence compared to the gradient descent. Finally, stochastic algorithms often provide a better convergence compared to deterministic algorithms. All the studied algorithms were implemented as a stand-alone library.

6.5. Software Engineering

Participants: Jocelyn Gate, 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). The interface has been improved:

- The visualization of the data graph has been improved. Users may now drag and drop models and parts between layers, as well as directly drag and drop files into SAMSON.
- The undo/redo stack can now be visualized.
- We have begun to work on selection and highlighting.

The software engineering process has been improved as well, in particular to help base and modules developers:

- We have reorganized the file hierarchy so that modules can have associated data.
- We have developed a system to build SAMSON automatically on virtual machines (e.g., ubuntu 12.04 32bit, ubuntu 12.04 64 bit, fedora 17 32 bit, etc.).
- Tools have been created to let modules developers easily write new modules.
- We have begun to develop a mechanism to make it easy to install and update SAMSON automatically.

We have also developed several *SAMSON apps* to test various concepts, including scripting, manipulating molecules with haptic feedback, etc. Figure 12 shows the current user interface of SAMSON.

We have deposited the first version of SAMSON's code base at the APP ("Agence de Protection des Programmes").

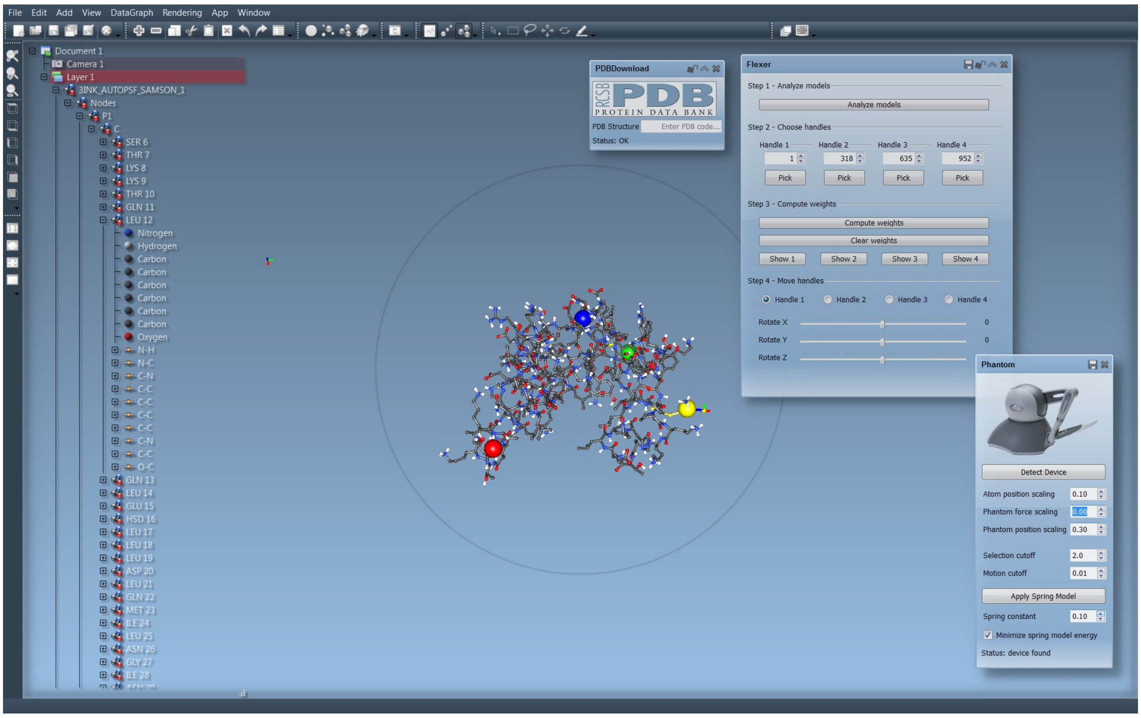


Figure 12. The current user interface of SAMSON, showing an app to download molecules directly from the Protein Data Bank, an app to deform molecules, and an app for haptic interaction. The data graph on the left shows the hierarchical structure of the data graph.

OPALE Project-Team

6. New Results

6.1. Mathematical analysis and control of macroscopic traffic flow models

6.1.1. Vehicular traffic

Participants: Maria Laura Delle Monache, Paola Goatin, Mauro Garavello [Piedmont University, Italy], Alexandre Bayen [UC Berkeley, CA, USA].

The activity in traffic flow modeling has being reinforced by the creation of the Associated Team ORESTE between OPALE and the UC Berkeley teams Mobile Millennium and Integrated Corridor Management (ICM) lead by Prof. A. Bayen (see http://www-sop.inria.fr/members/Paola.Goatin/ORESTE/index.html). In this framework, three PhD students from US visited Inria during August and September, and M.L. Delle Monache spent two and half months at UC Berkeley.

During this first year of common research we proposed a new junction model for ramp-metering in the continuous and discrete settings. We focused on a junction consisting in a mainline, an on-ramp and an off-ramp. In particular, we introduced a coupled PDE-ODE model, in which the PDE describes the evolution of the cars flow on the mainline 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. At the junction we imposed the maximization of the outgoing flux together with a fixed priority parameter for incoming roads. We were able to prove existence and uniqueness of the solution of the corresponding Riemann problem. This approach has then been extended to networks and discretized using the Godunov scheme. The corresponding discrete optimization problem has been solved using the Adjoint Method and it is now being implemented into a MATLAB code. This model will serve as starting point for a subsequent model for optimal rerouting, which includes multi-commodity flow and partial control.

Besides that, we studied a a coupled PDE-ODE system modeling the interaction of a large slow moving vehicle with the surrounding traffic flow. The model consists in a scalar conservation law with moving density constraint describing traffic evolution coupled with an ODE for the slow vehicle trajectory. The constraint location moves due to the surrounding traffic conditions, which in turn are affected by the presence of the slower vehicle, thus resulting in a strong non-trivial coupling. The existence result is given in [60].

The paper [41] is devoted to the study of a traffic flow model on a network composed by an arbitrary number of incoming and outgoing arcs connected together by a node with a buffer. We define the solution to the Riemann problem at the node and we prove existence and well posedness of solutions to the Cauchy problem.

6.1.2. Crowd motion

Participants: Nora Aïssiouene, Christophe Chalons [LJLL, UP7], Régis Duvigneau, Paola Goatin, Matthias Mimault, Massimiliano D. Rosini [ICM, Warsaw University, Poland], Nicolas Seguin [LJLL, UPMC], Monika Twarogowska.

The activity on in pedestrian flow modeling is reinforced by the doctoral thesis of M. Mimault, started in October, and the enrollment of M. Twagorowska on a post-doctoral position.

Concerning crowd motion modeling, we are interested in the optimization of facilities design, in order to maximize pedestrian flow and avoid or limit accidents due to panic situations. To this aim, we are now studying first and second order macroscopic models for crowd movements consisting in one or two scalar conservation law accounting for mass conservation and momentum balance, coupled with an Eikonal equation giving the flux direction depending on the density distribution. From the theoretical point of view, and as a first step, we are studying the problem in one space dimension (for applications, this case corresponds to a crowd moving in a corridor). In collaboration with M. Rosini (supported by the project CROM3, funded by the PHC Polonium 2011), we have established entropy conditions to select physically relevant solutions, and we have constructed explicit solutions for some simple initial data (these results are presented in [40]). We are now studying existence of solutions of the corresponding initial boundary value problem, using the wave-front tracking approach. In this framework, M. Mimault's internship was devoted to develop a MATLAB code based on wave-front tracking to compute the solutions of Hughes' model of pedestrian motion with generalized running cost. This model displays a non-classical dynamic at the splitting point between the two directions of motion. The wave-front tracking scheme provides us with reference solutions to test numerically the convergence of classical finite volume schemes, which do not treat explicitly the dynamics at the turning point (see [66]). The code can be downloaded at the following URL: http://www-sop.inria.fr/members/Paola.Goatin/wft.html

From the numerical point of view, we are implementing some macroscopic models in two space dimensions on triangular meshes on the Num3sis platform. This was partly done by N. El-Khatib (postdoc at Inria from January to August 2011), and is now being completed by M. Twarogowska, with the support of N. Aïssiouene. This will provide a performing numerical tool to solve the related optimization problems arising in the optimization of facilities design, such as the position and size of an obstacle in front of (before) a building exit in order to maximize the outflow through the door and avoid or limit over-compression.

Finally, in collaboration with C. Chalons and N. Seguin, we have generalized the results on conservation laws with local flux constraint obtained in [3], [5] to general flux functions and nonclassical solutions arising for example in pedestrian flow modeling. We first define the constrained Riemann solver and the entropy condition, which singles out the unique admissible solution. We provide a well posedness result based on wave-front tracking approximations and Kruzhkov doubling of variable technique. We then provide the framework to deal with nonclassical solutions and we propose a "front-tracking" finite volume scheme allowing to sharply capture classical and nonclassical discontinuities. Numerical simulations illustrating the Braess paradox are presented as validation of the method. The results are collected in [65].

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 discipline, such as structural mechanics.

Our approach to *competitive optimization* 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. This approach has been demonstrated over a test-case of aero-structural aircraft wing shape optimization, in which the eigensplit-based optimization reveals clearly superior [38].

While the two-discipline method is currently being applied to various complex physical multi-objective situations (see in particular 6.2.4 , 6.2.5 , 6.2.6), the method has been extended to situations involving more than two objectives when the initial point is Pareto-optimal. Then, a particular convex combination of the criteria is locally stationary, and the two-discipline strategy can be applied using this combination as preponderant criterion, and a particular other criterion as secondary one. Whence, the proposed split of territory produces a continuum of Nash equilibrium points *tangent* to the Pareto set. This theoretical result has been illustrated in the context of a simpler numerical experiment by E. Baratchart during his internship [4], see Fig. 2 .

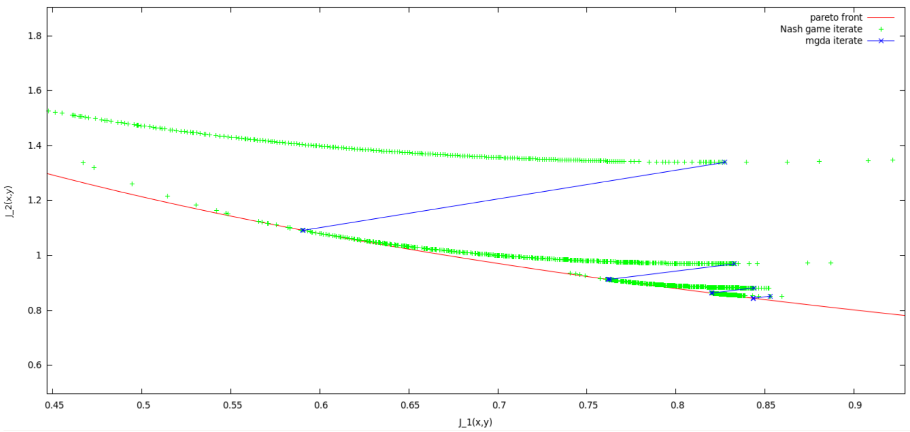


Figure 2. Combination of cooperative and competitive optimization algorithms: in red the Pareto set, in blue MGDA steps directed to the Pareto set, in green steps by Nash games with split of territory tangent to the Pareto set.

Our approach to *cooperative optimization* 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 [39] 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-optimal. 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 point on the Pareto set, at which a competitive optimization phase can possibly be launched on the basis of the local eigenstructure of the different Hessian matrices. This general formulation fosters several connected studies detailed in 6.2.1 .

6.2.1. Multiple-Gradient Descent Algorithm (MGDA)

Participants: Jean-Antoine Désidéri, Régis Duvigneau, Matteo Giacomini, 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.

In the original report [14], and in [39], we have introduced the notion of *Pareto-stationarity*, and given a first proof that it was the natural necessary condition for Pareto-optimality when the objective-functions are locally smooth in some open domain about the design-point. This report has been revised to provide a more rigorous, and extended proof. In particular, in the revised version [14] (version 3, 2012), the number of objective-functions n and the dimension of the design space compare arbitrarily. The objective-functions are assumed to be locally convex.

Additionally, we had established that MGDA converges to Pareto-stationary design-points. This had been confirmed by numerical experiments in which MGDA had been tested over a number of classical multi-objective optimization test-cases, and found successful to converge to Pareto-optimal solutions in situations of either convex or concave Pareto sets. Additionally, MGDA [57] and PAES [69] were found to have complementary merits, making a hybrid method promising.

The method was tested successfully in a domain partition model problem in which the sub-solutions to the Poisson equation are matched at the interfaces by minimization of the integral along the interface of the squared normal-derivative jump. This academic exercise has permitted to illustrate the importance of applying an appropriate scaling to the gradients prior to calculating the descent direction [61] [47]. This has led us to define, a novel form of MGDA, consisting of a direct algorithm [62] based on a Gram-Schmidt orthogonalization conducted with a special normalization. The direct method was found more accurate and more efficient. Subsequently, we proposed two enhancements [63], the first to define the order in which the gradients are introduced in the Gram-Schmidt process uniquely and to interrupt the process as soon as the current estimate of the search direction is proved to satisfy the descent property, and the second to optimally scale the gradients when the Hessians are known, or approximated (e.g. by the BFGS estimate).

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. 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 [55]. This more difficult problem has been proposed by Renault within the OMD2 ANR project.

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 6.6) 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: Jean-Antoine Désidéri, Régis Duvigneau, Jérémie Labroquère.

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, a numerical study is conducted to i) improve the understanding of controlled flows ii) develop a methodology to determine optimal control parameters by coupling the controlled flow simulation 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[37].

In this perspective, unsteady Reynolds Averaged Navier-Stokes equations are considered, with the Spalart-Allmaras turbulence closure. A numerical model for synthetic jets has been implemented to simulate the actuation[48], based on imposed velocity boundary conditions. Particular developments have then be carried out to include a noise term into Gaussian Process metamodels, which is used to filter errors arising from unsteady simulations/citelabroquere:hal-00742940. First results have demonstrated the feasibility of the proposed method. A systematic assessment of modeling and numerical errors is in progress, 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 to develop robust design tools for aircraft design 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 consisting of minimizing statistical quantities such as mean and variance of a cost function, typically the drag coefficient under lift constraint. MGDA is used for this purpose.

At present, analytical test cases have been tested, confirming the validity of our approach to identify the Pareto set.

One aspect of the problem is that the evaluation of these statistics and performing their optimization is very cost demanding. One solution could be, for aerodynamic design, to identify the most important variables to be treated as uncertain, possibly by the ANOVA approach, and construct adequate meta-models.

6.2.4. Aero-structural optimization

Participants: Gérald Carrier [Research Engineer, ONERA/DAAP], Jean-Antoine Désideri, Imane Ghazlane.

In industry, aircraft wings are designed by accounting for several multidisciplinary couplings. Certainly of greatest importance is the coupling, or concurrency, between aerodynamic optimization and structural design. At ONERA, in the former thesis of M. Marcelet, the aerodynamic gradient has been extended to account for (the main terms of) static fluid-structure interaction, commonly referred to as the “aeroelastic gradient”.

In her thesis, I. Ghazlane has extended M. Marcelet’s work to take into account, in the aeroelastic gradient, the terms originating from the differentiation of the wing-structural model. In this development, the wing structure is treated as an equivalent Euler-Bernoulli beam. These formal extensions have been validated by an extensive experimentation. Additionally, special post-processing procedures have been set up to evaluate accurately the various physical contributions to drag. As a result, a realistic aircraft wing optimization has been conducted using a configuration provided by Airbus France as initial design. I. Ghazlane defended successfully her doctoral thesis thesis in December 2012 [34].

Besides, I. Ghazlane has realized a two-objective optimization (drag and mass reduction) via a Nash game using our optimization platform FAMOSA. These results will be included in a common publication on Nash games in preparation.

6.2.5. 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 [68] for the calculation of the Whitham function corresponding to the lowest-boom (axisymmetric) shape. Method and results for more general geometries have been presented internationally in [50].

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. These results will be included in a common publication on Nash games in preparation.

6.2.6. 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. In the current work, 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 the twist angle along the wing is 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 a forthcoming AIAA Conference, and will also contribute to a common publication on Nash games in preparation.

6.2.7. Optimum design in naval hydrodynamics

Participants: Régis Duvigneau, Louis Blanchard.

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.

In collaboration with GALAAD Project-Team, 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[58]. 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.

6.3. Optimum design in structural mechanics

6.3.1. Shape Optimization in Multidisciplinary Non-Linear Mechanics

Participants: Aalae Benki, Jean-Antoine Désidéri, Abderrahmane Habbal.

In collaboration with the ArcelorMittal's Center for Research in Automotive and Applications, 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. In both cases, only arbitrary territory splitting was used. Application to large scale 3D industrial problems, and the study of intelligent territory splitting algorithms is ongoing.

6.3.2. Optimization of Addendum Surfaces in Stamping

Participants: Fatima Zahra Oujebbour, Jean-Antoine Désidéri, Abderrahmane Habbal.

Within the OASIS Consortium (ArcelorMittal, ErDF, Inria, UTC, EURODECISION, ESILV, NECS, Delta-CAD, SCILAB-DIGITEO), Opale Project leads the Optimization task. Our aim is to develop decentralized decision-making algorithms dedicated to find efficient solutions (Pareto optimal) in a complex multidisciplinary 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 thickness distribution.

We have successfully applied the NBI approach coupled to the hybrid SA+SPSA minimizer (Simulated Annealing with local search using the Simultaneous Perturbation Stochastic Approximation) to capture the Pareto front of a simple cross stamping of a high performance steel sheet. The use of cubic spline approximation of the costs (spring-back and failure criteria) turned out to be more reliable than e.g. a krigeage method.

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

6.4.1. Mathematical modeling of dorsal closure DC

Participants: Abderrahmane Habbal, Luis Almeida [University of Nice-Sophia Antipolis], Patrizia Bagnerini [Genova University], Fanny Serman [University of Nice-Sophia Antipolis], Stéphane Noselli [University of Nice-Sophia Antipolis], Glenn Edwards [Duke University].

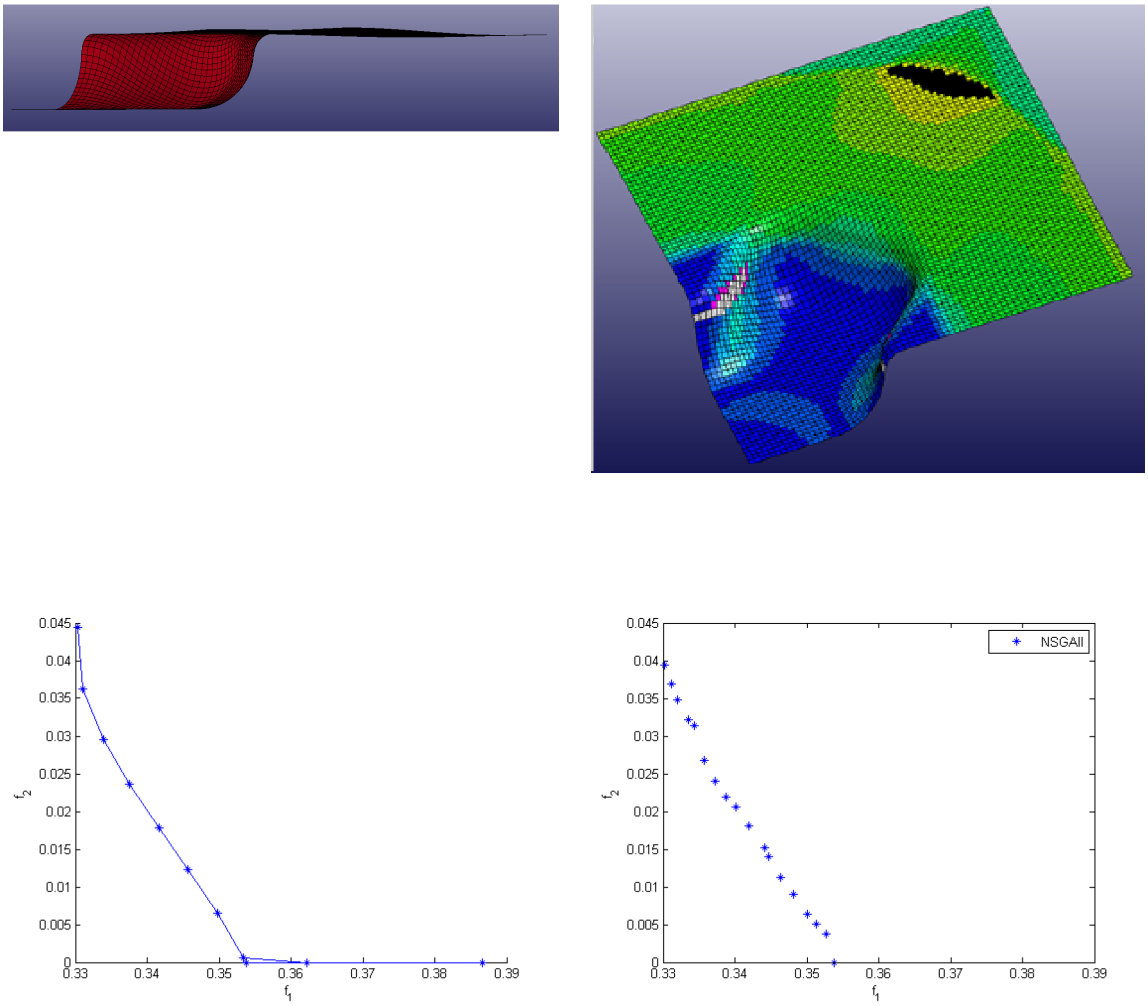


Figure 3. Multiobjective design of the stamping process of a high performance steel sheet. The costs are elastic spring-back (upper-left) and failure (upper-right). The Pareto front obtained by NNCM (lower-left) is compared to a NSGA-II one (lower-right).

A mathematical model for simulation of actin cable contraction, during wound closure for Drosophila embryo, which contains an extra term in addition to the curvature flow is developed. The basic mathematical model introduced and validated in [2] is extended in order to include the non-homogeneous wound healing or non-homogeneous dorsal closure The new model is obtained by adding extra terms that describe the particular process we want to model (lamellipodial crawling, granulation tissue contraction, extension of actin protrusions, epithelial resistance, etc.). We concentrate on the treatment of non-homogeneous forces, i.e. non-constant boundary terms which can be associated with a non-uniform cable, internal pull or zipping force due to the non-uniformity of the biological or physical properties of the boundary cells or of the connective tissue [35].

We also consider a particular yet major aspect of wound healing, namely the one related to the movement of wounded epithelial cell monolayers. The epithelial monolayer cell population, also referred to as cell-sheet, can be seen as a 2 dimensional structure, although it is well known that apical and basal sites play distinctive important roles during the migration, as well as the substrate itself. Immediately after a wound is created, the cells start to move in order to fill in the empty space. This movement, the wound closure, is a highly-coordinated collective behavior yielding a structured cohesive front, the wound leading edge. Even though wound closure involves biochemical and biomechanical processes, still far from being well understood, which are distributed over the whole monolayer, much specific attention was paid to the leading edge evolution, seen as the front of a traveling wave of the cell density function. We show that, for non inhibited wound assays, closure occurs at constant speed of the leading edge, a fact that is commonly shared by biologists and biomathematicians. But we also show that the leading edge may exhibit accelerated profiles, and that when inhibited, then the F-KPP has poor performances in modeling the leading edge dynamics.

6.5. Particular applications of simulation methods

6.5.1. Hermitian interpolation under uncertainties

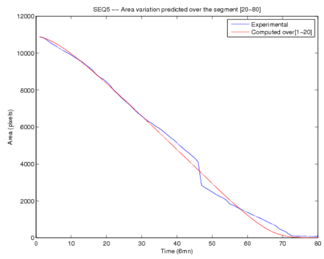
Participants: Jean-Antoine Désideri, Manuel Bompard [Doctoral Student, ONERA/DSNA until December 2011; currently post-doctoral fellow in Toulouse], Jacques Peter [Research Engineer, ONERA/DSNA].

In PDE-constrained global optimization, iterative algorithms are commonly efficiently accelerated by techniques relying on approximate evaluations of the functional to be minimized by an economical, but lower-fidelity model (meta-model), in a so-called Design of Experiment (DoE). Various types of meta-models exist (interpolation polynomials, neural networks, Kriging models, etc). Such meta-models are constructed by pre-calculation of a database of functional values by the costly high-fidelity model. In adjoint-based numerical methods, derivatives of the functional are also available at the same cost, although usually with poorer accuracy. Thus, a question arises : should the derivative information, available but known to be less accurate, be used to construct the meta-model or ignored ? As a first step to investigate this issue, we have considered the case of the Hermitian interpolation of a function of a single variable, when the function values are known exactly, and the derivatives only approximately, assuming a uniform upper bound ε on this approximation is known. The classical notion of best approximation has been revisited in this context, and a criterion introduced to define the best set of interpolation points. This set was identified by either analytical or numerical means. If $n+1$ is the number of interpolation points, it is advantageous to account for the derivative information when $\varepsilon \leq \varepsilon_0$, where ε_0 decreases with n, and this is in favor of piecewise, low-degree Hermitian interpolants. In all our numerical tests, we have found that the distribution of Chebyshev points is always close to optimal, and provides bounded approximants with close-to-least sensitivity to the uncertainties [56].

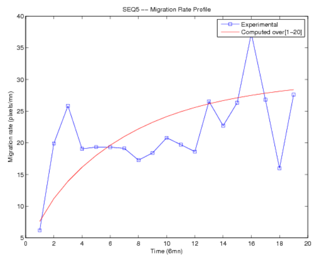
6.5.2. Mesh qualification

Participants: Jean-Antoine Désideri, Maxime Nguyen, Jacques Peter [Research Engineer, ONERA/DSNA].

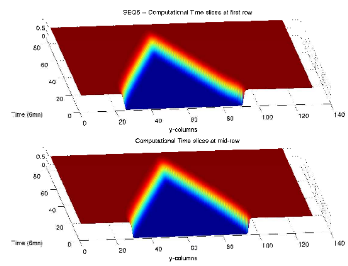
M. Nguyen Dinh is conducting a CIFRE thesis at ONERA supported by AIRBUS France. The thesis topic is the qualification of CFD simulations by anisotropic mesh adaption. Methods for refining the 2D or 3D structured mesh by node movement have been examined closely. Secondly, it is investigated how could the local information on the functional gradient $\|dJ/dX\|$ be exploited in a multi-block mesh context. This raises particular questions related to conservation at the interfaces.



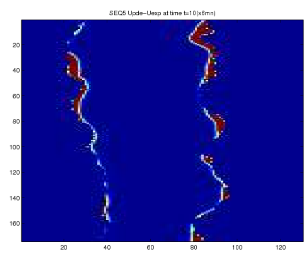
(a)



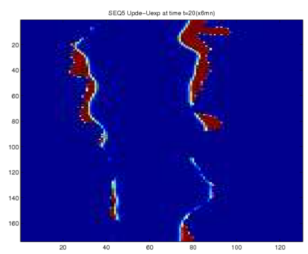
(b)



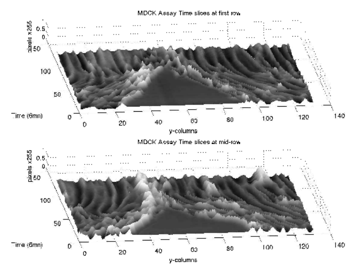
(c)



(d)



(e)



(f)

Figure 4. ***Sequence-5. Computational vs experimental wound evolution.*** *(a) Time variation of experimental (blue) versus computed (red) wound area (in pixels). (b) Time variation of the experimental (blue-dot) versus computed (red) migration rate (in pixels/mn). (c) Computed 3D XT view at first and mid-rows. (d) (e) (f) Traces of the difference between the experimental segmented and binarized cell-sheet images and the computed ones at different times, respectively 1hour (d), and 2hours (e) after the wounding. (f) Experimental 3D XT view at first and mid-rows.*

Several criteria have been assessed for mesh qualification in the context of inviscid-flow simulation and are currently being extended to the RANS context. These results have been presented internationally in the communication [54] and the publication [44].

6.5.3. Hybrid meshes

Participants: Sébastien Bourasseau, Jean-Antoine Désideri, Jacques Peter [Research Engineer, ONERA/DSNA], Pierre Trontin [Research Engineer, ONERA/DSNA].

S. Bourasseau has started a CIFRE thesis at ONERA supported by SNECMA. The thesis is on mesh adaption in the context of hybrid meshes, that is, made of both structured and unstructured regions. Again, the aim is to exploit at best the function gradient provided by the adjoint-equation approach. Preliminary experiments have been conducted on geometries of stator blade yielding the sensitivities to global shape parameters.

The on-going developments are related to the extension to the hybrid-mesh context of the full shape gradient in a 3D Eulerian flow computation.

6.5.4. Data Completion Problems Solved as Nash Games

Participants: Abderrahmane Habbal, Moez Kallel [University of Tunis].

The Cauchy problem for an elliptic operator is formulated as a two-player Nash game.

- Player (1) is given the known Dirichlet data, and *uses as strategy variable the Neumann condition* prescribed over the inaccessible part of the boundary.
- Player (2) is given the known Neumann data, and *plays with the Dirichlet condition* prescribed over the inaccessible boundary.
- The two players solve in parallel the associated Boundary Value Problems. Their respective objectives involve the *gap between the non used Neumann/Dirichlet known data and the traces of the BVP's solutions* over the accessible boundary, and are *coupled through a difference term*.

We prove the existence of a unique Nash equilibrium, which turns out to be the reconstructed data when the Cauchy problem has a solution. We also prove that the completion algorithm is stable with respect to noise. Many 3D experiments were performed which illustrate the efficiency and stability of our algorithm [42].

6.6. Isogeometric analysis and design

Participants: Louis Blanchard, Régis Duvigneau, Bernard Mourrain [Galaad Project-Team], Gang Xu [Galaad Project-Team].

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 all design tasks:

- the geometry is defined by NURBS surfaces;
- the computation domain is defined by NURBS volumes instead of meshes;
- the solution fields are obtained by using a finite-element approach that uses NURBS basis functions
- the optimizer controls directly NURBS control points.

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 GALAAD Project-Team, such as the development of methods for adaptive parameterization including an a posteriori error estimate[46], [45]. A collaborative work has also been carried out with the Technical University of Kaiserslautern, concerning the computation of shape gradients for linear elasticity problems[59].

POEMS Project-Team

6. New Results

6.1. Numerical methods for time domain wave propagation

6.1.1. Coupling Retarded Potentials and Discontinuous Galerkin Methods for time dependent wave propagation problems

Participant: Patrick Joly.

This topic is developed in collaboration with J. Rodriguez (Santiago de Compostela) in the framework of the contract ADNUMO with AIRBUS. The general objective was to use time-domain integral equations - or retarded potentials - as a tool for contructing transparent boundary conditions for wave problems in unbounded media, by coupling them to an inerior volumic method, namely the Discontinuous Galerkin (DG) method.

Since last year, our new goal is to extend the method proposed in a previous work for DG with central fluxes to the case of upwind fluxes, while preserving most of the good properties of the original method from both theoretical (stability via energy dissipation - instead of energy conservation) and practical points of view. We have designed a method that achieves this goal at the only prize of a small deterioration of the CFL condition. The method has been successfully implemented and the numerical results clearly emphasize the superiority of upwing fluxes for taking into account the convection terms in the linearized Euler equations in aeroacoustics, the privileged application.

At the same time, we have used similar ideas for treating physical boundary conditions involving differential (in time) impedance operators.

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

Participants: Aliénor Burel, Marc Duruflé, Patrick Joly.

This topic is the subject of the first part oh th PhD thesis of A. Burel. Its aim 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 context. Last year, a method has been proposed for solving the Dirichlet problem (clamped boundary), successfully analyzed and implemented. For free boundary conditions, we have proposed an original method considereing these boundary conditions as a perturbation of the Dirichlet conditions. The natural adaptation of the variational formulation used in the case of the Dirichlet problems presents nice theoretical properties and leads to satisfactory numerical results for the time harmonic problem. However, the implementation for the time dependent problem reveals severe instability phenomena that seem to be already present in the semi-discrete (in space) problem. In order to understand the cause of these instability (and possibly remedy them) we are currently performing the Kreiss analysis of the half-space problems in the case where Q_1 finite elements are used on the same uniform square grid for both P-waves and S-waves potentials.

6.1.3. Time domain analysis of Maxwell's equations in Lorentz materials

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

This is the time-domain counterpart of the research done at Poems about frequency domain analysis of metamaterials (see also the section 6.2.7) in the framework of the ANR Project Metamath. One fundamental question is the link between the two problems via the limiting amplitude principle, in particular in the cases where the time harmonic problem fails to be well posed problem in the standard framework. This occurs at certain frequencies (see section) when one considers a transmission problem between a Lorentz material and a standard one.

We are investigating this question 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.

6.1.4. Modeling and numerical simulation of a piano.

Participants: Juliette Chabassier, Marc Duruflé, Sébastien Imperiale, Patrick Joly.

The defense of the PhD thesis of Juliette Chabassier, in March, has marked one of the most spectacular achievements in Poems for the past years, concerning the "complete" physical and mathematical modeling of a grand piano and its computer simulation. This is the result of a quite interdisciplinary work in collaboration with Antoine Chaigne (UME, ENSTA). We refer the reader to the three previous activity reports of Poems for a more detailed description of the scientific developments that have led to the implementation of a parallel code for the simulation of the piano. Using this code, M. Duruflé and J. Chabassier have realized a bank of synthetic sounds that can be used for playing scoreboards (using MIDI files for instance). For more details, and also other additional information about the work, we refer the reader to the Web page : http://modelisation.piano.free.fr.

Although already quite satiafactory, the results obtained by the present version of the code show that there is still room for the improvement of our piano model. One of the ideas consists in improving the quality of the model for the hammers and that is why J. Chabassier and M. Duruflé have proposed an enriched model involving the virations of the hammer's shank. We expect to achieve further progress in this direction through our participation to the ITN (Initial Training Network) European project BATWOMAN (Basic Acoustics Training and Workprogram on Methodologies for Acoustics Network) that has been submitted lst November. This projects regroups 11 partners from 7 different contries and gathers academic people with industrials of the donain, including Steinway.

As a theoretical complement to the numerical developments, we have led a systematic theoretical study of the numerical method used in our code for computing string's vibrations. Our concern was to develop a new implicit time discretization, which is associated with finite element methods in space, in order to reduce numerical dispersion while allowing the use of a large time step. We proposed a new θ-scheme based on different θ-approximations for the flexural and shear terms of the equations, which allows to reduce numerical dispersion while relaxing the stability condition. In particular, we gave some insights of innovative proofs of stability by energy techniques that provide uniform estimates with respect to the CFL number. Theoretical results have been illustrated with numerical experiments corresponding to the simulation of a realistic piano string.

6.1.5. Numerical methods in electromagnetism

Participant: Patrick Ciarlet.

Collaborations with Eric Chung, Tang Fei Yu and Jun Zou (Chinese University of Hong Kong, China), Philippe Ciarlet (City University of Hong Kong, China) Haijun Wu (Nanjing University, China), Stefan Sauter and Corina Simian (Universität Zürich).

The numerical approximation of electromagnetic fields is still a very active branch of research. Below, three lines of work are briefly reported.

Edge finite elements are widely used in 2D/3D electromagnetics, however they approximate very weakly the divergence of the fields. In a recent work with H. Wu & J. Zou, we proposed a method that allows one to approximate the divergence accurately in H^{-s}-norms $(1/2 < s < 1)$.

Discontinuous Galerkin finite elements are also very popular, as they allow one to design fast (and accurate) methods to solve PDEs. Jointly with E. Chung and T. F. Yu, we designed a numerical method to solve the 2D/3D time-dependent Maxwell equations, using a high order staggered DG method in the spirit of those introduced by E. Chung and B. Engquist. The method has been analyzed on Cartesian meshes and its generalization to unstructured meshes is under way.

A few years ago, we proposed with Philippe Ciarlet a method to solve some problems in linear elasticity intrinsically. With S. Sauter, C. Simian and Philippe Ciarlet, we studied a similar approach that can be applied to 2D electrostatics. It consists in solving the problem in the electric field directly, using exact or local curl-free approximation of the field. Within this framework, we have been able to derive a general method that allows one to derive intrinsic conforming and non-conforming finite element spaces to compute the electrostatic potential. Generalization to 3D electrostatics and linear elasticity is under way.

6.2. Time-harmonic diffraction problems

6.2.1. Numerical computation of variational integral equation methods

Participants: Marc Lenoir, Nicolas Salles.

The dramatic increase of the efficiency of the variational integral equation methods for the solution of scattering problems must not hide the difficulties remaining for an accurate numerical computation of some influence coefficients, especially when the panels are close and almost parallel.

The formulas have been extended to double layer potentials and, for self influence coefficients, to affine basis functions. Their efficiency for the solution of Maxwell equations has been proved in the framework of a collaboration with CERFACS.

6.2.2. Formulation and Fast Evaluation of the Multipole Expansions of the Elastic Half-Space Fundamental Solutions

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 ongoing 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. 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.

6.2.3. Domain decomposition methods for time harmonic wave propagation

Participants: Francis Collino, Patrick Joly, Mathieu Lecouvez.

This work is motivated by a collaboration with the CEA-CESTA (B. Stupfel) through the PhD thesis of M. Lecouvez that has started at the beginning of the year.

We are interested in the diffraction of time harmonic electromagnetic waves by perfectly conducting objects covered by multi-layered (possibly thin) dielectric coatings. This problem is computationally hard when the size of the object is large (typically 100 times larger) with respect to the incident wavelength. In such a situation is to use a domain decomposition method in which each layer would contitute a subdomain. More precisely, we want to use a non overlaping iterative domain decomposition method based on the use of Robin type transmission conditions, a subject to which people at Poems gave substantial contributions in the 90's through the works of Collino, Desprès, 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. To overcome the disadvantage of dealing with completely nonlocal operators, we suggest to work with truncated kernels, i.e. with operators of the form (Γ represents one interface)

$$u(x) \quad \longrightarrow \quad \int_{\Gamma} K\,(\,|x-y|\,)\ \chi\left(\frac{|x-y|}{\lambda}\right)\ u(y)\ d\sigma(y)$$

where $K(|x|)$ is an appropriate singlar kernel (typically $K(|x|) = |x|^{-\gamma}$) and $\chi(\rho)$ an adequate smooth cut-off function. Playing with a few parameters such as the size of the support of χ, we expect to achieve an optimal compromise between the reduction of the number of iterations of the method and the cost of each iteration.

6.2.4. Time harmonic aeroacoustics

Participants: Anne-Sophie Bonnet-Ben Dhia, Jean-François Mercier.

We are still working on the numerical simulation of the acoustic radiation and scattering in presence of a mean flow. This is the object of the ANR project AEROSON, in collaboration with Florence Millot and Sébastien Pernet at CERFACS, Nolwenn Balin at EADS and Vincent Pagneux at the Laboratoire d'Acoustique de l'Université du Maine. Let us recall that our method combines, a Finite Element resolution of the augmented Galbrun equation and of the coupled vorticity transport equation, and the use of Perfectly Matched Layers (PML) to bound the computational domain. The main recent improvements concern the test of the method in presence of unstable modes.

When determining the aeroacoustics modes propagating in a flow, unstable modes exist for certain types of flows: when an inflection point exists in the velocity profile and when the shear in this point is strong enough. Such modes grow exponentially in space. Up to recently, our numerical simulations have been performed for stable flows. We have tested the behavior of PML in the presence of unstable modes, which usually convert a propagating field in a decaying field. Therefore we do not have a theoretical framework to characterize the behavior of PML in the presence of spatially growing modes but the various conducted numerical tests have shown that our numerical method is still able to select the outgoing solution, even in the presence of instabilities, if the attenuation in the PML is strong enough.

6.2.5. Multiple scattering in a duct

Participant: Jean-François Mercier.

This topis is developed in collaboration with Agnès Maurel (Langevin Institute ESPCI).
The objective of this work, part of the ANR Procomedia, is to develop analytical methods to describe the propagation of acoustic waves in 2D waveguides containing penetrable inclusions. Scatterers of arbitrary shape with a contrast in both density and sound speed are considered. A modal approach is adopted, in which the wave equation is projected onto the transverse modes of the homogeneous guide. For each mode a 1D wave equation is obtained with a source term which characterizes the scatterers and couples modes together. In weak scattering regime (small scatterers or low contrasts or low frequency), the Born approximation is used to solve analytically this family of coupled ODE. This gives an explicit prediction for the scatterered field, in particular the reflection and transmission coefficients are obtained in two cases of interest: periodically or randomly distributed scatterers. In both cases, expressions similar to those in free space (available only for low frequencies) are obtained without frequency limit, thanks to the presence of a shape factor sensitive to the geometry of the scatterers at high frequencies.

Recently the obtained analytical expressions have been exploited to develop a very simple imaging method in a heterogeneous waveguide. Measurements of low-frequency reflection and transmission allow to find the position of the object while the higher frequency measurements give access to the shape and to the physical characteristics of the scatterers. The results are good in the case of low contrast and small scatterers, for which the Born approximation is perfectly valid.

6.2.6. Localization in perturbed periodic metamaterials

Participant: Jean-François Mercier.

This topis is developed in collaboration with Agnès Maurel, Abdelwaheb Ourir (Langevin Institute ESPCI) and Vincent Pagneux (LAUM).

The aim of this work, part of the ANR Procomedia, is to study the propagation of electromagnetic waves through 1D perturbed periodic media. The attenuation length in a medium consisting of alternating materials of optical indices $n_1 > 0$ and $n_2 < 0$ (metamaterials) is determined. When such medium is randomly disturbed, the localization properties differ significantly from those obtained in a classical disturbed medium: in the homogeneous case $n_1 = n_2$, a random perturbation of the indices induces the Anderson localization with a strong field attenuation. In contrast, in the case $n_1 = -n_2$, it was recently shown that the introduction of disorder on the permittivities ϵ_1 and ϵ_2 gave rise to an "anomaly", the suppression of the Anderson localization. This anomaly results in a significant increase of the attenuation length l_N for large sample sizes N.

We have made two improvements to existing works: simple analytical expressions of the attenuation length have been determined, valid over a wide range of frequencies and of number of layers. In addition we considered realistic metamaterials by taking into account disorder in both the permittivity and the permeability μ. When only the permeability is disturbed (or only the permittivity), our analytical expression can explain the transition to the abnormal behavior when the number of layers increases. Furthermore we show that the anomaly is strongly affected when disturbances in permeability and permittivity are jointly considered: the coupling of the two effects is capable of reseting the usual localization.

6.2.7. Modeling of meta-materials in electromagnetism

Participants: Anne-Sophie Bonnet-Ben Dhia, Camille Carvalho, Patrick Ciarlet, Lucas Chesnel.

This topis is developed in collaboration with Eric Chung (Chinese Univ. of Hong Kong) and Xavier Claeys (Paris VI).

Meta-materials can be seen as particular media whose dielectric and/or magnetic constant are negative, at least for a certain range of frequencies. This type of behavior can be obtained, for instance, with particular periodic structures. Of special interest is 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. The year 2012 saw the completion of Lucas Chesnel PhD thesis. We present below the main results obtained these last three years. The first topic we considered a few years ago was: when is the (simplified) scalar model well-posed in the classical H^1 framework? It turned out this issue could be solved with the help of the so-called T-coercivity framework. While numerically, we proved that the (simplified) scalar model could be solved efficiently by the most “naive” discretization, still using T-coercivity. Recently, we have been able to provide sharp conditions for the T-coercivity to hold in general 2D and 3D geometries, which involve explicit estimates in simplified geometries together with localization arguments. We then analyzed the discretization of the scalar problem with a classical, H^1 conforming, finite element method, and proved the convergence under the same sharp conditions. We also showed that the problem can be solved with the help of a Discontinuous Galerkin discretization, which allows one to approximate both the field and its gradient (with E. Chung).

As a second topic, we investigated the case of a 2D corner which can be ill-posed (in the classical H^1 framework). Using the Mellin transform, we showed that a radiation condition at the corner has to be imposed to restore well-posedness (with X. Claeys). Indeed there exists 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 proposed a numerical approach to approximate the solution which consists in adding some PMLs in the neighbourhood of the corner.

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. Of course, these scalar problems involves sign-changing coefficients but they can be studied using simple scalar T-coercivity approach.
C. Carvalho started her PhD thesis this fall in the continuation of these works.

6.2.8. Numerical MicroLocal Analysis

Participants: Jean-David Benamou, Francis Collino, Simon Marmorat.

Numerical microlocal analysis of harmonic wavefields is based on a family of linear filters using Bessel functions and applied to wave data collected on a circle of fixed radius r_0 around the observation point x_0 where we want to estimate the Geometric Optics/ High Frequency components. The data can easily be reconstructed from more conventional line array or grid geometry. The output is an angular function presenting picks of amplitudes in the direction angles of rays.

The original NMLA algorithm relied on a local plane wave assumption for the data. For arbitrary waves, it meant linearization errors and accuracy limitations. Also, only the directions of the (multiple) rays are recovered but the traveltime and amplitudes are not reliably computed. We recently introduced a new "impedant" observable which allows to prove a stability theorem. Numerical results confirm that the new NMLA filter is robust to random and correlated noise.

Using asymptotic expansion on NMLA filtered point sources data, we designed a correction method for the angle which also estimates the wavefront curvature. It can be used to correct the linearization errors mentioned above and provides a second order correction in the Taylor approximation of the traveltime.

The parameters of the method (size of observation circle, discretization) are automatically optimized and a posteriori quantitative error on angles and curvature are available. Numerical studies validate the stability result and confirm the superior accuracy of the curvature corrected NMLA version over image processing methods.

When some bandwith is available we can also compute the traveltime. The amplitude remains polluted by phase errors. Its determination is still open.

6.3. Absorbing boundary conditions and absorbing layers

6.3.1. Evolution problems in perturbed infinite periodic media

Participant: Sonia Fliss.

For parabolic problems set in locally perturbed periodic media, we have developed an approach to determine the time-domain DtN operator. The principle is to apply the Laplace Transform in time to the equation and use the construction of the DtN operator for stationary equations. The main difficulty is the computation of the inverse of the Laplace Transform, more precisely to understand how to deal with the unbounded interval of integration and the choice of the discretization of the laplace variable. To deal with the first difficulty for waveguide problem, we have studied the asymptotic behavior of the DtN operator in the laplace domain when the laplace variable tends to $p_0 \pm \infty$. To deal with the second difficulty, we have used the Z-Transformation and its properties. The numerical study is still in progress. This work enters in the framework of the ANR PRoject MicroWave (Sonia Fliss is an external collaborator), in collaboration with Karim Ramdani (Institut Elie Cartan de Nancy, UMR CNRS 7502), Christophe Besse and Ingrid Violet (Laboratoire Paul Painlevé, UMR CNRS 8524).

6.3.2. New transparent boundary conditions for time harmonic acoustic problem in anisotropic media

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

This topis is developed in collaboration with Vahan Baronian (CEA). Many industrial applications require to check the quality of structures such as plates, for instance in aircraft design. A common way to inspect structures is to propagate ultrasonic waves and detect from the experimental results the presence or not of a defect or a crack. However, in aeronautics, structures are often complex media like anisotropic elastic plates for which the interpretation of this results is complicated. Therefore, efficient and accurate numerical methods of simulation are required. In our work, we want to study the diffraction of a time harmonic wave by a bounded defect in an anisotropic elastic media. In order to study the diffraction properties of the defect, we consider it in as infinite. Since the defect has an arbitrary geometry, we want to use a finite element method in a box that surround the defect. On the boundary of this artificial box, we need to find transparent conditions to simulate an infinite domain.

- We first have considered waveguides. The transparent boundary conditions are often written by using the so-called Dirichlet-to-Neumann maps which can be expressed thanks to a modal decomposition. However, classical iterative method does not converge necessarily. In this work, we introduce a new Dirichlet-to-Neumann operator which links the trace of the solution on a section of the waveguide to the normal trace on a different one. This operator can also be expressed analytically via a modal decomposition. Its main advantage is that, because of the overlapping, it becomes compact and this is exactly why we think an iterative resolution has more chance to converge. Other advantages will appear with the elasticity application. Indeed, in the formulation of the transparent boundary condition without overlapping, appears a lagrange multiplier which makes the resolution more costly. This additional unknown will be avoided with an overlap. For now, the theory is done for the scalar acoustic waveguide and the method has been implemented in the Melina code for the acoustic and the elastic case. The redaction of an article is in progress.

  item We then have studied scattering problem in locally perturbed anisotropic plate. The classical methods to derive transparent boundary conditions for acoustic isotropic media are based on the Green function (boundary integral formulation) or Fourier series (to determine DtN operator set on an artificial circle boundary). However, they cannot be extended for anisotropic elastic problems. Using a constructive method to determine transparent boundary conditions for periodic media developped in the laboratory, we were able to propose new exact boundary conditions which are adapted to anisotropic media and for which iterative method could converge rapidly. The numerical study is in progress for acoustic isotropic problem.

6.4. Waveguides, resonances, and scattering theory

6.4.1. Localized modes in periodic waveguides

Participants: Anne-Sophie Bonnet-Ben Dhia, Bérangère Delourme, Sonia Fliss, Sergei Nazarov, Elizaveta Vasilevskaia.

The general objective is the study of localized modes in locally perturbed periodic media. We investigate the existence theory of such modes as well as their numerical computations. We can distinguish two types of problems.

Numerical computation of guided modes in periodic media with line defects. We are interested in the propagation of guided modes that propagate in the direction of the line defect (which is parallel to one of the periodicity directions of the unperturbed medium) and decrease exponentially in the transverse directions. We aim at computing these modes and their dispersion relation. Last year, we developed a method based on the use of the DtN approach introduced in the PhD thesis of S. Fliss and the resolution of "operator pencil" eigenvalue problems. This year, in collaboration with Kersten Schmidt, we have made a numerical comparison of this new method with the more standard supercell method.

Existence of localized modes in closed periodic waveguides. We consider a propagation medium which is infinite and periodic in one space dimension and bounded in the transverse ones. We investigate the question of the influence of a local defect on the existence of localized modes. Once again this reduces to a selfadjoint eigenvalue problem in an unbounded domain.

The first problem that we studied is in the framework of the PostDoc of Bérangère Delourme. We have considered general locally perturbed periodic media for which we focus on determining sufficient conditions on the periodic media or the local defect so that it exists at least one eigenvalue below the essential spectrum of the underlying perfectly periodic operator. These sufficient conditions are based on Min-Max theory and an appropriate choice of test functions. We were able to validate these existence conditions thanks to the numerical method based on the use of DtN operators. For situations where the periodic "reference medium" is closed to a simple "limit medium" fo which all calculations can be made by hand, we show that these conditions could be really simple and explicit using perturbation theory and asymptotic expansions of the eigenvalues. We are investigating now the extension of this approach to sufficient conditions for existence of guided modes inside the essential spectrum.
The second case, that is investigated in the framework of the PhD thesis of E. Valisevskaia, is the case where the propagation medium is a thin structure (the thinness being characterized by the parameter ε) whose limit is a periodic graph. This is for instance the case of a symmetric ladder as illustrated by figure . If Neumann boundary conditions are considered, it is well known (see in particular the works by Exner, Kuchment) the the limit model when εtends to is the Helmholtz equation on the graph (1D Helmholtz equations on each branch competed by continuity and Kirchoff transimission conditions at each node) . For this limit problem, the underlying operator does not present any spectral gaps but can be written, due to the symmetry of the problem, as the sum of two operators, each of which having an infinity of spectral gaps. This allows us to look for eigenvalues in these spectral gaps, induced by symmetric and localized perturbations of the limit graph model. This can de done for instance by modifying (symetrically) the Kirchoff conditions on two symmetric nodes of the graph. In the limit process mentionned above, this would correspond to modifying the width of the rung that joins these two points in the original problem. First existence results have been obtained in this direction. In a further step, one can expect, by asymptotic analysis, to get corresponding existence results for the original problem, at least for ε small enough.

6.4.2. A new approach for the numerical computation of non linear modes of vibrating systems

Participants: Anne-Sophie Bonnet-Ben Dhia, Jean-François Mercier.

A collaboration with Cyril Touzé and François Blanc (Unité de Mécanique, ENSTA). The simulation of vibrations of large amplitude of thin plates or shells requires the expensive solution of a non-linear finite element model. The main objective of the proposed study is to develop a reliable numerical method which reduces drastically the number of degrees of freedom. The main idea is the use of the so-called non-linear modes to project the dynamics on invariant subspaces, in order to generate accurate reduced-order models. Cyril Touzé from the Unité de Mécanique of ENSTA has derived an asymptotic method of calculation of the non-linear modes for both conservative and damped systems. But the asymptotically computed solution remains accurate only for moderate amplitudes. This motivates the present study which consists in developing a numerical method for the computation of the non-linear modes, without any asymptotic assumption. This is the object of a collaboration with Cyril Touzé, and new results have been obtained during the post-doc of François Blanc in the Unité de Mécanique of ENSTA. The partial differential equations defining the invariant manifold of the non-linear mode are seen as a vectorial transport problem : the variables are the amplitude and the phase (a, φ) where the phase φ plays the role of the time. In the case of conservative systems, a finite difference scheme is used and an iterative algorithm is written, to take into account the 2π-periodicity in φ which is seen as a constraint. An adjoint state approach has been introduced to evaluate the gradient of the coast function. The method has been validated in a simple example with two degrees of freedom. Good agreement with an alternative method, the continuation of periodic solutions method, has been found. Currently the method is extended to the case of damped systems. The main difficulty is that, due to a change of variables, the 2π-periodicity does not hold anymore and new constraints more complicated to implement must be considered.

6.4.3. Harmonic wave propagation in locally perturbed periodic waveguide

Participants: Sonia Fliss, Patrick Joly.

We work on the expression and the asymptotic behaviour of the Green function for time harmonic wave equation in two-dimensional periodic waveguide. This enables us to define a radiation condition and show well-posedness of the Helmholtz equation set in a periodic waveguide. The redaction of an article is ongoing. This analysis is one of the main tool to solve inverse problems in locally perturbed periodic waveguide (see section 6.6.1) when the data are far field measurements of scattering problems.
One challenging perspective of this work is to extend these results to periodic problems in free space.

6.4.4. Finite element approximation of modes of elastic waveguides immersed in an infinite fluid

Participants: Anne-Sophie Bonnet-Ben Dhia, Cédric Doucet, Christophe hazard.

This work is developped in collaboration with Vahan Baronian (CEA). We are developping numerical tools to simulate ultrasonic non-destructive testing in elastic waveguides. This particular topic aims at finding an efficient way of coupling semi-analytical finite element methods and perfectly matched layers (PMLs) to compute modes of elastic waveguides embedded in an infinite fluid.
During our numerical investigations, we noticed that the semi-analytical mixed finite element formulation proposed in the PhD thesis of V. Baronian may lead to the computation of spurious modes. We overcame this problem in the following way: instead of approximating components of stress tensors by means of first-order finite elements of class $\mathcal{C}^0$, we decided to use zeroth-order discontinuous ones. This simple modification seems not only to stabilize the discretization step, but also to approximate modes more accurately in comparison with the classical semi-analytical finite element formulation. Last but not least, we observed a meaningful improvement of the approximation of the continuous spectrum of stretched operators related to PMLs. Besides, previous results (in the PhD thesis of B. Goursaud) about the best way of designing PMLs to simulate wave propagation in open acoustic waveguides have been confirmed by our numerical experiments on immersed elastic structures.
Further investigations need to be carried out to explain these phenomena. Especially, a theoretical analysis still remains to be done.

6.5. Asymptotic methods and approximate models

6.5.1. Effective boundary conditions for thin periodic coatings

Participants: Mathieu Chamaillard, Patrick Joly.

This topic is the object of a collaboration with Houssem Haddar. 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 of a flat layer of width delta (the reference configuration) that preserves the normals, which appears consistent with a manufactoring process. The electromagnetic parameters in the coating are then defined as the images through Φ_Γ of periodic functions in the reference configuration.

We have first considered the case of the scalar wave equation. 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

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

where B_Γ^1 and B_Γ^2 are second order tangential differential operators along Γ whose coefficients depend on both the geometrical characteristics of Γ (through the curvature tensor) and the material properties of the coating, through the resolution of particular 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. This new condition is expected to provide $O(\delta^3)$ accuracy. Its implementation and its rigorous analysis (error estimates) are ongoing.

6.5.2. Thin Layers in Isotropic Elastodynamics

Participants: Marc Bonnet, Aliénor Burel, Patrick Joly.

This research is developed in the framework the numerical modeling of non-destructive testing experiments using ultrasonic waves. Most realistis propagation media involves thin layers of resin (typically for gluing together different homogeneous media), which are, until now, difficult to take into account numerically, the principal issue being the very small space step needed for meshing such a thin layer. An idea to get rid of this complication is to use asymptotic analysis in order to establish effective transmission conditions. We have studied the simple model problem in two dimensions, with an infinite flat layer of thickness ε. Using a formal approach based on a scaling inside the layer and an power series expansion in ε solution as a polynomial in ε, we have established first and second order conditions. Energy techniques parmit to guaranty the stability of our approximation.

6.5.3. Homogenization and metamaterials

Participants: Sonia Fliss, Patrick Joly, Valentin Vinoles.

This topic is developpped in collaboration with Xavier Claeys (LJLL, Paris VI).
The mathematical modeling of electromagnetic metamaterials and the homogenization theory are intimately related because metamaterials are precisely constructed by a periodic assembly of small microstructures involving dielectric materials presenting a high contrast with respect to a reference medium. As a consequence, each microstructure behaves as a resonator which induces surprising properties to the effective or homogenized material such as negative permittivity and / or permeability at certain frequencies. The relevant theoretical approach to this question is the non standard (or high contrast) homogenization theory developed in particular in France by G. Bouchitté.

In the framework of the ANR Metamath, we wish to deepen this question by looking carefully at the treatment of boundaries and interfaces that are generally poorly taken into account by the first order homogenization. This is developed in collaboration with X. Claeys (Paris VI).

This question is already relevant for standard homogenization for which taking into account the presence of a boundary induces a loss of accuracy due to the inadequation of the standard homogenization approach to take into account the boundary layers induced by the boundary. Our objective is to construct approximate effective boundary conditions that would restore the desired accuracy.

With the PhD thesis of V. Vinoles, we aim at extending the previous approach to the treatment of metamaterials via high contrast homogenization. In particular, we intend to treat the challenging question of interfaces between metamaterials and standard materials (see also sections).

6.5.4. Asymptotic analysis and negative materials

Participants: Lucas Chesnel, Sergei Nazarov.

This topic is developpped in collaboration with Xavier Claeys (LJLL, Paris VI) and S.A. Nazarov (IPME RAS, St Petersburg, Russia).

One of the applications of negative materials (metals at optical frequencies or negative metamaterials) is the construction of subwavelength cavities. In this kind of application, the idea is to use the following result: an inclusion of a negative material in a positive material changes radically the spectrum of the Maxwell's operators. We demonstrated this result for the scalar operator in a configuration where a positive material contains a small negative inclusion whose size tends to zero. As a second topic, we proved an instability result for a configuration where the interface between the positive and the negative material has a rounded corner. It appears that the solution depends critically on the value of the rounding parameter and does not converge when the rounded corner tends to the actual corner. We also studied the spectrum of the scalar operator in this configuration. This spectrum does not converge but seems (for the moment, the proof is not complete) to oscillate like $\ln\delta$ where $\delta \to 0$ is the rounding parameter.

6.5.5. Modelling of non-homogeneous lossy coaxial cable for time domain simulation.

Participants: Geoffrey Beck, Sébastien Imperiale, Patrick Joly, Martina Novelinkova.

This topic, initiated at the end of the PhD thesis of S. Imperiale, has been the subject of the internship of M. Novelinkova and is the subject of the PhD thesis of G. Bech which started in October.

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. Doing so, we have been able to derive a generalized telegraphist's equation, a 1D wave equation with additional time convolution terms that results from the conjugated effect of electromagnetic losses and heterogeneity of the cross section. This new model has been fully justified through error estimates. We are currently working on a higher order generalized telegraphist's equation that would include dispersive effects through nonlocal capacity and inductance operators.

From the pratical point of view, a code that computes the coefficients (including the convolution kernel) of the effective model and solves the generalized telegraphist's equation has been implemented. It has been exploited to measure the presence of localized defects on the propagation of electromagnetic waves. This application has been motivated by the ANR project SODDA, in collaboration with CEA-LETI, about the non destructive trsting of networks of electric cables (a subject that we are investigating in collaboration with M. Sorine from Inria Rocquencourt).

6.5.6. Elastic wave propagation in strongly heterogeneous media

Participants: Patrick Joly, Simon Marmorat.

This subject enters our long term collaboration with CEA-LIST on the development on numerical methods for time-domain non destructive testing experiments using ultra-sounds. This is also the subject of the PhD thesis of Simon Marmorat. Our objective is to develop an efficient numerical approach for the propagation of elastic waves in a medium which is made of many small inclusions / heterogeneities embedded in a smooth (or piecewise smooth) background medium, without any particular assumption (such as periodicity) on the spatial distribution of these heterogeneities. Our idea is to exploit the smallness of the inclusions (with respect to the wavelength in the background medium) to derive a simplified approximate model in which each inclusion would be described by very few parameters (functions of time) coupled to the displacement field in background medium for which we could use a computational mesh that ignores the presence of the heterogeneities. For deriving such a model. we intend to use and adapt the asymptotic methods previously developed at Poems (such as matched asymptotic expansions).

6.5.7. Multiple scattering by small scatterers

Participants: Maxence Cassier, Christophe Hazard.

We consider the scattering of an acoustic time-harmonic wave by an arbitrary number of sound-soft obstacles located in a homogeneous medium. When the size of the obstacles is small compared with the wavelength, the numerical simulation of such a problem by classical methods (e.g., integral equation techniques or methods based on a Dirichlet-to Neumann map) can become highly time-consuming, particularly when the number of scatterers is large. In this case, the use of an asymptotic model may reduce considerably the numerical cost. Such a model was introduced by Foldy and Lax in the middle of the last century to study multiple isotropic scattering in a medium which contains randomly distributed small scatterers. Their asymptotic model is based on the fact that the scattered wave can be approximated by a wave emitted by point sources placed at the centers of the scatterers; the amplitudes of the sources are calculated by solving a linear system which represents the interactions between the scatterers. Nowadays, the FoldyñLax model is still used in numerous physical and numerical applications to approximate the scattered wave in a deterministic media. But to the best of our knowledge, there was no mathematical justification of this asymptotic model. We have proposed such a justification which provides local error estimates for the two-dimensional problem in the case of circular obstacles. An article on this subject has been accepted and will be published in Wave Motion in January 2013.

6.6. Imaging and inverse problems

6.6.1. Sampling methods in waveguides

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

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 from the scattered fields which correspond to the incident fields formed by the Floquet modes. The corresponding numerical implementation was the subject of the Master internship of Mathieu Guenel who obtained some first promising results.
Secondly, going back to the homogeneous waveguide in the acoustic case, we have started a study of the sampling methods in the time domain. This will be 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.

6.6.2. The exterior approach to retrieve obstacles

Participant: Laurent Bourgeois.

This theme is a collaboration with Jérémi Dardé from IMT (Toulouse).
We have adapted the exterior approach developped for the Laplace equation to the Stokes system. The aim is to find a fixed Dirichlet obstacle in a fluid which is governed by the Stokes system with the help of boundary measurements. 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. In particular, we have introduced two different mixed formulations of quasi-reversibility for the ill-posed Stokes systems in order to use standard Lagrange finite elements.

6.6.3. Inverse scattering with generalized impedance boundary conditions

Participants: Laurent Bourgeois, Mathieu Chamaillard, Nicolas Chaulet.

This work is a collaboration between POEMS and DEFI projects (more precisely Houssem Haddar) and constitutes the subject of the PhD thesis of N. Chaulet, which was defended on the 27/11/2012. We are concerned with 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.

During this last year, we complemented our previous work in two directions. First, 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.

Meanwhile, we studied the application of non linear optimization techniques to solve the inverse problem for the $3D$ Maxwell's equations. The main advantage of this type of method is that they can be applied with much less data than the Factorization method. Nevertheless, we had to compute the partial derivatives of the electromagnetic field with respect to the parameters we want to reconstruct. In our case, these parameters are the coefficients that define the impedance operator and the shape of the obstacle. We characterized these derivatives in the case where the GIBC is defined by a second order surface operator. The applicability of such methods has been illustrated by some numerical experiments in dimension 3 in which we reconstructed the shape of the scatterer as well as the coefficients that characterize the impedance operator. As demonstrated in the two dimensional case, we think that the GIBCs could be efficiently used to identify the shape of coated objects as well as the parameters of the coating in the $3D$ Maxwell case.

6.6.4. Linear sampling methods in the time domain

Participant: Simon Marmorat.

This work is developed in collaboration with H. Haddar (DEFI, Inria Saclay) and A. Lechleiter (Bremen University). We are concerned with the inverse problem of reconstructing obstacles from the knowledge of scattered acoustic waves in the time domain. We tackle this problem using a linear sampling method that directly acts on time domain data: this imaging technique yields a picture of the scatterer by solving a linear operator equation involving the measured data for many right-hand sides given by singular solutions to the wave equation. We have illustrated the method on numerical examples and have shown a good behaviour with respect to aperture (the quality of reconstruction is better than in the frequency case in the case of limited aperture) and the ability of simultaneously reconstructing obstacles with different boundary conditions among the Dirichlet, Neumann and Robin-Fourier ones.

6.6.5. Space-time focusing on unknown scatterers

Participants: Maxence Cassier, Patrick Joly, Christophe Hazard.

This topic concerns the studies started two years ago about time-reversal in the context of Maxence Cassier's thesis. The main question is to generate a time-dependent wave that focuses on one given scatterer not only in space, but also in time. Our recent works concern two items. On one hand, we have proposed a way to construct such a focusing wave which does not require an a priori knowledge of the location of the obstacle. This wave is represented by a suitable superposition of the eigenvectors of the so-called time-reversal operator in the frequency domain. Numerical results show the focusing properties of such a wave. On the other hand, we try to understand how to translate the physical idea of ìfocusingî into mathematical terms. We proposed and and implemented energy criterion which can be used in numerical experiments in order to evaluate the quality of the focus.

6.6.6. Asymptotic analysis of the interior transmission eigenvalues related to coated obstacles

Participant: Nicolas Chaulet.

This work is a collaboration with Fioralba Cakoni from the University of Delaware (USA) and Houssem Haddar from the DEFI project. The interior transmission eigenvalues play an important role in the area of inverse scattering problems. These eigenvalues can actually be determined by multi-static far field data. Thus, they could be used for non destructive testing. We focused on the case where the obstacle is a perfectly conducting body coated by some thin dielectric material. We derived and justified the asymptotic expansion of the first interior transmission eigenvalue with respect to the thickness of the coating for the TM electromagnetic polarization. This expansion provided interesting qualitative information about the behavior of these eigenvalues and also gave an explicit formula to compute the thickness of the coating.

6.6.7. Interior transmission problem

Participants: Anne-Sophie Bonnet-Ben Dhia, Lucas Chesnel, Jérémi Firozaly.

This work is a collaboration with F. Cakoni from the University of Delaware (U.S.) and H. Haddar from the DEFI project at Inria Saclay. The interior transmission problem plays an important role in the inverse scattering theory for inhomogeneous media. In particular, it arises when one is interested in the reconstruction of an inclusion embedded in a background medium from multi-static measurements of diffracted fields at a given frequency. Physically, it is important to prove that, for a given frequency, there are no waves which do not scatter. Mathematically, this last property boils down to state that the frequency is not a transmission eigenvalue, that is, an eigenvalue of the interior transmission problem. An important issue is to prove that transmission eigenvalues form at most a discrete set with infinity as the only accumulation point. This is not straightforward because the operator associated with this problem exhibits a sign changing in its principal part and its study is not standard. Using the T-coercivity approach, we proved the discreteness under relatively weak assumptions both for the scalar and Maxwell cases. In particular, the simple technique we proposed allows to treat cases, which were not covered by existing methods, where the difference between the inclusion index and the background index changes sign. Now, we are trying to understand the fundamental links which exist between this problem and the transmission problem between a positive and a negative material. In some configurations, the study of the interior transmission problems leads to consider the operator $\Delta(\sigma\Delta\cdot) : H_0^2(\Omega) \to H^{-2}(\Omega)$ where Ω is the domain and σ is a coefficient which changes sign on Ω. During the internship of Jérémy Firozaly, we proved that this operator exhibits properties very different from the operator $\mathrm{div}(\sigma\nabla\cdot) : H_0^1(\Omega) \to H^{-1}(\Omega)$.

6.6.8. Flaw identification using elastodynamic topological derivative

Participants: Marc Bonnet, Rémi Cornaggia.

In collaboration with Cédric Bellis (Columbia Univ. USA), Bojan 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). Current investigations focus on justifying 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.

6.6.9. Topological derivative in anisotropic elasticity

Participant: Marc Bonnet.

In collaboration with Gabriel Delgado (CMAP, Ecole Polytechnique).
Following up on previous work on the topological derivative (TD) of displacement-based cost functionals in anisotropic elasticity, a TD formula has been derived 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 remains finite no matter how small the inclusion size. 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.

6.6.10. Energy functionals for elastic medium reconstruction using transient data

Participant: Marc Bonnet.

In collaboration with Wilkins Aquino (Cornell 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, a fact 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 large FE models, making the time-domain ECR functional a worthwhile tool for medium identification.

6.7. Other topics

6.7.1. Fast non-overlapping Schwarz domain decomposition methods for the neutron diffusion equation

Participant: Patrick Ciarlet.

A collaboration with Erell Jamelot (CEA Saclay/DEN).
Investigating numerically the steady state of a nuclear core reactor can be very expensive, in terms of memory storage and computational time. In order to address both requirements, one can use a domain decomposition method, which is then implemented on a parallel computer.
We model the problem using a mixed approach, which involves a scalar flux and a vector current. The equivalent variational formulation is then discretized with the help of Raviart-Thomas-Nédélec finite elements. The domain decomposition method is based on the Schwarz iterative algorithm with Robin interface conditions to handle communications. This method is analyzed from the continuous to the discrete point of views: well-posedness, convergence of the finite element method, optimality of the parameter appearing in the Robin interface condition and algorithms. Numerical experiments carried out on realistic 3D configurations using the APOLLO3©code (of CEA/DEN) show the parallel efficiency of the algorithm.

SCIPORT Team

6. New Results

6.1. Automatic Differentiation and parallel codes

Participants: Valérie Pascual, Laurent Hascoët, Hubert Alcin, Jean Utke [Argonne National Lab. (Illinois, USA)], Uwe Naumann [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.

This year, we have presented our strategy [16] to extend Data-Flow analysis to Message-Passing communication. This strategy is specially designed for a program representation like that of TAPENADE, i.e. based on a Call-Graph whose nodes are indeed Flow-Graphs. This representation makes it easier to implement analyses in a way that is both context-sensitive and flow-sensitive. Our strategy also relies on the fixed-point implementation of the analyses, which uses a "wait-list".

At the same time, we continue the design of a adjoint-mode AD adapted to MPI communication. In our framework of AD by source transformation, we have pushed far in the direction of static data-flow analyses and static source transformation of individual MPI calls. We obtained results on classical cases of message-passing [38]. However, experience shows [11] that general usage of message-passing defies static analysis. A purely static analysis and transformation must resort too often to conservative choices, yielding a poor efficiency.

As a consequence, we are now going in the direction of a more dynamic, run-time treatment of adjoint MPI calls. This means designing a wrapper library "AMPI" on top of MPI, that takes care during execution of the adjoint code of the bookkeeping to send the adjoint messages in the reverse direction. This wrapper library should also be independent from the particular AD tool, as it will be used not only with TAPENADE but with the tools developed at Argonne and RWTH Aachen.

6.2. Finer control on AD transformation

Participants: Valérie Pascual, Laurent Hascoët.

We explore methods to provide the AD end-user with a better control on the AD transformation. We want to organize a progressive AD process in which the end-user can choose among a set of available AD code optimizations. In a first stage, the end-user may deactivate most of these optimizations, thus obtaining a differentiated code that is easier to understand and hopefully more robust. If problems do occur, this differentiated code is easier to debug with the debugging tools that we provide. In the next stages, the end-user may progressively turn the optimizations on, and at the same time check that the derivatives remain correct.

Another goal closely related is the comparison and evaluation of the existing corpus of AD code optimizations. TAPENADE is one of the AD tools that incorporate most of AD optimizations proposed in litterature. If a few missing optimizations are included, TAPENADE with its relatively large set of validation applications can be the common ground for a credible evaluation of the benefit brought by each optimization.

In this direction, we have extended TAPENADE to turn some classical optimizations that were automatically applied into optional optimizations. The emblematic example is activity analysis. This required some code cleanup. Also, we are extending TAPENADE to give the option of "association by address" instead of "association by name". This means bundling each variable with its derivative into a structured object, instead of creating new variables with new names to hold the derivatives. Which option is better is a difficult question, related to memory locality issues. This extension will allow us to make accurate measurements on our set of validation codes. This is also a step towards a better collaboration of TAPENADE with overloading-based AD tools, that natively use association by address.

6.3. Formal specification of AD

Participant: Laurent Hascoët.

There is very little formal specification of AD as a program transformation, and consequently no formal proof of its correctness. Correctness of tangent AD is problematic: if defined as equivalence of the tangent program semantics with the mathematical derivative of the semantics of the original code, correctness is mostly granted for simple staight-line programs, and in general not granted for programs with control. Therefore formal proofs of correctness appear unreachable at present. Fortunately, there is little concern about the practical relevance of tangent AD. The confidence of end-users regarding tangent AD is justified by everyday experience.

Adjoint-mode AD poses a different challenge. The adjoint AD transformation is by no means simple nor intuitive. Its specification is informal, so that end-users of AD cannot gain a strong confidence in the process. Moreover, the constant quest for efficiency of the adjoint code has introduced a number of improvements and tradeoffs that are defined informally. These improvements make the adjoint code intricate and sometimes interact to cause subtle bugs. On the other hand, the good news is that the difference between the adjoint code and the tangent code only lies in the order of the derivatives computations and not in their nature. A formal proof of semantic equivalence is thus conceivable.

The first step towards such a proof is a formal specification of both tangent-mode and adjoint-mode AD, including the specification of the program static data-flow analyses that the transformations require. We have provided this specification in terms of Data-Flow equations for the analyses, and in terms of Structural Operational Semantics (more precisely Natural Semantics) for the AD transformations themselves [19]. This specification will be the basis for future formal proofs of equivalence between tangent AD and adjoint AD.

6.4. Resolution of linearised systems

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

Increased sophistication of solution algorithms pose a challenge to Automatic Differentiation. Time-stepping iterations create numerous updates of the iterated solution vector. Other additional nonlinear iterative processes occur such as:

- the evaluation of an optimal step, which results at least from a homographic function of the unknown,
- the orthonormalisation of the updates (Gram-Schmidt method, Hessenberg method).

Adjoint-mode AD applied to these algorithms produces a "linearised iterative algorithm" which is transposed and therefore follows the original iterations in the reverse order, needing each of the iterated state solution vectors. One such extreme case is the simulation of unsteady phenomena with implicit numerical schemes: simulating high Reynolds turbulent flows by a Large Eddy Simulation (LES) and RANS-LES models requires hundreds of thousands time steps, each of them involving a modern iterative solution algorithm. This is the case targetted by the 4-year ANR project "ECINADS", jointly with university of Montpellier 2, the Institut de Mécanique des fluides de Toulouse and Lemma company, started in 2009.

In ECINADS, we design more efficient solution algorithms and we examine the questions risen by their adjoint differentiation. Our goal is practical scalability of the direct simulation and of its adjoint on a large number of processors. ECINADS also addresses the scalable solution of new approximations.

In 2012, the novel three-level method studied by H. Alcin on a model problem has been extended to compressible viscous flows by B. Koobus and C. Moussaed from university of Montpellier.

Hubert Alcin, Bruno Koobus, Olivier Allain and Alain Dervieux published their work on a two-level Schwarz algorithm in IJNMFD [12]. H. Alcin has presented his work in the Parallel CFD conference of Altlanta [14]. H. Alcin wrote his thesis [11], defended in december, on the three main subjects of ECINADS: the two- and three-level Schwarz algorithms, Automatic Differentiation and mesh adaptation.

6.5. Automatic Differentiation of a CFD code

Participants: Hubert Alcin, Valérie Pascual, Laurent Hascoët, Alain Dervieux.

The ECINADS workplan includes the building of an adjoint state for a CFD kernel. We have chosen AIRONUM 5.1 , a real life kernel that combines two particular features:

- it uses intensively the Fortran95 dynamic memory allocation
- it uses MPI parallelization.

This work is reported in H. Alcin's PhD [11].

6.6. Perturbation Methods

Participants: Alain Dervieux, Laurent Hascoët.

In the context of the European project NODESIM-CFD (ended 2010), the contribution of Sciport involved mainly the derivation of perturbation methods and reduced order models for the management of uncertainties. These methods rely on Taylor series with second-order terms. The production of second derivative code is obtained through repeated application of Automatic Differentiation. Three strategies can be applied to obtain (elements of) the Hessian matrix, named Tangent-on-Tangent, Tangent-on-Adjoint, and Adjoint-on-Tangent. These new methods are promoted through short courses, e.g. by Alain Dervieux at an ERCOFTAC session (Chatou, 15-16 mai 2012). The application and extension of these methods are part of a FP7 proposal (Proposal UMRIDA, nov. 2012).

6.7. Control of approximation errors

Participants: Frédéric Alauzet [GAMMA team, Inria-Rocquencourt], Estelle Mbinky [GAMMA team, Inria-Rocquencourt], Olivier Allain [Lemma], Alexandre Carabias, Hubert Alcin, Alain Dervieux.

This is a joint research between Inria teams Gamma (Rocquencourt), Sciport, Castor and the Lemma company. Gamma brings mesh and approximation expertise, Sciport brings adjoint methods, and CFD applications are developed by CASTOR and Lemma.

The resolution of the optimum problem using adjoint-mode AD can be used in a slightly different context than optimal shape design, namely mesh adaptation. This will be possible if we can map the mesh adaptation problem into a differentiable optimal control problem. To this end, we express the mesh adaptation problem in a purely functional form: the mesh is reduced to a continuous property of the computational domain named the continuous metric. We minimize a continuous model of the error resulting from that metric. Thus the search of an adapted mesh is transformed into the search of an optimal metric.

In 2012, this activity is amplifying. A work on goal-oriented mesh adaptation for unsteady Euler flows submitted to the journal JCP has been accepted and published [13]. Its extension to the compressible Navier-Stokes model has been developed in 2D [22] and in 3D [11]. A further extension to Large Eddy Simulation has been defined and developed in the WOLF demonstrator. A communication at ECCOMAS (Vienna) has been presented and papers are being written for publication in journal.

The method is being extended to a third-order approximation, the Vertex-CENO. This approximation was defined collaboratively between university of Montpellier, IMM-Moscow and Sciport. A more accurate version is studied by Alexandre Carabias. A new mesh adaptation theory involving error estimates and criteria has been developed by Gamma and Sciport. The extension of the multiscale adaptation method is considered by Estelle Mbinky at Rocquencourt and has been presented at ECCOMAS (Vienna). The extension of the goal-oriented method is considered by Alexandre Carabias and first results were presented at ECCOMAS (Vienna). A cooperation with CEMEF and university of Nice is considered and a ERC common proposal, CMILE, has been built. Anisotropic mesh adaptation allows for better convergence towards continuous solutions, and in particular more accurate a posteriori error estimates and correctors. The synergy between correctors and mesh adaptation is the subject of a joint contribution (Gamma and Sciport) for the FP7 UMRIDA proposal (nov. 2012).

SIMPAF Project-Team

6. New Results

6.1. Interactions of Macro- and Microscopic scales

6.1.1. Homogenization methods

We have obtained three types of results regarding the homogenization theory and its applications. The first series of results is related to nonlinear elasticity. In [44], A. Gloria has proved the convergence of a discrete model for rubber towards a nonlinear elasticity theory in collaboration with R. Alicandro and M. Cicalese. This analysis has motivated the study of a specific random point set to model the stochastic network of polymer chains, namely the random parking measure, and results have been obtained by A. Gloria and M. Penrose (University of Bath) in [42]. The numerical simulation of the model with the random parking measure has been addressed by A. Gloria, P. La Tallec and M. Vidrascu (project team REO) in [21], and the comparisons with mechanical experiments are promising, A related inverse problem is currently under investigation by M. de Buhan, A. Gloria, P. Le Tallec, and M. Vidrascu.

A second type of results concerns a quantitative theory of stochastic homogenization of discrete linear elliptic equations. A breakthrough has been obtained by A. Gloria and F. Otto (MPI Leipzig) in [63] and [24], who gave the first optimal variance estimate of the energy density of the corrector field for stochastic discrete elliptic equations. The proof makes extensive use of a spectral gap estimate and of deep elliptic regularity theory, bringing in fact the probabilistic arguments to a minimum. This analysis has enabled A. Gloria to propose efficient numerical homogenization methods, both in the discrete and continuum settings [62], [20], see the review article [33]. In [23], A. Gloria and J.-C. Mourrat has pushed the approach forward and introduced new approximation formulas for the homogenized coefficient. In [22] they have considered a more probabilistic approach and given a complete error analysis of a Monte-Carlo approximation of the homogenized coefficients in the discrete case. Work in progress concerns the generalization of the results on discrete elliptic equations to the continuum case.

The third direction of research concerns the periodic homogenization of a coupled elliptic/parabolic system arising in the modelling of nuclear waste storage. This work is in collaboration with the French agency ANDRA. A. Gloria, T. Goudon, and S. Krell have made a complete theoretical analysis of the problem, derived effective equations, and devised an efficient method to solve the effective problem numerically, based on the reduced basis approach, see [41]. This subject has been pushed forward by Z. Habibi in collaboration with ANDRA.

6.1.2. Statistical physics : molecular dynamics

In [28], the analysis of constrained molecular dynamics is proposed, with associated numerical schemes.

In [29], the pobabilistic derivation of the chemotaxis equation from the individual motion of bacteriae have been carried out. In [30], a numerical method with asymptotic variance reduction have been proposed.

6.2. Plasmas

We investigated a projective integration scheme for a kinetic equation in the limit of vanishing mean free path, in which the kinetic description approaches a diffusion phenomenon. The scheme first takes a few small steps with a simple, explicit method, such as a spatial centered flux/forward Euler time integration, and subsequently projects the results forward in time over a large time step on the diffusion time scale. We showed that, with an appropriate choice of the inner step size, the time-step restriction on the outer time step is similar to the stability condition for the diffusion equation, whereas the required number of inner steps does not depend on the mean free path. We also provided a consistency result. The presented method is asymptotic-preserving, in the sense that the method converges to a standard finite volume scheme for the diffusion equation in the limit of vanishing mean free path. This is a joint work with G. Samaey (K. U. Leuven) [27].

6.3. Finite element and finite volume methods

6.3.1. Control in fluid mechanics

Recently, open and closed active flow control were carried out in order to study the flow behavior over a backward-facing step in a transitional regime. It was done either by a global frequency destabilization at the entry of the domain, or by a local blowing or suction through the lower and upper parts of the step by the use of small jets ([58], E. Creusé, A. Giovannini (IMFT Toulouse) and I. Mortazavi (MC2 Inria EPI, Bordeaux)). The numerical computations were based on a vortex-in-cell method. Such controls were shown to be efficient in reducing the average recirculation length value, the global flow energy, as well as the global flow enstrophy. We have now in mind to apply such a strategy on cavity-stent flows, in order to study the effect of passive and/or active control on the average emptying time of the cavity, corresponding to a lot of possible industrial or health applications (combustion, blood circulation in arteries,...).
Passive as well as active control were also performed on the "Ahmed body geometry", which can be considered as a first approximation of a vehicle profile. This work was carried out in collaboration with the EPI Inria MC2 team in Bordeaux (C.H. Bruneau, I. Mortazavi and D. Depeyras), as well as with Renault car industry (P. Gillieron). We recently combined active and passive control strategies in order to reach efficient results, especially concerning the drag coefficient, for two and three dimensional simulations [51]. We recently worked on a 25° rear-window configuration of the Ahmed body, for which the 3D-effects are very important and have to be considered in the numerical simulations [9]. Moreover, the effect of the vortices dynamics on the drag coefficient of a square Ahmed body was adressed [53], as well as the impact of several Ahmed bodies on the same road [52].

In another field of applications, a work was performed with the TEMPO Laboratory of Valenciennes. The objective of this collaboration was to study the pressure wave generated by high-speed trains entering tunnels in order to improve the shape of the tunnel sections.

6.3.2. Numerical Methods for viscous flows

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 [11]. We are also concerned with the numerical simulation of certain multi-fluids flows, which in particular arises in the modelling of powdersnow 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 [38]. In order to answer these questions, we have developed a MATLAB code (NS2DDV-M, see the softwares section), a Fortran code and a C++ code.

6.3.3. A posteriori error estimators for finite element methods

A recent work, in collaboration with S. Nicaise (LAMAV, Valenciennes), was devoted to the derivation of some so-called "reconstruction estimators" based on gradient averaging, in order to provide lower and upper bounds of the error arising from a discontinuous Galerkin approximation of a diffusion problem [59].

At the same time, some equilibrated-type estimators were developed for the Reissner-Mindlin system arising in solid mechanics applications, for conforming and locking-free approximations, in the context of the PhD. of É. Verhille.

At last, a collaboration with the "Laboratoire d'électrotechnique et d'électronique de puissance de Lille (L2EP)" began two years ago, to derive a residual-based a posteriori error estimator for the Maxwell system in its vectorial and scalar potential formulation A/Φ (PhD of Z. Tang). The objective was to obtain a mathematical rigorous error indicator, in order to couple it with the automatic mesh generator used by EDF for very practical issues.

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 found 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 [17], [18], [32], [31], [65], obtained in the context of the Ph-D thesis of Zuqi Tang [2]. Then, other results about reconstructed a posteriori error estimators were obtained for Discontinuous Galerkin methods, applied to convection-reaction-diffusion equations [16].

6.4. Numerical anlaysis of Schrödinger equations

6.4.1. Absorbing boundary conditions

C. Besse continues his collaboration with X. Antoine (EPI Corida) and P. Klein. They construct in [3] some classes of absorbing boundary conditions for the two-dimensional Schrödinger equation with a time and space varying exterior potential and for general convex smooth boundaries. The construction is based on asymptotics of the inhomogeneous pseudodifferential operators defining the related Dirichlet-to-Neumann operator. Furthermore, a priori estimates are developed for the truncated problems with various increasing order boundary conditions. They propose in [34] some suitable discretization schemes of these ABCs and prove some semi-discrete stability results. Furthermore, the full numerical discretization of the corresponding initial boundary value problems is considered and simulations are provided to compare the accuracy of the different ABCs.

6.4.2. Semi-classical limit of the nonlinear Schrödinger equation

C. Besse works with R. Carles and F. Méhats (EPI Ipso). They consider in [36] the semiclassical limit for the nonlinear Schrödinger equation. They introduce a phase/amplitude representation given by a system similar to the hydrodynamical formulation, whose novelty consists in including some asymptotically vanishing viscosity. They 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. They propose a second order numerical scheme which is asymptotic preserving. Before singularities appear in the limiting Euler equation, they 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 Schrödinger equation.

6.4.3. Analysis and numerical simulation of the Schrödinger equation

The linear or nonlinear Schrödinger equation with potential is one of the basic equations of quantum mechanics and it arises in many areas of physical and technological interest, e.g. in quantum semiconductors, in electromagnetic wave propagation, and in seismic migration. The Schrödinger equation is the lowest order one-way approximation (paraxial wave equation) to the Helmholtz equation and is called Fresnel equation in optics, or standard parabolic equation in underwater acoustics. The solution of the equation is defined on an unbounded domain. If one wants to solve such a whole space evolution problem numerically, one has to restrict the computational domain by introducing artificial boundary conditions. So, the objective is to approximate the exact solution of the whole-space problem, restricted to a finite computational domain. A review article [45] was written this year to describe and compare the different current approaches of constructing and discretizing the transparent boundary conditions in one and two dimensions. However, these approaches are limited to the linear case (or nonlinear with the classical cubic nonlinearity: an article written was dedicated to this case this year [49]) and constant potentials. Therefore, in collaboration with X. Antoine (IECN Nancy and Inria Lorraine), we proposed to P. Klein to study, in her PhD thesis, the case of the Schrödinger equation with variable potentials. The study of the non-stationary one-dimensional case has already led to one publication [46] and some preliminary results in the stationary case are really promising. These cases are relevant since for example the equations appear in the Bose Einstein condensate with a quadratic potential.

This problem is obviously not limited to the Schrödinger equation and new developments are in progress on the Korteweg de Vries equation with M. Ehrhardt. This equation is more difficult to study due to its third order derivative in space.

Dispersive equations, such as the Schrödinger equation are also considered as boundary-value problems. For example, in [60], G. Dujardin studies the long time asymptotics of the solutions of linear Schrodinger equations considered as initial-boundary value problems on the half-line and on bounded intervals when the boundary data are periodic functions of time. G. Dujardin obtains theoretical results using a transformation method introduced by T. Fokas and provides several numerical experiments to support them.

6.5. Other contributions

6.5.1. Corrosion models

The Diffusion Poisson Coupled Model [47] 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 [12], 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 will be soon submitted for publication.

In [4], C. Chainais-Hillairet and coworkers have studied some numerical methods for the approximation of the DPCM model. The choice of the numerical methods is justified by a stability analysis and by the study of their numerical performance. These methods have been implemented in the code CALIPSO developed at ANDRA. Numerical experiments with real-life data show the efficiency of the developed methods.

6.5.2. Transparent boundary conditions for the Helmholtz equation

C. Besse and I. Violet start a collaboration with S. Fliss (Poems), J. Coatleven and K. Ramdani (Corida) to build transparent boundary conditions for the Helmholtz equation. They propose in [6] a strategy to determine the Dirichlet-to-Neumann (DtN) operator for infinite, lossy and locally perturbed hexagonal periodic media. They obtain 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. The second one is a Dirichlet-to-Dirichlet (DtD) type operator related to the symmetry properties of the problem. The half-space DtN operator is characterized via Floquet-Bloch transform, a family of elementary strip problems and a family of stationary Riccati equations. The DtD operator is the solution of an affine operator valued equation which can be reformulated as a non standard integral equation.

6.5.3. Analysis of subcycling techniques

Several physics situations involve phenomena which occur on very different time scales. A popular option to integrate the equations in time in this context is to use sub-cycling techniques, which allow to weaken the stability constraints. Several questions are still open for the asymptotic behavior of such methods, *e.g.* the preservation of equilibrium states. New results about the asymptotic orders if such methods have been derived on toy-model problems which allow a better understanding of these methods and their preservation of equilibrium states [40].

6.5.4. Phase transitions

We analyzed numerically a forward-backward diffusion equation with a cubic- like diffusion function, –emerging in the framework of phase transitions modelling– and its “entropy” formulation determined by considering it as the singular limit of a third-order pseudo-parabolic equation. Precisely, we proposed schemes for both the second and the third order equations, we discussed the analytical properties of their semi-discrete counter- parts and we compared the numerical results in the case of initial data of Riemann type, showing strengths and flaws of the two approaches, the main emphasis being put on the propagation of transition interfaces. This is a joint work with C. Mascia (Univ. La Sapienza) [25].

6.5.5. Modelling of the biological populations

We worked on two problems of biological populations: the understanding of the occurrence of collective behavior for large populations and the extinction probabilities in some population dynamics.

Several approaches are used in the modelling of collective behavior models for large populations of fish : we obtained results at the particle and kinetic levels for a model involving self-propulsion, friction and an attractive/repulsive potential. By introducing a new dimensionless setting, we identified five parameters that govern the possible asymptotic states for this system (clumps, spheres, dispersion, mills, rigid-body rotation, flocks) and performed a numerical analysis on the 3D particle-setting. Also, we described the kinetic system derived as the limit from the particle model as N tends to infinity; and we proposed, in 1D, a numerical scheme for the simulations, and performed a numerical analysis devoted to trying to recover asymptotically patterns similar to those emerging for the equivalent particle systems, when particles originally evolved on a circle. this is a joint work with J. Rosado (UCLA) and F. Vecil (Univ. Valencia) [43].

The extinction probabilities of a flower population may be modelled by an imhomogeneous random walk on the positive quadrant. On the one hand, introducing the generating function, that solves a PDE, we computed an explicit solution. On the other hand, we compared stochastic and deterministic resolutions of the random walk. This is a joint work with K. Raschel (Univ. Tours), V. C. Tran (Univ. Lille 1) [26].

APICS Project-Team

6. New Results

6.1. Source recovery problems

Participants: Laurent Baratchart, Sylvain Chevillard, Juliette Leblond, Ana-Maria Nicu.

The works presented here are done in collaboration with Maureen Clerc and Théo Papadopoulo from the Athena EPI, with Doug Hardin and Edward Saff from Vanderbilt University (Nashville, USA), and with Abderrazek Karoui (Univ. Bizerte, Tunisie) and Jean-Paul Marmorat (Centre de mathématiques appliquées (CMA), École des Mines de Paris).

This section in dedicated to 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 a common problem to both which has been recently achieved, see [37],[29], [39].These are sums of (distributional) derivatives of Sobolev functions vanishing on the boundary.

6.1.1. Application to EEG

In 3-D, functional or clinical active regions in the cortex are often represented by pointwise sources that have to be localized from measurements on the scalp of a potential satisfying a Laplace equation (EEG, electroencephalography). In the work [4] 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. A milestone in a long-haul research on the behaviour of poles of best rational approximants of fixed degree to functions with branch points has been reached this year [14], which shows that the technique carries over to finitely many sources (see section 4.2). In this connection, a dedicated software "FindSources3D" (see section 5.6) has been developed, in collaboration with the team Athena [16], [26].

Further, it appears that in the rational approximation step of these schemes, *multiple* poles possess a nice behaviour with respect to the branched singularities. This is due to the very basic physical assumptions on the model (for EEG data, one should consider *triple* poles). Though numerically observed in [16], there is no mathematical justification so far why these multiple poles have such strong accumulation properties, which remains an intriguing observation.

Issues of robust interpolation on the sphere from incomplete pointwise data are also under study in order to improve numerical accuracy of our reconstruction schemes. Spherical harmonics, Slepian bases and related special functions are of special interest (thesis of A.-M. Nicu [13], [67]), while other techniques should be considered as well.

Also, magnetic data from MEG (magneto-encephalography) will soon become available, which should enhance the accuracy of source recovery algorithms.

It turns out that discretization issues in geophysics can also be approached by these approximation techniques. Namely, in geodesy or for GPS computations, one may need to get a best 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 a physicist colleague (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

Magnetic sources localization from observations of the field away from the support of the magnetization is an issue under investigation in a joint effort with the Math. department of Vanderbilt University and the Earth Sciences department at MIT. The goal is to recover the 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).

The magnetization operator is the Riesz potential of the divergence of the magnetization. The problem of recovering a thin plate magnetization distribution from measurements of the field in a plane above the sample lead us to an analysis of the kernel of this operator, which we characterized in various function and distribution spaces (arbitrary compactly supported distributions or derivatives of bounded functions). For this purpose, we introduced a generalization of the Hodge decomposition in terms of Riesz transforms and showed that a thin plate magnetization is "silent" (i.e. in the kernel) if the normal component is zero and the tangential component is divergence free. In particular, we show that a unidirectional non-trivial magnetization with compact support cannot be silent. The same is true for bidirectional magnetizations if at least one of the directions is nontangential. We also proved that any magnetization is equivalent to a unidirectional. We did introduce notions of being silent from above and silent from below, which are in general distinct. These results have been reported in a paper to appear [37].

We currently work on Fourier based inversion techniques for unidirectional magnetizations, and Figures 5 , 6 , 7 and 8 show an example of reconstruction. A joint paper with our collaborators from VU and MIT is being written on this topic.

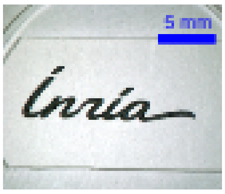


Figure 5. Inria's logo were printed on a piece of paper. The ink of the letters "In" were magnetized along a direction D_1. The ink of the letters "ria" were magnetized along another direction D_2 (almost orthogonal to D_1).

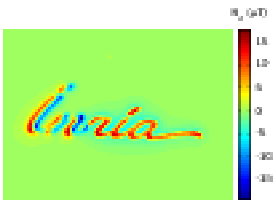


Figure 6. The Z-component of the magnetic field generated by the sample is measured by a SQUID microscope. The measure is performed 200μm above the sample.

For more general magnetizations, the severe ill-posedness of reconstruction challenges discrete Fourier methods, one of the main problems being the truncation of the observations outside the range of the SQUID measurements. We look forward to develop extrapolation techniques in the spirit of step 1 in section 3.1 .

6.2. Boundary value problems, generalized Hardy classes

Participants: Laurent Baratchart, Slah Chaabi, Juliette Leblond, Dmitry Ponomarev.

This work has been performed in collaboration with Yannick Fischer from the Magique3D EPI (Inria Bordeaux, Pau).

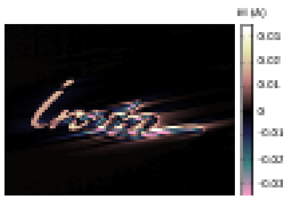


Figure 7. The field measured in Figure 6 is inversed, assuming that the sample is unidimensionally magnetized along the direction D_1. The letters "In" are fairly well recovered while the rest of the letters is blurred (because the hypothesis about the direction of magnetization is false for "ria").

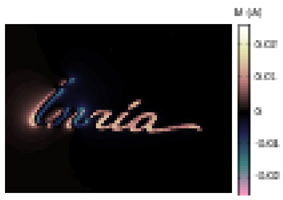


Figure 8. The field measured in Figure 6 is inversed, assuming that the sample is unidimensionally magnetized along the direction D_2. The letters "ria" are fairly well recovered while the rest of the letters is blured (because the hypothesis about the direction of magnetization is false for "In").

In collaboration with the CMI-LATP (University Aix-Marseille I), the team considers 2-D diffusion processes with variable conductivity. In particular its complexified version, the so-called *conjugate* or *real Beltrami equation*, was investigated. In the case of a smooth domain, and for Lipschitz conductivity, we analyzed the Dirichlet problem for solutions in Sobolev and then in Hardy classes [5].

Their traces merely lie in L^p $(1 < p < \infty)$ of the boundary, a space which is suitable for identification from pointwise measurements. Again these traces turn out to be dense on strict subsets of the boundary. This allows us 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 .

We generalized the construction to finitely connected Dini-smooth domains and $W^{1,q}$-smooth conductivities, with $q > 2$ [35]. The case of an annular geometry is the relevant one for the application to plasma shaping mentioned below [58], [35]. The application that initially motivated this work came from free boundary problems in plasma confinement (in tokamaks) for thermonuclear fusion. This work was initiated in collaboration with the Laboratoire J. Dieudonné (University of Nice).

In the transversal section of a tokamak (which is a disk if the vessel is idealized into a torus), the so-called poloidal flux is subject to some conductivity equation outside the plasma volume for some simple explicit smooth conductivity function, while the boundary of the plasma (in the Tore Supra tokamak) is a level line of this flux [54]. Related magnetic measurements are available on the chamber, which furnish incomplete boundary data from which one wants to recover the inner (plasma) boundary. This free boundary problem (of Bernoulli type) can be handled through the solutions of a family of bounded extremal problems in generalized Hardy classes of solutions to real Beltrami equations, in the annular framework [35].

In the particular case at hand, the conductivity is $1/x$ and the domain is an annulus embedded in the right half-plane. We obtained a basis of solutions (exponentials times Legendre functions) upon separating variables in toroidal coordinates. This provides a computational setting to solve the extremal problems mentioned before, and was the topic of the PhD thesis of Y. Fischer [58], [27]. In the most recent tokamaks, like Jet or ITER, an interesting feature of the level curves of the poloidal flux is the occurrence of a cusp (a saddle point of the poloidal flux, called an X point), and it is desirable to shape the plasma according to a level line passing through this X point for physical reasons related to the efficiency of the energy transfer. We established well-posedness of the Dirichlet problem in weighted L^p classes for harmonic measure on piecewise smooth domains without cusps, thereby laying ground for such a study. This issue is next in line, now that the present approach has been validated numerically on Tore Supra data, and the topic of the PhD thesis of D. Ponomarev.

The PhD work of S. Chaabi is devoted to further aspects of Dirichlet problems for the conjugate Beltrami equation. On the one hand, a method based on Foka's approach to boundary value problems, which uses Lax pairs and solves for a Riemann-Hilbert problem, has been devised to compute in semi explicit form solutions to Dirichlet and Neumann problems for the conductivity equation satisfied by the poloidal flux. Also, for more general conductivities, namely bounded below and lying in $W^{1,s}$ with $s \geq 2$, parameterization of solutions to Dirichlet problems on the disk by Hardy function was achieved through Bers-Nirenberg factorization. Note the conductivity may be unbounded when $s = 2$, which is completely new. Two papers are being prepared reporting on these topics.

Finally, note that the conductivity equation can be expressed like a static Schrödinger equation, for smooth enough conductivity coefficients. This provides a link with the following results recently set up by D. Ponomarev, who recently join the team for his PhD. 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 such setting, Helmholtz equation is approximated by a linear Schrödinger equation with one of spatial coordinates being an evolutionary variable. Explicit comparison of the solutions in the whole half-space allows to establish global justification of the Schrodinger model for sufficiently smooth pulses [73]. This phenomenon can also be described by a nonstationary model that relies on the spatial nonlinear Schrödinger (NLS) equation with the time-dependent refractive index. A toy problem is considered in [71], 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. The NLS approximation is derived from a 2-D quasilinear wave equation, for small time intervals and smooth initial data. Numerical simulations illustrate the approximation result in the 1-D case.

6.3. Circuit realisations of filter responses: determination of canonical forms and exhaustive computations of constrained realisations

Participant: Fabien Seyfert.

This work has been done in collaboration with Smain Amari (Royal Military College, Kingston, Canada), Jean Charles Faugère (SALSA EPI, Inria Rocquencourt), Giuseppe Macchiarella (Politecnico di Milano, Milan, Italy), Uwe Rosenberg (Design and Project Engineering, Osterholz-Scharmbeck, Germany) and Matteo Oldoni (Politecnico di Milano, Milan, Italy).

We continued our work on the circuit realizations of filters' responses with mixed type (inductive or capacitive) coupling elements and constrained topologies [1]. For inline circuits, methods based on sequential extractions of electrical elements are best suited due to their computational simplicity. On the other hand, for circuits with no inline topology ,such methods are inefficient while algebraic methods (based on a Groebner basis) can be used, but at high computational cost. In order to tackle large order circuits, our approach is to decompose them into connected inline sections, which can be directly realized by extraction techniques, and into complex sections, where algebraic methods are needed for realization. In order to do this, we started studying the synthesis of filter responses by means of circuits with reactive non-resonating nodes (dangling resonators) [22]. Links of this topic with Potapov's factorization of J-inner functions are currently being investigated.

In this connection, sensitivity analysis of the electrical response of a filter with respect to the electrical parameters of the underlying circuit has been published in collaboration with the University of Cartagena and ESA [20]. We essentially proved that the total electrical sensitivity of a filters' response does not depend on the coupling topology of the underlying circuit: the latter however controls the distribution of this sensitivity within each resonator.

6.4. 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 (Politecnico di Milano, Milan, Italy).

6.4.1. 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:

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

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 [62] when the interpolation frequencies lie in the *open* left half-plane. We conjecture that existence and uniqueness of the solution still holds in our case, where interpolation takes place on the boundary, provided r has no roots on the imaginary axis. Numerical experiments based on continuation techniques tend to corroborate our belief: efforts now focus on a mathematical proof. The derived numerical tools have already been used to successfully to design multiplexer's responses in collaboration with CNES and Xlim, thereby initiating a collaboration with Xlim on co-integration of filters and antennas.

6.4.2. De-embedding of multiplexers

Let S be the measured scattering matrix 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-embedding question we raise is the following: given S and T, is it possible to retrieve the F_k's ? The answer to this question depends of course of the admissible class of filters. For the simplest case where no assumption is made (except reciprocity), we showed that the problem has a unique solution for $N > 3$ and for generic T, while for $N = 2$ the solution space at each frequency point has real dimension 2. This redundancy can be explained by the existence of "ghost" or "silent" components that can hide behind the junction: when being chained to the junction these components do not affect its response. We also experienced that the generic behaviour for $N > 3$ is rather theoretical, as usual junctions are often made of chained T-junctions: in this non generic case (which is rather generic in practice !) some "silent" component still exists for $N > 3$. Additional hypotheses, such as rationality with prescribed degree for F_k, are currently being studied and already yielded results for the case $N = 3$ [21].

This work is pursued in collaboration with Thales Alenia Space, Politecnico di Milano, Xlim and CNES in particular within the contract CNES-Inria on compact N-port synthesis (see section 7.1).

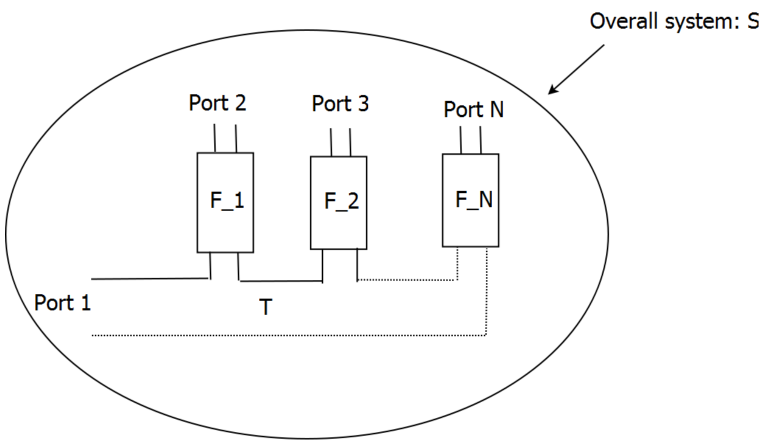


Figure 9. Multiplexer made of a junction T and filtering devices $F_1, F_2 \cdots F_N$

6.5. 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.

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 2011, 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.

In 2012, we focused on the kind of instabilities that these ideal systems can exhibit. We showed that a circuit can be unstable, although it has 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. This pathological example is unrealistic, though, because it assumes 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. Under this simple assumption, we proved that the class of transfer functions of realistic circuits is much smaller than in previous situation. In fact, 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. An article is currently being written on the subject.

6.6. Best constrained analytic approximation

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

This work is performed in collaboration with Jonathan Partington (Univ. Leeds, UK).

Continuing effort is being paid by the team to carry over the solution to bounded extremal problems of section 3.3.1 to various settings. We mentioned already in section 6.2 the extension to 2-D diffusion equations with variable conductivity for the determination of free boundaries in plasma control and the development of a generalized Hardy class theory. We also investigate the ordinary Laplacian in $\mathbb{R}^3$, where targeted applications are to data transmission step for source detection in electro/magneto-encephalography (EEG/MEG, see section 6.1).

Still, questions about the behaviour of solutions to the standard bounded extremal problems (P) of section 3.3.1 deserve attention. We realized this year that Slepian functions are eigenfunctions of truncated Toeplitz operators in 2-D. This can be used to quantify robustness properties of our resolution schemes in H^2 and to establish error estimates, see [25]. Moreover we considered additional interpolation constraints [28], as a simplified but already interesting issue, before getting at extremal problems for generalized analytic functions in annular non-smooth domains. The latter arise in the context of plasma shaping in tokamaks like ITER, and will be the subject of the PhD thesis of D. Ponomarev.

In another connection, weighted composition operators on Lebesgue, Sobolev, and Hardy spaces appear in changes of variables while expressing conformal equivalence of plane domains. A universality property related to the existence of invariant subspaces for these important classes of operators has been established in [19]. Additional density properties also allow one to handle some of their dynamical aspects (like cyclicity).

6.7. Rational Approximation for fitting Non-Negative EPT densities

Participants: Martine Olivi, Fabien Seyfert.

This work has been done in collaboration with Bernard Hanzon and Conor Sexton from Univ. Cork.

The problem is to fit a probability density function on a large set of financial data. The model class is the set of non-negative EPT (Exponential-Polynomials-Trigonometric) functions which provides a useful framework for probabilistic calculation as illustrated in the link http://www.2-ept.com/2-ept-literature.html. Moreover, an EPT function can alternatively be interpreted as the impulse response of a continuous time stable system whose Laplace transform is a rational transfer function. This interpretation allows us to approach this problem using approximation tools developed by the team. The very context brings up a classical, as yet essentially unsolved difficulty in rational approximation, namely preservation of positivity. This is known to be a hard issue. Our work, initiated in 2011, resulted this year in an improved approach for checking non-negativity of an EPT function. These results have been presented at the 16th IFAC Conference on System Identification [23]. The proposed method was demonstrated on the positive daily Dow Jones Industrial Average (DJIA) log returns over 80 years.

6.8. Rational and meromorphic approximation

Participant: Laurent Baratchart.

This work has been done in collaboration with Herbert Stahl (TFH Berlin) and Maxim Yattselev (Univ. Oregon at Eugene, USA).

We completed and published this year the proof of an important result in approximation theory, namely the counting measure of poles of best H^2 approximants (more generally: of critical points) 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 [14]. The proof requires showing existence and uniqueness of a compact set of minimal weighted logarithmic capacity in a field, outside of which the function is single-valued. Structure of this contour, along with error estimates, also come out of the proof. The result is in fact valid for functions that are Cauchy integrals of Dini-smooth functions on such a contour. We rely in addition on asymptotic interpolation estimates from [63].

This result warrants source recovery techniques used in section 6.1.1 .

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. In the case of 4 branchpoints, expressing the computation of Padé approximants in terms of the solution to a Riemann-Hilbert problem on the Riemann surface of the function, we proved that the pole behaviour generically shows deterministic chaos [49].

6.9. 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 2012 is the following:

- Publication of a work about the implementation of functions erf and erfc in multiple precision and with correct rounding [15]. It corresponds to a work initially begun in the Arénaire team and finished in the Caramel team. The goal of this work is to show on a representative example the different steps of the rigorous implementation of a function in multiple precision arithmetic (choice of a series approximating the function, choice of the truncation rank and working precision used for the computation, roundoff analysis, etc.). The steps are described in such a way that they can easily be reproduced by someone who would like to implement another function. Moreover, it is showed that the process is very regular, which suggests that it (or at least large parts of it) could be automated.
- In the same field of multiple precision arithmetic, and with Marc Mezzarobba (Aric team), we proposed an algorithm for the efficient evaluation of the Airy $\mathrm{Ai}(x)$ function when x is moderately large [57]. Again, this work deals with a representative example, with the idea of trying to automate

the process as a future work. 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.

- Finally, a more general endeavor is to develop a tool that helps developers of libms in their task. This is performed by the software Sollya [2], developed in collaboration with C. Lauter (Université Pierre et Marie Curie) and M. Joldeş (Uppsala University). During year 2012, a large effort has been made in view of the release of version 4.0 (to come in 2013). This effort (of about 400 commits in the svn repository of the project) is mainly intended to provide a library version of Sollya, as well as a robust test suite for the tool. As a matter of course, it allowed us to detect and fix a dozen of bugs.

[2] 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. Other works consist of analysing kinematic restitution laws based on the use of the kinetic energy metric. We also performed an analysis of the rocking block motion in terms of the kinetic angles between the two unilateral constraints. Results are in [21], [22] [55]. 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 [20].

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 simplcity 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 [18]. In [23] we have provided a tutorial on similar types of systems like relay systems, and their relationships with other formalisms like complementarity systems, or switching dynamical systems. This follows in fact a research program proposed in [4].

6.3. Optimization

6.3.1. Optimization algorithms for large-scale machine learning problems, and applications in computer vision

Participant: Jérôme Malick.

This collaboration with Zaid Harchaoui (Inria, LEAR Team) has been growing since summer 2010. It also involves Miro Dudik (Microsoft Research NYC) and a student who just started his PhD in october 2012 (after his master with us).

The explosion of data that we are experiencing (Big Data) lead us to huge-scale learning problems, new challenges for statistical learning and numerical optimisation algorithms. For example, the new databases for image categorization are large-scale in the three dimensions (large number of exemples, high-dimension feature description, and large number of categories). The resulting learning problem is out of reach by standard optimization problems.

We developped a new approach exploiting the hidden underlying lower-dimension structure of this big data. We proposed a new family of algorithms (of the type coordinate results, or conditional gadient), whose iterations have an algorithmic complexity lower that an order compared to standard methods. For example, applied to learning problems with trace-norm penalization, our algorithm [26] exploit the atomic decomposition of the norm and compute only an approximate largest singular vector pair (instead of the whole singular value decomposition). Promising results [27] have been obtained on the image database Imagenet, where we show significant improvements compare to the state-of-the-art approaches (one-vs-rest strategies).

6.3.2. Semidefinite programming and combinatorial optimization

Participants: Nathan Krislock, Jérôme Malick.

We have worked with Frederic Roupin (Prof. at Paris XIII) on the use of semidefinite programming to solve combinatorial optimization problems to optimality. Within exact resolution schemes (branch-and-bound), "good" bounds are those with a "good" balance between tightness and computing times.

We proposed a new family of semidefinite bounds for 0-1 quadratic problems with linear or quadratic constraints [50]. The paradigm is to trade computing time for a (small) deterioration of the quality of the usual semidefinite bounds, in view of enhancing this efficiency in exact resolution schemes. Extensive numerical comparisons et tests showed the superior quality of our bounds, when embedded within branch-and-bound shemes, on standard test-problems (unconstrained 0-1 quadratic problems, heaviest k-subgraph problems, and graph bisection problems).

We have embedded the new bounds within branch-and-bound algorithms to solve 2 standard combinatorial optimization problems to optimality.

- *Max-cut.* We developed [34] 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 ([52]) on the large test-problems.
- *Heaviest k-subgraph problems*. Our previous work [51] takes advantage of the new bounds in their basic form to prune very well in the search tree. Its performances are then comparable with the best method (based on convex quadratic relaxation using CPLEX as an engine). Adapting and incorporating the tehniques we developped for the max-cut problem, we propose in [35] an big improveement 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).

Finally, we have worked on making our data sets available online together with a web interface for our solvers. We have also started working on a generic online semidefinite-based solver for binary quadratic problems using the generality of [50]. All this is publicly available on line at http://lipn.univ-paris13.fr/BiqCrunch/.

6.3.3. Unified theory of inaccurate bundle methods

Participants: Claude Lemaréchal, Welington Oliveira.

Convergence of bundle methods is an intricate subject. The situation is even worse in the inexact case, where many variants exist, each with its specific *ad hoc* proof techniques.

With C. Sagastizábal (Rio de Janeiro), we have developed a synthetic theory to single out the successive steps when proving convergence of a generic algorithm, as well as the specific hypotheses that they need. Our pattern covers all variants published so far and suggests a new one. The corresponding paper is being finalized.

6.3.4. Stabilizing marginal prices in electricity production

Participants: Claude Lemaréchal, 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 [48]. However, the computed optimal dual variables show a noisy and unstable behaviour, that could prevent their use as price indicator. We propose a simple and controllable way to stabilize the dual optimal solutions, by penalizing the total variation of the prices [36]. Our illustrations on the daily electricity production optimization of EDF show a strinking stabilization at a negligible cost.

6.4. Robotics

6.4.1. Hierarchic QP solver

Participants: Pierre-Brice Wieber, Dimitar Dimitrov.

We are working in collaboration with the LAAS-CNRS and the CEA-LIST on solving multi-objective Quadratic Programs with Lexicographic ordering: Hierarchic QPs [47]. The focus this year has been on enabling fast computations in the case of time-varying Hierarchic QPs through warm-starting the active set method. This has been possible by developing an active set method for lexicographic multi-objective ordering [44], [45]. The main difference with respect to classical active set methods is in the use of a "lexicographic" (sometimes called "multi-dimensional") Lagrange multiplier.

6.4.2. Modeling of human balance in public transports

Participants: Pierre-Brice Wieber, Zohaib Aftab.

Zohaib Aftab finished his PhD thesis in collaboration with IFSTTAR (previously INRETS) on modeling human balance in public transports. A Model Predictive Control scheme has been developed for the prediction of recovery motions, including ankle and hip strategies as well as stepping with adaptive step locations and timings [37]. This MPC scheme has been validated against a balance recovery scenario found in the biomechanics literature [38].

6.4.3. Model Predictive Control for Biped Walking

Participants: Pierre-Brice Wieber, Andrei Herdt, Jory Lafaye.

In collaboration with the DLR in Munich, we designed an MPC scheme for biped walking based on the "Capture Point". This is just a simple change of variable $\xi = x + \frac{1}{\omega}\dot{x}$ that transforms the second-order dynamics of the Center of Mass x of the robot into a cascade of two first-order dynamics, one stable and one unstable. This MPC scheme has been evaluated successfully on the DLR biped robot [49].

Since fast computations are always a key objective for feedback controllers, we designed a change of variable in the underlying QP in order to expose the specific structure between time-varying and time-invariant parts of the Hessian matrix and compute its Cholesky decomposition in an efficient way by pre-computing the decomposition of the time-invariant part.

6.5. Computational Toxicology

Participant:

It is now well recognized that toxicology has entered a new era. Previously mainly based on animal testing, toxicology is now turning to in vitro and in silico experiments. To assess the risk of chemicals but also to gather and to interpret the massive amounts of experimental data generated by modern toxicology, the development of mathematical and computational tools are essential. An important element in risk assessment of chemicals is the human bioaccumulative potential. We developed a predictive tool for human bioaccumulation assesment using a physiologically based toxicokinetic model [53].

6.6. Computational Biology

Participant:

Biological oscillations have attracted widespread interest from experimentalists, with the *in vivo* design of synthetic oscillators, and from mathematicians, with the study of limit cycles. Oscillations in protein concentrations or gene expression are supposed to be involved in the generation of the rhythms observed in the cell. In many situations, oscillations are originated by negative feedback loops. In [54] we have studied the oscillatory regimes of a negative feedback oscillator and derived the probability of having oscillations.

6.7. Mechanical rods

6.7.1. High-order models of mechanical rods

Participants: Florence Bertails-Descoubes, Romain Casati.

Reduced-coordinates models for rods such as the articulated rigid body model or the super-helix model [39] 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-coordinates 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 we investigated the clothoidal case ($d = 1$) in the 2d case [19], relying on Romberg numerical integration. This 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. All these results will we submitted for publication early 2013.

6.7.2. Inverse modeling of mechanical rods

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

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 [43] we noted that reduced-coordinates models such as the super-helix are well-suited for static inversion in presence of gravity. The main difficulty then amounts to fitting a piecewise helix to an arbitrary input curve. This year in A. Derouet-Jourdan's PhD's thesis, we solved this problem by extending to 3d the floating tangents algorithm introduced in 2d in [43]. 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 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. This result was submitted for publication to Computer-Aided Geometric Design in Spring, and is currently under minor revision.

6.8. High-accuracy time-stepping schemes

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 fist proposed to improve the global order of accuracy over periods when the evolution is sufficiently smooth by mixing standard higher order schemes for Differential Algebraic equations and the Moreau–Jean's scheme [16]. We also proposed self-adapting schemes by applying time–discontinuous Galerkin methods to the measure differential equation in [24]. 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 [17]. Finally, the energetic behavior of the standard Moreau–Jean scheme has been addressed in [25] by developing a Newmark–type scheme for nonsmooth dynamics.

6.9. 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. Necessary and sufficient conditions for disspativity preservation after the time-discretization are derived (preservation of the stioarge function, the supply rate and the dissipation function). The possible state jumps are also analyzed [46]. It is shown that excepted when the system is state lossless and theta = 0.5, the conditions are very stringent.

6.9.1. Multivalued Lur'e dynamical systems

Participant: Bernard Brogliato.

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 [40]. The results in [42] extend those in [41] with an accurate characterization of the maximal monotonicity of the central operator of these systems. Concrete and verifiable criteria are provided for the above classes (complementarity, relay systems).

COMMANDS Project-Team

6. New Results

6.1. Optimal control of partial differential equations

6.1.1. Optimal control of a semilinear parabolic equation with singular arcs

Participant: Frédéric Bonnans.

This paper, published as Inria report 8099 [25], develops a theory of singular arc, and the corresponding second order necessary and sufficient conditions, for the optimal control of a semilinear parabolic equation with scalar control applied on the r.h.s. We obtain in particular an extension of Kelley's condition, and the characterization of a quadratic growth property for a weak norm.

6.2. Trajectory optimization

6.2.1. First and second order optimality conditions for optimal control problems of state constrained integral equations

Participants: Frédéric Bonnans, Xavier Dupuis.

In this work performed with Constanza De La Vega (U. Buenos Aires), and published as Inria report 7961 [26], we deal with optimal control problems of integral equations, with initial-final and running state constraints. The order of a running state constraint is defined in the setting of integral dynamics, and we work here with constraints of arbitrary high orders. First and second-order necessary conditions of optimality are obtained, as well as second-order sufficient conditions.

6.2.2. Sensitivity analysis for relaxed optimal control problems with final-state constraints

Participants: Frédéric Bonnans, Laurent Pfeiffer.

In this work, performed with Oana Serea (U. Perpignan), and published as Inria report 7977 [27], we compute a second-order expansion of the value function of a family of relaxed optimal control problems with final-state constraints, parameterized by a perturbation variable. The sensitivity analysis is performed for controls that we call R-strong solutions. They are optimal solutions with respect to the set of feasible controls with a uniform norm smaller than a given R and having an associated trajectory in a small neighborhood for the uniform norm. In this framework, relaxation enables us to consider a wide class of perturbations and therefore to derive sharp estimates of the value function.

6.2.3. Sensitivity analysis for the outages of nuclear power plants

Participants: Frédéric Bonnans, Laurent Pfeiffer.

In this work, performed with Kengy Barty (EDF), and published as Inria report 7884 [24]. Nuclear power plants must be regularly shut down in order to perform refueling and maintenance operations. The scheduling of the outages is the first problem to be solved in electricity production management. It is a hard combinatorial problem for which an exact solving is impossible.

Our approach consists in modelling the problem by a two-level problem. First, we fix a feasible schedule of the dates of the outages. Then, we solve a low-level problem of optimization of elecricity production, by respecting the initial planning. In our model, the low-level problem is a deterministic convex optimal control problem.

Given the set of solutions and Lagrange multipliers of the low-level problem, we can perform a sensitivity analysis with respect to dates of the outages. The approximation of the value function which is obtained could be used for the optimization of the schedule with a local search algorithm.

6.2.4. Optimization of the anaerobic digestion of microalgae in a coupled process

Participant: Pierre Martinon.

In this work in collaboration with Terence Bayen (U. Monptellier) and Francis Mairet (Inria Sophia), submitted to ECC13 [30], we study the maximization of the production of methane in a bioreactor coupling an anaerobic digester and a culture of micro-algae limited by light. The decision parameter is the dilution rate which is chosen as a control, and we enforce periodic constraints in order to repeat the same operation every day. The system is gathered into a three-dimensional system taking into account a day-night model of the light in the culture of micro-algae. Applying Pontryagin maximum principle, the necessary conditions on optimal trajectories indicate that the control consists of bang and/or singular arcs. We provide numerical simulations by both direct and indirect methods, which show the link between the light model and the structure of optimal solutions.

6.3. Stochastic programming

6.3.1. Solving multi-stage stochastic mixed integer linear programs by the dual dynamic programming approach

Participants: Frédéric Bonnans, Zhihao Cen.

In this work performed in the framework of the PhD thesis of Zhihao Cen, and published as an Inria report RR-7868 [29], We consider a model of medium-term commodity contracts management. Randomness takes place only in the prices on which the commodities are exchanged, whilst state variable is multi-dimensional, and decision variable is integer. In our previous article, we proposed an algorithm based on the quantization of random process and a dual dynamic programming type approach to solve the continuous relaxation problem. In this paper, we study the multi-stage stochastic mixed integer linear program (SMILP) and show the difficulty when using dual programming type algorithm. We propose an approach based on the cutting plane method combined with the algorithm in our previous article, which gives an upper and a lower bound of the optimal value and a sub-optimal integer solution. Finally, a numerical test on a real problem in energy market is performed.

6.3.2. Two methods of pruning Benders' cuts and their application to the management of a gas portfolio

Participant: Laurent Pfeiffer.

This report, coauthored with R. Apparigliato and S. Auchapt (Gdf Suez), and published as Inria report 8133 [31], describes a gas portfolio management problem, which is solved with the SDDP (Stochastic Dual Dynamic Programming) algorithm. We present some improvements of this algorithm and focus on methods of pruning Benders' cuts, that is to say, methods of picking out the most relevant cuts among those which have been computed. Our territory algorithm allows a quick selection and a great reduction of the number of cuts. Our second method only deletes cuts which do not contribute to the approximation of the value function, thanks to a test of usefulness. Numerical results are presented.

6.4. Hamilton-Jacobi approach

6.4.1. Hamilton-Jacobi equations in singular domains

Participants: Zhiping Rao, Hasnaa Zidani.

A good deal of attention has been devoted to the analysis of Hamilton–Jacobi equations adapted to unconventional domains, particularly in view of application to control problems and traffic models. The topic is new and capable of interesting developments, the results so far obtained have allowed to clarify under reasonable assumptions, basic items as the right notion of viscosity solution to be adopted and the validity of comparison principles.

- The work [19], co-authored with C. Imbert (LAMA, U. Paris-Est) and R. Monneau (Cermics, ENPC), focuses on a Hamilton-Jacobi approach to junction problems with applications to traffic flows. More specifically, the paper is concerned with the study of a model case of first order Hamilton-Jacobi equations posed on a *junction*, that is to say the union of a finite number of half-lines with a unique common point. The main result is a comparison principle. We also prove existence and stability of solutions. The two challenging difficulties are the singular geometry of the domain and the discontinuity of the Hamiltonian. As far as discontinuous Hamiltonians are concerned, these results seem to be new. They are applied to the study of some models arising in traffic flows. The techniques developed here provide new powerful tools for the analysis of such problems.

- This work deals with deterministic control problems where the dynamic can be completely different in multi-complementary domains of the space IR^d. As a consequence, the dynamics 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 and what is the right Bellman Equation associated to this problem?. In the case of finite horizon problems without runing cost, a jonction condition is derived on the interfaces, and a precise viscosity notion is provided in a paper in progress. Moreover, a uniqueness result of a viscosity solution is shown.

6.4.2. A general Hamilton-Jacobi framework for nonlinear state-constrained control problems

Participants: Olivier Bokanowski, Hasnaa Zidani.

This work [10], co-authored with Albert Altarovici, deals with deterministic optimal control problem with state constraints and nonlinear dynamics. It is known for such a problem that the value function is in general discontinuous and its characterization by means of an HJ equation requires some controllability assumptions involving the dynamics and the set of state constraints. Here, we first adopt the viability point of view and look at the value function as its epigraph. Then, we prove that this epigraph can always be described by an auxiliary optimal control problem free of state constraints, and for which the value function is Lipschitz continuous and can be characterized, without any additional assumptions, as the unique viscosity solution of a Hamilton-Jacobi equation. The idea introduced in this paper bypasses the regularity issues on the value function of the constrained control problem and leads to a constructive way to compute its epigraph by a large panel of numerical schemes. Our approach can be extended to more general control problems. We study in this paper the extension to the infinite horizon problem as well as for the two-player game setting. Finally, an illustrative numerical example is given to show the relevance of the approach.

6.4.3. State-constrained optimal control problems of impulsive differential equations

Participants: Nicolas Forcadel, Zhiping Rao, Hasnaa Zidani.

The research report [35] presents a study on optimal control problems governed by measure driven differential systems and in presence of state constraints. The first result shows that using the graph completion of the measure, the optimal solutions can be obtained by solving a reparametrized control problem of absolutely continuous trajectories but with time-dependent state-constraints. The second result shows that it is possible to characterize the epigraph of the reparametrized value function by a Hamilton-Jacobi equation without assuming any controllability assumption

6.4.4. Level-set approach for reachability analysis of hybrid systems under lag constraints

Participants: Giovanni Granato, Hasnaa Zidani.

The study in [36] aims at characterizing a reachable set of a hybrid dynamical system with a lag constraint in the switch control. The setting does not consider any controllability assumptions and uses a level-set approach. The approach consists in the introduction of an adequate hybrid optimal control problem with lag constraints on the switch control whose value function allows a characterization of the reachable set. The value function is in turn characterized by a system of quasi-variational inequalities (SQVI). We prove a comparison principle for the SQVI which shows uniqueness of its solution. A class of numerical finite differences schemes for solving the system of inequalities is proposed and the convergence of the numerical solution towards the value function is studied using the comparison principle. Some numerical examples illustrating the method are presented. Our study is motivated by an industrial application, namely, that of range extender electric vehicles. This class of electric vehicles uses an additional module *the range extender* as an extra source of energy in addition to its main source a high voltage battery. The methodolgy presented in [36] is used to establish the maximum range of a Hybrid vehicle, see [22].

6.5. Collision avoidance and motion planning

6.5.1. Collision analysis for a UAV

Participants: Anna Désilles, Hasnaa Zidani.

The *Sense and Avoid* capacity of Unmanned Aerial Vehicles (UAV) is one of the key elements to open the access to airspace for UAVs. In order to replace a pilot's *See and Avoid* capacity such a system has to be certified "as safe as a human pilot on-board". The problem is to prove that an unmanned aircraft equipped with a S&A system can comply with the actual air transportation regulations. A paper in progress aims to provide mathematical and numerical tools to link together the safety objectives and sensors specifications. Our approach starts with the natural idea of a specified "safety volume" around the aircraft: the safety objective is to guarantee that no other aircraft can penetrate this volume. We use a general reachability and viability concepts to define nested sets which are meaningful to allocate sensor performances and manoeuvring capabilities necessary to protect the safety volume. Using the general framework of HJB equations for the optimal control and differential games, we give a rigorous mathematical characterization of these sets. Our approach allows also to take into account some uncertainties in the measures of the parameters of the incoming traffic. We also provide numerical tools to compute the defined sets, so that the technical specifications of a S&A system can be derived in accordance with a small set of intuitive parameters. We consider several dynamical models corresponding to the different choices of maneuvers (lateral, longitudinal and mixed). Our numerical simulations show clearly that the nature of used maneuvers is an important factor in the specifications of sensor's performances.

6.6. Numerical methods for HJ equations

6.6.1. An adaptive sparse grid semi-lagrangian scheme for first order Hamilton-Jacobi Bellman equations

Participant: Olivier Bokanowski.

The paper [14], co-authored with M. Griebel (Fraunhofer SCAI & Univ. Bonn), J. Garcke and I. Klopmpaker (TUB, Berlin) proposes a semi-Lagrangian scheme using a spatially adaptive sparse grid to deal with non-linear time-dependent Hamilton-Jacobi Bellman equations. We focus in particular on front propagation models in higher dimensions which are related to control problems. We test the numerical efficiency of the method on several benchmark problems up to space dimension $d = 8$, and give evidence of convergence towards the exact viscosity solution. In addition, we study how the complexity and precision scale with the dimension of the problem.

6.6.2. A discontinuous Galerkin scheme for front propagation with obstacles

Participant: Olivier Bokanowski.

In [33], co-authored with C.-W. Shu (Brown Univ.) and Y. Cheng (Michigan Univ.), some front propagation problems in the presence of obstacles are analysed. We extend a previous work (Bokanowski, Cheng and Shu, SIAM J. Scient. Comput., 2011), to propose a simple and direct discontinuous Galerkin (DG) method adapted to such front propagation problems. We follow the formulation of (Bokanowski, Forcadel and Zidani, SIAM J. Control Optim. 2010), leading to a level set formulation driven by $\min(u_t + H(x, \nabla u), u - g(x)) = 0$, where $g(x)$ is an obstacle function. The DG scheme is motivated by the variational formulation when the Hamiltonian H is a linear function of ∇u, corresponding to linear convection problems in the presence of obstacles. The scheme is then generalized to nonlinear equations, written in an explicit form. Stability analysis is performed for the linear case with Euler forward, a Heun scheme and a Runge-Kutta third order time discretization using the technique proposed in (Zhang and Shu, SIAM J. Control and Optim., 2010). Several numerical examples are provided to demonstrate the robustness of the method. Finally, a narrow band approach is considered in order to reduce the computational cost.

6.6.3. Semi-Lagrangian discontinuous Galerkin schemes for some first and second order PDEs

Participant: Olivier Bokanowski.

Explicit, unconditionally stable, high order schemes for the approximation of some first and second order linear, time-dependent partial differential equations (PDEs) are proposed in [34], in collaboration with G. Simarmata (internship 2011, currently in RI dep. of Rabobank). The schemes are based on a weak formulation of a semi-Lagrangian scheme using discontinuous Galerkin elements. It follows the ideas of the recent works of Crouseilles, Mehrenberger and Vecil (2010) and of Qiu and Shu (2011), for first order equations, based on exact integration, quadrature rules, and splitting techniques. In particular we obtain high order schemes, unconditionally stable and convergent, in the case of linear second order PDEs with constant coefficients. In the case of non-constant coefficients, we construct "almost" unconditionally stable second order schemes and give precise convergence results. The schemes are tested on several academic examples, including the Black and Scholes PDE in finance.

CORIDA Project-Team

6. New Results

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

In [38], a new characteristics method for the discretization of the two dimensional fluid-rigid body problem is proposed in the case of different densities for the fluid and the solid. Convergence results are obtained for a fully-discrete finite element scheme.

In [35], controllability results are obtained for a low Reynolds number swimmer. The swimmer is undergoing radial and axi-symmetric deformations in order to propel itself in a viscous fluid.

The aim of the paper [51] is to tackle the time optimal controllability of an (n+1)-dimensional nonholonomic integrator. A full description of the optimal control and optimal trajectories are explicitly obtained.

In [25], we the interaction between a viscous incompressible fluid and an elastic structure immersed in the fluid.

In [30], weconsider the model composed by a rigid body immersed into a n incompressible perfect fluid and analyze the regularity of the trajectory of the rigid body and of the fluid particles.

In [39], we study the motion of a rigid body with a cavity filled with a viscous liquid.

In [34], we analyze a model of vesicle moving into a viscous incompressible fluid.

In [27], we obtain the identifiability of a rigid body moving in a stationary viscous fluid.

In [40] we study a mathematical model for the dynamics of vesicle membranes in a 3D incompressible viscous fluid. we show that, given $T > 0$, for initial data which are small (in terms of T), these solutions are defined on $[0, T]$ (almost global existence).

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

In [21] and [20], we propose an asymptotic analysis for the simple layer potential for multiple scattering at low frequencies.

In [19] we propose some strategies to solve numerically the difficult problem of multiple scattering by a large number of disks at high frequency. To achieve this, we combine a Fourier series decomposition with the EFIE integral equation. Numerical examples will be presented to show the efficiency of our method.

In [32], we are concerned with the convergence analysis of the iterative algorithm for solving initial data inverse problems from partial observations that has been recently proposed in Ramdani et al. More precisely, we provide a complete numerical analysis for semi-discrete (in space) and fully discrete approximations derived using finite elements in space and an implicit Euler method in time. The analysis is carried out for abstract Schrödinger and wave conservative systems with bounded observation (locally distributed).

In [23], 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 [18], we investigate absorbing boundary conditions for the two-dimensional Schrödinger equation with a time and space varying exterior potential.

6.3. Observality, controllability and stabilzation in the time domain

In [17] we consider N Euler-Bernoulli beams and N strings alternatively connected to one another and forming a chain beginning with a string. We study the strong and polynomial stabilities of this system on this network and the spectrum of the corresponding conservative system.

In [37] we study the asymptotic behavior of the solution of the non-homogeneous elastic systems with voids and a thermal effect. Our main results concern strong and polynomial stabilities (since this system suffers of exponential stability).

In [12], we consider the approximation of two coupled wave equations with internal damping. Our goal is to damp the spurious high frequency modes by introducing a numerical viscosity term in the approximation schemes and prove the exponential or polynomial decay of the discrete scheme.

In [13], we show similar results as in [12] for an abstract second order evolution equations.

In [44] we consider a class of infinite dimensional systems involving a control function u taking values in $[0, 1]$ and we prove, when u is given in an appropriate feedback form and the system satisfies appropriate observability assumptions, that the system is weakly stable. The main example concerns the analysis and stabilization of a model of Boost converter connected to a load via a transmission line.

In [46] we present a course on stabilization of hyperbolic equations given at a CIME session on Control of PDE's in Italy in July 2010, including well-known results, together with recent ones including nonlinear stabilization, memory-damping and stabilization of coupled systems by a reduced number of controls. In particular, we present the optimal-weight convexity method (Alabau-Boussouira 2005, 2010) in both the finite dimensional and infinite dimensional framework and give applications to semi-discretization of hyperbolic PDE's.

In [41], we consider stabilization of coupled systems of wave-type, with localized couplings and either localized internal closed loop controls or boundary control. We establish polynomial decay rates for coupling and damping regions which do not intersect in the one-dimensional case. We also derive results in the multi-dimensional case, under multiplier type conditions for both the coupling and damping regions. The novelty and difficulty is to consider localized couplings.

In [15], we give a constructive proof of Gibson's stability theorem, some extension and further positive and negative applications of this result.

In [36] we prove that the boundary controls for the heat equation have the bang-bang property, at least in rectangular domains. This result is proved by combining methods from traditionally distinct fields: the Lebeau-Robbiano strategy for null controllability and estimates of the controllability cost in small time for parabolic systems, on one side, and a Remez-type inequality for Muntz spaces and a generalization of Turan's inequality, on the other side.

In [16] we prove exact controllability for symmetric coupled wave equations by a single control in the case of coupling and control regions which do not intersect. For this, we use and extend the two-level energy method introduced by Alabau-Boussouira (2001, 2003). Using transmutation, we derive null controllability results for coupled parabolic and Schrödinger equations. This is the first positive quantitative result, in a multi-dimensional framework with control and coupling regions with empty intersection.

In [14], we prove controllability results for abstract systems of weakly coupled N evolution equations in cascade by a reduced number of boundary or locally distributed controls ranging from a single up to N-1 controls. We give applications to cascade coupled systems of N multi-dimensional hyperbolic, parabolic and diffusive (Schrödinger) equations. The results are valid for control and coupling regions which do not necessarily intersect.

In [22], we study two notions of controllability, called respectively radial controllability and directional controllability. We prove that for families of linear vector fields, the two notions are actually equivalent.

In [24] we solve an optimization problem in convex geometry which, despite its seeming simplicity, offers a nice variety of solutions, some of them being unexpectable.

The paper [28] is devoted to prove that the union of two identical balls minimizes a non linear eigenvalue (related to the generalized Wirtinger inequality) among sets of given volume.

In [33] is considered a problem in population dynamics where we investigate the question of optimal location of the zone of control.

In [26], we give a rigorous proof, valid also for unbounded operators, of the widely used “rotating wave approximations” for bilinear Schrödinger equations.

In [42], we exploit the results of [26] on standard examples of bilinear quantum systems.

DISCO Project-Team

6. New Results

6.1. Algorithmic study of linear functional systems

Participants: Alban Quadrat, Thomas Cluzeau [ENSIL, Univ. Limoges], Daniel Robertz [Univ. Aachen].

In [108], 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 [110]. 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 involved spectral sequence arguments as is done in the literature of modern algebra [82], [83]. To our knowledge, the algorithm obtained in [34] 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.

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. In [13], Serre's reduction problem is studied for underdetermined linear systems of partial differential equations with either polynomial, formal power series or analytic coefficients and with holonomic adjoints in the sense of algebraic analysis [82], [83]. These linear partial differential systems are proved to be equivalent to a linear partial differential equation. In particular, an analytic linear ordinary differential system with at least one input is equivalent to a single ordinary differential equation. In the case of polynomial coefficients, we give an algorithm which computes the corresponding linear partial differential equation.

The connection between Serre's reduction and the decomposition problem [90], which aims at finding an equivalent linear functional system which is defined by a block diagonal matrix of functional operators, is algorithmically studied in [92].

In [111], algorithmic versions of Statford's results [114] (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. 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 equivalently to a linear system of partial differential in 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.

6.2. Boundary value problems for linear ordinary integro-differential equations

Participants: Alban Quadrat, Georg Regensburger.

In [61], 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 [81] 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. Finally, system-theoretic interpretations of these results are given and illustrated on integro-differential equations.

In [78], we develop linear algebra results needed for generalizing the composition of boundary problems to singular ones. We consider generalized inverses of linear operators and study the question when their product in reverse order is again a generalized inverse. This problem has been studied for various kinds of generalized inverses, especially for matrices. Motivated by our application to boundary problems, we use implicit representation of subspaces via “boundary conditions” from the dual space and this approach gives a new representation of the product of generalized inverses. Our results apply to arbitrary vector spaces and for Fredholm operators, the corresponding computations reduce to finite-dimensional problems, which is crucial for our implementation for boundary problem for linear ordinary differential equations.

In collaboration with Li Guo and Markus Rosenkranz [77], we study algebraic aspects of integro-differential algebras and their relation to so-called differential Rota-Baxter algebras. We generalize this concept to that of integro-differential algebras with weight. Based on free commutative Rota-Baxter algebras, we investigate the construction of free integro-differential algebras with weight generated by a regular differential algebra. The explicit construction is not only interesting from an algebraic point of view but is also an important step for algorithmic extensions of differential algebras to integro-differential algebras (compare with the related construction and the implementation of integro-differential polynomials in [72]). In this paper, we review also the construction of integro-differential operators, the algorithms for regular boundary problems and a prototype implementation in the Theorema system.

In [11], we adapt our factorization technique for boundary problems to study ruin probabilities and related quantities in renewal risk theory. The analysis is based on boundary problems for linear ordinary differential equations (on the half bounded interval from zero to infinity) with variable coefficients and the corresponding factorization of Green’s operators. With this approach, we obtain closed-form and asymptotic expressions for discounted penalty functions under the more realistic assumption that the premium income depends on the present surplus of the insurance portfolio.

6.3. Symbolic methods for developing new domain decomposition algorithms

Participants: Thomas Cluzeau [ENSIL, Univ. Limoges], Victorita Dolean [Univ. Nice - Sophia-Antipolis], Frédéric Nataf [CNRS, Paris 6], Alban Quadrat.

Some algorithmic aspects of systems of partial differential equations based simulations can be better clarified by means of symbolic computation techniques. This is very important since numerical simulations heavily rely on solving systems of partial differential equations. For the large-scale problems we deal with in today’s standard applications, it is necessary to rely on iterative Krylov methods that are scalable (i.e., weakly dependent on the number of degrees on freedom and number of subdomains) and have limited memory requirements. They are preconditioned by domain decomposition methods, incomplete factorizations and multigrid preconditioners. These techniques are well understood and efficient for scalar symmetric equations (e.g., Laplacian, biLaplacian) and to some extent for non-symmetric equations (e.g., convection-diffusion). But they have poor performances and lack robustness when used for symmetric systems of partial differential equations, and even more so for non-symmetric complex systems (fluid mechanics, porous media, ...). As a general rule, the study of iterative solvers for systems of partial differential equations as opposed to scalar partial differential equations is an underdeveloped subject. In [76], we aim at building new robust and efficient solvers, such as domain decomposition methods and preconditioners for some linear and well-known systems of partial differential equations based on algebraic techniques (e.g., Smith normal forms, Gröbner basis techniques, D-modules).

6.4. Noncommutative geometry approach to infinite-dimensional systems

Participant: Alban Quadrat.

In [105], [104], [103], 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 [107] 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 [105], [104], [103], we show that every stabilizable system and their stabilizing controllers naturally admit geometric structures such as connections, curvatures, Chern classes, ... These results developed in [59] 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.

6.5. Stabilization of time-delay systems

Participants: Alban Quadrat, Arnaud Quadrat [SAGEM, MASSY].

In [60], we study the stabilization problem of a linear system formed by a simple integrator and a time-delay. We show that the stabilizing controllers of such a system can be be rewritten as the closed-loop system defined by the stabilizing controllers of the simple integrator and a distributed delay. This result is used to study tracking problems appearing in the study of inertially stabilized platforms for optical imaging systems.

6.6. Stabilization of MISO fractional systems with delays

Participants: Catherine Bonnet, Le Ha Vy Nguyen.

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 are derived in [51]. On the other hand, right coprime factorizations exist, and we have obtained explicit expressions for several particular cases of the studied systems.

6.7. Stability analysis of (fractional) neutral systems with commensurate delays

Participants: Catherine Bonnet, Andre Fioravanti [UNICAMP], Le Ha Vy Nguyen.

Neutral time-delay systems may have chains of poles asymptotic to the imaginary axis. As the chains approach the axis, some systems are H_∞-unstable even though all the poles are in the left-half plane. For a class of such systems, H_∞-stability conditions were presented in [84]. While systems with no more than one chain of poles asymptotic to a set of points on the imaginary axis were exhaustedly studied, only a particular case of systems with multiple chains were considered. We continue the stability analysis for more general cases of the latter systems. Primary results on pole locations are obtained [53], [52]. Based on these results, H_∞-stability conditions have also been derived.

6.8. Matrix Norm Approach for Control of Linear Time-Delay Systems

Participants: Catherine Bonnet, André Fioravanti [UNICAMP], José Claudio Geromel [UNICAMP], Silviu Niculescu.

In [94], we have treated the time-delay linear systems control design in the framework of complete and partial information. We were able to find linear controllers that increase the first stability window imposing at the same time that the delay-free system is stable using some properties about the norms of the state-space matrices. Our method treated the design problem by numeric routines based on Linear Matrix Inequalities (LMI) arisen from classical linear time invariant system theory coupled together with a unidimensional search. Both the state and output feedback design, were solved. We have this year tried our method on a 'high-dimensional' example for which no existing direct method would be computationnally feasible.

6.9. Interval observer

Participants: Frederic Mazenc, Silviu Niculescu, Thach Ngoc Dinh, Olivier Bernard [Inria - Sophia-Antipolis], Eric Walter [CNRS - L2S - Supelec], Michel Kieffer [CNRS - L2S - Supelec].

We made several progresses in the domain of the construction of state estimators called interval observers.
1) We presented the design of families of interval observers for continuous-time linear systems with a point-wise delay after showing that classical interval observers for systems without delays are not robust with respect to the presence of delays and that, in general, for linear systems with delay, the classical interval observers endowed with a point-wise delay are unstable. We proposed a new type of design of interval observers enabling to circumvent these obstacles. It incorporates distributed delay terms [26].

2) We considered a family of continuous-time systems that can be transformed through a change of coordinates into triangular systems. By extensively using this property, we constructed interval observers for nonlinear systems which are not cooperative and not globally Lipschitz. For a narrower family of systems, the interval observers possess the Input to State Stability property with respect to the bounds of the uncertainties [42], [21].

3) For the first time, we addressed in [44] the problem of constructing interval observers for discrete-time systems. Under a strong assumption, we proposed time-invariant interval observers for a very broad family of systems. In a second step, we have shown that, for any time-invariant exponentially stable discrete-time linear system with additive disturbances, time-varying exponentially stable discrete-time interval observers can be constructed. The latter result relies on the design of time-varying changes of coordinates which transform a linear system into a nonnegative one.

4) We considered continuous-time linear systems with additive disturbances and discrete-time measurements. First, we constructed a standard observer, which converges to the state trajectory of the linear system when the maximum time interval between two consecutive measurements is sufficiently small and there are no disturbances. Second, we constructed interval observers allowing to determine, for any solution, a set that is guaranteed to contain the actual state of the system when bounded disturbances are present [46].

6.10. New reduction model approach

Participants: Frederic Mazenc, Silviu Niculescu, Mounir Bekaik, Dorothee Normand-Cyrot [CNRS - L2S - Supelec], Claudio de Persis [Sapienza University of Rome], Miroslav Krstic [Univ. of California].

We considered several distinct problems entailing to the reduction model approach. Let us recall that this technique makes it possible to stabilize systems with arbitrarily large pointwise or distributed delay.

1) We proposed 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 [28], [50].

2) For linear systems with pointwise or distributed delays in the inputs which are stabilized through the reduction approach, we proposed a new technique of construction of Lyapunov-Krasovskii functionals. These functionals allow us to establish the ISS property of the closed-loop systems relative to additive disturbances [27], [49].

3) We proposed a solution to the problem of stabilizing nonlinear systems with input with a constant pointwise delay and state-dependent sampling. It relies on a recursive construction of the sampling instants and on a recent variant of the classical reduction model approach. The state feedbacks that are obtained do not incorporate distributed terms [43].

6.11. Analysis of neutral systems

Participants: Frederic Mazenc, Hiroshi Ito [Kyushu Institute of Technology].

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 [22], [45].

2) We extended the previous result to the problem of deriving the iISS property for dynamical networks with neutral, retarded and communication delay [41].

6.12. Hyperbolic systems

Participants: Frederic Mazenc, Christophe Prieur [GIPSA-Lab CNRS].

We considered a family of time-varying hyperbolic systems of balance laws. The partial differential equations of this family can be stabilized by selecting suitable boundary conditions. For the stabilized systems, the classical technique of construction of Lyapunov functions provides a function whose derivative along the trajectories of the systems may be not negative definite. In order to obtain a Lyapunov function with a negative definite derivative along the trajectories, we transform this function through a so-called "strictification" approach, which gives a time-varying strict Lyapunov function. It allows us to establish asymptotic stability in the general case and a robustness property with respect to additive disturbances of Input-to-State Stability type [32].

6.13. Time-varying systems with delay

Participants: Frederic Mazenc, Silviu Niculescu, Mounir Bekaik, Michael Malisoff [Departement of Mathematics - LSU].

1) We solved aproblem of state feedback stabilization of time-varying feedforward systems with a pointwise delay in the input. The approach 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 is illustrated through a tracking problem for a model for high level formation flight of unmanned air vehicles [48], [24].

2) We addressed the problem of stabilizing systems belonging to a family of time-varying nonlinear systems with distributed input delay through state feedbacks without retarded term. The approach we adopted is based on a new technique that is inspired by the reduction model technique. The control laws we obtained are nonlinear and time-varying. They globally uniformly exponentially stabilize the origin of the considered system. We illustrate the construction with a networked control system [25].

6.14. Positive invariance for time delay systems

Participants: Sorin Olaru [correspondent], Silviu Niculescu [CNRS (LSS)], Georges Bitsoris [University of Patras, Greece].

A new concept of positive invariance has been established in the original state space for discrete time dynamical systems. Furthermore, the necessary and sufficient algebraic condition for such properties have been derived allowing a direct test using basic linear programming arguments. In a recent work, the rigid positive invariance has been relaxed toward a cyclic invariant concept [18].

6.15. Predictive control for networked control systems

Participants: Sorin Olaru [correspondent], Silviu Niculescu [CNRS (LSS)], Warody Lombardi [INSA Lyon].

The work on the networked control system modeling lead to the establishement of a solid framework based on linear difference inclusion. Subsequently via set invariance and optimization based techniques, a design procedure has been proposed to deal with the real time constrained feedback control. Is worth to be mentioned that the robust feasibility and control performances are enforced via inverse optimality principles [19].

6.16. Reduced order H_∞-controllers synthesis with explicit constraints handling

Participants: Guillaume Sandou [correspondent], Gilles Duc [Suplec (E3S), Control Department], Mohamed Yagoubi [Ecole des Mines de Nantes].

Efficient dedicated methods have been developed for Hinfinity controller synthesis. However, such methods require translating the design objectives using weighting filters, whose tuning is not easy; in addition they lead to high order controllers which have to be reduced. Previous works have dealt with these two problems separately with the help of Particle Swarm Optimization: optimization of filter tunings for a full order synthesis and reduced order synthesis with fixed filters. In recent works, we have considered the solution to both problems in one shot. The constraints of the problem are explicitly taken into account in the synthesis problem, thanks to the use of Particle swarm optimization which does not require any specific expression for costs and constraints [63].

6.17. Robust optimization for energy management

Participants: Guillaume Sandou [correspondent], Philippe Dessante [Suplec (E3S), Energy Department], Marc Petit [Suplec (E3S), Energy Department].

The optimization of energy networks and the solution to Unit Commitment problems are one of the main collaborations between the Control and Energy Departments of Supelec. Robust optimization has been used to take into account the uncertainties which are observed on the consumer demand, the cost function, and the maximum capacity [66], [73].

6.18. Firefly optimization for the synthesis of controllers and the identification of systems

Participants: Guillaume Sandou [correspondent], Alfonso Goches Sanchez [Suplec (E3S), Control Department].

Firefly optimization is a new optimization algorithm which has appeared in 2009. This algorithm belongs to the class of metaheuristic algorithms. As such algorithms can optimized any cost and functions, firefly optimization has been tested for the optimization of PID controllers (with no reformulations of specifications) and the identification of nonlinear systems.

6.19. Receding horizon based controllers for the energy management in complex systems

Participants: Guillaume Sandou [correspondent], Sorin Olaru, Silviu Niculescu, Emmanuel Witrant [Gips-Lab, Grenoble].

The use of receding horizon based controllers is a good trend to extend the optimization results of a complex system in a closed loop framework. To prove the viability and the efficiency of the approach, several real life examples have been tested. Among them are the district heating networks and the mining ventilation system.

6.20. Particle Swarm Optimization for the optimization of feasibility domain volumes

Participants: Guillaume Sandou [correspondent], Mohamad-Taki Asghar [Suplec (E3S), Control Department].

It is a well-known fact that using mu-analysis for the computation of a guaranteed stability domain gives the largest hyper-rectangle included in the real stability domain (which is impossible to compute). However, the results strongly depend on the choice which has been made for the nominal system and the parameterization of the uncertainties. In this study, these choices are considered as optimization variables. The goal is now to find the best parameterization of the problem to get the largest stability domain. The optimization has been done using Particle Swarm Optimization.

6.21. Model of reaction networks

Participants: Georg Regensburger, Stefan Müller [RICAM, Linz].

In [100], we propose a notion of generalized mass action systems that could serve as a more realistic model for reaction networks in intracellular environments; classical mass action systems capture chemical reaction networks in homogeneous and dilute solutions. We show that several results of chemical reaction network theory carry over to the case of generalized mass action kinetics. Our main result gives conditions for the existence of a unique positive steady state for arbitrary initial conditions and independent of rate constants in this generalized setting. The conditions are formulated in terms of sign vectors (oriented matroids) of the stoichiometric and kinetic-order subspace and face lattices of related cones. We also give necessary and sufficient conditions for multistationarity, which is an important property in many applications, for example, in connection with cell differentiation.

6.22. Control of aircraft dynamics

Participants: Frederic Mazenc, Michael Malisoff [Departement of Mathematics - LSU], Aleksandra Gruszka [Departement of Mathematics - LSU].

We have worked on several models describing physical devices.

1) We studied a kinematic model that is suitable for control design for high level formation flight of UAVs [16], [40]. We designed controllers that give robust global tracking for a wide class of reference trajectories in the sense of input-to-state stability while satisfying amplitude and rate constraints on the inputs.

2) We studied feedback tracking problems for the planar vertical takeoff and landing (PVTOL) aircraft dynamics, which is a benchmark model in aerospace engineering. We provided a survey of the literature on the model. Then we constructed new feedback stabilizers for the PVTOL tracking dynamics. The novelty of our work is in the boundedness of our feedback controllers and their applicability to cases where the velocity measurements may not be available, coupled with the uniform global asymptotic stability and uniform local exponential stability of the closed loop tracking dynamics, and the input-to-state stable performance of the closed loop tracking dynamics with respect to actuator errors [15].

3) We solved a stabilization problem for an important class of feedback controllers that arise in curve tracking problems for robotics. Previous experimental results suggested the robust performance of the control laws under perturbations. Consequently, we used input-to-state stability to prove predictable tolerance and safety bounds that ensure robust performance under perturbations and time delays. Our proofs are based on an invariant polygon argument and a new strict Lyapunov function design [20].

6.23. Study of chemostat models

Participants: Frederic Mazenc, Michael Malisoff [Departement of Mathematics - LSU].

We provided a study of chemostat models in which two or more species compete for two or more limiting nutrients. First we considered the case where the nutrient flow and species removal rates and input nutrient concentrations are all given positive constants. In that case, we used Brouwer fixed point theory to give conditions guaranteeing that the models admit globally asymptotically stable componentwise positive equilibrium points. For cases where the dilution rate and input nutrient concentrations can be selected as controls, we used Lyapunov methods to prove that many different possible componentwise positive equilibria can be made globally asymptotically stable. We demonstrated our methods in simulations [23].

6.24. Modeling and control of Acute Myeloid Leukemia

Participants: José Luis Avila Alonso, 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 Niculescu, Hitay Özbay [Bilkent University, Ankara, Turkey], Ruoping Tang [INSERM Paris (Team18 of UMR 872) Cordeliers Research Centre and St. Antoine Hospital, Paris].

We have continued this year our work on modeling healthy and pathological hematopoiesis [36]. A. Ballesta has performed some experiments on patient fresh cell cultures in order to identify parameters of our model of acute myeloblastic leukemia (AML). To evaluate therapies, she also considered patient fresh cell cultures under anticancer drugs.

GECO Team

6. New Results

6.1. New results: geometric control

We start by presenting some results on the design of motion planning and tracking algorithms.

- In [10] we present an iterative steering algorithm for nonholonomic systems (also called driftless control-affine systems) and we prove its global convergence under the sole assumption that the Lie Algebraic Rank Condition (LARC) holds true everywhere. That algorithm is an extension of the one introduced in [65] for regular systems. The first novelty here consists in the explicit algebraic construction, starting from the original control system, of a lifted control system which is regular. The second contribution of the paper is an exact motion planning method for nilpotent systems, which makes use of sinusoidal control laws and which is a generalization of the algorithm described in [83] for chained-form systems.
- [6] and [5] are about motion planning for kinematic systems, and more particularly ε-approximations of non-admissible trajectories by admissible ones. This is done in a certain optimal sense. The resolution of this motion planing problem is showcased through the thorough treatment of the ball with a trailer kinematic system, which is a non-holonomic system with flag of type $(2, 3, 5, 6)$.

Application-oriented results about motion planning are contained in [15]. The paper proposes in particular a strategy for providing Unmanned Aerial Vehicles with a certain degree of autonomy, via autonomous planification/replanification strategies.

Let us list some new results in sub-Riemannian geometry and hypoellitpic diffusion.

- In [1] we study the Radon-Nikodym derivative of the spherical Hausdorff measure with respect to a smooth volume for a regular sub-Riemannian manifold . We prove that this is the volume of the unit ball in the nilpotent approximation and it is always a continuous function. We then prove that up to dimension 4 it is smooth, while starting from dimension 5, in corank 1 case, it is C^3 (and C^4 on every smooth curve) but in general not C^5. These results answer to a question addressed by Montgomery about the relation between two intrinsic volumes that can be defined in a sub-Riemannian manifold, namely the Popp and the Hausdorff volume. If the nilpotent approximation depends on the point (that may happen starting from dimension 5), then they are not proportional, in general.
- In [9] we study the Laplace–Beltrami operator on generalized Riemannian structures on orientable surfaces for which a local orthonormal frame is given by a pair of vector fields that can become collinear. Under the assumption that the structure is 2-step Lie bracket generating, we prove that the Laplace–Beltrami operator is essentially self-adjoint and has discrete spectrum. As a consequence, a quantum particle cannot cross the singular set (i.e., the set where the vector fields become collinear) and the heat cannot flow through the singularity.
- For an equiregular sub-Riemannian manifold M, Popp's volume is a smooth volume which is canonically associated with the sub-Riemannian structure, and it is a natural generalization of the Riemannian one. In [4] we prove a general formula for Popp's volume, written in terms of a frame adapted to the sub-Riemannian distribution. As a first application of this result, we prove an explicit formula for the canonical sub-Laplacian, namely the one associated with Popp's volume. Finally, we discuss sub-Riemannian isometries, and we prove that they preserve Popp's volume. We also show that, under some hypotheses on the action of the isometry group of M, Popp's volume is essentially the unique volume with such a property.

- In [21], for a sub-Riemannian manifold provided with a smooth volume, we relate the small time asymptotics of the heat kernel at a point y of the cut locus from x with roughly "how much" y is conjugate to x. This is done under the hypothesis that all minimizers connecting x to y are strongly normal, i.e. all pieces of the trajectory are not abnormal. Our result is a refinement of the one of Leandre $4t\log p_t(x,y)\to -d^2(x,y)$ for $t\to 0$, in which only the leading exponential term is detected. Our results are obtained by extending an idea of Molchanov from the Riemannian to the sub-Riemannian case, and some details we get appear to be new even in the Riemannian context. These results permit us to obtain properties of the sub-Riemannian distance starting from those of the heat kernel and vice versa. For the Grushin plane endowed with the Euclidean volume we get the expansion $p_t(x,y)\sim t^{-5/4}\exp\left(-d^2(x,y)/4t\right)$ where y is reached from a Riemannian point x by a minimizing geodesic which is conjugate at y. In [22] we investigate the small time heat kernel asymptotics on the cut locus on the class of two-spheres of revolution, which is the simplest class of 2-dimensional Riemannian manifolds different from the sphere with nontrivial cut-conjugate locus. We determine the degeneracy of the exponential map near a cut-conjugate point and present the consequences of this result to the small time heat kernel asymptotics at this point. These results give a first example where the minimal degeneration of the asymptotic expansion at the cut locus is attained.
- In [24] we studied normal forms for 2-dimensional almost-Riemannian structures. The latter 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. In [24] 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 analyse the cut locus from the singular set and we prove that it is not smooth either. A good candidate happens 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.

6.2. New results: quantum control

New results have been obtained for the control of the bilinear Schrödinger equation.

- In [16] we obtained a sufficient condition for approximate controllability of the bilinear discrete-spectrum Schrödinger equation exploiting the use of more than one control. The controllability result extends to simultaneous controllability, approximate controllability in H^s, and tracking in modulus. The result is more general than those present in the literature even in the case of one control and permits to treat situations in which the spectrum of the uncontrolled operator is very degenerate (e.g. multiple eigenvalues or presence of equal gaps among eigenvalues). These results are applied to the case of a rotating polar linear molecule in the space, driven by three external fields. A remarkable property of this model is the presence of infinitely many degeneracies and resonances in the spectrum preventing the application of the results in the literature.
- In [19] we present a constructive method to control the bilinear Schrödinger equation by means of

two or three controlled external fields. The method is based on adiabatic techniques and works if the spectrum of the Hamiltonian admits eigenvalue intersections, with respect to variations of the controls, and if the latter are conical. We provide sharp estimates of the relation between the error and the controllability time.

- In [18] we consider the minimum time population transfer problem for a two level quantum system driven by two external fields with bounded amplitude. The controls are modeled as real functions and we do not use the Rotating Wave Approximation. After projection on the Bloch sphere, we tackle the time-optimal control problem with techniques of optimal synthesis on 2-D manifolds. Based on the Pontryagin Maximum Principle, we characterize a restricted set of candidate optimal trajectories. Properties on this set, crucial for complete optimal synthesis, are illustrated by numerical simulations. Furthermore, when the two controls have the same bound and this bound is small with respect to the difference of the two energy levels, we get a complete optimal synthesis up to a small neighborhood of the antipodal point of the starting point.

6.3. New results: neurophysiology

- In [17] we study the global properties of an optimal control model of geometry of vision due to Petitot, Citti and Sarti. In particular, we consider the problem of minimizing $\int_0^L \sqrt{\xi^2 + K^2(s)}\, ds$ for a planar curve having fixed initial and final positions and directions. The total length L is free. Here s is the variable of arclength parametrization, $K(s)$ is the curvature of the curve and $\xi > 0$ a parameter. The main feature of the problem is that, if for a certain choice of boundary conditions there exists a minimizer, then this minimizer is smooth and has no cusp. However, not for all choices of boundary conditions there is a global minimizer. We study existence of local and global minimizers for this problem. We prove that if for a certain choice of boundary conditions there is no global minimizer, then there is neither a local minimizer nor a stationary curve (geodesic). We give properties of the set of boundary conditions for which there exists a solution to the problem. Finally, we present numerical computations of this set.
- In [2] we studied the general problem of reconstructing the cost from the observation of trajectories, in a problem of optimal control. It is motivated by the problem of determining what is the cost minimized in human locomotion. This applied question is very similar to the following applied problem, concerning HALE drones: one would like them to decide by themselves for their trajectories, and to behave at least as a good human pilot. These starting points are the reasons for the particular classes of control systems and of costs under consideration. To summarize, our conclusion is that in general, inside these classes, three experiments visiting the same values of the control are needed to reconstruct the cost, and two experiments are in general not enough. The method is constructive. The proof of these results is mostly based upon the Thom's transversality theory.

6.4. New results: switched systems

- In [12] we study the phenomenon of polynomial instability of switched systems. Stability properties for continuous-time linear switched systems are at first determined by the (largest) Lyapunov exponent associated with the system, which is the analogue of the joint spectral radius for the discrete-time case. We provided a characterization of marginally unstable systems, i.e., systems for which the Lyapunov exponent is equal to zero and such that there exists an unbounded trajectory. We also analyzed the asymptotic behavior of their trajectories. Our main contribution consists in pointing out a resonance phenomenon associated with marginal instability. In the course of our study, we derived an upper bound of the state at time t, which is polynomial in t and whose degree is computed from the resonance structure of the system. We also derived analogous results for discrete-time linear switched systems.
- The paper [13] is concerned with the stability of planar linear singularly perturbed switched systems of the type $\dot{x}(t) = \sigma(t)A_1^\epsilon x(t) + (1-\sigma(t))A_2^\epsilon x(t)$, where $\sigma : [0, +\infty) \to \{0, 1\}$, A_1^ϵ and A_2^ϵ are real matrices which represent singularly perturbed modes. By ϵ we denote here the parameter of

singular perturbation. We propose a characterization of the stability properties of such singularly perturbed switched systems based on the results given in [47]. More generally, we study transitions as ϵ varies and we restrict their number and nature. Finally, we compare the results obtained in this way with the Tikhonov-type results for differential inclusions obtained in the literature.

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

$$\sup_{y \in S} a(x,y) + u(y) = \lambda + u(x), \quad \forall x \in S, \tag{1}$$

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 [64], 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 :

$$u = \sup_{w \in \mathcal{M}_m} w + \mu_u(w) \quad , \tag{2}$$

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 (§6.1.4) 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 [64], 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 remarkable examples of metric spaces (§6.1.4) or 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.

Dans [116], on a établi des résultats de type Denjoy-Wolff pour l'étude asymptotique de la valeur d'un jeu répété, lorsque l'horizon tend vers l'infini. On s'intéresse pour cela plus généralement au "taux de fuite" $\rho(f) = \lim_{k\to\infty} d(x, f^k(x))/k$ où f est une application contractante au sens large pour une "métrique" d sur un espace X. Dans le cas des jeux, X est l'espace des fonctions continues sur l'ensemble des états, f est l'opérateur de Shapley, la métrique d est la norme sup (ou une métrique faible, non-symmétrique, comme $d(x, y) = \max_i (x_i - y_i)$), et $\rho(f)$ représente le maximum du paiement moyen quand l'état initial varie. On a montré, que si l'espace X est de courbure négative en un sens faible (Busemann), alors il existe une horofonction h telle que $h \circ f \geq h + \rho(f)$. Ceci entraîne par exemple, lorsque l'espace d'état est compact, l'existence d'un état dont la valeur croît linéairement avec un taux $\rho(f)$, lorsque l'horizon croît. On a travaillé cette année à la généralisation de ce résultat au temps continu (semigroupes associés à des équations d'Hamilton-Jacobi-Isaacs).

Par ailleurs, dans un travail avec J. Bolte (eprint récent [43]), on s'est intéressé, dans le cas où X est de dimension finie, à l'existence de la limite $\lim_k f^k(x)/k$ (vecteur de paiement moyen). On montre que cette 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

In [116], we established Denjoy-Wolff type results for the asymptotic behaviour of the value of a zero-sum game, when the horizon tends to infinity. To this end, we consider more generally the "escape rate" $\rho(f) = \lim_{k\to\infty} d(x, f^k(x))/k$ where f is a nonexpansive self-map of a "metric" space (X, d). In the case of games, X is the space of continuous functions on the set of states, f is the Shapley operator, and d is the sup-norm (or a weak, non-symmetric, metric like $d(x, y) = \max_i (x_i - y_i)$), and $\rho(f)$ represents the "maximal mean payoff", the maximum being taken over all possible initial states. We showed that if the space X is of nonpositive curvature in a mild sense (Busemann), then, there exists a horofunction h such that $h \circ f \geq h + \rho(f)$. This implies in particular, when the space state is compact, the existence of an initial state from which the value grows linearly with a rate $\rho(f)$, as a function of the horizon. We worked this year on the generalisation of this result to the continuous time case (semigroups associated to Hamilton-Jacovi-Isaacs PDE).

Moreover, in a joint work with J. Bolte (recent eprint [43]), we considered the case in which X is finite dimensional, and studied the existence of the limit $\lim_k f^k(x)/k$ (mean payoff vector). We showed 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 étudions le groupe des isométries pour la métrique de Hilbert. De La Harpe [181] a donné plusieurs conjectures relatives à ce groupe. Nous conjecturons 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. Nous avons démontré précédemment cette conjecture lorsque le domaine est un polytope [135].

Dans le cas général, on peut prouver, en utilisant les horo-fonctions, que si il existe une bijection entre deux cônes homogéne de degré -1, antitone, et d'inverse antitone, ces deux cônes sont symétriques. Nous essayons maintenant de montrer que toute isométrie de Hilbert sur un domaine convexe est la version projective d'un automorphisme linéaire du cône sur le domaine, ou d'une bijection du cône, homogéne de degré -1, qui est antitone et d'inverse antitone. Ce résultat pemettrait de compléter la preuve de la conjecture proposée plus haut.

L'état actuel de l'étude de ce problème est résumé dans un article de Walsh [41] (chapître d'un "handbook on the Hilbert geometry" à paraître).

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 investigating the isometries of the Hilbert geometry. De La Harpe [181] has previously made several conjectures about the isometry group of this space. We conjecture 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. We have previously proved that this conjecture is true in the case of a polytope domain [135].

In the general case, we can now prove, using horofunctions, that if a bijection between cones is homogeneous of degree -1, order inverting, and has an order inverting inverse, then both cones are symmetric. We are working on showing that every Hilbert isometry on a convex domain arises by considering projectively either a linear automorphism on the cone over the domain, or a homogeneous -1, order inverting bijection on this cone with order inverting inverse. Establishing this result would complete our proof of the above conjecture.

The current state of knowledge about this problem has been summarized in a paper by Walsh [41] that will appear as a chapter in a forthcoming handbook on the Hilbert geometry.

6.1.4. Espace de Teichmüller/Teichmüller space

Participant: Cormac Walsh.

L'espace de Teichmüller d'une surface est un espace métrique composé des structures conformes de cette surface. On peut le voir comme l'ensemble des classes d'équivalence des métriques riemanniennes de cette surface, où deux métriques sont équivalentes si il existe une application conforme homotope à l'identité qui envoie l'une des métriques sur l'autre.

Il existe plusieurs métriques naturelles sur l'espace de Teichmüller. Nous avons travaillé précédemment sur la métrique Lipschitz de Thurston et avons prouvé [174] que l'horo-frontière de cet espace métrique était la frontière de Thurston.

Néanmoins, la métrique la plus utilisées ur l'espace de Teichmüller est la métrique de Teichmüller. L'horo-frontière de cet espace métrique n'est autre que la frontière déja introduite dans la littérature sous le nom de frontière de Gardiner–Masur. Nous étudions cette frontière, en particulier nous donnons explicitement ses points de Busemann [55].

Par la suite, nous avons l'intention d'utiliser cette propriété afin d'étudier les sous-groupes du groupe modulaire, qui est le groupe des isométries de la métrique de Teichmüller.

English version

An interesting metric space is the Teichmüller space of a surface. This is the space of conformal structures on the surface. One may think of it as the space of equivalence classes of Riemannian metrics on the surface, where two such metrics are regarded as being equivalent if there is a conformal map on the surface taking one to the other that is homotopic to the identity.

There are several natural metrics on Teichmüller space. Previously, we have worked with Thurston's stretch metric and have shown [174] that the horofunction boundary with this metric is just the usual Thurston boundary.

However, the most commonly used metric on Teichmüller space is Teichmüller's metric. The horofunction boundary of this metric space turns out to be the same as a previously defined boundary, called the Gardiner–Masur boundary. We have been investigating this boundary. In particular, we have managed to work out explicitly its Busemann points [55].

In future work, we intend to apply this knowledge to study subgroups of the mapping class group, which is the isometry group of the Teichmüller metric.

6.1.5. Consensus non-commutatif et contraction d'opérateurs de Kraus/Noncommutative consensus and contraction of Kraus maps

Participants: Stéphane Gaubert, Zheng Qu.

Dans un travail récent [44], 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),

$$\kappa(P) := 1 - \min_{i,j} \sum_{s=1}^{n} \min(P_{is}, P_{js}).$$

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

$$T(x) = \sum_k a_k x a_k^* \qquad \text{avec} \qquad \sum_k a_k a_k^* = I \ .$$

English version

In a recent work [44], 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

$$T(x) = \sum_k a_k x a_k^* \qquad \text{with} \qquad \sum_k a_k a_k^* = I \ .$$

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 [98]. 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 [68], [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.* [147]). 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 [67] et aux systèmes à événements discrets [101], dans lesquelles la manipulation de tels polyèdres est le goulot d'étranglement.

Dans un travail de X. Allamigeon, S. Gaubert, et R. Katz [69], on étend le théorème de McMullen au cas tropical: ce dernier caractérise le nombre maximal de points extrêmes d'un polyèdre, en fonction du nombre d'inégalités qui le définissent et de sa dimension. Nous montrons que la même borne est valide dans le cas tropical (à une modification triviale près). Cependant, le calcul de la borne optimale est encore ouvert dans ce cas.

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 [112]. Dans un travail réalisé par X. Allamigeon et R. Katz [48], et effectué en partie lors d'une visite de R. Katz à Inria (juillet 2011), 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 [98]. 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 (débuté lors d'une visite de ce dernier à Inria en novembre 2012), 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 [99]. Celle-ci assure qu'étant donné un polytope tropical pur, il existe un polytope *lift* sur les séries de Puiseux, dont les demi-espaces associés aux faces se "tropicalisent" en une représentation par demi-espaces du polytope tropical initial.

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 [98]. 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.* [147]). 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 [67] and discrete event systems [101], in which computing such polyhedra turns out to be the bottleneck.

In a work of X. Allamigeon, S. Gaubert, and R. Katz [69], we extend the McMullen upper bound theorem to the tropical case. This theorem characterises the maximal number of extreme points of a polyhedron, as a function of the number of inequalities defining it, and of the dimension. We show that the same bound is valid in the tropical case (up to a trivial modification). However, computing the optimal bound is an open problem in this case.

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 [112]. In a work of X. Allamigeon and R. Katz [48], partly done during the visit of R. Katz at Inria (July 2011), 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 [98]. 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 (started during a visit of the latter at Inria in Novembre 2012), 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 [99]. 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.

6.2.2. Convexes max-plus et jeux avec paiements ergodiques/Max-plus convex sets and mean payoff games

Participants: Marianne Akian, Xavier Allamigeon, Stéphane Gaubert, Alexander Guterman [Moscow State University], Ricardo Katz [Conicet, Argentine], Sergei Sergeev [Birmingham, UK].

Dans un travail d'Akian, Gaubert et Guterman [15], on a montré un résultat d'équivalence entre les jeux ergodiques à somme nulle et les systèmes d'inégalités max-plus linéaires: décider la non-vacuité d'un polyèdre tropical est équivalent à vérifier si un jeu déterministe à somme nulle a un paiement moyen par unité de temps positif ou nul. Plus généralement, la même question pour un jeu stochastique à somme nulle est équivalente à vérifier si un convexe tropical (non-polyédral, i.e., défini par un système infini d'inégalités) est vide. Ces résultats sont démontrés à l'aide de techniques de théorie de Perron-Frobenius non-linéaire. Ils sont ensuite appliqués à l'étude de l'indépendance linéaire dans le semi-anneau tropical.

Le résultat de [15] a eu plusieurs retombées.

Dans un travail de Gaubert et Sergeev [24], on réduit le problème spectral tropical de type faisceaux, $Ax = \lambda Bx$, à un jeu paramétrique (ce qui permet de calculer le spectre en temps pseudo-polynômial).

Enfin, dans un travail de Gaubert, Katz, et Sergeev [22], on développe un algorithme de programmation linéaire tropicale (pseudo-polynômial) basé sur cette correspondance avec les jeux répétés.

English version

In a work by Akian, Gaubert and Guterman [15], we showed the equivalence mean payoff games and max-plus linear inequalities: testing whether a tropical polyhedron is non-empty is equivalent to checking whether a mean payoff deterministic game is winning. More generally, checking whether a mean payoff stochastic game is winning is equivalent to checking the non-emptyness of a tropical convex set defined by an infinite family of inequalities. These results are established using techniques of non-linear Perron-Frobenius theory. Then, they are applied to the study of linear independence over the tropical semiring.

The equivalence established in [15] had several consequences.

In a work of Gaubert and Sergeev [24], the tropical spectral problem for matrix pencils, $Ax = \lambda Bx$, is reduced to a parametric game (which allows one to compute the spectrum in pseudo-polynomial time).

Finally, in a work of Gaubert, Katz, and Sergeev [22], a (pseudo-polynomial) tropical linear programming algorithm is developed, based on the same correspondence with mean payoff games.

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

$$\max(a, b) \leq \epsilon \log(e^{a/\epsilon} + e^{b/\epsilon}) \leq \epsilon \log(2) + \max(a, b) \quad . \tag{3}$$

L'utilisation de ces propriétés a déjà conduit dans le passé aux travaux sur les perturbations de valeurs propres [60], [59], [58], ou sur les grandes déviations [1], [62]. 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 [60], [59], [58], or on large deviations [1], [62]. 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 [LRI, Paris Sud].

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 [58], [59], on montrait notamment que l'ordre de grandeur des valeurs propres d'un faisceau matriciel est donné (sous des conditions de non-dégénerescence) 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 [47], qui a été présenté dans [36]. 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 [58], [59], we shown 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 [47], which has been presented in [36]. Now we compute the order of magnitude of the eigenvalues of a matrix polynomial by using the tropical roots of the polynomial the coefficients of which are obtained by applying a norm to the coefficients of the 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.

Lors de son stage de M2 dans l'équipe, Andrea Marchesini a obtenu 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 [108] 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 [59] ou les idées de Murota [148].

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.

English version

During his M2 internship in the team, Andrea Marchesini has obtained 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 [108] 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 [59] or ideas of Murota [148].

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.

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 en novembre 2011, 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. Paul Poncet donnait en particulier une caractérisation des mesures maxitives régulières à valeurs dans un domaine, qui raffinait le théorème de décomposition des mesures maxitives établi dans [153]. Ces résultats font maintenant l'objet de [54].

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. Un article concernant le cas des semi-treillis [53] a été soumis.

Enfin la troisième et dernière partie qui traitait des semi-groupes inverses dans une tentative d'unification de l'algèbre usuelle et de l'algèbre tropicale fait l'objet de l'article [31].

On sait que les résultats sur les convexes tropicaux de dimension infinie de [154], qui se déduisent soit des résultats correspondants sur les semi-treillis, soit de résultats de théorie des mesures maxitives de la première partie de la thèse [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 in November 2011, 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. Paul Poncet gave in particular a characterization of domain valued maxitive measures that are regular, which improved the decomposition theorem of maxitive measures stated in [153]. These results are now gathered in [54].

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. A manuscript concerning the case of semilattices [53] has been submitted.

The third and last part which studied inverse semigroups in an attempt to unify usual and tropical algebras is presented in [31].

We know that the results on infinite dimensional tropical convex sets of [154], which are deduced either from the corresponding results on semilattices, or from the results on maxitive measures of the first part of the thesis manuscript, 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. Méthodes multigrilles pour le contrôle stochastique et les jeux répétés à somme nulle/Multigrid methods for stochastic control and repeated zero sum games

Participants: Marianne Akian, Sylvie Detournay.

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 [87]. 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.

Or, la méthode multigrille est l'une des rares méthodes permettant de résoudre, au moins dans les bons cas, des systèmes linéaires en un temps de l'ordre de la taille du système. De plus, alors que la méthode multigrille classique ne s'applique qu'à des discrétisations d'équations aux dérivées partielles elliptiques, la méthode multigrille algébrique (voir par exemple [164]) peut s'appliquer à tout système linéaire présentant des propriétés de monotonie (principe du maximum ou système avec M-matrice).

L'association entre méthodes multigrilles et itérations sur les politiques avait déjà été utilisée et étudiée dans le cas de problèmes de contrôle stochastique actualisé (voir par exemple [57], [65]), ainsi que dans le cas d'un algorithme d'itération sur les politiques simplifié pour le contrôle ergodique (voir par exemple [5]), mais pour lequel il n'existe pas de preuve de convergence. La méthode multigrille algébrique avait été récemment associée à des méthodes d'apprentissage (voir par exemple [180]). Nous l'avions aussi testée dans le cas de l'itération sur les politiques pour des problèmes de jeux à somme nulle actualisés au cours du stage de Shantanu Gangal en 2007.

La thèse de Sylvie Detournay a eu pour but 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 [87] et une méthode multigrille algèbrique, afin de résoudre des problèmes de jeux à somme nulle dégénérés, éventuellement posés directement sous forme discrète. Au cours de sa thèse, Sylvie Detournay a codé l'ensemble des algorithmes en C, en faisant appel éventuellement à des librairies existantes en particulier les méthodes multigrilles algèbriques d'Yvan Notay. L'ensemble des codes nouveaux est déposé sur le projet "pigames" de la gforge et sera disponible librement.

Une première partie de la thèse [11] qui a été publiée dans [14] concerne le cas non dégénéré (actualisé). Elle comprend en particulier des tests sur des discrétisations d'équations aux dérivées partielles d'Hamilton-Jacobi-Bellman ou d'Isaacs, ou d'inéquations variationnelles.

Le reste de la thèse concerne le cas de problèmes avec critère moyen en temps. Sylvie Detournay a en particulier implémenté et raffiné l'algorithme proposé par Cochet-Terrasson et Gaubert [87], 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 [87], et avec les détails d'implémentation) et les preuves de sa convergence sont regroupés dans le manuscrit [45] écrit avec Jean Cochet-Terrasson et Stéphane Gaubert.

Ces travaux ont aussi conduit à l'introduction dans [11] d'une nouvelle méthode multigrille multiplicative pour le calcul de la mesure invariante de chaînes de Markov irréductibles, qui consiste en l'application de l'algorithme d'itération sur les politiques combiné aux méthodes multigrilles algèbriques au problème de contrôle optimal (à un joueur) avec critère moyen en temps obtenu par transformation log-exp du système linéaire initial. Cette méthode a été testée et comparée aux méthodes multigrilles multiplicatives existantes.

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 [87]. 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.

For the solution of large size linear systems, the state of art consists of multigrid methods which are often able to solve systems in linear time. Whereas multigrid methods can only be applied to systems that come from discretizations of elliptic partial differential equations, algebraic multigrid methods (see for instance [164]) can be applied to any linear system with monotonicity properties (discrete maximum principle or system with a M-matrix).

The association of multigrid methods with policy iteration has been used and studied in the case of discounted stochastic control problems (see for instance [57], [65]), or in the case of a simplified policy iteration algorithm for ergodic control (see for instance [5]), but for which no proof of convergence is known. Some recent work combines the algebraic multigrid method with learning methods [180]. We also tested it in the case of policy iterations for discounted zero-sum two-player games, during the internship of Shantanu Gangal in 2007.

The aim of the PhD thesis of Sylvie Detournay was to develop and study 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 [87] and an algebraic multigrid method (AMG). During her thesis, Sylvie Detournay coded all algorithms in C, using eventually existing librairies in particular the algebraic multigrid libray of Yvan Notay. All new algorithms belong to the gforge project “pigames” and will be distributed openly.

A first part of the thesis manuscript [11], which has published in [14], concerns the nondegenerate (discounted) case. It contains in particular some tests on discretisations of Hamilton-Jacobi-Bellman or Isaacs partial differential equations or variational inequalities.

The rest of the thesis concerns the case of problems with mean-payoff criteria. In particular, Sylvie Detournay has implemented and refined the algorithm proposed by Cochet-Terrasson and Gaubert [87], 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 [87], with implementation details), and convergence proofs are gathered in the article [45] with Jean Cochet-Terrasson and Stéphane Gaubert.

These works also led to the introduction in [11] of a new multiplicative AMG method for computing invariant measures of irreducible Markov chains. This method consists of the application of the policy iteration algorithm combined with AMG method to the optimal control (or one player) problem with mean-payoff criteria obtained after a log-exp transformation of the initial linear system. It has been tested and compared with previous multiplicative AMG methods.

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 [67], [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, M. Joswig et S. Gaubert, nous nous intéressons aux problèmes de programmation linéaire tropicale. Nous définissons un analogue tropical de la méthode du simplexe. L’algorithme repose sur une technique de pivotage entièrement combinatoire entre deux points de base, se fondant sur la notion d’hypergraphes tangents.

English version

X. Allamigeon, S. Gaubert, and E. Goubault, have developed in [67], [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, M. Joswig and S. Gaubert, we study the problems of tropical linear programming. We define a tropical analog of simplex algorithm. It relies on a pivoting technique between two basis points, which is entirely combinatorial, and which involves the notion of tangent hypergraphs.

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 [17], 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], [176], [175], [156], [157], [158], [103], [74], 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 [17], 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], [176], [175], [156], [157], [158], [103], [74], 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, porte sur le développement de méthodes tropicales en programmation dynamique approchée.

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 [114]. 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 $d_T(A, B) = \| \log \operatorname{spec} (A^{-1}B) \|_\infty$, 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 [51] 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 réalisée récemment par Z. Qu.

English version

The PhD work of Zheng Qu is supervised by S. Gaubert and S. Tang, it aims in particular at developing tropical methods in approximate dynamic programming.

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 [114]. 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 $d_T(A,B) = \| \log \operatorname{spec}(A^{-1}B)\|_\infty$, 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 [51] 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 applied recently these results to the analysis of a method of reduction of the curse of dimensionality, introduced by McEneaney.

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 [40], [18], [77] 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 [106].

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 [40], [18], [77] 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 [106].

6.5.3. Équations aux dérivées partielles en dynamique des populations/Partial differential equations arising in population dynamics

Participants: Sepideh Mirrahimi, Stéphane Gaubert.

Nous étudions la limite en temps long de dynamiques des populations structurées. Il s'agit de l'étude asymptotique de l'équation suivante

$$\partial_t n_\varepsilon - \varepsilon \Delta n_\varepsilon = \frac{n_\varepsilon}{\varepsilon} R(x, I_\varepsilon), \quad I_\varepsilon(t) := \int \psi(x) n_\varepsilon(x,t) dx. \tag{4}$$

Il est connu qu'asymptotiquement, lorsque le taux de mutation est petit et en temps long, la solution de cette équation se concentre en une masse de Dirac en un point de maximum de $R(\cdot, I_M)$, avec $I_M = \lim_{t\to\infty} \lim_{\varepsilon\to 0} I(t)$. Un tel point s'appelle ESS (Evolutionary stable strategy) en dynamiques adaptatives. On s'intéresse à savoir, dans le cas où le problème admet plusieurs ESS (qui correspondent à des points de maximum de R), vers quel ESS la densité va converger en temps grand. Nous essayons de répondre à cette question en supposant que le taux de mutations est important (comme dans le cas des cellules cancéreuses). Nous voudrions déterminer la limite suivante: $\lim_{\varepsilon\to 0} \lim_{t\to\infty} n_\varepsilon(x,t)$. Une conjecture est que la limite est une masse de Dirac en un point x_M où x_M est le point de maximum de $R(\cdot, I_M)$ au voisinage duquel $R(x, I_M)$ est plus plat (une fonction F dépendant de la hessienne de R est maximisée en x_M). Celle-ci est motivée d'une part par un travail de M. Akian, R. Bapat et S. Gaubert, montrant à l'aide d'outils de théorie spectrale max-plus qu'une propriété analogue est vraie en dimension finie (convergence du vecteur propre de Perron de matrices dont les coefficients sont de la forme $\exp(A_{ij}/\varepsilon)$), et d'autre part par des travaux reliés en théorie de KAM faible (les points de maximum de R correspondent à l'ensemble d'Aubry projeté). L'objectif est donc ici de déterminer quel vecteur propre du problème ergodique est sélectionné à la limite visqueuse.

Nous avons déjà identifié la limite lorsque le taux de mutations tend vers 0 ($\varepsilon \to 0$) en partant de la solution stationnaire de (12). Il nous reste à démontrer que la solution de (12) converge en temps long vers la solution stationnaire. L'analogue discret de ce problème est également une question ouverte à laquelle on s'intéresse.

English version

We study the long-time asymptotic behaviour of structured population models. We consider specially the PDE (12). It is known that asymptotically, when the mutation rate is small, and the time horizon is large, the solution of this equation concentrates to a Dirac mass at a maximum point of $R(\cdot, I_M)$, with $I_M = \lim_{t\to\infty} \lim_{\varepsilon\to 0} I(t)$. Such a limit point is called ESS (Evolutionary stable strategy) in the field of adaptative dynamics. We are interested to know, when there are several ESS (corresponding to several points of maximum of R), to which ESS the density will converge as the horizon tends to infinity. We are studying this question in particular when the mutation rate is large (as in the case of tumor cells), leading to compute the following limit: $\lim_{\varepsilon\to 0} \lim_{t\to\infty} n_\varepsilon(x,t)$. We made a conjecture that the limit is a Dirac mass at a point x_M where among the points of maximum of $R(\cdot, I_M)$, x_M is the one at which $R(x, I_M)$ is the "flatest" (an auxiliary function F depending on the Hessian of R is maximized at point x_M). This is motivated on the one hand by a previous work of M. Akian, R. Bapat and S. Gaubert, showing, through max-plus spectral theory, that an analogous property does hold in finite dimension (convergence of the Perron eigenvector of matrices with coefficients $\exp(A_{ij}/\varepsilon)$), and on the other hand, by related works in weak KAM theory (the points of maximum of R correspond to the projected Aubry set); these works determine the eigenvector of the ergodic problem which is selected by the viscous limit.

We already identified the limit when the mutation rate tends to 0 ($\varepsilon \to 0$), starting from the stationnary solution of (12). We still need to show that the solution of (12) does converge in large time to the stationnary solution. Even the discrete analogue of this problem is an open issue, which we are studying.

6.5.4. Analyse statique de programmes et itération sur les politiques/Static analysis of computer programs and policy iteration

Participants: Assale Adjé [LSV, ENS Cachan], Stéphane Gaubert, Eric Goubault [CEA].

On applique ici des méthodes de théorie des jeux et d'optimisation (analyse convexe abstraite, programmation convexe et non convexe) aux problèmes de point fixe intervenant en analyse statique de programme. On a introduit dans [13] un nouveau domaine en analyse statique, qui étend au cas non-linéaire le domaine des "gabarits" introduit par Manna, Sankaranarayanan, and Sipma [166]. Ce domaine permet de représenter des ensembles accessibles non-convexes (définis par un nombre fini d'inégalités prises dans un dictionnaire). Ceci permet d'intégrer en particulier des informations liées à l'existence de fonctions de Lyapunov, qui sont souvent connues dans les applications issues de l'ingénierie. Nous avons montré dans [13] que des invariants (expérimentalement précis) pouvaient être obtenus en couplant l'itération sur les politiques avec des relaxations de Shor (relaxations SDP de problèmes quadratiques non-convexes), ce qui fournit des abstractions précises de certains programmes numériques (ex: filtres avec seuils).

Un problème important consiste à déterminer le plus petit point fixe (l'algorithme de [13] fournit un point fixe, qui peut ne pas être minimal). Ce problème est abordé dans [26], où l'approche de [13] est comparée avec une approche duale développée par Gawlitza et Seidl.

English version

We apply methods from game theory and optimization (generalized duality, convex and non convex programming) to the fixed point problems arising in static analysis of programs by abstract interpretation. We introduced in [13] a new domain in static analysis, which extends to nonlinear cases the "templates" introduced by Manna, Sankaranarayanan, and Sipma [166]. This domain allows one to represent accessible sets that are non convex. These are defined by finitely many inequalities taken from a dictionnary. This allows one to use in particular the information provided by Lyapunov functions, which are often known in applications arising from engineering. We showed in [13] that experimentally accurate invariants can be obtained by coupling policy iteration with Shor relaxation (SDP relaxation of convex programming problems). This yields accurate abstractions of some numerical programs, like linear filters with thresholds.

An important problem consists in determining the smallest fixed point (the algorithm of [13] yields a possibly non minimal fixed point). This problem is addressed in [26], in which the approach of [13] is compared with a dual approach developed by Gawlitza and Seidl.

6.5.5. Optimisation du référencement sur la toile/Optimization of web referencing

Participants: Marianne Akian, Mustapha Bouhtou [Orange Labs], Olivier Fercoq, Stéphane Gaubert.

La thèse d'O. Fercoq [12], co-encadrée par M. Akian, M. Bouhtou, et S. Gaubert, financée par un CRE d'Orange Labs, avait pour but d'appliquer des méthodes d'optimisation et de théorie des jeux à l'optimisation de services en lignes. On a tout d'abord étudié le problème de l'optimisation du référencement, que l'on formalise en se donnant par exemple un ensemble d'hyperliens et de ressources obligatoires, dont la nature et la position sur le site web sont déterminées à l'avance par le concepteur. Cet ensemble forme en quelque sorte le squelette du site web. On se donne aussi un ensemble d'hyperliens ou de ressources facultatives, pour lesquels le concepteur du site a certains degrés de liberté (le lien ou le contenu peut être mis sur une page plutôt qu'une autre, voire être omis).

Dans [20], on aborde le problème de l'optimisation du "Pagerank" dans ce cadre, en appliquant des techniques de décision Markovienne classiques et sous-contraintes. Le problème peut en effet se ramener à un problème de contrôle ergodique ou de contrôle ergodique sous contraintes (ergodiques), selon que les contraintes sur les hyperliens sont locales à chaque page ou font intervenir plusieurs pages. On traite à la fois le cas relaxé où les probabilités de passage d'une page à une autre peuvent être des réels positifs quelconques (on peut par exemple supposer que cette probabilité dépend de la position et des caractères utilisés pour l'hyperlien correspondant) et le cas discret où ces probabilités sont uniformes parmis celles qui sont strictement positives (comme dans la modélisation classique conduisant au calcul du Pagerank). On montre que cette famille de problèmes correspondent à des problèmes de programmation dynamique avec un nombre exponentiel de contrôles, mais où les polytopes des mesures de probabilités de transition admettent des oracles de séparation polynômiaux. On obtient de la sorte des résultats de complexité, ainsi que, sous certaines hypothèses, des algorithmes adaptés à des instances de grande taille, couplant programmation dynamique et relaxation Lagrangienne. Ces algorithmes ont été testés sur un fragment du graphe du web.

Un critère de référencement classique, alternatif au pagerank, est donné par le vecteur propre de Perron, comme dans le cas de l'algorithme "HITS" de Kleinberg. O. Fercoq a abordé le problème associé d'optimisation du référencement, qui se révèle plus difficile que celui du pagerank, en raison de l'absence de propriété de convexité. Cependant, il a développé un algorithme rapide et creux (basé sur des propriétés de rang 1 d'opérateurs intervenant dans le calcul de dérivées du critère) permettant de calculer un optimum local du référencement [106].

O. Fercoq a aussi donné un algorithme analogue pour optimiser le score "HOTS" de Tomlin [38]. Cependant, la convergence de l'algorithme original de HOTS n'avait jamais été prouvée. Dans [50], O. Fercoq a identifié le taux de convergence de l'algorithme et de plusieurs de ses variantes grâce à des techniques d'applications contractantes au sens large et aux propriétés des problèmes de flot d'entropie maximale dans un réseau.

La thèse de Fercoq comprend aussi un algorithme de classement permettant de déterminer les pages de Spam parmi un ensemble de pages douteuses, supposant connues un autre ensemble de pages repertoriées comme spam [33]. Cet algorithme exploite les techniques développées pour l'optimisation du PageRank [33].

English version

The goal of the PhD work [12] of O. Fercoq, cosupervised by M. Akian, M. Bouhtou, and S. Gaubert, and supported by a research contract (CRE) of Orange Labs, was to apply optimization and game theory methods to the optimization of online services. We started by investigating the problem of the optimization of referencing, which we modelled by considering a family of compulsory hyperlinks and resources (fixed in advance by the website designer, these constitute the "skeletton" of the website) and also a family of facultative hyperlink or resources (some links may be ommited or some other links may be added).

In [20], we are approaching the problem of the pagerank optimization in this framework, by applying usual and constrained Markov decision processes techniques. This problem can indeed be reduced to an ergodic control problem without or with (ergodic) constraints, depending on the fact that hyperlinks constraints are local to each web page or depend on several web pages. We study the relaxed problem where the transition probabilities from one page to another may be any positive real (one may assume for instance that this probability depends on the position and type used for the corresponding hyperlink), as well as the discrete problem where these probabilities are uniform among the positive ones (as in the usual modelisation leading to the Pagerank). We show that these problems can be reduced to dynamic programming problems with exponentially many discrete actions, in which however the polytopes of transition probability measures admit polynomial time separation oracles. We derive from this approach polynomial time complexity results, as well as under some additional assumption, scalable algorithms (adapted to large web graphs), coupling dynamic programming and Lagrange relaxation. The latter have been tested on a real subgraph of the web.

A classical alternative ranking relies on the Perron eigenvector, as in the case of the algorithm "HITS" by Kleinberg. O. Fercoq treated the associated optimisation problem, which turns out to be harder than in the pagerank case, due to the lack of convexity properties. However, he developed a fast (sparse) algorithm, exploiting the rank 1 properties of operators appearing when computing the derivative of the objective function, allowing one to compute a local optimum [106].

O. Fercoq also developed a similar method to optimize Tomlin's "HOTS" score [38]. However, the convergence of the original HOTS algorithm was not proved. In [50], O. Fercoq has computed the convergence rate of the algorithm and of several of its variants, using techniques of nonexpansive mappings and properties of problems of flow with maximal entropy in a network.

The PhD thesis of Fercoq also comprises a ranking algorithm allowing one to detect spam pages [33] among dubious pages, starting from a seed (set of pages which are surely known to be spam). This algorithm relies on the Pagerank optimization techniques of [33].

6.5.6. Gestion du revenu appliquée à la tarification de services données/Yield management applied to pricing of data services

Participants: Mustapha Bouhtou [Orange Labs], Jean-Baptiste Dumont, Stéphane Gaubert.

Le travail de thèse CIFRE de J-B. Dumont, supervisée par M. Bouhtou et S. Gaubert, porte sur la tarification de services data et la gestion des ressources dans les réseaux mobiles. Celle-ci est abordée à l'aide de techniques de contrôle et d'optimisation stochastique. Dumont a développé un modèle de tarification, permettant d'analyser des mécanismes incitant les clients à reporter leur demande en dehors des periodes les plus chargées.

English version

The CIFRE PhD work of J-B. Dumont is jointly supervised by M. Bouhtou and S. Gaubert. It deals with the pricing of data services and resource allocation in mobile networks. This is addressed through stochastic control and stochastic optimization techniques. Dumont developed a model of pricing, in order to analyse incitations for customers to move their demand from loaded to less loaded time periods.

6.5.7. Vérification de systèmes temps-réels/Verification of real-time systems

Participants: Xavier Allamigeon, Uli Fahrenberg [IRISA], Stéphane Gaubert, Ricardo Katz [Conicet], Axel Legay [IRISA], Søren Ravn [Aalborg University].

Dans [140], 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 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.

Un autre problème important survenant dans cette application est l'élimination rapide de vecteurs linéairement dépendants (au sens tropical). Pendant son stage à Inria et au CEA (avril-juillet 2012) supervisé par X. Allamigeon, S. Gaubert et E. Goubault, S. Ravn a implémenté un algorithme dont la complexité est reliée à la taille du résultat (*output-sentive complexity*). Il a également implémenté une interface entre la bibliothèque TPLib et l'outil VerifyTAPN (https://launchpad.net/verifytapn).

English version

Lu, Madsen, Milata, Ravn, Fahrenberg and Larsen have shown in [140] 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 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.

Another important problem arising in this application is the fast elimination of linearly dependent vectors (in the tropical sense). During its internship at Inria and CEA (April-July 2012) supervised by X. Allamigeon, S. Gaubert and E. Goubault, S. Ravn has implemented an output-sensitive algorithm to eliminate such vectors. He has also implemented an interface between the library TPLib and the model-checker VerifyTAPN (https://launchpad.net/verifytapn).

MCTAO Team

5. New Results

5.1. 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.

5.1.1. 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, feedback classification in relation with the relaxation times of the species. This activity has been the object of two publications [5], [4], and a conference talk [14] on feedback classification in the contrast problem, that will be followed by a journal article.

John Marriott will defend his Phd thesis on this topic, august 28, 2013; This will be followed by a two day conference on quantum control systems with applications, supported by a NSF grant and by the Engineering Department (P.E. Crouch).

5.1.2. Experimental aspects

Participants: Bernard Bonnard, Olivier Cots, Dominique Sugny [Univ. de Bourgogne], Steffan Glaser [TU München].

As said in section 4.2 , our work on this problem is based on experiments conducted in Prof. S. Glaser in Munich. Experiments using our techniques and measuring the improvement between materials that have an importance in medicine, like oxygenated and de-oxygenated blood have been conducted successfully, see [7], [9].

5.1.3. Numerical aspects

Participants: Bernard Bonnard, Olivier Cots, Jean-Baptiste Caillau.

In december, Pierre Martinon and Mathieu Caeys visited our group. This launhes a collaboration whose objective is to compare the direct and indirect methods in the contrast problem (implemented in the Bocop and Hampath sofwares) and use LMI techniques to get a global bound on the problem (in the contrast problem there are many local optima and the global optimality is a complicated issue)-also O. Cots visited R. Zidani (COMMANDS team) to investigate the use of numerical HJB techniques in the problem. This collaboration will allow to compare in a physical important problem the various available numerical methods in optimal control.

5.2. 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 applications in optimal control to compute the global optimum and in optimal transport where regularity properties of the map in the Monge problem is related to convexity properties of the tangent injectivity domains. This shows also the transverse part of the team: [3] complete the previous results obtained with Rifford [33] ; the paper [20] analyses the conjugate and cut loci in Serret-Andoyer metrics and dynamics of spin particles with Ising coupling, and is a first step towards the computation of conjugate and cut loci on left invariant Riemannian and SR- metrics in S0(3) with applications for instance to the attitude control problem of a spacecraft. The submitted paper [19] concerns the analysis of singular metrics on surfaces in relation with the average orbital transfer problem.

5.3. Averaging in control

Participants: Bernard Bonnard, Helen-Clare Henninger, Jean-Baptiste Pomet.

A reference paper on the construction and properties of an “average control system” [2] is to be published; 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.

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. Helen Henninger’s PhD aims at going much further in this direction and then apply this local study to real missions, possibly in a three-body environment.

5.4. Optimal transport

Participants: Ludovic Rifford, Alice Erlinger, Ahed Hindawi, Alessio Figalli, Bernard Bonnard, Jean-Baptiste Caillau, Lionel Jassionesse, Robert Mc Cann [U. of Toronto].

This year has seen new results or starting directions in many areas of optimal cotrol.

- The very general condition for continuity of the transport map given in [47] motivated exploration of conditions for convexity of the tangent injectivity domain [10], [3] on. Lionel Jassionnesse’s PhD is in part devoted to Ma-Tudinger-Wang tensor that also plays an important role in this matter.
- In Ahed Hindawi’s PhD [1], defended this year, results in optimal transport for sub-Riemannian costs (see the survey [16]) are generalized to costs coming from optimal control problems with quadratic cost and a drift.
- Alice Erlinger’s PhD, joint with University of Toronto is exploring Optimal Transport’s application to modeling in economics

5.5. Applications of control methods to lDynamical systems

Participants: Ludovic Rifford, Ayadi Lazrag, Riccardo Ruggiero, Alessio Figalli, Rafael Ruggiero [PUC, Rio de Janeiro].

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 See [11], [13], [21].

Ayadi Lazrag’s PhD also deals with such problems

NECS Project-Team

6. New Results

6.1. Communication and control co-design for networked systems

6.1.1. Energy-aware communication and control co-design in wireless networked control systems

Participants: C. Canudas de Wit [Contact person], N. Cardoso de Castro, F. Garin, D. Quevedo [Newcastle Univ., Australia].

This work is the topic of the PhD thesis of N. Cardoso de Castro [12]. 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, as we had pointed out in the review paper [63], 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 [31] or over a finite receding horizon [32].

6.1.2. System-theoretic analysis of modern error correcting codes (serial turbo codes)

Participants: F. Garin [Contact person], G. Como [Lund Univ., Sweden], F. Fagnani [Polit. Torino, Italy].

Serial turbo codes are a family of codes for error correction in point-to-point digital communication. The encoder can be described as the composition of three linear maps, the intermediate one being a permutation (called interleaver) while the inner and outer one are convolutional codes, i.e., linear dynamical systems where state, input and output belong to a vector space over the finite field $GF(2)$. The decoding is performed with iterative low-complexity algorithms which give a good approximation of the optimal maximum-likelihood (ML) decoder. Using system-theoretic properties of the constituent convolutional codes and probabilistic arguments, we study the average and the typical behavior of ensembles of such codes (with fixed convolutional codes, and random interleaver), asymptotically in the block-length [18]. We disprove the common conjecture that the typical behavior concentrates around the average: indeed, the average error decays polynomially in the block-length N, while the typical code has a faster error decay (exponential in some fractional power of N); however, the typical-code analysis confirms the same design parameters for the convolutional codes that were already suggested by the study of the ensemble average: free distance of the outer encoder, and effective free distance of the inner encoder.

6.2. Networked systems and Graph analysis

6.2.1. Observability in consensus networks

Participants: A. Kibangou [Contact person], C. Commault [Gipsa-Lab].

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 in [70] for paths and circular graphs where the study was carried out based on rules on number theory. Herein, we have considered families of graphs admitting an association scheme [62] 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 [79]. Based on the so-called Bose-Mesner algebra [60], 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 so-called 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. In particular, we have shown that observability is ensured in such graphs only if $DK \geq N-1$ where D is the number of classes of the association scheme, N the number of nodes, and K the valency of the graph, i.e. the cardinality of the neighborhood.

6.2.2. Distributed graph discovery

Participants: A. Kibangou [Contact person], F. Garin [Contact person], C. Commault [Gipsa-Lab], D. Tran, D. Varagnolo [KTH], K.H. Johansson [KTH].

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. Two approaches have been developed. For the first one [38], based on properties of the observability matrix, we have shown that Laplacian eigenvalues can be recovered by solving a local eigenvalue decomposition on an appropriately constructed matrix of observed data. Unlike FFT based methods recently proposed in the literature (see [65], [73]), in our proposed method we are also able to estimate the multiplicities of the eigenvalues. However, this method is only applicable to networks having nodes with sufficient storage and computation capabilities. That's why we have proposed a second method requiring much less computation and storage capabilities in [76]. Based on a recent result showing that the average consensus matrix can be factored in D Laplacian based consensus matrices, where D stands for the number of nonzero distinct Laplacian eigenvalues [40], we have shown how carrying out such a factorization in a fully distributed way. The proposed solution results on a distributed solution of a constrained consensus problem.

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 algorithms. This is particularly difficult in the case when the agents do not have or do not want to disclose their identifiers (IDs), either for technological reasons (in time-varying self-organized networks, assigning unique identifiers to agents is a challenge) or for privacy concerns. In a recent work [78] the authors proposed an algorithm which allows each agent to find an estimate of the number of agents in the network, in an anonymous way. Such an algorithm is based on the generation of pseudo-random numbers, on some consensus algorithms (for distributed computation either of average or of maximum), and on statistical inference. In our work [37], we show how the same algorithm, with some minor modifications, can provide more information: approximations of each node's eccentricity, of the graph diameter and of the graph radius. We study the quality of such approximations, providing tight bounds on the error.

6.3. Distributed methods for control

6.3.1. Distributed control

Participants: A. Seuret [Contact person], G. Rodrigues de Campos, L. Brinon-Arranz, D.V. Dimarogonas [KTH], K.H. Johansson [KTH].

Another particular effort has been provided to the design of distributed control laws for multi-agents systems. Three main contributions have been produced and can be summarized as follows.

In [44], a new consensus algorithms for heterogeneous multi-agent systems is provided. A control strategy based on a consensus algorithm which is decoupled from the original systems is proposed. Consequently, its major advantage remains in the separation of the stability analysis of each subsystem and the distributed control algorithm. It is shown that our method allows using classical distributed consensus algorithms such as simple integrator consensus (with or without delay) and distributed consensus filter algorithms.

For many multi-robot applications it is interesting to impose a particular configuration for the robotic agents. This paper discusses the design and analysis of a distributed algorithm for the compact deployment of agents, where the behavior of each vehicle is only dependent on local information. The objective of the paper [72] is to achieve the most compact formation possible. To solve this problem we propose, in a first step, two uncorrelated controllers: one designed for dispersion with connectivity maintenance and a second designed to minimize inter-agent angles. An improved controller including variable gains, particularly designed to avoid singular configurations, is also provided. Lastly, we propose a sequential strategy composed of the two previously mentioned controllers and a stability analysis based on hybrid systems theory. Finally, some simulation results for different configurations supporting our theoretical results are presented.

6.3.2. Collaborative source seeking control

Participants: C. Canudas [Contact person], R. Fabbiano, F. Garin.

The problem of source localization consists in finding the point or the spatial region from which a quantity of interest is being emitted; this goal can be pursued by one or several agents possibly cooperating each other. 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.

Within the FeedNetBack European project, we have addressed the problem of collaborative source seeking with a fleet of autonomous underwater vehicles (UAVs). This topic was explored in the PhD thesis of Lara Brinon [61], where a solution was proposed, based on circular formations with the center of the formation following a 2-dimensional movement in the direction of the gradient of the source. The gradient computation was achieved through an approximation using the point-wise measurements from the various vehicles.

In a more recent work [29], we leave temporarily aside all issues of coordination and communication failures well-addressed in [61], and we focus on the gradient computation formula. Under some assumptions on the source emission (isotropic diffusive source in steady-state, whose solution satisfies the Laplace equation), we show that there is an exact integral formula (based on the Poisson integral of harmonic functions) for the computation of the gradient at the center of a circle, using pointwise measurements along the circumference. This approach has two main advantages: it can be generalized in three (or more) dimensions, and it allows to compute also higher-order derivatives, which allow to find higher-order control laws, useful e.g. for non-holonomic vehicles. A relevant property is that such an integral formula exploits mathematical properties of the source density distribution (the fact that it is harmonic), but does not require the knowledge of an explicit expression for the density function. This makes our approach different from the main source-seeking techniques present in the literature, which 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.

The latter work is part of the research of Ruggero Fabbiano during his Ph.D. studies.

6.3.3. Distributed real-time Simulation of numerical models

Participants: D. Simon [Contact person], A. Ben Khaled [IFPEN], M. Ben Gaid [IFPEN].

The need of quick innovation in the automotive domain made simulation necessary at early stages of the development cycle. Vehicles and powertrains are complex systems where different domains are involved. Representative phenomenological models of powertrains have been developed and have been used in the design phase under domain dedicated tools. However, their use for controls validation using Model-In-the-Loop (MIL) and Hardware-In-the-Loop (HIL) was prevented due to performance limitation of widely used single-solver/single-core simulation approaches.

Multicore simulation for complex systems has been studied with a focus on simulation duration speedup. The methodology of parallelization across the model has been selected for such problem where strong interactions between the model components are observed. The current study showed that decoupling the model parts by relaxing their data dependencies is promising in term of simulation speed (by increasing the parallelism) and results accuracy. Besides, tests results on engine model showed that, with the model partitioning, it is possible to use efficiently variable-step solvers thanks to the decrease of the number of discontinuities, so the number of integration interrupts, in each subsystem [26].

Further work will investigate in the combination of the use of variable-step solvers in split model with the use of multicore architecture for parallel computing, in order to improve the simulation speedup while keeping results accuracy under control.

6.4. Distributed average consensus algorithms

6.4.1. Finite-time average consensus protocols

Participants: A. Kibangou [Contact person], 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 majority of the 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. 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 [40], [39]. 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 [65], [73], [76]). In [77], 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. Unlike the method in [40], the factor matrices are not necessarily symmetric and the number of these factor matrices is exactly equal to the diameter of the graph.

6.4.2. Quadratic indices for performance evaluation of consensus algorithms

Participants: F. Garin [Contact person], S. Zampieri [Università di Padova], E. Lovisari [Università di Padova and Lund Univ.].

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. Examples of various relevant costs can be found in the book chapter [66] and in the references therein.

We are interested in evaluating the effect of the topology of the communication graph on performance, in particular for large-scale graphs. Motivated by the study of wireless sensor networks, our main objective is to understand the limitations which arise when agents are limited to truly local interactions, i.e., the neighborhoods are determined by being 'near' in a geometric (Euclidean) way, differently from graphs with few but possibly 'distant' connections, such as in small world models. At first [19] we consider graphs which are regular lattices (infinite lattices, or grids on tori, or grids on hyper-cubes), which are examples of geometrically local interactions, but also have a very rich structure: their symmetries allow to exploit powerful algebraic tools, such as the discrete Fourier transform over rings, to compute their eigenvalues, and then find bounds on the associated costs. Then, we extend the results to a more general class of graphs, thus showing that the behavior of lattices is mainly due to the local nature of interactions and not to the spatial invariance (the richness of the automorphism group). To do so, we exploit the analogy between reversible Markov chains and resistive electrical networks, which allows to study some perturbed grids, with less regularity but still exhibiting the same dimension-dependent asymptotic behavior. This latter work is part of the Ph.D. thesis of E. Lovisari at University of Padova, Italy, and the topic of a journal paper in preparation.

6.5. Distributed Estimation and Data fusion

6.5.1. Distributed joint state and input estimation

Participants: A. Kibangou [Contact person], F. Garin [Contact person], A. Esna Ashari.

Three consensus-based distributed algorithms have been developed for joint state and input estimation in discrete-time systems. The methods are proper substitutes for distributed Kalman filter in the case in which there are additive faults to the system. Previously developed centralized estimation methods have been reformulated so that the estimator can be used for distributed sensor networks. These new forms are similar to the information form of Kalman filter [34], [35]. The new forms can be used to propose distributed algorithms based on the consensus of the nodes on calculation of some matrices and vectors. Also a second algorithm is proposed, based on the consensus of the local estimators on local state estimations. This algorithm has less computation effort than the first, but gives a sub-optimal solution in the sense of covariance error. Finally, a third method based on covariance intersection method for diffusing local estimations was proposed in addition. This method also provides a sub-optimal solution. Compared with the second approach, the diffusion of local data is less complicated, however it requires more message communication between nodes.

6.5.2. Data fusion approaches for motion Capture by Inertial and Magnetic Sensors

Participants: H. Fourati [Contact person], A. Makni.

We are interested to motion capture (or attitude) by fusing Inertial and Magnetic Sensors. In [17], we present a viable quaternion-based Complementary Observer (CO) which is designed for rigid body attitude estimation. We claim that this approach is an alternative one to overcome the limitations of the Extended Kalman Filter (EKF). 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. These results are promising for human motion applications, in particular future ambulatory monitoring. The estimated attitude is used to reconstitute the linear acceleration, linear velocity and finally the 3D position from a usual integration procedure (in the case of foot motion) [36]. The problem of attitude estimation is also recently studied within the PhD thesis of Aida Makni. Our goal is to develop a new attitude estimation methods in the case of aerial vehicles (hexa-rotors) by the use of intermittent measures of gyroscopes with the goal to reduce the energy consumption and to gain in the autonomy of the battery.

6.6. Stability and control design of asynchronous interconnected systems

6.6.1. New approaches for stability analysis of time-delay systems

Participants: A. Seuret [Contact person], F. Gouaisbaut.

A particular attention has been paid to the stability analysis of time delay systems. Indeed delays represent a classical phenomenon which appears in networked control systems cite. This corresponds to the fact that data are not transmitted instantaneously from one node to its neighbors. In this context some effort has been provided in order to reduce the conservatism of the stability conditions. This works represents some fundamental researches to develop accurate stability conditions to networked control systems. More especially we produced a paper [45] which addresses the stability problem of linear time delay system. In the literature, the most popular approach to tackle this problem relies on the use of Lyapunov-Krasovskii functionals. Many results have proposed new functionals and techniques for deriving less and less conservative stability conditions. Nevertheless, all these approaches use the same trick, the well-known Jensen's inequality which generally induces some conservatism difficult to overcome. In light of those observations, we propose to reduce the conservatism of Lyapunov-Krasovskii functionals by introducing new classes of integral inequalities called Wirtinger's inequalities. This integral type inequality is firstly shown to encompass Jensen's inequality and is then employed to derive new stability conditions. To this end, a slightly modified Lyapunov functional is proposed. Several examples illustrate the effectiveness of our methodology. Further efforts on this topics have been provided and several improved articles are now submitted to servals journals.

6.6.2. Stability and control of asynchronous sampled-data systems

Participants: A. Seuret [Contact person], C. Briat [ETHZ], J. Gomes Da Silva Jr. [UFRGS], M. M. Peet [Illinois Institute of Technology].

Sampled-data systems have been extensively studied in the literature and the references therein. It is now reasonable to design controllers which guarantee the robustness of the solutions of a closed-loop system under periodic samplings. However the case of asynchronous samplings still leads to several open problems. This corresponds to the realistic situation where the difference between two successive sampling instants is time-varying. Several articles drive the problem of time-varying periods based on a discrete-time approach, input delay approach using the framework of Lyapunov-Krasovskii theorem, using the small gain theorem or the analysis of impulsive systems. These last approaches are very relevant to this problem because they cope with time-varying sampling periods as well as with uncertain systems in a simple manner. Nevertheless, these sufficient conditions are still more conservative than discrete-time approaches. In [24], we proposed a novel approach to assess stability of continuous linear systems with sampled-data inputs. The method, which is based on a particular type of functionals, called 'looped-functionals' provided easy tractable stability conditions for the continuous-time model. This method has been extended to various cases dealing with sampled-data systems. Indeed a method to constructs such class of functionals using the Sum of Squares framework was developed in [23]. Another extensions was also proposed in order to include saturations in the actuators [21]. Extensions to the case of communication delays and asynchronous samplings was also provided in [22].

Based on this new type of Lyapunov functional, several works have been provided in the more general context of hybrid system. Indeed sampled-data systems can be seen as a particular type of hybrid systems. This has been provided in several study done by A.R. Teel, Dragan Nesic and many other researchers. Thus the idea was to show that the previous approach was also able to provide efficient stability conditions for impulsive systems [16], [27], [28], [54] or switched systems [53].

6.6.3. Event-based control

Participants: A. Seuret [Contact person], N. Marchand [Gipsa-Lab], C. Prieur [GIPSA-Lab], S. Durand [CINVESTAV].

Usually feedback laws are implemented in a periodic fashion on digital hardware. The main reason for using this periodicity in the hardware comes from the difficulties to analyze the stability of aperiodic or asynchronous systems. However it also seems natural to hold the same control input longer if the system behaves in a suitable way or shorter if the system requires an updated input. In [9], an algorithm is suggested to sample the control input based on the behavior of a Lyapunov-like function. This algorithm is called event-triggered since the Lyapunov-like function directly depends on the state of the systems. Using a Lyapunov-like function, two algorithms for the design of event-triggered algorithm are designed. It is assumed that a stabilizing controller for the continuous control system is given. Both event-triggered algorithms need to consider a closed-loop system with a mixed discrete/continuous dynamics (namely this is a hybrid system). Some numerical simulations illustrate the stability properties of both algorithms. In a future work, the performance issue should be analyzed. It is remarked that the event-triggered algorithms have a different performance. The first one seems to ensure a good speed of convergence on numerical simulations, whereas the second event-triggered algorithm allows less jumps and thus needs to compute less often the control variables. The advantages and disadvantages of each algorithm will be studied more precisely in a future work, for a theoretical point of view (e.g. by estimating a priori the number of switches), or on applications (to understand which algorithm is better depending on the application). Regarding this remark a journal paper has been submitted to IMA Journal of Mathematic Control and Information lately in 2012.

6.6.4. *Feedback under slacken real-time*

Participants: D. Simon [Contact person], A. Seuret, P. Andrianiaina [AIRBUS].

Robustness in control usually deals with the plant's parameter uncertainties, but the insensitivity or adaptability w.r.t. timing deviations from the theoretical pattern, such as jitter or deadlines misses can be exploited. The interesting point is that a feedback control system which is robust w.r.t. the plants parameters uncertainties is also robust, to some extent, w.r.t. timing deviations. Hence a feedback control system is not as hard as it is often considered in the literature, but should be better considered as *weakly hard*, i.e. able to tolerate specified timing deviations without leaving its requested performance [46].

A weakened implementation scheme for real-time feedback controllers is proposed to reduce the conservatism due to traditional worst-cases considerations. To save wasted computing resources, new real-time scheduling scenarios allowed for reducing the time slots allocated to control tasks below the value of the Worst Case Execution Time which is traditionally used to implement embedded control software. The stability of the control system under occasional deadlines miss is assessed using robustness arguments, using Lyapunov-Krasovskii functionals and LMIs solving based on [10]. The methodology has been successfully assessed for a fighter aircraft pitch controller, which show that the stability of the plant can be kept (and even improved) using the new scheduling schemes using less computing resources than traditional implementations [25], [11].

6.6.5. *Varying sampling for LPV systems*

Participants: D. Simon [Contact person], O. Sename, E. Roche.

In the context of network-controlled systems the idea of using varying control intervals naturally arises when the available computing power devoted to feedback control is limited, e.g. in embedded systems. It can be easily shown that decreasing the control frequency directly decreases the amount of computing needed for control. However, the stability of the feedback controller under varying sampling must be assessed for all the allowed variations of the sampling intervals [8].

The Linear Fractional Transform (LFR) formulation is widely used in robust analysis to study the influence of the plant's uncertain parameters on the stability and performances of a closed-loop system. Usually it is used to build a parameter dependent model of a dynamical system, depending on a known set of parameters. Here the set of varying parameters has been extended with the sampling interval of the control system, thus allowing to handle both varying sampling and plants uncertainties in a single framework (Figure 6).

Here, P_d is a on-line discretized model of the plant, Δ represents the uncertain parameters of the plant and δ is the variation of the sampling interval around its nominal value. From this model a robust controller can be synthesized, enforcing the control system stability for all variations of the sampling interval inside a predefined range.

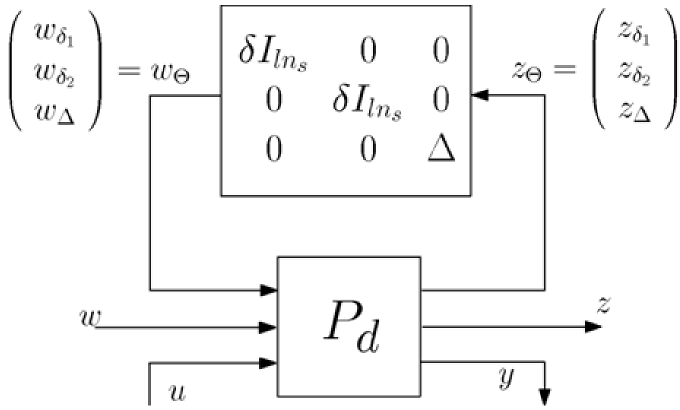


Figure 6. LFR system depending on system parameters and sampling interval variations

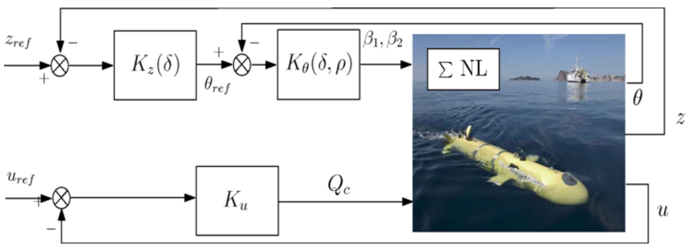


Figure 7. Control of an AUV

The approach have been successfully applied to the pitch and altitude control of a non-linear autonomous underwater vehicle, where the source of sampling variations comes from the altitude ultrasonics sensors [43]. However the approach still suffers from conservatism for which improvements using full block multipliers, or parameter-dependent Lyapunov functions, have been investigated [58].

6.7. Vehicular transportation systems

6.7.1. 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 [30], 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. Simulation results exhibit that the measured densities obtained from the traffic simulator Aimsun and the estimated densities agree closely. In [69], 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 [68].

6.7.2. Traffic control

Participants: C. Canudas de Wit [Contact person], D. Pisarski.

The problem of equilibrium points for the Cell Transmission Model was studied in [42]. The structure of equilibrium sets was analyzed in terms of model parameters and boundary conditions. The goal was to determine constant input flows, so that the resultant steady state of vehicle density was uniformly distributed along a freeway. The necessary and sufficient conditions for the existence of one-to-one relation between input flow and density were derived. The equilibrium sets were described by formulas that allow to design a desired balanced density. A numerical example for the case of a two-cell system was presented. In [41], the problem of optimal balancing of traffic density distributions was explored. The optimization was carried out over the sets of equilibrium points for the Cell Transmission Traffic Model. The goal was to find the optimal balanced density distribution, that maximizes both the Total Travel Distance and the total input flow. The optimization was executed in two steps. At the first step, a nonlinear problem to find a uniform density distribution that maximizes the Total Travel Distance was solved . The second step was to solve a quadratic problem reflecting the trade-off between density balance and input flow maximization. At both steps, decomposition methods were used. The computational algorithms associated to such a problem were given. Finally, in [71], the application of the idea of optimal balancing of traffic density distribution was presented. It was implemented to the Grenoble South Ring in the context of the Grenoble Traffic Lab. The traffic on the ring is represented by the Cell Transmission Model that was tuned by using real data and Aimsun micro-simulator. A special attention was paid to the calibration of a flow merging model. A large-scale optimization problem was solved by using advanced combinatorial procedures. The main difficulties in the implementation as well as the limitations of the designed software were highlighted. Finally, the results of different traffic scenarios on the Grenoble South Ring were presented.

6.7.3. Vehicle control for disabled people

Participants: C. Canudas de Wit [Contact person], V. Ciarla, J. Dumon, F. Quaine [UJF], V. Cahouet [UJF].

The typical architecture of an Electric Power Assistance Steering (EPAS) system includes a static map to provide the correct amplification to the drivers exerted torque. In literature, it is generally known as booster curve. This work concerns the study of the amplification criteria, that are commonly used to these booster curves. The basic concepts of the Electric Power Steering (EPS) systems with a realistic model for the friction contact, that acts on the wheels are discussed. A relation between the assistance and the driver's torque is provided, under the hypothesis of a position-oriented control of the movement and the Stevens' power law [33]. In current works, we want to modify the general architecture of the EPAS system for people driving with two arms. For this purpose, we insert two additional blocks: the first one provides an estimation of the gravitational torque due to the weight of the driver's arm while the second gets as inputs the total driver's torque and the estimated gravitational torque in order to update the driver's torque with the gravitational torque. The updated measure is then given as input to the booster curve for deriving the correct assistance.

6.7.4. 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, corresponding to different levels of energy consumption; therefore, there is 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, but 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 travel time of vehicles in the road network. If all the vehicles can communicate with one another and with the active infrastructure (traffic lights), we can imagine benefits for each of the two problems which can be considered as a whole: on the one hand, for vehicles, 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. More importantly, the traffic manager can send instructions to the vehicle. The aim of the research is to evaluate the potential in terms of energy saving and traffic improvement made possible by communicating vehicle. This work is carried out in collaboration with IFP in the framework of a CIFRE thesis.

NON-A Project-Team

5. New Results

5.1. Model-free control

Participants: Cédric Join, Samer Riachy.

The achievements obtained in 2012 are as follows:

- The model-free control approach is applied to a complex nonlinear model describing the dynamics of a traffic flow in [24]. The robustness with respect to external disturbances is shown by numerical simulations.
- Model-free control is applied to a magnetic bearing in [56], which is a quite important industrial device. The experimental results are compared to those obtained via other control techniques.
- ”Model-free” control and the related ”intelligent” proportional-integral controllers are successfully applied to freeway ramp metering control in [47]. Implementing the proposed control strategy is straightforward. Numerical simulations need the identification of quite complex quantities like the free flow speed and the critical density. This is achieved due to new estimation techniques, where the differentiation of noisy signals plays a key role.

5.2. Algebraic technique for estimation, differentiation and its applications

Participants: Cédric Join, Mamadou Mboup, Wilfrid Perruquetti, Rosane Ushirobira, Olivier Gibaru.

Elementary techniques from operational calculus, differential algebra, and noncommutative 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:

- The paper [30] proposes an algebraic method to fault diagnosis for uncertain linear systems. The main advantage of this new approach is to realize fault diagnosis only from knowledge of input and output measurements without identifying explicitly model parameters. Using tools and results of algebraic identification and pseudospectra analysis, the issues of robustness of the proposed approach compared to the model order and noise measurement are examined.
- The aim of [79], [84] is to develop an algebraic approach to estimate human posture in the sagittal plane using inertial measurement unit providing accelerations and angular velocities. For this purpose the issue of the estimation of the amplitude, frequency and phase is addressed for a biased and noisy sum of three sinusoidal waveform signals on a moving time horizon. Since the length of the time window is small, the estimation must be done within a fraction of the signal’s period. The problem is solved via algebraic techniques.
- An application of algebraic estimation approach for estimation of option pricing and dynamic hedging is given in [66].
- A model-based online fault-diagnosis scheme for an electromagnetically supported plate is presented in [73] as an example of a nonlinear and open-loop unstable system. First, residuals for sensor as well as for actuator faults are generated using algebraic derivative estimators. Then, the robust detection and isolation of step-like sensor and actuator faults is presented.
- The paper [57] uses the extreme value theory for threshold selection in a previously proposed algebraic spike detection method. The algebraic method characterizes the occurrence of a spike by an irregularity in the neural signal and devises a nonlinear (Volterra) filter which enhances the presence of such irregularities.

- The papers [39], [40] generalize the algebraic method from the integer order to the fractional order for estimating the fractional order derivatives of noisy signals. The proposed fractional order differentiator is deduced from the Jacobi orthogonal polynomial filter and the Riemann-Liouville fractional order derivative definition. Exact and simple formula for this differentiator is given where an integral formula involving Jacobi polynomials and the noisy signal is used without complex mathematical deduction. Hence, it can be used both for continuous-time and discrete-time models. The comparison between our differentiator and the recently introduced digital fractional order Savitzky-Golay differentiator is given in numerical simulations so as to show its accuracy and robustness with respect to corrupting noises.

5.3. Observability and observer design for nonlinear systems

Participants: Jean-Pierre Barbot, Wilfrid Perruquetti, Gang Zheng, Denis Efimov.

Observability analysis and observer design are important issues in the field of control theory. Some recent results are listed below:

- The problem of observer design for fault detection in a class of nonlinear systems subject to parametric and signal uncertainties is studied in [22]. The design procedure includes formalized optimization of observer free parameters in terms of trade-offs for fault detection performance and robustness to external disturbances and model uncertainties. The technique makes use of some monotonicity conditions imposed on the estimation error dynamics. Efficiency of the proposed approach is demonstrated through the Oscillatory Failure Case in aircraft control surface servo-loops.
- An algorithm for the frequency and bias identification of a harmonic signal is presented in [14], [15]. The solution is based on an adaptive observer technique and the hybrid systems method.
- An influence of a singular manifold of non observable states on reconstruction of chaotic attractors is analysed in [25]. The probability of visits of the observability singularity manifold and the relative time spent in the observability singularity manifold are introduced.
- In [36], the cluster structured sparse signals are investigated. Under the framework of Bayesian compressive sensing, a hierarchical Bayesian model is employed to model both the sparse prior and cluster prior, then Markov Chain Monte Carlo (MCMC) sampling is implemented for the inference. Unlike the state-of-the-art algorithms, which are also taking into account the cluster prior, the proposed in [36] algorithm solves the inverse problem automatically–prior information on the number of clusters and the size of each cluster is unknown.
- The papers [54], [86], [87] present a new approach for observer design for a class of nonlinear singular systems which can be transformed into a special normal form. The interest of the proposed form is to facilitate the observer synthesis for the studied nonlinear singular systems. Necessary and sufficient geometrical conditions are deduced in order to guarantee the existence of a diffeomorphism, which transforms the studied nonlinear singular systems into the proposed normal form.
- The paper [85] investigates the observer design problem of for linear switched system with disturbance jumps. Detection of active sub-system and finite time estimation of states are respectively discussed. A switched finite time observer is proposed to guarantee the finite time convergence independent of the disturbance jumps.
- The paper [71], [72] proposes a new observer scheme for chaotic and hyperchaotic systems. Firstly, a classical impulsive observer is investigated for Lorenz chaotic system. This approach is based on sufficient conditions for stability of impulsive dynamical systems. After, an hybrid observer is proposed for hypoerchaotic systems. In the paper [70], a new method of strange attractor identification, under sparse measurement, is proposed this method is based on the concept of compressive sensing. For this, some particular impulsive observers have been presented with a decision scheme linked to diagnosis method, the identification of the strange attractor and state observation are done.

- The problem of state reconstruction for nonlinear differential-algebraic systems with unknown inputs is studied in [51].
- In the paper [26] the design of observers for nonlinear systems with unknown, time-varying, bounded delays, on both state and input for a class of nonlinear systems is proposed. Furthermore, the feasibility of the proposed strategy is illustrated by a numerical example.

5.4. Sliding mode control estimation

Participants: Jean-Pierre Barbot, Wilfrid Perruquetti, Denis Efimov, Thierry Floquet.

Sliding mode algorithms are very popular for finite-time estimation and regulation. The recent results obtained by the group are as follows:

- The issues of a higher order sliding mode controller realization under actuator saturation and quantization have been analysed in [37]. The zig-zag solutions are introduced and analysed.
- The problem of design of interval observers for linear-parameter-varying systems, containing non detectable or non strongly observable parts, is addressed in [18], [63], [62] applying the higher order sliding mode algorithms. Application of sliding mode observers leads to accuracy improvement in the system.
- In [32] an anomaly signal detection in communication networks is studied by control theory techniques. Several classes of sliding mode observers are proposed for a fluid flow model of the transmission control protocol (TCP)/internet protocol network. Comparative simulations via network simulator NS-2 show the enhancement brought by a higher order sliding mode observer. The efficiency of this observer opens the way toward observing traffics with real TCP flow characteristics.
- In [80], [42], [41] the problem of continuous and discrete state estimation for a class of linear switched systems is studied. The class of systems under study can contain non-minimum phase zeros in some of their "operating modes". The conditions for exact reconstruction of the discrete state are given using structural properties of the switched system. The state-space is decomposed into the strongly observable part, the nonstrongly observable part and the unobservable part, to analyze the effect of the unknown inputs. A state observer based on high-order sliding-mode and Luenberger-like observers is proposed. For the case when the exact reconstruction of the state cannot be achieved, the ultimate bounds on the estimation errors are provided. In [41] this technique has been applied to fault detection in switched systems.
- The paper [55] aims, firstly to highlight the possibility of recovering a message included in a chaotic continuous time delay system, secondly to show that it is possible to use the third order sliding mode in order to recover directly all the states and the unknown input (message), thirdly to illustrate the robustness of the proposed observer with respect to a noisy signal. This work is based on the concept of left invertibility and recent advances in sliding mode observers.
- The problem of estimation of discrete and continuous states for switched systems applying higher order sliding mode observers and projection is investigated in the papers [68], [67].

5.5. Non-linear, Sampled and Time-delay systems

Participants: Jean-Pierre Richard, Lotfi Belkoura, Gang Zheng, Denis Efimov, Wilfrid Perruquetti.

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:

- A new type of stability is introduced and its equivalent Lyapunov characterization is presented in [16]. The problem of global stability for the compact set composed of all invariant solutions of a nonlinear system (several equilibriums, for instance) is studied. It is shown that several well-known multi-stable systems satisfy this new stability property.

- A new state-dependent sampling control is proposed in [23], [65], which enlarges the sampling intervals of state feedback control. The case of linear time invariant systems with time delays is considered that guarantees the exponential stability of the system origin for a chosen decay rate. The approach is based on LMIs obtained from the sufficient Lyapunov-Razumikhin stability conditions.
- Nonlinear feedback design for fixed-time stabilization of linear control systems is studied in [31]. Nonlinear control algorithms of two types are presented for uncertain linear plants. Controllers of the first type are stabilizing polynomial feedbacks that allow to adjust a guaranteed convergence time of system trajectories into selected neighborhood of the origin independently on initial conditions. Controllers of the second type are modifications of the second order sliding mode control algorithms. They provide global finite-time stability of the closed-loop system and allow to adjust a guaranteed settling time independently on initial conditions. Control algorithms are presented for both single-input and multi-input systems.
- The problem of natural wave control is addressed in [17], which involves steering a lattice of oscillators towards a desired natural (i.e. zero-input) assignment of energy and phase across the lattice. This problem is formulated and solved for lattices of linear oscillators via a passivity-based approach.
- The verification problems for transition systems enriched with a metric structure is analysed in [27]. The main novelty compared to an algorithm presented recently by Lerda et al. [2008] consists in introducing a tuning parameter, which improves the performance drastically. A procedure that allows one to prove unbounded safety from the result of the bounded safety algorithm via a refinement step is also established. The algorithm to handle bounded liveness verification is adapted.
- The problem of finite-time output stabilization of the double integrator is addressed in [52] applying the homogeneity approach. A homogeneous controller and a homogeneous observer are designed (for different degree of homogeneity) ensuring the finite-time stabilization. Their combination under mild conditions is shown to stay homogeneous and finite-time stable as well.
- The notes [76], [77] are dedicated to the stability analysis of bilinear sampled-data systems, controlled via a linear state feedback static controller. A zero order hold device is used. The purpose is to find a constructive way to calculate the maximum allowable sampling period (MASP) that guarantees the local stability of the system. The proposed stability conditions are formulated as linear matrix inequalities (LMI).
- The works [75], [74] concern the adaptation of sampling times for linear time invariant systems controlled by state feedback. Complementary to various works that guarantee stabilization independently of changes in the sampling rate, there the conditions to design stabilizing sequences of sampling instants is provided. In order to reduce the number of these sampling instants, a dynamic scheduling algorithm optimizes, over a given sampling horizon, a sampling sequence depending on the system state value. The proofs are inspired on switched system techniques combining Lyapunov functions and LMI optimization.
- The mechanism of entrainment to natural oscillations in a class of (bio)mechanical systems described by linear models is investigated in [61]. A nonlinear control strategy (based on the speed gradient control algorithm) is analyzed providing the system oscillation in resonance mode with a natural frequency. It ensures an energy-optimal entrainment performance robustly against perturbations in system parameters in a finite time.
- The paper [29] considers a networked control loop, where the plant is a "slave" part, and the remote controller and observer constitute the "master". Since the performance of Networked Control Systems (NCS) depends on the Quality of Service (QoS) available from the network, a controller is designed that takes into account qualitative information on the QoS in real time.
- In the paper [50], the theory of non-commutative rings allows determining whether or not there exists an equation called algebraically essential in order to estimate the delay on a nonlinear system. From this equation, it is shown that this equation is generally not enough to guarantee the delay estimation, thus the notion of persistent signal with respect to delay estimation is introduced.

Furthermore, based on the definitions of algebraically essential equation and of persistent signal, a delay estimation algorithm is proposed. Some simulation results have been presented in order to highlight the robustness (with respect to measurement noise) of the proposed algorithm.

- The problem of algebraic identifiability for linear and nonlinear dynamical systems is considered in [88].

5.6. Interval control and estimation

Participants: Denis Efimov, Wilfrid Perruquetti.

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 apply the interval observer techniques, which generate an estimate on the interval of the admissible values of the state at the current instant of time. The recent results are listed below:

- The problem of output stabilization of a class of nonlinear systems subject to parametric and signal uncertainties is studied in [20], [21]. First, an interval observer is designed estimating the set of admissible values for the state. Next, it is 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 linear-parameter-varying systems without assumption that the vector of scheduling parameters is available for measurements.
- The problem of interval observer design for a class of observable nonlinear systems is studied in [33]. It is shown that under some mild conditions a Hurwitz matrix can be transformed to a Hurwitz and Metzler one using a real similarity transformation.
- The work [64] is devoted to interval observer design 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 that under some mild conditions the cooperativity of an LTV system can be ensured by a static linear transformation of coordinates. The case of a time-varying transformation for periodic systems is considered in the work [64].
- The problem of actuator fault detection for flat systems using the sliding-mode differentiation and the interval constraint satisfaction technique has been analysed in [43].

5.7. Applications

Participants: Jean-Pierre Richard, Jean-Pierre Barbot, Mamadou Mboup, Gang Zheng, Denis Efimov, Wilfrid Perruquetti, Olivier Gibaru, Samer Riachy.

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:

- The global stabilization of a ball & beam through saturated control, which imposes restrictions on the reactivity of the closed loop, is studied in [91], [81]. A modified design for the classical ball & beam system is presented. The beam is driven by two actuators. In comparison to the classical system, this design offers an additional degree of freedom, which is the vertical motion of the beam. We show that the new design offers the possibility to get rid of the closed loop low reactivity restriction. Two nonlinear controllers to steer the trajectories of the system towards a final desired position are proposed.
- In papers [48], [49] a new class of power converters is studied (Parallel Multicell Chopper). The topology of these chopper is based on a combination of n switching cells interconnected via independent inductors. This type of choppers is a new DC/DC static power converter which has an output current equals to n times the source current where n is the number of cells . After recalling the dynamical equations of the converter, its hybrid dynamical behavior and properties are highlighted. This particular hybrid system induces new and difficult control problems, such problem can be tackled by a new control concept based on Petri net.

- The paper [69] addresses the problem of power management of a hydrogen fuel cell system combined with super capacitors under high load variations in an electric vehicle. The singular perturbation theory is used for the control and coordination of two converters. The Lyapunov theory is used for analysis.
- Combined feedforward/feedback control algorithm for highly nonlinear systems was proposed on the basis of the approximating hybrid model in [28]. The designed MIMO controller enables simultaneous control of the air-to-fuel ratio and torque for injector automobile engines. The theoretical results were validated experimentally with physical cars.
- A spike sorting method for multi-channel recordings is proposed in [35]. The proposed method uses an iterative application of Independent Component Analysis (ICA) algorithm and a deflation technique in two nested loops. The results suggest that the proposed solution significantly improves the performance of ICA in spike sorting.
- In the paper [83] an algorithm for a particular change-point detection problem is proposed, where the frequency band of the signal changes at some points in the time axis. Apart from detecting the change-points, the proposed algorithm is also able to estimate the frequency bands. The main idea of the algorithm is to consider a simple local bandlimited model to represent the input signal in each sliding time window.
- The papers [60], [58], [59] present a new sensorless parameter identification method for permanent magnet stepper motors. Current sensors are assumed available, but position and velocity sensors are not. Data is obtained with open-loop voltage commands at multiple speeds. A new reference frame is proposed that presents advantages similar to the standard $d-q$ frame, but without the need for a position sensor. The method exploits carefully derived linear parameterizations and a least-squares algorithm. In one case, overparameterization is resolved using elimination theory. Overall, the parameters identified using the new procedure are found to be very close to those obtained with position sensors. The approach is potentially applicable to other types of synchronous motors as well.
- In the paper [78], an improvement of the dynamic accuracy of a flexible robot joint is addressed. Based on the observation of the measured axis deformation, a simplified elastic joint model is deduced. In the first step, the non-linear model component's is analyzed and identified in the cases of the gravity bias and the friction term. In the second step, a non asymptotically algebraic fast identification of the oscillatory behavior of the robot axis is introduced. Finally, the performances of the identification approach are exploited in order to improve the dynamic accuracy of a flexible robot axis. This is done experimentally by the combination of the adaptation of the jerk time profile to reduce the end-point vibration and the model-based precompensation of the end-point tracking error.
- Localizability of unicycle mobiles robots is analysed in [82] from an algebraic point of view. A sensibility study leads to a new fusion algorithm in the multi landmark case using as a basis the posture differentiation based estimator.
- The problem of early detection of oscillatory failures for aircrafts is addressed in [38]. The proposed solution is based on a finite-time sliding-mode differentiator and a hybrid optimization scheme.
- The H_∞ control design under time-varying delays and uncertainties, which ensures the stability and performance (synchronization/transparency) between the master and slave manipulators, is proposed in [46], [44], [45]. The design of the controller based on a proposed control scheme, which is performed by using LMI optimization based on Lyapunov-Krasovskii functionals and H_∞ control theory.

CLASSIC Project-Team

5. New Results

5.1. Contributions earlier to 2012 but only published in 2012

Participants: Gérard Biau, Vincent Rivoirard, Gilles Stoltz, Olivier Catoni.

We do not discuss here the contributions provided by [16], [17], [11], [13], [14], [15], [18], since they were achieved in 2011 or earlier (but only published this year due to the reviewing and publishing process). Also, the book [25] (whose first edition was published in 2009) was augmented and revised for its second edition, published this year.

5.2. Extended journal versions written in 2012 of conference papers published in 2011

Participants: Sébastien Gerchinovitz, Gilles Stoltz.

We wrote extended journal papers of some conference papers discussed in previous annual activity reports; they correspond to refences [32], [19], [20].

5.3. Bayesian methods

Participants: Gérard Biau, Vincent Rivoirard.

5.3.1. The ABC method

Approximate Bayesian Computation (ABC for short) is a family of computational techniques which offer an almost automated solution in situations where evaluation of the posterior likelihood is computationally prohibitive, or whenever suitable likelihoods are not available. In the paper [29] Gérard Biau and his coauthors analyze the procedure from the point of view of k-nearest neighbor theory and explore the statistical properties of its outputs. They discuss in particular some asymptotic features of the genuine conditional density estimate associated with ABC, which is a new interesting hybrid between a k-nearest neighbor and a kernel method.

5.3.2. Semi-parametric version of the Bernstein-von Mises theorem

In [22], Vincent Rivoirard and Judith Rousseau study the asymptotic posterior distribution of linear functionals of the density by deriving general conditions to obtain a semi-parametric version of the Bernstein-von Mises theorem. The special case of the cumulative distributive function evaluated at a specific point is widely considered. In particular, they show that for infinite dimensional exponential families, under quite general assumptions, the asymptotic posterior distribution of the functional can be either Gaussian or a mixture of Gaussian distributions with different centering points. This illustrates the positive but also the negative phenomena that can occur for the study of Bernstein-von Mises results. In [22] Vincent Rivoirard and Judith Rousseau use convergence rates on Besov spaces established in [23].

5.4. Sequential learning

Participants: Pierre Gaillard, Gilles Stoltz.

5.4.1. Bandit problems

The article [30] revisits asymptotically optimal results of Lai and Robbins, Burnetas and Katehakis in a non-asymptotic way. A preliminary attempt was mentioned in the 2011 annual report; it was concerned (essentially) with the case of Bernoulli distributions over the arms. We achieve here the stated optimality of the regret bounds for larger models: regular exponential families; finitely supported distributions.

5.4.2. Theoretical results for the prediction of arbitrary sequences

We generalize and unify in [24] several notions of regret under a same banner: these include adaptive regret (regret against a fixed convex combination on subintervals of the time); shifting regret (regret against a slowly evolving target sequence of convex combinations); and discounted regret (when the instances are weighted with weights depending on how recent the instances are). We recover and sometimes improve some earlier bounds.

5.4.3. Forecasting of the production data of oil reservoirs

We applied our sequential aggregation techniques to a new data set, with IFP Energies nouvelles as a partner. The goal was to aggregate in a sequential fashion the forecasts made by some (about 100) base experts in order to predict some behaviors (gas/oil ratio, cumulative oil extracted, water cut) of the exploitation of some oil wells. Results were obtained with the help of an intern, Charles-Pierre Astolfi, and are described in the technical report [27] (to be transformed into a regular journal / conference paper next year).

5.5. Regression, classification, regression methods

Participants: Gérard Biau, Olivier Catoni, Ilaria Giulini.

5.5.1. Metric-based decision procedures

We know now that a good part of the statistical performance of regression and classification algorithms relies on the metric chosen to represent the proximity between the data points. Throughout his work, Gérard Biau became convinced that, well beyond the traditional distances, (dis)similarities and other self-reproducing kernel metrics, it is now necessary to attempt to define proximities generated by the sample itself. These metrics are inevitably random and probabilistic, and force us to rethink the nature of the estimates, as shown for example in the preliminary article [12].

5.5.2. Unsupervised classification in reproducing kernel Hilbert spaces

In her PhD started in September 2012, Ilaria Giulini uses dimension free estimates of the principal components of an i.i.d. sample of points in a Reproducing Kernel Hilbert Space to derive new unsupervised clustering algorithms based on the idea of dimension reduction by nonlinear coordinate smoothing along aggregated principal components. The dimension free estimates are obtained using PAC-Bayes bounds derived from thresholded exponential moments.

5.6. Sparsity and ℓ_1–regularization

Participant: Vincent Rivoirard.

5.6.1. For multivariate Hawkes processes

Motivated by statistical problems in neuroscience, Vincent Rivoirard and his coauthors study in [31] non-parametric inference for multivariate Hawkes processes depending on an unknown function to be estimated by linear combinations of a fixed dictionary. To select coefficients, they propose a Lasso-type methodology where data-driven weights of the penalty are derived from new Bernstein-type inequalities for martingales. Oracle inequalities are established under assumptions on the Gram matrix of the dictionary. Non-asymptotic probabilistic results are proven, which allows them to check these assumptions by considering general dictionaries based on histograms, Fourier or wavelet bases. They finally carry out a simulation study and compare their methodology with the adaptive Lasso procedure proposed by Zou. They observe an excellent behavior of their procedure with respect to the problem of supports recovery. Unlike adaptive Lasso of Zou, their tuning procedure is proven to be robust with respect to all the parameters of the problem, revealing its potential for concrete purposes in neuroscience, but also in other fields.

5.6.2. In the spherical convolution model

In [21], Thanh Mai Pham Ngoc and Vincent Rivoirard consider the problem of estimating a density of probability from indirect data in the spherical convolution model. They aim at building an estimate of the unknown density as a linear combination of functions of an overcomplete dictionary. The procedure is devised through a well-calibrated ℓ_1–penalized criterion. The dictionary approach allows to combine various bases and thus enhances estimates sparsity. They provide an oracle inequality under global coherence assumptions. Moreover, the calibrated procedure that they put forward gives very satisfactory results in the numerical study when compared with other procedures.

5.6.3. For semiparametric nonlinear mixed-effects models

Semiparametric nonlinear mixed-effects models (SNMMs) have been proposed as an extension of nonlinear mixed-effects models (NLMMs). These models are a good compromise and retain nice features of both parametric and nonparametric models resulting in more flexible models than standard parametric NLMMs. In [28], Vincent Rivoirard and his coauthors propose new estimation strategies in SNMMs. They propose a Lasso-type method to estimate the unknown nonlinear function. They derive oracle inequalities for this nonparametric estimator. They combine the two approaches in a general estimation procedure that they illustrate with simulations and through the analysis of a real data set of price evolution in on-line auctions.

5.7. Computational linguistics

Participants: Olivier Catoni, Thomas Mainguy.

In a forthcoming paper, Olivier Catoni and Thomas Mainguy study a new statistical model to learn the syntactic structure of natural languages from a training set made of written sentences. This model learns a new type of stochastic grammar and defines a statistical model on sentences. Global constraints are enforced, that set the approach apart from the family of Markov models. On the other hand, the grammar model generates outputs through a split and merge stochastic process that is more elaborate than the production rules defining a context free grammar. Experiments made on small corpora are very encouraging. Working on large corpora will require to speed up the algorithms used to implement the model as well as some code optimization.

DOLPHIN Project-Team

6. New Results

6.1. On Optimizing a Bi-objective Flowshop Scheduling Problem in Uncertain Environment

Participants: Arnaud Liefooghe, Laetitia Jourdan, El-Ghazali Talbi

Existing models from scheduling often over-simplify the problems appearing in real-world industrial situations. The original application is often reduced to a single-objective one, where the presence of uncertainty is neglected. In [23], we focus on multi-objective optimization in uncertain environments. A bi-objective flowshop scheduling problem with uncertain processing times is considered. An indicator-based evolutionary algorithm is proposed to handle these two difficulties (multiple objectives and uncertain environment) at the same time. Four different strategies, based on uncertainty-handling quality indicators, are proposed in the paper. Computational experiments are performed on a large set of instances by considering different scenarios with respect to uncertainty. We show that an uncertainty-handling strategy is a key issue to obtain good-quality solutions, and that the algorithm performance is strongly related to the level of uncertainty over the environmental parameters.

6.2. New Price settings models in the energy field

Participants: L. Brotcorne, S. Afsar

The electricity supply industry is facing in many countries a restructuring process towards deregulation and competition. In that context classical marginal cost based approaches based on estimation of cost production function and demand functions are not well-suited anymore. Indeed, the energy prices have to be defined not only to retrieve the production costs but also in order to take into account the consumer behavior. Consumers make their choice of service, or of energy provider in order to minimize their disutility values. Failing to recognize that may lead to tremendous lack on revenues. In order to capture this hierarchical decision process where a leader (the energy provider) takes explicitly into account the reaction of a follower (the consumers) in his decision process. The energy pricing problems addressed in this are modeled as bilevel programs.

6.3. Bi-level formulation for a Long-Distance Freight Transportation Problem

Participants: M. Diaby, L. Brotcorne, E.-G. Talbi.

A company wants to convey different types of products from origin i to points of destination j. It can deliver the goods itself or hire a transport company, and subcontract part of the application. The transport company must offer attractive prices while aiming to maximize its profit. The aim of this problem is to determine rates that allow the carrier to maximize its revenues and remain affordable for the customer. The problem is modeled as a bilevel program at the first level, the carrier (leader) wants to maximize its revenues; at the second level, the client. An exact and an evolutionary solution approaches are developped.

6.4. On Local Search for Bi-objective Knapsack Problems

Participant: A. Liefooghe.

In [26], a local search approach is proposed for three variants of the bi-objective binary knapsack problem, with the aim of maximizing the total profit and minimizing the total weight. First, an experimental study on a given structural property of connectedness of the efficient set is conducted. Based on this property, a local search algorithm is proposed and its performance is compared against exact algorithms in terms of running time and quality metrics. The experimental results indicate that this simple local search algorithm is able to find a representative set of optimal solutions in most of the cases, and in much less time than exact algorithms.

6.5. Convergent methods based on aggregation in mathematical models

Participant : François Clautiaux

We designed several algorithms to aggregate variables in integer linear programs. Our methods first solve aggregated models, and converge to the optimal solution of the initial problem by iteratively refining the model.

The first method applies on a large network flow models that use a pseudo-polynomial number of variables. It is based on an initial aggregation of the vertices of the model and its iterative refinement using different optimization techniques. This led to dramatical improvements for a special case of vehicle routing problem. We proposed several theoretical results regarding convergence, suitable discretizations, wort-case analysis and approximation algorithms [44].

The second method applies on column generation approaches for the cutting-stock problem. Our algorithm links groups of dual variables by linear constraints, leading to a problem of smaller dimension, whose solutions are dual-feasible for the initial problem. The corresponding "inner approximation" is iteratively refined by splitting the groups into smaller groups until an optimal dual solution is found. This method allows to produce a valid lower bound at each iteration, which is not the case for classical column-generation schemes [58].

6.6. Investigating the Optimization Goal of Indicator-Based Multiobjective Search

Participant from DOLPHIN: Dimo Brockhoff; External Participants: Heike Trautmann and Tobias Wagner (TU Dortmund University, Germany)

Using a quality indicator in the environmental selection step of evolutionary multiobjective optimization (EMO) algorithms to indicate which solutions shall be kept in the algorithms' population and which should be deleted, introduces a certain search bias. Instead of an “arbitrary” subset of the Pareto front, such (quality) indicator based search algorithms aim at approximating the set of μ solutions that optimizes a given indicator, for which the term *optimal μ-distribution* has been introduced [63]. Also for performance assessment with respect to a given indicator, knowledge about the optimal μ-distributions is helpful as interpreting the *achieved* indicator values with respect to the best *achievable* value becomes possible. For the hypervolume indicator, several results on these optimal μ-distributions are known [63], [62], [75], [69], [70], [61] [64], but the understanding of the optimization goal for other indicators is less developed. Recently, we started to investigate the optimal μ-distributions, both theoretically and numerically, for the so-called $R2$ indicator [79]—another often recommended quality indicator [90]. Instead of the binary version of [79] that takes two solution sets and assigns them a certain quality, we thereby investigated an equivalent unary indicator where one (reference) set is always fixed.

First experiments for problems with two objectives and connected Pareto fronts have been presented in [37] which won the best paper award within the EMO track at GECCO'2013 [5]. Further investigations on problems with disconnected Pareto fronts have been submitted to the Evolutionary Computation journal [72]. We also studied in more detail how the parameters of the $R2$ indicator such as the ideal point or the distribution of weight vectors can be used to change the optimization goal [86] and correspondingly proposed the algorithm $R2$-EMOA which is able to steer the search towards preferred regions of the Pareto front by optimizing the $R2$ indicator directly in its environmental selection [85], [72].

6.7. Runtime Analyses of Interactive Evolutionary Algorithms

Participant from DOLPHIN: Dimo Brockhoff; External Participants: Manuel López-Ibáñez (Université Libre de Bruxelles, Belgium), Boris Naujoks (Cologne University of Applied Sciences, Germany), and Gunter Rudolph (TU Dortmund University, Germany)

[5] See http://www.sigevo.org/gecco-2012/papers.html.

If a decision maker (DM) expresses preferences, e.g., towards certain points or regions of the search space, during the algorithm run, we call such an algorithm *interactive*. Interactive algorithms are frequently used in the field of multi-criteria decision making, but theoretical results on interactive evolutionary multiobjective algorithms (EMOAs) have not been derived until recently. In [36], we started to analyze interactive versions of an evolutionary algorithm with plus-selection and a population size of one, the so-called iRLS and $i(1+1)$EA. On two pseudo-boolean problems, recently used for theoretically analyzing EMOAs, we could prove upper bounds on the expected runtime of the two mentioned algorithms and on the number of times, the DM is asked about his/her preferences until the most-preferred search point is found. The analyzes showed that the internal value function of the DM has a strong, non-desired influence on the algorithms' runtimes and that the number of questions to the DM are too high for a practical relevant algorithm. It is an open question which algorithm designs are necessary to circumvent these two drawbacks.

6.8. Benchmarking of CMA-ES Variants for Numerical Blackbox Optimization

Participant from DOLPHIN: Dimo Brockhoff; External Participants: Anne Auger and Nikolaus Hansen (Inria Saclay - Ile-de-France)

The covariance matrix adaptation evolution strategy (CMA-ES) is one of the state-of-the-art optimization algorithms for numerical single-objective blackbox optimization [81], [80] [67]. Previously, we proposed to use so-called mirrored mutations to generate new candidate solutions in evolution strategies which turned out to increase the convergence rate for certain variants [71], [65], [66]. Another recent approach to speed up the CMA-ES is to perform an active (i.e. negative) covariance matrix update [60]. In [32], [35], [34], [33], we tested empirically how the combination of mirrored mutations and active CMA-ES perform on the COCO framework [77], [78]. It turned out that both concepts complement each other well without a significant decrease in performance on any of the 24 test functions. Moreover, the main improvement over the standard CMA-ES could be shown to come from the active covariance matrix adaptation while the addition of mirrored mutations only slightly improves the algorithm.

6.9. Self-adaptive method for a three-objective vector-packing problem

Participants: Nadia Dahmani, François Clautiaux, El-Ghazali Talbi

We introduced a new multi-objective packing problem (MOBPP), in which we optimize the number of bins, the maximum weight of a bin, and the loading balancing. We studied the impact and the combination of two complementary decoding strategies for this problem. A feature of our work is to insert the parameters of the decoders in the representation of the solution. It leads to self-adaptive meta-heuristics, where the algorithm iteratively adapts the parameters during the search. We embedded our approaches in a local search and an evolutionary algorithm for the MOBPP. A comprehensive set of experiments were performed on various benchmarks inspired from the literature. Results confirm that our methods lead to more effective muti-objective metaheuristics for this problem.

6.10. Multiple Neighborhood Exploration Through Adaptive Search

Participants: Bilel Derbel, Houda Derbel, El-Ghazali Talbi, Hiba Yahyaoui

Variable neighborhood descent (VND) and its several variants are based on the systemic change of neighborhoods within the search. It is well known that the performance of a VND-like algorithm highly depends on the order/way the neighborhoods are alternated. In this work, we focus on designing new meta-strategies for deciding what neighborhood structure to apply through the search. Two new approaches are proposed to tackle this issue. In the first approach [41], we model the search by considering the neighborhood tree induced by alternating the use of different structures within a local search descent. We investigate the issue of designing a search strategy operating at the neighborhood tree level by exploring different paths of the tree in a heuristic way. We show that allowing the search to 'backtrack' to a previously visited solution and resuming the iterative variable neighborhood descent by 'pruning' the already explored neighborhood branches leads to the design of effective and efficient search heuristics. In the second approach, we investigate deterministic and randomized adaptive strategies for selecting the next neighborhood to apply at runtime. The adaptive strategies are based on computing a reward for each neighborhood with respect to the observed average ratio of solution quality and time cost.

6.11. CoBRA: A cooperative coevolutionary algorithm for bi-level optimization

Participants: François Legillon, Arnaud Liefooghe, El-Ghazali Talbi

In [43] we present CoBRA, a new evolutionary algorithm, based on a coevolutionary scheme, to solve bi-level optimization problems. It handles population-based algorithms on each level, each one cooperating with the other to provide solutions for the overall problem. Moreover, in order to evaluate the relevance of CoBRA against more classical approaches,a new performance assessment methodology, based on rationality, is introduced. An experimental analysis is conducted on a bi-level distribution planning problem, where multiple manufacturing plants deliver items to depots, and where a distribution company controls several depots and distributes items from depots to retailers. The experimental results reveal significant enhancements, particularly over the lower level, with respect to a more classical approach based on a hierarchical scheme.

6.12. Neutrality in the Graph Coloring Problem

Participants: Marie-Eléonore Marmion, Aymeric Blot, Laetitia Jourdan, and Clarisse Dhaenens

The graph coloring problem is often investigated in the literature. Many insights about the existence of many neighboring solutions with the same fitness value are raised but as far as we know, no deep analysis of this neutrality has ever been conducted in the literature. We have quantified the neutrality of some hard instances of the graph coloring problem. This neutrality property has to be detected as it impacts the search process. Indeed, local optima may belong to plateaus that represents a barrier for local search methods. We also aim at pointing out the interest of exploiting neutrality during the search. Therefore, a generic local search dedicated to neutral problems (NILS) and previously tested on flowshop problems, is performed and tested on several hard instances. Results show that taking into account neutrality allows to obtain better results than when not considering it.

6.13. Local Search in the Context of Classification Rule Mining

Participants: Julie Jacques, Laetitia Jourdan, Clarisse Dhaenens

Many multi-objective algorithms have been proposed to solve the classification rule mining problem; the vast majority of them are based on genetic algorithms. We propose an algorithm, MOCA - Multi-Objective Classification Algorithm -, to solve this problem. The originality of MOCA is to be a dominance-based multi-objective local search (DMLS) using a Pittsburgh representation of rules. We evaluated several DMLS implementations and neighborhood operators on literature datasets and one real dataset. Then we compared the best obtained algorithm against several efficient approaches of the literature. The experiments show that the proposed approach is very competitive in comparison to other algorithms tested. Moreover, our approach is able to deal with very large real datasets and manages to have a good accuracy.

6.14. MOCA-I: discovering rules and guiding decision maker in the context of partial classification in large and imbalanced datasets

Participants: Julie Jacques, Laetitia Jourdan, Clarisse Dhaenens

In this work we focus on the modeling and the implementation as a multi-objective optimization problem of a Pittsburgh classification rule mining algorithm adapted to large and imbalanced datasets, as encountered in hospital data. Indeed hospital data comes with problems such as class imbalance, volumetry or inconsistency, and optimization approaches have to take into account such specificities. We present MOCA-I, an adaptation of MOCA dedicated to this kind of problems. We propose its implementation as a dominance-based local search in opposition to existing multi-objective approaches based on genetic algorithms. We associate to this algorithm an original post-processing method based on the ROC curve to help the decision maker to choose the most interesting set of rules. Our approach is currently compared to state-of-the-art classification rule mining algorithms (both classic approaches such as C4.5 and optimization approaches), giving as good or better preliminary results, using less parameters. Moreover, our approach has been compared to C4.5 and C4.5-CS on a real dataset (hospital data) with a larger set of attributes, giving the best results. The complete evaluation is still going on.

6.15. A method to combine combinatorial optimization and statistics to mine high-throughput genotyping data

Participants : Julie Hamon, Clarisse Dhaenens, Julien Jacques (MODAL)

In the context of genomic analysis (collaboration with Genes Diffusion), dealing with high-throughput genotyping data, the objective of our study is to select a subset of SNPs (single nucleotide polymorphisms) explaining a trait of interest. We propose a method combining combinatorial optimization and statistics to extract a subset of interesting SNPs. The combinatorial part aims at exploring in an efficient way the large search space induced by the large number of possible subsets and statistics are used to evaluate the selection. We propose a first method based on an ILS (iterated local search) and using a regression. Three criteria used to evaluate the quality of the regression are compared. One of them (the k-fold validation) shows better performance. We also compare this approach to classical statistical approaches on simulated datasets. Results are promising as the proposed approach outperforms most of these statistical approaches [51].

6.16. Design and implementation of performance or energy-aware parallel optimization algorithms

Problems in practice are nowadays becoming more and more complex and time-intensive and their resolution requires to harness more and more computational resources. In parallel, the recent advances in hardware architecture enable to provide such required tremendous computational power through massively multi-core and GPU infrastructures. Such huge amount of cores is often provided through heterogeneous single or multi-clusters. The exploitation of such infrastructures clearly poses two fundamental and conflictual issues which are two major challenging perspectives of the Dolphin project that have been investigated during the 2012 year: (1) *Performance-aware issue*: how to design, implement and validate efficient and effective algorithms for such target machines to solve large size combinatorial optimization problems? ; (2) *Energy-aware issue*: using a large amount of computational resources for the deployment of large scale algorithms is energy-consuming. Therefore, the second issue is how to deal with the performance issue with a minimized cost in terms of energy consumption?
To deal with these issues, we have proposed new approaches summarized in the following sections.

6.16.1. Design and implementation of performance-aware optimization algorithms

In order to allow one to solve large size combinatorial optimization problems, we have revisited the design and implementation of meta-heuristics and exat (B&B) algorithms for two major hardware platforms: heterogeneous multi and many-core clusters and computational grids including multiple clusters.

- **Multi-core GPU-based hybrid meta-heuristics** - *Participants: T-V. Luong, N. Melab and E-G. Talbi.*

In [28], we have revisited the design and implementation of respectively single-solution and population-based meta-heuristics for single-core CPU coupled with a GPU device. We have investigated and proposed a new guidline for combining multi-core and GPU computing for hybrid meta-heuristics. Efficient approaches have been proposed for CPU-GPU data transfer optimization and task repartition between the GPU device and the CPU cores. Extensive experiments have been performed on an 8-core CPU coupled with a GPU card using Ant colonnies combined with a local serach applied to the Quadratic Assignment Problem (QAP). The reported results show that the use of multi-core computing, in addition to GPU computing, provides a performance improvement of up to 75%.

- **GPU-accelerated Branch-and-Bound algorithms** - *Participants: I. Chakroun and N. Melab.*
  Branch-and-Bound (B&B) algorithms are based on an implicit enumeration of a dynamically built tree-based search space. Pruning tree nodes (sub-problems) is traditionally used as a powerful mechanism to reduce the size of the explored search space. Such mechanism requires to perform the bounding operation which consists in applying a lower bound function to the generated sub-problems. Preliminary experiments performed on the Flow-Shop scheduling problem (FSP) have shown that the bounding operation consumes over 98% of the execution time of the B&B algorithm. Therefore, we have investigated the use of GPU computing as a major complementary way to speed up the search. We have revisited the design and implementation of the parallel bounding model for FSP on GPU accelerators dealing with two major issues: (1) thread divergence caused by the highly irregular nature of the explored tree and the SIMD execution model of GPU ; (2) data access optimization required for mapping efficiently different data structures on the hierarchy of memories provided in the GPU device. In [14], we have proposed a GPU-based parallel bounding model together with a data refactoring approach to deal with thread divergence. In [45] (an extended version submitted to the CCPE journal is being revised), we have proposed an efficient data optimization strategy based on a deep analysis of the complexity of the different data structures of the FSP lower bound algorithm in terms of memory size and access latency. The different proposed approaches for the two issues have been extensively experimented using and Nvidia Tesla C2050 GPU card. Compared to a CPU-based execution, accelerations up to more than $\times 100$ are achieved for large problem instances.
- **Peer-to-peer Branch-and-Bound algorithms** - *Participants: T-T. Vu, B. Derbel and N. Melab.*
  To deal with dynamic load balancing in large scale distributed systems, we have proposed in [50] to organize computing resources following a logical peer-to-peer overlay and to distribute the load according to the so-defined overlay. We have used a tree as a logical structure connecting distributed nodes and we balance the load according to the size of induced subtrees. We have conducted extensive experiments involving up to 1000 computing cores and provided a throughout analysis of different properties of our generic approach for two different applications, namely, the standard Unbalanced Tree Search and the more challenging parallel Branch-and-Bound algorithm. Substantial improvements are reported in comparison with the classical random work stealing and two finely tuned application specific strategies taken from the literature.

6.16.2. Design and implementation of energy-aware optimization algorithms

- Participants: Y. Kessaci, N. Melab and E-G. Talbi.
Cloud computing is an emerging computer science paradigm of distributed computing in which applications, data and infrastructures are proposed as a service that can be consumed in a ubiquitous, flexible and transparent way. Cloud computing brings with it such benefits via cloud managers which hide to the user some complex and challenging issues such as scheduling. However, the solutions to these issues provided in cloud managers are sometimes limited. For instance, the scheduling approach proposed in many cloud managers like OpenNebula is limited regarding the criteria taken into account. Energy consumption, which is highly critical for many applications such as High Performance Computing (HPC), is rarely considered. In [42] (selected for a special issue of FGCS journal) , we have addressed energy-aware scheduling of energy and time-consuming applications for cloud infrastructures. We have proposed a multi-start parallel

local search heuristic for cloud managers (EMLS-ONC) with the focus put on OpenNebula. EMLS-ONC has been experimented using different (VMs) arrival scenarii and different hardware infrastructures. The results show that EMLS-ONC outperforms the scheduler provided in OpenNebula by a significant margin in terms of energy consumption and number of scheduled VMs.

GEOSTAT Project-Team

6. New Results

6.1. Multiresolution analysis and optimal inference for high resolution ocean dynamics and ocean/atmosphere fluxes

Participants: Hussein Yahia [correspondant], Véronique Garçon, Oriol Pont, Joel Sudre, Christine Provost, Antonio Turiel, Christoph Garbe, Claire Pottier, Boris Dewitte.

A $p_{CO_2}^{ocean}$ signal computed as an output from the ROMS coupled physical/biogeochemical simulation model possesses the characteristics of the presence of a multiscale organization, typical of turbulence, which can be evidenced by the computation of singularity spectra. The multiscale organization is related to the cascading properties of intensive variables acquired from the underlying system. We show how to perform inference along the scales in order to build higher resolution of $p_{CO_2}^{ocean}$ maps. Figure 4 illustrates clearly one of the main ideas implemented in this study: coherent structures of $p_{CO_2}^{ocean}$ and SST (Sea Surface Temperature) signals are related, and the LPEs, which are dimensionless quantities recording transition strengths in a signal, encode properly the multiscale transitions.

Figure 4. Local Predictability Exponents (LPEs) of ROMS-simulated $p_{CO_2}^{ocean}$ signal (left) and of corresponding SST (Sea Surface Temperature) generated signal (right). Transitions are are visually and quantitatively correlated, although not the same.

We perform a linear regression test:

$$\mathcal{S}(p_{CO_2}^{ocean})(x) = a(x)\mathcal{S}(SST)(x) + b(x)\mathcal{S}(CHLa)(x) + c(x) \quad (5)$$

with $\mathcal{S}(p_{CO_2}^{ocean})(x)$: LPE of $p_{CO_2}^{ocean}$ at x, $\mathcal{S}(SST)(x)$: LPE of SST at x, $\mathcal{S}(CHLa)(x)$: LPE of CHLa signal at x (CHLa: ocean colour data, corresponding to chlorophyl concentration). Tests are conducted over a period of 10 years on ROMS simulated data, with images corresponding to 128×128 pixels for the high resolution and 32×32 for the low resolution. There is one data every 10 days. In figure 5 we compare the functional dependencies of $p_{CO_2}^{ocean}$ vs. SST and CHLa with those of the corresponding LPEs: the original signals are physical variables of different dimensions, with complex undetermined functional dependencies. On the contrary, the dimensionless LPEs of these variables, which record the multiscale transitions, display clearly a much simpler dependency, approximated at satisfactory precision by a linear regression.

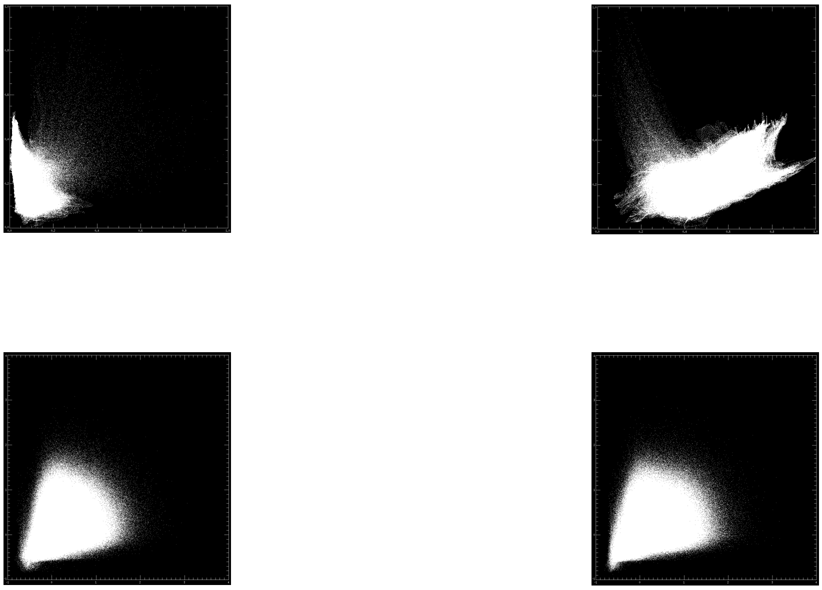


Figure 5. Pictures indicating the nature of the functional dependencies of $p_{CO_2}^{ocean}$ vs. CHLa (top left), of $p_{CO_2}^{ocean}$ vs. SST (top right), of $\mathcal{S}(p_{CO_2}^{ocean})$ vs $\mathcal{S}(CHLa)$ (bottom left) and of $\mathcal{S}(p_{CO_2}^{ocean})$ vs $\mathcal{S}(SST)$ (bottom right). The dependencies are computed on a 10-year ROMS simulation dataset, with a time frequency of one every 10 days.

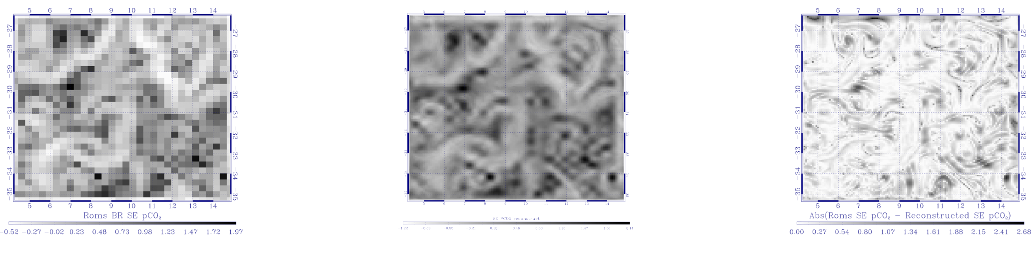


Figure 6. Left : the low resolution version of LPEs for $\mathcal{S}(p_{CO_2}^{ocean})$. Middle: result of the reconstruction. Right: absolute difference map between the ROMS generated high resolution LPEs and the reconstructed.

We prove the feasibility of a reconstruction by computing the high resolution LPEs $\mathcal{S}(p_{CO_2}^{ocean})(x)$ from their low resolution counterparts and an effective multiresolution analysis, using only an approximation of the optimal wavelet in the form of a Battle-Lemarié 3-31 mother wavelet. We show in figure 6 the results obtained by inference along the scales. The reconstructed LPEs of $p_{CO_2}^{ocean}$ are in good correspondence with the original high resolution signal.

- Related publications: [15], [16], [24], [14].

6.2. Singularity analysis and reconstructible systems

Participants: Oriol Pont [correspondant], Hussein Yahia, Antonio Turiel.

The local singularity exponents of a signal are directly related to the distribution of information in it. This fact implies that accurate evaluation of such exponents opens the door to signal reconstruction and characterisation of the dynamical parameters of the process originating the signal. Many practical implications arise in a context of digital signal processing, since the information on singularity exponents is usable for compact encoding, reconstruction and inference. The evaluation of singularity exponents in a digital context is not straightforward and requires the calculation of the Unpredictable Point Manifold of the signal. In this work, we present an algorithm for estimating the values of singularity exponents at every point of a digital signal of any dimension. We show that the key ingredient for robust and accurate reconstructibility performance lies on the definition of multiscale measures in the sense that they encode the degree of singularity and the local predictability at the same time. See figure 7 .

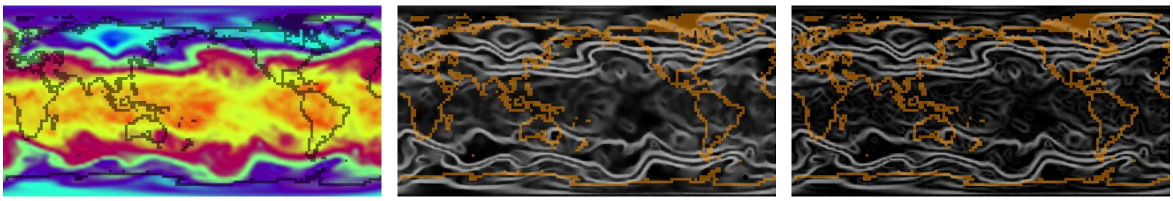


Figure 7. Left: 876576th hour slice of ERA-40 artificially rescaled 4x with bicubic interpolation for the purpose of clarity of illustration. Middle: singularity exponents calculated only in the space. Some rescaling artefacts visibly appear but without significant disturbance of the fine structure details. Right: singularity exponents calculated in the space-time domain. Notice the increased degree of detail when the temporal information is taken into account.

- Related publication: [13].

6.3. Multiscale analysis of the heart electric potential: describing atrial fibrillation

Participants: Oriol Pont [correspondant], Hussein Yahia, Rémi Dubois.

The cardiac electrical activity is a complex system, for which nonlinear signal-processing is required to characterize it properly. In this context, an analysis in terms of singularity exponents is shown to provide compact and meaningful descriptors of the structure and dynamics. In particular, singularity components reconstruct the epicardial electric potential maps of human atria, inverse-mapped from surface potentials; such approach describe sinus-rhythm dynamics as well as atrial flutter and atrial fibrillation. See figure 2 .

- Related publications: [12], [20], [23].

6.4. Edges, transitions and criticality

Participants: Suman Maji [correspondant], Hussein Yahia.

In this work, various notions of edges encountered in digital image processing are reviewed in terms of compact representation (or completion). We show that critical exponents defined in Statistical Physics lead to a much more coherent definition of edges, consistent across the scales in acquisitions of natural phenomena, such as high resolution natural images or turbulent acquisitions. Edges belong to the multiscale hierarchy of an underlying dynamics, they are understood from a statistical perspective well adapted to fit the case of natural images. Numerical computation methods for the evaluation of critical exponents in the non-ergodic case are recalled, which apply for the vast majority of natural images. We study the framework of reconstructible systems in a microcanonical formulation, show how it redefines edge completion, and how it can be used to evaluate and assess quantitatively the adequation of edges as candidates for compact representations. We study with particular attention the case of turbulent data, in which edges in the classical sense are particularly challenged. Tests are conducted and evaluated on a standard database for natural images. We test the newly introduced compact representation as an ideal candidate for evaluating turbulent cascading properties of complex images, and we show better reconstruction performance than the classical tested methods. See figure 8
.

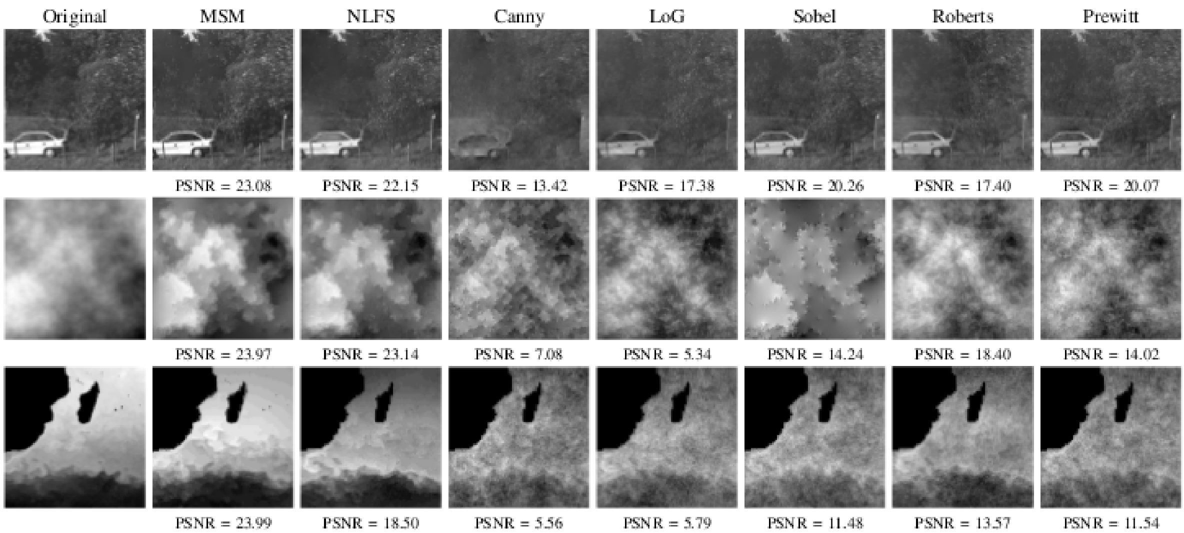


Figure 8. From left to right in each line: an original input image, and the reconstruction performed on the outputs resulting from various edge detection algorithms, showing the superiority of edge pixels computed from the Microcanonical Multiscale Formalism (column MSM). Note that NLFS [32], which is based on nonlinear filtering, performs the best after MSM.

6.5. Reconstruction of Optical phase from acquired sub-image gradients

Participants: Suman Maji [correspondant], Hussein Yahia, Thierry Fusco.

Turbulence in the Earth's atmosphere leads to a distortion in the planar wavefront from outer space resulting in a phase error. This phase error is responsible for the refractive blurring of images accounting to the loss in spatial resolution power of ground based telescopes. The common mechanism used to remove phase error from incoming wavefront is Adaptive Optics (AO). In AO systems, an estimate of the phase error is obtained from the gradient measurements of the wavefront collected by a Hartmann-Shack (HS) sensor. The correction estimate is then passed through a servo-control loop to a deformable mirror which compensates for the loss in resolution power. In this work, we propose a new approach to reconstructing the phase error from the HS

Table 1: Evaluation of the reconstructed phase under different levels of noise.

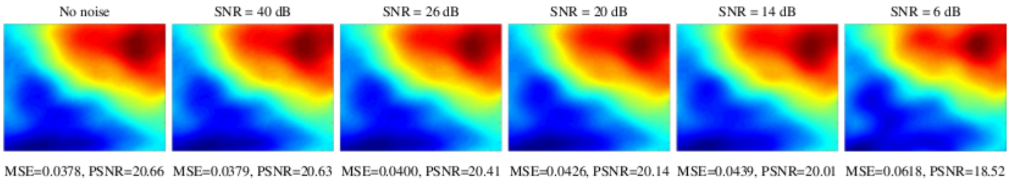


Table 2: Evaluation of the reconstructed phase using log power spectrum (**row 1**) and atmospheric structure functions (**row 2**).

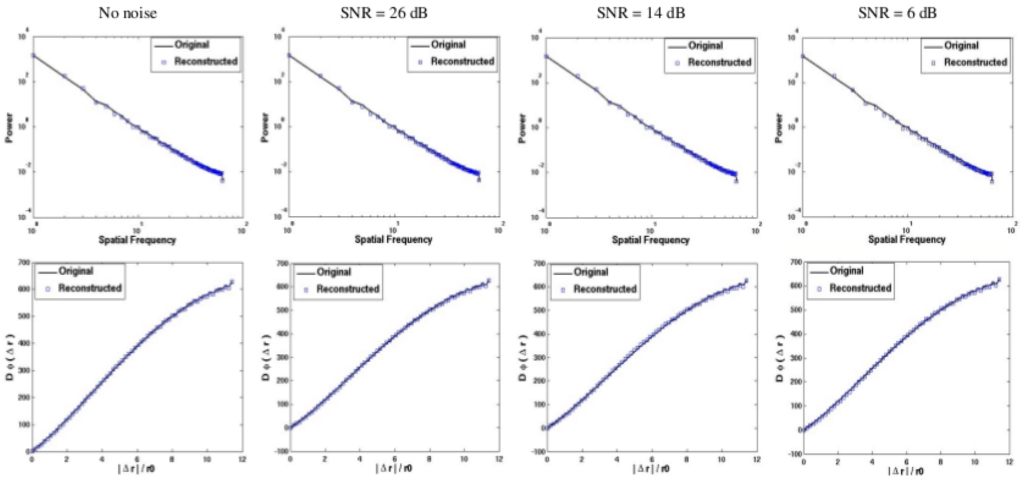


Figure 9. Results showing the robustness of the multiscale phase reconstruction algorithm for Adaptive Optics (AO) under various conditions of noise.

gradient measurements using the MMF. We also validate the results using standard validation techniques in Adaptive Optics (log power spectrum, structure functions). See figure 9 .

- Related publications: [18], [19].

6.6. Discriminative learning for Automatic speaker recognition

Participants: Reda Jourani [correspondant], Khalid Daoudi, Régine André-Obrecht, Driss Aboutajdine.

We continued our work aiming at developing efficient versions of Large Margin Gaussian Mixture Models (LM-GMM) for speaker identification. We developed a new and efficient learning algorithm and evaluated it on NIST-SRE'2006 data. The results show that, combined with the channel compesentation technique SFA, this new algorithm outperforms the state-of-the-art discriminative method GMM-supervectors SVM combined with NAP compensatation.

- Related publication: [10].

6.7. Speech Analysis

Participants: Vahid Khanagha [correspondant], Khalid Daoudi, Hussein Yahia, Oriol Pont.

- Development of a GCI detection algorithm (Vahid Khanagha, Khalid Daoudi, Hussein Yahia). According to the aerodynamic theory of voicing, the excitation source for voiced speech sounds is represented as glottal pulses, which to a first approximation, can be considered to occur at discrete instants of time. This major excitation usually coincides with the Glottal Closure Instants (the GCIs). The precise detection of GCIs has found many applications in speech technology: accurate estimation of vocal tract system, pitch marking of speech for pitch synchronous speech processing algorithms, conversion of pitch and duration of speech recordings, prosody modification and synthesis. We use the MMF for detection of these physically important instants. To do so, we study the correspondence of the Most Singular Manifold with the physical production mechanism of the speech signal and we show that this subset can be used for GCI detection. We show that, in clean speech, our algorithm has similar performance to recent methods and, in noisy speech, it significantly outperforms state-of-the-art methods. Indeed, as our algorithm is based on both time domain and inter-scale smoothings, it provides higher robustness against many types of noises. In the mean-time, the high geometrical resolution of singularity exponents prevents the accuracy to be compromised. Moreover, the algorithm extracts GCIs directly from the speech signal and does not rely on any model of the speech signal (such as the autoregressive model in linear predictive analysis). See figure 10 .
- Development of an efficient algorithm for sparse Linear Prediction Analysis (Vahid Khanagha, Khalid Daoudi). We address the problem of sparse Linear Prediction (LP) analysis, which involves the estimation of vocal tract model such that the corresponding LP residuals are as sparse as possible: for voiced sounds, one desires the residual to be zero all the time, except for few impulses at GCIs. Sparse Linear Prediction Analysis (LPA) problem has recently got much scientific attention and its classical solutions suffer from computational and algorithmic complexties. We introduce a simple closed-form solution in this chapter which is based on the minimization of weighted l_2-norm of residuals. The weighting function plays the most important role in our solution in maintaining the sparsity of the resulting residuals. We use our MSM-based GCI detector to extract from the speech signal itself, the points having the potential of attaining largest norms of residuals and then we construct the weighting function such that the prediction error is relaxed on these points. Consequently, the weighted l_2-norm objective function can be efficiently minimized by the solution of normal equations of liner least squares problem. The choice of our MSM-based GCI detector is particularly justified, considering the fact that most of the successful GCI detection methods actually use LP residuals for their detection and hence, they cannot be used for constraining the LP problem. Our algorithm is completely independent of any model that might be assumed for speech signal. We will see that when compared to classical techniques, our simple algorithm provides better sparseness

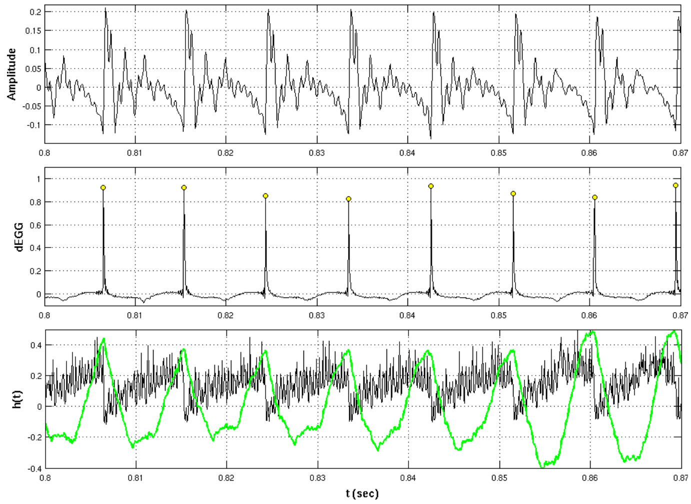


Figure 10. Top: a voiced segment of the speech signal taken from KED database. Middle: the differenced Electro-Glotto-Graph signal which serves for extraction of reference GCI points. The peaks are marked with yellow circles as the reference GCIs. Bottom: singularity exponents are shown by black color and an auxiliary functional showing changes in DC level of exponents is shown in green. The local minima of singularity exponents within each positive half-period of the auxiliary functional are taken as GCIs.

properties and does not suffer from usual instabilities. We also present an experiment to show how such sparse solution may result in more realistic estimates of the vocal tract by decoupling of the contributions of the excitation source from that of the vocal tract filter. See figure 11 .

- Multi-pulse estimation of speech excitation source (Vahid Khanagha, Khalid Daoudi). In the GCI detector algorithm, the cardinality of MSM was restricted to one sample per pitch period. We then proceed to study the significance of MSMs of higher cardinalities, in the framework of multi-pulse estimation of voiced sound excitation source. Multi-pulse source coding has been widely used and studied within the framework of Linear Predictive Coding (LPC). It consists in finding a sparse representation of the excitation source (or residual) which yields a source-filter reconstruction with high perceptual quality. The MultiPulse Excitation (MPE) method is the first and one of the most popular techniques to achieve this goal. MPE provides a sparse excitation sequence through an iterative Analysis-by-Synthesis procedure to find the position and amplitudes of the excitation source in two stages: first the location of pulses are estimated one at a time by minimization of perceptually wieghted reconstruction error. In the second stage, the amplitude of these pulses are jointly re-optimized to find the optimal pulse values. Using the MSM, we propose a novel approach to find the locations of the multi-pulse sequence that approximates the speech source excitation. We consider locations of MSM points as the locations of excitation impulses and then, the amplitude of these impulses are computed using the second stage of the classical MPE coder by minimization of the spectrally weighted mean squared error of reconstruction. The multi pulse sequence is then fed to the classical LPC synthesizer to reconstruct speech. Our algorithm is more efficient than classical methods, while providing the same level of perceptual quality as the classical MPE method. See figure 12 .
- Speech representation based local singularity analysis (Vahid Khanagha, Khalid Daoudi, Hussein Yahia, Oriol Pont). Precise estimation of singularity exponents unlocks the determination a collection of points inside the complex signal which are considered as the least predictable points (the MSM). This leads to the associated compact representation and reconstruction. This work presents the very first steps in establishing the links between the MSM and the speech signal. To do so, we make slight modifications to the formalism so as to adapt it to the particularities of the speech signal. Indeed,

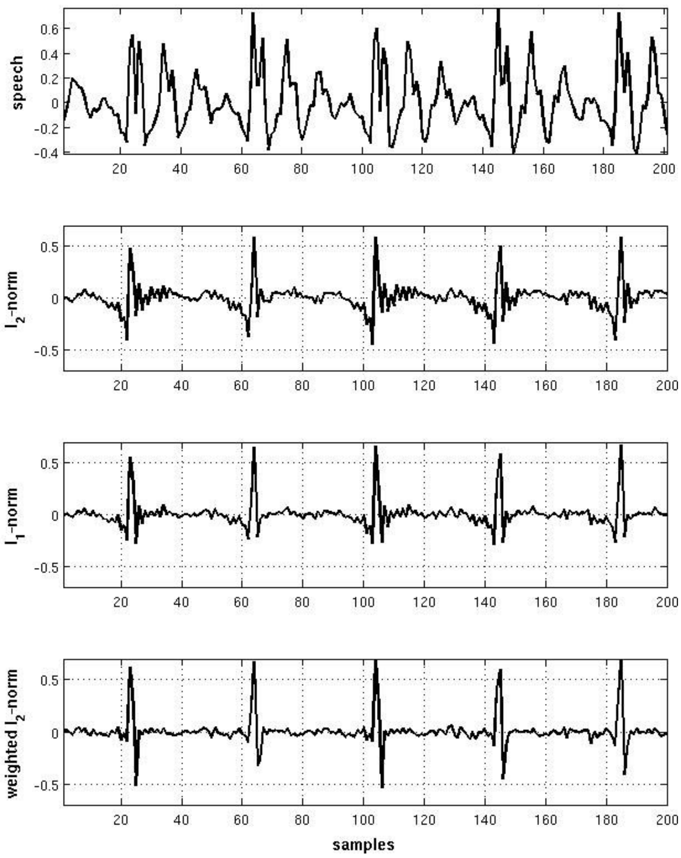


Figure 11. The residuals of the LP analysis obtained from different optimization strategies.

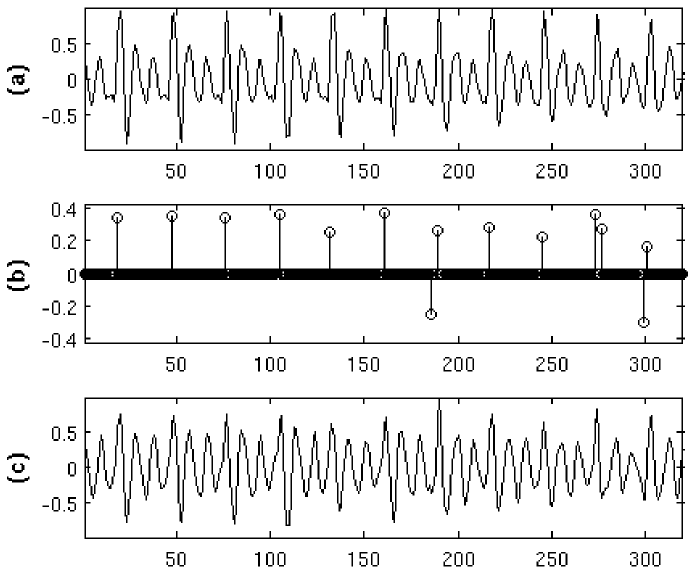


Figure 12. (a) a 40 ms segment of stationary voiced speech, (b) the MSM excitation sequence using 7 pulses per 20 ms and (c) the corresponding reconstructed signal.

the complex intertwining of different dynamics in speech (added to purely turbulent descriptions) suggests the definition of appropriate multi-scale functionals that might influence the evaluation of SEs, hence resulting in a more parsimonious MSM. We present a study that comforts these observations: we show that an alternative multi-scale functional does lead to a more parsimonious MSM from which the whole speech signal can be reconstructed with good perceptual quality. As MSM is composed of a collection of irregularly spaced samples, we use a classical method for the interpolation of irregularly spaced samples, called the Sauer-Allebach algorithm, to reconstruct the speech signal from its MSM. We show that by using this generic algorithm [and even by slight violation of its conditions] high quality speech reconstruction can still be achieved from a MSM of low cardinality. This shows that the MSM formed using the new multi-scale functional we define, indeed can give access to a subset of potentially interesting points in the domain of speech signal. Finally, in order to show the potential of this parsimonious representation in practical speech processing applications, we quantize and encode the MSM so as to develop a waveform coder. See figure 13 .

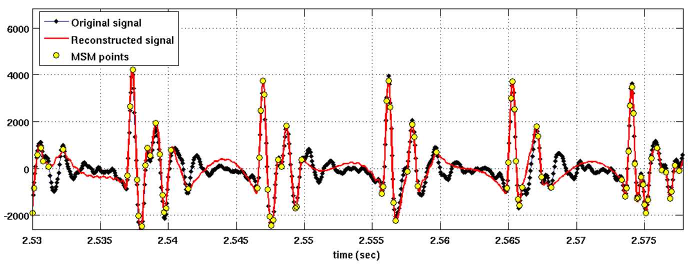


Figure 13. Waveforms of the original signal and the reconstructed signal. Samples belonging to MSM are marked with yellow circles.

- Related publications: [10], [17], [11].

6.8. Reconstruction and gradient-based video editing

Participants: Hicham Badri [correspondant], Hussein Yahia, Driss Aboutajdine.

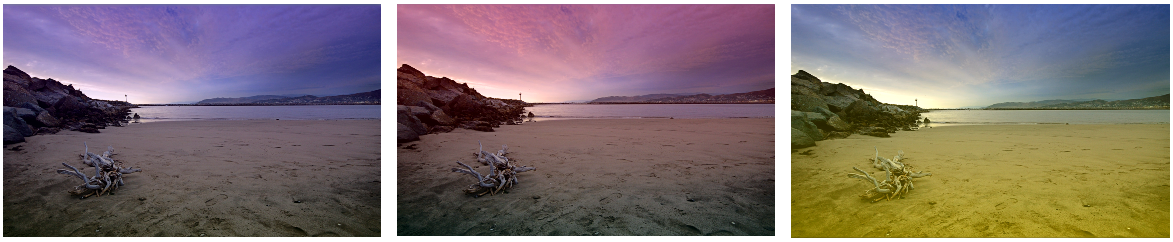


Figure 14. From left to right: original image and examples of non-photoralistic rendering.

Figure 15. Top left: original image. Top right: object removal with FFT-reconstruction algorithm. Botton left: object removal with MVC (Mean Value Coordinates) algorithm. Bottom right: object removal by numerical solving of Poisson equation.

Gradient-domain methods have become a standard for many computational photography applications including object cloning, panorama stitching and non-photorealistic rendering. Integration from a vector field is required to perform gradient-domain-based applications and this operation must be fast enough for interactive editing. The most popular way to perform this integration is known as the Poisson equation and requires solving a large linear system that becomes more costly as the region of interest becomes larger. We propose to use an FFT-based solution and the framework of reconstructible systems instead of performing interactive local/global editing in the gradient domain on the CPU/GPU for both images and videos. See figures 14 , 15 .

- Related publication: [21].

MISTIS Project-Team

6. New Results

6.1. Mixture models

6.1.1. Taking into account the curse of dimensionality

Participant: Stéphane Girard.

Joint work with: Bouveyron, C. (Université Paris 1), Fauvel, M. (ENSAT Toulouse)

In the PhD work of Charles Bouveyron (co-advised by Cordelia Schmid from the Inria LEAR team) [53], 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]. Also, the description of the R package is published in [11]. Our recent work consists in adding a kernel in the previous methods to deal with nonlinear data classification [27], [45].

6.1.2. Robust mixture modelling using skewed multivariate 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). In such cases, the multivariate student t distribution is motivated as a heavy-tailed alternative to the multivariate Gaussian distribution. The additional flexibility of the multivariate t comes from introducing an additional degree of freedom parameter (dof) which can be viewed as a robust tuning parameter.

A useful representation of the t-distribution is as a so-called *infinite mixture of scaled Gaussians* or *Gaussian scale mixture*,

$$p(y;\mu,\Sigma,\theta) = \int_0^\infty \mathcal{N}_M(y;\mu,\Sigma/w)\; f_W(w;\theta)\;\mathrm{d}w \qquad (6)$$

where $\mathcal{N}_M(\,.\,;\mu,\Sigma/w)$ denotes the M-dimensional Gaussian distribution with mean μ and covariance Σ/w and f_W is the probability distribution of a univariate positive variable W referred to as the weight variable. When f_W is a Gamma distribution $\mathcal{G}(\nu/2,\nu/2)$ where ν denotes the degrees of freedom, we recover the multivariate t distribution. The weight variable W in this case effectively acts to govern the tail behaviour of the distributional form from light tails ($\nu\to\infty$) to heavy tails ($\nu\to 0$) depending on the value of ν.

For many applications, the distribution of the data may also be highly asymmetric in addition to being heavy tailed (or affected by outliers). A natural extension to the Gaussian scale mixture case is to consider *location and scale Gaussian mixtures* of the form,

$$p(y;\mu,\Sigma,\theta)=\int_0^\infty \mathcal{N}_M(y;\mu+w\beta\Sigma,w\Sigma)\; f_W(w;\theta)\;\mathrm{d}w, \qquad (7)$$

where β is an additional M-dimensional vector parameter for skewness and the determinant of Σ equals 1 for parameter identifiability. When f_W is a Generalized Inverse Gaussian distribution ($GIG(y;\lambda,\delta,\gamma)$, we recover the family of Generalized Hyperbolic (GH) distributions. Depending on the parameter choice for the GIG, special cases of the GH family, include: the multivariate GH distribution with hyperbolic margins ($\lambda=1$); the normal inverse Gaussian distribution ($\lambda=-1/2$); the multivariate hyperbolic ($\lambda=\frac{M+1}{2}$) distribution; the hyperboloid distribution ($\lambda=0$); the hyperbolic skew-t distribution ($\lambda=-\nu,\gamma=0$); and the normal gamma distribution ($\lambda>0,\mu=0,\delta=0$)) amongst others. For applied problems, the most popular of these forms appears to be the Normal Inverse Gaussian (NIG) distribution, with extensive use in financial applications. Another distributional form allowing for skewness and heavy or light tails includes different forms of the multivariate skew-t. Most of these distributional forms are also able to be represented as *location and scale Gaussian mixtures*.

Although the above approaches provide for great flexibility in modelling data of highly asymmetric and heavy tailed form the above approaches assume f_W to be a univariate distribution and hence each dimension is governed by the same amount of tailweight. There have been various approaches to address this issue in the statistics literature for both symmetric and asymmetric distributional forms. In his work, [66] proposes a dependent bivariate t-distribution with marginals of different degrees of freedom but the tractability of the extension to the multivariate case is unclear. Additional proposals are reviewed in chapters 4 and 5 of [67] but these formulations tend to be appreciably more complicated, often already in the expression of the probability density function. Increasingly, there has been much research on copula approaches to account for flexible distributional forms but the choice as to which one to use in this case and the applicability to (even) moderate dimensions is also not clear. In general the papers take various approaches whose relationships have been characterized in the bivariate case by [73]. However, most of the existing approaches suffer either from the non-existence of a closed-form pdf or from a difficult generalization to more than two dimensions.

In this work, we show that the location and scale mixture representation can be further explored and propose a framework that is considerably simpler than those previously proposed with distributions exhibiting interesting properties. Using the normal inverse Gaussian distribution (NIG) as an example, we extend the standard *location and scale mixture of Gaussian representation* to allow for the tail behaviour to be set or estimated differently in each dimension of the variable space. The key elements of the approach are the introduction of multidimensional weights and a decomposition of the matrix Σ in (6) which facilitates the separate estimation and also allows for arbitrary correlation between dimensions. We outline an approach for maximum likelihood estimation of the parameters via the EM algorithm and explore the performance of the approach on several simulated and real data sets in the context of clustering.

6.1.3. Robust clustering for high dimensional data

Participants: Florence Forbes, Darren Wraith, Minwoo Lee.

For a clustering problem, a parametric mixture model is one of the popular approaches. Most of all, Gaussian mixture models are widely used in various fields of study such as data mining, pattern recognition, machine learning, and statistical analysis. The modeling and computational flexibility of the Gaussian mixture model makes it possible to model a rich class of density, and provides a simple mathematical form of cluster models.

Despite the success of Gaussian mixtures, the parameter estimations can be severely affected by outliers. By adding an additional degrees of freedom (dof) parameter, a robustness tuning parameter, the robust improvement in clustering has been achieved. Although adopting t distribution loses the closed-form solution, it is still tractable by representing t distribution as Gaussian scale mixture (GSM), which consists of a Gaussian random vector that is weighted by a hidden scaling variable. Recent work that uses the multivariate t distribution has showed the improved robustness.

Along with robustness from t distribution, for the practical use, efficient handling of a high dimensional data is critical. High dimensional data often make most of clustering methods perform poorly. To overcome the curse of dimensionality, Bouveyron et al. [54] proposed the model-based high dimensional data clustering (HDDC). HDDC searches the intrinsic dimension of each class with the BIC criterion or the scree-test of Cattell; this allows them to limit the number of parameters by taking into account only the specific subspace that each class is located. The parameterization makes HDDC not only computationally efficient but robust with respect to the ill-conditioning or the singularity of empirical covariance matrix.

This work proposes an approach that combines robust clustering with the HDDC. The use of the mixture of multivariate t distribution on the basis of HDDC develops robust high dimensional clustering methods that can capture various kinds of density models. Further, extending the mixture model with multiple t distributions for each dimension, we propose more flexible model that can be applicable to various data. We suggest a model-based approach for this method.

6.1.4. Partially Supervised Mapping: A Unified Model for Regression and Dimensionality Reduction

Participant: Florence Forbes.

Joint work with: Antoine Deleforge and Radu Horaud from the Inria Perception team.

We cast dimensionality reduction and regression in a unified latent variable model. We propose a two-step strategy consisting of characterizing a non-linear *reversed* output-to-input regression with a generative piecewise-linear model, followed by Bayes inversion to obtain an output density given an input. We describe and analyze the most general case of this model, namely when only some components of the output variables are observed while the other components are latent. We provide two EM inference procedures and their initialization. Using simulated and real data, we show that the proposed method outperforms several existing ones.

6.1.5. Variational EM for Binaural Sound-Source Separation and Localization

Participant: Florence Forbes.

Joint work with: Antoine Deleforge and Radu Horaud from the Inria Perception team.

We addressed the problem of sound-source separation and localization in real-world conditions with two microphones. Both tasks are solved within a unified formulation using supervised mapping. While the parameters of the direct mapping are learned during a training stage that uses sources emitting white noise (calibration), the inverse mapping is estimated using a variational EM formulation. The proposed algorithm can deal with natural sound sources such as speech which are known to yield sparse spectrograms, and is able to locate multiple sources both in azimuth and in elevation. Extensive experiments with real data show that the method outperform state-of-the-art both in separation and localization.

6.2. Statistical models for Neuroscience

6.2.1. Variational approach for the joint estimation-detection of Brain activity from functional MRI data

Participants: Florence Forbes, Lotfi Chaari, Thomas Vincent.

Joint work with: Michel Dojat (Grenoble Institute of Neuroscience) and Philippe Ciuciu from Neurospin, CEA in Saclay.

In standard within-subject analyses of event-related fMRI data, two steps are usually performed separately: detection of brain activity and estimation of the hemodynamic response. Because these two steps are inherently linked, we adopt the so-called region-based Joint Detection-Estimation (JDE) framework that addresses this joint issue using a multivariate inference for detection and estimation. JDE is built by making use of a regional bilinear generative model of the BOLD response and constraining the parameter estimation by physiological priors using temporal and spatial information in a Markovian model. In contrast to previous works that use Markov Chain Monte Carlo (MCMC) techniques to sample the resulting intractable posterior distribution, we recast the JDE into a missing data framework and derive a Variational Expectation-Maximization (VEM) algorithm for its inference. A variational approximation is used to approximate the Markovian model in the unsupervised spatially adaptive JDE inference, which allows automatic fine-tuning of spatial regularization parameters. It provides a new algorithm that exhibits interesting properties terms of estimation error and computational cost compared to the previously used MCMC-based approach. Experiments on artificial and real data show that VEM-JDE is robust to model mis-specification and provides computational gain while maintaining good performance in terms of activation detection and hemodynamic shape recovery. Main corresponding paper [13]

6.2.2. Hemodynamic-informed parcellation of fMRI data in a Joint Detection Estimation framework

Participants: Florence Forbes, Lotfi Chaari, Thomas Vincent.

Joint work with: Philippe Ciuciu from Team Parietal and Neurospin, CEA in Saclay.

Identifying brain hemodynamics in event-related functional MRI (fMRI) data is a crucial issue to disentangle the vascular response from the neuronal activity in the BOLD signal. This question is usually addressed by estimating the so-called Hemodynamic Response Function (HRF). Voxelwise or region-/parcelwise inference schemes have been proposed to achieve this goal but so far all known contributions commit to pre-specified spatial supports for the hemodynamic territories by defining these supports either as individual voxels or a priori fixed brain parcels. In this paper, we introduce a Joint Parcellation-Detection-Estimation (JPDE) procedure that incorporates an adaptive parcel identification step based upon local hemodynamic properties. Efficient inference of both evoked activity, HRF shapes and *supports* is then achieved using variational approximations. Validation on synthetic and real fMRI data demonstrate the JPDE performance over standard detection estimation schemes and suggest it as a new brain exploration tool. Corresponding papers [29], [28].

6.2.3. 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. 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 [25]. Corresponding paper [26].

6.2.4. Bayesian BOLD and perfusion source separation and deconvolution from functional ASL imaging

Participants: Florence Forbes, Thomas Vincent.

In the context of ARC AINSI project, joint work with: Philippe Ciuciu from Neurospin, CEA in Saclay.

In many neuroscience applications, the Arterial Spin Labeling (ASL) fMRI modality arises as a preferable choice to the standard BOLD modality due to its ability to provide a quantitative measure of the Cerebral Blood Flow (CBF). Such a quantification is central but generally performed without consideration of a specific modeling of the perfusion component in the signal often handled via standard GLM approaches using the BOLD canonical response function as regressor. In this work, we propose a novel Bayesian hierarchical model of the ASL signal which allows activation detection and both the extraction of a perfusion and a hemodynamic component. Validation on synthetic and real data sets from event-related ASL show the ability of our model to address the source separation and double deconvolution problems inherent to ASL data analysis.

6.2.5. Extraction of physiological components in functional ASL data

Participants: Florence Forbes, Thomas Vincent, Lotfi Chaari, Marc Guillotin.

In the context of ARC AINSI project, joint work with: Jan Warnking (Grenoble Institute of Neuroscience) and Philippe Ciuciu from Neurospin, CEA in Saclay.

The internship of Marc Guillotin has been supported by Le pole Cognition de Grenoble.

The goal of this work was to investigate Independent component analysis techniques to identify the part of the ASL signal due to physiological sources such as respiratory and cardiac components. Once identified those physiological components should be removed to produce an uncontaminated ASL signal. This preliminary work showed that the physiological effects were affecting all signal components and were therefore not easy to extract without removing some of the useful signal. More experiments should be made on real data from the GIN.

6.2.6. Comparison of processing workflows for ASL data analysis

Participant: Thomas Vincent.

In the context of ARC AINSI project, joint work with: Michel Dojat (Grenoble Institute of Neuroscience), Philippe Ciuciu from Neurospin, CEA in Saclay, Remi Dubujet, Elise Bannier, Isabelle Courouge, Christian Barillot, Camille Maudet from EPI Visages in Rennes.

We assessed and compared the performance of different ASL processing pipelines in order to promote one using specific indexes (Contrast to noise ratio, partial volume effect, et). We proposed to assess the impact of the pipelines based on the quality of the final corrected ASL images using a common set of subjects for all workflows. We leaned on the expertise of the Visages and GIN teams on ASL, and first started from existing attempts made in the teams. At the moment, there is a striking lack of such guidelines. The recent toolbox ASLtbx proposes a number of procedures that are based on very standard tools (e.g. SPM) and do not make use of more efficient approaches from more recent literature. Similarly, in the BIRN project, processing pipelines are mentioned but none are currently available.

6.3. Markov models

6.3.1. Spatial risk mapping for rare disease with hidden Markov fields and variational EM

Participants: Florence Forbes, Senan James Doyle.

Joint work with: Lamiae Azizi, David Abrial and Myriam Garrido from INRA Clermont-Ferrand-Theix.

Current risk mapping models for pooled data focus on the estimated risk for each geographical unit. A risk classification, *i.e.* grouping of geographical units with similar risk, is then necessary to easily draw interpretable maps, with clearly delimited zones in which protection measures can be applied. As an illustration, we focus on the Bovine Spongiform Encephalopathy (BSE) disease that threatened the bovine production in Europe and generated drastic cow culling. This example features typical animal disease risk analysis issues with very low risk values, small numbers of observed cases and population sizes that increase the difficulty of an automatic classification. We propose to handle this task in a spatial clustering framework using a non standard discrete hidden Markov model prior designed to favor a smooth risk variation. The model parameters are estimated using an EM algorithm and a mean field approximation for which we develop a new initialization strategy appropriate for spatial Poisson mixtures. Using both simulated and our BSE data, we show that our strategy performs well in dealing with low population sizes and accurately determines high risk regions, both in terms of localization and risk level estimation.

Main corresponding paper [14].

6.3.2. Spatial modelling of biodiversity from high-througput 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 EPI Bamboo

Biodiversity has been acknowledged as a vital ressource for ecosystem health and stability, faced with an unprecedented global decline. In order to be effective, conservation actions need to be based on reliable and fast analysis. Recent advances in DNA sequencing methods now enable DNA-based identification of multiple species from only few, even potentially degraded environmental samples (metabarcoding.org, [74]). This offers a new way of biodiversity assessment and is of particular interest where large-scale individual-based diversity assessment is difficult, for example in tropical environments. Due to their comparatively low demand in cost and effort, these methods are characterized by their high throughput; they are expected to produce vast amounts of data as they gain in popularity over the coming years. The specific properties of these data (e.g. bias from sequencing errors, notion of species) and their high dimensionality provides new statistical and computational challenges for biodiversity assessment. This project aims at extending existing summary statistics to be used with data from metabarcoding surveys and, where this is not adequate, to develop new methodology. A special focus is on the spatial mapping of biodiversity and the co-occurrence of species. In a first instance, we investigate spatial clustering algorithms based on Markov random fields (software SpaCEM3, http://spacem3.gforge.inria.fr/) to identify regions of high species occurrence as well as structured additive regression models and their implementation to estimate cross-correlations between species occurrences in space [61], [72], [71]. At present, results have been derived in form of species occurrence maps, which take into account pairwise cross-correlation, and interaction graphs.

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 dependencies 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 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. The graph building stage was based on exploring the space of possible chain graph models, which required defining a notion of neighbourhood of these graphs. A parametric distribution was associated with each graph. It was obtained by combining families of univariate and multivariate distributions or regression models. These were chosen by selection model procedures among different parametric families.

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. 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)

The aim of this work was to characterize genetic determinisms of the alternation of flowering in apple tree progenies. 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. Post-Reflow Automated Optical Inspection of Lead Defects

Participants: Florence Forbes, Kai Qin, Huu Giao Nguyen, Darren Wraith, Ludovic Leau-mercier.

This is joint work with VI-Technology in the context of the IVP project.

Quality and throughput in printed circuit board (PCB) assembly lines constitute a continuous challenge, especially when placing smaller components on boards that are becoming increasingly dense. Automated optical inspection (AOI) technology allows PCB assembly lines to keep operating at a high throughput while visually inspecting production quality in term of paste deposits, mounted components and solder joints in an automatic and non-contact manner. In the AOI, high definition cameras precisely move in both X- and Y-direction to scan the device under test lit by special lighting techniques, e.g. light-emitting diode (LED) lighting. The captured images are then analyzed using specific inspection algorithms to identify defects. The AOI systems can be placed at several stages during the manufacturing process, such as bare board inspection, solder paste inspection, pre-reflow inspection and post-reflow inspection, which usually need some time to be programmed via offline learning of verified boards and expert expertise before online inspection starts. Vi TECHNOLOGY (VIT) offers a wide range of AOI solutions to increase productivity throughout electronics manufacturing lines while enhancing the quality of products. Post-reflow AOI is implemented after the reflow procedure in PCB assembly lines to enable inspection of the major post-reflow defects. This work focus on certain types of post-reflow defects occurring on leaded components, i.e. lifted lead, no solder, excess of solder, contamination on lead, insufficient solder, bad wedding and dry joint. We aim at developing efficient post-reflow lead defect detection approaches by synergizing image analysis, pattern recognition, machine learning, and statistics techniques to improve performance of VIT commercial post-reflow AOI solutions from two aspects: 1) Reducing both detection escape rate and false detection rate; 2) Minimizing programming efforts. The exact nature of the work is confidential.

6.4.2. An Improved CUDA-Based Implementation of Differential Evolution on GPU

Participants: Kai Qin, Florence Forbes.

Modern GPUs enable widely affordable personal computers to carry out massively parallel computation tasks. NVIDIA's CUDA technology provides a wieldy parallel computing platform. Many state-of-the-art algorithms arising from different fields have been redesigned based on CUDA to achieve computational speedup. Differential evolution (DE), as a very promising evolutionary algorithm, is highly suitable for parallelization owing to its data parallel algorithmic structure. However, most existing CUDA based DE implementations suffer from excessive low-throughput memory access and less efficient device utilization. This work presents an improved CUDA-based DE to optimize memory and device utilization: several logically-related kernels are combined into one composite kernel to reduce global memory access; kernel execution configuration parameters are automatically determined to maximize device occupancy; streams are employed to enable concurrent kernel execution to maximize device utilization. Experimental results on several numerical problems demonstrate superior computational time efficiency of the proposed method over two recent CUDA-based DE and the sequential DE across varying problem dimensions and algorithmic population sizes.

This work was nominated for the best paper award (finalist) in the Digital Entertainment Technologies and Arts / Parallel Evolutionary Systems session of the Genetic and Evolutionary Computation Conference 2012 (GECCO12) conference [33].

6.4.3. Augmented cumulative distribution networks for multivariate extreme value modelling

Participants: Stéphane Girard, Gildas Mazo, Florence Forbes.

Max-stable distribution functions are theoretically grounded models for modelling multivariate extreme values. However they suffer from some striking limitations when applied to real data analysis due to the intractability of the likelihood when the number of variables becomes high. Cumulative Distribution Networks (CDN's) have been introduced recently in the machine learning community and allow the construction of max-stable distribution functions for which the density can be computed. Unfortunately, we show in this work that the dependence structure expected in the data may not be accurately reflected by max-stable CDN's. To face this limitation, we therefore propose to augment max-stable CDN's with the more standard Gumbel max-stable distribution function in order to enrich the dependence structure [32].

6.4.4. Modelling extremal events

Participants: Stéphane Girard, Jonathan El-Methni, El-Hadji Deme.

Joint work with: Guillou, A. and Gardes, L. (Univ. Strasbourg).

We introduced a new model of tail distributions depending on two parameters $\tau \in [0,1]$ and $\theta > 0$. This model includes very different distribution tail behaviors from Fréchet and Gumbel maximum domains of attraction. In the particular cases of Pareto type tails ($\tau = 1$) or Weibull tails ($\tau = 0$), our estimators coincide with classical ones proposed in the literature, thus permitting us to retrieve their asymptotic normality in an unified way. The first year of the PhD work of Jonathan El-methni has been dedicated to the definition of an estimator of the parameter τ. This permits the construction of new estimators of extreme quantiles. The results are published in [17]. Our future work will consist in proposing a test procedure in order to discriminate between Pareto and Weibull tails.
We are also 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 [64], [63]). This work is in collaboration with El-Hadji Deme, a PhD student from the Université de Saint-Louis (Sénégal). El-Hadji Deme obtained a one-year mobility grant to work within the Mistis team on extreme-value statistics. The results are submitted for publication [49]. We also proposed reduced-bias estimators of the Proportional Hazard Premium for heavy-tailed distributions. The results are submitted for publication [50].

6.4.5. Conditional extremal events

Participants: Stéphane Girard, Gildas Mazo, Jonathan El-methni.

Joint work with: L. Gardes, Amblard, C. (TimB in TIMC laboratory, Univ. Grenoble I) and Daouia, A. (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 [59] 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) and the tail of the distribution is heavy, we focus on kernel methods [18]. We extension to all kind of tails in investigated in [15].

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.

More future work will include the study of multivariate and spatial extreme values. With this aim, a research on some particular copulas [1] has been initiated with Cécile Amblard, since they are the key tool for building multivariate distributions [69]. The PhD theses of Jonathan El-methni and Gildas Mazo should address this issue too.

6.4.6. Level sets estimation

Participant: Stéphane Girard.

Joint work with: Guillou, A. and Gardes, L. (Univ. Strasbourg), Stupfler, G. (Univ. Strasbourg) and Daouia, A. (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].
In collaboration with A. Daouia, we investigate the application of such methods in econometrics [42], [48]: 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 the PhD thesis of Gilles Stupfler (co-directed by Armelle Guillou and Stéphane Girard), 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 [19], [20], [21].

6.4.7. Quantifying uncertainties on extreme rainfall estimations

Participant: Stéphane Girard.

Joint work with: Carreau, J. (Hydrosciences Montpellier), Gardes, L. (univ. Strasbourg) and Molinié, G. from Laboratoire d'Etude des Transferts en Hydrologie et Environnement (LTHE), France.

Extreme rainfalls are generally associated with two different precipitation regimes. Extreme cumulated rainfall over 24 hours results from stratiform clouds on which the relief forcing is of primary importance. Extreme rainfall rates are defined as rainfall rates with low probability of occurrence, typically with higher mean return-levels than the maximum observed level. For example Figure 2 presents the return levels for the Cévennes-Vivarais region that can be obtained. It is then of primary importance to study the sensitivity of the extreme rainfall estimation to the estimation method considered.

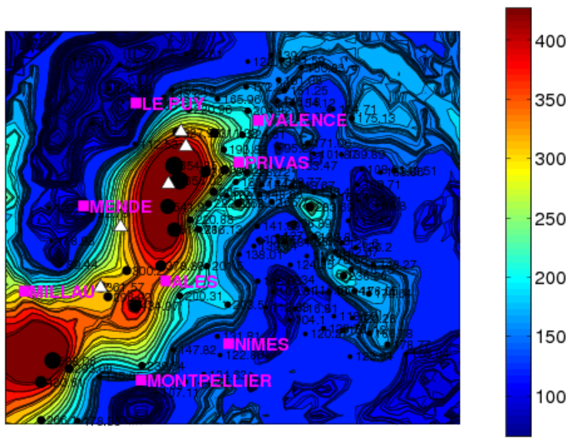


Figure 2. Map of the mean return-levels (in mm) for a period of 10 years.

The obtained results are published in [12].

6.4.8. Retrieval of Mars surface physical properties from OMEGA hyperspectral images.

Participant: Stéphane Girard.

Joint work with: Douté, S. from Laboratoire de Planétologie de Grenoble, France and Saracco, J (University 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) [47]. We have also defined an adaptive version of the method which is able to deal with block-wise evolving data streams [46].

6.4.9. Statistical modelling development for low power processor.

Participant: Stéphane Girard.

Joint work with: A. Lombardot and S. Joshi (ST Crolles).

With scaling down technologies to the nanometer regime, the static power dissipation in semiconductor devices is becoming more and more important. Techniques to accurately estimate System On Chip static power dissipation are becoming essential. Traditionally, designers use a standard corner based approach to optimize and check their devices. However, this approach can drastically underestimate or over-estimate process variations impact and leads to important errors.

The need for an effective modeling of process variation for static power analysis has led to the introduction of Statistical static power analysis. Some publication state that it is possible to save up to 50% static power using statistical approach. However, most of the statistical approaches are based on Monte Carlo analysis, and such methods are not suited to large devices. It is thus necessary to develop solutions for large devices integrated in an industrial design flow. Our objective to model the total consumption of the circuit from the probability distribution of consumption of each individual gate. Our preliminary results are published in [23].

MODAL Project-Team

6. New Results

6.1. Model for conditionally correlated categorical data

Participants: Christophe Biernacki, Matthieu Marbac-Lourdelle, Vincent Vandewalle.

An extension of the latent class model is proposed for clustering categorical data by relaxing the classical class conditional independence assumption of variables. In this model, variables are grouped into inter-independent and intra-dependent blocks in order to consider the main intra-class correlations. The dependence between variables grouped into the same block is taken into account by mixing two extreme distributions, which are respectively the independence and the maximum dependence ones. In the conditionally correlated data case, this approach is expected to reduce biases involved by the latent class model and to produce a meaningful model with few additional parameters. The parameters estimation by maximum likelihood is performed by an EM algorithm while a MCMC algorithm avoiding combinatorial problems involved by the block structure search is used for model selection. Applications on sociological and biological data sets bring out the proposed model interest. These results strengthen the idea that the proposed model is meaningful and that biases induced by the conditional independence assumption of the latent class model are reduced. This model was used in September for software components data set of Philippe Merle (ADAM Team Inria Lille).

A conference paper [26] and a poster workshop [35] have been presented. A preprint has been also written [45]. Furthermore, an R package is currently under development.

6.2. Model-based clustering for multivariate partial ranking data

Participants: Christophe Biernacki, Julien Jacques.

The first model-based clustering algorithm dedicated to multivariate partial ranking data has been developed in [43]. This is an extension of the (ISR) model for ranking data published in [4]. The proposed algorithm has allowed to exhibit regional alliances between European countries in the Eurovision contest, which are often suspected but never proved.

6.3. A new probability distribution for ordinal data

Participants: Christophe Biernacki, Julien Jacques.

In [21], a probability distribution for univariate ordinal data is proposed from a stochastic dichotomic search algorithm in a sorting table. Interest of this approach is to give a specific model for ordinal data, without any reference to numerical or nominal data, as it is often the case. The resulting distribution is governed by a position and a dispersion parameter, and is easily estimated by using an EM algorithm.

6.4. Clustering and variable selection in regression

Participants: Christophe Biernacki, Julien Jacques, Loic Yengo.

The works presented in [28] address the issue of simultaneous linear regression and clustering of predictors. A new framework is proposed that both sidesteps optimization challenges and improves prediction performance. In that framework, 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.

6.5. Mixture of Gaussians with Missing Data

Participants: Christophe Biernacki, Vincent Vandewalle.

The generative models allow to handle with 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 in [18] to improve the distance estimation by fitting a mixture of Gaussian distribution instead of a considering only one Gaussian component. An extension of the previous work including the high setting has been submitted in Neurocomputing journal. 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. We are working on the theoretical characterization of this behaviour around a degenerated solution.

6.6. Transfer 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 [37]. This is a joint work with Alexandre Lourme.

A book chapter about transfer learning (including clustering, classification and regression) has been also published [37]. It is a joint work with Farid Beninel, Charles Bouveyron, Julien Jacques and Alexandre Lourme.

6.7. 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 work is was presented as a poster to workshop [31] and is also a preprint [41] currently in revision in an international journal. This is a joint work with Alexandre Lourme.

6.8. Decorrelating variables in high dimension for linear regression

Participants: Christophe Biernacki, Clément Thery.

Databases from the steel industry are often large (very long process with many parameters) and have strong correlations between variables. Some variables may be written directly in terms of other via physical models or related by definition. Moreover the process, which is specific to the type of finished product, conditions most of the process parameters and therefore induces strong correlations between variables. The main idea is to consider some form of sub-regressions models, some variables defining others. We can then remove temporarily some of the variables to overcome ill-conditioned matrices inherent in linear regression and then reinject the deleted information, based on the struc- ture that links the variables. The final model therefore takes into account all the variables but without suffering from the consequences of correlations between variables or high dimension. This research is placed in a steel industry context (Arcelor-Mittal Dunkerque).

The work has been presented to a conference [27] and as a poster to a workshop [36]. It is a joint work with Gaétan Loridant from Arcelor-Mittal.

6.9. Model-based clustering for multivariate functional data

Participants: Julien Jacques, Cristian Preda.

We developed in [19] an extension of the model-based clustering algorithm for univariate functional data proposed in [20], [23], [11] to the case of multivariate functional data. For this, multivariate functional principal components analysis is defined and a parametric mixture model is proposed and estimated by an EM-like algorithm. Results on simulated and real datasets have shown the efficiency of the proposed method.

6.10. A method to combine combinatorial optimization and statistics to mine high-throughput genotyping data

Participants: Julie Hamon, Julien Jacques, Clarisse Dhaenens.

In the context of genomic analysis (collaboration with Genes Diffusion), dealing with high-throughput genotyping data, the objective of our study is to select a subset of SNPs (single nucleotide polymorphisms) explaining a trait of interest. We propose in [33] and [32] a method combining combinatorial optimization and statistics to extract a subset of interesting SNPs. The combinatorial part aims at exploring in a efficient way the large search space induced by the large number of possible subsets and statistics are used to evaluate the selection. We propose a first method based on an ILS (iterated local search) and using a regression. Three criteria used to evaluate the quality of the regression are compared. One of them (the k-fold validation) shows better performance. We also compare this approach to classical statistical approaches on simulated datasets. Results are promising as the proposed approach outperforms most of these statistical approaches.

6.11. Wavelet based clustering using mixed effects functional models

Participant: Guillemette Marot.

Curve clustering in the presence of inter-individual variability has longly been studied, especially using splines to account for functional random effects. However splines are not appropriate when dealing with high-dimensional data and can not be used to model irregular curves such as peak-like data. We propose a wavelet based clustering procedure ([6]) and apply it to high dimensional data. We suggest a dimension reduction step based on wavelet thresholding adapted to multiple curves and using an appropriate structure for the random effect variance, we ensure that both fixed and random effects lie in the same functional space even when dealing with irregular functions that belong to Besov spaces. In the wavelet domain, our model resumes to a linear mixed-effects model that can be used for a model-based clustering algorithm and for which we develop an EM- algorithm for maximum likelihood estimation. An R package curvclust implementing this procedure has been posted this year to the CRAN, the official website of the R software.

6.12. Comparison of normalisation procedures in RNA-sequencing before differential analysis

Participant: Guillemette Marot.

The continuing technical improvements and decreasing cost of next-generation sequencing technologies have made RNA sequencing (RNA-seq) a popular choice for gene expression studies. Several methods for the normalization of RNAseq data (removal of errors due to the small number of samples, corrections for sequence composition) have been proposed in recent years. With the Statomique Consortium, we have compared seven normalisation methods, discarded two out of them (although still widely used). We give practical recommendations on the appropriate normalization method to be used and its impact on the differential analysis of RNA-seq data in the paper ([14]).

6.13. Change point detection algorithm

Participant: Alain Célisse.

We develop a new change-point detection algorithm where focus is given to detect changes in the whole distribution of data. This challenging problem is addressed by use of kernels which enable us to deal with non-vectorial data of aby type (graphs, DNA sequences, etc). A preprint has been submitted ([46]).

6.14. Cross validation algorithms

Participant: Alain Célisse.

The performance of Cross-validation (CV) algorithms are assessed for estimating the risk as well as for model selection. Whereas optimality of leave-one-out (LOO) cross-validation is proved for risk estimation, it is no longer the case for model selection. In the latter setup, conditions are derived that lead to optimality for leave-p-cross-validation (LPO) when p is larger than 1. See for details [47].

6.15. Stochastic Block Model

Participant: Alain Célisse.

The convergence of maximum likelihood and variational estimators in a random graph model called Stochastic Block model is addressed. To the best of our knowledge, these are the first results providing consistency for maximum likelihood and variational estimators in that model. See [5].

6.16. Approximations for scan statistics.

Participants: Alexandru Amarioarei, Cristian Preda.

Accurate approximations for the distribution of extremes of 1-dependent stationary sequences are developed (see [38]). Viewed as maximum of some particular sequence of 1-dependent random variables, we provide sharp error bounds and approximations for the distribution of the three-dimensional scan statistics (see [39]). The Binomial and Poisson models are considered.

REALOPT Project-Team

6. New Results

6.1. Theoretical and Methodological Developments

Participants: Andrew Miller, Arnaud Pêcher, Pierre Pesneau, Ruslan Sadykov, Gautier Stauffer, François Vanderbeck.

We made progress in the development of theory and algorithms in the area of "Reformulation and Decomposition Approaches for MIP", "Mixed Integer Nonlinear Programming", and "Polyhedral Combinatorics and Graph Theory".

6.1.1. Column Generation for Extended Formulations

Working in an extended variable space allows one to develop tight reformulations for mixed integer programs. However, the size of the extended formulation grows rapidly too large for a direct treatment by a MIP-solver. Then, one can work with inner approximations defined and improved by generating dynamically variables and constraints. The alternative considered in [21] is an inner approximation obtained by generating dynamically the variables of the extended formulation. It assumes that the extended formulation stems from a decomposition principle. Then one can implement column generation for the extended formulation using Dantzig-Wolfe decomposition paradigm. Pricing subproblem solutions are expressed in the variables of the extended formulation and added to the current restricted version of the extended formulation along with the subproblem constraints that are active for the subproblem solutions.

Our paper [21] revisits the column-and-row generation approach, which is viewed herein as a generalization of standard column generation, the latter being based on a specific subproblem extended formulation. This generic view not only highlights the scope of applicability of the method, but it also leads to a more general termination condition than the traditional reduced cost criteria and to theoretically stronger dual bounds. We highlight a key benefit of the latter: 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. The results illustrate the stabilization effect resulting from column disaggregation and recombinations that is shown to have a cumulative effect when used in combination with a standard stabilization technique.

6.1.2. Primal Heuristics for Branch-and-Price

Primal heuristics have become an essential component in mixed integer programming (MIP). Generic heuristic paradigms of the literature remain to be extended to the context of a column generation solution approach. Our goal is to derive black-box primal heuristics for use in Branch-and-Price approaches. This requires extending primal heuristic paradigms to the context of dynamic generation of the variables of the model. We highlight an important fact: such generic tools typically performs better than problem specific meta-heuristics, in terms of solution quality and computing times. Based on our application specific experience with these techniques [55], [57], [72], [73], and on a review of generic classes of column generation based primal heuristics, in [49], we are developing a full blown review of such techniques, completed with new methods and an extensive numerical study. This research is being carried on in collaboration with the members of the associated team project, SAMBA [27] [30].

As a Dantzig-Wolfe reformulation is typically tighter than the original compact formulation, techniques based on rounding its linear programming solution have better chance to yield good primal solutions. The aggregated information built into the column definition and the price coordination mechanism provide a global view at the solution space that may be lacking in somewhat more "myopic" approaches based on compact formulations. However, the dynamic generation of variables requires specific adaptation of heuristic paradigms. Our contribution [30] lies in proposing simple strategies to get around these technical issues. We initially concentrate on "diving" methods and consider their combination with "sub-MIPing", relaxation induced neighborhood search, truncated backtracking using a Limited Discrepancy Search. These add-ons serves as local-search or diversification/intensification mechanisms. The methods are numerically tested on standard models such as Cutting Stock, Vertex Coloring, Generalized Assignment, Lot-Sizing, and Vehicle Routing problems. We further extend this research by combining the "diving" method mentioned above with the "feasibility pump" approach [27]. We show how this combination can be implemented in a context of dynamically defined variables, and we report on numerically testing "feasibility pump" for cutting stock and generalized assignment problems.

6.1.3. Stabilization techniques for column generation

Within the SAMBA project, we are collaboratively studying techniques to accelerate the convergence of column generation algorithms [25]. This techniques exploit Lagrangian duality theory. By revisiting all the alternative approaches to solving the Lagrangian dual, we identify suitable combinations of paradigms.

We also bridge the gap with techniques used in the dual framework of cut generation that have their unexploited counterpart for column generation [32], [29]. Cutting plane algorithmic strategies translate into stabilization procedures for column generation. We establish the link between the in-out separation procedure and dual price smoothing techniques for column generation. In this framework, we develop generic convergence proofs and effective smoothing auto-regulating strategies that avoids the need for parameter tuning. We further improve performance of such stabilization by hybridization with an ascent method. This work might inspire novel cut separation strategies.

6.1.4. Stable sets in claw-free graphs

A *stable set* is a set of pairwise non adjacent vertices in a graph and a graph is *claw-free* when no vertex contains a stable set of size three in its neighborhood. Given weights on the vertices, the stable set problem (a NP-hard problem in general) consists in selecting a set of pairwise non adjacent vertices maximizing the sum of the selected weights. The stable set problem in claw-free graphs is a fundamental generalization of the classic matching problem that was shown to be polynomial by Minty in 1980 (G. Minty. *On maximal independent sets of vertices in claw-free graphs*. J. Combinatorial Theory B, 28:284-304 (1980)). However, in contrast with matching, the polyhedral structure (i.e. the integer hull of all stable sets in a claw-free graph) is not very well understood and thus providing a 'decent' linear description of this polytope has thus been a major open problem in our field.

We proposed a new algorithm to find a maximum weighted stable set in a claw-free graph [38] whose complexity is now drastically better than the original algorithm by Minty (n^3 versus n^6, where n is the number of vertices). We also provided a description of the polyhedra in an extended space (i.e. using additional artificial variables) and an *efficient procedure* to separate over the polytope in polynomial-time [26]. Beside those main contributions, we published another papers on the strongly minimal facets of the polytope.

6.1.5. The Circular-Chromatic number

Another central contribution of our team concerns the chromatic number of a graph (the minimum number of independent stable sets needed to cover the graph). We proved that the chromatic number and the clique number of some superclasses of perfect graphs is computable in polynomial time [17].

We investigated the circular-chromatic number. It is a well-studied refinement of the chromatic number of a graph (designed for problems with periodic solutions): the chromatic number of a graph is the integer ceiling of its circular-chromatic number. Xuding Zhu noticed in 2000 that circular cliques are the relevant circular counterpart of cliques, with respect to the circular chromatic number, thereby introducing circular-perfect graphs, a super-class of perfect graphs.

We proved that the clique and chromatic numbers of circular-perfect graphs is computable in polynomial time [16], thereby extending Grötschel, Lovász and Schrijver's result to the whole family of circular-perfect graphs. We gave closed formulas for the Lovász Theta number of circular-cliques (previously, closed formulas were known for circular-cliques with clique number at most 3 only), and derived from them that the circular-chromatic number of circular-perfect graphs is computable in polynomial time [24].

6.2. Model Specific Developments and Applications

Participants: Andrew Miller, Arnaud Pêcher, Pierre Pesneau, Ruslan Sadykov, Gautier Stauffer, François Vanderbeck.

The models on which we made progress can be partitioned in three areas: "Packing and Covering Problems", "Network Design and Routing", and "Planning, Scheduling, and Logistic Problems".

6.2.1. Bin-Packing with Conflicts

The bin-packing problem consists in finding the minimum number of bin of fixed size one needs to pack a set of items of different sizes. We studied a generalization of this problem where items can be in conflicts and thus cannot be put together in the same bin. We show in [20] that the instances of the literature with 120 to 1000 items can be solved to optimality with a generic Branch-and-Price algorithm, such as our prototype BaPCod, within competitive computing time. Moreover, we solved to optimality all the 37 open instances. The approach involves generic primal heuristics, generic branching, but a specific pricing procedure.

6.2.2. Using graph theory for solving orthogonal knapsack problems

We investigated the orthogonal knapsack problem, with the help of graph theory. The multi-dimensional orthogonal packing problem (OPP) is defined as follows: given a set of items with rectangular shapes, the problem is to decide whether there is a non-overlapping packing of these items in a rectangular bin. The rotation of items is not allowed. A powerful characterization of packing configurations by means of interval graphs was introduced by Fekete and Schepers using an efficient representation of all geometrically symmetric solutions by a so called *packing class* involving one *interval graph* (whose complement admits a transitive orientation: each such orientation of the edges corresponds to a specific placement of the forms) for each dimension. Though Fekete & Schepers' framework is very efficient, we have however identified several weaknesses in their algorithms: the most obvious one is that they do not take advantage of the different possibilities to represent interval graphs.

In [12], [11], we give two new algorithms: the first one is based upon matrices with consecutive ones on each row as data structures and the second one uses so-called MPQ-trees, which were introduced by Korte and Mohring to recognize interval graphs. These two new algorithms are very efficient, as they outperform Fekete and Schepers' on most standard benchmarks.

6.2.3. Inventory routing and logistics problems

Inventory routing problems combine the optimization of product deliveries (or pickups) with inventory control at customer sites. in [13], we considered the planning of single product pickups over time: each site accumulates stock at a deterministic rate; the stock is emptied on each visit. Our objective is to minimize a surrogate measure of routing cost while achieving some form of regional clustering by partitioning the sites between the vehicles. The fleet size is given but can potentially be reduced. Planning consists in assigning customers to vehicles in each time period, but the routing, i.e., the actual sequence in which vehicles visit customers, is considered as an "operational" decision. We developed a truncated branch-and-price algorithm. This exact optimization approach is combined with rounding and local search heuristics to yield both primal solutions and dual bounds that allow us to estimate the deviation from optimality of our solution. We were confronted with the issue of symmetry in time that naturally arises in building a cyclic schedule (cyclic permutations along the time axis define alternative solutions). Central to our approach is a state-space relaxation idea that allows us to avoid this drawback: the symmetry in time is eliminated by modeling an average behavior. Our algorithm provides solutions with reasonable deviation from optimality for large scale problems (260 customer sites, 60 time periods, 10 vehicles) coming from industry. The subproblem is interesting in its own right: it is a multiple-class integer knapsack problem with setups. Items are partitioned into classes whose use implies a setup cost and associated capacity consumption.

6.2.4. Scheduling

Cross docking terminals allow companies to reduce storage and transportation costs in a supply chain. At these terminals, products of different types from incoming trucks are unloaded, sorted, and loaded to outgoing trucks for delivery. In [19], we focus on the operational activities at a cross docking terminal with two doors: one for incoming trucks and another one for outgoing trucks. We consider the truck scheduling problem with the objective to minimize the storage usage during the product transfer inside the terminal. Our interest in this problem is mainly theoretical. We show that it is NP-hard in the strong sense even if there are only two product types. For a special case with fixed subsequences of incoming and outgoing trucks, we propose a dynamic programming algorithm, which is the first polynomial algorithm for this case. The results of numerical tests of the algorithm on randomly generated instances are also presented.

In [18], we consider the scheduling jobs in parallel, i.e., jobs can be executed on more than one processor at the same time. With the emergence of new production, communication and parallel computing system, the usual scheduling requirement that a job is executed only on one processor has become, in many cases, obsolete and unfounded. In this work, we consider the NP-hard problem of scheduling malleable jobs to minimize the total weighted completion time (or mean weighted flow time). For this problem, we introduce the class of "ascending" schedules in which, for each job, the number of machines assigned to it cannot decrease over time while this job is being processed. We prove that, under a natural assumption on the processing time functions of jobs, the set of ascending schedules is dominant for the problem. This result can be used to reduce the search space while looking for an optimal solution.

Currently, we are working on a scheduling application at a port. For this application, an equipment routing task scheduling problem [28] has been formulated, where a set of tasks needs to be performed. Tasks require equipment of different types. A particularity of the problem is that an equipment needs to be moved to the actual locations of tasks which use this equipment. So, there are both scheduling and routing decisions are to be taken simultaneously.

6.2.5. One warehouse multi-retailer problem

The *One-Warehouse Multi-retailer problem (OWMR)* is a very important NP-hard inventory control problem arising in the distribution of goods when one central warehouse is supplying a set of final retailers facing demand from customers. In [22], we provide a simple and fast 2-approximation algorithm for this problem (i.e. an algorithm ensuring a deviation by a factor at most two from the optimal solution). This result is both important in practice and in theory as it allows to approximate large real-world instances of the problem (we implemented this algorithm at IBM and it is within 10% of optimality in practice) and the techniques we developed appear to apply to more general settings. We are extending our results to other inventory control problems.

6.3. Software prototypes, Generic Developments and Specific Tools

Participants: Romain LeGuay, Pierre Pesneau, Ruslan Sadykov, François Vanderbeck.

6.3.1. BaPCod - a generic branch-and-price code

The development of the prototype software platform is supported by our junior engineer, Romain Leguay. He developed a new interface with the underlying MIP solver allowing multiple solvers to be called in the same run. He then re-organized the svn depository and a web distribution platform in view of the increasing number if users to whom Romain offers precious support. Romain has then redesigned parts of the code in the perspective of its parallelization and contributed to designing a pseudo modeling language for a friendly user interface. The emphasis is currently on enhancing the code performance in particular through rapid access data structure. Romain also participates to the setting up of stabilization and preprocessing algorithms.

The software platform BaPCod is continuously improved to include all the methodological features that arise from our research, in particular in our collaborative project with Brazil: SAMBA. BaPCod serves there as a proof-of-concept code and is useful for the transfer of knowledge between the parties, including the company GAPSO (a Brazilian spin-up launched by these academics).

SELECT Project-Team

6. New Results

6.1. Model selection in Regression and Classification

Participants: Gilles Celeux, Mohammed El Anbari, Clément Levrard, Erwan Le Pennec, Lucie Montuelle, Pascal Massart, Caroline Meynet, Jean-Michel Poggi, Adrien Saumard.

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 [6] 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.

In collaboration with Marie-Laure Martin-Magniette (URGV et UMR AgroParisTech/INRA MIA 518) and Cathy Maugis (INSA Toulouse) Gilles Celeux has extended their variable selection procedure for model-based clustering and supervised classification to deal with high dimensional data sets with a backward selection procedure which is more efficient that the previous forward selection procedure in this context. Moreover they have analysed the differences between the model-based approach and geometrical approach to select variable for clustering. Through numerical experiments, they showed the advantage of the model-based appraoch when many variables are highly correlated. These variable selection procedures are in particular used for genomics applications which is the result of a collaboration with researchers of of URGV (Evry Genopole).

Caroline Meynet provided an ℓ_1-oracle inequality satisfied by the Lasso estimator with the Kullback-Leibler loss in the framework of a finite mixture of Gaussian regressions model for high-dimensional heterogeneous data where the number of covariates may be much larger than the sample size. In particular, she has given a condition on the regularization parameter of the Lasso to obtain such an oracle inequality. This oracle inequality extends the ℓ_1-oracle inequality established by Massart and Meynet in the homogeneous Gaussian linear regression case. It is deduced from a finite mixture Gaussian regression model selection theorem for ℓ_1-penalized maximum likelihood conditional density estimation, which is inspired from Vapnik's method of structural risk minimization and from the theory on model selection for maximum likelihood estimators developed by Massart.

From an practical point of view, Caroline Meynet has introduced a procedure to select variables in model-based clustering in a high-dimensional context. In order to tackle with the problem of high-dimension, she has proposed to first use the Lasso in order to select different sets of variables and then estimate the density by a standard EM algorithm by reducing the inference to the linear space of the selected variables by the Lasso. Numerical experiments show that this method can outperform direct estimation by the Lasso.

In collaboration with Jean-Patrick Baudry (Paris 6) and Margarida Cardoso, Ana Ferreira and Maria-José Amorim (Lisbon University], Gilles Celeux has proposed an approach to select, in the model-based clustering context, a model and a number of clusters in order to get a partition which both provides a good fit with the data and is related to the external categorical variables. This approach makes use of the integrated joint likelihood of the data, the partition derived from the mixture model and the known partitions. It is worth noticing that the external categorical variables are only used to select a relevant mixture model. Each mixture model is fitted by the maximum likelihood methodology from the observed data. Numerical experiments illustrate the promising behaviour of the derived criterion [29].

Since September 2008, Pascal Massart is the cosupervisor with Frédéric Chazal (GEOMETRICA) of the thesis of Claire Caillerie (GEOMETRICA). The project intends to explore and to develop new researches at the crossing of information geometry, computational geometry and statistics.

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 seperately. 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.

Adrien saumard has worked on the theoretical validation of the slope heuristics, a practical method of penalties calibration derived in a Gaussian setting by Birgé and Massart in 2006 and extended to bounded M-estimation by Arlot and Massart in 2010. He was able to prove the validity of this heuristics in bounded heteroscedastic regression with random design when the considered models where linear spans made of piecewise polynomials. A preliminary work on a fixed model was necessary and published in [9], while the validation of the slope heuristics itself - as well as the validation of a cross-validation approach - can be found in a preprint.

6.2. Statistical learning methodology and theory

Participants: Gilles Celeux, Christine Keribin, Erwan Le Pennec, Pascal Massart, Lucie Montuelle, Jean-Michel Poggi, Adrien Saumard, Solenne Thivin.

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.

Gilles Celeux, Christine Keribin and the Ph D. student Vincent Brault continue their work on the Latent Block Model (LBM). They compared several model selection criteria for binary tables [19]. However, the SEM-VEM Gibbs algorithm used to estimate LBM is subject to spurious solutions (empty clusters). To tackle this drawback, they have proposed to use Bayesian inference through Gibbs Sampling and studied the influence of the calibration of non informative prior distributions. They showed on numerical experiment the advantages of coupling Gibbs sampling with a Variational Bayes algorithm to get pointwise estimators [17]. Furthermore, they extended the previous studies from binary to categorical data [32].

Christine Keribin has proposed to compare, on genomics applications, the use of LBM with other methodologies (variable selection procedure of Maugis and Martin Magniette, component analysis). She supervised an internship (Master 1) on the use of principal component analysis for gene expression data (Inria funding). This has been done on data of the SONATA project (leaded by URGV - Evry Genopole), in collaboration with Marie-Laure Martin-Magniette.

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 test approach based on the test decision theory. A key issue is to learn good discrimant features and their probabilistic properties. So far, they have worked on cloud images given by Thales. They focus on a Markovian modeling of the clouds.

Considering the case of maximum likelihood density estimation on histograms, Adrien saumard has investigated both theory and methodology. On the one hand, he has shown that AIC is twice the minimal penalty in the sense of Birgé and Massart, which by consequence implies the asymptotic optimality of the slope heuristics based on a linear shape. On the other hand, he investigated the methodology of the small to moderate sample size setting in this case. The robustness of the slope heurisitics compared to AIC is shown on simulated examples and a new overpenalization of Akaike's criterion is proposed, which outperforms the criterion AICc of

Hurvitch and Tsai and shows comparable results to the procedure proposed by Birgé and Rozenholc in 2006. The benefits of the derived procedure here is its theoretical background and interpretation. This work is still in process and some of the results can be found in a preprint.

6.3. Reliability and Computer Experiments

Participants: Yves Auffray, Gilles Celeux, Rémy Fouchereau, Shuai Fu.

In the computer experiments field, the goal is to approximate an expensive black box function from a limited number of evaluations. The choice of these evaluations i.e. the choice of a design of (computer) experiments is a major issue.

Following the previous work of the past three years, Shuai Fu has concluded her Ph.D thesis under the direction of Gilles Celeux [1]. This year, the work was focused on controlling four main error quantities, in order to validate the methodology in the industrial framework. More precisely, the DAC criterion (Data Agreement Criterion), which has been proposed for assessing the relevance of the design of experiments (DOE) and the prior choice with the observed data was applied to a complex hydrological model, coding and testing the relevant algorithms [30]. For the purpose of controlling the emulator error in an adaptive kriging algorithm, two Bayesian criteria have been proposed for searching and adding new points into the current DOE. The computation time remains important, which makes the method meaningful only in the case where we have a really time-consuming code.

In the framework of a CIFRE convention with Snecma-SAFRAN Rémy Fouchereau has started a thesis on the modeling of fatigue damage for Inco718 supervised by Gilles Celeux. Inco718 is a Zinc-based alloy. To determine its minimum lifetime, a lot of stress tests are made. The alloy lifetimes are reported as function of the stress. The aim is to propose a stochastic models for fatigue lifetime prediction based on a fracture mechanics-based approach. A mixture model with a lognormal component and a sum of two lognormals components is considered. Since the sum of two or more lognormal distribution is not closed form, inference on this model needs Monte Carlo integration within the EM algorithm. Thus, we have provided engineers with a probabilistic tool for reliability design of mechanical parts, but also with a diagnostic tool for material elaboration.

6.4. Statistical analysis of genomic data

Participant: Gilles Celeux.

In collaboration with Florence Jaffrezic and Andrea Rau (INRA, département de génétique animale) Gilles Celeux initiated modelling genomics networks from RNA-seq data. It was the subject of the internship of Mélina Gallpin who is starting a thesis on this subject. To day the performance of overdispersed Poisson models has been investigated. The results are somewhat poor especially for large numbers of genes.

6.5. Curves classification, denoising and forecasting

Participants: Émilie Devijver, Pascal Massart, Jean-Michel Poggi.

In collaboration with Farouk Mhamdi and Meriem Jaidane (ENIT, Tunis, Tunisia), Jean-Michel Poggi proposeda 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.

In collaboration with Mina Aminghafari (Amirkabir University, Teheran), Jean-Michel Poggi made uses of wavelets in a statistical forecasting purpose for time series. Recent approaches involve wavelet decompositions in order to handle non stationary time series. They study and extended an approach proposed by Renaud et al., to estimate the prediction equation by direct regression of the process on the Haar non-decimated wavelet coefficients depending on its past values. The new variants are used first for stationary data and after for stationary data contaminated by a deterministic 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 is strongly related to the use of wavelets together with curves clustering in order to perform accurate load comsumption forecasting. The thesis develops methodological and applied aspects linked to the electrical context as well as theoretical ones by introducing exogeneous variables in the context of nonparametric forecasting time series.

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 Emilie 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 his 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.

SEQUEL Project-Team

6. New Results

6.1. Decision-making Under Uncertainty

6.1.1. Reinforcement Learning

Transfer in Reinforcement Learning: a Framework and a Survey [56]

Transfer in reinforcement learning is a novel research area that focuses on the development of methods to transfer knowledge from a set of source tasks to a target task. Whenever the tasks are *similar*, the transferred knowledge can be used by a learning algorithm to solve the target task and significantly improve its performance (e.g., by reducing the number of samples needed to achieve a nearly optimal performance). In this chapter we provide a formalization of the general transfer problem, we identify the main settings which have been investigated so far, and we review the most important approaches to transfer in reinforcement learning.

Online Regret Bounds for Undiscounted Continuous Reinforcement Learning [44]

We derive sublinear regret bounds for undiscounted reinforcement learning in continuous state space. The proposed algorithm combines state aggregation with the use of upper confidence bounds for implementing optimism in the face of uncertainty. Beside the existence of an optimal policy which satisfies the Poisson equation, the only assumptions made are Holder continuity of rewards and transition probabilities.

Semi-Supervised Apprenticeship Learning [23]

In apprenticeship learning we aim to learn a good policy by observing the behavior of an expert or a set of experts. In particular, we consider the case where the expert acts so as to maximize an unknown reward function defined as a linear combination of a set of state features. In this paper, we consider the setting where we observe many sample trajectories (i.e., sequences of states) but only one or a few of them are labeled as experts' trajectories. We investigate the conditions under which the remaining unlabeled trajectories can help in learning a policy with a good performance. In particular, we define an extension to the max-margin inverse reinforcement learning proposed by Abbeel and Ng (2004) where, at each iteration, the max-margin optimization step is replaced by a semi-supervised optimization problem which favors classifiers separating clusters of trajectories. Finally, we report empirical results on two grid-world domains showing that the semi-supervised algorithm is able to output a better policy in fewer iterations than the related algorithm that does not take the unlabeled trajectories into account.

Fast Reinforcement Learning with Large Action Sets Using Error-Correcting Output Codes for MDP Factorization [31] [48]

The use of Reinforcement Learning in real-world scenarios is strongly limited by issues of scale. Most RL learning algorithms are unable to deal with problems composed of hundreds or sometimes even dozens of possible actions, and therefore cannot be applied to many real-world problems. We consider the RL problem in the supervised classification framework where the optimal policy is obtained through a multiclass classifier, the set of classes being the set of actions of the problem. We introduce error-correcting output codes (ECOCs) in this setting and propose two new methods for reducing complexity when using rollouts-based approaches. The first method consists in using an ECOC-based classifier as the multiclass classifier, reducing the learning complexity from O(A2) to O(Alog(A)) . We then propose a novel method that profits from the ECOC's coding dictionary to split the initial MDP into O(log(A)) separate two-action MDPs. This second method reduces learning complexity even further, from O(A2) to O(log(A)) , thus rendering problems with large action sets tractable. We finish by experimentally demonstrating the advantages of our approach on a set of benchmark problems, both in speed and performance.

Analysis of Classification-based Policy Iteration Algorithms [13]

We introduce a variant of the classification-based approach to policy iteration which uses a cost-sensitive loss function weighting each classification mistake by its actual regret, i.e., the difference between the action-value of the greedy action and of the action chosen by the classifier. For this algorithm, we provide a full finite-sample analysis. Our results state a performance bound in terms of the number of policy improvement steps, the number of rollouts used in each iteration, the capacity of the considered policy space (classifier), and a capacity measure which indicates how well the policy space can approximate policies that are greedy w.r.t. any of its members. The analysis reveals a tradeoff between the estimation and approximation errors in this classification-based policy iteration setting. Furthermore it confirms the intuition that classification-based policy iteration algorithms could be favorably compared to value-based approaches when the policies can be approximated more easily than their corresponding value functions. We also study the consistency of the algorithm when there exists a sequence of policy spaces with increasing capacity.

Minimax PAC-Bounds on the Sample Complexity of Reinforcement Learning with a Generative Model [5] [24]

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 $\gamma \in [0,1)$ only $O(N \log(N/\delta)/[(1-\gamma)^3 \epsilon^2])$ state-transition samples are required to find an ϵ-optimal estimation of the action-value function with the probability (w.p.) $1-\delta$. Further, we prove that, for small values of ϵ, an order of $O(N \log(N/\delta)/[(1-\gamma)^3 \epsilon^2])$ samples is required to find an ϵ-optimal policy w.p. $1-\delta$. We also prove a matching lower bound of $\Omega(N \log(N/\delta)/[(1-\gamma)^3 \epsilon^2])$ 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 $1/(1-\gamma)$ 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 $1/(1-\gamma)$.

Optimistic planning in Markov decision processes [25]

The reinforcement learning community has recently intensified its interest in online planning methods, due to their relative independence on the state space size. However, tight near-optimality guarantees are not yet available for the general case of stochastic Markov decision processes and closed-loop, state-dependent planning policies. We therefore consider an algorithm related to $AO*$ that optimistically explores a tree representation of the space of closed-loop policies, and we analyze the near-optimality of the action it returns after n tree node expansions. While this optimistic planning requires a finite number of actions and possible next states for each transition, its asymptotic performance does not depend directly on these numbers, but only on the subset of nodes that significantly impact near-optimal policies. We characterize this set by introducing a novel measure of problem complexity, called the near-optimality exponent. Specializing the exponent and performance bound for some interesting classes of MDPs illustrates the algorithm works better when there are fewer near-optimal policies and less uniform transition probabilities.

Risk Bounds in Cost-sensitive Multiclass Classification: an Application to Reinforcement Learning [61]

We propose a computationally efficient classification-based policy iteration (CBPI) algorithm. The key idea of CBPI is to view the problem of computing the next policy in policy iteration as a classification problem. We propose a new cost-sensitive surrogate loss for each iteration of CBPI. This allows us to replace the non-convex optimization problem that needs to be solved at each iteration of the existing CBPI algorithms with a convex one. We show that the new loss is classification calibrated, and thus is a sound surrogate loss, and find a calibration function (i.e., a function that represents the convergence rate of the true loss in terms of the convergence rate of the surrogate-loss) for this loss. To the best of our knowledge, this is the first calibration result (with convergence rate) in the context of multi-class classification. As a result, we are able to extend the theoretical guarantees of the existing CBPI algorithms that deal with a non-convex optimization at each iteration to our convex and efficient algorithm, and thereby, obtain the first computationally efficient and theoretically sound CBPI algorithm.

Least-Squares Methods for Policy Iteration [55]

Approximate reinforcement learning deals with the essential problem of applying reinforcement learning in large and continuous state-action spaces, by us- ing function approximators to represent the solution. This chapter reviews least-squares methods for policy iteration, an important class of algorithms for approxi- mate reinforcement learning. We discuss three techniques for solving the core, pol- icy evaluation component of policy iteration, called: least-squares temporal difference, least-squares policy evaluation, and Bellman residual minimization. We introduce these techniques starting from their general mathematical principles and detailing them down to fully specified algorithms. We pay attention to online variants of policy iteration, and provide a numerical example highlighting the behavior of representative offline and online methods. For the policy evaluation component as well as for the overall resulting approximate policy iteration, we provide guarantees on the performance obtained asymptotically, as the number of processed samples and executed iterations grows to infinity. We also provide finite-sample results, which apply when a finite number of samples and iterations is considered. Finally, we outline several extensions and improvements to the techniques and methods reviewed

On Classification-based Approximate Policy Iteration [53]

Efficient methods for tackling large reinforcement learning problems usually exploit special structure, or regularities, of the problem at hand. For example, classification-based approximate policy iteration explicitly controls the complexity of the policy space, which leads to considerable improvement in convergence speed whenever the optimal policy is easy to represent. Conventional classification-based methods, however, do not benefit from regularities of the value function, because they typically use rollout-based estimates of the action-value function. This Monte Carlo-style approach for value estimation is data-inefficient and does not generalize the estimated value function over states. We introduce a general framework for classification-based approximate policy iteration (CAPI) which exploits regularities of both the policy and the value function. Our theoretical analysis extends existing work by allowing the policy evaluation step to be performed by any reinforcement learning algorithm (including temporal-difference style methods), by handling nonparametric representations of policies, and by providing tighter convergence bounds on the estimation error of policy learning. In our experiments, instantiations of CAPI outperformed powerful purely value-based approaches.

Conservative and Greedy Approaches to Classification-based Policy Iteration [37]

The existing classification-based policy iteration (CBPI) algorithms can be divided into two categories: *direct policy iteration* (DPI) methods that directly assign the output of the classifier (the approximate greedy policy w.r.t. the current policy) to the next policy, and *conservative policy iteration* (CPI) methods in which the new policy is a mixture distribution of the current policy and the output of the classifier. The conservative policy update gives CPI a desirable feature, namely the guarantee that the policies generated by this algorithm improve at each iteration. We provide a detailed algorithmic and theoretical comparison of these two classes of CBPI algorithms. Our results reveal that in order to achieve the same level of accuracy, CPI requires more iterations, and thus, more samples than the DPI algorithm. Furthermore, CPI may converge to suboptimal policies whose performance is not better than DPI's.

A Dantzig Selector Approach to Temporal Difference Learning [36]

LSTD is a popular algorithm for value function approximation. Whenever the number of features is larger than the number of samples, it must be paired with some form of regularization. In particular, l1-regularization methods tend to perform feature selection by promoting sparsity, and thus, are well- suited for high-dimensional problems. However, since LSTD is not a simple regression algorithm, but it solves a fixed-point problem, its integration with l1-regularization is not straightforward and might come with some drawbacks (e.g., the P-matrix assumption for LASSO-TD). In this paper, we introduce a novel algorithm obtained by integrating LSTD with the Dantzig Selector. We investigate the performance of the proposed algorithm and its relationship with the existing regularized approaches, and show how it addresses some of their drawbacks.

Finite-Sample Analysis of Least-Squares Policy Iteration [14]

In this paper, we report a performance bound for the widely used least-squares policy iteration (LSPI) algorithm. We first consider the problem of policy evaluation in reinforcement learning, that is, learning the value function of a fixed policy, using the least-squares temporal-difference (LSTD) learning method, and report finite-sample analysis for this algorithm. To do so, we first derive a bound on the performance of the LSTD solution evaluated at the states generated by the Markov chain and used by the algorithm to learn an estimate of the value function. This result is general in the sense that no assumption is made on the existence of a stationary distribution for the Markov chain. We then derive generalization bounds in the case when the Markov chain possesses a stationary distribution and is β-mixing. Finally, we analyze how the error at each policy evaluation step is propagated through the iterations of a policy iteration method, and derive a performance bound for the LSPI algorithm.

Approximate Modified Policy Iteration [47]

Modified policy iteration (MPI) is a dynamic programming (DP) algorithm that contains the two celebrated policy and value iteration methods. Despite its generality, MPI has not been thoroughly studied, especially its approximation form which is used when the state and/or action spaces are large or infinite. In this paper, we propose three implementations of approximate MPI (AMPI) that are extensions of well-known approximate DP algorithms: fitted-value iteration, fitted-Q iteration, and classification-based policy iteration. We provide error propagation analyses that unify those for approximate policy and value iteration. On the last classification-based implementation, we develop a finite-sample analysis that shows that MPI's main parameter allows to control the balance between the estimation error of the classifier and the overall value function approximation.

Bayesian Reinforcement Learning [57]

This chapter surveys recent lines of work that use Bayesian techniques for reinforcement learning. In Bayesian learning, uncertainty is expressed by a prior distribution over unknown parameters and learning is achieved by computing a posterior distribution based on the data observed. Hence, Bayesian reinforcement learning distinguishes itself from other forms of reinforcement learning by explicitly maintaining a distribution over various quantities such as the parameters of the model, the value function, the policy or its gradient. This yields several benefits: a) domain knowledge can be naturally encoded in the prior distribution to speed up learning; b) the exploration/exploitation tradeoff can be naturally optimized; and c) notions of risk can be naturally taken into account to obtain robust policies.

6.1.2. Multi-arm Bandit Theory

Learning with stochastic inputs and adversarial outputs [15]

Most of the research in online learning is focused either on the problem of adversarial classification (i.e., both inputs and labels are arbitrarily chosen by an adversary) or on the traditional supervised learning problem in which samples are independent and identically distributed according to a stationary probability distribution. Nonetheless, in a number of domains the relationship between inputs and outputs may be adversarial, whereas input instances are i.i.d. from a stationary distribution (e.g., user preferences). This scenario can be formalized as a learning problem with stochastic inputs and adversarial outputs. In this paper, we introduce this novel stochastic-adversarial learning setting and we analyze its learnability. In particular, we show that in a binary classification problem over an horizon of n rounds, given a hypothesis space H with finite VC-dimension, it is possible to design an algorithm that incrementally builds a suitable finite set of hypotheses from H used as input for an exponentially weighted forecaster and achieves a cumulative regret of order $O(\sqrt{nVC(H)\log n})$ with overwhelming probability. This result shows that whenever inputs are i.i.d. it is possible to solve any binary classification problem using a finite VC-dimension hypothesis space with a sub-linear regret independently from the way labels are generated (either stochastic or adversarial). We also discuss extensions to multi-class classification, regression, learning from experts and bandit settings with stochastic side information, and application to games.

A Truthful Learning Mechanism for Multi-Slot Sponsored Search Auctions with Externalities [35]

Sponsored search auctions constitute one of the most successful applications of *microeconomic mechanisms*. In mechanism design, auctions are usually designed to incentivize advertisers to bid their truthful valuations and, at the same time, to assure both the advertisers and the auctioneer a non–negative utility. Nonetheless, in sponsored search auctions, the click–through–rates (CTRs) of the advertisers are often unknown to the auctioneer and thus standard incentive compatible mechanisms cannot be directly applied and must be paired with an effective learning algorithm for the estimation of the CTRs. This introduces the critical problem of designing a learning mechanism able to estimate the CTRs as the same time as implementing a truthful mechanism with a revenue loss as small as possible compared to an optimal mechanism designed with the true CTRs. Previous works showed that in single–slot auctions the problem can be solved using a suitable exploration–exploitation mechanism able to achieve a per–step regret of order $O(T^{-1/3})$ (where T is the number of times the auction is repeated). In this paper we extend these results to the general case of contextual multi–slot auctions with position– and ad–dependent externalities. In particular, we prove novel upper–bounds on the revenue loss w.r.t. to a VCG auction and we report numerical simulations investigating their accuracy in predicting the dependency of the regret on the number of rounds T, the number of slots K, and the number of advertisements n.

Regret Bounds for Restless Markov Bandits [43]

We consider the restless Markov bandit problem, in which the state of each arm evolves according to a Markov process independently of the learner's actions. We suggest an algorithm that after T steps achieves $\widetilde{O}(\sqrt{T})$ regret with respect to the best policy that knows the distributions of all arms. No assumptions on the Markov chains are made except that they are irreducible. In addition, we show that index-based policies are necessarily suboptimal for the considered problem.

Online allocation and homogeneous partitioning for piecewise constant mean approximation [42]

In the setting of active learning for the multi-armed bandit, where the goal of a learner is to estimate with equal precision the mean of a finite number of arms, recent results show that it is possible to derive strategies based on finite-time confidence bounds that are competitive with the best possible strategy. We here consider an extension of this problem to the case when the arms are the cells of a finite partition P of a continuous sampling space X in Rd. Our goal is now to build a piecewise constant approximation of a noisy function (where each piece is one region of P and P is fixed beforehand) in order to maintain the local quadratic error of approximation on each cell equally low. Although this extension is not trivial, we show that a simple algorithm based on upper confidence bounds can be proved to be adaptive to the function itself in a near-optimal way, when |P| is chosen to be of minimax-optimal order on the class of alpha-Holder functions.

The Optimistic Principle applied to Games, Optimization and Planning: Towards Foundations of Monte-Carlo Tree Search [17]

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.

Kullback-Leibler Upper Confidence Bounds for Optimal Sequential Allocation [6]

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.

Minimax strategy for Stratified Sampling for Monte Carlo [8]

We consider the problem of stratified sampling for Monte-Carlo integration. We model this problem in a multi-armed bandit setting, where the arms represent the strata, and the goal is to estimate a weighted average of the mean values of the arms. We propose a strategy that samples the arms according to an upper bound on their standard deviations and compare its estimation quality to an ideal allocation that would know the standard deviations of the strata. We provide two pseudo-regret analyses: a distribution-dependent bound of order $O(n^{-3/2})$ that depends on a measure of the disparity of the strata, and a distribution-free bound $O(n^{-4/3})$ that does not. We also provide the first problem independent (minimax) lower bound for this problem and demonstrate that MC-UCB matches this lower bound both in terms of number of samples n and in terms of number of strata K. Finally, we link the pseudo-regret with the difference between the mean squared error on the estimated weighted average of the mean values of the arms, and the optimal oracle strategy: this provides us also with a problem dependent and a problem independent rate for this measure of performance and, as a corollary, asymptotic optimality.

Upper-Confidence-Bound Algorithms for Active Learning in Multi-Armed Bandits [7]

In this paper, we study the problem of estimating uniformly well the mean values of several distributions given a finite budget of samples. If the variance of the distributions were known, one could design an optimal sampling strategy by collecting a number of independent samples per distribution that is proportional to their variance. However, in the more realistic case where the distributions are not known in advance, one needs to design adaptive sampling strategies in order to select which distribution to sample from according to the previously observed samples. We describe two strategies based on pulling the distributions a number of times that is proportional to a high-probability upper-confidence-bound on their variance (built from previous observed samples) and report a finite-sample performance analysis on the excess estimation error compared to the optimal allocation. We show that the performance of these allocation strategies depends not only on the variances but also on the full shape of the distributions.

Bandit Algorithms boost motor-task selection for Brain Computer Interfaces [32] [10]

Brain-computer interfaces (BCI) allow users to "communicate" with a computer without using their muscles. BCI based on sensori-motor rhythms use imaginary motor tasks, such as moving the right or left hand, to send control signals. The performances of a BCI can vary greatly across users but also depend on the tasks used, making the problem of appropriate task selection an important issue. This study presents a new procedure to automatically select as fast as possible a discriminant motor task for a brain-controlled button. We develop for this purpose an adaptive algorithm, *UCB-classif*, based on the stochastic bandit theory. This shortens the training stage, thereby allowing the exploration of a greater variety of tasks. 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. Comparing the proposed method to the standard practice in task selection, for a fixed time budget, *UCB-classif* leads to an improved classification rate, and for a fixed classification rate, to a reduction of the time spent in training by 50%.

Adaptive Stratified Sampling for Monte-Carlo integration of Differentiable functions [26]

We consider the problem of adaptive stratified sampling for Monte Carlo integration of a differentiable function given a finite number of evaluations to the function. We construct a sampling scheme that samples more often in regions where the function oscillates more, while allocating the samples such that they are well spread on the domain (this notion shares similitude with low discrepancy). We prove that the estimate returned by the algorithm is almost similarly accurate as the estimate that an optimal oracle strategy (that would know the variations of the function *everywhere*) would return, and provide a finite-sample analysis.

Risk-Aversion in Multi-Armed Bandits [46]

In stochastic multi-armed bandits the objective is to solve the exploration-exploitation dilemma and ultimately maximize the expected reward. Nonetheless, in many practical problems, maximizing the expected reward is not the most desirable objective. In this paper, we introduce a novel setting based on the principle of risk-aversion where the objective is to compete against the arm with the best risk-return trade-off. This setting proves to be intrinsically more difficult than the standard multi-arm bandit setting due in part to an exploration risk which introduces a regret associated to the variability of an algorithm. Using variance as a measure of risk, we introduce two new algorithms, we investigate their theoretical guarantees, and we report preliminary empirical results.

Bandit Theory meets Compressed Sesing for high dimensional Stochastic Linear Bandit [27]

We consider a linear stochastic bandit problem where the dimension K of the unknown parameter θ is larger than the sampling budget n. In such cases, it is in general impossible to derive sub-linear regret bounds since usual linear bandit algorithms have a regret in $O(K\sqrt{n})$. In this paper we assume that θ is S-sparse, i.e. has at most S non-zero components, and that the space of arms is the unit ball for the L_2 norm. We combine ideas from Compressed Sensing and Bandit Theory and derive an algorithm with a regret bound in $O(S\sqrt{n})$. We detail an application to the problem of optimizing a function that depends on many variables but among which only a small number of them (initially unknown) are relevant.

Thompson Sampling: an Asymptotically Optimal Finite Time Analysis [38]

The question of the optimality of Thompson Sampling for solving the stochastic multi-armed bandit problem had been open since 1933. In this paper we answer it positively for the case of Bernoulli rewards by providing the first finite-time analysis that matches the asymptotic rate given in the Lai and Robbins lower bound for the cumulative regret. The proof is accompanied by a numerical comparison with other optimal policies, experiments that have been lacking in the literature until now for the Bernoulli case.

Regret bounds for Restless Markov Bandits [43]

We consider the restless Markov bandit problem, in which the state of each arm evolves according to a Markov process independently of the learner's actions. We suggest an algorithm that after T steps achieves $O(\sqrt{T})$ regret with respect to the best policy that knows the distributions of all arms. No assumptions on the Markov chains are made except that they are irreducible. In addition, we show that index-based policies are necessarily suboptimal for the considered problem.

Minimax number of strata for online Stratified Sampling given Noisy Samples [28]

We consider the problem of online stratified sampling for Monte Carlo integration of a function given a finite budget of n noisy evaluations to the function. More precisely we focus on the problem of choosing the number of strata K as a function of the budget n. We provide asymptotic and finite-time results on how an oracle that has access to the function would choose the number of strata optimally. In addition we prove a lower bound on the learning rate for the problem of stratified Monte-Carlo. As a result, we are able to state, by improving the bound on its performance, that algorithm MC-UCB, is minimax optimal both in terms of the number of samples n and the number of strata K, up to a $\log(nK)$ factor. This enables to deduce a minimax optimal bound on the difference between the performance of the estimate output by MC-UCB, and the performance of the estimate output by the best oracle static strategy, on the class of Holder continuous functions, and up to a factor $\log(n)$.

Best Arm Identification: A Unified Approach to Fixed Budget and Fixed Confidence [33]

We study the problem of identifying the best arm(s) in the stochastic multi-armed bandit setting. This problem has been studied in the literature from two different perspectives: fixed budget and fixed confidence. We propose a unifying approach that leads to a meta-algorithm called unified gap-based exploration (UGapE), with a common structure and similar theoretical analysis for these two settings. We prove a performance bound for the two versions of the algorithm showing that the two problems are characterized by the same notion of complexity. We also show how the UGapE algorithm as well as its theoretical analysis can be extended to take into account the variance of the arms and to multiple bandits. Finally, we evaluate the performance of UGapE and compare it with a number of existing fixed budget and fixed confidence algorithms.

6.2. Statistical Analysis of Time Series

6.2.1. Prediction of Sequences of Structured and Unstructured Data

Reducing statistical time-series problems to binary classification [45]

We show how binary classification methods developed to work on i.i.d. data 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. The algorithms that we construct for solving these problems are based on a new metric between time-series distributions, which can be evaluated using binary classification methods. Universal consistency of the proposed algorithms is proven under most general assumptions. The theoretical results are illustrated with experiments on synthetic and real-world data.

6.2.2. Hypothesis Testing

Testing composite hypotheses about discrete ergodic processes [21]

Given a discrete-valued sample $X_1, \cdots, X_n$ we wish to decide whether it was generated by a distribution belonging to a family H_0, or it was generated by a distribution belonging to a family H_1. In this work we assume that all distributions are stationary ergodic, and do not make any further assumptions (in particular, no independence or mixing rate assumptions). We find some necessary and some sufficient conditions, formulated in terms of the topological properties of H_0 and H_1, for the existence of a consistent test. For the case when H_1 is the complement of H_0 (to the set of all stationary ergodic processes) these necessary and sufficient conditions coincide, thereby providing a complete characterization of families of processes membership to which can be consistently tested, against their complement, based on sampling. This criterion includes as special cases several known and some new results on testing for membership to various parametric families, as well as testing identity, independence, and other hypotheses.

Uniform hypothesis testing for finite-valued stationary processes [22]

Given a discrete-valued sample $X_1, \cdots, X_n$ we wish to decide whether it was generated by a distribution belonging to a family H_0, or it was generated by a distribution belonging to a family H_1. In this work we assume that all distributions are stationary ergodic, and do not make any further assumptions (e.g. no independence or mixing rate assumptions). We would like to have a test whose probability of error (both Type I and Type II) is uniformly bounded. More precisely, we require that for each ϵ there exist a sample size n such that probability of error is upper-bounded by ϵ for samples longer than n. We find some necessary and some sufficient conditions on H_0 and H_1 under which a consistent test (with this notion of consistency) exists. These conditions are topological, with respect to the topology of distributional distance.

6.2.3. Change Point Analysis

Locating Changes in Highly Dependent Data with Unknown Number of Change Points [39]

The problem of multiple change point estimation is considered for sequences with unknown number of change points. A consistency framework is suggested that is suitable for highly dependent time-series, and an asymptotically consistent algorithm is proposed. In order for the consistency to be established the only assumption required is that the data is generated by stationary ergodic time-series distributions. No modeling, independence or parametric assumptions are made; the data are allowed to be dependent and the dependence can be of arbitrary form. The theoretical results are complemented with experimental evaluations.

6.2.4. Clustering Time Series, Online and Offline

Online Clustering of Processes [40]

The problem of online clustering is considered in the case where each data point is a sequence generated by a stationary ergodic process. Data arrive in an online fashion so that the sample received at every time-step is either a continuation of some previously received sequence or a new sequence. The dependence between the sequences can be arbitrary. No parametric or independence assumptions are made; the only assumption is that the marginal distribution of each sequence is stationary and ergodic. A novel, computationally efficient algorithm is proposed and is shown to be asymptotically consistent (under a natural notion of consistency). The performance of the proposed algorithm is evaluated on simulated data, as well as on real datasets (motion classification).

Incremental Spectral Clustering with the Normalised Laplacian [52]

Partitioning a graph into groups of vertices such that those within each group are more densely connected than vertices assigned to different groups, known as graph clustering, is often used to gain insight into the organization of large scale networks and for visualization purposes. Whereas a large number of dedicated techniques have been recently proposed for static graphs, the design of on-line graph clustering methods tailored for evolving networks is a challenging problem, and much less documented in the literature. Motivated by the broad variety of applications concerned, ranging from the study of biological networks to graphs of scientific references through to the exploration of communications networks such as the World Wide Web, it is the main purpose of this paper to introduce a novel, computationally efficient, approach to graph clustering in the evolutionary context. Namely, the method promoted in this article is an incremental eigenvalue solution for the spectral clustering method described by Ng. et al. (2001). Beyond a precise description of its practical implementation and an evaluation of its complexity, its performance is illustrated through numerical experiments, based on datasets modelling the evolution of a HIV epidemic and the purchase history graph of an e-commerce website.

6.2.5. Online Semi-Supervised Learning

Learning from a Single Labeled Face and a Stream of Unlabeled Data [41]

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.

6.3. Statistical Learning and Bayesian Analysis

6.3.1. Non-parametric Methods for Function Approximation

Linear Regression with Random Projections [16]

We investigate a method for regression that makes use of a randomly generated subspace G_P (of finite dimension P) of a given large (possibly infinite) dimensional function space F, for example, $L_2([0,1]^d)$. G_P is defined as the span of P random features that are linear combinations of a basis functions of F weighted by random Gaussian i.i.d. coefficients. We show practical motivation for the use of this approach, detail the link that this random projections method share with RKHS and Gaussian objects theory and prove, both in deterministic and random design, approximation error bounds when searching for the best regression function in G_P rather than in F, and derive excess risk bounds for a specific regression algorithm (least squares regression in G_P). This paper stresses the motivation to study such methods, thus the analysis developed is kept simple for explanations purpose and leaves room for future developments.

6.3.2. Nonparametric Bayesian Estimation

DPM pour l'inférence dans les modèles dynamiques non linéaires avec des bruits de mesure alpha-stable [50]

Stable random variables are often use to model impulsive noise; Recently it has be shown that communication at very high frequency suffer from such a noise. Stable noise cannot however be considered as usual noise in estimation processes because the variance does not usually exists nor an analytic expression for the probability density function. In this work we show how to manage such a problem using a bayesian nonparametric approach. We develop a Sequential Monte Carlo based algorithm to realize the estimation in a non linear dynamical system. The measurement noise is a non-stationnary stable process and it is modeled using a Dirichlet Process Mixture.

6.3.3. Random Finite Sets for Multisensor Multitarget Tracking

Multi-sensor PHD filtering with application to sensor management [2]

The aim of multi-object filtering is to address the multiple target detection and/or tracking problem. This thesis focuses on the Probability Hypothesis Density (PHD) filter, a well-known tractable approximation of the Random Finite Set (RFS) filter when the observation process is realized by a single sensor. The first part proposes the rigorous construction of the exact multi-sensor PHD filter and its simplified expression, without approximation, through a joint partitioning of the target state space and the sensors. With this new method, the exact multi-sensor PHD can be propagated in simple surveillance scenarii. The second part deals with the sensor management problem in the PHD framework. At each iteration, the Balanced Explorer and Tracker (BET) builds a prediction of the posterior multi-sensor PHD thanks to the Predicted Ideal Measurement Set (PIMS) and produces a multi-sensor control according to a few simple operational principles adapted to surveillance activities

6.4. Applications

6.4.1. Signal Processing

Dirichlet Process Mixtures for Density Estimation in Dynamic Nonlinear Modeling: Application to GPS Positioning in Urban Canyons [19]

In global positioning systems (GPS), classical localization algorithms assume, when the signal is received from the satellite in line-of-sight (LOS) environment, that the pseudorange error distribution is Gaussian. Such assumption is in some way very restrictive since a random error in the pseudorange measure with an unknown distribution form is always induced in constrained environments especially in urban canyons due to multipath/masking effects. In order to ensure high accuracy positioning, a good estimation of the observation error in these cases is required. To address this, an attractive flexible Bayesian nonparametric noise model based on Dirichlet process mixtures (DPM) is introduced. Since the considered positioning problem involves elements of non-Gaussianity and nonlinearity and besides, it should be processed on-line, the suitability of the proposed modeling scheme in a joint state/parameter estimation problem is handled by an efficient Rao-Blackwellized particle filter (RBPF). Our approach is illustrated on a data analysis task dealing with joint estimation of vehicles positions and pseudorange errors in a global navigation satellite system (GNSS)-based localization context where the GPS information may be inaccurate because of hard reception conditions.

Dislocation detection in field environments: A belief functions contribution [20]

Dislocation is defined as the change between discrete sequential locations of critical items in field environments such as large construction projects. Dislocations on large sites of materials and critical items for which discrete time position estimates are available represent critical state changes. The ability to detect dislocations automatically for tens of thousands of items can ultimately improve project performance significantly. Detecting these dislocations in a noisy information environment where low cost radio frequency identification tags are attached to each piece of material, and the material is moved sometimes only a few meters, is the main focus of this study. We propose in this paper a method developed in the frame of belief functions to detect dislocations. The belief function framework is well-suited for such a problem where both uncertainty and imprecision are inherent to the problem. We also show how to deal with the calculations. This method has been implemented in a controlled experimental setting. The results of these experiments show the ability of the proposed method to detect materials dislocation over the site reliably. Broader application of this approach to both animate and inanimate objects is possible.

Towards dictionary learning from images with non Gaussian noise [29]

We address the problem of image dictionary learning from noisy images with non Gaussian noise. This problem is difficult. As a first step, we consider the extreme sparse code given by vector quantization, i.e. each pixel is finally associated to 1 single atom. For Gaussian noise, the natural solution is K-means clustering using the sum of the squares of differences between gray levels as the dissimilarity measure between patches. For non Gaussian noises (Poisson, Gamma,...), a new measure of dissimilarity between noisy patches is necessary. We study the use of the generalized likelihood ratios (GLR) recently introduced by Deledalle et al. 2012 to compare non Gaussian noisy patches. We propose a K-medoids algorithm generalizing the usual Linde-Buzo-Gray K-means using the GLR based dissimilarity measure. We obtain a vector quantization which provides a dictionary that can be very large and redundant. We illustrate our approach by dictionaries learnt from images featuring non Gaussian noise, and present preliminary denoising results.

6.4.2. Medical Applications

Outlier detection for patient monitoring and alerting. [12]

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.

6.4.3. Web Mining

Managing advertising campaigns – an approximate planning approach [11]

We consider the problem of displaying commercial advertisements on web pages, in the "cost per click" model. The advertisement server has to learn the appeal of each type of visitor for the different advertisements in order to maximize the profit. Advertisements have constraints such as a certain number of clicks to draw, as well as a lifetime. This problem is thus inherently dynamic, and intimately combines combinatorial and statistical issues. To set the stage, it is also noteworthy that we deal with very rare events of interest, since the base probability of one click is in the order of 10^4. Different approaches may be thought of, ranging from computationally demanding ones (use of Markov decision processes, or stochastic programming) to very fast ones.We introduce NOSEED, an adaptive policy learning algorithm based on a combination of linear programming and multi-arm bandits. We also propose a way to evaluate the extent to which we have to handle the constraints (which is directly related to the computation cost). We investigate the performance of our system through simulations on a realistic model designed with an important commercial web actor.

ICML Exploration & Exploitation challenge: Keep it simple! [18]

Recommendation has become a key feature in the economy of a lot of companies (online shopping, search engines...). There is a lot of work going on regarding recommender systems and there is still a lot to do to improve them. Indeed nowadays in many companies most of the job is done by hand. Moreover even when a supposedly smart recommender system is designed, it is hard to evaluate it without using real audience which obviously involves economic issues. The ICML Exploration & Exploitation challenge is an attempt to make people propose efficient recommendation techniques and particularly focuses on limited computational resources. The challenge also proposes a framework to address the problem of evaluating a recommendation algorithm with real data. We took part in this challenge and achieved the best performances; this paper aims at reporting on this achievement; we also discuss the evaluation process and propose a better one for future challenges of the same kind.

6.4.4. Games

CLOP: Confident Local Optimization for Noisy Black-Box Parameter Tuning [30]

Artificial intelligence in games often leads to the problem of parameter tuning. Some heuristics may have coefficients, and they should be tuned to maximize the win rate of the program. A possible approach is to build local quadratic models of the win rate as a function of program parameters. Many local regression algorithms have already been proposed for this task, but they are usually not robust enough to deal automatically and efficiently with very noisy outputs and non-negative Hessians. The CLOP principle, which stands for Confident Local OPtimization, is a new approach to local regression that overcomes all these problems in a simple and efficient way. CLOP discards samples whose estimated value is confidently inferior to the mean of all samples. Experiments demonstrate that, when the function to be optimized is smooth, this method outperforms all other tested algorithms.

6.5. Other Results

Sequential approaches for learning datum-wise sparse representations [9]

In supervised classification, data representation is usually considered at the dataset level: one looks for the “best” representation of data assuming it to be the same for all the data in the data space. We propose a different approach where the representations used for classification are tailored to each datum in the data space. One immediate goal is to obtain sparse datum-wise representations: our approach learns to build a representation specific to each datum that contains only a small subset of the features, thus allowing classification to be fast and efficient. This representation is obtained by way of a sequential decision process that sequentially chooses which features to acquire before classifying a particular point; this process is learned through algorithms based on Reinforcement Learning. The proposed method performs well on an ensemble of medium-sized sparse classification problems. It offers an alternative to global sparsity approaches, and is a natural framework for sequential classification problems. The method extends easily to a whole family of sparsity-related problems which would otherwise require developing specific solutions. This is the case in particular for cost-sensitive and limited-budget classification, where feature acquisition is costly and is often performed sequentially. Finally, our approach can handle non-differentiable loss functions or combinatorial optimization encountered in more complex feature selection problems.

Multiple Operator-valued Kernel Learning [60]

Positive definite operator-valued kernels generalize the well-known notion of reproducing kernels, and are naturally adapted to multi-output learning situations. This paper addresses the problem of learning a finite linear combination of infinite-dimensional operator-valued kernels which are suitable for extending functional data analysis methods to nonlinear contexts. We study this problem in the case of kernel ridge regression for functional responses with an lr-norm constraint on the combination coefficients. The resulting optimization problem is more involved than those of multiple scalar-valued kernel learning since operator-valued kernels pose more technical and theoretical issues. We propose a multiple operator-valued kernel learning algorithm based on solving a system of linear operator equations by using a block coordinatedescent procedure. We experimentally validate our approach on a functional regression task in the context of finger movement prediction in brain-computer interfaces.

SIERRA Project-Team

6. New Results

6.1. A Stochastic Gradient Method with an Exponential Convergence Rate for Strongly-Convex Optimization with Finite Training Sets

Participants: Francis Bach, Mark Schmidt, Nicolas Le Roux [correspondant].

In [21], we propose a new stochastic gradient method for optimizing the sum of a finite set of smooth functions, where the sum is strongly convex. While standard stochastic gradient methods converge at sublinear rates for this problem, the proposed method incorporates a memory of previous gradient values in order to achieve a linear convergence rate. In a machine learning context, numerical experiments indicate that the new algorithm can dramatically outperform standard algorithms, both in terms of optimizing the training objective and reducing the testing objective quickly.

6.2. Convex Relaxation for Combinatorial Penalties

Participants: Francis Bach, Guillaume Obozinski [correspondant].

In [15], we propose an unifying view of several recently proposed structured sparsity-inducing norms. We consider the situation of a model simultaneously (a) penalized by a set- function de ned on the support of the unknown parameter vector which represents prior knowledge on supports, and (b) regularized in Lp-norm. We show that the natural combinatorial optimization problems obtained may be relaxed into convex optimization problems and introduce a notion, the lower combinatorial envelope of a set-function, that characterizes the tightness of our relaxations. We moreover establish links with norms based on latent representations including the latent group Lasso and block-coding, and with norms obtained from submodular functions.

6.3. Kernel change-point detection

Participant: Sylvain Arlot [correspondant].

In [16], we tackle the change-point problem with data belonging to a general set. We propose a penalty for choosing the number of change-points in the kernel-based method of Harchaoui and Cappé (2007). This penalty generalizes the one proposed for one dimensional signals by Lebarbier (2005). We prove it satisfies a non-asymptotic oracle inequality by showing a new concentration result in Hilbert spaces. Experiments on synthetic and real data illustrate the accuracy of our method, showing it can detect changes in the whole distribution of data, even when the mean and variance are constant. Our algorithm can also deal with data of complex nature, such as the GIST descriptors which are commonly used for video temporal segmentation.

Collaboration with Alain Celisse (University Lille 1; Inria Lille, MODAL team) and Zaïd Harchaoui (Inria Grenoble, LEAR team).

6.4. On the Equivalence between Herding and Conditional Gradient Algorithms

Participants: Francis Bach [correspondant], Simon Lacoste-Julien, Guillaume Obozinski.

In [5], we show that the herding procedure of Welling (2009) takes exactly the form of a standard convex optimization algorithm–namely a conditional gradient algorithm minimizing a quadratic moment discrepancy. This link enables us to invoke convergence results from convex optimization and to consider faster alternatives for the task of approximating integrals in a reproducing kernel Hilbert space. We study the behavior of the different variants through numerical simulations. The experiments indicate that while we can improve over herding on the task of approximating integrals, the original herding algorithm tends to approach more often the maximum entropy distribution, shedding more light on the learning bias behind herding.

6.5. V-fold cross-validation and V-fold penalization in least-squares density estimation

Participant: Sylvain Arlot [correspondant].

In [22], we study V-fold cross-validation for model selection in least-squares density estimation. The goal is to provide theoretical grounds for choosing V in order to minimize the least-squares risk of the selected estimator. We first prove a non asymptotic oracle inequality for V-fold cross-validation and its bias-corrected version (V-fold penalization), with an upper bound decreasing as a function of V. In particular, this result implies V-fold penalization is asymptotically optimal. Then, we compute the variance of V-fold cross-validation and related criteria, as well as the variance of key quantities for model selection performances. We show these variances depend on V like $1 + 1/(V - 1)$ (at least in some particular cases), suggesting the performances increase much from $V = 2$ to $V = 5$ or 10, and then is almost constant. Overall, this explains the common advice to take $V = 10$—at least in our setting and when the computational power is limited—, as confirmed by some simulation experiments.

Collaboration with Matthieu Lerasle (CNRS, University Nice Sophia Antipolis).

6.6. Machine learning for Neuro-imaging

Participants: Fabian Pedregosa [correspondant], Francis Bach, Guillaume Obozinski.

In the course of the year 2011-2012 two articles where submitted and accepted in international workshops. The first published article, **Improved brain pattern recovery through ranking approaches** ([12]) was presented at the 2nd International Workshop on Pattern Recognition in NeuroImaging in London, July 2012 and proposes a new approach for the problem of estimating the coefficients of a generalized linear model with monotonicity constraint. For this, we explore the use of ranking techniques, which are popular in the context of information retrieval but novel for medical imaging applications.

The second published article, **Learning to rank from medical imaging data** ([11]) uses the same techniques as the previous article to solve a more fundamental problem, that is, to predict a quantitative (and potentially non-linear) variable from a set of noisy measurements. We show on simulations and two fMRI datasets that this approach is able to predict the correct ordering on pairs of images, yielding higher prediction accuracy than standard regression and multiclass classification techniques.

Collaboration with the Parietal project-team (A. Gramfort, B. Thirion, G. Varoquaux)

6.7. SiGMa: Simple Greedy Matching for Aligning Large Knowledge Bases

Participant: Simon Lacoste-Julien [correspondant].

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. In [20], 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 which leverages both the structural information from the relationship graph as well as flexible similarity measures between entity properties in a greedy local search, thus making it scalable. Despite its greedy nature, our experiments indicate that SiGMa can efficiently match some of the world's largest knowledge bases with high precision. We provide additional experiments on benchmark datasets which demonstrate that SiGMa can outperform state-of-the-art approaches both in accuracy and efficiency.

Collaboration with Konstantina Palla, Alex Davies, Zoubin Ghahramani (Machine Learning Group, Department of Engineering, University of Cambridge); Gjergji Kasneci (Max Planck Institut fur Informatik); Thore Graepel (Microsoft Research Cambridge).

6.8. Block-Coordinate Frank-Wolfe Optimization for Structural SVMs

Participants: Simon Lacoste-Julien [correspondant], Mark Schmidt.

In [19], 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 the same 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, this yields an online algorithm that has the same low iteration complexity as primal stochastic subgradient methods. However, unlike stochastic subgradient methods, the stochastic 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.

Collaboration with Martin Jaggi (Centre de Mathématiques Appliquées, Ecole Polytechnique); Patrick Pletscher (Machine Learning Laboratory, ETH Zurich).

6.9. A convex relaxation for weakly supervised classifiers

Participants: Armand Joulin [correspondant], Francis Bach.

In [8], we introduce a general multi-class approach to weakly supervised classification. Inferring the labels and learning the parameters of the model is usually done jointly through a block-coordinate descent algorithm such as expectation-maximization (EM), which may lead to local minima. To avoid this problem, we propose a cost function based on a convex relaxation of the soft-max loss. We then propose an algorithm specifically designed to efficiently solve the corresponding semidefinite program (SDP). Empirically, our method compares favorably to standard ones on different datasets for multiple instance learning and semi-supervised learning, as well as on clustering tasks.

6.10. Multi-Class Cosegmentation

Participants: Armand Joulin [correspondant], Francis Bach.

Bottom-up, fully unsupervised segmentation remains a daunting challenge for computer vision. In the cosegmentation context, on the other hand, the availability of multiple images assumed to contain instances of the same object classes provides a weak form of supervision that can be exploited by discriminative approaches. Unfortunately, most existing algorithms are limited to a very small number of images and/or object classes (typically two of each). In [9], we propose a novel energy-minimization approach to cosegmentation that can handle multiple classes and a significantly larger number of images. The proposed cost function combines spectral- and discriminative-clustering terms, and it admits a probabilistic interpretation. It is optimized using an efficient EM method, initialized using a convex quadratic approximation of the energy. Comparative experiments show that the proposed approach matches or improves the state of the art on several standard datasets.

Collaboration with the Willow project-team (J. Ponce).

6.11. A latent factor model for highly multi-relational data

Participants: Nicolas Le Roux, Guillaume Obozinski [correspondant].

Many data such as social networks, movie preferences or knowledge bases are multi-relational, in that they describe multiple relations between entities. While there is a large body of work focused on modeling these data, modeling these multiple types of relations jointly remains challenging. Further, existing approaches tend to breakdown when the number of these types grows. In [7], we propose a method for modeling large multi relational datasets, with possibly thousands of relations. Our model is based on a bilinear structure, which captures various orders of interaction of the data, and also shares sparse latent factors across different relations. We illustrate the performance of our approach on standard tensor-factorization datasets where we attain, or outperform, state-of-the-art results. Finally, a NLP application demonstrates our scalability and the ability of our model to learn efficient and semantically meaningful verb representations.

Collaboration with R. Jenatton (CMAP, Ecole Polytechnique) and Antoine Bordes (CNRS, Université de Technologie de Compiégne).

6.12. Semi-supervised NMF with time-frequency annotations for single-channel source separation

Participants: Francis Bach, Augustin Lefèvre [correspondant].

In [10], we formulate a novel extension of nonnegative matrix factorization (NMF) to take into account partial information on source-specific activity in the spectrogram. Results on single-channel source separation show that time-frequency annotations allow to disambiguate the source separation problem, and learned annotations open the way for a completely unsupervised learning procedure for source separation with no human intervention.

Collaboration with C. Févotte (Laboratoire traitement et communication de l'information (LTCI), CNRS: UMR5141 - Institut Télécom - Télécom ParisTech).

TAO Project-Team

6. New Results

6.1. Realistic step sizes for optimization algorithms

Many theoretical results about objective improvement in the process of continuous optimization rely on the assumption that the steps of the algorithm are infinitesimally small, the only situation in which theoretical guarantees of improvement can be given. Y. Akimoto and Y. Ollivier have waived the necessity for such an assumption in a whole class of continuous optimization algorithms, thanks to the use of information geometry [20]. This takes theory closer to the practice of actual optimization algorithms.

6.2. Noisy Optimization Bounds with Constant Noise Variance

Many bounds in noisy evolutionary optimization are based on low variance assumptions (in particular, variance of noise converging to 0 close to the optima). Other bounds in the optimization literature consider difficult objective functions. We prove some new bounds, in the following setting[55]:

- without assuming that the variance is going to zero at the optimum;
- following some debates on the COCO mailing list (see 5.4), assuming that sampling far from the optimum (we had earlier results without this assumption; new results emphasize the contrast).

6.3. Extensions of Upper Confidence Trees

We developed extensions of Upper Confidence Trees to continuous or large domains (states and/or actions) and to domains with high expertise or strong structure[37], [31], [38] (incidentally realizing performances on MineSweeper); we recently submitted a proof of a variant of UCT with consistency proof in the continuous domains (both actions and random variables are allowed to be continuous). Another extension is to the difficult setting with no possibility to “undo” a decision or duplicate a state; see [63]. Yet another extension aims at multi-objective optimization [56].

6.4. Mixing myopic fast algorithms and asymptotically optimal algorithms

We made several works based on combining in sequential decision making:

- a fast algorithm providing quickly good heuristic results;
- an asymptotically optimal, too slow for real size problems.

Results are published in [31] and [38], outperforming the state of the art for MineSweeper in reasonable time; an application to energy has been done, and a new one is under work (see Section 4.1). We believe that this diea of combining fast approximate solutions and slow asymptotically optimal algorithms is a key for improving the state of the art in high dimensional combinatorial planning and that our results on MineSweeper and moderate size energy problem are a solid first step in this direction.

6.5. Adaptive Metropolis with Online Relabeling

In [23] we proposed a novel adaptive MCMC algorithm named AMOR (Adaptive Metropolis with Online Relabeling) for efficiently simulating from permutation-invariant targets occurring in, for example, Bayesian analysis of mixture models. An important feature of the algorithm is to tie the adaptation of the proposal distribution to the choice of a particular restriction of the target to a domain where label switching cannot occur. The algorithm relies on a stochastic approximation procedure for which we design a Lyapunov function that formally defines the criterion used for selecting the relabeling rule. This criterion reveals an interesting connection with the problem of optimal quantifier design in vector quantization which was only implicit in previous works on the label switching problem. In benchmark examples, the algorithm turns out to be fast-converging and efficient at selecting meaningful non-trivial relabeling rules to allow accurate parameter inference. In [24] the algorithm was applied to a synthetic mixture model inspired by the muonic water Cherenkov signal of the surface detectors in the Pierre Auger Experiment.

6.6. Reinforcement learning for frugal cascade learning

In [32] we propose an algorithm that builds sparse decision DAGs (directed acyclic graphs) from a list of base classifiers provided by an external learning method such as AdaBoost. The basic idea is to cast the DAG design task as a Markov decision process. Each instance can decide to use or to skip each base classifier, based on the current state of the classifier being built. The result is a sparse decision DAG where the base classifiers are selected in a data-dependent way. The method has a single hyperparameter with a clear semantics of controlling the accuracy/speed trade-off. The algorithm is competitive with state-of-the-art cascade detectors on three object-detection benchmarks, and it clearly outperforms them when there is a small number of base classifiers. Unlike cascades, it is also readily applicable for multi-class classification. Using the multi-class setup, we show on a benchmark web page ranking data set that we can significantly improve the decision speed without harming the performance of the ranker. Beside outperforming classical cascade designs on benchmark data sets, the algorithm also produces interesting deep structures where similar input data follows the same path in the DAG, and subpaths of increasing length represent features of increasing complexity.

ALEA Project-Team

6. New Results

6.1. Bayesian Nonparametric models for ranked data and bipartite graphs.

In [20], the author develops a novel Bayesian nonparametric model for random bipartite graphs. The model is based on the theory of completely random measures and is able to handle a potentially infinite number of nodes. It is shown that the model has appealing properties and in particular it may exhibit a power-law behavior. Posterior characterization, a generative process for network growth, and a simple Gibbs sampler for posterior simulation are derived. The model is shown to be well fitted to several real-world social networks.

In [21], we develop a Bayesian nonparametric extension of the popular Plackett-Luce choice model that can handle an infinite number of choice items. Our framework is based on the theory of random atomic measures, with the prior specified by a gamma process. We derive a posterior characterization and a simple and effective Gibbs sampler for posterior simulation. We develop a time-varying extension of our model, and apply it to the New York Times lists of weekly bestselling books.

6.2. A new model for polychotomous data

Multinomial logistic regression is one of the most popular models for modelling the effect of explanatory variables on a subject choice between a set of specified options. This model has found numerous applications in machine learning, psychology or economy. Bayesian inference in this model is non trivial and requires, either to resort to a Metropolis-Hastings algorithm, or rejection sampling within a Gibbs sampler. In [19], we propose an alternative model to multinomial logistic regression. The model builds on the Plackett-Luce model, a popular model for multiple comparisons. We show that the introduction of a suitable set of auxiliary variables leads to an Expectation-Maximization algorithm to find Maximum A Posteriori estimates of the parameters. We further provide a full Bayesian treatment by deriving a Gibbs sampler, which only requires to sample from highly standard distributions. We also propose a variational approximate inference scheme. All are very simple to implement. One property of our Plackett-Luce regression model is that it learns a sparse set of feature weights. We compare our method to sparse Bayesian multinomial logistic regression and show that it is competitive, especially in presence of polychotomous data.

6.3. 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 in [37] 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.

6.4. Evolutionnary algorithms and genetic programming

In [22], we consider the identification of a nonlinear system modelled by a nonlinear output error (NOE) model when the system output is disturbed by an additive zero-mean white Gaussian noise. In that case, standard on-line or off-line least squares methods may lead to poor results. Here, our approach is based on evolutionary algorithms. Although their computational cost can be higher than the above methods, these algorithms present some advantages, which often lead to an effortless optimisation. Indeed, they do not need an elaborate formalisation of the problem. When their parameters are correctly tuned, they avoid to get stuck at a local optimum. To take into account the influence of the additive noise, we investigate different approaches and we suggest a whole protocol including the selection of a fitness function and a stop rule. Without loss of generality, simulations are provided for two nonlinear systems and various signal-to-noise ratios.

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. The paper [17] 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. In [23] and [24], 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.

In [32], the goal 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.

6.5. Moderate Deviations for Mean Field Particle Models

The article [40] is concerned with moderate deviation principles of a general class of mean eld type interacting particle models. We discuss functional moderate deviations of the occupation measures for both the strong - topology on the space of fi nite 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.

6.6. Bifurcating autoregressive processes

In [42], 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.

In [46], we study 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.

In [47], 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.

6.7. Durbin-Watson statistic and first order autoregressive processes

In [45], 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.

In [51], 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.

6.8. 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 [50], 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.

6.9. 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. In [49], 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.

6.10. A Robbins-Monro procedure for a class of models of deformation

The paper [48] deals with the statistical analysis of several data sets as- sociated 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 esti- mates 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.

6.11. Individual load curves intraday forecasting

A dynamic coupled modelling is investigated to take temperature into account in the individual energy consumption forecasting. The objective in [44] 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. On the length of one–dimensional reactive paths

Participants: Frédéric Cérou, Arnaud Guyader, Florent Malrieu.

See 3.3 and 4.2 .

This is a collaboration with Tony Lelièvre (ENPC).

Motivated by some numerical observations on molecular dynamics simulations, we analyze metastable trajectories in a very simple setting, namely paths generated by a one-dimensional overdamped Langevin equation for a double well potential. More precisely, we are interested in so–called reactive paths, namely trajectories which leave definitely one well and reach the other one. The aim of [32] is to precisely analyze the distribution of the lengths of reactive paths in the limit of small temperature, and to compare the theoretical results to numerical results obtained by a Monte Carlo method, namely the multi–level splitting approach.

5.2. Long time behavior of piecewise–deterministic Markov processes

Participant: Florent Malrieu.

This is a collaboration with Michel Benaïm (université de Neuchâtel), Stéphane Le Borgne (IRMAR) and Pierre–André Zitt (université de Marne–la–Vallée).

5.2.1. Quantitative ergodicity for some switched dynamical systems

We provide quantitative bounds for the long time behavior of a class of piecewise deterministic Markov processes with state space $R^d \times E$ where E is a finite set. The continuous component evolves according to a smooth vector field that switches at the jump times of the discrete coordinate. The jump rates may depend on the whole position of the process. Under regularity assumptions on the jump rates and stability conditions for the vector fields we provide explicit exponential upper bounds for the convergence to equilibrium in terms of Wasserstein distances [13]. As an example, we obtain convergence results for a stochastic version of the Morris–Lecar model of neurobiology.

5.2.2. On the stability of planar randomly switched systems

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 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. The paper [29] can be viewed as a probabilistic counterpart of the paper [36] by Baldé, Boscain and Mason.

5.2.3. Qualitative properties of certain piecewise deterministic Markov processes

We study a class of piecewise deterministic Markov processes with state space $R^m \times E$ where E is a finite set. The continous component evolves according to a smooth vector field that it switched at the jump times of the discrete coordinate. The jump rates may depend on the whole position of the process. Working under the general assumption that the process stays in a compact set, we detail a possible construction of the process and characterize its support, in terms of the solutions set of a differential inclusion. We establish results on the long time behaviour of the process, in relation to a certain set of accessible points, which is shown to be strongly linked to the support of invariant measures. Under Hörmander–type bracket conditions, we prove that there exists a unique invariant measure and that the processes converges to equilibrium in total variation. Finally we give examples where the bracket condition does not hold, and where there may be one or many invariant measures, depending on the jump rates between the flows [30].

5.3. Quantitative long time behavior of an ergodic variant of the telegraph process

Participant: Florent Malrieu.

This is a collaboration with Joaquin Fontbona (University of Chile) and Hélène Guérin (IRMAR).

Motivated by stability questions on piecewise deterministic Markov models of bacterial chemotaxis, we study the long time behavior of a variant of the classic telegraph process having a non–constant jump rate that induces a drift towards the origin. We compute its invariant law and show exponential ergodicity, obtaining a quantitative control of the total variation distance to equilibrium at each instant of time. These results [15] rely on an exact description of the excursions of the process away from the origin and on the explicit construction of an original coalescent coupling for both velocity and position. Sharpness of the obtained convergence rate is discussed.

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 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 [28] is to provide quantitative estimates for the exponential convergence to equilibrium, in terms of the total variation and Wasserstein distances.

5.5. Convergence results for approximate Bayesian computation

Participants: Frédéric Cérou, Arnaud Guyader.

This is a collaboration with Gérard Biau (ENS and université Pierre et Marie Curie).

Approximate Bayesian computation (ABC for short) is a family of computational techniques which offer an almost automated solution in situations where evaluation of the posterior likelihood is computationally prohibitive, or whenever suitable likelihoods are not available. In [31], we analyze the procedure from the point of view of k-nearest neighbor theory and explore the statistical properties of its outputs. We discuss in particular some asymptotic features of the genuine conditional density estimate associated with ABC, which is a new interesting hybrid between a k-nearest neighbor and a kernel method. These are among the very few results on the convergence of ABC, and our assumptions on the underlying probability distribution are minimal.

5.6. Soft level splitting for rare event estimation

Participants: Frédéric Cérou, Arnaud Guyader.

See 3.3 and 4.2 .

This is a collaboration with Nicolas Hengartner (Los Alamos).

It is well established now that one can use adaptive splitting levels to compute the conditional probabilities of nested sets. To get an efficient algorithm, the probability of a set given the previous one should be always the same, which is approximately achieved adaptively by using the empirical cdf (cumulative distribution function) of the scores. The way to proceed is to fix a probability of success p_0, and then choose the p_0 quantile of the current scores. Here we investigate whether, by using the whole cdf, and not only one quantile, we can design an algorithm with better performance. The main trick is a transformation to have a sample of exponential variables. This would require the knowledge of the cdf of the cost, which is obviously unvailable, but we can replace it by the empirical cdf of the sample at the previous level. The complete theoretical study of this algorithm is still to be done, but we have illustrated by some examples that it can lead to significantly better results than the standard splitting procedure with the same number of intermediate levels.

5.7. Decoding fingerprints using the Markov chain Monte Carlo method

Participants: Frédéric Cérou, Arnaud Guyader.

This is a collaboration with Teddy Furon (Inria Rennes, project–team TEXMEX).

The paper [22] proposes a new fingerprinting decoder based on the Markov chain Monte Carlo (MCMC) method. A Gibbs sampler generates groups of users according to the posterior probability that these users could have forged the sequence extracted from the pirated content. The marginal probability that a given user pertains to the collusion is then estimated by a Monte Carlo method. The users having the biggest empirical marginal probabilities are accused. This MCMC method can decode any type of fingerprinting codes. This paper is in the spirit of the *learn and match* decoding strategy: it assumes that the collusion attack belongs to a family of models. The expectation–maximization algorithm estimates the parameters of the collusion model from the extracted sequence. This part of the algorithm is described for the binary Tardos code and with the exploitation of the soft outputs of the watermarking decoder. The experimental body considers some extreme setups where the fingerprinting code lengths are very small. It reveals that the weak link of our approach is the estimation part. This is a clear warning to the *learn and match* decoding strategy.

5.8. Iterative isotone regression

Participants: Arnaud Guyader, Nicolas Jégou.

This is a collaboration with Nicolas Hengartner (Los Alamos) and Eric Matzner–Løber (université de Rennes 2), and with Alexander B. Németh (Babeş Bolyai University) and Sándor Z. Németh (University of Birmingham).

The current collaboration on nonparametric regression focuses on a novel nonparametric regression technique that applies ideas borrowed from iterative bias reduction to estimating functions of bounded variations. This work has emerged from the joint supervision of Nicolas Jégou's PhD thesis by Arnaud Guyader, Nick Hengartner and Eric Matzner-Løber.

A geometric approach has been investigated, as an extension of some ideas developed in the thesis. The current work [33] proposes and analyzes a novel method for estimating a univariate regression function of bounded variation. The underpinning idea is to combine two classical tools in nonparametric statistics, namely isotonic regression and the estimation of additive models. A geometrical interpretation enables us to link this iterative method with Von Neumann's algorithm. Moreover, making a connection with the general property of isotonicity of projection onto convex cones, we derive another equivalent algorithm and go further in the analysis. As iterating the algorithm leads to overfitting, several practical stopping criteria are also presented and discussed.

5.9. Detection issues in track–before–detect

Participants: François Le Gland, Alexandre Lepoutre.

See 4.1 .

This is a collaboration with Olivier Rabaste (ONERA Palaiseau).

Track–before–detect refers to situations where the target SNR is so low that it is practically impossible to detect the presence of a target, using a simple thresholding rule. In such situations, the solution is to keep all the information available in the raw radar data and to address directly the tracking problem, using a particle filter with a binary Markov variable that models the presence or absence of the target. The choice of the proposal distribution is crucial here, and an efficient particle filter is proposed [24] that is based on a relevant proposal distribution built from detection and estimation considerations, that aims at extracting all the available information from the measurements. The proposed filter leads to a dramatically improved performance as compared with particle filters based on the classical proposal distribution, both in terms of detection and estimation. A further improvement, in terms of detection performance, is to model the problem as a quickest change detection problem [70] in a Bayesian framework. In this context, the posterior distribution of the first time of appearance of the target is a mixture where each component represents the hypothesis that the target appeared at a given time. The posterior distribution is intractable in practice, and it is proposed [23] to approximate each component of the mixture by a particle filter. It turns out that the mixture weights can be computed recursively in terms of quantities that are provided by the different particle filters. The overall filter yields good performance as compared with classical particle filters for track–before–detect.

5.10. Estimation of conflict probability

Participants: François Le Gland, Damien–Barthélémy Jacquemart.

See 3.3 and 4.2 .

This is a collaboration with Jérôme Morio (ONERA Palaiseau).

In [16], the conflict probability between aircraft in uncontrolled airspace is estimated using the importance splitting method, and this algorithm is applied on realistic situations of aircraft conflict. The current work aims at designing efficient intermediate regions at a reasonnable computational cost, or alternatively at introducing weights to compensate for a simple but suboptimal design of the intermediate regions.

5.11. Minimum volume set for a rare event

Participants: François Le Gland, Rudy Pastel.

See 3.3 and 4.2 .

This is a collaboration with Jérôme Morio (ONERA Palaiseau).

The paper [19] first reviews the principle of minimum volume set estimation of a given probability level for a multidimensional density, a strategy that provides a sound solution to the multidimensional quantile issue. It then describes an importance sampling algorithm that is suitable for this kind of estimation problems, and provides simulation results for the estimation of the impact zone of a space launcher. The current work aims at designing an importance splitting method that would be more efficient for extreme quantiles.

5.12. Laplace and sequential Monte Carlo methods in Bayesian filtering

Participants: François Le Gland, Paul Bui–Quang.

This is a collaboration with Christian Musso (ONERA Palaiseau).

The Laplace method is a deterministic technique to approximate integrals, and it has been widely used in Bayesian statistics, e.g. to compute posterior means and variances [72]. The approximation is consistent as the observations sample size goes to infinity or as the observation noise intensity goes to zero, and the main condition to apply the method is that the model should be identifiable. The aim of [21] is to combine SMC methods and the Laplace method in order to better approximate the posterior density in nonlinear Bayesian filtering. At each stage of the proposed algorithm, a first approximate density is build from the current population of particles, then an accurate estimate of the posterior mean and covariance matrix is obtained using the Laplace method, and these estimates are used to shift and rescale the population of particles. Overall, this procedure could be interpreted as another design of an importance distribution that takes the observations into account. The current work aims at using the Laplace method to cope with *weight degeneracy* in particle filtering, a phenomenon that typically occurs when the observation noise is small, which is precisely the situation where the Laplace method is efficient.

5.13. Wind–wave modelling

Participant: Valérie Monbet.

This is a collaboration with Pierre Ailliot (UBO).

Climate change will bring large changes to the mean climate, and especially to climate extremes, over the coming decades. Computationally expensive global climate model (GCM) projections provide good information about future mean changes. Computationally efficient, yet physically consistent, statistical models of weather variables (stochastic weather generators) allow us to explore the frequency and severity of weather and climate events in much greater detail. When deployed as a complement to GCMs, stochastic weather generators provide a much richer picture of the future, allowing us to better understand, evaluate and manage future weather and climate risks, especially for renewal energy. In this context we are developing a space time model for wind fields in the North–East Atlantic, based on a conditionally transformed Gaussian state space model.

5.14. Sequential data assimilation: ensemble Kalman filter vs. particle filter

Participants: François Le Gland, Valérie Monbet.

Surprisingly, very little was known about the asymptotic behaviour of the ensemble Kalman filter [44], [45], [46], whereas on the other hand, the asymptotic behaviour of many different classes of particle filters is well understood, as the number of particles goes to infinity. Interpreting the ensemble elements as a population of particles with mean–field interactions, and not only as an instrumental device producing an estimation of the hidden state as the ensemble mean value, it has been possible to prove the convergence of the ensemble Kalman filter, with a rate of order $1/\sqrt{N}$, as the number N of ensemble elements increases to infinity [62]. In addition, the limit of the empirical distribution of the ensemble elements has been exhibited, which differs from the usual Bayesian filter. The next step 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.

CQFD Project-Team

5. New Results

5.1. Singularly Perturbed Discounted Markov Control Processes in a General State Space

Participant: François Dufour.

Markov decision processes, optimal control, infinite discounted expected cost, optimal control, singular perturbation

In this work, it is studied the asymptotic optimality of discrete-time Markov Decision Processes (MDP's in short) with general state space and action space and having weak and strong interactions. The idea in this work is to consider a MDP with general state and action spaces and to reduce the dimension of the state space by considering an averaged model. This formulation is often described by introducing a small parameter $\epsilon > 0$ in the definition of the transition kernel, leading to a singularly perturbed Markov model with two time scales. Our objective is twofold. First it is shown that the value function of the control problem for the perturbed system converges to the value function of a limit averaged control problem as ϵ goes to zero. In the second part of this work, it is proved that a feedback control policy for the original control problem defined by using an optimal feedback policy for the limit problem is asymptotically optimal. Our work extends existing results of the literature in the following two directions: the underlying MDP is defined on general state and action spaces and we do not impose strong conditions on the recurrence structure of the MDP such as Doeblin's condition.

These results have been obtained in collaboration with Oswaldo Luis Do Valle Costa from Escola Politécnica da Universidade de São Paulo, Brazil.

It has been published in SIAM Journal of Control and Optimization [16].

5.2. The expected total cost criterion for Markov decision processes under constraints: a convex analytic approach.

Participant: François Dufour.

Markov decision process, expected total cost criterion, constraints, linear programming, occupation measure

This work deals with discrete-time Markov Decision Processes (MDP's) under constraints where all the objectives have the same form of an expected total cost over the infinite time horizon. The existence of an optimal control policy is discussed by using the convex analytic approach. We work under the assumptions that the state and action spaces are general Borel spaces and the model is non-negative, semi-continuous and there exists an admissible solution with finite cost for the associated linear program. It is worth noting that, in contrast with the classical results of the literature, our hypotheses do not require the MDP to be transient or absorbing. Our first result ensures the existence of an optimal solution to the linear program given by an occupation measure of the process generated by a randomized stationary policy. Moreover, it is shown that this randomized stationary policy provides an optimal solution to this Markov control problem. As a consequence, these results imply that the set of randomized stationary policies is a sufficient set for this optimal control problem. Finally, our last main result states that all optimal solutions of the linear program coincide on a special set with an optimal occupation measure generated by a randomized stationary policy. Several examples are presented to illustrate some theoretical issues and the possible applications of the results developed in the paper.

These results have been obtained in collaboration with Alexey Piunovskiy from Department. of Mathematical Sciences, The University of Liverpool, United Kingdom and with Masayuki Horiguchi form the Department of Mathematics, Faculty of Engineering, Kanagawa University, Japan.

It has been published in Advances in Applied Probability [17] and in the invited session of the 25th conference EURO 2012 [27]

5.3. Approximation of Infinite Horizon Discounted Cost Markov Decision Processes

Participant: François Dufour.

Markov decision processes, infinite horizon discounted cost criterion, approximation and discretization

In this work, we deal with a discrete-time infinite horizon Markov decision process with locally compact Borel state and action spaces, and possibly unbounded cost function. Based on Lipschitz continuity of the elements of the control model, we propose a state and action discretization procedure for approximating the optimal value function and an optimal policy of the original control model. We provide explicit bounds on the approximation errors.

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 the book Optimization, Control, and Applications of Stochastic Systems. In Honor of Onésimo Hernandez-Lerma [52].

5.4. Continuous Control of Piecewise Deterministic Markov Processes with Long Run Average Cost

Participant: François Dufour.

Piecewise-deterministic Markov Processes, long-run average cost, optimal control, integro-differential optimality equation

The main goal of this work is to derive sufficient conditions for the existence of an optimal control strategy for the long run average continuous control problem of piecewise deterministic Markov processes (PDMP's) taking values in a general Borel space and with compact action space depending on the state variable. In order to do that we apply the so-called vanishing discount approach to obtain a solution to an average cost optimality inequality (ACOI) associated to the long run average cost problem. Our main assumptions are written in terms of some integro-differential inequalities related to the so-called expected growth condition, and geometric convergence of the post-jump location kernel associated to the PDMP.

These results have been obtained in collaboration with Oswaldo Luis Do Valle Costa from Escola Politécnica da Universidade de São Paulo, Brazil.

It has been published in the book Stochastic Processes, Finance and Control. A Festschrift in Honor of Robert J. Elliott [51].

5.5. Optimal stopping for partially observed piecewise-deterministic Markov processes

Participants: Adrien Brandejsky, Benoîte de Saporta, François Dufour.

We have investigated an optimal stopping problem under partial observation for piecewise-deterministic Markov processes (PDMP) both from the theoretical and numerical points of view. PDMP's have been introduced by Davis [73] as a general class of stochastic models. They form a family of Markov processes involving deterministic motion punctuated by random jumps. One important property of a PDMP, relevant for the approach developed in this paper, is that its distribution is completely characterized by the embedded discrete time Markov chain $(Z_n, S_n)_{n\in\mathbb{N}}$ where Z_n is the n-th post-jump location and S_n is the n-th inter-jump time. We consider the following optimal stopping problem for a partially observed PDMP $(X_t)_{t\geq 0}$. Roughly speaking, the observation process $(Y_t)_{t\geq 0}$ is a point process defined through the embedded discrete time Markov chain $(Z_n, S_n)_{n\in\mathbb{N}}$. The inter-arrival times are given by $(S_n)_{n\in\mathbb{N}}$ and the marks by a noisy function of $(Z_n)_{n\in\mathbb{N}}$. For a given reward function g and a computation horizon $N \in \mathbb{N}$, we study the following optimal stopping problem

$$\sup_{\sigma \le T_N} \mathbb{E}\left[g(X_\sigma)\right],$$

where T_N is the N-th jump time of the PDMP $(X_t)_{t\geq 0}$, σ is a stopping time with respect to the natural filtration $\mathcal{F}^o = (\mathcal{F}^o_t)_{t\geq 0}$ generated by the observations $(Y_t)_{t\geq 0}$.

A general methodology to solve such a problem is to split it into two sub-problems. The first one consists in deriving the filter process given by the conditional expectation of X_t with respect to the observed information $\mathcal{F}^o_t$. Its main objective is to transform the initial problem into a completely observed optimal stopping problem where the new state variable is the filter process. The second step consists in solving this reformulated problem, the new difficulty being its infinite dimension. Indeed, the filter process takes values in a set of probability measures.

Our work is inspired by [92] which deals with an optimal stopping problem under partial observation for a Markov chain with finite state space. The authors study the optimal filtering and convert their original problem into a standard optimal stopping problem for a continuous state space Markov chain. Then they propose a discretization method based on a quantization technique to approximate the value function. However, their method cannot be directly applied to our problem for the following main reasons related to the specificities of PDMPs.

Firstly, PDMPs are continuous time processes. Then, it appears natural to work with the embedded Markov chain $(Z_n, S_n)_{n\in\mathbb{N}}$. In addition, we assume that $(Z_n)_{n\in\mathbb{N}}$ takes finitely many values. However, an important difficulty is that the structure of stopping time remains intrinsically continuous. Consequently, our problem cannot be converted into a fully discrete time problem.

Secondly, the distribution of a PDMP combines both absolutely continuous and singular components. This is due to the existence of forced jumps when the process hits the boundary of the state space. As a consequence the derivation of the filter process is not straightforward. In particular, the absolute continuity hypothesis **(H)** of [92] does not hold.

Thirdly, in our context the reformulated optimization problem is not standard, unlike in [92]. Indeed, although we obtain a reformulation similar to an optimal stopping problem for a fully observed PDMP, it involves the Markov chain $(\Pi_n, S_n)_{n\in\mathbb{N}}$ that is not the embedded Markov chain of some PDMP. Therefore, a new derivation of dynamic programming equations is required as we cannot use the results of [81]. In particular, one needs to derive fine properties of the structure of the $(\mathcal{F}^o_t)_{t\geq 0}$-stopping times. Moreover, we construct an ϵ-optimal stopping time.

Finally, a natural way to proceed with the numerical approximation is then to follow the ideas developed in [92] [8] namely to replace the filter Π_n and the inter-jump time S_n by some finite state space approximations in the dynamic programming equation. However, a noticeable difference from [8] lies in the fact that the dynamic programming operators therein were Lipschitz continuous whereas our new operators are only Lipschitz continuous between some points of discontinuity. We overcome this drawback by splitting the operators into their restrictions onto their continuity sets. This way, we obtain not only an approximation of the value function of the optimal stopping problem but also an ϵ-optimal stopping time with respect to the filtration $(\mathcal{F}^o_t)_{t\geq 0}$ that can be computed in practice.

This work is submitted for publication [60] and presented in an invited international conference [26].

5.6. Predictive maintenance for the heated hold-up tank

Participants: Benoîte de Saporta, François Dufour, Huilong Zhang.

A complex system is inherently sensitive to failures of its components. One must therefore determine maintenance policies in order to maintain an acceptable operating condition. Optimizing the maintenance is a very important problem in the analysis of complex systems. It determines when it is best that maintenance tasks should be performed on the system in order to optimize a cost function: either maximize a performance function or conversely minimize a loss function. Moreover, this optimization must take into account the random nature of failures and random evolution and dynamics of the system.

The example considered here is the maintenance of the heated hold-up tank, a well know test case for dynamic reliability, see e.g. [75], [89], [90], [94]. 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 rate of the components depends on the temperature, the position of the three components monitors the liquid level in the tank, and in turn, the liquid level determines the temperature. The main characteristic of this system is that it can be modeled by a stochastic hybrid process, where the discrete and continuous parts interact in a closed loop. As a consequence, simulating this process and computing related reliability indices has been a challenge for the dynamic reliability community. To our best knowledge, optimization of maintenance policies for the heated hold-up tank has not been addressed yet in the literature.

The only maintenance operation considered here is the complete replacement of all the failed components and the system restarts in its initial equilibrium state. Partial repairs are not allowed. Mathematically, this problem of preventive maintenance corresponds to a stochastic optimal stopping problem as explained by example in the book of Aven and Jensen [68]. It is a difficult problem because of the closed loop interactions between the state of the components and the liquid level and temperature. A classical approach consists in using condition-based maintenance (CBM) to act on the system based on its current state and before its failure. One can for example calculate the remaining useful life (RUL) of the system and the preventive replacement is carried out when the deterioration level exceeds a certain threshold or enters in a certain state [96], [80]. Our approach also takes into account the current state of the process, but our decision rule is not based on damage accumulation nor does it correspond to hitting some threshold. Instead, it involves a performance function that reflects that the longer the system is in a functioning state the better.

The dynamics of the heated hold-up tank can be modeled by a piecewise deterministic Markov process (PDMP), see [94]. Therefore, our maintenance problem boils down to an optimal stopping problem for PDMP's. PDMP's are a class of stochastic hybrid processes that has been introduced by Davis [73] in the 80's. These processes have two components: a Euclidean component that represents the physical system (e.g. temperature, pressure, ...) and a discrete component that describes its regime of operation and/or its environment. Starting from a state x and mode m at the initial time, the process follows a deterministic trajectory given by the laws of physics until a jump time that can be either random (e.g. it corresponds to a component failure or a change of environment) or deterministic (when a magnitude reaches a certain physical threshold, for example the pressure reaches a critical value that triggers a valve). The process restarts from a new state and a new mode of operation, and so on. This defines a Markov process. Such processes can naturally take into account the dynamic and uncertain aspects of the evolution of the system. A subclass of these processes has been introduced by Devooght [75] for an application in the nuclear field. The general model has been introduced in dynamic reliability by Dutuit and Dufour [79].

As illustrated above, it is crucial to have an efficient numerical tool to compute the optimal maintenance time in practical cases. To this aim, a general numerical approach was developed in [8]. It was first applied to an example of maintenance of a metallic structure subject to corrosion, without closed loop interactions or deterministic jumps, and with a simple cost function that did not depend on time, see [23]. The objective of the present paper is to further demonstrate the high practical power of the theoretical methodology described in [8], by applying it to the more challenging heated hold-up tank problem. The cost function chosen here is also more complex as it takes into account both continuous components as well as the running time. More precisely, we propose to compute the optimal cost as well as a quasi-optimal stopping rule, which is the date when the maintenance should be performed. As a by-product of our procedure, the distribution of the optimal maintenance dates is also obtained, as well as the distributions of the liquid level and temperature at the chosen maintenance date.

This work is submitted for publication [66] and presented in an international conference [32].

5.7. Efficient simulation of the availability of a feedwater control system

Participants: Benoîte de Saporta, François Dufour, Huilong Zhang.

In the reliability modeling of complex control systems, classical methodologies such as even-trees/fault-trees or Petri nets may not represent adequately the dynamic interactions existing between the physical processes (modeled by continuous variables) and the functional and dysfunctional behavior of its components (modeled by discrete variables). We have proposed a framework for modeling and simulation of a water level control system in the steam generator (SG) in the secondary circuit of a nuclear power plant. A similar benchmark system was described by the U.S. Nuclear Regulatory Commission [67] to compare two approaches to dynamic reliability: DFM (Dynamic Flowgraph Methodology) and Markov/CCMT (Cell-to-Cell Mapping Technique). But the report released by the NRC is not sufficient to reconstruct a realistic model. We have developed a complete benchmark case. The behavioral model of SG is obtained from a linearized model published in 2000 by EDF [87]. Detailed description of the components, failure modes and control laws of the principal components is presented. For modeling the system, we use the piecewise deterministic Markov processes (PDP) framework [73] and for implementation we chose Simulink associated with Stateflow. PDP's offer a very general modeling framework to deal with dynamic reliability problems; Simulink is a good tool to simulate non linear differential equations and their controller, while Stateflow implementation is appropriate for finite state machine descriptions of different components.

In our benchmark system, four physical processes are considered: feedwater flowrate, steam flow, narrow range water level and wide range water level. A PID controller is used to maintain the water level within limits of set-points. The system is composed of seven components: 1 passive system representing vapor transport system, 3 extraction pumps, 2 feeding turbopumps, and 1 waterflow regulation valve. The functional and dysfunctional behaviors and the failure rates of each component are based on operational experience. In 2012, we have further improved our simulator by taking captors (and their possible failures) into account.

This work was presented in an international conference [36], a national conference [39] and is published as a book chapter [49].

5.8. 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. 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. Why? A smart operator, if provided information about target's position and velocity and a sound propagation code can find a good trajectory. If we- now consider a submarine surrounded by several targets, it is clear that a human operator will have great difficulty to find the best route.

This work was presented in an international conference [35].

5.9. Statistical study od asymmetry in cell lineage data

Participants: Benoîte de Saporta, Anne Gégout-Petit.

This work proposes a rigorous methodology to study cell division data consisting in several observed genealogical trees of possibly different shapes. For instance, [93] filmed 94 colonies of Escherichia coli cells dividing between four and nine times. We propose a new rigorous approach to take into account all the available information. Indeed, we propose an inference based on a finite fixed number of replicated trees when the total number of observed cells tends to infinity. We use the missing data asymmetric BAR model introduced by [7]. In this approach, the observed genealogies are modeled with a two-type Galton Watson (GW) process. However, we propose a different least-squares estimator for the parameters of the BAR process that does not correspond to the single-tree estimators averaged on the replicated trees. We also propose an estimator of the parameters of the GW process specific to our binary tree structure and not based simply on the observation of the number of cells of each type in each generation.

Our procedure allows us to fully take into account missing observations, data from different trees as well as the dependence structure within genealogical trees. It also enables us to use all the information available without the drawbacks of low accuracy for estimators or low power for tests on small single trees. We study the consistency and asymptotic normality of our estimators and derive asymptotic confidence intervals as well as Wald's type tests to investigate the asymmetry of the data for both the BAR and GW processes. Our results are applied to the Escherichia coli data of [93].

This work is in collaboration with Laurence Marsalle (Lille 1 University). It is submitted for publication [65] and was presented in an international conference [33].

5.10. Random coefficient bifurcating autoregressive processes

Participants: Benoîte de Saporta, Anne Gégout-Petit.

In the 80's, Cowan and Staudte [72] introduced Bifurcating Autoregressive processes (BAR) as a parametric model to study cell lineage data. A quantitative characteristic of the cells (e.g. growth rate, age at division) is recorded over several generations descended from an initial cell, keeping track of the genealogy to study inherited effects. As a cell usually gives birth to two offspring by division, such genealogies are naturally structured as binary trees. BAR processes are thus a generalization of autoregressive processes (AR) to this binary tree structure, by modeling each line of descent as a first order AR process, allowing the environmental effects on sister cells to be correlated. Statistical inference for the parameters of BAR processes has been widely studied, either based on the observation of a single tree growing to infinity [72], [85], [83], [95] or on a large number of small independent trees [86], [84].

Various extensions of the original model have been proposed, but to our best knowledge, only two papers [71] and [70] deal with random coefficient BAR processes. In the former by Bui and Huggins it is explained that random coefficients BAR processes can account for observations that do not fit the usual BAR model. For instance, the extra randomness can model irregularities in nutrient concentrations in the media in which the cells are grown. In this work, we propose a new model for random coefficient BAR processes (R-BAR). It is more general than that of Bui and Huggins, as the random variables are not supposed to be Gaussian, they may not have moments of all order and correlation between all the sources of randomness are allowed. Moreover, we propose an asymmetric model in the continuance of [82], [69], [74], [70], [7], [24] in the context of missing data. Indeed, experimental data are often incomplete and it is important to take this phenomenon into account for the inference. We model the structure of available data by a Galton Watson tree, instead of a complete binary tree. Our model is close to that developed in [70], but the assumptions on the noise process are different as we allow correlation between the two sources of randomness but require higher moments because of the missing data and because we do not use a weighted estimator. The main difference is that the model in [70] is fully observed, whereas ours allows for missing observations.

Our approach for the inference of our model is also different from [71], [70]. As we cannot use maximum likelihood estimation, we propose modified least squares estimators as in [91]. The originality of our approach is that it combines the bifurcating Markov chain and martingale approaches. Bifurcating Markov chains (BMC) were introduced in [82] on complete binary trees and further developed in [74] in the context of missing data on Galton Watson trees. BAR models can be seen as a special case of BMC. This interpretation allows us to establish the convergence of our estimators. A by-product of our procedure is a new general result for BMC on Galton Watson trees. Indeed, in [82], [74] the driven noise sequence is assumed to have moments of all order. Here, we establish new laws of large numbers for polynomial functions of the BMC where the noise sequence only has moments up to a given order. The strong law of large numbers [78] and the central limit theorem for martingales have been previously used in the context of BAR processes and adapted to special cases of martingales on binary trees. In this paper, we establish a general law of large numbers for square integrable martingales on Galton Watson binary trees. This result is applied to our R-BAR model to obtain sharp convergence rates and a quadratic strong law for our estimators.

This work is in collaboration with Laurence Marsalle (Lille 1 University). It is submitted for publication [64].

5.11. Hidden Markov Model for the detection of a degraded state in an optronic equipment

Participants: Camille Baysse, Anne Gégout-Petit, Jérôme Saracco.

As part of optimizing the reliability, Thales Optronics now includes systems that examine the state of its equipment. This function is performed by HUMS (Health & Usage Monitoring System). We hope to implement a program based on these observations that can determine the lifetime of this optronic equipment. Our study focuses on a simple example of HUMS. As part of our research, we are interested in a variable called "time-to cold" noted TMF, which reflects the state of system. Using this information about this variable, we seek to detect as soon as possible a degraded state and propose maintenance before failure. For this we use a hidden Markov model. The state of our system at time t is then modeled by a Markov chain X_t. However we do not observe directly this chain but indirectly through the TMF, a noisy function of this chain. Thanks to filtering equations, we obtained results on the probability that an equipment breaking down at time t, knowing the history of the TMF until this moment. We have subsequently studied this methodology with simulated data. Then finally we applied these results on the analysis of our real data and we have checked that the results are consistent with the reality. So using this method could allow the company to recall equipments which are estimated in deteriorated state and do not control those estimated in stable state. Thales Optronics could improve its maintenance system and reduce its cost function.

This work is a part of the CIFRE PhD of Camille Baysse also supervised for the Thales part by Didier Bihannic and Michel Prenat. It was presented in an national conference [38] and is submitted for publication in an national per-reviewed journal [58].

5.12. Predictive maintenance for an optronic equipment

Participants: Camille Baysse, Benoîte de Saporta, Anne Gégout-Petit, Jérôme Sarraco.

After the problem of detection of a degraded state, we have tackled the problem of predictive maintenance for an optronic equipment. For this we model the state of the system by a PDMP (state with three possible values and cumulative time of use). In this framework, we reformulate the problem of maintenance of optimization in an optimal stopping problem maximizing a criteria about time of use without failure. In this framework, we can use known results developed in the CQFD team on optimal control [8], [23]. We have extensively studied the problem with simulated data, computed grid of quantization and optimal policy for the real problem. This results will be implemented by Thales in HUMS of optronic equipment.

This work was presented in an national conference [38] and an abstract is accepted for publication in an international conference with papers.

5.13. Non parametric estimation of the jump rate for non-homogeneous marked renewal processes

Participants: Romain Azaïs, François Dufour, Anne Gégout-Petit.

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. The methodology is illustrated by a numerical example. It is the object of a paper [57] to appear in the Annales de l'Intitut Poincaré

5.14. Non parametric estimation of conditional distribution of the interjumping times for piecewise Markov processes

Participants: Romain Azaïs, François Dufour, Anne Gégout-Petit.

This work gives 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 example illustrates the behavior of our estimator. This work is the object of a paper [56] submitted for publication

5.15. Stochastic modelling and simulation of fatigue crack propagation using piecewise-deterministic Markov processes

Participants: Romain Azaïs, Anne Gégout-Petit.

Fatigue crack propagation is a stochastic phenomenon in nature due to the inherent uncertainties coming from material properties, environmental conditions and loads. Stochastic processes offer an appropriate framework for modelling crack propagation since it is intended to include sources variabilities. In this work, we propose to model crack propagation mechanism with Piecewise Deterministic Markov Process (PDMP) using usual random crack laws. Conventional laws proposed in the literature seem inadequate for describing the whole fatigue crack trajectory mainly when the crack extends in a rapid manner. To overcome this drawback, a new modelling is proposed that consists in using more than one law as each one is more suitable for a specific phase during crack propagation. Regime-switching models seem very attractive and with our modelling assessed crack growth rates and crack lengths are very close to experimental values. Moreover, behaviour just before failure is well captured and can be discussed. Empirical curves from literature are used to adjust the parameters associated to the proposed modelling. Statistical observations and numerical simulations show the efficiency of the proposed approach to model and to simulate fatigue crack growth. This work has been presented in an international congress [34] and is the object of a paper which will be submitted very soon.

5.16. Statistical Analysis of Grapevine Mortality Associated with Esca or Eutypa Dieback Foliar Expression

Participant: Anne Gégout-Petit.

Esca and Eutypa dieback are two major wood diseases of grapevine in France. Their widespread distribution in vineyards leads to vine decline and to a loss in productivity. However, little is known either about the temporal dynamics of these diseases at plant level, and equally, the relationships between foliar expression of the diseases and vine death is relatively unknown too. . To investigate these questions, we surveyed the vines of six vineyards cv. Cabernet Sauvignon in the Bordeaux region, by recording foliar symptoms, dead arms and dead plants from 2004 to 2010. In 2008, 2009 and 2010, approximately five percent of the asymptomatic vines died but the percentage of dead vines which had previously expressed esca foliar symptoms was higher, and varied between vineyards. A logistic regression model was used to select the previous years of symptomatic expression associated with vine mortality. The mortality of esca is always associated with the foliar symptom expression of the year preceding vine death. One or two other earlier years of expression frequently represented additional risk factors. The Eutypa dieback symptom was also a risk factor of death, superior or equal to that of esca. The study of the internal necroses of vines expressing esca or Eutypa dieback is discussed in the light of these statistical results. This work has been presented in an international congress [44] and is the object of a submitted paper.

5.17. MonteCarlo test for two patterns of point processes on a grid

Participants: Anne Gégout-Petit, Marie Chavent, Amaury Labenne.

In order to compare two patterns of distribution of symptomatic or dead vines in a same vineyard but for two consecutive years, we have developed a Monte Carlo test. First we estimate the intensity of occurrence of disease in one of the pattern, then we simulate n realizations i.i.d. of this intensity and compute the associate likelihoods in order to build an interval that cover $(1-\alpha)$ per cent of the realizations. The test reject the equality of repartition if the likelihood computed with the second pattern is not included in this interval. We have made simulations and applied this test to the repartition of esca in vineyard. This work has been presented in a national workshop on software R [46].

5.18. Multivariate Analysis for the detection of the effect of a treatment

Participant: Anne Gégout-Petit.

The aim of this work is to give some statistical rules to determine if a patient is meeting a given treatment (a BD here). The criterium commonly used to determine if a patient is meeting a BD treatment is based only on one physiological parameter : if this parameter increases, the patient is meeting. But now, many physiological parameters are measured in routine and it seems that a patient could have a global amelioration of his health state due to the treatment without an increase of the single used parameter.

Using standard multivariate analysis techniques, and classification, we have proposed criteria to discriminate groups of patients different in regard of their response to treatment. This work will be used by physiologists to propose new criteria for the measure of the effect of a BD treatment. It is in collaboration with physiologists from Bordeaux and Nantes universities and is the object of a submitted paper in a international peer-reviewed journal in the domain of pneumology .

5.19. A hidden renewal model for monitoring aquatic systems biosensors

Participants: Romain Azaïs, Raphaël Coudret.

This work aims at modeling signals of oysters' openings over time using a four-state renewal process. Two of them are of particular interest and correspond to instants when the animals are open or closed. An estimator of the cumulative jump rate of this process is provided. It relies on observations of the jumps between the four states. Here these measures are not available but the observed signal takes ranges of real values according to this underlying process. A procedure to estimate a probability density function that summarizes the information of the signal is explained. This leads to estimate the hidden renewal process and then its cumulative jump rate for each oyster. A classification of these functions for a group of oysters discriminate them according to their assumed health status. Such a diagnosis is essential when using these animals as biosensors for water quality assessment. This work is a joint work with Gilles Durrieu from Université de Bretagne Sud and in collaboration with UMR CNRS 5805 EPOC.

5.20. A recursive nonparametric estimator for the transition kernel of a piecewise-deterministic Markov process

Participant: Romain Azaïs.

We investigate a nonparametric approach to provide a recursive estimator of the transition density of a non-stationary piecewise-deterministic Markov process, from only one observation of the path within a long time. In this framework, we do not observe a Markov chain with transition kernel of interest. Fortunately, one may write the transition density of interest as the ratio of the invariant distributions of two embedded chains of the process. Our method consists in estimating these invariant measures. We state a result of consistency under some general assumptions about the main features of the process. A simulation study illustrates the well asymptotic behavior of our estimator. This work is the object of a paper [55] submitted for publication.

5.21. A new sliced inverse regression method for multivariate response

Participants: Jérôme Saracco, Raphaël Coudret.

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 e ffective dimension reduction (EDR) space without requiring a prespeci ed parametric model. The convergence at rate square root of 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.

These results have been obtained in collaboration with Stéphane Girard (Inria Rhône Alpes).

The paper is under revision for possible publication in CSDA [63].

5.22. Comparison of kernel density estimators with assumption on number of modes

Participants: Jérôme Saracco, Raphaël Coudret.

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.

These results have been obtained in collaboration with Gilles Durrieu (Université Bretagne-Sud).

The paper is under revision for possible publication in Communications in Statistics - Simulation and Computation [62].

5.23. A new approach on recursive and non-recursive SIR methods

Participant: Jérôme Saracco.

We consider a semiparametric single index regression model involving a p-dimensional quantitative covariable x and a real dependent variable y. A dimension reduction is included in this model via an index $x'\beta$. Sliced inverse regression (SIR) is a well-known method to estimate the direction of the Euclidean parameter β which is based on a ”slicing step” of y in the population and sample versions. The goal of this paper is twofold. On the one hand, we focus on a recursive version of SIR which is also suitable for multiple indices model. On the other hand, we propose a new method called SIRoneslice when the regression model is a single index model. The SIRoneslice estimator of the direction of β is based on the use of only one ”optimal” slice chosen among the H slices. Then, we provide its recursive version.We give an asymptotic result for the SIRoneslice approach. Simulation study shows good numerical performances of the SIRoneslice method and clearly exhibits the main advantage of using recursive versions of the SIR and SIRoneslice methods from a computational time point of view. A real dataset is also used to illustrate the approach. Some extensions are discussed in concluding remarks. The proposed methods and criterion have been implemented in R and the corresponding codes are available from the authors.

These results have been obtained in collaboration with Bernad Bercu (Université Bordeaux 1) and Thi Mong Ngoc Nguyen (Université de Strasbourg).

The paper has been published in the Journal of the Korean Statistical Society [11].

5.24. On the asymptotic behavior of the Nadaraya-Watson estimator associated with the recursive SIR method

Participant: Jérôme Saracco.

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.

These results have been obtained in collaboration with Bernad Bercu (Université Bordeaux 1) and Thi Mong Ngoc Nguyen (Université de Strasbourg) .

The paper is submitted [59].

5.25. Comparison of sliced inverse regression approaches for underdetermined cases

Participants: Jérôme Saracco, Raphaël Coudret.

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 RSIR and 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 eQTL.

These results have been obtained in collaboration with Benoit Liquet (Université Bordeaux 2) . The paper is submitted .

5.26. Orthogonal rotation in PCAMIX

Participants: Marie Chavent, Jérôme Saracco.

Kiers (1991) considered the orthogonal rotation in PCAMIX, a principal component method for a mixture of qualitative and quantitative variables. PCAMIX includes the ordinary Principal Component Analysis (PCA) and Multiple Correspondence Analysis (MCA) as special cases. In this work, we give a new presentation of PCAMIX where the principal components and the squared loadings are obtained from a Singular Value Decomposition. The loadings of the quantitative variables and the principal coordinates of the categories of the qualitative variables are also obtained directly. In this context, we propose a computationaly efficient procedure for varimax rotation in PCAMIX and a direct solution for the optimal angle of rotation. A simulation study shows the good computational behavior of the proposed algorithm. An application on a real data set illustrates the interest of using rotation in MCA. All source codes are available in the R package “PCAmixdata”.

These results have been obtained in collaboration with Vanessa Kuentz of IRSTEA (UR ABDX).

It has been published in Advances in Data Analysis and Classification [15] and presented in the context of application in cultural sociology in the Premières Rencontres R [42].

5.27. A sliced inverse regression approach for data stream

Participants: Marie Chavent, Jérôme Saracco.

In this work, we focus on data arriving sequentially by block 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 in pooling all the observed blocks and estimate the EDR direction by the SIR (Sliced Inverse Regression) method. But some disadvantages appear in practice such as the storage of the blocks and the running time for high dimensional data. To overcome these drawbacks, we propose an adaptive SIR estimator of based on the SIR approach for a stratified population developed by Chavent et al. (2011). The proposed approach is faster both from computational complexity and running time points of view, and provides data storage benefits. We show the consistency of our estimator at the root-n rate and give its asymptotic distribution. We propose an extension to multiple indices model. We also provide a graphical tool in order to detect if a drift occurs in the EDR direction or if some aberrant blocks appear in the data stream. In a simulation study, we illustrate the good numerical behavior of our estimator. One important advantage of this approach is its adaptability to changes in the underlying model. Finally we apply it on real data concerning the estimation of Mars surface physical properties.

This work is under revision in Statistics and Computing [61].

5.28. ClustOfVar: An R Package for the Clustering of Variables

Participants: Marie Chavent, Jérôme Saracco.

Clustering of variables is as a way to arrange variables into homogeneous clusters, i.e., groups of variables which are strongly related to each other and thus bring the same information. These approaches can then be useful for dimension reduction and variable selection. Several specific methods have been developed for the clustering of numerical variables. However concerning qualitative variables or mixtures of quantitative and qualitative variables, far fewer methods have been proposed. The R package ClustOfVar was specifically developed for this purpose. The homogeneity criterion of a cluster is defined as the sum of correlation ratios (for qualitative variables) and squared correlations (for quantitative variables) to a synthetic quantitative variable, summarizing “as good as possible” the variables in the cluster. This synthetic variable is the first principal component obtained with the PCAMIX method. Two clustering algorithms are proposed to optimize the homogeneity criterion: iterative relocation algorithm and ascendant hierarchical clustering. We also propose a bootstrap approach in order to determine suitable numbers of clusters. We illustrate the methodologies and the associated package on small datasets.

These results have been obtained in collaboration with Vanessa Kuentz of IRSTEA (UR ABDX).

It has been published in Journal of Statistical Softwares [14]. The study of the inclusion of environment by the farmer with ClustOfVar has been presented in the Premières Rencontres R and in [45]

5.29. Divisive Monothetic Clustering for Interval and Histogram-valued Data

Participant: Marie Chavent.

In this paper we propose a divisive top-down clustering method designed for interval and histogram-valued data. The method provides a hierarchy on a set of objects together with a monothetic characterization of each formed cluster. At each step, a cluster is split so as to minimize intra-cluster dispersion, which is measured using a distance suitable for the considered variable types. The criterion is minimized across the bipartitions induced by a set of binary questions. Since interval-valued variables may be considered a special case of histogram-valued variables, the method applies to data described by either kind of variables, or by variables of both types. An example illustrates the proposed approach.

These results have been obtained in collaboration with Paula Brito of Porto University and presented in ICPRAM'2012 [31].

5.30. Classification of EEG signals by an evolutionary algorithm

Participants: Marie Chavent, Laurent Vézard.

The goal is to predict the alertness of an individual by analyzing the brain activity through electroencephalographic data (EEG) captured with 58 electrodes. Alertness is characterized 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.

These results have been obtained in collaboration with Pierrick Legrand of ALEA Inria team.

It has been published in Journal des Nouvelles Technologies [25] and presented in COMPSTAT 2012 [47].

5.31. Variable selection by genetic algorithm for the study of alertness states.

Participants: Marie Chavent, Laurent Vézard.

The aim of this work is to predict the state of alertness of an individual (binary variable, "normal" or "relaxed") from the study of brain activity (electroencephalographic signals EEG) collected with a limited number of electrodes. In fact, the set up of electrodes during the EEG signal acquisition is time consuming and these electrodes are correlated. In our study, 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 based on the study of the contingent negative variation (CNV), 19 subjects were retained in the study. A CSP (Common Spacial Pattern) coupled to a linear discriminant analysis were used to build a decision rule and thus predict the alertness of the participants. A genetic algorithm was used to determine a subset of electrodes of size p '(where p' <p, where p = 58 is the number of electrodes). This presentation will present the CSP in the general framework and will introduce innovations made to this method. The genetic algorithm will be described proposed and recent results will be presented.

These results have been obtained in collaboration with Pierrick Legrand of ALEA Inria team.

It has been presented in the Journée Évolutionnaire Thématique, 23éme édition [48].

5.32. Handling Missing Values with Regularized Iterative Multiple Correspondence Analysis

Participant: Marie Chavent.

A common approach to deal with missing values in multivariate exploratory data analysis consists in minimizing the loss function over all non-missing elements. This can be achieved by EM-type algorithms where an iterative imputation of the missing values is performed during the estimation of the axes and components. This paper proposes such an algorithm, named iterative multiple correspondence analysis, to handle missing values in multiple correspondence analysis (MCA). This algorithm, based on an iterative PCA algorithm, is described and its properties are studied. We point out the over tting problem and propose a regularized version of the algorithm to overcome this major issue. Finally, performances of the regularized iterative MCA algorithm (implemented in the R-package named missMDA) are assessed from both simulations and a real dataset. Results are promising with respect to other methods such as the missing-data passive modi ed margin method, an adaptation of the missing passive method used in Gini's Homogeneity analysis framework.

It has been published in Journal of Classification [21].

I4S Team

6. New Results

6.1. identification of linear systems

6.1.1. Modular identification and damage detection for large structures

Participants: Michael Döhler, Laurent Mevel.

Subspace identification algorithms are efficient for output-only eigenstructure identification of linear MIMO systems. The problem of merging sensor data obtained from moving and nonsimultaneously recorded measurement setups under varying excitation is considered. To address the problem of dimension explosion, when retrieving the system matrices of the complete system, a modular and scalable approach is proposed. Adapted to a large class of subspace methods, observability matrices are normalized and merged to retrieve global system matrices [12].

6.1.2. Fast multi order subspace identification algorithm

Participants: Michael Döhler, Laurent Mevel.

Subspace methods have proven to be efficient for the identification of linear time-invariant systems, especially applied to mechanical, civil or aeronautical structures in operation conditions. Therein, system identification results are needed at multiple (over-specified) model orders in order to distinguish the true structural modes from spurious modes using the so-called stabilization diagrams. In this paper, new efficient algorithms are derived for this multi-order system identification with subspace-based identification algorithms and the closely related Eigensystem Realization Algorithm. It is shown that the new algorithms are significantly faster than the conventional algorithms in use. They are demonstrated on the system identification of a large-scale civil structure [11], [15].

6.1.3. Evaluation of confidence intervals and computation of sensitivities for subspace methods

Participants: Michael Döhler, Laurent Mevel.

In Operational Modal Analysis, the modal parameters (natural frequencies, damping ratios and mode shapes) obtained from Stochastic Subspace Identification (SSI) of a structure, are afflicted with statistical uncertainty. Uncertainty computation schemes have been developed.This approach has been validated on large scale examples[16].

6.1.4. Subspace methods in frequency domain

Participants: Philippe Mellinger, Michael Döhler, Laurent Mevel.

In Operational Modal Analysis (OMA) of large structures it is often needed to process output-only sensor data from multiple non-simultaneously recorded measurement setups, where some reference sensors stay fixed, while the others are moved between the setups. A standard approach to process the data together for global system identification is to transfer the data into frequency domain and merge it there. However, this only works if the unmeasured ambient excitation remains stationary throughout all setups. As the ambient excitation can be different from setup to setup, the amplitude of the measured data can be different as well and the data has to be normalized. Recently, a method has been developed for covariance- and data-driven Stochastic Subspace Identification (SSI) to automatically normalize and merge the data from multiple setups in order to obtain the global modal parameters (natural frequencies, damping ratios, mode shapes), instead of doing the SSI for each setup separately. In this paper, we adapt this approach to multi-setup SSI in frequency domain, where we use spectra data instead of time series data. We demonstrate the advantages of the new merging approach in the frequency domain and apply it to a relevant industrial large scale example, where we compare the estimation results of the modal parameters between the time and frequency domain approaches [24].

6.1.5. Subspace Identification for Linear Periodically Time-varying Systems

Participant: Ahmed Jhinaoui.

In this paper, an extension of the output-only subspace identification, to the class of linear periodically time-varying (LPTV) systems, is proposed. The goal is to identify a useful information about the system's stability using the Floquet theory which gives a necessary and sufficient condition for stability analysis. This information is retrieved from a matrix called the monodromy matrix, which is extracted by some simultaneous singular value decomposition (SVD) and from a resolution of a least squares criterion. The method is, finally, illustrated by a simulation of a model of a helicopter with hinged-blades rotor and a prototype of the same model. The method is then applied to data from a real wind turbine [22], [19], [20].

6.2. damage detection for mechanical structures

6.2.1. Damage detection and localisation

Participants: Michael Döhler, Luciano Marin, 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 some empirically defined threshold. In this paper, we show how the derivation of the uncertainty of the state space system can be used to derive uncertainty on the damage localization residuals and help to decide about the damage location [23].

6.2.2. Robust subspace damage detection

Participants: Michael Döhler, Laurent Mevel.

Subspace methods enjoy some popularity, especially in mechanical engineering, where large model orders have to be considered. In the context of detecting changes in the structural properties and the modal parameters linked to them, some subspace based fault detection residual has been recently proposed and applied successfully. However, most works assume that the unmeasured ambient excitation level during measurements of the structure in the reference and possibly damaged condition stays constant, which is not possible in any application. This work addresses the problem of robustness of such fault detection methods. A subspace-based fault detection test is derived that is robust to excitation change but also to numerical instabilities that could arise easily in the computations [17], [26].

6.2.3. Input-Output Subspace-Based Fault Detection

Participant: Laurent Mevel.

Subspace-based fault detection method using input-output information is developed in this paper. In some practical applications, the environment noise is the only input that excites the system. Although the statistical properties of the noise might be estimated, the value of the noise is not usually available at each time instance. The traditional subspace fault detection is already developed for such situations. In several other applications, measured inputs are applied to the system or even the stochastic noise might be measurable. While it is still possible to use the traditional output-only detection method, it is reasonable to expect that the application of extra input information together with the output data improves the detection. Several computation issues are discussed in this paper to include input data in the detection method, correctly. Simulation results show the efficiency of using the input information to improve the quality of fault detection [18].

6.2.4. Structural Reliability Updating with Stochastic Subspace Damage Detection Information

Participant: Michael Döhler.

Damage detection algorithms as a part of Structural Health Monitoring (SHM) are widely applied in research and industry and have shown their capabilities to efficiently detect structural damages. These algorithms usually compare a model from a safe reference state of a structure to vibration data from a possibly damaged state. For such a comparison, special properties of real vibration data introduce uncertainties, such as low signal-to-noise ratios, non-stationary or nonwhite ambient excitation, non-linear behavior and many more. Recently, statistical damage detection algorithms based on stochastic subspace identification have been proposed that take into account the uncertainties in the data. Building upon the uncertainty modeling, the next step in the view of the authors is to utilize damage detection algorithm information in the context of the structural reliability theory. Therefore, this paper introduces an approach for the updating of the structural reliability with damage detection algorithm information. Two steps are described namely the determination of a probability of detection (PoD) distribution function for damage detection algorithms accounting for the relevant uncertainties and the concept of Bayesian updating of the structural reliability. The introduced approaches are applied in generic examples. In this way the potential of the utilization of damage detection system information for more reliable structural systems are demonstrated [27].

6.3. Instability monitoring of aeronautical structures

6.3.1. Instability monitoring for LPTV systems

Participants: Laurent Mevel, Ahmed Jhinaoui.

Most subspace-based methods enabling instability monitoring are restricted to the linear time-invariant (LTI) systems. In this paper, a new subspace method of instability monitoring is proposed for the linear periodically time-varying (LPTV) case. For some LPTV systems, the system transition matrices may depend on some parameter and are also periodic in time. A certain range of values for the parameter leads to an unstable transition matrix. Early warning should be given when the system gets close to that region, taking into account the time variation of the system. Using the theory of Floquet, some symptom parameter of stability- or residual- is defined. Then, the parameter variation is tracked by performing a set of parallel cumulative sum (CUSUM) tests. Finally, the method is tested on a simulated model of a helicopter with hinged blades, for monitoring the ground resonance phenomenon [21]. It follows the work on linear systems for aircraft monitoring done previously [14].

6.3.2. Optimal input design for identification and detection

Participant: Laurent Mevel.

This paper considers the problem of auxiliary input design for subspace-based fault detection methods. In several real applications, particularly in the damage detection of mechanical structures and vibrating systems, environment noise is the only input to the system. In some applications, white noise produces low quality output data for the subspace-based fault detection method. In those methods, a residual is calculated to detect the fault based on the output information. However, some modes of the system may not influence the outputs and the residual appropriately if the input is not exciting enough for those modes. In this paper, the method of "rotated inputs" is implemented to excite the system modes. In addition to produce a residual more sensitive to the weak modes, it is possible to detect system order changes due to the fault using the rotated inputs. Simulation results demonstrate the efficiency of injecting the auxiliary input to improve the subspace-based fault detection methodology. [13]. This work is funded by FP7-NMP Large Scale Integrated Project IRIS.

MATHRISK Team

5. New Results

5.1. Dynamic risk measures and BSDEs with jumps

The standard approach of mathematical quantification of financial risk in terms of Value at Risk has serious deficiencies. This has motivated a systematic analysis of risk measures which satisfy some minimal requirements of coherence and consistency. The theory of risk measures has been first developed in [54] in the coherent case and then extended in various directions (convex, dynamic, law-invariant) (see e.g. [70], [68], [93], [69]). We are extending this theory, in particular in the case of markets with possible random jumps and model ambiguity, and investigate various types of optimization problems involving risk measures.

Mathematical techniques for the treatment of such problems are based on non linear expectations, backward stochastic differential equations (BSDEs), stochastic control, stochastic differential games.

In the Brownian case, links between dynamic risk measures and Backward Stochastic Differential Equations (BSDEs) have been established (see, among others, [57]). A. Sulem and M.-C. Quenez are exploring these links in the case of stochastic processes with jumps. To this purpose, we have recently extended some comparison theorems for BSDEs with jumps given in [90], and provided a representation theorem of convex dynamic risk measures induced by BSDEs with jumps (see [44]). Optimization of dynamic risk measures leads to stochastic differential games or to optimal control problems for coupled systems of forward-backward stochastic differential equations (FBSDEs). They can be studied by stochastic maximum principles [100] or by transforming them into controlled Backward Stochastic Partial Differential Equations (BSPDEs). We address these questions in collaboration with B. Øksendal (Oslo university) and T. Zhang (Manchester University).

The numerical study of (F)BSDEs with jumps is especially demanding in high dimensions and collaboration has started on these issues with J. Lelong (ENSIMAG) and C. Labart (Université de Savoie).

5.2. Stochastic Differential Games

In many situations, controls are chosen by several agents who interact in various ways. To handle such cases one may use the theory of SDGs. This applies to model uncertainty problems, which can be regarded as a zero-sum game between the agent and the "market" and risk minimization, with risk represented via dynamic risk measures. More general non-zero sum games, involving several players, possibly with asymmetric information or delay will be studied.

An interesting new application of the theory of stochastic differential games, is the issue of *Public Private Partnership* which is a mechanism for a community to outsource the construction of public equipment. The community agrees to pay a rent to the contractor in order to cover the depreciation of the equipment, the maintenance costs and the financial costs. We want to model such partnerships and to compute and compare Nash equilibria and Stackelberg equilibria when the community is the leader. We would also like to investigate whether the community aversion to debt may lead it to enter such a partnership even this is more costly than constructing and managing the equipment by itself.

5.3. Optimal control of Stochastic Partial Differential equations (SPDEs)

SPDEs appear in the modeling of a number of situations: for example, in dynamic pollution models, in financial models involving interest rate derivatives, in systemic risk modeling. The research issues include optimal control of SPDEs and nonlinear filtering theory, stochastic control of forward-backward systems of SPDEs with imperfect and/or asymmetric information, optimal stochastic control of mean-field systems of SPDEs. We have started to study singular control of SPDEs. We plan to give a method for solving optimal control problems for general, possibly non-Markovian systems of FBSDEs by means of BSPDEs with jumps and associated comparison theorems.

5.4. Optimal stopping

Our research on optimal stopping problems covers the analysis of free boundaries in optimal stopping problems for multidimensional stochastic processes with jumps (Thesis of A. Bouselmi, supervised by D. Lamberton). Numerical issues are also be investigated (Monte Carlo methods, quantization methods, methods based on Malliavin calculus). Even in diffusion models, a realistic dividend modeling introduces jumps in the dynamics : at the dividend dates the spot value of the stock undergoes a jump equal to minus the dividend amount. We plan to take into account this feature in optimal stopping problems (Thesis of M. Jeunesse, supervised by B. Jourdain).

The pricing of American options with irregular payoff such as, for instance, binary options, leads to challenging mathematical problems. Some theoretical properties of optimal stopping problems with irregular payoffs have already been obtained. We now plan to focus on the Markovian case by using viscosity solutions and numerical analysis techniques.

In [45], we study optimal stopping problems for (non necessarily) convex dynamic risk measures induced by BSDEs with jumps and establish their connections with *Reflected* BSDEs with jumps. Such problems are related to optimal stopping for non linear expectations, which has been recently studied by [58] in the convex case only. We also address the case of model ambiguity and its relation with mixed control/optimal stopping problems.

5.5. Analysis of stochastic processes with jumps

The use of stochastic processes with jumps in financial modeling has been constantly increasing in the recent years. Simulation of these processes raises specific difficulties. A PhD thesis (V. Rabiet, adviser: V. Bally) has started on regularity properties of the law of multi-dimensional processes with jumps and on sensitivity analysis of derivative products with singular payoffs in such models.

5.6. Monte-Carlo methods

5.6.1. Adaptive variance reduction methods.

Stochastic algorithms [52], [53], [80], [63], [81], [27] or, more recently, direct stochastic optimization [73] proved to be a promising path to automatic variance reduction methods. Direct stochastic optimization techniques are easier to use in practice, avoiding completely any manual tuning needed for stochastic algorithms. This method is well understood (see [73]) only in the Gaussian case and for regular functions. We plan to extend the algorithms and prove rigorous results in non Gaussian cases with financial applications in view for jumps models (see [77], [76], [75]).

5.6.2. Monte-Carlo methods for calibration.

The interest for models combining local and stochastic volatility has been growing recently. Indeed, the local volatility model is not rich enough to efficiently deal with complex derivatives. A popular model is the so called Heston model, in which the volatility process solves a square-root stochastic differential equation (just as in the Cox-Ingersoll-Ross model for interest rate modeling). The thesis of L. Abbas-Turki [12](advisers: D. Lamberton and B. Lapeyre) concentrates on the multi-dimensional Heston model. For these models, numerical aspects are very demanding and we plan to use Monte-Carlo methods using advanced parallel devices (GPU clusters,...) both for price computations and calibration procedures. The thesis of Abbas-Turki is supported by the *Pôle de Compétitivité Finance Innovation* within the consortium *CrediNext*.

5.7. Systemic Risk

We extend the model in [51] in two major ways: First, study the optimal intervention strategy by a lender of last resort that would minimize the size of contagion under budget constraints. Second, allow our model not to be constrained to a single type of financial distress and model jointly insolvency and illiquidity. The interplay of these two mechanisms yields a more potent type of contagion than just the mechanical balance-sheet insolvency type of contagion [85], [92]. In [35], we have started to tackle these issues. This study can be enriched in many different manners.

Benjamin Jourdain and Agnès Sulem have organized a CEA-EDF-Inria school (70 participants) on the issues of Systemic risk and quantitative risk management in October 15-17 2012. (http://bit.ly/finance_inria). A special issue on "Systemic Risk" of the journal *Statistics and Risk Modeling* with B. Jourdain and A. Sulem as guest editors will be published in 2013.

REGULARITY Project-Team

6. New Results

6.1. A multifractional Hull and White model

Participants: Joachim Lebovits, Jacques Lévy Véhel.

In collaboration with Sylvain Corlay (Paris 6 University).

We have considered the following model, which is an extension of the fractional Hull and White model proposed in [55]: under the risk-neutral measure, the forward price of a risky asset is the solution of the S.D.E.

$$\begin{aligned} dF_t &= F_t \sigma_t dW_t, \\ d\ln(\sigma_t) &= \theta\left(\mu - \ln(\sigma_t)\right)dt + \gamma_h d^{\diamond} B_t^h + \gamma_\sigma dW_t^\sigma, \quad \sigma_0 > 0, \theta > 0, \end{aligned}$$

where B_t^h is a multifractional Brownian motion with regularity function h, and W_t, W_t^σ are standard Brownian motions. This SDE is interpgreted in the Wick-Itô sense.

Using functional quantization techniques, it is possible to compute numerically implied forward start volatilities for this model. Using an adequate h function estimated from SP500 data, we have shown that this model is able to reproduce to some extent the volatility surface observed on the market [34].

6.2. Markov characterization of the set-indexed Lévy process

Participant: Erick Herbin.

In collaboration with Prof. Ely Merzbach (Bar Ilan university, Israel).

In [21], the class of set-indexed Lévy processes is considered using the stationarity property defined for the set-indexed fractional Brownian motion in [20]. The general framework of Ivanoff-Merzbach allows to consider standard properties of stochastic processes (e.g. martingale and Markov properties) in the set-indexed context. Processes are indexed by a collection $\mathcal{A}$ of compact subsets of a metric space $\mathcal{T}$ equipped with a Radon measure m, which satisfies several stability conditions. Each process $\{X_U;\ U \in \mathcal{A}\}$ is assumed to admit an increment process $\{\Delta X_C;\ C \in \mathcal{C}\}$ defined as an additive extension of X to the collections $\mathcal{C}_0 = \{U \setminus V;\ U, V \in \mathcal{A}\}$ and

$$\mathcal{C} = \left\{ U \setminus \bigcup_{1 \le i \le n} V_i;\ n \in \mathbf{N}; U, V_1, \cdots, V_n \in \mathcal{A} \right\}.$$

A set-indexed process $X = \{X_U;\ U \in \mathcal{A}\}$ is called a *set-indexed Lévy process* if the following conditions hold

1. $X_{\varnothing'} = 0$ almost surely, where $\varnothing' = \bigcap_{U \in \mathcal{A}} U$.
2. the increments of X are independent: for all pairwise disjoint $C_1, \cdots, C_n$ in $\mathcal{C}$, the random variables $\Delta X_{C_1}, \cdots, \Delta X_{C_n}$ are independent.
3. X has m-stationary $\mathcal{C}_0$-increments, i.e. for all integer n, all $V \in \mathcal{A}$ and for all increasing sequences $(U_i)_i$ and $(A_i)_i$ in $\mathcal{A}$, we have

$$[\forall i,\ m(U_i \setminus V) = m(A_i)] \Rightarrow (\Delta X_{U_1 \setminus V}, \cdots, \Delta X_{U_n \setminus V}) \stackrel{(d)}{=} (\Delta X_{A_1}, \cdots, \Delta X_{A_n})$$

4. X is continuous in probability: if $(U_n)_{n \in \mathbf{N}}$ is a sequence in $\mathcal{A}$ such that

$$\overline{\bigcup_n \bigcap_{k \geq n} U_k} = \bigcap_n \overline{\bigcup_{k \geq n} U_k} = A \in \mathcal{A}$$

then

$$\lim_{n \to \infty} P\left\{|X_{U_n} - X_A| > \epsilon\right\} = 0$$

On the contrary to previous works of Adler and Feigin (1984) on one hand, and Bass and Pyke (1984) one the other hand, the increment stationarity property allows to obtain explicit expressions for the finite-dimensional distributions of a set-indexed Lévy process. From these, we obtained a complete characterization in terms of Markov properties.

Among the various definitions for Markov property of a SI process, we considered the $\mathcal{Q}$-Markov property. A collection $\mathcal{Q}$ of functions

$$\begin{aligned} \mathbf{R} \times \mathcal{B}(\mathbf{R}) &\to \mathbf{R}_+ \\ (x, B) &\mapsto Q_{U,V}(x, B) \end{aligned}$$

where $U, V \in \mathcal{A}(u)$ are s.t. $U \subseteq V$, is called a *transition system* if the following conditions are satisfied:

1. $Q_{U,V}(\bullet, B)$ is a random variable for all $B \in \mathcal{B}(\mathbf{R})$.
2. $Q_{U,V}(x, \bullet)$ is a probability measure for all $x \in \mathbf{R}$.
3. For all $U \in \mathcal{A}(u)$, $x \in \mathbf{R}$ and $B \in \mathcal{B}(\mathbf{R})$, $Q_{U,U}(x, B) = \delta_x(B)$.
4. For all $U \subseteq V \subseteq W \in \mathcal{A}(u)$,

$$\int_{\mathbf{R}} Q_{U,V}(x, dy) Q_{V,W}(y, B) = Q_{U,W}(x, B).$$

A transition system $\mathcal{Q}$ is said

- *spatially homogeneous* if for all $U \subset V$,

$$\forall x \in \mathbf{R}, \forall B \in \mathcal{B}(\mathbf{R}), \quad Q_{U,V}(x, B) = Q_{U,V}(0, B - x);$$

- *m-homogeneous* if $Q_{U,V}$ only depends on $m(V \setminus U)$,
  i.e. $\forall U, V, U', V' \in \mathcal{A}(u)$ such that $U \subset V$ and $U' \subset V'$,

$$m(V \setminus U) = m(V' \setminus U') \Rightarrow Q_{U,V} = Q_{U',V'}.$$

A set-indexed process $X := \{X_U;\ U \in \mathcal{A}\}$ is called *$\mathcal{Q}$-Markov* if $\forall U, V \in \mathcal{A}(u), U \subseteq V$

$$\forall B \in \mathcal{B}(\mathbf{R}), \quad P[\Delta X_V \in \Gamma \mid \mathcal{F}_U] = Q_{U,V}(\Delta X_U; \Gamma),$$

where $(\mathcal{F}_U)_{U \in \mathcal{A}(u)}$ is the minimal filtration of the process X.

Balan-Ivanoff (2002) proved that any SI process with independent increments is a $\mathcal{Q}$-Markov process with a spatially homogeneous transition system. The following result proved in [21] shows that the converse is true.

Theorem *Let $X = \{X_U;\ U \in \mathcal{A}\}$ be a set-indexed process with definite increments. The two following assertions are equivalent:*

1. *X is a $\mathcal{Q}$-Markov process with a spatially homogeneous transition system $\mathcal{Q}$;*
2. *X has independent increments.*

This result is strengthened in the following characterization of set-indexed Lévy processes as Markov processes with homogeneous transition systems.
Theorem *Let $X = \{X_U;\ U \in \mathcal{A}\}$ be a set-indexed process with definite increments and satisfying the stochastic continuity property.*

The two following assertions are equivalent:

1. *X is a set-indexed Lévy process ;*
2. *X is a $\mathcal{Q}$-Markov process such that $X_\varnothing = 0$ and the transition system $\mathcal{Q}$ is spatially homogeneous and m-homogeneous.*

Consequently, if $\mathcal{Q}$ is a transition system which is both spatially homogeneous and m-homogeneous, then there exists a set-indexed process X which is a $\mathcal{Q}$-Markov process.

6.3. Local Hölder regularity of Set-Indexed processes

Participants: Erick Herbin, Alexandre Richard.

In the set-indexed framework of Ivanoff and Merzbach ([62]), stochastic processes can be indexed not only by $\mathbf{R}$ but by a collection $\mathcal{A}$ of subsets of a measure and metric space $(\mathcal{T}, d, m)$, with some assumptions on $\mathcal{A}$. In we introduce and study some assumptions (A_1) and (A_2) on the metric indexing collection $(\mathcal{A}, d_{\mathcal{A}})$ in order to obtain a Kolmogorov criterion for continuous modifications of SI stochastic processes. Under this assumption, the collection is totally bounded and a set-indexed process with good incremental moments will have a modification whose sample paths are almost surely Hölder continuous, for the distance $d_{\mathcal{A}}$. Once this condition is established, we investigate the definition of Hölder coefficients for SI processes. We shall denote $\widetilde{\alpha}_X(t)$ and $\alpha_X(t)$ for the local and pointwise Hölder exponents of X at t, and $\widetilde{\alpha}_X(t)$ and $\alpha_X(t)$ for their deterministic counterpart in case X is Gaussian.

In [18], a set-indexed extension for fractional Brownian motion has been defined and studied. A mean-zero Gaussian process $\mathbf{B}^H = \left\{\mathbf{B}^H_U, U \in \mathcal{A}\right\}$ is called a *set-indexed fractional Brownian motion (SIfBm for short)* on $(\mathcal{T}, \mathcal{A}, m)$ if

$$\forall U, V \in \mathcal{A}, \quad \mathbf{E}\left[\mathbf{B}^H_U \mathbf{B}^H_V\right] = \frac{1}{2}\left[m(U)^{2H} + m(V)^{2H} - m(U \bigtriangleup V)^{2H}\right], \tag{8}$$

where $H \in (0, 1/2]$ is the index of self-similarity of the process.

In [12], $\widetilde{\alpha}_X$ and $\widetilde{\alpha}_X$ have been determined for the particular case of an SIfBm indexed by the collection $\{[0,t];\ t \in \mathbf{R}^N_+\} \cup \{\varnothing\}$, called the *multiparameter fractional Brownian motion*. If X denotes the $\mathbf{R}^N_+$-indexed process defined by $X_t = \mathbf{B}^H_{[0,t]}$ for all $t \in \mathbf{R}^N_+$, it is proved that for all $t_0 \in \mathbf{R}^N_+$, $\widetilde{\alpha}_X(t_0) = H$ and with probability one, for all $t_0 \in \mathbf{R}^N_+$, $\widetilde{\alpha}_X(t_0) = H$. A theorem of allows one to extend these results to SIfBm indexed by a more general class than the sole collection of rectangles of $\mathbf{R}^N_+$.

Theorem 0.1 Let $\mathbf{B}^H$ be a set-indexed fractional Brownian motion on $(\mathcal{T}, \mathcal{A}, m)$, $H \in (0, 1/2]$. Assume that the subclasses $(\mathcal{A}_n)_{n \in \mathbf{N}}$ satisfy Assumption (A_1).
Then, the local and pointwise Hölder exponents of $\mathbf{B}^H$ at any $U_0 \in \mathcal{A}$, defined with respect to the distance d_m or any equivalent distance, satisfy

$$\mathbf{P}\left(\forall U_0 \in \mathcal{A},\ \widetilde{\alpha}_{\mathbf{B}^H}(U_0) = H\right) = 1$$

and if Assumption (A_2) holds,

$$\mathbf{P}\left(\forall U_0 \in \mathcal{A},\ \alpha_{\mathbf{B}^H}(U_0) = H\right) = 1.$$

Consequently, since the collection $\mathcal{A}$ of rectangles of $\mathbf{R}_+^N$ with m the Lebesgue measure satisfies (A_1) and (A_2), we obtained a new result on a classical multiparameter process: the multiparameter fractional Brownian motion $\mathbf{B}^H$ satisfy, for $T \in \mathbf{R}_+^N$:

$$\mathbf{P}\left(\forall t \in [0,T],\ \alpha_{\mathbf{B}^H}([0,t]) = \widetilde{\alpha}_{\mathbf{B}^H}([0,t]) = H\right) = 1.$$

6.4. Separability of Set-Indexed Processes

Participant: Alexandre Richard.

A classical result states that any (multiparameter) stochastic process has a separable modification, thus ensuring the measurability property of the sample paths. We extend this result to set-indexed processes.
Let $(T, \mathcal{O})$ be a topological space. We assume that this space is *second-countable*, ie there exists a countable subset $\widetilde{\mathcal{O}} \subseteq \mathcal{O}$ such that any open set of $\mathcal{O}$ can be expressed as a union of elements of $\widetilde{\mathcal{O}}$.

A process $\{X_t, t \in T\}$ is *separable* if there exists an at most countable set $S \subset T$ and a null set Λ such that for all closed sets $F \subset \mathbf{R}$ and all open set $O \in \mathcal{O}$,

$$\{\omega : X_s(\omega) \in F \text{forall} s \in O \cap S\} \setminus \{\omega : X_s(\omega) \in F \text{forall} s \in O\} \subset \Lambda.$$

This definition is different of the one found in [57], where the space is “linear", in that this author considers the previous equation only when O is an interval. It happens that this notion needs not be defined in a general topological space. However when restricted to a vector space, our definition implies the previous one.

Theorem 0.2 (Doob's separability theorem) Any T-indexed stochastic process $X = \{X_t;\ t \in T\}$ has a separable modification.

If T is an indexing collection in the sense of [62], the topology induced by the distance d_T has to be second-countable. This happens for instance when (T, d_T) is totally bounded, which is the case in

6.5. An increment type set-indexed Markov property

Participant: Paul Balança.

[1] investigates a new approach for the definition of a set-indexed Markov property, named $\mathcal{C}$-*Markov*. The study is based on Merzbach and Ivanoff's set-indexed formalism, i.e. $\mathcal{A}$ denotes a set-indexed collection and $\mathcal{C}$ the family of increments $C = A \setminus B$, where $A \in \mathcal{A}$ and $B \in \mathcal{A}(u)$ (finite unions of sets from $\mathcal{A}$). Moreover, for any $C = A \setminus B$, $B = \cup_{i=1}^k A_i$, $\mathcal{A}_\mathbf{C}$ is defined as the following subset of $\mathcal{A}$:

$$\mathcal{A}_\mathbf{C} = \{U \in \mathcal{A}_\ell;\ U \not\subseteq B^\circ\} := \{U_C^1, \cdots, U_C^p\}, \qquad \text{where } p = |\mathcal{A}_\mathbf{C}|$$

and $\mathcal{A}_\ell$ corresponds to the semilattice $\{A_1 \cap \cdots \cap A_k, \cdots, A_1 \cap A_2, A_1 \cdots, A_k\} \subset \mathcal{A}$. The notation $\mathbf{X_C}$ refers to a random vector $\mathbf{X_C} = \left(X_{U_C^1}, \cdots, X_{U_C^p}\right)$. Similarly, $\mathbf{x_C}$ is used to denote a vector of variables $(x_{U_C^1}, \cdots, x_{U_C^p})$.

Then, an E-valued set-indexed process $(X_A)_{A \in \mathcal{A}}$ is said to be $\mathcal{C}$-*Markov* with respect to a filtration $(\mathcal{F}_A)_{A \in \mathcal{A}}$ if it is adapted to $(\mathcal{F}_A)_{A \in \mathcal{A}}$ and if it satisfies

$$\mathbb{E}[f(X_A)\,|\,\mathcal{G}^*_C] = \mathbb{E}[f(X_A)\,|\,\mathbf{X_C}] \quad \mathbb{P}\text{-a.s.} \tag{9}$$

for all $C = A \setminus B \in \mathcal{C}$ and any bounded measurable function $f : E \to \mathbf{R}$. The sigma-algebra $\mathcal{G}^*_C$ is usually called the strong history of $(\mathcal{F}_A)_{A\in\mathcal{A}}$ and is defined as $\mathcal{G}^*_C = \bigvee_{A\in\mathcal{A}, A\cap C=\varnothing} \mathcal{F}_A$.

The $\mathcal{C}$-Markov approach has several advantages compared to existing set-indexed Markov literature (mainly $\mathcal{Q}$-Markov described in [48]). It appears to be a natural extension of the classic one-parameter Markov property. In particular, the concept of transition system can easily extended to our formalism: for any $\mathcal{C}$-Markov process X, one can defined $\mathcal{P} = \{P_C(\mathbf{x_C}; \mathrm{d}x_A); C \in \mathcal{C}\}$ as

$$\forall \mathbf{x_C} \in E^{|\mathcal{A}_\mathbf{C}|}, \Gamma \in \mathcal{E}; \quad P_C(\mathbf{x_C}; \Gamma) := \mathbb{P}(X_A \in \Gamma \,|\, \mathbf{X_C} = \mathbf{x_C}).$$

A $\mathcal{C}$-transition system $\mathcal{P}$ happens to satisfy a set-indexed Chapman-Kolmogorov equation,

$$\forall C \in \mathcal{C},\ A' \in \mathcal{A}; \qquad P_C f = P_{C'} P_{C''} f \quad \text{where} \quad C' = C \cap A',\ C'' = C \setminus A' \tag{10}$$

and f is a bounded measurable function.

Similarly to the classic Markovian theory, is is proved in [1] that the initial distribution μ and $\mathcal{P}$ characterize entirely the law of a $\mathcal{C}$-Markov process, and that conversely, for any initial law and any $\mathcal{C}$-transition system, a corresponding canonical set-indexed $\mathcal{C}$-Markov process can be constructed. $\mathcal{C}$-Markov processes enjoy several other properties such as

1. Projections on elementary flows are Markovian;
2. Conditional independence of natural filtrations;
3. Strong Markov property.

The class of set-indexed Lévy processes defined and studied in [21] offers examples of $\mathcal{C}$-Markov processes whose transition probabilities correspond to

$$\forall C = A \setminus B \in \mathcal{C}, \quad \forall \Gamma \in \mathcal{E}; \quad P_C(\mathbf{x_C}; \Gamma) = \mu^{m(C)}(\Gamma - \Delta x_B), \tag{11}$$

where m is a measure on $\mathcal{T}$ and μ the infinitely divisible probability measure that characterizes the Lévy process. We note that the transition system related the $\mathcal{Q}$-Markov property has a different form, even if it is related.

Another non-trivial example of $\mathcal{C}$-Markov process is the set-indexed Ornstein-Uhlenbeck process that has been introduced and studied in [32]. It is a Gaussian Markovian process whose transition densities are given by

$$p_C(\mathbf{x_C}; y) = \frac{1}{\sigma_C\sqrt{2\pi}} \exp\left[-\frac{1}{2\sigma_C^2}\left(y - e^{-\lambda m(A)}\left[\sum_{i=1}^n (-1)^{\varepsilon_i}\, x_{U_C^i}\, e^{\lambda m(U_C^i)}\right]\right)^2\right], \tag{12}$$

where λ and σ are positive parameters, m is a measure on $\mathcal{T}$ and

$$\sigma_C^2 = \frac{\sigma^2}{2\lambda}\left(1 - e^{-2\lambda m(A)}\left[\sum_{i=1}^n (-1)^{\varepsilon_i} e^{2\lambda m(U_C^i)}\right]\right).$$

In the particular case of multiparameter processes, corresponding to the indexing collection $\mathcal{A} = \{[0,t]; t \in \mathbf{R}_+^N\}$, the $\mathcal{C}$-Markov formalism is related to several existing works. It generalizes the two-parameter $*$-Markov property introduced in [53] and also embraces the multiparameter Markov property investigated recently in [68]. Finally, under some Feller assumption on the transition system, a multiparameter $\mathcal{C}$-Markov process is proved to admit a modification with right-continuous sample paths.

6.6. Fine regularity of Lévy processes

Participant: Paul Balança.

This ongoing work focuses on the fine regularity of one-parameter Lévy processes. The main idea of this study is to use the framework of stochastic 2-microlocal analysis (introduced and developed in [16],[33]) to refine sample paths results obtained in [65].

The latter describes entirely the multifractal spectrum of Lévy processes, i.e. the Hausdorff geometry of level sets $(E_h)_{h \in \mathbf{R}_+}$ of the pointwise exponent. These are usually called the *iso-Hölder sets* of X and are given by

$$E_h = \{t \in \mathbf{R} : \alpha_{X,t} = h\} \quad \text{for every } h \in \mathbf{R}_+ \cup \{+\infty\}.$$

The multifractal spectrum is itself defined as the localized Hausdorff dimension of the previous sets, i.e.

$$d_X(h,V) = \dim_{\mathcal{H}}(E_h \cap V) \quad \text{for every } h \in \mathbf{R}_+ \cup \{+\infty\} \text{ and } V \in \mathcal{O} \text{ (open sets in } \mathbf{R}). \tag{13}$$

[65] states that under a mild assumption on the Lévy measure π, a Lévy process X with no Brownian component almost surely satisfies

$$\forall V \in \mathcal{O}; \quad d_X(h,V) = \begin{cases} \beta h & \text{if } h \in [0, 1/\beta]; \\ -\infty & \text{if } h \in (1/\beta, +\infty], \end{cases} \tag{14}$$

where the Blumenthal-Getoor exponent β is given by

$$\beta = \inf\left\{\delta \geq 0 : \int_{\mathbf{R}^d} \left(1 \wedge \|x\|^\delta\right) \pi(\mathrm{d}x) < \infty\right\}. \tag{15}$$

Since classic multifractal analysis focuses on the pointwise exponent, it is natural from our point of view to integrate the 2-microlocal frontier into this description. More precisely, we focus on the dichotomy usual/unusual regularity, corresponding to the sets $(\widetilde{E}_h)_{h \in \mathbf{R}_+}$ and $(\widehat{E}_h)_{h \in \mathbf{R}_+}$:

$$\widetilde{E}_h = \{t \in E_h : \forall s' \in \mathbf{R};\ \sigma_{X,t}(s') = (h + s') \wedge 0\} \quad \text{and} \quad \widehat{E}_h = E_h \setminus \widetilde{E}_h.$$

The collection $(\widetilde{E}_h)_{h \in \mathbf{R}_+}$ represents times at which the 2-microlocal behaviour is rather common (i.e. the slope is equal to one), whereas at points which belong $(\widehat{E}_h)_{h \in \mathbf{R}_+}$, the 2-microlocal frontier has an unusual form.

Then, our main result states that sample paths of a Lévy process X with no Brownian component almost surely satisfy

$$\forall V \in \mathcal{O}; \quad \dim_{\mathcal{H}}(\widetilde{E}_h \cap V) = \begin{cases} \beta h & \text{if } h \in [0, 1/\beta]; \\ -\infty & \text{if } h \in (1/\beta, +\infty]. \end{cases} \tag{16}$$

Furthermore, the collection of sets $(\widehat{E}_h)_{h\in\mathbf{R}_+}$ enjoys almost surely

$$\forall V \in \mathcal{O}; \quad \dim_{\mathcal{H}}(\widehat{E}_h \cap V) \leq \begin{cases} 2\beta h - 1 & \text{if } h \in (1/2\beta, 1/\beta)\,; \\ -\infty & \text{if } h \in [0, 1/2\beta] \cup [1/\beta, +\infty]. \end{cases} \tag{17}$$

These results clearly extend those obtained in [65] since we know that the pointwise exponent is completely characterize by the 2-microlocal frontier. Moreover, it also proves that from a Hausdorff dimension point of view, the common regularity is a 2-microlocal frontier with a slope equal to one.

Nevertheless, equation (15) also exhibits some unusual behaviours, corresponding to times $(\widehat{E}_h)_{h\in\mathbf{R}_+}$, that are not captured by the classic multifractal spectrum. The existence of such particular times highly depends on the structure of the Lévy measure, and not only the value of the Blumenthal-Getoor exponent which is therefore not sufficient to characterize entirely the fine regularity. This last aspect of the study illustrates the fact that 2-microlocal analysis is an interesting tool for the study of stochastic processes' regularity since some sample paths' properties can not be captured by common tools such as Hölder exponents.

6.7. A class of self-similar processes with stationary increments in higher order Wiener chaoses.

Participant: Benjamin Arras.

Self similar processes with stationary increments (SSSI processes) have been studied for a long time due to their importance both in theory and in practice. Such processes appear as limits in various renormalisation procedures [69]. In applications, they occur in various fields such as hydrology, biomedicine and image processing. The simplest SSSI processes are simply Brownian motion and, more generally, Lévy stable motions. Apart from these cases, the best known such process is probably fractional Brownian motion (fBm). A construction of SSSI processes that generalizes fBm to higher order Wiener chaoses was proposed in [73]. These processes read

$$\forall t \in \mathbb{R}_+ \quad X_t = \int_{\mathbb{R}^d} h_t^H(x_1, ..., x_d) dB_{x_1} ... dB_{x_d}$$

where h_t^H verifies:

1. $h_t^H \in \widehat{L}^2(\mathbb{R}^d)$,
2. $\forall c > 0, \quad h_{ct}^H(cx_1, ..., cx_d) = c^{H-\frac{d}{2}} h_t^H(x_1, ..., x_d)$,
3. $\forall \rho \geq 0, \quad h_{t+\rho}^H(x_1, ..., x_d) - h_t^H(x_1, ..., x_d) = h_\rho^H(x_1 - t, ..., x_d - t)$.

In [41], we define a class of such processes by the following multiple Wiener-Itô integral representation:

$$X_t^\alpha = \int_{\mathbb{R}^d} \left[||\mathbf{t}^* - \mathbf{x}||_2^{H-\frac{d}{2}} - ||\mathbf{x}||_2^{H-\frac{d}{2}} \right] dB_{x_1} ... dB_{x_d} \tag{18}$$

where $t \in [0,1]$, $\mathbf{t}^* = (t, ..., t)$ and $\alpha = H - 1 + \frac{d}{2}$. When $d = 1$, this is just fBm. In order to study the local regularity of this class of processes as well as the asymptotic behaviour at infinity, we use wavelet's methods. More precisely, following ideas from [46], we obtain the following wavelet-like expansion:
Almost surely,

$$\forall t \in [0,1] \quad X_t^\alpha = \sum_{j\in\mathbb{Z}} \sum_{\mathbf{k}\in\mathbb{Z}^d} \sum_{\epsilon\in E} 2^{-jH} \left[I^{\alpha+1}(\psi^{(\epsilon)})(2^j \mathbf{t}^* - \mathbf{k}) - I^{\alpha+1}(\psi^{(\epsilon)})(-\mathbf{k}) \right] I_d(\psi_{j,\mathbf{k}}^{(\epsilon)}).$$

From this representation, we get several results about this class of processes. Namely:

- There exists a strictly positive random variable A_d of finite moments of any order and a constant, $b_d > 1$, such that:

$$\forall \omega \in \Omega^* \quad \sup_{(s,t)\in[0,1]} \frac{|X_t^\alpha(\omega) - X_s^\alpha(\omega)|}{|t-s|^H (\log(b_d + |t-s|^{-1}))^{\frac{d}{2}}} \leq A_d(\omega).$$

- There exists a strictly positive random variable B_d of finite moments of any order and a constant $c_d > 3$, such that:

$$\forall \omega \in \Omega^* \quad \sup_{t\in\mathbb{R}_+} \frac{|X_t^\alpha(\omega)|}{(1+|t|)^H (\log\log(c_d + |t|))^{\frac{d}{2}}} \leq B_d(\omega).$$

Using an estimate from [54], we compute the uniform almost sure pointwise Hölder exponent of X^α defined by:

$$\gamma_{X^\alpha}(t) = \sup\{\gamma > 0 : \quad \limsup_{\rho\to 0} \frac{|X_{t+\rho}^\alpha - X_t^\alpha|}{|\rho|^\gamma} < +\infty\}.$$

We get the following result:
Almost surely,

$$\forall t \in (0,1), \;\; \gamma_{X^\alpha}(t) = H.$$

In the last part of [41], we give general bounds on the Hausdorff dimension of the range and graphs of multidimensional anisotropic SSSI processes defined by multiple Wiener integrals. Let $Y_t^H = \gamma(H,d) I_d(h_t^H)$ where $\gamma(H,d)$ is a normalizing positive constant such that $\mathbb{E}[|Y_1^H|^2] = 1$. Let $\frac{1}{2} < H_1 \leq ... \leq H_N < 1$. Let $\{\mathbb{Y}_t^H\}$ be the multidimensional process defined by:

$$\{\mathbb{Y}_t^H\} = \{(Y_t^{H_1}, ..., Y_t^{H_N}) : t \in \mathbb{R}_+\}$$

where the coordinates are independent copies of the process Y_t^H. Following classical ideas from [78] and using again the estimate from [54], we obtain:
Almost surely,

$$dim_{\mathcal{H}} R_E(\mathbb{Y}^H) \geq \min\left(N; \frac{dim_{\mathcal{H}} E + \frac{\sum_{j=1}^k (H_k - H_j)}{d}}{H_k}, k = 1, ..., N\right),$$

$$dim_{\mathcal{H}} Gr_E(\mathbb{Y}^H) \geq \min\left(\frac{dim_{\mathcal{H}} E + \frac{\sum_{j=1}^k (H_k - H_j)}{d}}{H_k}, k = 1, ..., N, dim_{\mathcal{H}} E + \sum_{i=1}^N \frac{(1-H_i)}{d}\right).$$

And,

$$dim_{\mathcal{H}} R_E(\mathbb{Y}^H) \leq \min\left(N; \frac{dim_{\mathcal{H}} E + \sum_{j=1}^{k}(H_k - H_j)}{H_k}, k = 1, ..., N\right),$$

$$dim_{\mathcal{H}} Gr_E(\mathbb{Y}^H) \leq \min\left(\frac{dim_{\mathcal{H}} E + \sum_{j=1}^{k}(H_k - H_j)}{H_k}, k = 1, ..., N; dim_{\mathcal{H}} E + \sum_{i=1}^{N}(1 - H_i)\right).$$

where $E \subset \mathbb{R}_+$.

6.8. Economic growth models

Participants: Jacques Lévy Véhel, Lining Liu.

In collaboration with D. La Torre, University of Milan.

We study certain economic growth models where we add a source of randomness to make the evolution equations more realistic. We have studied two particular models:

- An augmented Uzawa-Lucas growth model where technological progress is modelled as the solution of a stochastic differential equation driven by a Lévy or an additive process. This allows for a more faithful description of reality by taking into account discontinuities in the evolution of the level of technology. In details, we consider a closed economy in which there is single good which is produced by combining physical capital $K(t)$ and human capital $H(t)$. The laws of motions of $K(t)$ and $H(t)$ are:

$$\dot{K}(t) = A(t)^{\gamma}[u(t)H(t)]^{\xi}K(t)^{1-\xi-\gamma} - \beta_K K(t) - C(t), \tag{19}$$

$$K(0) = K_0;$$

$$\dot{H}(t) = (\eta(1 - u(t)) - \beta_H)H(t), \tag{20}$$

$$H(0) = H_0,$$

where $A(t)$ is the level of technology, $H(t)$ is the total stock of human capital, $u(t)$ is the proportion to the production of good, $\gamma \in (0,1)$, $\xi \in (0,1)$ and $1 - \xi - \gamma \in (0,1)$ are the shares of income accruing to $A(t)$, $u(t)H(t)$ and $K(t)$, respectively, $\beta_K \in [0,1]$ is the constant rate of depreciation of physical capital, $\beta_H \in [0,1]$ is the rate of depreciation of human capital and $\eta \geq 0$ is the productivity of human capital.

We assume that the level of technology evolves according to the following stochastic differential equation:

$$dA(t) = \mu A(t)dt + \sigma A(t)dW(t) + \delta \int A(t^-)z(\widetilde{N}(dt, dz) - \nu(dt, dz)), \tag{21}$$

where $\mu \in \mathbb{R}$ is the drift rate, $\sigma > 0$ is the volatility, $0 \leq \delta \leq 1$, W is a standard Brownian motion and $\widetilde{N}$ is Poisson random measure with intensity measure ν which satisfies

$$\lim_{s\to t^+}\frac{1}{s-t}\int_t^s\int_{-1}^1 z^2\nu(dz,dx)+\lim_{s\to t^+}\frac{1}{s-t}\int_t^s\int_1^\infty z\nu(dz,dx)<\infty,$$

and

$$\int_0^t\int_{-1}^1 z^2\nu(dz,dx)+\int_0^t\int_1^\infty z\nu(dz,dx)<\infty,$$

for $t>0$.

With a CIES utility function, the optional inter-temporal decision problem can be formulated as

$$\max_{[C,u]}\mathbb{E}\left[\int_0^\infty \frac{C(t)^{1-\phi}-1}{1-\phi}e^{-\rho t}dt\right], \tag{22}$$

where $\rho>0$ is the rate of time preference and $\phi>0$. We denote $V(H,K,A)$ the maximum value function associated with the stochastic optimisation problem. For given t, the maximum expect utility up to time t obtained when applying the stochastic control $[C(t),u(t)]$ is defined by

$$V(H(t),K(t),A(t))=\max_{[C,u]}\mathbb{E}\left[\int_0^t \frac{C(x)^{1-\phi}-1}{1-\phi}e^{-\rho x}dx\right]. \tag{23}$$

We have been able to solve this program under some simplifying assumptions. Numerical simulations allow one to assess precisely the effect of (tempered) multistable noise on the model.

- A stochastic demographic jump shocks in a multi-sector growth model with physical and human capital accumulation. This models allows one to take into account sudden changes in population size, due for instance to wars or natural catastrophes. The laws of motions of physical capital $K(t)$ and human capital $H(t)$ are:

$$\dot{K}(t)=AM(t)^{1-\xi-\beta}[u(t)H(t)]^\beta K(t)^\xi-\eta_K K(t)-c(t)M(t), \tag{24}$$

$$\dot{H}(t)=B(1-u(t))H(t)-\eta_H H(t), \tag{25}$$

with initial conditions $K(0)=K_0$ and $H(0)=H_0$, where $M(t)$ is the population size, $H(t)$ is the human capital, $u(t)$ is the share of human capital employed in production, $\beta\in(0,1)$, $\xi\in(0,1)$ and $1-\xi-\beta\in(0,1)$ are the shares accruing to $M(t)$, $u(t)H(t)$ and $K(t)$, respectively, $\eta_K\in[0,1]$ is the constant rate of depreciation of physical capital, $\eta_H\in[0,1]$ is the rate of depreciation of human capital and $A\geq 0$, $B\geq 0$ are the productivities of physical capital and human capital.

We assume that the population size evolves according to the following stochastic differential equation:

$$dM(t)=\mu M(t)dt+\sigma M(t)dW(t)+\delta\int M(t^-)z(\widetilde{N}(dt,dz)-\nu(dt,dz))$$

with initial condition $M(0)=M_0$, where $\mu\in\mathbb{R}$ is the drift rate, $\sigma>0$ is the volatility, $0\leq\delta\leq 1$, W is a standard Brownian motion and $\widetilde{N}$ is Poisson random measure with intensity measure $\nu(dt,dz)$.

Here again, we are able to solve an optimisation program under some simplifying assumptions. This sheds light on the effect of demographic shocks on macroeconomic growth.

TOSCA Project-Team

6. New Results

6.1. Probabilistic numerical methods, stochastic modelling and applications

Participants: Mireille Bossy, Nicolas Champagnat, Julia Charrier, Julien Claisse, Madalina Deaconu, Samuel Herrmann, James Inglis, Antoine Lejay, Sylvain Maire, Sebastian Niklitschek Soto, Nicolas Perrin, Denis Talay, Etienne Tanré, Denis Villemonais, Laurent Violeau.

6.1.1. Published works and preprints

- In collaboration with P.-E. Jabin (University of Maryland), J.-F. Jabir and J. Fontbona (CMM and Universidad de Chile, Santiago de Chile), M. Bossy have studied the link between the Lagrangian version of divergence free constraint (and the uniform density constraint), with an additional potential term in the Lagrangian equation, having some similarity with the role of the Eulerian pressure term. They obtained the local existence of analytical solutions to an incompressible Lagrangian stochastic model in periodic domain. The paper is in positive revision for publication in *Communications in Partial Differential Equations* [33]. http://hal.inria.fr/hal-00691712
- N. Champagnat worked with A. Lambert (Univ. Paris 6) on splitting trees with Poissonian mutations. Assuming that each mutation is neutral and gives a new type in the population, they obtained in [13], [14] large time convergence results on the sizes of the largest families and the ages of the oldest families in the population. http://hal.inria.fr/inria-00515481, http://hal.inria.fr/inria-00616765. In collaboration with Mathieu Richard (Ecole Polytechnique, Palaiseau), they also extended some of these results to the case of splitting trees with mutations occuring at birth of individuals [15], http://hal.inria.fr/hal-00736036.
- N. Champagnat obtained with P. Diaconis (Stanford Univ.) and L. Miclo (Univ. Toulouse 3) the full spectral decomposition of the transition matrix of two-dimensional Markov chains $(X_n, Y_n)_{n\geq 0}$ in $\mathbb{Z}_+^2$, without immigration or mutation, which are *neutral* in the sense that $(X_n + Y_n)_{n\geq 0}$ is a Markov process. Because of the specific form of the eigenvectors, they were also able to characterize all the Dirichlet eigenvectors in subdomains of $\mathbb{Z}_+^2$ of the form $\{(i,j) \in \mathbb{Z}_+^2 : i + j \geq d\}$ for all $d \geq 0$. As an application, they could determine the quasi-stationary and quasi-limiting distributions of such processes [12], http://hal.inria.fr/hal-00672938.
- N. Champagnat studied with F. Campillo (EPI MODEMIC, Inria Sophia Antipolis — Méditerrannée) individual based models of clonal plants where plants interact through the network formed by the rizhomes or stolons linking plants. In the limit of large population, they obtained a PDE governing the dynamics of population densities in space [11], http://hal.inria.fr/hal-00723209.
- M. Deaconu and S. Herrmann introduced a new method for the simulation of the hitting times of nonlinear boundaries for Bessel processes. This method combines the method of images and the random walk on spheres method. They construct the so called walk on moving spheres algorithm. This approach can be applied for the hitting time of a given level for the Cox-Ingersoll-Ross process and thus be used in models coming from finance and neuroscience [17], http://hal.inria.fr/hal-00636056/en. This work is part of the ANR MANDy project.
- J. Inglis and E. Tanré studied with F. Delarue and S. Rubenthaler (Univ. Nice – Sophia Antipolis) the global solvability of a networked system of integrate-and-fire neurons proposed in the neuroscience literature. In the mean-field limit the equation resembles a McKean-Vlasov equation, but is highly non-standard and previous attempts at rigorous analysis were not satisfactory. They here bridge this gap, and shed light on a surprisingly complicated problem [35], http://hal.inria.fr/hal-00747565.

- A. Lejay continued his long term investigations on probabilistic interpretations and Monte Carlo simulations of interfaces conditions, such as ones arising in discontinuous media. With G. Pichot (IRISA, Rennes), he has developed a series of tests and benchmarks regarding one-dimensional Monte Carlo methods, such as the ones proposed in [19], http://hal.inria.fr/hal-00649170. He has also developed a new family of stochastic diffusion processes, called the *snapping out Brownian motion*, in order to take into account an interface condition where the concentration of the fluid is proportional to its gradient. Finally, A. Lejay and S. Maire also proposed new methods and tested a few ones to deal with the locally isotropic case for multidimensional problems [18], http://hal.inria.fr/hal-00689581.
- With A. Kohatsu-Higa (Ristumeikan University) and K. Yasuda (Hosei university), A. Lejay has continued his work [25] on the simulation of SDE with a discontinuous drift. http://hal.inria.fr/hal-00670123
- With L. Coutin (University of Toulouse), A. Lejay has developed an appropriate framework to deal with linear rough differential equations, extending some results (Magnus formula, Dyson series...) to this case. Using theses properties, they have studied the sensitivites of solutions of rough differential equations with respect to the signal, the vector field or the starting point. They have provided new results such as the Hölder continuity of the derivative of the so called Itô map which transforms a rough path to the solution of a rough differential equation [34]. http://hal.inria.fr/hal-00722900
- S. Maire and C. Prissette (Univ. du Sud – Toulon – Var) have developed in [21] a stochastic algorithm to solve Sudoku puzzles using estimation of distribution coupled with restart techniques. http://hal.inria.fr/inria-00591852
- S. Maire and E. Tanré have generalised the spectral methods for elliptic PDEs developed in [42], [43] to the case of pure Neumann boundary conditions. Some additional difficulties occur because the stochastic representation of the solutions is defined only up to an additive constant and as a limit involving local time approximations [40]. By taking into account these additional properties, they still obtained a spectral matrix having a condition number converging to one [36]. http://hal.inria.fr/hal-00677529
- C. Graham (Ecole Polytechnique) and D. Talay wrote the first volume [27] of their series of books published by Springer on the Foundations of Stochastic Simulations. They started to write the second volume.
- D. Villemonais wrote with S. Méléard (École Polytechnique) a survey on quasi-stationary distributions and Q-processes for stochastic models of population dynamics. This survey also contains a detailed numerical study of the behaviour of classical models with extinction [23]. http://hal.inria.fr/hal-00653834
- 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 [39]. http://hal.inria.fr/hal-00681601
- D. Villemonais proved in [38] 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. http://hal.archives-ouvertes.fr/hal-00598085

6.1.2. Other works in progress

- 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 also 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 the exponential ergodicity of the Q-process. This work is currently being written.

- N. Champagnat and D. Villemonais work on time-reversal of absorbed processes, which allow to characterize the path to extinction in extinct populations which are known to be non-extinct at some time in the past. They plan to apply these results on practical ecological situations.
- 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 and an infinite-horizon optimal control problem on a birth-death process. He is currently working on a finite-horizon optimal control problem on a branching-diffusion process. In addition, he is working on modelling of a pH-mediated cancer treament.
- M. Deaconu and S. Herrmann continue the study of the hitting times for Bessel processes in the situation of noninteger dimensions and also in the application of this method to the simulation of the Brownian hitting time,
- M. Deaconu starts a collaboration with L. Beznea (Simion Stoilow Institute of Mathematics of the Romanian Academy) on coagulation-fragmentation models and their connection with branching processes.
- M. Deaconu studies in collaboration with F. Nobile and F. Tesei (EPFL) a pollution model by using hitting times of stochastic processes.
- S. Herrmann and E. Tanré worked on a scheme to construct an efficient algorithm to simulate the first hitting time of curves by a one dimensional Brownian motion. They apply the result to estimate the spiking time of leaky integrate fire models in neuroscience. This work is part of the ANR MANDy project.
- S. Larnier joined the team in September as a post-doctoral researcher and began working with A. Lejay on data assimilation in order to predict the ocean wave energy from the knowledge of near-shore incoming waves. They started a collaboration on video data with R. Almar (LEGOS, Toulouse) and R. Cienfuegos (Pontificia Universidad Católica de Chile).
- S. Maire works with M. Simon (Mainz Univ.) on electrical impedance tomography problems using new Monte Carlo schemes that deal with Robin and transmission boundary conditions.
- S. Maire develops with I. Dimov (Bulgarian academy of sciences) a Monte Carlo method called the walk on equations to solve linear systems of algebraic equations.
- S. Niklitschek has continued his PhD. work under the supervision of D. Talay. They were able to extended their first work in which they gave a probabilistic interpretation of a parabolic equation with discontinuous drift and proved the weak rate of convergence of the Euler method using the accurate pointwise estimates obtained for the derivatives of the solution, to the case in which both drift and diffusion coefficients are discontinuous. Both results are consistent with each other, and also with the results obtained by M. Martinez and D. Talay in [22].
- N. Perrin continued his PhD. on stochastic methods in molecular dynamics under the supervision of M. Bossy, N. Champagnat and D. Talay. This year, he studied a stochastic interpretation of parabolic PDEs with divergence form operators involved in the Poisson-Boltzmann PDE of molecular dynamics, and the associated numerical Monte Carlo method. He also continued his study of a method due to P. Malliavin (French Academy of Science) based on the Fourier analysis of covariance matrices with delay in order to identify the fast and slow components of a molecular dynamics.
- P. Guiraud (University of Valparaiso) 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 noiseless model does not have synchronization.
- P. Orio (Centro Interdisciplinario de Neurociencia de Valparaiso) and E. Tanré work on the comparison of global properties of the solution of mathematical models and the associated measurements obtained by experiments.

- 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 (MOISE team, Inria Sophia Antipolis – Méditerranée, Montpellier). Laurent studied this year the rate of convergence of the Nadaraya-Watson conditional estimator for "linear" kinetic processes. He is currently working on the rate of convergence of the particle approximation of kinetic conditional McKean-Vlasov stochastic models.
- P-E. Jabin and D. Talay continue to develop their innovating approach, which combines stochastic analysis and PDE analysis, for the time varying Hamilton-Jacobi-Bellman-McKean-Vlasov equations of the Lasry and Lions mean-field stochastic control theory.
- D. Talay is working with J. Bion-Nadal (Ecole Polytechnique) on applications of risk measures to the calibration of stochastic models, with N. Touzi (Ecole Polytechnique) on the stochastic control of stochastic differential equations with weighted local times, and with O. Bardou (GDF) on Edgeworth expansions for the Central Limit Theorem for Brownian martingales whose integrands depend on ergodic diffusion processes.

6.2. Financial Mathematics

Participants: Mireille Bossy, Paul Charton, Dalia Ibrahim, Denis Talay, Etienne Tanré.

- Mireille Bossy, in collaboration with H. Quinteros (Univ. Chile) worked on the rate of convergence of non Lipschitz diffusion processes discretized with the symetrized Milstein scheme. Under the same kind of hypotheses than in [41] on the symetrized Euler scheme, they obtained the expected improvement of the strong rate of convergence, when the diffusion coefficient is of the form $\sigma(x) = x^\alpha$, with $\alpha \in [1/2, 1[$.

  A preprint is being written.
- P. Charton continued his PhD. under the supervision of M. Deaconu and A. Lejay. He studied some storage strategies for wind farms.
- **Mathematical modelling for technical analysis techniques** Since November 2009, D. Ibrahim has been working on her PhD. thesis on Mathematical modeling of technical analysis in finance, under supervision of D. Talay and E. Tanré. The aim of her work is to study the performances of a technical analysis tool designed to detect changes in the volatility term: The Bollinger Bands. She studied the performances of this indicator in a modified Black-Scholes model such that the volatility is equal to σ_0 up to a random time τ, independent of the Brownian motion governing the prices. After τ, the volatility is equal to σ_1. She proved that Bollinger Bandwidth indicator can detect the time change (at which the volatility changes its value), in the case of small and large volatilities. She has also exhibited a mathematical optimal allocation strategy, by decomposing the initial allocation problem into an allocation problem before the change time τ and an allocation problem after τ, in order to circumvent some technical problems brought from the change of volatility.

  This work is part of the contract with FINRISK.
- In collaboration with C. Michel (CA-CIB) and V. Reutenauer (Citi), D. Talay and E. Tanré worked on the
  - the study of the liquidity risk in the interest rate options market;
  - the minimization of the hedging error in interest rates Gaussian models by means of strategies designed in an effective way by using stochastic optimization algorithms.
- P. Protter (Columbia University) and D. Talay continue to work on bubbles time evolution models, which leads them to try to extend Feller's results on explosion times for stochastic differetential equations.