



RESEARCH CENTER  
**Bordeaux - Sud-Ouest**

FIELD

Activity Report 2013

# Section New Results

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## LFANT Project-Team

## 6. New Results

### 6.1. Class groups and other invariants of number fields

**Participants:** Karim Belabas, Jean-Paul Cerri, Pierre Lezowski.

In collaboration with E. Friedman, K. Belabas presented in [22] a new algorithm to compute the residue at  $s = 1$  of the Dedekind zeta function of a number field, conditional on GRH. This improves on previous results of Eric Bach [31] by a useful constant factor. Such an estimate is one of the two key analytic ingredients to Buchmann's class group algorithm, the other being the existence (under GRH) of an explicit set of small generators [33].

In collaboration with F. Thorne, H. Cohen worked on Dirichlet series associated to cubic and quartic fields with given resolvent. In [23] they give an explicit formula for the Dirichlet series  $\sum_K |\Delta(K)|^{-s}$ , where the sum is over isomorphism classes of all cubic fields whose quadratic resolvent field is isomorphic to a fixed quadratic field  $k$ . This is a sequel to previous work of Cohen and Morra, where such formulæ are proved in a more general setting, in terms of sums over characters of certain groups related to ray class groups. Here, the analysis is carried further and they prove explicit formulæ for these Dirichlet series over  $\mathbb{Q}$ . As an application, they compute tables of the number of  $S_3$ -sextic fields  $K$  with discriminant ranging up to  $10^{23}$ . An accompanying PARI/GP implementation is available.

In [24], they give an explicit formula for the Dirichlet series  $\sum_K |\Delta(K)|^{-s}$ , where this time the sum is over isomorphism classes of all quartic fields whose cubic resolvent field is isomorphic to a fixed cubic field  $k$ . This work is a sequel to an unpublished preprint of Cohen, Diaz y Diaz, and Olivier.

The papers by H. Cohen on Haberland's formula and numerical computation of Petersson scalar products and by A. Angelakis and P. Stevenhagen on imaginary quadratic fields with isomorphic abelian Galois groups, which were presented at the ANTS-X conference, were published in [17], [16].

### 6.2. Number and function fields

**Participants:** Athanasios Angelakis, Jean-Marc Couveignes, Karim Belabas.

In collaboration with Reynald Lercier, Jean-Marc Couveignes presents in [12] a randomised algorithm that on input a finite field  $K$  with  $q$  elements and a positive integer  $d$  outputs a degree  $d$  irreducible polynomial in  $K[x]$ . The running time is  $d^{1+o(1)} \times (\log q)^{5+o(1)}$  elementary operations. The  $o(1)$  in  $d^{1+o(1)}$  is a function of  $d$  that tends to zero when  $d$  tends to infinity. And the  $o(1)$  in  $(\log q)^{5+o(1)}$  is a function of  $q$  that tends to zero when  $q$  tends to infinity. In particular, the complexity is quasi-linear in the degree  $d$ .

The book of surveys "Explicit methods in number theory. Rational points and Diophantine equations" [19] edited by K. Belabas with contributions from K. Belabas, F. Beukers, P. Gaudry, W. McCallum, B. Poonen, S. Siksek, M. Stoll and M. Watkins presents the state of the art of the use of explicit methods in arithmetic geometry to solve diophantine problems.

### 6.3. Quaternion algebras

**Participants:** Jean-Paul Cerri, Pierre Lezowski, Aurel Page.

In a joint work with J. Chaubert ([11]), J.-P. Cerri and P. Lezowski have studied totally definite quaternion fields over number fields which are Euclidean, that is to say that they admit a left or right Euclidean order. In particular, they have established the complete list of totally definite and Euclidean quaternion fields over real quadratic number fields. In this list, all fields are in fact norm-Euclidean. The proofs are both theoretic and algorithmic.

A. Page uploaded a new version of his article [30] on the computation of arithmetic Kleinian groups, incorporating comments from the referee.

## 6.4. Complex multiplication and modularity

**Participants:** Jean-Marc Couveignes, Andreas Enge, Nicolas Mascot, Enea Milio, Aurel Page, Damien Robert.

H. Ivey-Law has been implementing efficient algorithms to compute Hilbert class polynomials and modular polynomials for various modular functions, as well as various supplementary algorithms required by, or based on, these two primary components. These algorithms form an important and time-critical part of algorithms used to select elliptic curves for use in cryptographic applications.

The implementation is based on algorithms for these tasks published by A. Sutherland and his collaborators. It includes, more specifically, algorithms to compute Hilbert class polynomials for various different modular functions over  $\mathbb{Z}$  or  $\mathbb{Z}/M\mathbb{Z}$ , modular polynomials for various different modular functions over  $\mathbb{Z}$ ,  $\mathbb{Z}/M\mathbb{Z}$ , and/or pre-instantiated at a particular point. The supplementary algorithms include functionality for computing equations for isogenies between elliptic curves and equations for their codomains, for manipulating, interrogating and traversing isogeny volcanoes, for computing minimal polycyclic presentations of abstract groups, for testing supersingularity of  $j$ -invariants, for accessing optimised equations of the modular curve  $X_1(N)$  for  $N \leq 50$ , for finding elliptic curves with a given trace or a given endomorphism ring, for calculating the endomorphism ring of a given elliptic curve, for computing the action of the torsor  $\text{Cl}(\mathcal{O})$  on the set of elliptic curves with endomorphism ring  $\mathcal{O}$  and for enumerating the kernel of the map  $\text{Cl}(\mathbb{Z} + N\mathcal{O}) \rightarrow \text{Cl}(\mathcal{O})$ .

These algorithms are implemented in an experimental branch of PARI/GP, and will be integrated in the public version soon.

A. Enge and R. Schertz determine in [13] under which conditions singular values of multiple  $\eta$ -quotients of square-free level, not necessarily prime to 6, yield class invariants, that is, algebraic numbers in ring class fields of imaginary-quadratic number fields. It turns out that the singular values lie in subfields of the ring class fields of index  $2^{k'-1}$  when  $k' \geq 2$  primes dividing the level are ramified in the imaginary-quadratic field, which leads to faster computations of elliptic curves with prescribed complex multiplication. The result is generalised to singular values of modular functions on  $X_0^+(p)$  for  $p$  prime and ramified.

The paper of R. Cosset and D. Robert [25] presenting an algorithm for computing isogenies between principally polarised abelian surface has been accepted for publication in Mathematics of Computation. This paper explains, given the theta coordinates of the points of a maximal isotropic kernel of the  $\ell$ -torsion, how to compute the corresponding isogeny. It also gives formulæ for the conversion between theta coordinates and Mumford coordinates.

The paper by K. Lauter and D. Robert on Improved CRT Algorithm for Class Polynomials in Genus 2, which was presented at the ANTS-X conference, was published in [18].

A. Enge and E. Thomé describe in [14] a quasi-linear algorithm for computing Igusa class polynomials of Jacobians of genus 2 curves via complex floating-point approximations of their roots. After providing an explicit treatment of the computations in quartic CM fields and their Galois closures, they pursue an approach due to Dupont for evaluating  $\vartheta$ -constants in quasi-linear time using Newton iterations on the Borchartd mean. They report on experiments with the implementation CMH and present an example with class number 20016.

N. Mascot's article on computing modular Galois representations [15] has been published in Rendiconti del Circolo Matematico di Palermo. This article describes an algorithm to compute Galois representations attached to a newform, and to deduce the Fourier coefficients of this newform modulo a small prime.

E. Milio has implemented R. Dupont's algorithms [38] in PARI/GP. With them, he has calculated the three modular polynomials in genus 2 and level 2 defined by Streng's version of Igusa modular forms and a modular polynomial of genus 2 and level 3 coming from theta modular forms.

## 6.5. Elliptic curve cryptology

**Participants:** Jean-Marc Couveignes, Andreas Enge, Damien Robert.

Couveignes and Lercier study in [26] the problem of parameterisations by radicals of low genus algebraic curves. They prove that for  $q$  a prime power that is large enough and prime to 6, a fixed positive proportion of all genus 2 curves over the field with  $q$  elements can be parameterised by 3-radicals. This results in the existence of a deterministic encoding into these curves when  $q$  is congruent to 2 modulo 3. Deterministic encodings into curves are useful in numerous situations, for instance in discrete logarithm cryptography. The parameterisation found by Couveignes and Lercier is in some sense the first generic one for genus 2 curves.

A software for this method is in preparation.

The survey [21], published in the *Handbook of Finite Fields*, presents the state of the art of the use of elliptic curves in cryptography.

## 6.6. Pairings

**Participants:** Andreas Enge, Damien Robert.

In [27], A. Enge gives an elementary and self-contained introduction to pairings on elliptic curves over finite fields. For the first time in the literature, the three different definitions of the Weil pairing are stated correctly and proved to be equivalent using Weil reciprocity. Pairings with shorter loops, such as the ate,  $\text{ate}_i$ , R-ate and optimal pairings, together with their twisted variants, are presented with proofs of their bilinearity and non-degeneracy. Finally, different types of pairings are reviewed in a cryptographic context. The article can be seen as an update chapter to [40].

With D. Lubicz, D. Robert has worked on extending the algorithm to compute Weil and Tate pairings using theta functions from [42] to the ate and optimal ate pairings in [29]. The result includes how to compute the Miller functions with theta functions, but also how to generalise ate and optimal ate pairings to Kummer varieties. In contrast to preceding algorithms using Miller functions which needed a geometric interpretation of the addition law and worked with Jacobians, this new algorithm uses only the algebraic Riemann relations and works on any abelian variety (provided with a theta structure). This algorithm has been implemented using AVISOGENIES.

## ALEA Project-Team

# 6. New Results

## 6.1. Sparsity-Promoting Bayesian Dynamic Linear Models

Sparsity-promoting priors have become increasingly popular over recent years due to an increased number of regression and classification applications involving a large number of predictors. In time series applications where observations are collected over time, it is often unrealistic to assume that the underlying sparsity pattern is fixed. We propose an original class of flexible Bayesian linear models for dynamic sparsity modelling. The proposed class of models expands upon the existing Bayesian literature on sparse regression using generalized multivariate hyperbolic distributions. The properties of the models are explored through both analytic results and simulation studies. We demonstrate the model on a financial application where it is shown that it accurately represents the patterns seen in the analysis of stock and derivative data, and is able to detect major events by filtering an artificial portfolio of assets.

## 6.2. Evolutionary algorithms and genetic programming

The regularity of a signal can be numerically expressed using Hölder exponents, which characterize the singular structures a signal contains. In particular, within the domains of image processing and image understanding, regularity-based analysis can be used to describe local image shape and appearance. However, estimating the Hölder exponent is not a trivial task, and current methods tend to be computationally slow and complex. This work presents an approach to automatically synthesize estimators of the pointwise Hölder exponent for digital images. This task is formulated as an optimization problem and Genetic Programming (GP) is used to search for operators that can approximate a traditional estimator, the oscillations method. Experimental results show that GP can generate estimators that achieve a low error and a high correlation with the ground truth estimation. Furthermore, most of the GP estimators are faster than traditional approaches, in some cases their runtime is orders of magnitude smaller. This result allowed us to implement a real-time estimation of the Hölder exponent on a live video signal, the first such implementation in current literature. Moreover, the evolved estimators are used to generate local descriptors of salient image regions, a task for which a stable and robust matching is achieved, comparable with state-of-the-art methods. In conclusion, the evolved estimators produced by GP could help expand the application domain of Hölder regularity within the fields of image analysis and signal processing.

One of the main open problems within Genetic Programming (GP) is to meaningfully characterize the difficulty (or hardness) of a problem. The general goal is to develop predictive tools that can allow us to identify how difficult a problem is for a GP system to solve. On this topic, we identify and compare two main approaches that address this question. We denote the first group of methods as Evolvability Indicators (EI), which are measures that attempt to capture how amenable the fitness landscape is to a GP search. The best examples of current EIs are the Fitness Distance Correlation (FDC) and the Negative Slope Coefficient (NSC). The second, more recent, group of methods are what we call Predictors of Expected Performance (PEP), which are predictive models that take as input a set of descriptive attributes of a particular problem and produce as output the expected performance of a GP system. The experimental work presented here compares an EI, the NSC, and a PEP model for a GP system applied to data classification. Results suggest that the EI fails at measuring problem difficulty expressed by the performance of the GP classifiers, an unexpected result. On the other hand, the PEP models show a very high correlation with the actual performance of the GP system. It appears that while an EI can correctly estimate the difficulty of a given search, as shown by previous research on this topic, it does not necessarily capture the difficulty of the underlying problem that GP is intended to solve. Conversely, while the PEP models treat the GP system as a computational black-box, they can still provide accurate performance predictions.

Another research area is to predict the alertness of an individual by analyzing the brain activity through electroencephalographic data (EEG) captured with 58 electrodes. Alertness is characterized here as a binary variable that can be in a "normal" or "relaxed" state. We collected data from 44 subjects before and after a relaxation practice, giving a total of 88 records. After a pre-processing step and data validation, we analyzed each record and discriminate the alertness states using our proposed "slope criterion". Afterwards, several common methods for supervised classification ( $k$  nearest neighbors, decision trees (CART), random forests, PLS and discriminant sparse PLS) were applied as predictors for the state of alertness of each subject. The proposed "slope criterion" was further refined using a genetic algorithm to select the most important EEG electrodes in terms of classification accuracy. Results shown that the proposed strategy derives accurate predictive models of alertness.

### **6.3. Moderate Deviations for Mean Field Particle Models**

Our team is interested with moderate deviation principles of a general class of mean field type interacting particle models. We discuss functional moderate deviations of the occupation measures for both the strong - topology on the space of finite and bounded measures as well as for the corresponding stochastic processes on some class of functions equipped with the uniform topology. Our approach is based on an original semigroup analysis combined with stochastic perturbation techniques and projective limit large deviation methods.

### **6.4. Bifurcating autoregressive processes**

We investigate the asymptotic behavior of the least squares estimator of the unknown parameters of random coefficient bifurcating autoregressive processes. Under suitable assumptions on inherited and environmental effects, we establish the almost sure convergence of our estimates. In addition, we also prove a quadratic strong law and central limit theorems. Our approach mainly relies on asymptotic results for vector-valued martingales together with the well-known Rademacher-Menchov theorem.

We study also the asymptotic behavior of the weighted least square estimators of the unknown parameters of random coefficient bifurcating autoregressive processes. Under suitable assumptions on the immigration and the inheritance, we establish the almost sure convergence of our estimators, as well as a quadratic strong law and central limit theorems. Our study mostly relies on limit theorems for vector-valued martingales.

Finally, we study the asymptotic behavior of the weighted least squares estimators of the unknown parameters of bifurcating integer-valued autoregressive processes. Under suitable assumptions on the immigration, we establish the almost sure convergence of our estimators, together with the quadratic strong law and central limit theorems. All our investigation relies on asymptotic results for vector-valued martingales.

### **6.5. Durbin-Watson statistic and first order autoregressive processes**

We investigate moderate deviations for the Durbin-Watson statistic associated with the stable first-order autoregressive process where the driven noise is also given by a first-order autoregressive process. We first establish a moderate deviation principle for both the least squares estimator of the unknown parameter of the autoregressive process as well as for the serial correlation estimator associated with the driven noise. It enables us to provide a moderate deviation principle for the Durbin-Watson statistic in the easy case where the driven noise is normally distributed and in the more general case where the driven noise satisfies a less restrictive Chen-Ledoux type condition.

We investigate the asymptotic behavior of the Durbin-Watson statistic for the general stable  $p$ -order autoregressive process when the driven noise is given by a first-order autoregressive process. We establish the almost sure convergence and the asymptotic normality for both the least squares estimator of the unknown vector parameter of the autoregressive process as well as for the serial correlation estimator associated with the driven noise. In addition, the almost sure rates of convergence of our estimates are also provided. Then, we prove the almost sure convergence and the asymptotic normality for the Durbin-Watson statistic. Finally, we propose a new bilateral statistical procedure for testing the presence of a significative first-order residual autocorrelation and we also explain how our procedure performs better than the commonly used Box-Pierce and Ljung-Box statistical tests for white noise applied to the stable autoregressive process, even on small-sized samples.



In a recent paper (to appear hal-00677600), we investigate the asymptotic behavior of the maximum Likelihood estimators of the unknown parameters of positive recurrent Ornstein-Uhlenbeck processes driven by Ornstein-Uhlenbeck processes.

## **6.6. Ornstein-Uhlenbeck process with shift**

We investigate the large deviation properties of the maximum likelihood estimators for the Ornstein-Uhlenbeck process with shift. We estimate simultaneously the drift and shift parameters. On the one hand, we establish a large deviation principle for the maximum likelihood estimates of the drift and shift parameters. Surprisingly, we find that the drift estimator shares the same large deviation principle as the one previously established for the Ornstein-Uhlenbeck process without shift. Sharp large deviation principles are also provided. On the other hand, we show that the maximum likelihood estimator of the shift parameter satisfies a large deviation principle with a very unusual implicit rate function.

## **6.7. Markovian superquadratic BSDEs**

In [Stochastic Process. Appl., 122(9):3173-3208], the author proved the existence and the uniqueness of solutions to Markovian superquadratic BSDEs with an unbounded terminal condition when the generator and the terminal condition are locally Lipschitz. In [8], we prove that the existence result remains true for these BSDEs when the regularity assumptions on the generator and/or the terminal condition are weakened.

## **6.8. Non-Asymptotic Analysis of Adaptive and Annealed Feynman-Kac Particle Models**

Sequential and Quantum Monte Carlo methods, as well as genetic type search algorithms can be interpreted as a mean field and interacting particle approximations of Feynman-Kac models in distribution spaces. The performance of these population Monte Carlo algorithms is strongly related to the stability properties of nonlinear Feynman-Kac semigroups. We analyze these models in terms of Dobrushin ergodic coefficients of the reference Markov transitions and the oscillations of the potential functions. Sufficient conditions for uniform concentration inequalities w.r.t. time are expressed explicitly in terms of these two quantities. We provide an original perturbation analysis that applies to annealed and adaptive FK models, yielding what seems to be the first results of this kind for these type of models. Special attention is devoted to the particular case of Boltzmann-Gibbs measures' sampling. In this context, we design an explicit way of tuning the number of Markov Chain Monte Carlo iterations with temperature schedule. We also propose and analyze an alternative interacting particle method based on an adaptive strategy to define the temperature increments.

## **6.9. A Robbins-Monro procedure for a class of models of deformation**

We are interested with the statistical analysis of several data sets associated with shape invariant models with different translation, height and scaling parameters. We propose to estimate these parameters together with the common shape function. Our approach extends the recent work of Bercu and Fraysse to multivariate shape invariant models. We propose a very efficient Robbins-Monro procedure for the estimation of the translation parameters and we use these estimates in order to evaluate scale parameters. The main pattern is estimated by a weighted Nadaraya-Watson estimator. We provide almost sure convergence and asymptotic normality for all estimators. Finally, we illustrate the convergence of our estimation procedure on simulated data as well as on real ECG data.

## **6.10. Individual load curves intraday forecasting**

A dynamic coupled modelling is investigated to take temperature into account in the individual energy consumption forecasting. The objective is both to avoid the inherent complexity of exhaustive SARIMAX models and to take advantage of the usual linear relation between energy consumption and temperature for thermosensitive customers. We first recall some issues related to individual load curves forecasting. Then,

we propose and study the properties of a dynamic coupled modelling taking temperature into account as an exogenous contribution and its application to the intraday prediction of energy consumption. Finally, these theoretical results are illustrated on a real individual load curve. The authors discuss the relevance of such an approach and anticipate that it could form a substantial alternative to the commonly used methods for energy consumption forecasting of individual customers.

## BACCHUS Team

## 6. New Results

### 6.1. Residual distribution schemes for steady problems

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

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

### 6.2. Curved meshes

**Participants:** Rémi Abgrall, Cécile Dobrzynski [Corresponding member], Algiane 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 stretched, this can be quite challenging since, in addition, we want that the mesh keep a structure, in particular for boundary layers. Using tools explored in iso-geometrical analysis, we have been able to construct a software computing curved meshes (in 2D and 3D), while keeping as much as possible the structure of the mesh and guaranteeing that the generated mesh is suitable to CFD simulation (all elements have a positive Jacobian). This software is being used for high order computations with the IDIHOM project. The full paper has been accepted in IJNMF and will be published in 2014.

### 6.3. Hypoelastic models

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

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

### 6.4. Penalisation methods using unstructured meshes

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

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

## 6.5. Unsteady problem

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

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

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

## 6.6. Uncertainty Quantification

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

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

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

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

## 6.7. Robust Design Optimization

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

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

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

## 6.8. Multiphase flows

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

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

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

## 6.9. Depth averaged free surface modeling

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

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

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

## 6.10. Self healing composites modeling

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

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

## 6.11. Parallel remeshing

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

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

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

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

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



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

## 6.12. Graph remapping

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

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

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

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

### 6.13. Sparse matrix reordering for ILU solvers

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

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

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

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

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

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

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

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

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

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



## CAGIRE Team

## 6. New Results

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

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

### 6.2. Low Mach number flows simulations issues

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

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

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

## **CONCHA Project-Team**

### **6. New Results**

#### **6.1. New result 1**

## CQFD Project-Team

## 6. New Results

### 6.1. Nonparametric estimation of the jump rate for non-homogeneous marked renewal processes.

**Participants:** Romain Azais, François Dufour, Anne Gégout-Petit.

Non-homogeneous marked renewal process, nonparametric estimation, jump rate estimation, Nelson-Aalen estimator, asymptotic consistency, ergodicity of Markov chains

This work is devoted to the nonparametric estimation of the jump rate and the cumulative rate for a general class of non-homogeneous marked renewal processes, defined on a separable metric space. In our framework, the estimation needs only one observation of the process within a long time. Our approach is based on a generalization of the multiplicative intensity model, introduced by Aalen in the seventies. We provide consistent estimators of these two functions, under some assumptions related to the ergodicity of an embedded chain and the characteristics of the process. A numerical example illustrates our theoretical results.

It has been published in *Ann. Inst. H. Poincaré Probab. Statist.* [16].

### 6.2. Nonparametric estimation of the conditional distribution of the inter-jumping times for piecewise-deterministic Markov processes

**Participants:** Romain Azais, François Dufour, Anne Gégout-Petit.

Piecewise-deterministic Markov process, ergodicity of Markov chains, nonparametric estimation, jump rate estimation, Nelson-Aalen estimator, asymptotic consistency

In this work, we present a nonparametric method for estimating the conditional density associated to the jump rate of a piecewise-deterministic Markov process. In our framework, the estimation needs only one observation of the process within a long time interval. Our method relies on a generalization of Aalen's multiplicative intensity model. We prove the uniform consistency of our estimator, under some reasonable assumptions related to the primitive characteristics of the process. A simulation study illustrates the behavior of our estimator.

It has been accepted for publication in *Scandinavian Journal of Statistics* [17].

### 6.3. Finite Linear Programming Approximations of constrained discounted Markov decision processes

**Participant:** François Dufour.

Constrained Markov decision processes, linear programming approach to control problems, quantization, approximation of Markov decision processes

We consider a Markov decision process (MDP) with constraints under the total expected discounted cost optimality criterion. We are interested in proposing approximation methods of the optimal value of this constrained MDP. To this end, starting from the linear programming (LP) formulation of the constrained MDP (on an infinite-dimensional space of measures), we propose a finite state approximation of this LP problem. This is achieved by suitably approximating a probability measure underlying the random transitions of the dynamics of the system. Explicit convergence orders of the approximations of the optimal constrained cost are obtained. By exploiting convexity properties of the class of relaxed controls, we reduce the LP formulation of the constrained MDP to a finite-dimensional static optimization problem, that can be used to obtain explicit numerical approximations of the corresponding optimal constrained cost. A numerical application illustrates our theoretical results.

These results have been obtained in collaboration with Tomas Prieto-Rumeau, Department of Statistics and Operations Research, UNED, Madrid, Spain.

It has been published in SIAM Journal of Control and Optimization [25].

## 6.4. Stochastic Approximations of Constrained Discounted Markov Decision Processes

**Participant:** François Dufour.

Constrained Markov decision processes; Linear programming approach to control problems; Approximation of Markov decision processes

We consider a discrete-time constrained Markov decision process under the discounted cost optimality criterion. The state and action spaces are assumed to be Borel spaces, while the cost and constraint functions might be unbounded. We are interested in approximating numerically the optimal discounted constrained cost. To this end, we suppose that the transition kernel of the Markov decision process is absolutely continuous with respect to some probability measure  $\mu$ . Then, by solving the linear programming formulation of a constrained control problem related to the empirical probability measure  $\mu_n$  of  $\mu$ , we obtain the corresponding approximation of the optimal constrained cost. We derive a concentration inequality which gives bounds on the probability that the estimation error is larger than some given constant. This bound is shown to decrease exponentially in  $n$ . Our theoretical results are illustrated with a numerical application based on a stochastic version of the Beverton-Holt population model.

These results have been obtained in collaboration with Tomas Prieto-Rumeau, Department of Statistics and Operations Research, UNED, Madrid, Spain.

It has been accepted for publication in Journal of Mathematical Analysis and Applications [26].

## 6.5. The expected total cost criterion for Markov decision processes under constraints

**Participant:** François Dufour.

Markov decision process, expected total cost criterion, constraints, linear programming, occupation measure

In this work, we study discrete-time Markov decision processes (MDPs) with constraints when all the objectives have the same form of expected total cost over the infinite time horizon. Our objective is to analyze this problem by using the linear programming approach. Under some technical hypotheses, it is shown that if there exists an optimal solution for the associated linear program then there exists a randomized stationary policy which is optimal for the MDP, and that the optimal value of the linear program coincides with the optimal value of the constrained control problem. A second important result states that the set of randomized stationary policies provides a sufficient set for solving this MDP. It is important to notice that, in contrast with the classical results of the literature, we do not assume the MDP to be transient or absorbing. More importantly, we do not impose the cost functions to be non-negative or to be bounded below. Several examples are presented to illustrate our results.

These results have been obtained in collaboration with Alexey Piunovskiy from Department. of Mathematical Sciences.

It has been published in Advances in Applied Probability [24].

## 6.6. Optimal stopping for piecewise-deterministic Markov processes and applications

**Participants:** Adrien Brandejsky, Benoîte de Saporta, François Dufour, Huilong Zhang.

We worked further on numerical methods for optimal stopping of PDMPs. On the one hand, we applied our numerical method to compute an optimal maintenance date to the test case of the heated hold-up tank. The system consists of a tank containing a fluid whose level is controlled by three components: two inlet pumps and one outlet valve. A thermal power source heats up the fluid. The failure rates of the components depends on the temperature, the position of the three components monitors the liquid level in the tank and the liquid level determines the temperature. Therefore, this system can be modeled by a hybrid process where the discrete (components) and continuous (level, temperature) parts interact in a closed loop. We model the system by a piecewise deterministic Markov process, propose and implement a numerical method to compute the optimal maintenance date to repair the components before the total failure of the system. This work is published in [30].

On the other hand, we investigated the optimal stopping problem under partial observations for PDMPs. We first obtain a recursive formulation of the optimal filter process and derive the dynamic programming equation of the partially observed optimal stopping problem. Then, we propose a numerical method, based on the quantization of the discrete-time filter process and the inter-jump times, to approximate the value function and to compute an  $\epsilon$ -optimal stopping time. We prove the convergence of the algorithms and bound the rates of convergence. This work is published in [20].

## 6.7. Stochastic control for underwater optimal trajectories

**Participants:** Benoîte de Saporta, François Dufour, Huilong Zhang.

This work aims to compute optimal trajectories for underwater vehicles evolving in a given environment to accomplish some tasks. This is an optimal control problem. In real context, available inputs are not perfectly known. Hence a stochastic approach seems to be needed, coupled with the outputs of the tracking algorithms. Markov decision processes (MDPs) constitute a general family of controlled stochastic processes suitable for the modeling of sequential decision-making problems. The analysis of MDPs leads to mathematical and computational problems. The corresponding theory has reached a rather high degree of maturity, although the classical tools (such as value iteration, policy iteration, linear programming, and their various extensions) are generally hardly applicable in practice. Hence, solving MDPs numerically is an awkward and important problem. The method is applied to control a submarine which wants to well detect one or several targets and only has the information given by the tracking algorithms from the sonar observations [47].

## 6.8. Modeling of cell division data

**Participants:** Benoîte de Saporta, Anne Gégout-Petit.

This work is in collaboration with Laurence Marsalle (Univ. Lille 1).

A rigorous methodology is proposed to study cell division data consisting in several observed genealogical trees of possibly different shapes. The procedure takes into account missing observations, data from different trees, as well as the dependence structure within genealogical trees. Its main new feature is the joint use of all available information from several data sets instead of single data set estimation, to avoid the drawbacks of low accuracy for estimators or low power for tests on small single trees. The data is modeled by an asymmetric bifurcating autoregressive process and possibly missing observations are taken into account by modeling the genealogies with a two-type Galton-Watson process. Least-squares estimators of the unknown parameters of the processes are given and symmetry tests are derived. Results are applied on real data of *Escherichia coli* division and an empirical study of the convergence rates of the estimators and power of the tests is conducted on simulated data. This work is to appear in [29].

We have also presented a new model of asymmetric bifurcating autoregressive process with random coefficients. We couple this model with a Galton-Watson tree to take into account possibly missing observations. We propose least-squares estimators for the various parameters of the model and prove their consistency, with a convergence rate, and asymptotic normality. We use both the bifurcating Markov chain and martingale approaches and derive new results in both these frameworks. This work is to appear in [28].

## 6.9. Numerical method for the filtering of Markov jump linear systems

**Participants:** Benoîte de Saporta, Eduardo Costa.

We are interested in efficient pre-computations of the solutions of Markov switching Riccati equations. These equations are matrix-valued and naturally arise in control or filtering problems for Markov jump linear systems. It is crucial for applications to be able to compute the filter in real time, although the solutions to Riccati equations are slow to compute. Hence the need for pre-computations, taking into account the random possible changes of regimes. We propose a numerical method based on the discretization by quantization of the underlying Markov chain.

## 6.10. Optimization of the assembly line of the future European launcher

**Participants:** Benoîte de Saporta, François Dufour, Christophe Nivot.

In collaboration with Astrium space transportation, we have started working on the optimization of the assembly line of the future European launcher. We have started with a simplified model with five components to be assembled in workshops liable to breakdowns. We have modeled the problem using the Markov Decision Processes (MDP) framework and built a simulator of the process in order to run an optimization procedure

## 6.11. A variable clustering approach for the typology of units: a survey on farming and environment

**Participants:** Jérôme Saracco, Marie Chavent.

A survey on farming and environment dealing with the current transformations of the farmer job is considered. We propose to replace the usual data mining strategy which consists of applying Multiple Correspondence Analysis by a variable clustering approach. Clustering of variables aims at lumping together variables which are strongly related to each other and thus bring the same information. The ClustOfVar approach used in this paper provides at the same time groups of variables and their associated synthetic variables. In this algorithm, the homogeneity criterion of a cluster is defined by the squared Pearson correlation for the quantitative variables and by the correlation ratio for the qualitative variables. The step of variable clustering enables to get synthetic variables that can be read as a gradient. In our case study, values correspond to some relevant groupings of categories. This enables to interpret and name easily the synthetic variables. Trends in the opinion of farmers are thus highlighted with the variable clustering approach. Then we clarify these first results by applying a clustering method on the scores of the individuals measured by the synthetic variables. At the sociological level, the supply provided by the synthetic variables to interpret the clusters of farmers is obvious.

These results have been obtained in collaboration with Vanessa Kuentz from Irstea, UR ADBX.

They have been published in Journal de la Société Française de Statistique [31].

## 6.12. Multiple Facctorial Analysis for mixed data type

**Participants:** Jérôme Saracco, Marie Chavent, Amaury Labenne.

Multiple Factor Analysis (MFA) originally proposed by Escofier and Pages in 1982 is a method dedicated to the study of a set of  $n$  individuals described by groups of quantitative variables. Later, this method was extended to take into account groups of qualitative variables (Pages, 1983) then simultaneously quantitative groups and qualitative groups (Pages, 2002). However, this method does not currently take into account mixed groups, that is to say containing both quantitative and qualitative variables. The aim of our study is to propose sustainable development indicators by integrating the aspect of quality of life. For that, we are confronted with the analysis of groups of variables with quantitative and qualitative variables. In this work, we propose an extension of the MFA method, called MFAMIX, for the multiple factor analysis of mixed groups of variables. This approach relies on a combination of AFM and PCAMIX method that allows the analysis of mixed data. MFAMIX method is presented using a singular value decomposition and illustrated on socio-economic data about the quality of life.

These results have been obtained in collaboration with Vanessa Kuentz from Irstea, UR ADBX.

They have been presented in two national conferences [43], [41].

### 6.13. Detecting mental states of alertness with genetic algorithm variable selection

**Participants:** Marie Chavent, Laurent Vézard.

The objective of the present work is to develop a method able to automatically determine mental states of vigilance; i.e., a person's state of alertness. Such a task is relevant to diverse domains, where a person is expected or required to be in a particular state. For instance, pilots or medical staffs are expected to be in a highly alert state, and this method could help to detect possible problems. In this paper, an approach is developed to predict the state of alertness ("normal" or "relaxed") from the study of electroencephalographic signals (EEG) collected with a limited number of electrodes. The EEG of 58 participants in the two alertness states (116 records) were collected via a cap with 58 electrodes. After a data validation step, 19 subjects were retained for further analysis. A genetic algorithm was used to select an optimal subset of electrodes. Common spatial pattern (CSP) coupled to linear discriminant analysis (LDA) was used to build a decision rule and thus predict the alertness of the participants. Different subset sizes were investigated and the best result was obtained by considering 9 electrodes (correct classification rate of 73.68

These results have been obtained in collaboration with Pierrick Legrand from Alea Inria team and Leonardo Trujillo from Instituto Tecnológico de Tijuana.

This work has been presented in a international IEEE conference [38].

### 6.14. ClustOfVar : an R package for dimension reduction via clustering of variables. Application in supervised classification and variable selection in gene expressions data

**Participants:** Marie Chavent, Jérôme Saracco.

The main goal of this work is to tackle the problem of dimension reduction for high-dimensional supervised classification. The motivation is to handle gene expression data. The proposed method works in 2 steps. First, one eliminates redundancy using clustering of variables, based on the R-package ClustOfVar. This first step is only based on the exploratory variables (genes). Second, the synthetic variables (summarizing the clusters obtained at the first step) are used to construct a classifier (e.g. logistic regression, LDA, random forests). We stress that the first step reduces the dimension and gives linear combinations of original variables (synthetic variables). This step can be considered as an alternative to PCA. A selection of predictors (synthetic variables) in the second step gives a set of relevant original variables (genes). Numerical performances of the proposed procedure are evaluated on gene expression datasets. We compare our methodology with LASSO and sparse PLS discriminant analysis on these datasets.

This work is a collaboration with Robin Genuer from SISTM Inria team and Benoit Liquet from University of Queensland.

This work has been presented in a international workshop on Statistical Methods for (post)-Genomics Data (SMPGD 2013) [42].

### 6.15. A sliced inverse regression approach for data stream

**Participants:** Jérôme Saracco, Marie Chavent.

This work is in collaboration with Stéphane Girard (Inria Grenoble Alpes), Benoît Liquet (MRC, Cambridge University), Vanessa Kuentz (Irstea) and Thi Mong Gnoc Nguyen (Univ. de Strasbourg).



In this work, we focus on data arriving sequentially by blocks in a stream. A semiparametric regression model involving a common EDR (Effective Dimension Reduction) direction is assumed in each block. Our goal is to estimate this direction at each arrival of a new block. A simple direct approach consists of pooling all the observed blocks and estimating the EDR direction by the SIR (Sliced Inverse Regression) method. But in practice, some disadvantages appear such as the storage of the blocks and the running time for large sample sizes. To overcome these drawbacks, we propose an adaptive SIR estimator of based on the optimization of a quality measure. The corresponding approach is faster both in terms of computational complexity and running time, and provides data storage benefits. The consistency of our estimator is established and its asymptotic distribution is given. An extension to multiple indices model is proposed. A graphical tool is also provided in order to detect changes in the underlying model, i.e., drift in the EDR direction or aberrant blocks in the data stream. A simulation study illustrates the numerical behavior of our estimator. Finally, an application to real data concerning the estimation of physical properties of the Mars surface is presented.

This work is to appear in [21].

## **6.16. Comparison of Kernel Density Estimators with Assumption on Number of Modes**

**Participant:** Jérôme Saracco.

This work is in collaboration with Bernard Bercu (Univ. Bretagne Sud) and Thi Mong Gnoc Nguyen (Univ. de Strasbourg).

In this work, we investigate the asymptotic behavior of the Nadaraya-Watson estimator for the estimation of the regression function in a semiparametric regression model. On the one hand, we make use of the recursive version of the sliced inverse regression method for the estimation of the unknown parameter of the model. On the other hand, we implement a recursive Nadaraya-Watson procedure for the estimation of the regression function which takes into account the previous estimation of the parameter of the semiparametric regression model. We establish the almost sure convergence as well as the asymptotic normality for our Nadaraya-Watson estimator. We also illustrate our semiparametric estimation procedure on simulated data.

This work is to appear in [19].

## **6.17. Comparison of Kernel Density Estimators with Assumption on Number of Modes**

**Participants:** Jérôme Saracco, Raphaël Coudret.

This work is in collaboration with Gilles Durrieu (Univ. Bretagne Sud).

A data-driven bandwidth choice for a kernel density estimator called critical bandwidth is investigated. This procedure allows the estimation to have as many modes as assumed for the density to estimate. Both Gaussian and uniform kernels are considered. For the Gaussian kernel, asymptotic results are given. For the uniform kernel, an argument against these properties is mentioned. These theoretical results are illustrated with a simulation study which compare the kernel estimators that rely on critical bandwidth with another one which uses a plug-in method to select its bandwidth. An estimator that consists in estimates of density contour clusters and takes assumptions on number of modes into account is also considered. Finally, the methodology is illustrated using environment monitoring data.

This work is to appear in [22].

## **6.18. Comparison of sliced inverse regression approaches for underdetermined cases**

**Participants:** Jérôme Saracco, Raphaël Coudret.

This work is in collaboration with Benoît Liquet (MRC, Cambridge University).

Among methods to analyze high-dimensional data, the sliced inverse regression (SIR) is of particular interest for non-linear relations between the dependent variable and some indices of the covariate. When the dimension of the covariate is greater than the number of observations, classical versions of SIR cannot be applied. Various upgrades were then proposed to tackle this issue such as regularized SIR (RSIR) and sparse ridge SIR (SR-SIR), to estimate the parameters of the underlying model and to select variables of interest. In this paper, we introduce two new estimation methods respectively based on the QZ algorithm and on the Moore-Penrose pseudo-inverse. We also describe a new selection procedure of the most relevant components of the covariate that relies on a proximity criterion between submodels and the initial one. These approaches are compared with RSIR and SR-SIR in a simulation study. Finally we applied SIR-QZ and the associated selection procedure to a genetic dataset in order to find markers that are linked to the expression of a gene. These markers are called expression quantitative trait loci (eQTL).

This work was presented in a national conference [23] and is to appear in [37].

## 6.19. Conditional Quantile Estimation through Optimal Quantization

**Participants:** Jérôme Saracco, Isabelle Charlier.

This work is in collaboration with Davy Paindaveine (Univ. Libre de Bruxelles).

In this work, we construct a nonparametric estimator of conditional quantiles of  $Y$  given  $X$  via optimal quantization. In a first step, we propose to approximate conditional quantiles thanks to optimal quantization in  $L^p$ -norm, consisting in discretizing  $X$  and  $Y$  thanks to some optimal grids of size  $N$ . We state a result of convergence of this approximation toward the true conditional quantile. The estimator was implemented in **R** in order to evaluate its numerical behavior and to compare it with existing estimators. A simulation study illustrates the good behavior of our estimator. The practical choice of  $N$  is discussed. We apply our approach to a real data set.

This work was presented in a national conference [35].

## 6.20. Estimation of water consumption based on survey techniques using an automatic meter reading sample

**Participant:** Jérôme Saracco.

This work is in collaboration with Karim Claudio (LyRE), Vincent Couallier (Univ. de Bordeaux) and Yves Le Gat (Irstea).

Automatic water meters reading are, nowadays, the best technology for real time knowledge of water consumption. At an hydraulic sector scale, a complete equipment permits to know the total consumption of a finite size population, for a time scale as small as the hour. However its cost for generalization is sometimes unbearable for the collectivity, for whom sampling techniques have to be set up. In a objective of a total consumption estimation, this article describes and compares standard methods of survey techniques and propose to retain a methodology for implementation of an operational sample and to calibrate the corresponding total estimator.

This work was presented in a national conference [36] and an associated paper is currently in revision.

## 6.21. Hidden Markov Model for the detection of a degraded operating mode of optronic equipment

**Participants:** Camille Baysse, Anne Gégout-Petit, Jérôme Saracco.

This work is in collaboration with Didier Bihannic (Thales Optronics) and Michel Prenat (Thales Optronics).

As part of optimizing the reliability, Thales Optronics now includes systems that examine the state of its equipment. The aim of this work is to use hidden Markov Model to detect as soon as possible a change of state of optronic equipment in order to propose maintenance before failure. For this, we carefully observe the dynamic of a variable called “cool down time” and noted Tmf, which reflects the state of the cooling system. Indeed, the Tmf is an observation of the hidden state of the system. This one is modeled by a Markov chain and the Tmf is a noisy function of it. Thanks to filtering equations, we obtain results on the probability that an appliance is in degraded state at time  $t$ , knowing the history of the Tmf until this moment. We have evaluated the numerical behavior of our approach on simulated data. Then we have applied this methodology on our real data and we have checked that the results are consistent with the reality. This method can be implemented in a HUMS (Health and Usage Monitoring System). This simple example of HUMS would allow the Thales Optronics Company to improve its maintenance system. This company will be able to recall appliances which are estimated to be in degraded state and do not control too early those estimated in stable state.

This work is to appear in [18].

## 6.22. A new sliced inverse regression method for multivariate response

**Participants:** Jérôme Saracco, Raphaël Coudret.

This work is in collaboration with Stéphane Girard (Inria Grenoble Alpes).

We consider a semiparametric regression model of a  $q$ -dimensional multivariate response  $y$  on a  $p$ -dimensional covariate  $x$ . In this paper, a new approach is proposed based on sliced inverse regression for estimating the effective dimension reduction (EDR) space without requiring a prespecified parametric model. The convergence at rate  $\sqrt{n}$  of the estimated EDR space is shown. We discuss the choice of the dimension of the EDR space. The numerical performance of the proposed multivariate SIR method is illustrated on a simulation study. Moreover, we provide a way to cluster components of  $y$  related to the same EDR space. One can thus apply properly multivariate SIR on each cluster instead of blindly applying multivariate SIR on all components of  $y$ . An application to hyperspectral data is provided.

This work is currently under revision, see [48].

## 6.23. An introduction to dimension reduction in nonparametric kernel regression

**Participant:** Jérôme Saracco.

This work is in collaboration with Stéphane Girard (Inria Grenoble Alpes).

Nonparametric regression is a powerful tool to estimate nonlinear relations between some predictors and a response variable. However, when the number of predictors is high, nonparametric estimators may suffer from the curse of dimensionality. In this chapter, we show how a dimension reduction method (namely Sliced Inverse Regression) can be combined with nonparametric kernel regression to overcome this drawback. The methods are illustrated both on simulated datasets as well as on an astronomy dataset using the **R** software.

This work was presented in “School in Astrostatistics” (Annecy, October, 21-25, 2013) and is to appear as a chapter in book intilted *Methods and Applications of Regression in Astrophysics* in 2014.

## GEOSTAT Project-Team

### 6. New Results

#### 6.1. Nonlinear dynamics and Mild Therapeutic Hypothermia (MTH)

**Participants:** Binbin Xu [correspondant], Oriol Pont, Hussein Yahia, Ihu Liryc.

The neurological damage after cardiac arrest constitutes a big challenge of hospital discharge. The mild therapeutic hypothermia (MTH) ( $34^{\circ}\text{C}$  -  $32^{\circ}\text{C}$ ) has shown its benefit to reduce this type of damage. However, it can have many adverse effects, among which the cardiac-arrhythmia-generation-a-posteriori (CAGP) can represent up to 34%. So it's important to understand the mechanism of CAGP in order to improve this therapy. Our study with a cardiac culture in vitro showed that at  $35^{\circ}\text{C}$  the CAGP can be induced. Spiral waves, commonly considered as a sign of cardiac arrhythmia, are observed. The process of MTH can be represented by a Pitchfork bifurcation, which could explain the different ratio of arrhythmia among the adverse effects after this therapy. This nonlinear dynamics suggests that a variable speed of cooling / rewarming, especially when passing  $35^{\circ}\text{C}$ , would help to decrease the ratio of post-hypothermia arrhythmia and then improve the hospital output. See figures 5 , 6 .



Figure 5. Phase space reconstruction for extracellular potential signals at  $37^{\circ}\text{C}$ ,  $35^{\circ}\text{C}$  and  $33^{\circ}\text{C}$ .

Publications: [33], [35], [39].

#### 6.2. Characterizing cardiac arrhythmias and their mechanisms by means of nonlinear and robust methods

**Participants:** Oriol Pont [correspondant], Binbin Xu, Hussein Yahia, Ihu Liryc.



Figure 6. Illustration of Bifurcation or Trifurcation (type Pitchfork) of hypothermia effect.

Nonlinear analysis provides appropriate tools to characterize cardiac dynamics. Singularity analysis and phase-space reconstruction are physically meaningful complexity measures with minimal assumptions on the underlying models. These methods are based on effective descriptions derived from first principles, and as a consequence, parameters are robustly estimated. We have validated this approach on ECG, endocavitary catheter measures and electrocardiographic maps.

Key parameters vary infrequently and exhibit sharp transitions, which show where information concentrates and correspond to actual dynamical regime changes. Singularity exponents sift a simple fast dynamics from its slow modulation. In space domain, extreme values highlight arrhythmogenic areas. We observe a correspondence of time lag fluctuations of phase-space reconstructions with atrial fibrillation episodes in the same way as with the dynamical changes coming from singularity exponents. This characterization of information transitions could be used in the regularization of inverse-problem mapping of electrocardiographic epicardial maps. Furthermore, this opens the way for improved model-independent complexity descriptors to be used in non-invasive, automatic diagnosis support and ablation guide for electrical insulation therapy, in cases of arrhythmias such as atrial flutter and fibrillation.

Publications: [34], [29], [32], [37], [21].

### 6.3. Multifractal Deep Convolutional Pooling for Robust Texture Discrimination

**Participants:** Hicham Badri [correspondant], Hussein Yahia, Khalid Daoudi.

A robust and fast affine invariant texture classification system is presented. The new approach consists first in filtering the input image with multiple wavelet filters of different scales and orientations followed by a dual-pooling operation to increase the local invariance. The process is repeated for different wavelet sets and multiple image resolutions. This can be seen as a deep convolutional network where the outputs correspond to the pooling responses. The next step consists in extracting a robust affine invariant descriptor based on the scale invariance prior observed in natural images ; a multifractal log exponent histogram is calculated for each output node of the network. These log- histograms are combined to form the main descriptor. The final step consists in features post-processing based on the sparse wavelet coefficients prior to reduce the influence of small perturbations. For the training, we propose a combination of the generative PCA classifier with multiclass SVMs which improves classification rates. We also propose to use multi-illumination and multi-scale training ; two simple strategies to significantly boost classification results when dealing with small and homogeneous training sets. Experiments demonstrate that the proposed solution outperforms existing methods on three challenging public benchmark datasets.

Work submitted to CVPR 2014.

## 6.4. Nonlinear reconstruction of optical phase perturbed by atmospheric turbulence in Adaptive Optics

**Participants:** Suman Maji [correspondant], Hussein Yahia, Thierry Fusco.

A new approach to wavefront phase reconstruction in Adaptive Optics (AO) from the low-resolution gradient measurements provided by a wavefront sensor, using a nonlinear approach derived from the Microcanonical Multiscale Formalism (MMF). MMF comes from established concepts in statistical physics, it is naturally suited to the study of multiscale properties of complex natural signals, mainly due to the precise numerical estimate of geometrically localized critical exponents, called the singularity exponents. These exponents quantify the degree of predictability, locally, at each point of the signal domain, and they provide information on the dynamics of the associated system. We show that multiresolution analysis carried out on the singularity exponents of a high-resolution turbulent phase (obtained by model or from data) allows a propagation along the scales of the gradients in low-resolution (obtained from the wavefront sensor), to a higher resolution. We compare our results with those obtained by linear approaches, which allows us to offer an innovative approach to wavefront phase reconstruction in Adaptive Optics.

Supporting grant: Conseil Régional Aquitaine project and funding *OPTAD*.

PhD thesis defended: Suman Kumar Maji, *Multiscale Methods in Signal Processing for Adaptive Optics*, University Bordeaux-1, PhD defended on November 14th, 2013, supervisor: H. Yahia [14].

Publications: [19], [20], [28], [14].

## 6.5. Nonlinear Speech Analysis

**Participants:** Vahid Khanagha [correspondant], Khalid Daoudi, Safa Mrad, Nicolas Vinuesa, Blaise Bertrac.

1. *MMF for speech analysis* : we continued our research on the adaptation and application of the MMF to speech analysis and started a research theme on pathological voice analysis. We proposed a novel compact representation of speech which consists in reconstructing a speech signal from its most singular manifold. This leads us to build a speech waveform coder which outperforms the G.726 standard. We then used our recently developed algorithm for Glottal Closure Instants (GCI) detection to improve the performance of our sparse linear prediction method. We also used this algorithm to develop new acoustic perturbation measures for normal/pathological voice classification.
2. *Matching pursuit for speech analysis* : we first showed that the Gabor dictionary is actually more efficient than the Gammatone dictionary for speech coding using the matching pursuit (MP) algorithm. This result mitigates some famous findings on the neural coding at the human auditory nerve. Second, we showed that one single parameter, derived from MP decomposition of speech, allows discrimination between normal and dysphonic voices with an accuracy which is significantly higher than all existing methods.

Supporting grant: Inria CORDIS.

PhD thesis defended: Vahid Khanagha *Novel Multiscale Methods for Nonlinear Speech Analysis*, University Bordeaux-1, PhD defended on January 16th, 2013, supervisors: K. Daoudi and H. Yahia [13].

Publications: [17], [27], [41], [40], [44].

## 6.6. Discriminative learning for Automatic speaker recognition

**Participants:** Khalid Daoudi [correspondant], Reda Jourani, Régine André Obrecht, Driss Aboutajdine.

We proposed a speaker identification which combines SVM and Large Margin Gaussian Mixture Models (LM-GMM) which outperforms the performance of our LM-GMM system.

Publication: [26].

## 6.7. Learning Multifractal Structures in Images

**Participants:** Hicham Badri [correspondant], Hussein Yahia, Driss Aboutajdine.

Learning dictionaries has become a powerful tool in many image processing applications. However, standard learning methods such as K-SVD and Online learning do not take into account the structure of the patches : each patch is expressed as a linear combination of atoms of one global dictionary. We present a new dictionary learning method which takes into account the nature of each patch by performing a multifractal decomposition of the image. As a result, each fractal set will have a specific dictionary and each dictionary contains atoms of a certain singularity degree. Each patch can therefore be expressed much more efficiently compared to global dictionary learning methods. Current experiments in image denoising show that the proposed method outperforms the global dictionary learning methods.

Work in progress.

## 6.8. Super resolution maps of partial pressure $pCO_2$ between the ocean and the atmosphere

**Participants:** Hussein Yahia [correspondant], Véronique Garçon (laboratoire d'Etudes En Géophysique Et Océanographie Spatiales (legos)), Joël Sudre (laboratoire d'Etudes En Géophysique Et Océanographie Spatiales (legos)), Christoph Garbe (university Of Heidelberg), Christophe Maes (laboratoire d'Etudes En Géophysique Et Océanographie Spatiales (legos)), André Butz (karlsruhe Institute Of Technology (kit)), Boris Dewitte (laboratoire d'Etudes En Géophysique Et Océanographie Spatiales (legos)), Isabelle Dadou (université Paul Sabatier).

Multiresolution analysis computed on singularity exponents estimated from physical variables is used to produce submesoscale (pixel size: 4 kms) of partial pressures  $pCO_2$  maps between the ocean and the atmosphere. Low resolution  $pCO_2$  information coming from models and data is propagated across the scale of the specific multiresolution analysis to infer super resolution  $pCO_2$  maps. Validation with model outputs and boat campaigns.

Supporting grant: OceanFlux project.

Publications: [30], [38].

## 6.9. Turbulent ocean dynamics at super resolution: validation

**Participants:** Hussein Yahia [correspondant], Véronique Garçon, Joël Sudre.

Synoptic determination of ocean circulation using data acquired from space, with a coherent depiction of its turbulent characteristics, from large scale ocean circulation down to super resolution of remote sensing optical sensors, remains a fundamental challenge in Oceanography. This determination has the potential of revealing all aspects of the ocean's dynamic variability on a wide range of spatio-temporal scales and will enhance our understanding of ocean-atmosphere exchanges at super resolution, as required in the present context of climate change. We show a 4-year time series of spatial super resolution (4 kms) turbulent ocean dynamics generated from satellite data using emerging nonlinear physics, low resolution dynamics and super resolution oceanic sea surface temperature data. The method at its core consists in propagating across the scales the low resolution dynamics in a multi resolution analysis computed on adimensional critical transition information. The resulting vector field is validated with Lagrangian buoy data at super resolution obtained from NASA Global Drifter Program.

A movie showing the evolution of turbulent ocean dynamics around South Africa in the Agulhas current has been made with the help and support of Inria DIRCOM project (C. Blonz, P.-O. Gaumin).

Supporting grant: ICARODE project.

Publications: [30], [38].

## 6.10. Upwelling

**Participants:** Ayoub Tamim [correspondant], Khalid Daoudi, Hussein Yahia, Joël Sudre.

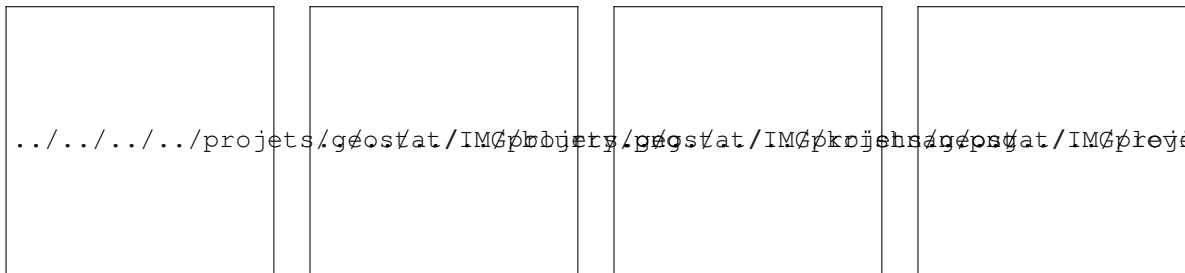
Based on fuzzy clustering, we developed a new algorithm for the segmentation of upwelling regions in the southern atlantic Moroccan coast using Sea Surface temperature images. This method has the advantage of being more efficient and more accurate than a state-of-the-art method. It is followed by a work under way of determining oriented contours using the MMF.

Publication: [31].

## 6.11. Combining Local and Non-Local Priors For Image Deconvolution

**Participants:** Hicham Badri [correspondant], Hussein Yahia.

Non-blind deconvolution consists in recovering a sharp latent image from a blurred image with a known kernel. Deconvolved images usually contain unpleasant artifacts due to the ill-posedness of the problem even when the kernel is known. Making use of natural sparse priors has shown to reduce ringing artifacts but handling noise remains limited. On the other hand, non-local priors have shown to give the best results in image denoising. We propose in this project to combine both local and non-local priors in one framework. By studying the distribution of the singularity exponents as well as the distribution of the eigenvalues of similar patches, we show that the blur increases the self-similarity within an image and thus makes the non-local prior a good choice for denoising blurred images. The blurred image is denoised using only the self-similarities within the image, without any prior specific to the blur, via low rank estimation. However, denoising introduces outliers which are not Gaussian and should be well modeled. Experiments show that our method produces a much better image reconstruction both visually and empirically compared to some popular methods. See figure 7 . Work in progress.



(a) Blurred and Noisy,  $\sigma = 2\%$  (b) Krishnan (NIPS 2009) (c) Levin (SIGGRAPH 2007) (d) Proposed

Figure 7. Various deconvolution results. The proposed method produces a much better reconstruction ; note the background noise in the methods (b) and (c). The PSNR is higher with our method 29.56 dB compared to the methods (b) 27.22 dB and (c) 28.11 dB.

## 6.12. Fast Multi-Scale Detail Decomposition via Accelerated Iterative Shrinkage

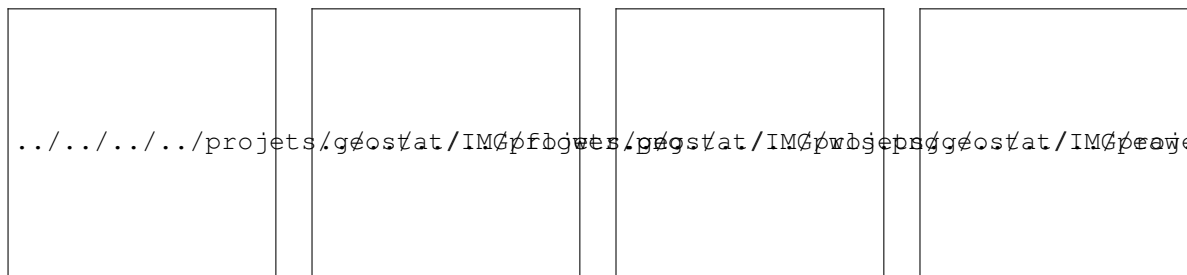
**Participants:** Hicham Badri [correspondant], Hussein Yahia, Driss Aboutajdine.

Edge-aware smoothing is one of the most important operations in computer graphics and vision. It is the building-block for a wide range of applications including : smoothing, detail manipulation, HDR tone-mapping, to cite a few. However, good quality edge-aware smoothing operators are relatively slow. We present a fast solution for performing high-quality edge-aware smoothing, particularly efficient for edge manipulation applications. Our strategy to perform smoothing consists in using a half-quadratic solver with a non-convex sparsity-inducing norm, accelerated using a first order approximation. First, we show how to solve optimization problems with complex non-convex norms using a first order proximal estimation. This step is of



paramount importance not just for smoothing, but for many applications requiring the use non-convex norms. Secondly, we design two norms inspired by natural image statistics. We incorporate these norms with a first order proximal estimation to design the main smoothing operator. Finally, we propose a warm-start solution to accelerate the solver. Experiments show that our method produces high quality results, sometimes better than some state-of-the-art methods, with reduced processing time. We demonstrate the performance of the proposed approach on various applications such as smoothing, multi-scale detail manipulation of low and high dynamic range images as well as high definition video manipulation. See figure 8 .

Work presented at SIGGRAPH Asia 2013 (technical brief), Hong Kong [24].



(a)

(b)

(c)

(d)

Figure 8.

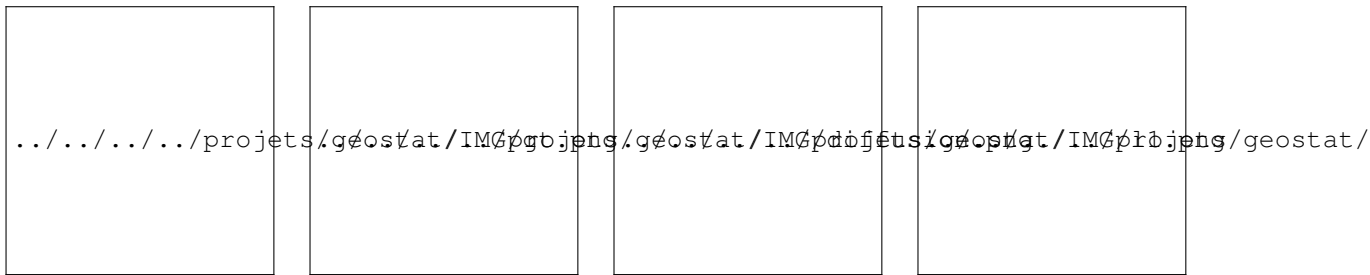
*Detail manipulation example. The proposed method produces a high-quality result with reduced processing time. From left to right:(a) Input, (b) WLS, (c) EAW, (d) Proposed method.*

### 6.13. Robust Surface Reconstruction via Triple Sparsity

**Participants:** Hicham Badri [correspondant], Hussein Yahia, Driss Aboutajdine.

Reconstructing a surface/image from corrupted gradient fields is a crucial step in many imaging applications where a gradient field is subject to both noise and unlocalized outliers, resulting typically in a non-integrable field. The methods presented so far can only handle a small amount of outliers and noise due to the limited performance of their models. We present in this project a powerfull method for robust surface reconstruction. The proposed formulation is based on a triple sparsity prior : a sparse prior on the residual gradient field and a double sparse prior on the surface itself. A double prior corrects the outliers in the field, while the third sparsity prior smooths the surface to reduce the noise. We develop an efficient alternate minimization strategy to solve the proposed optimization problem. The method is able to recover a good quality surface from severely corrupted gradients thanks to its ability to handle both noise and outliers. We demonstrate the performance of the proposed method on synthetic and real data. Experiments show that the proposed solution outperforms some existing methods in the three possible cases : noise only, outliers only and mixed noise/outliers. See figure 9 .

Work submitted to CVPR 2014.



(a) Ground-truth

(b) Diffusion (ECCV 2006)

(c)  $l_1$ -norm (CVPR09)

(d) Proposed

*Figure 9. Photometric stereo reconstruction from noisy images. The proposed method produces a much better reconstruction compared to two state-of-the-art methods.*

## MC2 Project-Team

# 6. New Results

## 6.1. Cancer modelling

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

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

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

- Cell Migration modelling:

The collaboration with IECB (University of Bordeaux) has continued with the postdoctoral 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. Poinard has been invited at Osaka in february by Prof. Suzuki. A model describing the destruction of the extracellular matrix by the MMP enzyme, and then the cell migration has been obtained. R. Mahumet, a PhD student of Prof. Suzuki is developing a code to simulate the model.

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

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

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

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

## 6.2. Newtonian fluid flows simulations and their analysis

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

Recent developments on multiphase flows have been performed. We are able to simulate water/air interactions with interface regularization. The interface with a boat is also taken into account. See <http://www.math.u-bordeaux1.fr/~mbergman> for simulations.

We are also able to compute the strong (implicit) fluid structure interactions between the fluid and an elastic medium. For instance we have simulated a fish with an elastic tail and highlighted the fact that a given flexibility of tail allows to increase significantly the swimming efficiency.

- Turbulence flow on an hemisphere : Participants: Charles-Henri Bruneau, Patrick Fischer (MCF Bordeaux 1), Yong Liang Xiang (PostDoc)

ANR Cyclobulle lead by Hamid Kellay Soap hemi-bubble film experiments have shown some links between the formation of vortices when the hemi-bubble is heated at the equator and the formation of tornados in the earth atmosphere. Two-dimensional simulations using a stereographic map are used to compare to these experimental results and confirm the results when Coriolis force and heat source terms are added.

- Compressible flows: Immersed boundary methods. We are concerned with immersed boundary methods, i.e., integration schemes where the grid does not fit the geometry, and among this class of methods, more specifically with cartesian grid methods, where the forcing accounting for the presence of boundaries is performed at the discrete level. We have developed a simple globally second order scheme inspired by ghost cell approaches to solve compressible flows, inviscid as well as viscous. In the fluid domain, away from the boundary, we use a classical finite-volume method based on an approximate Riemann solver for the convective fluxes and a centered scheme for the diffusive term. At the cells located on the boundary, we solve an ad hoc Riemann problem taking into account the relevant boundary condition for the convective fluxes by an appropriate definition of the contact discontinuity speed. This method can easily be implemented in existing codes and is suitable for massive parallelization. It has been validated in two dimensions for Euler and Navier-Stokes equations, and in three dimensions for Euler equations. The order of convergence is two in  $L^2$  norm for all variables, and between one and two in  $L^\infty$  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 unknowns 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 conditions 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 characteristics which satisfy a vectorial transport equation. We derive the associated fluid-structure models for incompressible and compressible media. The equations are discretized on a cartesian mesh with finite differences and finite volumes schemes. The applications concern the bio-locomotions and the study of air-elastic interaction.
- Vortex methods : The aim of this work is to couple vortex methods with the penalization methods in order to take advantage from both of them. This immersed boundary approach maintains the efficiency of vortex methods for high Reynolds numbers focusing the computational task on the rotational zones and avoids their lack on the no-slip boundary conditions replacing the vortex sheet method by the penalization of obstacles. This method that is very appropriate for bluff-body flows is validated for the flow around a circular cylinder on a wide range of Reynolds numbers. Its validation is now extended to moving obstacles (axial turbine blades) and three-dimensional bluff-bodies (flow around a sphere). See [72]. Moreover, using the global properties of the penalization method, this technique permits to include porous media simultaneously in the flow computation. We aim to adapt the porous media flows to our new method and to apply it in order to implement passive control techniques using porous layers around bluff-bodies.
- Domain decomposition : Domain decomposition methods are a way to parallelize the computation of numerical solutions to PDE. To be efficient, domain decompositions methods should converge independently on the number of subdomains. The classical convergence result for the additive Schwarz preconditioner with coarse grid is based on a stable decomposition. The result holds for discrete versions of the Schwarz preconditioner, and states that the preconditioned operator has a uniformly bounded condition number that depends only on the number of colors of the domain decomposition, and the ratio between the average diameter of the subdomains and the overlap width. Constants are usually non explicit and are only asserted to depend on the "shape regularity" of the domain decomposition.

two years ago, we showed the result holds the additive Schwarz preconditioner can also be defined at the continuous level and provided completely explicit 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 explicitly and are independent of the ratio between the diameter of the largest subdomain and the diameter of the smallest subdomain.

This year, we have studied explored new coarse spaces algorithms for domain decomposition methods. Coarse spaces are necessary to get a scalable algorithm whose convergence speed does not deteriorate when the number of subdomains increases. For domains decomposition methods with discontinuous iterates, we showed that continuous coarse spaces can never be an optimal choice. As an alternative, we introduced both the use of discontinuous coarse spaces(DCS) and a new coarse space algorithm using these discontinuous coarse spaces.

### 6.3. Flow control and shape optimization

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

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

## REALOPT Project-Team

# 6. New Results

## 6.1. Extending the column generation paradigm

Building on our technical review [89] of methods for solving the Lagrangian Dual (with an analysis of the scope for hybridization) we have worked on methodologies that can be understood as an extension of the column generation approach in [22]. Working in an extended variable space allows one to develop tighter reformulations for mixed integer programs. To handle the size of the extended formulation, one can work with inner approximations defined and improved by generating dynamically variables and constraints. This so-called "column-and-row generation" procedure is revisited here in a unifying presentation that generalizes the column generation algorithm and extends to the case of working with an approximate extended formulation. A key benefit of this approach is that lifting pricing problem solutions in the space of the extended formulation permits their recombination into new subproblem solutions and results in faster convergence. The interest of the approach is evaluated numerically on machine scheduling, bin packing, generalized assignment, and multi-echelon lot-sizing problems. We compare a direct handling of the extended formulation, a standard column generation approach, and the "column-and-row generation" procedure. Within the Samba project we further showed that this stabilization offered by the recombination of solutions is complementary and adds up to stabilization techniques based on smoothing that were developed within Samba. These techniques have been applied in [26], [29].

## 6.2. Interior point cutting plane strategy revisited for column generation

In [89], we identify what are the stabilization features that are built into variants of subgradient algorithms and polyhedral approaches. In [27], we further compare their theoretical performance and discuss their combination. Stabilization procedures for column generation can be viewed as cutting plane strategies in the dual. Exploiting the link between in-out separation strategies and dual price smoothing techniques for column generation, we derive a generic bound convergence property for algorithms using a smoothing feature. Such property adds to existing in-out asymptotic convergence results. In our study on In-Out Separation and Column Generation Stabilization by Dual Price Smoothing, we note that our convergence property adds to existing in-out asymptotic convergence results. Beyond theoretical convergence, we describe in [88] a proposal for effective finite convergence in practice and we develop a smoothing auto-regulating strategy that makes the need for parameter tuning obsolete. Practical speed-up convergence that are observed go from 20% to 500%. These contributions turn stabilization by smoothing into a general purpose practical scheme that can be used into a generic column generation procedure. We conclude the paper by showing that the approach can be combined with an ascent method, leading to improved performances. Such combination might inspire novel cut separation strategies.

## 6.3. A MILP approach to minimize the number of late jobs with and without machine availability constraints

The study in [13] investigates scheduling problems that occur when the weighted number of late jobs that are subject to deterministic machine availability constraints have to be minimized. These problems can be modeled as a more general job selection problem. Cases with resumable, non-resumable, and semi-resumable jobs as well as cases without availability constraints are investigated. The proposed efficient mixed integer linear programming approach includes possible improvements to the model, notably specialized lifted knapsack cover cuts. The method proves to be competitive compared with existing dedicated methods: numerical experiments on randomly generated instances show that all 350-job instances of the test bed are closed for the well-known problem  $1|r_i|\sum w_i U_i$ . For all investigated problem types, 98.4% of 500-job instances can be solved to optimality within one hour.



## 6.4. Multidimensional dual-feasible functions

Dual-feasible functions have been used in the past to compute lower bounds and valid inequalities for different combinatorial optimization and integer programming problems. Until now, all the dual-feasible functions proposed in the literature were 1-dimensional functions. In [11] we extended the principles of dual-feasible functions to the  $m$ -dimensional case by introducing the concept of vector packing dual-feasible function. We explored the theoretical properties of these functions in depth, and we proposed general schemes for generating some instances of these functions. Additionally, we proposed and analyzed different new families of vector packing dual-feasible functions. All the proposed approaches were tested extensively using benchmark instances of the 2-dimensional vector packing problem. Our computational results showed that these functions can approximate very efficiently the best lower bounds for this problem.

## 6.5. New branch-and-price methods for variants of bin packing problems

We proposed branch-and-price methods for two variants of the well-known bin-packing problem.

The bin packing problem with conflicts consists in packing items in a minimum number of bins of limited capacity while avoiding joint assignments of items that are in conflict. The study in [21] demonstrates that a generic implementation of a Branch-and-Price algorithm using specific pricing oracle yields comparatively good performance for this problem. We use our black-box Branch-and-Price solver BaPCod, relying on its generic branching scheme and primal heuristics. We developed a dynamic programming algorithm for pricing when the conflict graph is an interval graph, and a depth-first-search branch-and-bound approach for pricing when the conflict graph has no special structure. The exact method was tested on instances from the literature where the conflict graph is an interval graph, as well as harder instances that we generated with an arbitrarily conflict graph and larger number of items per bin. Our computational experiment report sets new benchmark results for this problem, closing all open instances of the literature in one hour of CPU time.

In the bin-packing with fragile objects, we are given a set of objects, each characterized by a weight and a fragility, and a large number of uncapacitated bins. Our aim is to find the minimum number of bins needed to pack all objects, in such a way that in each bin the sum of the object weights is less than or equal to the smallest fragility of an object in the bin. The problem is known in the literature as the Bin Packing Problem with Fragile Objects, and appears in the telecommunication field, when one has to assign cellular calls to available channels by ensuring that the total noise in a channel does not exceed the noise acceptance limit of a call. In [10], we propose a branch-and-bound and several branch-and-price algorithms for the exact solution of the problem, and improve their performance by the use of lower bounds and tailored optimization techniques. In addition we also develop algorithms for the optimal solution of the related knapsack problem with fragile objects. We conduct an extensive computational evaluation on the benchmark set of instances, and show that the proposed algorithms perform very well.

## 6.6. Freight railcar routing

In some countries, the activities of managing railroads and managing a fleet of freight railcars are separated by a law. A state-owned company is in charge of the first activity. The control of freight railcars is separated between several independent companies. The main objective of such company is an effective management of its railcars. As these companies are commercial, the goal is to maximize the profit from the usage of their railcars. The profit of a company is mainly determined by the difference between the total gain it receives from satisfying requests for delivery of goods in railcars and the costs it pays to the state-owned company for exploiting the railroad network.

Consequently, the main optimization problem that every freight railcar management company faces can be formulated as follows. We need 1) to choose a set of transportation demands between stations in a railroad network, and 2) to fulfill these demands by appropriately routing the set of available railcars, while maximizing the total profit. We formulate this problem as a multi-commodity flow problem in a large space-time graph. Three approaches are proposed to solve the Linear Programming relaxation of this formulation: direct solution by an LP solver, a column generation approach based on the path reformulation, and a “column generation for

extended formulations” approach [22]. In the latter, the multi-commodity flow formulation is solved iteratively by dynamic generation of arc flow variables. Three approaches have been tested on a set of real-life instances provided by one of the largest freight rail transportation companies in Russia. Instances with up to 10 millions of arc flow variables were solved within minutes of computational time [29], [39].

## 6.7. Reliable Service Allocation in Clouds with Memory and Capacity Constraints

In [25] we consider allocation problems that arise in the context of service allocation in Clouds. More specifically, on the one part we assume that each Physical Machine (denoted as PM) is offering resources (memory, CPU, disk, network). On the other part, we assume that each application in the IaaS Cloud comes as a set of services running as Virtual Machines (VMs) on top of the set of PMs. In turn, each service requires a given quantity of each resource on each machine where it runs (memory footprint, CPU, disk, network). Moreover, there exists a Service Level Agreement (SLA) between the Cloud provider and the client that can be expressed as follows: the client requires a minimal number of service instances which must be alive at the end of the day, with a given reliability (that can be converted into penalties paid by the provider). In this context, the goal for the Cloud provider is to find an allocation of VMs onto PMs so as to satisfy, at minimal cost, both capacity and reliability constraints for each service. In this paper, we propose a simple model for reliability constraints and we prove that it is possible to derive efficient heuristics.

## 6.8. On the Theta number of powers of cycle graphs

In [17] we give a closed formula for Lovász’s theta number of the powers of cycle graphs  $C_k^d$  and of their complements, the circular complete graphs  $K_{k/d}$ . As a consequence, we establish that the circular chromatic number of a circular perfect graph is computable in polynomial time. We also derive an asymptotic estimate for the theta number of  $C_k^d$ .

## 6.9. Strong chromatic index of planar graphs with large girth

Let  $\Delta$  be an integer. In [18], we prove that every planar graph with maximum degree  $\Delta$  and girth at least  $10\Delta + 46$  is strong  $(2\Delta - 1)$ -edge-colorable, that is best possible (in terms of number of colors) as soon as  $G$  contains two adjacent vertices of degree  $\Delta$ . This improves the best previous result when  $\Delta \geq 6$ .

## 6.10. Computing clique and chromatic number of circular-perfect graphs in polynomial time

A main result of combinatorial optimization is that clique and chromatic number of a perfect graph are computable in polynomial time (Grötschel et al. in *Combinatorica* 1(2):169–197,1981). Perfect graphs have the key property that clique and chromatic number coincide for all induced subgraphs; in [19] we address the question whether the algorithmic results for perfect graphs can be extended to graph classes where the chromatic number of all members is bounded by the clique number plus one. We consider a well-studied superclass of perfect graphs satisfying this property, the circular-perfect graphs, and show that for such graphs both clique and chromatic number are computable in polynomial time as well. In addition, we discuss the polynomial time computability of further graph parameters for certain subclasses of circular-perfect graphs. All the results strongly rely upon Lovász’s Theta function.

## 6.11. Computing the clique number of a-perfect graphs in polynomial time

A main result of combinatorial optimization is that clique and chromatic number of a perfect graph are computable in polynomial time (Grötschel, Lovasz and Schrijver 1981). This result relies on polyhedral characterizations of perfect graphs involving the stable set polytope of the graph, a linear relaxation defined by clique constraints, and a semi-definite relaxation, the Theta-body of the graph. A natural question is whether the algorithmic results for perfect graphs can be extended to graph classes with similar polyhedral properties.

In [20] we consider a superclass of perfect graphs, the  $\alpha$ -perfect graphs, whose stable set polytope is given by constraints associated with generalized cliques. We show that for such graphs the clique number can be computed in polynomial time as well. The result strongly relies upon Fulkerson's antiblocking theory for polyhedra and Lovasz's Theta function.

## CARMEN Team

## 6. New Results

### 6.1. Mathematical models

- *Mathematical derivation of a bilayer surface model of the atria using asymptotic analysis methods [28], [16]*

We derived rigorously, by using asymptotic analysis tools, a bilayer model of atrial electrophysiology. Starting with a 3D model of atrial tissue that includes two layers with distinct electrophysiological characteristics and with an aspect ratio of  $\epsilon$ , we obtained an asymptotic equivalent model when  $\epsilon \rightarrow 0$  made up of two surface models coupled by a coupling term. The bilayer model describes the evolution of the mean in the thickness of the 3D potential in each layer. This approach is an improvement of the classical surface model of cardiac electrophysiology, because it guarantees a higher convergence speed, and allows to take into account transmural heterogeneities. We numerically implemented the 3D and bilayer models and compared it to the classical surface model. We observed a second order accuracy of the bilayer model and drastically reduced computational times respectively to the 3D model.

- *Formal derivation of a macroscopic model of propagation that includes the non linear behavior of gap junctions [16]*

A macroscopic model of electrical propagation that take into account the non linear conductivity of the gap junction is obtained by a formal homogenization method. We derived a one dimensional macroscopic model which diffusive tensor varies in time. We compared this macroscopic model with a cell-to-cell propagation. This is an very important improvement of existing models that only consider a linear cell-to-cell coupling. The introduction of this non linear phenomenon in homogenized models gives a simulation tool to investigate the impact of the microscopic nonlinear mechanisms on the macroscopic propagation.

- *Influence of periodic diffusive inclusions on the bidomain model [29]*

We present a new mathematical model of the electric activity of the heart. In the standard bidomain model we can distinguish the intra- and the extracellular space with different conductivities for excitable cells and the fibrotic tissue around them. The main drawback is that it assumes the existence of excitable cells everywhere in the heart, while it is known that there exist non small regions where fibroblasts take place. The fibroblasts are equally distributed and since they are non excitable cells, they can be considered as a diffusive part. Hence we extend the standard bidomain model as follows: we assume that we have periodic alternation of the healthy tissue (linear bidomain model) and fibrotic extracellular space (diffusive part). We use homogenisation techniques to derive our macroscopic partial differential equations. Interestingly, we obtain again a bidomain type model with modified conductivities that involve the volume fraction of the diffusive domain. Preliminary numerical experiments will conclude on the influence of these diffusive inclusions.

### 6.2. Construction of numerical models

- *Implementation of an accurate bilayer model of human atria, including realistic geometry and qualitative fibre direction [19], [21], [16]*

We introduce a bilayer model of the human atria. We set a specific mathematical model based on two surface monodomain problems coupled by a coupling term. We recalled convergence results of the bilayer model towards a 3D model for thin tissues, we formalized an optimization method to set the coupling coefficient and we present two different asymptotically equivalent numerical implementation of the model. We then present a geometrically and electrophysiologically accurate

model of the atrial heterogeneities, including two layers of fibre directions and ionic function heterogeneities based on histological and modelling works. We assess the physiological relevance of the model during a sinus wave and we check the occurrence of three-dimensional electrical behaviour such as slight electrical dissociation. This bilayer model is able to take into account transmural heterogeneities only accessible since then with full 3D models, while keeping the low computational load associated with surface models. It is then a light and relevant tool for long-lasting simulations designed to investigate atrial arrhythmia.

- *Personalization method of the bilayer model to registrate the geometry to a patient dependant geometry [16]*

If the generic atrial bilayer model developed in [21] allows to conduct general experiments, greater customization of the model is necessary to carry out more specific studies on a given patient. We present a methodology to obtain a patient-dependant model containing the geometry of the patient, a generic fibrous organization and an image of the patient's fibrosis obtained by late-enhancement MRI. This is a common work with the clinical team of the CHU du Haut-Lévêque (H. Cochet and P. Jaïs) and the Asclepios Inria team.

The methodology is based on a registration method developed by Durrleman et al. [34] that allows to register surfaces : the generic model is registrated towards a patient-specific geometry (work by M. Sermseant and R. Cabrera-Lozoya, Asclepios Team). The fibre organisation is transported by the same linear local transformations. The late-enhancement is projected on the model to take into account the complex patient-specific fibrotic repartition. A similar methodology was presented by McDowell et al. [37]. However, the authors took as a starting point a three-dimensional geometry and a different methodology to registrate the geometry. The work presented here is therefore innovative.

- *Faster solvers for cardiac electro-physiology problems [27]*

There are many applications in cardiac electro-physiology where computational time is the main requirement to fulfill, even by sacrificing accuracy. Some techniques were investigated in this direction, in order to obtain a break-even point between accuracy and speed. The complete problem involves solving some ODEs on each mesh node and inverting large sparse matrices, often ill-conditioned.

We first designed a method based on the Proper Orthogonal Decomposition (POD) technique: we project the linear system onto a well-chosen orthogonal basis of smaller dimension while still solving the ODES. We tried the method on both the bidomain and monodomain equations, and extended the tests on an HPC machine, in order to observe scalability performances. There is no improvement for the monodomain equations because its linear systems are well-conditioned. For the bidomain equations, the CPU time decreases by a factor of 10 between the full and reduced models, and better scalability performances.

We secondly developed an eikonal model, in view of serious games applications for the Medic Activ project. The Dijkstra algorithm is used to solve the eikonal equation and the transmembrane potential is determined by the solution of a Mitchell-Schaeffer model on each mesh node. Some modifications were introduced to take into account re-excitability and allox re-entrant waves. Compared by the algorithm proposed by [38], the transmembrane potential comes from the solution of an underlying model, not through an approximation. This represent an innovation, to our knowledge not present in literature.

### 6.3. Medical applications of numerical models

- *Influence of Transmural Slow-Conduction Zones on the Long-Time Behaviour Of Atrial Arrhythmia. A Numerical Study with a Human Bilayer Atrial Model. [20], [31], [16]*

Atrial fibrosis is known to be a factor in the perpetuation of atrial arrhythmia. Despite the thinness of atrial tissue, the fibrosis distribution may not be homogeneous through the entire thickness of the atria. The aim of this study is twofold. 1) We want to elucidate the respective influences of a

transmural and a non-transmural distribution of fibrosis, described as a slow conduction zone, on the perpetuation of a rotor-like arrhythmic episode, compared to a control situation. 2) We aim to assess which is the more efficient ablation protocol between a) a lesion-box ablation, b) an ablation line connecting the fibrotic zone to the closest anatomical obstacle, c) ablation spots.

We used a bilayer monodomain representation of the atria that included transmural heterogeneities of fibre organisation, and an arrhythmic scenario composed of a rotor initiated near the pulmonary veins. This model allowed long simulations for a sustainable computational load. We observed that when the fibrosis was transmural, the centre of the rotor was anchored in the slow conduction zone and was stable during a 10 seconds simulation, whereas the other simulations showed meandering rotors that disappeared after a few seconds. In our model framework, only a transmural fibrosis distribution had a stabilizing effect on reentrant circuits. Furthermore, the lesion-box ablation and the line ablation were able to stop the arrhythmia, unlike the spot lesions. The bilayer model proved to be a good trade-off between accuracy and speed for observing the influence of transmural heterogeneities on atrial arrhythmia over long periods.

- *Effects of L-type Calcium channel and hERG blockers on the electrical activity of the human heart: A simulation study.*

Class III and IV drugs affect cardiac hERG (IKr) and L-type calcium (ICaL) channels, resulting in complex alterations in repolarization with both anti and pro-arrhythmic consequences. Interpretation of their effects on cellular and ECG-based biomarkers for risk stratification is challenging. As pharmaceutical compounds often exhibit multiple ion channel effects, our goal is to investigate the simultaneous effect of ICaL and IKr block on human ventricular electrophysiology from ionic to ECG level. ECG simulations show that ICaL block results in shortening of the QT interval, ST elevation and reduced T wave amplitude, caused by reduction in APD and AP amplitude during the plateau phase, and in repolarization times. In contrast, IKr block results in QT prolongation and reduced T wave amplitude. Combined ICaL and IKr block are combined, the degree of ICaL block strongly determines QT interval whereas the effect of IKr block is more pronounced on the T wave amplitude.

## 6.4. Inverse problems

- *A Steklov-Poincaré approach to solve the inverse problem in electrocardiography [23]*

In the cardiac electrophysiology imaging community the most widely used approach to solve the inverse problem is the least square formulation with different Tikhonov regularizations. Clinicians are not yet fully satisfied by the technology that solves the inverse problem. Reformulating the inverse problem could bring new techniques to solve it. In this paper we use the Steklov-Poincaré formulation of the Cauchy problem in order to solve the inverse problem in electrocardiography imaging. We present in this work the technique and an algorithm of gradient descent. We also show numerical results based on simulated synthetic data.

- *A machine learning regularization of the inverse problem in electrocardiography imaging [22]*

Radio-frequency ablation is one of the most efficient treatments of atrial fibrillation. The idea behind it is to stop the propagation of ectopic beats coming from the pulmonary vein and the abnormal conduction pathways. Medical doctors need to use invasive catheters to localize the position of the triggers and they have to decide where to ablate during the intervention. ElectroCardioGraphy Imaging (ECGI) provides the opportunity to reconstruct the electrical potential and activation maps on the heart surface and analyze data prior to the intervention. The mathematical problem behind the reconstruction of heart potential is known to be ill posed. In this study we propose to regularize the inverse problem with a statistically reconstructed heart potential, and we test the method on synthetically data produced using an ECG simulator.

- *Inverse problem in electrocardiography via factorization method of boundary value problems : How to reconstruct epicardial potential maps from measurements on the torso ? [26]*

We are working on a new approach for solving the inverse problem of electrocardiography. This approach is based on an invariant embedding method: the factorization method of boundary values problems [35]. The idea is to embed the initial problem into a family of similar problems on subdomains bounded by a moving boundary from the torso skin to the epicardium surface. For the direct problem this method provides an equivalent formulation with two Cauchy problems evolving on this moving boundary and which have to be solved successively in opposite directions. This method calculates Neumann-Dirichlet and Dirichlet-Neumann operators on this moving boundary that satisfy Riccati equations. Regarding the inverse problem, mathematical analysis allows to write an optimal estimation of the epicardial potential based on a quadratic criterion. Then, the ill-posed behaviour of the inverse problem can be analyzed and a better regularization and discretization of the problem can be proposed. One of the advantages of this method is the computation of the potential at different times during cardiac cycle: it is not necessary to repeat the resolution of all the equations at every time. In a first time the simpler case of a cylinder is considered. In a second time the method is applied to the 3D model of concentric spheres. The next step will be to use 3D deformed surfaces.

- *Reconstruction of 3D depolarization wavefronts from surface optical mapping images [33]*

Starting from the diffusion-absorption equation of light in a tissue we solved the forward problem for excitation light using the FreeFem++ software ([www.freefem.org/ff++](http://www.freefem.org/ff++)). We first considered a spherical wave front expanding in time: the tissue is depolarized inside the sphere. This choice allowed us to locate the position of the excitation. Using this representation of the wavefront, we obtained in silico data. We defined a functional to minimize and implemented the BFGS method to solve the inverse problem. We tested our method on in silico data and obtained good results. We next compared our results with an approach developed by Khait [36] and found that our method is more accurate and that we have less restrictions for the convergence of the method. We modified the wave front into ellipsoid in order to start working on experimental data.

## MAGIQUE-3D Project-Team

## 6. New Results

### 6.1. Inverse Problems

#### 6.1.1. Reconstruction of an elastic scatterer immersed in a homogeneous fluid

**Participants:** H el ene Barucq, Rabia Djellouli,  Elodie Est ecahandy.

The determination of the shape of an obstacle from its effects on known acoustic or electromagnetic waves is an important problem in many technologies such as sonar, radar, geophysical exploration, medical imaging and nondestructive testing. This inverse obstacle problem (IOP) is difficult to solve, especially from a numerical viewpoint, because it is ill-posed and nonlinear. Its investigation requires as a prerequisite the fundamental understanding of the theory for the associated direct scattering problem, and the mastery of the corresponding numerical solution methods.

In this work, we are interested in retrieving the shape of an elastic obstacle from the knowledge of some scattered far-field patterns, and assuming certain characteristics of the surface of the obstacle. The corresponding direct elasto-acoustic scattering problem consists in the scattering of time-harmonic acoustic waves by an elastic obstacle  $\Omega^s$  embedded in a homogeneous medium  $\Omega^f$ , that can be formulated as follows:

$$\begin{aligned}
 \Delta p + (\omega^2/c_f^2)p &= 0 && \text{in } \Omega^f \\
 \nabla \cdot \sigma(u) + \omega^2 \rho_s u &= 0 && \text{in } \Omega^s \\
 \omega^2 \rho_f u \cdot n &= \partial p / \partial n + \partial e^{i(\omega/c_f)x \cdot d} / \partial n && \text{on } \Gamma \\
 \sigma(u)n &= -pn - e^{i(\omega/c_f)x \cdot d} n && \text{on } \Gamma \\
 \lim_{r \rightarrow +\infty} r (\partial p / \partial r - i(\omega/c_f)p) &= 0 && 
 \end{aligned} \tag{1}$$

where  $p$  is the fluid pressure in  $\Omega^f$  whereas  $u$  is the displacement field in  $\Omega^s$ , and  $\sigma(u)$  represents the stress tensor of the elastic material.

This boundary value problem has been investigated mathematically and results pertaining to the existence, uniqueness and regularity can be found in [92] and the references therein, among others. We have obtained a new result proving the well-posedness of the problem when the fluid-solid interface is only lipschitzian. This has been published in the Journal of Mathematical Analysis and Applications [20]. We then propose a solution methodology based on a regularized Newton-type method for solving the IOP. The proposed method is an extension of the regularized Newton algorithm developed for solving the case where only the Helmholtz equation is involved, that is the acoustic case by impenetrable scatterers [86]. The direct elasto-acoustic scattering problem defines an operator  $F : \Gamma \rightarrow p_\infty$  which maps the boundary  $\Gamma$  of the scatterer  $\Omega^s$  onto the far-field pattern  $p_\infty$ . Hence, given one or several measured far-field patterns  $\tilde{p}_\infty(\hat{x})$ , corresponding to one or several given directions  $d$  and wavenumbers  $k$ , one can formulate IOP as follows:

$$\text{Find a shape } \Gamma \text{ such that } F(\Gamma)(\hat{x}) = \tilde{p}_\infty(\hat{x}); \quad \hat{x} \in S^1.$$

At each Newton iteration, we solve the forward problem using a finite element solver based on discontinuous Galerkin approximations, and equipped with high-order absorbing boundary conditions. We have first characterized the Fr chet derivatives of the scattered field and the characterization has been published in the Journal of Inverse and Ill-posed problems [18]. It is worth noting that they are solutions to the same boundary value problem as the direct problem with other transmission conditions. This work has been the object of several talks [63], [50], [36]. Elodie Est ecahandy has defended her PhD thesis [14] in September 2013 and two papers will be submitted soon.



### 6.1.2. *hp-adaptive inversion of magnetotelluric measurements*

**Participants:** H el ene Barucq, Julien Alvarez Aramberri, David Pardo.

The magnetotelluric (MT) method is a passive electromagnetic exploration technique. It makes use of natural electric fields which propagate permanently into the Earth. Electric fields induce magnetic waves which can be detected at the surface to produce a map of the subsurface from the determination of the resistivity distribution. Magnetotelluric method is based on the mathematical relation between the magnetic and telluric variations which involve the electric resistivity of the subsurface. It is particularly relevant for the detection of metallic ores and for the study of geothermal sites. It is also used for oil and gas exploration because it provides information on sedimentary basins. It performs well on depth scales varying between a few tens of meters to hundred of kilometers, following the pioneering works of Tikhonov and Cagniard. Magnetotelluric measurements are governed by polarized Maxwell's equations in such a way that Helmholtz equations have to be solved. The geological mapping is constructed from the solution of an Inverse problem which requires computing the Impedance and/or the Resistivity distributions. In this work, we assimilate Earth with a horizontally layered model with possible 2D heterogeneities. Both the size of the direct problem and the required computational times may be excessively large. Indeed, on the one hand, the model of the source requires defining a horizontally sufficiently large thick plate to avoid undesirable effects that could take place around the edges. On the other hand, the inversion of MT measurements typically requires the computation of an accurate solution at the receivers located at different positions. Since traditional hp-goal oriented techniques [98], [97] provide an accurate solution in one single point, we use a multi-goal-oriented algorithm [99] to obtain accurate solutions at all receivers. To get accurate quantities at several positions, it is necessary to increase the size of the mesh. This induces high computational costs in particular because the solution of the inverse problem is based on reiterated solutions of the direct problem. To decrease the computational costs required to perform the inversion, we propose an adaptive multi-dimensional inversion algorithm, which consists in increasing step by step the dimension in which the direct problem and the inversion are solved. At first step, we compute the 1D primary field with a semi-analytical solution and we invert the 1D problem. After that, we introduce the 2D heterogeneities. Regarding the direct problem, we compute the secondary field, thereby, drastically reducing the size of the computational domain for this problem. Then, we perform the inversion using the solution to the 1D Inverse Problem as a regularization term, increasing the robustness of the inversion algorithm.

#### 6.1.2.1. *Reverse Time Migration with Elastic Wave Equations*

**Participants:** H el ene Barucq, Henri Calandra, Julien Diaz, J er ome Luquel.

Even if RTM has enjoyed the tremendous progresses of scientific computing, its performances can still be improved, in particular when applied to strong heterogeneous media. In this case, images have been mainly obtained by using direct arrivals of acoustic waves and the transition to elastic waves including multiples is not obvious, essentially because elastic waves equations are still more computationally consuming. We have thus chosen to consider high-order Discontinuous Galerkin Methods which are known to be well-adapted to provide accurate solutions based upon parallel computing. Now, one of the main drawback of RTM is the need of storing a huge quantity of information which is prohibitive when using elastic waves. For that purpose, we apply the Griewank algorithm [88] following Symes' ideas [101] for the acoustic RTM. The idea is to find a compromise between the number of wave equations to solve and the number of numerical waves that we have to store. This is the so-called Optimal Checkpointing. By reducing the occupancy of the memory, RTM should be efficient even when using elastic waves. The next step is the derivation of accurate imaging conditions, which could take advantage of all the information contained in the elastic wavefield. For acoustic media, Claerbout [83] proposed an imaging condition which is widely used and turns out to be sufficient to accurately reproduce interfaces. But Claerbout conditions do not take wave conversions into account and, since P-wave and S-wave interact with each other, it might be relevant to use an imaging condition including these interactions. This has been done successfully by J. Tromp and C. Morency [102] for seismology applications based upon the inversion of the global Earth. Their approach is based upon the adjoint state and it involves sensitivity kernels which are defined from the propagated and the back-propagated fields. Now, it has been shown in [93] that full wave form inversions using these sensitivity kernels may be polluted by numerical

artifacts. One solution is to use a linear combination of the sensitivity kernels to delete artifacts. In this work, we propose then a new imaging condition which construction is inspired from [93] with some approximations required to keep admissible computational costs. We illustrate the properties of the new imaging condition on industrial benchmarks like the Marmousi model. In particular, we compare the new imaging condition with other imaging conditions by using as criteria the quality of the image and the computational costs required by the RTM. The results will be presented at the 2014 ECCOMAS conference in Barcelona.

## 6.2. Modeling

### 6.2.1. Implementation of a non-reflecting boundary condition on ellipsoidal boundary

**Participants:** H el ene Barucq, Anne-Ga elle Saint-Guirons, S ebastien Tordeux.

The modeling of wave propagation problems using finite element methods usually requires the truncation of the computational domain around the scatterer of interest. Absorbing boundary conditions are classically considered in order to avoid spurious reflections. This year we have proposed and tested a formulation which allows to take into account with no extra-cost a quasi-exact radiation condition based on a non local Dirichlet to Neumann operator.

### 6.2.2. Modeling of small heterogeneities in the context of the time domain wave equation

**Participants:** Vanessa Mattesi, S ebastien Tordeux.

We have proposed an approximate model to take into account small heterogeneities for the three dimensional time dependent wave equation. One of the most important result of this work is the generalization of the multipole theory (classically written for the Helmholtz equation) to the wave equation. This work has been presented at Waves 2013 and at JSA 2013 [58], [39]

### 6.2.3. A new modified equation approach for solving the wave equation

**Participants:** H el ene Barucq, Henri Calandra, Julien Diaz, Florent Ventimiglia.

In order to obtain high-order time-schemes, we are considering an alternative approach to the ADER schemes and to the modified equation technique described in section 3.2 . The two first steps of the construction of the schemes are similar to the previous schemes : we apply a Taylor expansion in time to the solution of the wave equation and we replace the high-order derivatives with respect to the time by high order space operators, using the wave equation. The difference is that we do not use auxiliary variables and we choose to discretize directly the high-order operators in space. These operators can not be discretized by classical finite elements. For the discretization of the biharmonic operator in an homogeneous acoustic medium, both C1 finite elements, such as the Hermite ones, and Discontinuous Galerkin Finite Elements (DGFE) can be used, while in a discontinuous medium, or for higher-order operators, DGFE should be preferred [80]. We have applied this method to the second order wave equation [15] and the numerical results showed that this technique induced less computational burden than the modified equation scheme or the ADER scheme.

In the framework of the PhD thesis of Florent Ventimiglia, we have extended the new method involving  $p$ -harmonic operator to the first order formulation of the acoustic wave equation, which is the formulation discretized in the DIVA platform of TOTAL. In this case, the high order operators in space are not powers of the Laplace operator but powers of the gradient. Hence, we also had to adapt the space discretization, and we have extended the DG formulation with centered fluxes proposed in [87] to higher order operators. A numerical analysis of performance in 2D indicates that, for a given accuracy, this method requires less computational costs and less storage than the High-Order ADER Scheme. These results have been presented to the SMAI conference [49], Waves 2013 [61], Numerico IV [61] and HF2013 [34]. A paper has been accepted in ESAIM Proceedings [49].

### 6.2.4. Constructing and using Absorbing Boundary Conditions

#### 6.2.4.1. Higher Order On-Surface Radiation Conditions for elastic scatterers

**Participants:** H el ene Barucq, Chokri Bekkey, Juliette Chabassier, Julien Diaz.

The numerical simulation of wave propagation is generally performed by truncating the propagation medium and the team works on new Absorbing Boundary Conditions (ABCs), trying to improve the performance of existing conditions. As we explained at Section 3.2, item **Boundary conditions**, we are developing ABCs for curved boundaries, based on the full factorization of the wave equation. These ABCs should take propagating, grazing and evanescent waves into account. In [17], we have considered the issue of constructing high-order ABCs taking into account both propagating and evanescent waves for the Helmholtz equation. In case of the simulation of acoustic waves diffracted by a solid immersed in a fluid, we investigate the performance of the new ABCs when used as On-Surface Radiation Conditions. The ABCs are set directly on the boundary of the solid. The unbounded problem is then replaced by a problem involving an acoustic pressure computed on the surface of the solid only. Preliminary results have been obtained by considering the toy problem where the scatterer is a disk. Analytic solutions are then available and we show that taking into account evanescent waves in the ABC could improve the accuracy of classical ABCs by two orders of magnitude at mid-frequency range, for  $ka$  between 1 and 100,  $k$  being the frequency and  $a$  the typical size of the diffracting obstacle. These results have been presented to the Waves 2013 conference [47].

#### 6.2.4.2. Radiation boundary condition at high frequency

**Participants:** Hélène Barucq, Elodie Estécahandy, Juliette Chabassier, Julien Diaz.

Regarding the solution of the Helmholtz equation at high frequency with finite element methods, it is current to refine the mesh in order to limit the effect of numerical pollution. It is then interesting to dispose of radiation boundary conditions which do not require to set the artificial boundary far from the scatterer. In this work, we have investigated the possibility of bringing closer the artificial boundary when standard conditions are enhanced by the modeling of grazing waves. The preliminary results we obtained show that this new ABC outperforms classical ABCs at high-frequency, for  $ka > 50$ , and that it is highly accurate, even when the boundary is very close to the scatterer. These results have been presented to the Waves 2013 conference [45]. Now, the next step is to consider an ABC taking the three types of waves into account.

#### 6.2.4.3. Absorbing Boundary Conditions for Tilted Transverse Isotropic Elastic Media

**Participants:** Hélène Barucq, Lionel Boillot, Henri Calandra, Julien Diaz.

The simulation of wave propagation in geophysical media is often performed in domains which are huge compared to the wavelengths of the problem. It is then necessary to reduce the computational domain to a box. When considering acoustic or elastic isotropic media, this can be done by applying an Absorbing Boundary Condition (ABC) or by adding a Perfectly Matched Layer (PML). However, a realistic representation of the Earth subsurface must include anisotropy and, in particular, the so-called Tilted Transverse Isotropy. Perfectly Matched Layers are known to be unstable for this kind of media and, to the best of our knowledge, no ABC have been proposed yet. We have thus proposed a low-order ABC for TTI media. The construction is based on comparing and then connecting the slowness curves for isotropic and elliptic TTI waves. Numerical experiments illustrate the performance of the new ABC. They are performed by integrating the ABC in a DG formulation of Elastodynamics. When applied in a TTI medium, the new ABC performs well with the same level of accuracy than the standard isotropic ABC set in an isotropic medium. The condition demonstrates also a good robustness when applied for large times of simulation. These results have been presented to the Smai and to the Waves conferences [67], [68] and a paper has been submitted.

#### 6.2.5. Modeling of the damping factor of Multiperforated plates

**Participants:** Estelle Piot, Vincent Popie, Sébastien Tordeux.

Multiperforated plates are classically used as a damping material. Melling has proposed in [94] a model to estimate the energy dissipated by these devices. However its well-known result should be corrected by a factor two to fit with experimental data. We have proposed a correct way to compute the energy dissipated by the multiperforated plates. This work has been presented at the Fifth International Scientific Conference and Young Scientists School "Theory and Computational Methods for Inverse and Ill-posed Problems.

#### 6.2.6. Performance Assessment of IPDG for the solution of an elasto-acoustic scattering problem

**Participants:** Hélène Barucq, Rabia Djellouli, Élodie Estécahandy.

We present a solution methodology for the direct elasto-acoustic scattering problem that falls in the category of Discontinuous Galerkin methods. The method distinguishes itself from the existing methods by combining high-order Discontinuous Galerkin approximations, local stabilizations for the coupled problem and the use of curved element edges on the boundaries. We present some numerical results that illustrate the salient features and highlight the performance of the proposed solution methodology on the resonance phenomenon existing in the elastic scatterer for simple geometries such as circles. Moreover, the designed method ensures a convergence order with a gain of two order of magnitude compared to polygonal boundaries, and a potential to address both mid- and high-frequency regimes. These results have been accepted for publication in International Journal for Numerical Methods in Engineering [19].

### 6.2.7. On the influence of curvature on transmission conditions

**Participants:** H el ene Barucq, Martin Gander, Yingxiang Xu.

Domain decomposition methods are both highly successful parallel solvers and also important modeling tools, since problems in subdomains can be treated by adapted methods to the physics in each subdomain. Subdomain boundaries are therefore rarely straight lines. The focus of this paper is to study the influence of curvature on transmission conditions used in optimized Schwarz methods. For straight interfaces and simple geometries, optimized interface conditions are typically determined using Fourier analysis. Asymptotically, these optimized conditions are still valid for curved interfaces. Since however the curvature is the most important information for a smooth curve, we want to study in this paper if and how the interface curvature influences the constants in the optimized parameters.

We consider the model problem

$$(\Delta - \eta)u = f, \quad \text{on } \Omega = \mathbb{R}^2, \quad \eta > 0, \quad (2)$$

and we require the solution to decay at infinity. We decompose  $\Omega$  into two overlapping subdomains  $\Omega_1 = (-\infty, a(y)) \times \mathbb{R}$  and  $\Omega_2 = (b(y), \infty) \times \mathbb{R}$ , where  $\Gamma_1$  given by  $a(y)$  and  $\Gamma_2$  given by  $b(y)$  are smooth curves satisfying  $a(y) \geq b(y)$ . A general parallel Schwarz algorithm is then given by

$$\begin{aligned} (\Delta - \eta)u_i^n &= f && \text{in } \Omega_i, \\ \mathcal{B}_i(u_i^n) &= \mathcal{B}_i(u_j^{n-1}) && \text{on } \Gamma_i, \quad 1 \leq i \neq j \leq 2, \end{aligned} \quad (3)$$

where  $\mathcal{B}_i, i = 1, 2$ , are transmission conditions to be chosen. If  $\mathcal{B}_i, i = 1, 2$  are chosen as  $\partial_{n_i} + DtN_i$ , with  $DtN_i$  the Dirichlet to Neumann operators, the iterates will converge in two steps. These operators are however non-local, and thus difficult to use in practice. Therefore, local approximations are used in optimized Schwarz methods. We presented two different approaches to take the curvature of interfaces into account in the transmission conditions of optimized Schwarz methods: micro-local analysis, and analysis using a circular model problem. In both cases, we obtained curvature dependent transmission conditions. A preliminary comparison shows that the transmission conditions based on optimization perform better on the model problem, and that it could be important to take the curvature into account in transmission conditions. In our opinion it is however essential to do a more thorough theoretical and numerical study on more general geometry, where micro-local analysis is still applicable, before we can definitely draw conclusions. This work has been published in the peer-reviewed proceedings of the conference Decomposition Methods in Science and Engineering XXI [51].

### 6.2.8. Operator Based Upscaling for Discontinuous Galerkin Methods

**Participants:** H el ene Barucq, Th eophile Chaumont, Christian Gout.

Realistic numerical simulations of seismic wave propagation are difficult to handle because they must be performed in strongly heterogeneous media. Two different scales must then be taken into account. Indeed, the medium heterogeneities are currently very small compared to the characteristic dimensions of the propagation medium. To get accurate numerical solutions, engineers are then forced to use meshes that match the finest scale representing the heterogeneities. Meshing the whole domain with a fine grid leads then to huge linear systems and the computational cost of the numerical method is then too high to consider 3D realistic simulations. To dispose of a numerical method allowing to represent the heterogeneity of the medium accurately while computing on a coarse grid is thus relevant. This is the challenge of multiscale approaches like homogenization or upscaling. The ultimate objective of this work is to develop a software package for the Helmholtz equation set in heterogeneous domains. We focus on the operator-based upscaling method. Operator-based upscaling methods were first developed for elliptic flow problems (see [81]) and then extended to hyperbolic problems (see [90], [104], [103]). Operator-based upscaling method consists in splitting the solution into a coarse and a fine part. The coarse part is defined on a coarse mesh while the fine part is computed on a fine mesh. In order to speed up calculations, artificial boundary conditions (ABC) are imposed. By enforcing suitable ABCs on the boundary of every cells of the coarse mesh, calculations on the fine grid can be carried out locally. The coarse part is next computed globally on the coarse mesh. Operator-based upscaling methods were so far developed in joint with standard finite element discretization strategy. In this work, we investigate the idea of combining an operator based upscaling method with discontinuous Galerkin finite element methods (DGFEM). During this year, we have performed the mathematical analysis of the Helmholtz equation set in a domain represented by a discontinuous velocity. The analysis has been achieved both for the continuous and the discretized problem which is based on a quadrature scheme which allows to take the discontinuities of the velocity into account. We get new stability results for stratified-like domains and numerical experiments show that in case of industrial benchmarks, the quadrature scheme leads to lower computational costs with a very good level of accuracy. A paper is in preparation and the results will be presented at the 2014 ECCOMAS conference in Barcelona.

### **6.2.9. Efficient solution methodology based on a local wave tracking strategy for high-frequency Helmholtz problems.**

**Participants:** Mohamed Amara, Sharang Chaudhry, Julien Diaz, Rabia Djellouli, Steven Fiedler.

We have proposed a procedure for selecting basis function orientation to improve the efficiency of solution methodologies that employ local plane-wave approximations. The proposed adaptive approach consists of a local wave tracking strategy. Each plane-wave basis set, within considered elements of the mesh partition, is individually or collectively rotated to best align one function of the set with the local propagation direction of the field. Systematic determination of the direction of the field inside the computational domain is formulated as a minimization problem. As the resultant system is nonlinear with respect to the directions of propagation, the Newton method is employed with exact characterization of the Jacobian and Hessian. To illustrate the salient features and evaluate the performance of the proposed wave tracking approach, we present error estimates as well as numerical results obtained by incorporating the procedure into a prototypical plane-wave based approach, the least-squares method (LSM) developed by Monk and Wang [95]. The numerical results obtained for the case of a two-dimensional rigid scattering problem indicate that (a) convergence was achievable to a prescribed level of accuracy, even upon initial application of the tracking wave strategy outside the pre-asymptotic convergence region, and (b) the proposed approach reduced the size of the resulting system by up to two orders of magnitude, depending on the frequency range, with respect to the size of the standard LSM system. These results have been presented to the Waves 2013 [43] and in a Research Report [71]. A paper has been submitted.

### **6.2.10. Mesh Free Frontier-based Formulation (MF3) for High Frequency Helmholtz Problems.**

**Participants:** Mohamed Amara, Julien Diaz, Rabia Djellouli.

We have proposed a novel approach for solving efficiently Helmholtz problems. The proposed solution method employs a boundary-type formulation without however involving Green functions and/or incurring singular integrals. In addition, this approach does not necessitate the use of a mesh. For these reasons, the method is named Mesh Free Frontier-based Formulation (MF3). Furthermore, the sought-after field is locally approximated using a set of basis of functions that consists of a Bessel kind function computed at a prescribed finite set of points. The number of the functions determines mainly the size of the resulting system, the complexity, as well as the computational cost of the proposed method. Preliminary numerical results obtained in the case of 2D-Helmholtz problems in the high-frequency regime are presented to illustrate the computational efficiency of MF3 (the method delivers results with high accuracy level, about  $10^{-8}$  on the  $L^2$  relative error, while requiring the solution of small linear systems). In addition, these results tend to suggest that MF3 is pollution free. These results has been presented to two conferences [32], [44]. A paper is in preparation.

### **6.2.11. Energy based simulation of a Timoshenko beam in non-forced rotation. Application to the flexible piano hammer shank.**

**Participants:** Juliette Chabassier, Marc Duruflé.

A nonlinear model for a vibrating Timoshenko beam in non-forced unknown rotation is derived from the virtual work principle applied to a system of beam with mass at the end. The system represents a piano hammer shank coupled to a hammer head. An energy-based numerical scheme is then provided, obtained by non classical approaches. A major difficulty for time discretization comes from the nonlinear behavior of the kinetic energy of the system. Numerical illustrations are obtained by coupling this new numerical scheme to a global energy-preserving numerical solution for the whole piano. These numerical results show that the pianistic touch clearly influences the spectrum of the piano sound of equally loud isolated notes. These differences do not come from a possible shock excitation on the structure, nor from a changing impact point, nor a “longitudinal rubbing motion” on the string, since neither of these features are modeled in our study.

This work has been submitted for publication in Journal of Sound and Vibration [79]. discretization

### **6.2.12. Simulating the propagation of ultra short laser pulses in a dispersive non linear medium.**

**Participants:** Juliette Chabassier, Marc Duruflé, Nayla Herran.

This collaboration with CEA-CESTA aimed at evaluating the limits of validity of the MIRÓ software provided by CEA. The MIRÓ software implements the propagation of laser pulses with a non-linear Schrodinger-like equation obtained from Maxwell’s equations in non-linear dispersive medium, assuming that the pulse spectrum is narrow and the non-linearity small enough. When considering intense ultra-short pulses, the spectrum bandwidth and the amplitude of the pulse may violate the constitutive assumptions of the model used by MIRÓ. This collaboration began with the internship of Nayla Herran (march 2013- august 2013). During this internship, different alternative models have been explored, and some of them were able to provide a solution much more accurate than MIRÓ’s models. The comparisons between alternative models and MIRÓ’s model have been performed in 1-D on small cases, for which the reference solution could be obtained from a direct numerical simulation of non-linear Maxwell’s equations. An efficient and accurate solver for non-linear Maxwell’s equations has been implemented in Montjoie software. This solver uses high order finite element in space, and high order Runge-Kutta-Nystrom scheme in time. The space grid moves with respect to the group velocity such that the computational domain stays relatively small and centered around the pulse. Thanks to this solver, we have been able to validate the different models and compare them. These 1-D promising results encourage us to continue this collaboration in order to obtain efficient and accurate numerical methods in 3-D. Our desire is also to be able to perform realistic cases involving physically relevant phenomena.

### **6.2.13. Asymptotic Modeling for Elasto-Acoustics**

**Participants:** Julien Diaz, Victor Péron.

In the papers [31], [74], we derive equivalent conditions and asymptotic models for the diffraction problem of elastic and acoustic waves in a solid medium surrounded by a thin layer of fluid medium. Due to the thinness of the layer with respect to the wavelength, this problem is well suited for the notion of equivalent conditions and the effect of the fluid medium on the solid is as a first approximation local. We derive and validate equivalent conditions up to the fourth order for the elastic displacement. These conditions approximate the acoustic waves which propagate in the fluid region. This approach leads to solve only elastic equations. The construction of equivalent conditions is based on a multiscale expansion in power series of the thickness of the layer for the solution of the transmission problem.

Questions regarding the implementation of the conditions have been addressed carefully and the boundary conditions have been integrated without changing the structure of the code `Hou10ni`.

This work has been presented in two international conferences and Workshops : Workshop HPC-GA and WAVES'2013 [55].

A paper with numerical results for the elasto-acoustic problem with several configurations (a thin layer of variable thickness; coupling with an exterior "acoustic" medium) is in preparation.

#### 6.2.14. *Thin layer models for electromagnetics*

**Participants:** Marc Duruflé, Victor Péron, Clair Poignard.

We have considered the transmission of electromagnetic waves through a thin layer. This thin layer can be replaced by transmission conditions. Media with thin inclusions appear in many domains: geophysical applications, microwave imaging, biomedical applications, cell phone radiations, radar applications, non-destructive testing. Our application concerns also media for which the conductivity drops inside the layer, such that the low-frequency regime has a different behavior from the mid-frequency regime. Different models are compared for these two regimes, drawbacks and disadvantages of each model are detailed. This work has been accepted for publication [27].

#### 6.2.15. *Corner Asymptotics of the Magnetic Potential in the Eddy-Current Model*

**Participants:** Monique Dauge, Patrick Dular, Laurent Krähenbühl, Victor Péron, Ronan Perrussel, Clair Poignard.

The following results rely on a problematic developed in section 3.2 , item **Asymptotic modeling**.

In the paper [25], we describe the magnetic potential in the vicinity of a corner of a conducting body embedded in a dielectric medium in a bidimensional setting. We make explicit the corner asymptotic expansion for this potential as the distance to the corner goes to zero. This expansion involves singular functions and singular coefficients. We introduce a method for the calculation of the singular functions near the corner and we provide two methods to compute the singular coefficients: the method of moments and the method of quasi-dual singular functions. Estimates for the convergence of both approximate methods are proven. We eventually illustrate the theoretical results with finite element computations. The specific non-standard feature of this problem lies in the structure of its singular functions: They have the form of series whose first terms are harmonic polynomials and further terms are genuine non-smooth functions generated by the piecewise constant zeroth order term of the operator. This work has been presented in the international conference JSA 2013 [38].

#### 6.2.16. *Finite Element Subproblem Method*

**Participants:** Patrick Dular, Christophe Geuzaine, Laurent Krähenbühl, Victor Péron, Ronan Perrussel.

In the paper [26], we develop a finite element subproblem method to correct the inaccuracies proper to perfect conductor and impedance boundary condition models, in particular near edges and corners of conductors, for a large range of conductivities and frequencies. Successive local corrections, supported by fine local meshes, can be obtained from each model to a more accurate one, allowing efficient extensions of their domains of validity. This work has been presented in the international conference Compumag 2013 [57].

We develop also a finite element subproblem method for progressive eddy current modeling. The modeling of eddy currents in conductors is split into a sequence of progressive finite element subproblems. The source fields generated by the inductors alone are calculated at first via either the Biot-Savart law or finite elements. The associated reaction fields for each added conductive region, and in return for the source regions themselves when massive, are then calculated with finite element models, possibly with initial perfect conductor and/or impedance boundary conditions to be further corrected. The resulting subproblem method allows efficient solving of parameterized analyses thanks to a proper mesh for each subproblem and the reuse of previous solutions to be locally corrected. This work has been presented in the international conference ISEF'2013 [56].

## 6.3. High Performance methods for solving wave equations

### 6.3.1. Coupling the DG code with task programming libraries

**Participants:** Emmanuel Agullo, Lionel Boillot, Georges Bosilca, Henri Calandra.

Last year we optimized the DG code implemented in the DIVA platform of Total by reducing the number of communications between each processors. This optimization, coupled with the use of Hybrid MPI and OpenMP parallel programming has allowed to prove the scalability of the code up to 512 cores. We are now planning to extend these tests up to 4000 cores. However, preliminary results emphasized the limitations due to low level issues such as threads placement, data communications and cache utilization. Therefore, we are now considering the implementation in DIVA of task programming libraries such as StarPU (<http://runtime.bordeaux.inria.fr/StarPU/>) or DAGuE (<http://icl.cs.utk.edu/dague/index.html>). These libraries handle the low level issues directly at the runtime level and allow the programmer to focus on the algorithm itself. They are also provide a valuable help to improve the portability of the code from one architecture to another, which will allow us to port DIVA on heterogeneous architectures such as CPU/GPU and Intel Xeon Phi. We have already coupled DIVA and DAGuE on the Symmetric Multiprocessor System (SMP) of Plafirim (<https://plafirim.bordeaux.inria.fr>) and compared the performance of the code with MPI and an OpenMP implementations [66], [64].



## MAGNOME Project-Team

# 6. New Results

## 6.1. Adopting new computing paradigms

**Participants:** David James Sherman [correspondant], Pascal Durrens, Natalia Golenetskaya, Florian Lajus, Xavier Calcas.

Analyses in comparative genomics are characteristically forms of datamining in high-dimension sets of relations between genes and gene products. For every linear increase in genomic data, these relations can grow at worst geometrically.

Natalia Golenetskaya's thesis [12] developed an integrated architecture that we call *Tsvetok*, which combines a novel NoSQL storage schema, domain-specific Map-Reduce algorithms, and existing resources to efficiently handle the fundamentally data-parallel analyses encountered in comparative genomics [48], [42], [51]. Tsvetok components are deployed in MAGNOME's private cloud and have been extensively tested using data and use cases derived from log analyses of the Génolevures web resource. We designed Map-Reduce solutions for the principal whole-genome analyses used by MAGNOME for comparative genomics, in particular new distributed algorithms for systematic identification of gene fusion and fission events in eukaryote genomes, and large-scale consensus clustering for protein families. These examples illustrate two strategies that can be used to scale algorithms in a Map-Reduce setting [12].

1. Converting classical graph-based algorithms with message propagation: instead of traversing a graph, which would incur high latency, information is sent forward in waves, and synchronized later. Some of the intermediate computations may be redundant, but overall running time is minimized.
2. Iterative sampling strategies, which run the standard algorithm on carefully chosen subsets, and later compute a consensus of the intermediate results. The iterations may take some time to converge, but the individual instances can be run within one machine.

Florian Lajus extended the Magus software platform to use the NoSQL storage components in Tsvetok, and has validated it on a large collection of fungal genomes. Xavier Calcas is currently integrating the Galaxy platform <sup>8</sup> with Magus.

## 6.2. Improving inference of metabolic models

**Participants:** David James Sherman [correspondant], Pascal Durrens, Razanne Issa, Anna Zhukova.

The Pantograph approach uses an annotated “scaffold” (reference) model and a collection of complementary predictions of homology between scaffold genes and target genes. The basis of the method is a weighing of the homology evidence to decide whether a reaction that is present in the scaffold ought to be present in the target.

We have improved on the method in two ways. First, we model the implicit knowledge represented in the boolean formula of each gene association, to derive hypotheses about the explicit role of individual genes; for example, a gene association  $(S_1 \wedge S_2) \vee (S_1 \wedge S_3)$  may implicitly represent an enzyme complex formed from two subunits, the first encoded by gene  $S_1$ , and the second encoded by two paralogous genes  $S_2$  and  $S_3$  (figure 2). By using these hypotheses to rewrite gene associations, we improve the decision of whether a reaction is present in the target or not.

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<sup>8</sup><http://usegalaxy.org>



*Figure 1. General architecture of Tsvetok, showing the role of NoSQL (Apache Cassandra) and Map-Reduce (Apache Hadoop) paradigms*

Second, we have adopted an abductive strategy for inferring reactions. In this strategy we consider that it is the reactions that explain the genes observed in the target genome. In the corresponding abductive logic program, the observations are the genes in the target, the integrity constraints are the rules that rewrite gene associations, and the hypotheses to be abduced are the reactions in the model. The scaffold model is compiled into a set of facts and predicates that express the reactions, their gene associations, and the integrity constraint rules; the abducibles generate assertions that specific reactions are in the target model. Combined with the facts of the genes observed in the target, this program generates, through abduction, the set of target reactions that explain the greatest number of genes.

The advantage of this approach is that it can invent, through specialization, reactions that are not present *per se* in the scaffold model.



Figure 2. An explicit model that is one possible explanation of the gene association  $(S_1 \wedge S_2) \vee (S_1 \wedge S_3)$

### 6.3. Knowledge-based generalization of metabolic models

**Participants:** David James Sherman [correspondant], Pascal Durrens, Razanne Issa, Anna Zhukova.

There is an inherent tension between detail and understandability in large metabolic networks: detailed description of individual reactions is needed for simulation, but high-level views of reactions are needed for describing pathways in human terms. We defined knowledge-based methods that factor similar reactions into “generic” reactions in order to visualize a whole pathway or compartment, while maintaining the underlying model so that the user can later “drill down” to the specific reactions if need be [22], [23], [26] This method is available as a Python library from <http://metamogen.gforge.inria.fr/>.

Figures 3 and 4 illustrate model generation for *Yarrowia lipolytica* fatty acid oxidation in the peroxisome. Molecular species are represented as circular nodes, and the reactions as square ones, connected by edges to their reactants and products. Ubiquitous species (e.g. *oxygen*, *water*, *ATP*) are of smaller size and colored gray. Non-ubiquitous species are divided into fifteen equivalence classes and colored accordingly (red/blue for trivial species/reaction equivalence classes, different colors for non-trivial equivalence classes). The size of the model does not allow for readability of the species labels, thus we do not show them (figure 3).

The generalization algorithm identifies equivalent molecular species using an ontology, and groups together reactions that operate on the same abstract species. It finds the greatest generalization that preserves stoichiometry. The generalized model represents quotient species and reactions. For example, the violet *unsaturated FA-CoA* node is a quotient of *hexadec-2-enoyl-CoA*, *oleoyl-CoA*, *tetradecenoyl-CoA*, *trans-dec-2-enoyl-CoA*, *trans-dodec-2-enoyl-CoA*, *trans-hexacos-2-enoyl-CoA*, *trans-octadec-2-enoyl-CoA*, and *trans-tetradec-2-enoyl-CoA* (colored violet in figure 3). In a similar manner, the light-green *acCoA oxidase* quotient reaction, that converts *fatty acyl-CoA* (yellow) into *unsaturated FA-CoA* (violet), generalizes six corresponding light-green reactions of the initial model (figure 3).

The generalized model describes  $\beta$ -oxidation in a more generic way: as a transformation of *fatty acyl-CoA* (yellow) into *unsaturated FA-CoA* (violet), then into *hydroxy FA-CoA* (dark green), *3-oxo FA-CoA* (magenta), and back to *fatty acyl-CoA* (with a shorter carbon chain); while the specific model describes the same process in more details, specifying those reactions for each of the *fatty acyl-CoA* species presented in the organisms' cell (e.g. *decanoyl-CoA*, *dodecanoyl-CoA*, etc.). That is why the *beta-oxidation* chain of the reactions in the initial model, transforming step-by-step the *fatty-acyl-CoA* with the longest carbon chain into the one with the shortest chain, in the generalized model appears as a cycle (generalizing all the *fatty-acyl-CoAs* into one species, regardless the chain-length).

The specific model is appropriate for simulation, because it contains all of the precise reactions. The generalized model is suited for a human, because it reveals the main properties of the model and masks distracting details. For example, the generalized model highlights the fact that there is a particularity concerning *C24:0-CoA* (*stearoyl-CoA*) (red, inside the cycle): there exists a "shortcut" reaction (blue, inside the cycle), producing it directly from another *fatty acyl-CoA* (yellow), avoiding the usual four-reaction beta-oxidation chain, used for other *fatty acyl-CoAs*. This shortcut is not obvious in the specific model, because it is hidden among a plethora of similar-looking reactions.

## 6.4. Characterization of STAND protein families

**Participants:** David James Sherman, Pascal Durrens, Witold Dyrka [correspondant].

In collaboration with Sven Saupe and Mathieu Paoletti from IBGC Bordeaux (ANR Mykimun), we worked on characterization of the STAND protein family in the fungal phylum. We established an *in silico* screen based on state-of-the-art bioinformatic tools, which – starting from experimentally studied sequences from *Podospora anserina* – allowed us to determine the first systematic picture of fungal STAND protein repertoire (ms. in preparation). Most notably, we found evidence of extensive modularity of domain associations, and signs of concerted evolution within the recognition domain. Both results support the hypothesis that fungal STAND proteins, originally described in the context of vegetative incompatibility, are involved in a general fungal immune system. In addition, we investigated improved protein domain representations and elaborated a grammatical modelling method [15], which will be used to elucidate mechanisms of formation and operation of the STAND proteins.

## 6.5. Avoiding stiffness in BioRica

**Participants:** David James Sherman [correspondant], Joaquin Fernandez.

We previously formalized two strategies for integrating discrete control with continuous models, coefficient switches that control the parameters of the continuous model, and strong switches that choose different models [29], [27]. While these strategies have proved useful for modeling hybrid systems in biotechnology [31] and medicine [28], the resulting system model can be inefficient when the different subsystems evolve at very different time scales. In order to improve the efficiency of the resulting simulations, we investigated the use of Kofman's Quantized State Systems (QSS), and demonstrated that the QSS approach can be adapted to BioRica [13]. On the strength of this demonstration, we invited Joaquin Fernandez from Kofman's lab to Magnome. Joaquin had previously implemented an efficient library for QSS simulation, and during his stay succeeded in adapting it to our hybrid modeling framework. In his approach, SBML models with events are compiled into a hybrid model, using a variant of Modelica for surface syntax and using the QSS library for efficient simulation.



*Figure 3. Yarrowia lypolitica fatty acid oxidation model before generalization. Reactions of the specific model are divided into fifteen equivalence classes, represented by different colours*



*Figure 4. Generalization of the Yarrowia lipolytica fatty acid oxidation model, described as a transformation of fatty acyl-CoA (yellow) into unsaturated FA-CoA (violet), then into hydroxy FA-CoA (dark green), 3-oxo FA-CoA (magenta), and back to fatty acyl-CoA (with a shorter carbon chain)*

## 6.6. Applications in biotechnology and health

**Participants:** David James Sherman, Pascal Durrens [correspondant], Florian Lajus, Xavier Calcas.

Using MAGNOME's Magus system and YAGA software, we have successfully realized a full annotation and analysis of several groups of related genomes:

- Seven new genomes, provided to the Génolevures Consortium by the CEA–Génoscope (Évry), including two distant genomes from the *Saccharomycetales* were annotated using previously published Génolevures genomes.
- Twelve wine starter yeasts linked to fermentation efficiency.
- Five pathogenic (to human) and non pathogenic Nakaseomycetes.
- Two oleaginous strains with applications in biofuels.

**Winemaking yeasts.** In collaboration with partners in the ISVV, Bordeaux, we have assembled and analyzed 12 wine starter yeasts, with the goal of understanding genetic determinants of performance in wine fermentation. Analysis included identification of strain-specific gains and losses of genes linked both to niche specificity and to performance in industrial applications (article in prep.). A further combined analysis with 50 natural and industrial strains showed a pattern of introgression concentrated in industrial strains (article in prep.).

**Oleaginous yeasts.** In collaboration with Prof Jean-Marc Nicaud's lab at the INRA Grignon, we developed the first functional genome-scale metabolic model of *Yarrowia lipolytica*, an oleaginous yeast studied experimentally for its role as a food contaminant and its use in bioremediation and cell factory applications.

Using MAGNOME's Pantograph method (see section 5.2 ) we produced an accurate functional model for *Y. lipolytica*, MODEL1111190000 in BioModels <sup>9</sup>, that has been qualitatively validated against gene knockouts. This model has been enriched by Anna Zhukova with ontology terms from ChEBI and GO.

**Pathogenic yeasts.** A further group of five species, comprised of pathogenic and nonpathogenic species, was analyzed with the goal of identifying virulence determinants [39]. By choosing species that are highly related but which differ in the particular traits that are targeted, in this case pathogenicity, we are able to focus on the few hundred genes related to the trait [16]. The approximately 40,000 new genes from these studies were classified into existing Génolevures families as well as branch-specific families.

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<sup>9</sup><http://biomodels.net/>

## MNEMOSYNE Team

# 6. New Results

## 6.1. Overview

Though our view is systemic, our daily research activities are concerned with the design, at a given scale of description, of models of neuronal structures, each concerned with a specific learning paradigm. Of course, a major challenge is to keep in mind the systemic view, to put a specific emphasis on the way each neuronal structure communicates with the rest of the system and to highlight how the learning paradigm interplays with other memory systems.

Among the numerous loops involving the brain, the body and the environment, a basic grid of description corresponds to distinguish “Perception Loops”, the goal of which is to extract from the inner and outer world sensory invariants helpful to identify and evaluate the current state and to make predictions from previous learning, and “Action Loops”, the goal of which is to rely on this sensory, emotional and motivational information to decide, plan and trigger actions for the benefit of the body.

Presently, our team is engaged on the following topics: Concerning perception loops, we are firstly considering the role of the hippocampus and of the posterior cortex in learning high level sensory cues that contribute to pavlovian conditioning in the amygdala. Secondly, we are investigating the role of the thalamus in attentional shifts in the cortex. This latter topic relies on recent advances we made in the Keops ANR project (*cf.* § 7.1 ) on a model of the retina that we also sum up here. Concerning Action loops, we are preparing a critical analysis of the current views of the interactions between the prefrontal cortex and the basal ganglia. Finally, we also report here more methodological achievements.

## 6.2. Pavlovian conditioning

The fundamental role of the amygdala in pavlovian conditioning is widely acknowledged, both on the motor, autonomic and hormonal expression of pavlovian responses and on the learning of the associations between conditional and unconditioned stimuli. This year, we have proposed models showing in a systemic view how errors of prediction in the amygdala might trigger, by cholinergic hormonal expression, episodic learning in the hippocampus [17] and semantic learning and attentional shift in the posterior cortex [8]. On this basis, we are currently studying how emotional values of sensory information are dynamically encoded in the basolateral nucleus of the amygdala [11], to fit with the multiple requirements for this kind of information in the brain.

## 6.3. The thalamus is more than a relay

Many recent results in neuroscience indicate that the role of the thalamus in the brain is certainly more important than it used to be considered, particularly concerning its relation with the cortex. Interestingly, we considered this question as a side effect of our work in the Keops project (*cf.* § 7.1 ) with our chilean neuroscientist colleagues studying non standard ganglion cells in the retina. Our modeling [6] and bibliographic studies led us to propose a biologically-founded algorithm [13] for the interplay between the modulatory and driving connections between the thalamus and the cortex, in the case of the projection of these ganglion cells on the thalamus [14]. This study has been carried out with the strong constraint of proposing a system working on a real visual flow. In the near future, we aim at developing this original view of the thalamus in the more general case of its pulvinar associative nucleus, learning to route to the cortex multimodal information flows.



## **6.4. Eyes are really smarter than believed**

While it is known that the retina has not only standard ganglion cells devoted to contrast (parvo) or motion (magno) cues, but is able to perform sophisticated detection of spatial or temporal events in the visual scene (konio) [40], it was still to understand how such computation could be implemented as a robust effective processing of realistic natural image sequence and not only as a toy model of cartoonish stimuli. It has been shown in our group [19] that biologically plausible variational models of non-linear filtering coupled with optimized simple threshold mechanisms as derived from statistical learning mechanisms provides an efficient and realistic simulation of such non-standard retina output as observable at the level of konio-cells [14].

## **6.5. On the computational efficiency of Basal Ganglia models**

Many valuable models have been proposed to capture the richness of the fundamental relations between the basal ganglia and prominent brain structures including the prefrontal cortex, the hippocampus and the superior colliculus. To choose among them the mechanisms on which to build the design of the motor pole of our brain-inspired system, a fundamental issue is to evaluate the efficiency of these models in more realistic cases than the ones which are generally considered by the authors. For this reason, we are presently preparing a comparative study of models, including a model developed in our lab with neuroscientist colleagues [2], in the more realistic case of large sensory and motor flows.

## **6.6. From distributed computing to distributed computing**

One of the challenges in our systemic approach is to promote behaviors using distributed adaptive numerical computing that prevents (by definition) the specification of any behavior at a global level (no homunculus). This paradigm has been found to be very close to some class of problems in computer graphics where one tries to achieve a specific effect at the whole image level while the actual implementation is made at the pixel level (fragment). Transposing our expertise in distributed numerical computing, we thus experiment GPU programming (vertex/fragment programming) that offers hardware enforcement of distributed constraints: every fragment get the same program but their combination promotes a global image effect. This has been done for the case of text rendering [4] and dashed line rendering [5].

## CEPAGE Project-Team

## 6. New Results

### 6.1. Resource allocation and Scheduling

#### 6.1.1. *Broadcasting on Large Scale Heterogeneous Platforms under the Bounded Multi-Port Model*

**Participants:** Olivier Beaumont, Nicolas Bonichon, Lionel Eyraud-Dubois, Przemyslaw Uznanski.

In [17], we consider the problem of broadcasting a large message in a large scale distributed network under the multi-port communication model. We are interested in building an overlay network, with the aim of maximizing the throughput and minimizing the degree of the participating nodes. We consider a classification of participating nodes into two parts: open nodes that stay in the open-Internet and "guarded" nodes that lie behind firewalls or NATs, with the constraint that two guarded nodes cannot communicate directly. Without guarded nodes, we prove that it is possible to reach the optimal throughput with a quasi-optimal (up to a small additive increase) degree of the participating nodes. In presence of guarded nodes, we provide a closed form formula for the optimal cyclic throughput and we observe that the optimal solution may require arbitrarily large degrees. In the acyclic case, we propose an algorithm that reaches the optimal acyclic throughput with low degree. Then, we prove a worst case  $5/7$  ratio between the optimal acyclic and cyclic throughput and show through simulations that this ratio is on average very close to 1, what makes acyclic solutions efficient both in terms of throughput maximization and degree minimization.

#### 6.1.2. *Non Linear Divisible Load Scheduling*

**Participants:** Olivier Beaumont, Hubert Larchevêque.

Divisible Load Theory (DLT) has received a lot of attention in the past decade. A divisible load is a perfect parallel task, that can be split arbitrarily and executed in parallel on a set of possibly heterogeneous resources. The success of DLT is strongly related to the existence of many optimal resource allocation and scheduling algorithms, what strongly differs from general scheduling theory. Moreover, recently, close relationships have been underlined between DLT, that provides a fruitful theoretical framework for scheduling jobs on heterogeneous platforms, and MapReduce, that provides a simple and efficient programming framework to deploy applications on large scale distributed platforms. The success of both have suggested to extend their framework to non-linear complexity tasks. In [32], we show that both DLT and MapReduce are better suited to workloads with linear complexity. In particular, we prove that divisible load theory cannot directly be applied to quadratic workloads, such as it has been proposed recently. We precisely state the limits for classical DLT studies and we review and propose solutions based on a careful preparation of the dataset and clever data partitioning algorithms. In particular, through simulations, we show the possible impact of this approach on the volume of communications generated by MapReduce, in the context of Matrix Multiplication and Outer Product algorithms. (Joint work with Loris Marchal from ENS Lyon)

#### 6.1.3. *Reliable Service Allocation in Clouds*

**Participants:** Olivier Beaumont, Lionel Eyraud-Dubois, Hubert Larchevêque, Paul Renaud-Goud, Philippe Duchon.

In [30], we consider several reliability problems that arise when allocating applications to processing resources in a Cloud computing platform. More specifically, we assume on the one hand that each computing resource is associated to a capacity constraint and to a probability of failure. On the other hand, we assume that each service runs as a set of independent instances of identical Virtual Machines, and that the Service Level Agreement between the Cloud provider and the client states that a minimal number of instances of the service should run with a given probability. In this context, given the capacity and failure probabilities of the machines, and the capacity and reliability demands of the services, the question for the cloud provider is to find an allocation of the instances of the services (possibly using replication) onto machines satisfying all types of constraints during a given time period. The goal of this work is to assess the impact of the reliability constraint on the complexity of resource allocation problems. We consider several variants of this problem, depending on the number of services and whether their reliability demand is individual or global. We prove several fundamental complexity results (#P' and NP-completeness results) and we provide several optimal and approximation algorithms. In particular, we prove that a basic randomized allocation algorithm, that is easy to implement, provides optimal or quasi-optimal results in several contexts, and we show through simulations that it also achieves very good results in more general settings.

In [29], we extend this work to an energy minimisation framework, by considering two energy consumption models based on DVFS techniques, where the clock frequency of physical resources can be changed with a Dynamic Voltage and Frequency Scaling (DVFS) method. For each allocation problem and each energy model, we prove deterministic approximation ratios on the consumed energy for algorithms that provide guaranteed probability failures, as well as an efficient heuristic, whose energy ratio is not guaranteed.

In [37], we study the robustness of an allocation of Virtual Machines (VM) on a set of Physical Machines (PM) when the resource demand of the VMs can change over time. This may imply sometimes expensive "SLA violations", corresponding to some VM's consumption not satisfied because of overloaded PMs. Thus, while optimizing the global resource utilization of the PMs, it is necessary to ensure that at any moment a VM's need evolves, a few number of migrations (moving a VM from PM to PM) is sufficient to find a new configuration in which all the VMs' consumptions are satisfied. We modelize this problem using a fully dynamic bin packing approach and we present an algorithm ensuring a global utilization of the resources of 66%. Moreover, each time a PM is overloaded at most one migration is necessary to fall back in a configuration with no overloaded PM, and only 3 different PMs are concerned by required migrations that may occur to keep the global resource utilization correct. This allows the platform to be highly resilient to a great number of changes.

#### 6.1.4. *Splittable Single Source-Sink Routing on CMP Grids: A Sublinear Number of Paths Suffice*

**Participants:** Adrian Kosowski, Przemyslaw Uznanski.

In [44], we study single chip multiprocessors (CMP) with grid topologies, where a significant part of power consumption is attributed to communications between the cores of the grid. We investigate the problem of routing communications between CMP cores using shortest paths, in a model in which the power cost associated with activating a communication link at a transmission speed of  $f$  bytes/second is proportional to  $f^\alpha$ , for some constant exponent  $\alpha > 2$ . Our main result is a trade-off showing how the power required for communication in CMP grids depends on the ability to split communication requests between a given pair of node, routing each such request along multiple paths. For a pair of cores in a  $m \times n$  grid, the number of available communication paths between them grows exponentially with  $n, m$ . By contrast, we show that optimal power consumption (up to constant factors) can be achieved by splitting each communication request into  $k$  paths, starting from a threshold value of  $k = \Theta(n^{1/(\alpha-1)})$ . This threshold is much smaller than  $n$  for typical values of  $\alpha \approx 3$ , and may be considered practically feasible for use in routing schemes on the grid. More generally, we provide efficient algorithms for routing multiple  $k$ -splittable communication requests between two cores in the grid, providing solutions within a constant approximation of the optimum cost. We support our results with algorithm simulations, showing that for practical instances, our approach using  $k$ -splittable requests leads to a power cost close to that of the optimal solution with arbitrarily splittable requests, starting from the stated threshold value of  $k$ .

### 6.1.5. Maximum matching in multi-interface networks

**Participants:** Adrian Kosowski, Dominik Pajak.

In [26], we consider the standard matching problem in the context of multi-interface wireless networks. In heterogeneous networks, devices can communicate by means of multiple wireless interfaces. By choosing which interfaces to switch on at each device, several connections might be established. That is, the devices at the endpoints of each connection share at least one active interface. In the studied problem, the aim is to maximize the number of parallel connections without incurring in interferences. Given a network  $G = (V, E)$ , nodes  $V$  represent the devices, edges  $E$  represent the connections that can be established. If node  $x$  participates in the communication with one of its neighbors by means of interface  $i$ , then another neighboring node of  $x$  can establish a connection (but not with  $x$ ) only if it makes use of interface  $j \neq i$ . The size of a solution for an instance of the outcoming matching problem, that we call *Maximum Matching in Multi-Interface networks* (MMMI for short), is always in between the sizes of the solutions for the same instance with respect to the standard matching and its induced version problems. However, we prove that MMMI is NP-hard even for proper interval graphs and for bipartite graphs of maximum degree  $\Delta \geq 3$ . We also show polynomially solvable cases of MMMI with respect to different assumptions.

### 6.1.6. Parallel scheduling of task trees with limited memory

**Participant:** Lionel Eyraud-Dubois.

In a paper submitted to ACM TOPC, we have investigated the execution of tree-shaped task graphs using multiple processors. Each edge of such a tree represents some large data. A task can only be executed if all input and output data fit into memory, and a data can only be removed from memory after the completion of the task that uses it as an input data. Such trees arise, for instance, in the multifrontal method of sparse matrix factorization. The peak memory needed for the processing of the entire tree depends on the execution order of the tasks. With one processor the objective of the tree traversal is to minimize the required memory. This problem was well studied and optimal polynomial algorithms were proposed. We have extended the problem by considering multiple processors, which is of obvious interest in the application area of matrix factorization. With multiple processors comes the additional objective to minimize the time needed to traverse the tree, i.e., to minimize the makespan. Not surprisingly, this problem proves to be much harder than the sequential one. We study the computational complexity of this problem and provide inapproximability results even for unit weight trees. We design a series of practical heuristics achieving different trade-offs between the minimization of peak memory usage and makespan. Some of these heuristics are able to process a tree while keeping the memory usage under a given memory limit. The different heuristics are evaluated in an extensive experimental evaluation using realistic trees.

### 6.1.7. Point-to-point and congestion bandwidth estimation: experimental evaluation on PlanetLab

**Participants:** Lionel Eyraud-Dubois, Przemyslaw Uznanski.

In large scale Internet platforms, measuring the available bandwidth between nodes of the platform is difficult and costly. However, having access to this information allows to design clever algorithms to optimize resource usage for some collective communications, like broadcasting a message or organizing master/slave computations. In [54], we analyze the feasibility to provide estimations, based on a limited number of measurements, for the point-to-point available bandwidth values, and for the congestion which happens when several communications take place at the same time. We present a dataset obtained with both types of measurements performed on a set of nodes from the PlanetLab platform. We show that matrix factorization techniques are quite efficient at predicting point-to-point available bandwidth, but are not adapted for congestion analysis. However, a LastMile modeling of the platform allows to perform congestion predictions with a reasonable level of accuracy, even with a small amount of information, despite the variability of the measured platform.

### 6.1.8. Parallel Mining of Functional Dependencies

**Participants:** Sofian Maabout, Nicolas Hanusse.

The problem of extracting functional dependencies (FDs) from databases has a long history dating back to the 90's. Still, efficient solutions taking into account both material evolution, namely the advent of multicore machines, and the amount of data that are to be mined, are still needed. In [46] we propose a parallel algorithm which, upon small modifications, extracts (i) the minimal keys, (ii) the minimal exact FDs, (iii) the minimal approximate FDs and (iv) the Conditional functional dependencies (CFDs) holding in a table. Under some natural conditions, we prove a theoretical speed up of our solution with respect to a baseline algorithm which follows a depth first search strategy. Since mining most of these dependencies require a procedure for computing the number of distinct values (NDV) which is a space consuming operation, we show how sketching techniques for estimating the exact value of NDV can be used for reducing both memory consumption as well as communications overhead when considering distributed data while guaranteeing a certain quality of the result. Our solution is implemented in both shared, using C++ and OpenMP, and distributed memory, using Hadoop implementation of Map-Reduce. The experimental results show the efficiency and scalability of our proposal. Most notably, the theoretical speed ups are confirmed by the experiments.

### 6.1.9. Fast Skyline Query Evaluation with Skycuboids Materialization based on Functional Dependencies

**Participants:** Sofian Maabout, Nicolas Hanusse.

Ranking multidimensional data via different Skyline queries gives rise to the so called skycube structure. Most of previous work on optimizing the subspaces skyline queries have concentrated on full materialization of the skycube. Due to the exponential number of skylines one must pre-compute, the full materialization is unfeasible in practice. However, due to the non monotonic nature of skylines, there is no immediate inclusion relationship between the skycuboids when we have an inclusion of the dimensions. This makes the partial materialization harder. In this paper, we identify sufficient conditions for establishing inclusions between skycuboids thanks to the functional dependencies that hold in the underlying data. This leads to the characterization of a *minimal* set of skycuboids to be materialized in order to answer all the possible skyline queries without resorting to the underlying data. We conduct an extensive set of experiments showing that with the help of a small fraction of the skycube, we can efficiently answer all the possible skyline queries. In addition, our proposal turns to be helpful even in the full materialization setting. Indeed, thanks to the inclusions we identify, we devise a full materialization algorithm which outperforms state of the art skycube computation algorithms especially when data and dimensions get large. The results are reported in the technical report submitted to SIGMOD'14.

## 6.2. Compact Routing

### 6.2.1. On the Communication Complexity of Distributed Name-Independent Routing Schemes

**Participants:** Cyril Gavoille, Nicolas Hanusse, David Ilcinkas.

In [38], we present a distributed asynchronous algorithm that, for every undirected weighted  $n$ -node graph  $G$ , constructs name-independent routing tables for  $G$ . The size of each table is  $\tilde{O}(\sqrt{n})$ , whereas the length of any route is stretched by a factor of at most 7 w.r.t. the shortest path. At any step, the memory space of each node is  $\tilde{O}(\sqrt{n})$ . The algorithm terminates in time  $O(D)$ , where  $D$  is the hop-diameter of  $G$ . In synchronous scenarios and with uniform weights, it consumes  $\tilde{O}(m\sqrt{n} + n^{3/2} \min D, \sqrt{n})$  messages, where  $m$  is the number of edges of  $G$ .

In the realistic case of sparse networks of poly-logarithmic diameter, the communication complexity of our scheme, that is  $\tilde{O}(n^{3/2})$ , improves by a factor of  $\sqrt{n}$  the communication complexity of *any* shortest-path routing scheme on the same family of networks. This factor is provable thanks to a new lower bound of independent interest.

### 6.2.2. There are Plane Spanners of Maximum Degree 4

**Participant:** Nicolas Bonichon.

Let  $\mathcal{E}$  be the complete Euclidean graph on a set of points embedded in the plane. Given a fixed constant  $t \geq 1$ , a spanning subgraph  $G$  of  $\mathcal{E}$  is said to be a  $t$ -spanner of  $\mathcal{E}$  if for any pair of vertices  $u, v$  in  $\mathcal{E}$  the distance between  $u$  and  $v$  in  $G$  is at most  $t$  times their distance in  $\mathcal{E}$ . A spanner is *plane* if its edges do not cross.

We consider the question: “What is the smallest *maximum degree* that can be achieved for a *plane* spanner of  $\mathcal{E}$ ?” Without the planarity constraint, it is known that the answer is 3 which is thus the best known lower bound on the degree of any plane spanner. With the planarity requirement, the best known upper bound on the maximum degree is 6, the last in a long sequence of results improving the upper bound. In this work we show that there is a constant  $t \geq 1$  such that the complete Euclidean graph always contains a plane  $t$ -spanner of maximum degree 4 and make a big step toward closing the question. Our construction leads to an efficient algorithm for obtaining the spanner from Chew’s  $L_1$ -Delaunay triangulation.

## 6.3. Mobile Agents

### 6.3.1. Collision-Free Network Exploration

**Participants:** Ralf Klasing, Adrian Kosowski, Dominik Pajak.

A set of mobile agents is placed at different nodes of a  $n$ -node network. The agents synchronously move along the network edges in a *collision-free* way, i.e., in no round may two agents occupy the same node. In each round, an agent may choose to stay at its currently occupied node or to move to one of its neighbors. An agent has no knowledge of the number and initial positions of other agents. We are looking for the shortest possible time required to complete the collision-free *network exploration*, i.e., to reach a configuration in which each agent is guaranteed to have visited all network nodes and has returned to its starting location. In [34], we first consider the scenario when each mobile agent knows the map of the network, as well as its own initial position. We establish a connection between the number of rounds required for collision-free exploration and the degree of the minimum-degree spanning tree of the graph. We provide tight (up to a constant factor) lower and upper bounds on the collision-free exploration time in general graphs, and the exact value of this parameter for trees. For our second scenario, in which the network is unknown to the agents, we propose collision-free exploration strategies running in  $O(n^2)$  rounds for tree networks and in  $O(n^5 \log n)$  rounds for general networks.

### 6.3.2. Deterministic Rendezvous of Asynchronous Bounded-Memory Agents in Polygonal Terrains

**Participant:** Adrian Kosowski.

In [22], we deal with a more geometric variant of the rendezvous problem. Two mobile agents, modeled as points starting at different locations of an unknown terrain, have to meet. The terrain is a polygon with polygonal holes. We consider two versions of this rendezvous problem: exact RV, when the points representing the agents have to coincide at some time, and  $\epsilon$ -RV, when these points have to get at distance less than  $\epsilon$  in the terrain. In any terrain, each agent chooses its trajectory, but the movements of the agent on this trajectory are controlled by an adversary that may, e.g., speed up or slow down the agent. Agents have bounded memory: their computational power is that of finite state machines. Our aim is to compare the feasibility of exact and of  $\epsilon$ -RV when agents are anonymous vs. when they are labeled. We show classes of polygonal terrains which distinguish all the studied scenarios from the point of view of feasibility of rendezvous. The features which influence the feasibility of rendezvous include symmetries present in the terrains, boundedness of their diameter, and the number of vertices of polygons in the terrains.

### 6.3.3. Optimal Patrolling of Fragmented Boundaries

**Participant:** Adrian Kosowski.

Mobile agents in geometric scenarios are also studied in [33], where a set of mobile robots is deployed on a simple curve of finite length, composed of a finite set of vital segments separated by neutral segments. The robots have to patrol the vital segments by perpetually moving on the curve, without exceeding their maximum speed. The quality of patrolling is measured by the idleness, i.e., the longest time period during which any vital point on the curve is not visited by any robot. Given a configuration of vital segments, our goal is to provide algorithms describing the movement of the robots along the curve so as to minimize the idleness. Our main contribution is a proof that the optimal solution to the patrolling problem is attained either by the cyclic strategy, in which all the robots move in one direction around the curve, or by the partition strategy, in which the curve is partitioned into sections which are patrolled separately by individual robots. These two fundamental types of strategies were studied in the past in the robotics community in different theoretical and experimental settings. However, to our knowledge, this is the first theoretical analysis proving optimality in such a general scenario.

### 6.3.4. Fast Collaborative Graph Exploration

**Participants:** Adrian Kosowski, Dominik Pajak, Przemyslaw Uznanski.

In [35], we study the following scenario of online graph exploration. A team of  $k$  agents is initially located at a distinguished vertex  $r$  of an undirected graph. At every time step, each agent can traverse an edge of the graph. All vertices have unique identifiers, and upon entering a vertex, an agent obtains the list of identifiers of all its neighbors. We ask how many time steps are required to complete exploration, i.e., to make sure that every vertex has been visited by some agent. We consider two communication models: one in which all agents have global knowledge of the state of the exploration, and one in which agents may only exchange information when simultaneously located at the same vertex. As our main result, we provide the first strategy which performs exploration of a graph with  $n$  vertices at a distance of at most  $D$  from  $r$  in time  $O(D)$ , using a team of agents of polynomial size  $k = Dn^{1+\epsilon} < n^{2+\epsilon}$ , for any  $\epsilon > 0$ . Our strategy works in the local communication model, without knowledge of global parameters such as  $n$  or  $D$ . We also obtain almost-tight bounds on the asymptotic relation between exploration time and team size, for large  $k$ . For any constant  $c > 1$ , we show that in the global communication model, a team of  $k = Dn^c$  agents can always complete exploration in  $D(1 + \frac{1}{c-1} + o(1))$  time steps, whereas at least  $D(1 + \frac{1}{c} - o(1))$  steps are sometimes required. In the local communication model,  $D(1 + \frac{2}{c-1} + o(1))$  steps always suffice to complete exploration, and at least  $D(1 + \frac{2}{c} - o(1))$  steps are sometimes required. This shows a clear separation between the global and local communication models.

### 6.3.5. A $\tilde{O}(n^2)$ Time-Space Trade-off for Undirected $s$ - $t$ Connectivity

**Participant:** Adrian Kosowski.

The work [43] makes use of the Metropolis-type walks due to Nonaka et al. (2010) to provide a faster solution to the  $S$ - $T$ -connectivity problem in undirected graphs (USTCON). As the main result of this research, we propose a family of randomized algorithms for USTCON which achieves a time-space product of  $S \cdot T = \tilde{O}(n^2)$  in graphs with  $n$  nodes and  $m$  edges (where the  $\tilde{O}$ -notation disregards poly-logarithmic terms). This improves the previously best trade-off of  $\tilde{O}(nm)$ , due to Feige (1995). Our algorithm consists in deploying several short Metropolis-type walks, starting from landmark nodes distributed using the scheme of Broder et al. (1994) on a modified input graph. In particular, we obtain an algorithm running in time  $\tilde{O}(n + m)$  which is, in general, more space-efficient than both BFS and DFS. Finally, we show how to fine-tune the Metropolis-type walk so as to match the performance parameters (e.g., average hitting time) of the unbiased random walk for any graph, while preserving a worst-case bound of  $\tilde{O}(n^2)$  on cover time.

### 6.3.6. The multi-agent rotor-router on the ring: a deterministic alternative to parallel random walks

**Participants:** Ralf Klasing, Adrian Kosowski, Dominik Pajak.

The *rotor-router mechanism* was introduced as a deterministic alternative to the random walk in undirected graphs. In this model, an agent is initially placed at one of the nodes of the graph. Each node maintains a cyclic ordering of its outgoing arcs, and during successive visits of the agent, propagates it along arcs chosen according to this ordering in round-robin fashion. In [42], we consider the setting in which multiple, indistinguishable agents are deployed in parallel in the nodes of the graph, and move around the graph in synchronous rounds, interacting with a single rotor-router system. We propose new techniques which allow us to perform a theoretical analysis of the multi-agent rotor-router model, and to compare it to the scenario of parallel independent random walks in a graph. Our main results concern the  $n$ -node ring, and suggest a strong similarity between the performance characteristics of this deterministic model and random walks.

We show that on the ring the rotor-router with  $k$  agents admits a cover time of between  $\Theta(n^2/k^2)$  in the best case and  $\Theta(n^2/\log k)$  in the worst case, depending on the initial locations of the agents, and that both these bounds are tight. The corresponding expected value of cover time for  $k$  random walks, depending on the initial locations of the walkers, is proven to belong to a similar range, namely between  $\Theta(n^2/(k^2/\log^2 k))$  and  $\Theta(n^2/\log k)$ .

Finally, we study the limit behavior of the rotor-router system. We show that, once the rotor-router system has stabilized, all the nodes of the ring are always visited by some agent every  $\Theta(n/k)$  steps, regardless of how the system was initialized. This asymptotic bound corresponds to the expected time between successive visits to a node in the case of  $k$  random walks. All our results hold up to a polynomially large number of agents ( $1 \leq k < n^{1/11}$ ).

### 6.3.7. Efficient Exploration of Anonymous Undirected Graphs

**Participant:** Ralf Klasing.

In [41], we consider the problem of exploring an anonymous undirected graph using an oblivious robot. The studied exploration strategies are designed so that the next edge in the robot's walk is chosen using only local information. We present some current developments in the area. In particular, we focus on recent work on *equitable strategies* and on the *multi-agent rotor-router*.

### 6.3.8. Gathering radio messages in the path

**Participant:** Ralf Klasing.

In [19], we address the problem of gathering information in one node (sink) of a radio network where interference constraints are present: when a node transmits, it produces interference in an area bigger than the area in which its message can actually be received. The network is modeled by a graph; a node is able to transmit one unit of information to the set of vertices at distance at most  $dt$  in the graph, but when doing so it generates interferences that do not allow nodes at distance up to  $di$  ( $di \geq dt$ ) to listen to other transmissions. We are interested in finding a gathering protocol, that is an ordered sequence of rounds (each round consists of non-interfering simultaneous transmissions) such that  $w(u)$  messages are transmitted from any node  $u$  to a fixed node called the sink. Our aim is to find a gathering protocol with the minimum number of rounds (called *gathering time*). In [19], we focus on the specific case where the network is a path with the sink at an end vertex of the path and where the traffic is unitary ( $w(u) = 1$  for all  $u$ ); indeed this simple case appears to be already very difficult. We first give a new lower bound and a protocol with a gathering time that differ only by a constant independent of the length of the path. Then we present a method to construct incremental protocols. An incremental protocol for the path on  $n + 1$  vertices is obtained from a protocol for  $n$  vertices by adding new rounds and new calls to some rounds but without changing the calls of the original rounds. We show that some of these incremental protocols are optimal for many values of  $dt$  and  $di$  (in particular when  $dt$  is prime). We conjecture that this incremental construction always gives optimal protocols. Finally, we derive an approximation algorithm when the sink is placed in an arbitrary vertex in the path.

### 6.3.9. Computing Without Communicating: Ring Exploration by Asynchronous Oblivious Robots

**Participant:** David Ilcinkas.



In [24], we consider the problem of exploring an anonymous unoriented ring by a team of  $k$  identical, oblivious, asynchronous mobile robots that can view the environment but cannot communicate. This weak scenario is standard when the spatial universe in which the robots operate is the two-dimensional plane, but (with one exception) has not been investigated before for networks. Our results imply that, although these weak capabilities of robots render the problem considerably more difficult, ring exploration by a small team of robots is still possible. We first show that, when  $k$  and  $n$  are not co-prime, the problem is not solvable in general, e.g., if  $k$  divides  $n$  there are initial placements of the robots for which gathering is impossible. We then prove that the problem is always solvable provided that  $n$  and  $k$  are co-prime, for  $k \geq 17$ , by giving an exploration algorithm that always terminates, starting from arbitrary initial configurations. Finally, we consider the minimum number  $\rho(n)$  of robots that can explore a ring of size  $n$ . As a consequence of our positive result we show that  $\rho(n)$  is  $O(\log n)$ . We additionally prove that  $\Omega(\log n)$  robots are necessary for infinitely many  $n$ .

### 6.3.10. Worst-case optimal exploration of terrains with obstacles

**Participant:** David Ilcinkas.

A mobile robot represented by a point moving in the plane has to explore an unknown flat terrain with impassable obstacles. Both the terrain and the obstacles are modeled as arbitrary polygons. We consider two scenarios: the *unlimited vision*, when the robot situated at a point  $p$  of the terrain explores (sees) all points  $q$  of the terrain for which the segment  $pq$  belongs to the terrain, and the *limited vision*, when we require additionally that the distance between  $p$  and  $q$  is at most 1. All points of the terrain (except obstacles) have to be explored and the performance of an exploration algorithm, called its complexity, is measured by the length of the trajectory of the robot.

For unlimited vision we show in [21] an exploration algorithm with complexity  $O(P + D\sqrt{k})$ , where  $P$  is the total perimeter of the terrain (including perimeters of obstacles),  $D$  is the diameter of the convex hull of the terrain, and  $k$  is the number of obstacles. We do not assume knowledge of these parameters. We also prove a matching lower bound showing that the above complexity is optimal, even if the terrain is known to the robot. For limited vision we show exploration algorithms with complexity  $O(P + A + \sqrt{Ak})$ , where  $A$  is the area of the terrain (excluding obstacles). Our algorithms work either for arbitrary terrains (if one of the parameters  $A$  or  $k$  is known) or for  $c$ -fat terrains, where  $c$  is any constant (unknown to the robot) and no additional knowledge is assumed. (A terrain  $\mathcal{T}$  with obstacles is  $c$ -fat if  $R/r \leq c$ , where  $R$  is the radius of the smallest disc containing  $\mathcal{T}$  and  $r$  is the radius of the largest disc contained in  $\mathcal{T}$ .) We also prove a matching lower bound  $\Omega(P + A + \sqrt{Ak})$  on the complexity of exploration for limited vision, even if the terrain is known to the robot.

### 6.3.11. Exploration of the $T$ -Interval-Connected Dynamic Graphs: the Case of the Ring

**Participants:** David Ilcinkas, Ahmed Wade.

In [40], we study the  $T$ -interval-connected dynamic graphs from the point of view of the time necessary and sufficient for their exploration by a mobile entity (agent). A dynamic graph (more precisely, an evolving graph) is  $T$ -interval-connected ( $T \geq 1$ ) if, for every window of  $T$  consecutive time steps, there exists a connected spanning subgraph that is stable (always present) during this period. This property of connection stability over time was introduced by Kuhn, Lynch and Oshman (STOC 2010). We focus on the case when the underlying graph is a ring of size  $n$ , and we show that the worst-case time complexity for the exploration problem is  $2n - T - \Theta(1)$  time units if the agent knows the dynamics of the graph, and  $n + \frac{n}{\max\{1, T-1\}}(\delta - 1) \pm \Theta(\delta)$  time units otherwise, where  $\delta$  is the maximum time between two successive appearances of an edge.

### 6.3.12. Time vs. space trade-offs for rendezvous in trees

**Participant:** Adrian Kosowski.

In [23], we consider the rendezvous problem, in which two identical (anonymous) mobile agents start from arbitrary nodes of an unknown tree and have to meet at some node. Agents move in synchronous rounds: in each round an agent can either stay at the current node or move to one of its neighbors. We consider deterministic algorithms for this rendezvous task. We obtain a tight trade-off between the optimal time of completing rendezvous and the size of memory of the agents. For agents with  $k$  memory bits, we show that optimal rendezvous time is  $\Theta(n + n^2/k)$  in  $n$ -node trees. More precisely, if  $k \geq c \log n$ , for some constant  $c$ , we design agents accomplishing rendezvous in arbitrary trees of size  $n$  (unknown to the agents) in time  $O(n + n^2/k)$ , starting with arbitrary delay. We also show that no pair of agents can accomplish rendezvous in time  $o(n + n^2/k)$ , even in the class of lines of known length and even with simultaneous start. Finally, we prove that at least logarithmic memory is necessary for rendezvous, even for agents starting simultaneously in a  $n$ -node line.

## HIEPACS Project-Team

## 6. New Results

### 6.1. High-performance computing on next generation architectures

#### 6.1.1. Composing multiple StarPU applications over heterogeneous machines: a supervised approach

Enabling HPC applications to perform efficiently when invoking multiple parallel libraries simultaneously is a great challenge. Even if a uniform runtime system is used underneath, scheduling tasks or threads coming from different libraries over the same set of hardware resources introduces many issues, such as resource oversubscription, undesirable cache flushes or memory bus contention.

This paper presents an extension of **StarPU**, a runtime system specifically designed for heterogeneous architectures, that allows multiple parallel codes to run concurrently with minimal interference. Such parallel codes run within *scheduling contexts* that provide confined execution environments which can be used to partition computing resources. Scheduling contexts can be dynamically resized to optimize the allocation of computing resources among concurrently running libraries. We introduce a *hypervisor* that automatically expands or shrinks contexts using feedback from the runtime system (e.g. resource utilization). We demonstrate the relevance of our approach using benchmarks invoking multiple high performance linear algebra kernels simultaneously on top of heterogeneous multicore machines. We show that our mechanism can dramatically improve the overall application run time (-34%), most notably by reducing the average cache miss ratio (-50%).

This work is developed in the framework of Andra Hugo's PhD. These contributions have been presented at the international workshop on Accelerators and Hybrid Exascale Systems [19] in Boston.

#### 6.1.2. A task-based H-matrix solver for acoustic and electromagnetic problems on multicore architectures

$\mathcal{H}$ -Matrix is a hierarchical, data-sparse approximate representation of matrices that allows the fast approximate computation of matrix products,  $LU$  and  $LDL^T$  decompositions, inversion and more. This representation is suitable for the direct solution of large dense linear systems arising from the Boundary Element Method in  $O(N \log_2^\alpha(N))$  operations. This kind of formulation is widely used in the industry for the numerical simulation of acoustics and electromagnetism scattering by large objects. Applications of this approach include aircraft noise reduction and antenna siting at Airbus Group. The recursive and irregular nature of these  $\mathcal{H}$ -Matrix algorithms makes an efficient parallel implementation very challenging, especially when relying on a "Bulk Synchronous Parallel" paradigm. We have considered an alternative parallelization for multicore architectures using a task-based approach on top of a runtime system, namely **StarPU**. We have showed that our method leads to a highly efficient, fully pipelined computation on large real-world industrial test cases provided by Airbus Group.

This research activity has been conducted in the framework of the EADS-ASTRIUM, Inria, Conseil Régional initiative in collaboration with the **RUNTIME** Inria project, and is part of Benoit Lize's PhD.

#### 6.1.3. A task-based 3D geophysics application

Reverse Time Migration (RTM) technique produces underground images using wave propagation. A discretization based on the Discontinuous Galerkin (DG) method unleashes a massively parallel elastodynamics simulation, an interesting feature for current and future architectures. We have designed a task-based version of this scheme in order to enable the use of manycore architectures. At this stage, we have demonstrated the efficiency of the approach on homogeneous and cache coherent Non Uniform Memory Access (ccNUMA) multicore platforms (up to 160 cores) and designed a prototype version of a distributed memory version that can exploit multiple instances of such architectures. This work has been conducted in the context of the **DIP** Inria-Total strategic action in collaboration with the **MAGIQUE3D** Project-Team and thanks to the long-term visit of George Bosilca funded by TOTAL. George's expertise ensured an optimum usage of the **PaRSEC** runtime system onto which our task-based scheme has been ported.

This work was presented during a PRACE workshop [28] as well as during a TOTAL scientific event [29].

#### 6.1.4. Resiliency in numerical simulations

For the solution of systems of linear equations, various recovery-restart strategies have been investigated in the framework of Krylov subspace methods to address the situations of core failures. The basic underlying idea is to recover fault entries of the iterate via interpolation from existing values available on neighbor cores. The resulting results are reported in the research report [41] currently submitted to an international journal. In that resilience framework, we have extended the recovery-restart ideas to the solution of linear eigenvalue problems. Contrary to the linear system case, not only the current iterate can be interpolated but also part of the subspace where candidate eigenpairs are searched.

This work is developed in the framework of Mawussi Zounon's PhD funded by the ANR **RESCUE**. These contributions have been presented at the international workshop Sparse Days [27] in Toulouse. More details and results can be found in report RR-8324 [41]. Notice that these activities are also part of our contribution to the **G8 ESC** (Enabling Climate Simulation at extreme scale).

## 6.2. High performance solvers for large linear algebra problems

### 6.2.1. Parallel sparse direct solver on runtime systems

The ongoing hardware evolution exhibits an escalation in the number, as well as in the heterogeneity, of the computing resources. The pressure to maintain reasonable levels of performance and portability, forces the application developers to leave the traditional programming paradigms and explore alternative solutions. Algorithms, especially those in critical domains such as linear algebra, need to undergo invasive structural changes and be adapted to new programming paradigms to be in agreement with the latest hardware advances. **PaStiX** is a parallel sparse direct solver, based on a dynamic scheduler for modern hierarchical architectures. In this paper, we study the replacement of the highly specialized internal scheduler in **PaStiX** by two generic runtime frameworks: **PaRSEC** and **StarPU**. The tasks graph of the factorization step is made available to the two runtimes, providing them with the opportunity to optimize it in order to maximize the algorithm efficiency for a predefined execution environment. A comparative study of the performance of the **PaStiX** solver with the three schedulers on different execution contexts is performed. The analysis highlights the similarities from a performance point of view between the different execution supports. These results demonstrate that these generic DAG-based runtimes provide a uniform and portable programming interface across heterogeneous environments, and are, therefore, a sustainable solution for hybrid environments.

This work is developed in the framework of Xavier Lacoste's PhD funded by the ANR **ANEMOS**. These contributions have been presented at the international workshop Sparse Days [37] in Toulouse. More details and results can be found in report RR-8446 [46].

### 6.2.2. Hybrid parallel implementation of hybrid solvers

In the framework of the hybrid direct/iterative **MaPhyS** solver, we have designed and implemented an hybrid MPI-thread variant. More precisely, the implementation rely on the multi-threaded MKL library for all the dense linear algebra calculations and the multi-threaded version of **PaStiX**. Among the technical difficulties, one was to make sure that the two multi-threaded libraries do not interfere with each other. The resulting software prototype is currently experimented to study its new capability to get flexibility and trade-off between the parallel and numerical efficiency. Parallel experiments have been conducted on the Plafrim platform as well as on a large scale machine located at the USA DOE NERSC, which has a large number of CPU cores per socket.

This work is developed in the framework of the PhD thesis of Stojce Nakov funded by TOTAL. These contributions have been presented at the NVIDIA GPU Technology Conference [25] in San Jose.

### 6.2.3. Designing LU-QR hybrid solvers for performance and stability

New hybrid LU-QR algorithms for solving dense linear systems of the form  $Ax = b$  have been introduced. Throughout a matrix factorization, these algorithms dynamically alternate LU with local pivoting and QR elimination steps, based upon some robustness criterion. LU elimination steps can be very efficiently parallelized, and are twice as cheap in terms of flops, as QR steps. However, LU steps are not necessarily stable, while QR steps are always stable. The hybrid algorithms execute a QR step when a robustness criterion detects some risk for instability, and they execute an LU step otherwise. Ideally, the choice between LU and QR steps must have a small computational overhead and must provide a satisfactory level of stability with as few QR steps as possible. In this paper, we introduce several robustness criteria and we establish upper bounds on the growth factor of the norm of the updated matrix incurred by each of these criteria. In addition, we describe the implementation of the hybrid algorithms through an extension of the PaRSEC software to allow for dynamic choices during execution. Finally, we analyze both stability and performance results compared to state-of-the-art linear solvers on parallel distributed multicore platforms. These contributions have been presented at the international conference IPDPS [18] in Phoenix.

## 6.3. High performance Fast Multipole Method for N-body problems

Last year we have worked primarily on developing an efficient fast multipole method for heterogeneous architecture. Some of the accomplishments for this year include:

1. Implementation of the FMM of multicore machines using StarPU. A new parallel scheduler was developed for this purpose. We implemented a state-of-the-art OpenMP version of the code for benchmarking purposes. It was found that StarPU significantly outperforms OpenMP. Figures show the traces of an execution of the FMM algorithm with our priority scheduler for the cube (volume) and ellipsoid (surface) with 20 million particles on a 4 deca-core Intel Xeon E7-4870 machine.
2. Implementation of the FMM of heterogeneous machines (CPU+GPU) using StarPU. The FMM was also used to demonstrate the flexibility of StarPU for handling different types of processors. In particular we demonstrated in that application that StarPU can automatically select the appropriate version of a computational kernel (CPU or GPU version) and run it on the appropriate processor in order to minimize the overall runtime. Significant speed-up were obtained on heterogeneous platforms compared to multicore only processors.

These contributions have been presented in minisymposia at the SIAM conference on Computational Sciences and Engineering [23], [33] in Boston and at NVIDIA GPU Technology Conference [24]. More details and results can be found in report RR-8277 [40], our paper is accepted for publication in the SIAM Journal on Scientific Computing [11].

Concerning dynamics dislocations (DD) kernels, an efficient formulation of the isotropic elastic far-field interactions between dislocations has been developed. This formulation is suitable for any polynomial interpolation based Fast Multipole Method (FMM) and is currently being implemented in OptiDis.

Meanwhile a much lighter and faster interpolation scheme based on a uniform grid (i.e. Lagrange interpolation) and the Fast Fourier Transform (FFT) was implemented into ScalFMM. This last feature was introduced in order to overcome the expensive cost of the Chebyshev FMM in the range of low interpolation orders (up to approx. 10). This should significantly improve the performances of the far-field computation in DD simulations where tensorial kernels are involved but only relatively low interpolation orders are required. This work is developed in the framework of Pierre Blanchard's PhD funded by ENS.

## 6.4. Efficient algorithmic for load balancing and code coupling in complex simulations

### 6.4.1. Dynamic load balancing for massively parallel coupled codes

As a preliminary step related to the dynamic load balancing of coupled codes, we focus on the problem of dynamic load balancing of a single parallel code, with variable number of processors. Indeed, if the workload

varies drastically during the simulation, the load must be redistributed regularly among the processors. Dynamic load balancing is a well studied subject but most studies are limited to an initially fixed number of processors. Adjusting the number of processors at runtime allows to preserve the parallel code efficiency or to keep running the simulation when the current memory resources are exceeded. We call this problem, *MxN graph repartitioning*. We propose some methods based on graph repartitioning in order to rebalance the load while changing the number of processors. These methods are split in two main steps. Firstly, we study the migration phase and we build a “good” migration matrix minimizing several metrics like the migration volume or the number of exchanged messages. Secondly, we use graph partitioning heuristics to compute a new distribution optimizing the migration according to the previous step results. Besides, we propose a direct  $k$ -way partitioning algorithm that allows us to improve our biased partitioning. Finally, an experimental study validates our algorithms against state-of-the-art partitioning tools. Our algorithms are implemented in the **LBC2** library and have been integrated in the partitioning tools *Scotch* as a prototype.

This work is developed in the framework of Clément Vuchener’s PhD, that will be defended on February 2014. These contributions have been presented at the international conference *ParCo* [22] in Munchen.

Regarding the problem of dynamic balancing of parallel coupled codes, we start to reuse results on *MxN graph repartitioning*. Given two coupled codes  $A$  and  $B$ , the key idea is to develop an algorithm of *two-graph co-partitioning*, that partitions two *coupled* graphs  $G_A$  and  $G_B$  in respectively  $N_A$  and  $N_B$  with classic objectives (*i.e.*, balancing computational load and minimizing communication cost for each code) and that minimizes the number of messages exchanged between codes in the coupling phase.

This work is developed in the framework of Maria Predari’s PhD, that just started in october 2013.

#### 6.4.2. Graph partitioning for hybrid solvers

Nested Dissection has been introduced by A. George and is a very popular heuristic for sparse matrix ordering before numerical factorization. It allows to maximize the number of parallel tasks, while reducing the fill-in and the operation count. The basic standard idea is to build a “small separator”  $S$  of the graph associated with the matrix in order to split the remaining vertices in two parts  $P_0$  and  $P_1$  of “almost equal size”. The vertices of the separator  $S$  are ordered with the largest indices, and then the same method is applied recursively on the two sub-graphs induced by  $P_0$  and  $P_1$ . At the end, if  $k$  levels of recursion are done, we get  $2^k$  sets of independent vertices separated from each other by  $2^k - 1$  separators.

However, if we examine precisely the complexity analysis for the estimation of asymptotic bounds for fill-in or operation count when using Nested Dissection ordering, we can notice that the size of the halo of the separated sub-graphs (set of external vertices belonging to an old separator and previously ordered) plays a crucial role in the asymptotic behavior achieved. In the perfect case, we need halo vertices to be balanced among parts.

Considering now hybrid methods mixing both direct and iterative solvers such as **HIPS**, **MaPHyS**, obtaining a domain decomposition leading to a good balancing of both the size of domain interiors and the Scalable numerical schemes for scientific applications size of interfaces is a key point for load balancing and efficiency in a parallel context. This leads to the same issue: balancing the halo vertices to get balanced interfaces.

For this purpose, we revisit the algorithm introduced by Lipton, Rose and Tarjan which performed the recursion of nested dissection in a different manner: at each level, we apply recursively the method to the sub-graphs. But, for each sub-graph, we keep track of halo vertices. We have implemented that in the *Scotch* framework, and have studied its main algorithm to build a separator, called greedy graph growing.

This work is developed in the framework of Astrid Casadei’s PhD. These contributions have been presented at the international workshop on Nested Dissection [32] in Waterloo.

## 6.5. Application Domains

### 6.5.1. Dislocation dynamics simulations in material physics

This year we have focused on the hybrid parallelization of the OptiDis code. As dislocations move in their grain, they expand, shrink, collide and annihilate, which means that we are facing a extremely dynamic n-body problem. Also, we have introduced an adaptive cache conscious data structure to manage the dislocation mesh. Moreover, two main kernels, plugged in our **ScalFMM** library, was built to handle the pairwise force interactions and the collisions between dislocations. Finally the code is written using hybrid parallelism based on OpenMP tasks inside on node and MPI to exchange data between nodes. The code can run on both shared and distributed memories. Future works will mainly focus on tuning the code and manage dynamically this tuning to adapt to different kind of simulations and architectures. On the physical side, we have introduced more *split node* cases to simulate irradiated materials. Now we are able to run simulations with tens of thousand of dislocations in materials. Typically, our simulation box can hold lot of tiny dislocation loops such as those induced by radiation on materials, so we can observe how Frank-Read sources interact while they cross the field of loop defects.

This work is developed in the framework of Arnaud Etcheverry's PhD funded by the ANR **OPTIDIS**.

### 6.5.2. Co-design for scalable numerical algorithms in scientific applications

The study of the **thermo-acoustic stability of large combustion chambers** requires the solution of a nonlinear eigenvalue problem. The nonlinear problem is linearized using a fixed point iteration procedure. This leads to a sequence of linear eigenproblems which must be solved iteratively in order to obtain one nonlinear eigenpair. Therefore, efficient and robust parallel eigensolvers for the solution of linear problems have been investigated, and strategies to accelerate the solution of the sequence of linear eigenproblems have also been proposed. Among the numerical techniques that have been considered (Krylov-Schur, Implicitly Restarted Arnoldi, Subspace iteration with Chebyshev acceleration) the Jacobi-Davidson method was the best suited to be combined with techniques to recycle spectral information between the nonlinear iterations. The robustness of the parallel numerical techniques were illustrated on large problems with a few millions unknowns solved on a few tens of cores.

These results are part of the outcome of Pablo Salas PhD thesis that has been defended on November 15th.

The **Time-domain Boundary Element Method (TD-BEM)** has not been widely study but represent an interesting alternative to its frequency counterpart. Usually based on inefficient Sparse Matrix Vector-product (SpMV), we investigate other approaches in order to increase the sequential flop-rate. We have implement extremely efficient operator using intrinsic SIMD or even ASM64 instructions. We are using this novel approaches to parallelize both in shared and distributed memory and target execution on hundreds of clusters. All the implementations should be in high quality in the Software Engineering sense since the resulting library is going to be used by industrial applications.

This work is developed in the framework of Bérenger Bramas's PhD and contributes to the EADS-ASTRIUM, Inria, Conseil Régional initiative.

In a preliminary work, a **3D Cartesian SN solver** DOMINO has been designed and implemented using two nested levels of parallelism (multicore+SIMD) on shared memory computation nodes. DOMINO is written in C++, a multi-paradigm programming language that enables the use of powerful and generic parallel programming tools such as Intel TBB and Eigen. These two libraries allow us to combine multi-thread parallelism with vector operations in an efficient and yet portable way. As a result, DOMINO can exploit the full power of modern multi-core processors and is able to tackle very large simulations, that usually require large HPC clusters, using a single computing node. The very high Flops/Watt ratio of DOMINO makes it a very interesting building block for a future many-nodes nuclear simulation tool.

This work is developed in the framework of Salli Moustafa's PhD in collaboration with EDF. These contributions have been presented at the international conference on Supercomputing on Nuclear Applications [21] in Paris.

Concerning the numerical simulation of **the turbulence of plasma particules inside a tokamak**, two software tools, providing a post-mortem analysis, have been designed to manage the memory optimization of **GYSELA** [20]. The first one is a visualization tool. It plots the memory consumption of the code along an execution. This tool helps the developer to localize where happens the memory peak and to wonder how he can modify the code to decrease it. On the same graphic, the names of the allocated structures are labelled, which gives a significant hint on the modifications to apply. The second tool concerns the prediction of the peak memory. Given an input set of parameters, we can replay the allocations of the code in an offline mode. With this tool, we can deduce accurately the value of the memory peak and where it happens. Thank to this prediction we know which size of mesh is possible under a given architecture.

This work is carried on in the framework of Fabien Rozar's PhD in collaboration with CEA Cadarache.

In the first part of our research work concerning the parallel **aerodynamic code** FLUSEPA, an intermediate version based on the previous one has been developed. By using an hybrid OpenMP/MPI parallelism based on a domain decomposition, we achieved a faster version of the code and the temporal adaptive method used without bodies in relative motion has been tested successfully for real complex 3D-cases using up to 400 cores. Moreover, an asynchronous strategy for computing bodies in relative motion and mesh intersections has been developed and the test of this feature is currently in progress. The next step will be to design a new fully asynchronous code based on a task graph description to be executed on a modern runtime system like **StarPU**. This work is carried on in the framework of Jean-Marie Couteyen's PhD in collaboration with Astrium Les Mureaux.



## PHOENIX Project-Team

# 6. New Results

## 6.1. Design-Driven Development Methodology for Resilient Computing

Critical systems have to face changes, either to meet new user requirements or because of changes in the execution context. Often, these changes are made at runtime because the system is too critical to be stopped. Such systems are called *resilient systems*. They have to guarantee dependability despite runtime evolution. For example, in the domain of pervasive computing, building management systems (*e.g.*, anti-intrusion, fire protection system, access control) have to be resilient as they are in charge of people safety and have to run in a continuous way.

To mitigate faults at runtime, dependable systems are augmented with fault tolerance mechanisms such as replication techniques or degraded modes of operation. However, these mechanisms cover a large spectrum of areas ranging from hardware to distributed platforms, to software components. As a consequence, the need of fault-tolerance expertise is spread throughout the software development process, making it difficult to trace the dependability requirements. The fault tolerance mechanisms have to be systematically and rigorously applied in order to guarantee the conformance between the application runtime behavior and the dependability requirements. This integration becomes even more complex when taking into account runtime adaptation. Indeed, a change in the execution context of an application may require to adapt the fault tolerance mechanisms. For example, a decrease of the network bandwidth may require to change the replication mechanism for one requiring less network bandwidth (*e.g.*, Leader-Follower Replication instead of Primary-Backup Replication).

Without a clear separation of the functional and fault-tolerance concerns, ensuring dependability becomes a daunting task for programmers, whose outcome is unpredictable. In this context, design-driven development approaches are of paramount importance because the design drives the development of the application while ensuring the traceability of the dependability requirements. However, because most existing approaches are general purpose, their guidance is limited, causing inconsistencies to be introduced in the design and along the development process. This situation calls for an integrated development process centered around a conceptual framework that allows to guide the development process of a resilient application in a systematic manner.

In this work, we propose a novel approach that relies on a design language which is extended with fault-tolerance declarations. To further raise the level of abstraction, our development approach revolves around the Sense-Compute-Control paradigm. The design is then compiled into a customized programming framework that drives and supports the development of the application. To face up changes in the execution context, our development methodology relies on a component-based approach, allowing fine-grained runtime adaptation. This design-driven development approach ensures the traceability of the dependability requirements and preserves the separation of concerns, despite runtime evolution.

This work was funded by the Inria collaboration program (in french, actions de recherches collaboratives). The Serus ARC includes the Phoenix project-team (Bordeaux), the ADAM project-team (Lille) and the TSF-LAAS group (Toulouse). These accomplishments were part of Quentin Enard's PhD studies [14]. This work has been published at the International Conference on Component-based Software Engineering (CBSE'13) [23].

## 6.2. A Case for Human-Driven Software Development

Human-Computer Interaction (HCI) defines a range of principles and methodologies to design User Interfaces (UIs), aiming (1) to improve the interaction between users and computers, (2) to address how interfaces are implemented, leveraging techniques such as program generation and component architectures, and (3) to propose methods to evaluate and compare interfaces.

Despite the many successes of HCI, when it comes to software development, this domain expertise often does not go beyond guidelines (*e.g.*, ISO/TR 22411:2008 addressing the needs of the elderly and users with disabilities). Sometimes, guidelines are mapped into UI design artifacts. However, for a lack of tools, these artifacts remain contemplative. As a consequence, there exists a gap between UI design and software development. This gap is not typical of the HCI domain. Yet, its consequences are dramatically increasing in importance as software systems intertwine with our daily activities, both professional and domestic. Nowadays, a host of systems are playing a critical role for users in terms of safety, privacy, *etc.*

To bridge the gap between UI design and software development, our approach consists in making UI design a full-fledged dimension of software design. We introduce a language dedicated to designing UIs in a high-level manner, while capturing the key requirements of user interaction. We go beyond a contemplative approach and process a UI design artifact to produce a dedicated programming framework that supports the implementation of all the dimensions expressed in a design artifact. This programming framework guides the stakeholders during the development process, while ensuring the conformance between the UI design and its implementation over time.

This work has been published at the International Conference on Software Engineering (ICSE'13, NIER track) [21].

### **6.3. Technological Support for Self-Regulation of Children with Autism**

Children with Autism Spectrum Disorders (ASD) have difficulties to self-regulate emotions, impeding their inclusion in a range of mainstreamed environments. Self-regulating emotions has been shown to require recognizing emotions and invoking specific coping strategies.

In the context of the School+ research project, we have developed an application dedicated to self-regulating emotions in children with ASD. Ten children with ASD have experimentally tested this tablet-based application over a period of three months in a mainstreamed school. A collaborative learning approach, involving parents, teachers and a school aid, was used 1) to train students to operate the tablet and our application autonomously, and 2) to facilitate the adoption of our intervention tool.

This study shows that our application was successful in enabling students with ASD to self-regulate their emotions in a school environment. Our application helped children with autism to recognize and name their emotions, and to regulate them using idiosyncratic, parent-child, coping strategies, supported by multimedia contents.

This work is in the context of the School+ national research project funded by the French Ministry of National Education. This work is part of Charles Fage's PhD studies.

## **RUNTIME Project-Team**

# **6. New Results**

## **6.1. SIMD Analysis Support in MAQAO**

Either on ARM and x86 architectures, compilers and tools are needed for automatic and efficient vectorization. Although commercial compilers (e.g. IBM xlc, Intel icc, PGI pgcc) have made significant advances in auto-vectorization, a lot of source codes still remain too complicated for a compiler to vectorize, particularly when complex data structures are involved, or because of the lack of information at compile time. However, when vectorization fails, compilers leave the user with little clues about the cause of the failure, even though in certain cases moderate modifications could be applied on the source code to enable the compiler to vectorize.

Thus, the main objective for this work was to analyse SIMD vectorization potentials through loop detection. Parallelism detection is done through the instrumentation of the binary codes, capturing all memory streams in target loops and computing memory dependences using MAQAO. When combined to a static analysis for register dependences, this technique ensures that parallel slices of computation will be detected.

From a practical point of view, this work consists in the capture of the trace and its processing to extract memory reference patterns. To do so, we made use of the current state of the art MAQAO for instrumentation and trace capture on Intel architectures. We then implemented the dependence analysis on memory traces for performing loop pattern recognition. Finally, using this mechanism for loop pattern recognition, we can conclude about the vectorization potential of computation intensive loop nests. The dependence analysis does not depend on the target architecture, hence results computed for x86 architectures are valuable for ARM target as well.

## **6.2. NUMA-aware fine grain parallelization for multi-core architecture**

Today, popular frameworks like Intel TBB or OpenMP offer a task based programming interface that allows to easily parallelize algorithms in shared memory. We have proposed some improvements to these task-based parallelization frameworks in order to cope with the problem of expressing an algorithm with a suitable task grain size and with the problem of Non Uniform Memory Accesses that degrades performance. In its current prototype state, our framework does not fully automate the selection of an optimal grain size. However, it significantly helps the programmer by proposing a simple interface to deal with DAG coarsening.

We have shown the benefits of this work on the parallelization of a sparse ILU preconditioner which is a challenging application with respect to task grain tuning and NUMA effect to an Intel TBB implementation. To improve even more the NUMA aspects, we are working on improving the task scheduler with cache-aware hierarchical scheduling support using a similar approach as the one implemented in the Bubblesched thread scheduler.

## **6.3. Task scheduling over heterogeneous architectures**

We continued our work on extending STARPU to master exploitation of Heterogeneous Platforms through dynamic task scheduling, leading to the release of STARPU 1.1. We have extended our lightweight DSM to support out-of-core scheduling over disks. We have finished integrating STARPU with SIMGRID and obtained very accurate simulated times, which allows to experiment scheduling heuristics without having to actually execute the application on the target platform, thus tremendously reducing experimentation time and resource consumption.

We have modularized the scheduling part of STARPU, which permits to create complex schedulers by assembling simple scheduling components. This will allow theoreticians to work on writing the simple scheduling components without having to deal with the technical parts of the scheduling, performed in other scheduling components.

We have also collaborated with various research project to leverage the potential of STARPU: for instance, the PaStiX sparse matrix solver was ported over STARPU, so that we improved the dynamic task and management for applications with such fine-grain task size. This resulted with fair-enough performance on CPUs, compared to the hand-optimized static scheduler of PaStiX, and very promising performance on CPUs + GPUs. EADS ported its sparse hmatrix solver over STARPU, and we collaborated to work on adding STARPU support for communicating sparse data over MPI.

#### 6.4. Task Size Control with XcalableMP/StarPU

On the work sharing among GPUs and CPU cores on GPU equipped clusters, it is a critical issue to select the task computational weights suited to these heterogeneous computing resources. We have been developing a solution for this problem, based on the cooperation of a PGAS language named XcalableMP (developed at the University of Tsukuba) together with a runtime sytem named XMP-dev/StarPU building on the work of the University of Tsukuba and on the StarPU platform developed by the Inria Runtime Team. Through the development, we found the necessity of adaptive task weight control for the GPU/CPU work sharing to achieve the best performance for various application codes. In particular, the language was extended to add a new feature allowing to alter the task size to be assigned to these heterogeneous resources dynamically during application execution. As a result of performance evaluation on several benchmarks, we confirmed the proposed feature correctly works and perform well even for relatively small size of problems.

#### 6.5. Scheduling contexts for StarPU

Scheduling context is an extension of STARPU that allows multiple parallel codes to run concurrently with minimal interference. A scheduling context encapsulates an instance of the runtime system, and runs on top of a subset of the available processing units (i.e. regular cores or GPU accelerators). In order to maximize the overall efficiency of applications, contexts can be dynamically shrunk or expanded by a *hypervisor* that periodically gathers performance statistics inside each context (e.g. resource utilization, computation progress) and tries to determine how resources should be assigned to contexts so as to minimize the overall execution time. We have demonstrated the relevance of this approach using benchmarks invoking multiple high performance linear algebra kernels simultaneously on top of heterogeneous multicore machines. We have shown that our mechanism can dramatically improve the overall application run time (-34%), most notably by reducing the average cache miss ratio (-50%).

#### 6.6. Load-balancing with TreeMatch

In the context of the Joint Laboratory for Petascale Computing (JLPC) included Inria and the University of Illinois at Urbana, we developed two load balancers for Charm++.

The two load-balancers we wrote take into account both the computing power and the hierarchical topology depending on the fact that the application is compute-bound or communication-bound. This work is based on our TREEMATCH library that computes process placement in order to reduce an application communication costs based on the hardware topology. Compared to some other solutions based on weighted topologies (latency, bandwidth, ...), ours is fully dynamic because we use only a qualitative approach for our representation of the hardware architecture.

The first load balancer is designed for compute-bound applications as it favours the leveling of CPU loads. The second load balancer focuses on communication-bound applications as it first reduces the congestion on the upper links in the topology tree.

These two load balancers gave us improvements for some applications up to 10% of the execution time.

## **6.7. List scheduling in embedded systems taking into account memory constraints**

Video decoding and image processing in embedded systems are subject to strong resource constraints, particularly in terms of memory. List-scheduling heuristics with static priorities (HEFT, SDC, etc.) being the often-cited solution due to both their good performance and their low complexity, we propose a method aimed at introducing the notion of memory into them. Moreover, we show that through appropriate adjustment of task priorities and judicious resort to insertion-based policy, speedups up to 20% can be achieved. Lastly, we show that our technique allows to prevent deadlock and to substantially reduce the required memory footprint compared to classic list-scheduling heuristics.

## **6.8. NewMadeleine generic multi-threading**

The PIOMan progression engine utilized in NewMadeleine used to rely on the Marcel specific multi-threading library, with dedicated hooks and close co-operation between libraries. It restricted the target platforms and applications, and was considered as a constraint by users. We have designed mechanisms to make communication progress without hooks in the thread scheduler, able to run on any system with a pthread library. We have re-written PIOMan from the ground up to implement these mechanisms, and based on lock-free structures, with scalability in mind. A proof-of-concept port to the Intel Xeon Phi has been implemented in cooperation with the University of Tokyo, using the DCFA (Direct Communication Facility for manycore-based Accelerators) library to access InfiniBand boards from the Xeon Phi.

## FLOWERS Project-Team

## 6. New Results

### 6.1. Robotic and Computational Models of Human Development

#### 6.1.1. *Computational models of information-seeking, curiosity and attention*

**Participants:** Pierre-Yves Oudeyer, Manuel Lopes.

An associated team, called Neurocuriosity, was created between Flowers and the Cognitive Neuroscience lab of Jacqueline Gottlieb at Univ. Columbia, NY. The goal of this associated team is to investigate mechanisms of spontaneous exploration and learning in humans by setting up experiments allowing to confirm or falsify predictions made by computational models previously developed by the team. This constitutes a crucial collaboration between developmental robotics and cognitive neuroscience. This joint work already led to a major publication on curiosity and information seeking, in the prestigious Trends in Cognitive Science journal (impact factor: 16.5). [27]

**Abstract:** Intelligent animals devote much time and energy to exploring and obtaining information, but the underlying mechanisms are poorly understood. We review recent developments on this topic that have emerged from the traditionally separate fields of machine learning, eye movements in natural behavior, and studies of curiosity in psychology and neuroscience. These studies show that exploration may be guided by a family of mechanisms that range from automatic biases toward novelty or surprise to systematic searches for learning progress and information gain in curiosity-driven behavior. In addition, eye movements reflect visual information searching in multiple conditions and are amenable for cellular-level investigations. This suggests that the oculomotor system is an excellent model system for understanding information-sampling mechanisms.

##### 6.1.1.1. *Formalizing Imitation Learning*

**Participants:** Thomas Cederborg, Pierre-Yves Oudeyer.

An original formalization of imitation learning was elaborated. Previous attempts to systematize imitation learning has been limited to categorizing different types of demonstrator goals (for example defining success in terms of the sequential joint positions of a dance, or in terms of environmental end states), and/or been limited to a smaller subset of imitation (such as learning from tele-operated demonstrations). The formalism proposed attempts to describe a large number of different types of learning algorithms using the same notation. Any type of algorithm that modifies a policy based on observations of a human, is treated as an interpretation hypothesis of this behavior. One example would be an update algorithm that updates a policy, partially based on the hypothesis that the demonstrator succeeds at demonstrations with probability 0.8, or an update algorithm that assumes that a scalar value is an accurate evaluation of an action compared to the latest seven actions. The formalism aims to give a principled way of updating these hypotheses, either rejecting some of a set of hypotheses regarding the same type of behavior, or set of parameters of an hypothesis. Any learning algorithm that modifies policy based on observations of a human that wants an agent to do something or act in some way, is describable as an interpretation hypothesis. If the learning algorithm is static, this simply corresponds to an hypothesis that is not updated based on observations. A journal article [26].

##### 6.1.1.2. *Self-Organization of Early Vocal Development in Infants and Machines: The Role of Intrinsic Motivation*

**Participants:** Clément Moulin-Frier, Sao Mai Nguyen, Pierre-Yves Oudeyer.

We bridge the gap between two issues in infant development: vocal development and intrinsic motivation. We propose and experimentally test the hypothesis that general mechanisms of intrinsically motivated spontaneous exploration, also called curiosity-driven learning, can self-organize developmental stages during early vocal learning and explain several aspects observed in infants (Figure 20). We introduce a computational model of intrinsically motivated vocal exploration, which allows the learner to autonomously structure its own vocal experiments, and thus its own learning schedule, through a drive to maximize competence progress. This model relies on a physical model of the vocal tract, the auditory system and the agent's motor control, as well as vocalizations of social peers. We present computational experiments that show how such a mechanism can explain the adaptive transition from vocal self-exploration with little influence from the speech environment, to a later stage where vocal exploration becomes influenced by vocalizations of peers (Figure 21). Within the initial self-exploration phase, we show that a sequence of vocal production stages self-organizes, and shares properties with data from infant developmental psychology: the vocal learner first discovers how to control phonation, then focuses on vocal variations of unarticulated sounds, and finally automatically discovers and focuses on babbling with articulated proto-syllables (Figure 22). As the vocal learner becomes more proficient at producing complex sounds, imitating vocalizations of peers starts to provide high learning progress explaining an automatic shift from self-exploration to vocal imitation.

This work has been recently accepted in the journal *Frontiers in Psychology, Cognitive Science* [30].

#### 6.1.1.3. *Emergent Proximo-Distal Motor Development through Adaptive Exploration, applied to Reaching and Vocal Learning*

**Participants:** Freek Stulp, Pierre-Yves Oudeyer, Jules Brochard, Clément Moulin-Frier.

Life-long robot learning in the high-dimensional real world requires guided and structured exploration mechanisms. In this developmental context, we have investigated the use of the  $PI^2$ -CMAES episodic reinforcement learning algorithm, which is able to learn high-dimensional motor tasks through adaptive control of exploration. By studying  $PI^2$ -CMAES in a reaching task on a simulated arm, we observe two developmental properties. First, we show how  $PI^2$ -CMAES autonomously and continuously tunes the global exploration/exploitation trade-off, allowing it to re-adapt to changing tasks. Second, we show how  $PI^2$ -CMAES spontaneously self-organizes a maturational structure whilst exploring the degrees-of-freedom (DOFs) of the motor space. In particular, it automatically demonstrates the so-called *proximo-distal maturation* observed in humans: after first freezing distal DOFs while exploring predominantly the most proximal DOF, it progressively frees exploration in DOFs along the proximo-distal body axis. These emergent properties suggest the use of  $PI^2$ -CMAES as a general tool for studying reinforcement learning of skills in life-long developmental learning contexts. This work was published in the *Paladyn Journal of Behavioral Robotics* [36].

This model of emergent developmental freezing and unfreezing of degrees of freedom was then applied to infant vocal development. For this aim, we used an articulatory synthesizer which is a computer model of the human vocal tract and the ear. While testing different possibilities, the algorithm eventually creates learning structures, which are more efficient than random motor babbling. Using the algorithm with a vocal synthesizer, we show that it can reproduce a babbling infant's characteristic: the predominance of the jaw over the other articulators, namely the canonical babbling.

This is the first study to our knowledge of emergent maturation in speech. Without presupposing any biological or social constraint, we give a new explanation of the jaw predominance in babbling, based on freezing and freeing the degrees of freedom in an adaptive maturation scheme to improve learning. This provides an original hypothesis regarding the emergence of canonical babbling in infant vocal development.

This last work was performed during the internship of Jules Brochard in 2013 and a journal article is currently being written.

#### 6.1.2. *COSMO (“Communicating about Objects using Sensory-Motor Operations”): a Bayesian modeling framework for studying speech communication and the emergence of phonological systems*

**Participants:** Clément Moulin-Frier, Jean-Luc Schwartz, Julien Diard, Pierre Bessi re.



*Figure 20. Rapid view of the first year of infant vocal development.*





*Figure 21. Our model displays an adaptive transition from vocal self-exploration with little influence from the speech environment, to a later stage where vocal exploration becomes influenced by vocalizations of peers.*



Figure 22. Within the self-exploration phase, our model first discovers how to control phonation, then focuses on vocal variations of unarticulated sounds, and finally automatically discovers and focuses on babbling with articulated proto-syllables.

This work began with the PhD thesis of Clément Moulin-Frier at GIPSA-Lab, Grenoble, France, supervised by Jean-Luc Schwartz (GIPSA-Lab, CNRS), Julien Diard (LPNC, CNRS) and Pierre Bessière (College de France, CNRS). A few papers were finalized during his post-doc at FLOWERS in 2012. Firstly, an international journal paper based on the PhD thesis work of Raphael Laurent (GIPSA-Lab), extending Moulin-Frier’s model, was published [108], as well as a commentary in *Behavioral and Brain Sciences* [97]. Both these papers provide computational arguments based on a sensory-motor cognitive model to feed the age-old debate of motor vs. auditory theories of speech perception. Secondly, in another journal paper under the submission process, we attempt to derive some properties of phonological systems (the sound systems of human languages) from the mere properties of speech communication. We introduce a model of the cognitive architecture of a communicating agent, called COSMO (for “Communicating about Objects using Sensory-Motor Operations”) that allows expressing in a probabilistic way the main theoretical trends found in the speech production and perception literature. This allows a computational comparison of these theoretical trends, helping to identify the conditions that favor the emergence of linguistic codes. We present realistic simulations of phonological system emergence showing that COSMO is able to predict the main regularities in vowel, stop consonant and syllable systems in human languages.

This work is currently under consideration as a target article for a special issue in an international journal. Pierre-Yves Oudeyer joined this process as a member of the editing committee.

### 6.1.3. Recognizing speech in a novel accent: the Motor Theory of Speech Perception reframed

**Participants:** Clément Moulin-Frier, Michael Arbib.

Clément Moulin-Frier engaged this work with Michael Arbib during his 6-month visit in 2009 at the USC Brain Project, University of Southern California, Los Angeles, USA, during his PhD thesis at Gipsa-Lab, Grenoble. He continues to write a journal article during his post-doc in the Flowers team in 2012-2013. This paper has been published recently in *Biological Cybernetics* [29], in which we offer a novel computational

model of foreign-accented speech adaptation, together with a thorough analysis of its implications with respect to the motor theory of speech perception.

## 6.2. Life-Long Robot Learning and Development of Motor and Social Skills

### 6.2.1. Active Learning and Intrinsic Motivation

#### 6.2.1.1. Active Learning of Inverse Models with Goal Babbling

**Participants:** Adrien Baranes, Pierre-Yves Oudeyer.

We have continued to elaborate and study our Self-Adaptive Goal Generation - Robust Intelligent Adaptive Curiosity (SAGG-RIAC) architecture as an intrinsically motivated goal exploration mechanism which allows active learning of inverse models in high-dimensional redundant robots. Based on active goal babbling, this allows a robot to efficiently and actively learn distributions of parameterized motor skills/policies that solve a corresponding distribution of parameterized tasks/goals. The architecture makes the robot sample actively novel parameterized tasks in the task space, based on a measure of competence progress, each of which triggers low-level goal-directed learning of the motor policy parameters that allow to solve it. For both learning and generalization, the system leverages regression techniques which allow to infer the motor policy parameters corresponding to a given novel parameterized task, and based on the previously learnt correspondences between policy and task parameters.

We have conducted experiments with high-dimensional continuous sensorimotor spaces in three different robotic setups: 1) learning the inverse kinematics in a highly-redundant robotic arm, 2) learning omnidirectional locomotion with motor primitives in a quadruped robot [2324](#), 3) an arm learning to control a fishing rod with a flexible wire. We show that 1) exploration in the task space can be a lot faster than exploration in the actuator space for learning inverse models in redundant robots; 2) selecting goals maximizing competence progress creates developmental trajectories driving the robot to progressively focus on tasks of increasing complexity and is statistically significantly more efficient than selecting tasks randomly, as well as more efficient than different standard active motor babbling methods; 3) this architecture allows the robot to actively discover which parts of its task space it can learn to reach and which part it cannot.

This work was published in the journal *Robotics and Autonomous Systems* [\[25\]](#).

#### 6.2.1.2. Learning Exploration Strategies in Model-based Reinforcement Learning

**Participants:** Manuel Lopes, Todd Hester, Peter Stone, Pierre-Yves Oudeyer.

We studied how different exploration algorithms can be combine and selected at runtime. Typically the user must hand-tune exploration parameters for each different domain and/or algorithm that they are using. We introduced an algorithm called leo for learning to select among different exploration strategies on-line. This algorithm makes use of bandit-type algorithms to adaptively select exploration strategies based on the rewards received when following them. We show empirically that this method performs well across a set of five domains. In contrast, for a given algorithm, no set of parameters is best across all domains. Our results demonstrate that the leo algorithm successfully learns the best exploration strategies on-line, increasing the received reward over static parameterizations of exploration and reducing the need for hand-tuning exploration parameters [\[46\]](#).

#### 6.2.1.3. Active Inverse Reinforcement Learning through Generalized Binary Search

**Participants:** Manuel Lopes, Francisco Melo.

We contributed the first aggressive active learning algorithm for nonseparable multi-class classification. We generalize an existing active learning algorithm for binary classification [\[116\]](#) to the multi-class setting, and identify mild conditions under which the proposed method provably retains the main properties of the original algorithm, namely consistency and sample complexity. In particular, we show that, in the binary case, our method reduces to the original algorithm of [\[116\]](#). We then contribute an extension of our method to multi-label settings, identify its main properties and discuss richer querying strategies. We conclude the paper with two illustrative application examples. The first application features a standard text-classification problem. The second application scenario features a learning from demonstration setting. In both cases we demonstrate the advantage of our active sampling approach against random sampling. We also discuss the performance of the proposed approach in terms of the derived theoretical bounds.



*Figure 23. Experimenting SAGG-RIAC for learning an inverse model for omnidirectional locomotion of a quadruped robot. The quadruped robot is controlled using 24 dimensional motor synergies parameterized with 24 continuous values : 12 for the amplitudes and 12 others for the phases of a sinusoid tracked by each motor. Experiments consider a task space  $u, v, \alpha$  which corresponds to the 2D position and orientation of the quadruped.*



*Figure 24. Evolution of the quality of the learnt inverse model for the quadruped robot experiment, depending on various exploration strategies (measured as mean error over a set of uniformly distributed goals generated independantly from learning trials).*

#### 6.2.1.4. Exploration strategies in developmental robotics: a unified probabilistic framework

**Participants:** Clément Moulin-Frier, Pierre-Yves Oudeyer.

We present a probabilistic framework unifying two important families of exploration mechanisms recently shown to be efficient to learn complex non-linear redundant sensorimotor mappings. These two explorations mechanisms are: 1) goal babbling, 2) active learning driven by the maximization of empirically measured learning progress. We show how this generic framework allows to model several recent algorithmic architectures for autonomous exploration. Then, we propose a particular implementation using Gaussian Mixture Models, which at the same time provides an original empirical measure of the competence progress. Finally, we perform computer simulations on two simulated setups: the control of the end effector of a 7-DoF arm and the control of the formants produced by an articulatory synthesizer. We are able to reproduce previous results from [25] with the advantages of a clean and compact probabilistic framework to efficiently express, implement and compare various exploration strategies on developmental robotics setups.

This work was published in three international conferences [54], [56], [55].

#### 6.2.1.5. Autonomous Reuse of Motor Exploration Trajectories

**Participants:** Fabien Benureau, Pierre-Yves Oudeyer.

We developed an algorithm for transferring exploration strategies between tasks that share a common motor space in the context of lifelong autonomous learning in robotics. In such context sampling is costly, and exploration can take a long time before finding interesting, learnable data about a task. Our algorithm shows that we can significantly reduce sampling by reusing past data of other learned tasks, with no need of external knowledge or specific task structure. The algorithm does not transfer observations, or make assumptions about how the learning is conducted. Instead, only selected motor commands are transferred between tasks, chosen autonomously according to an empirical measure of learning progress. We show that on a wide variety of variations from a source task, such as changing the object the robot is interacting with or altering the morphology of the robot, this simple and flexible transfer method increases early performance significantly in the new task. We also investigate the limitation of this algorithm on specific situations.

This work has been published at ICDL, in Osaka [40].

### 6.2.2. Learning and optimization of motor policies

#### 6.2.2.1. Off-Policy Actor-Critic

**Participants:** Thomas Degris, Martha White, Richard Sutton.

Actor-critic architectures are an interesting candidate for learning with robots: they can represent complex stochastic policies suitable for robots, they can learn online and incrementally and their per-time-step complexity scales linearly with the number of learned weights. Moreover, interesting connections have been identified in the existing literature with neuroscience. Until recently, however, practical actor-critic methods have been restricted to the on-policy setting, in which the agent learns only about the policy it is executing.

In an off-policy setting, on the other hand, an agent learns about a policy or policies different from the one it is executing. Off-policy methods have a wider range of applications and learning possibilities. Unlike on-policy methods, off-policy methods are able to, for example, learn about an optimal policy while executing an exploratory policy, learn from demonstration, and learn multiple tasks in parallel from a single sensory-motor interaction with an environment. Because of this generality, off-policy methods are of great interest in many application domains.

We have presented the first actor-critic algorithm for off-policy reinforcement learning. Our algorithm is online and incremental, and its per-time-step complexity scales linearly with the number of learned weights. We have derived an incremental, linear time and space complexity algorithm that includes eligibility traces and empirically show better or comparable performance to existing algorithms on standard reinforcement-learning benchmark problems. This work was reproduced independently by Saminda Abeyruwan from the University of Miami.

### 6.2.2.2. Auto-Actor Critic

**Participant:** Thomas Degris.

As mentioned above, actor–critic architectures are an interesting candidate for robots to learn new skills in unknown and changing environments. However, existing actor–critic architectures, as many machine learning algorithms, require manual tuning of different parameters to work in the real world. To be able to systematize and scale-up skill learning on a robot, learning algorithms need to be robust to their parameters. The Flowers team has been working on making existing actor–critic algorithms more robust to make them suitable to a robotic setting. Results on standard reinforcement learning benchmarks are encouraging. This work will be submitted to international conference related with reinforcement learning. Interestingly, the methods developed in this work also offer a new formalism to think about different existing themes of Flowers research such as curiosity and maturational constraints.

### 6.2.2.3. Deterministic Policy Gradient Algorithms

Thomas Degris and colleagues from UCL and Deepmind have considered deterministic policy gradient algorithms for reinforcement learning with continuous actions. The deterministic policy gradient has a particularly appealing form: it is the expected gradient of the action-value function. This simple form means that the deterministic policy gradient can be estimated much more efficiently than the usual stochastic policy gradient. To ensure adequate exploration, we introduce an off-policy actor-critic algorithm that learns a deterministic target policy from an exploratory behaviour policy. We demonstrate that deterministic policy gradient algorithms can significantly outperform their stochastic counterparts in high-dimensional action spaces. [58]

### 6.2.2.4. Relationship between Black-Box Optimization and Reinforcement Learning

**Participant:** Freek Stulp.

Policy improvement methods seek to optimize the parameters of a policy with respect to a utility function. There are two main approaches to performing this optimization: reinforcement learning (RL) and black-box optimization (BBO). In recent years, benchmark comparisons between RL and BBO have been made, and there has been several attempts to specify which approach works best for which types of problem classes.

We have made several contributions to this line of research by: 1) Defining four algorithmic properties that further clarify the relationship between RL and BBO. 2) Showing how the derivation of ever more powerful RL algorithms displays a trend towards BBO. 3) Continuing this trend by applying two modifications to the state-of-the-art  $PI^2$  algorithm, which yields an algorithm we denote  $PI^{BB}$ . We show that  $PI^{BB}$  is a BBO algorithm, and, more specifically, that it is a special case of the state-of-the-art CMAES algorithm. 4) Demonstrating that the simpler  $PI^{BB}$  achieves similar or better performance than  $PI^2$  on several evaluation tasks. 5) Analyzing why BBO outperforms RL on these tasks. These contributions have been published on HAL [129], and in Paladyn: Journal of Behavioral Robotics [36].

### 6.2.2.5. Probabilistic optimal control: a quasimetric approach

**Participants:** Steve N’Guyen, Clément Moulin-Frier, Jacques Droulez.

During his previous post-doc at the Laboratoire de Physiologie de la Perception et de l’Action (College de France, Paris), Clément Moulin-Frier joined Jacques Droulez and Steve N’Guyen to work on an alternative and original approach of probabilistic optimal control called *quasimetric*. A journal paper was published in PLoS ONE in December 2013 [31], where the authors propose a new approach dealing with decision making under uncertainty.

## 6.2.3. Social learning and intrinsic motivation

### 6.2.3.1. Socially Guided Intrinsic Motivation for Skill Learning

**Participants:** Sao Mai Nguyen, Pierre-Yves Oudeyer.

We have explored how social interaction can bootstrap the learning of a robot for motor learning. We first studied how simple demonstrations by teachers could have a bootstrapping effect on autonomous exploration with intrinsic motivation by building a learner who uses both imitation learning and SAGG-RIAC algorithm [25], and thus designed the SGIM-D (Socially Guided Intrinsic Motivation by Demonstration) algorithm [32], [24], [32] [114], [111]. We then investigated on the reasons of this bootstrapping effect [113], to show that demonstrations by teachers can both enhance more tasks to be explored, as well as favor more easily generalized actions to be used. This analysis is generalizable for all algorithms using social guidance and goal-oriented exploration. We then proposed to build a strategic learner who can learn multiple tasks and with multiple strategies. An overview and theoretical study of multi-task, multi-strategy Strategic Learning is presented in [99]. We also forsook to build a learning algorithm for more natural interaction with the human users. We first designed the SGIM-IM algorithm so that it can determine itself when it should ask for help from the teacher while trying to explore autonomously as long as possible so as to use as little of the teacher's time as possible [112]. After tackling with the problem of how and when to learn, we also investigated an active learner who can determine who to ask for help: in the case of two teachers available, SGIM-IM can determine which strategy to adopt between autonomous exploration and learning by demonstration, and which teacher enhances most learning progress for the learner [115], and ask him for help.



Figure 25. Illustration of SGIM-D and SGIM-IM algorithms

While the above results have been shown in simulation environments: of a simple deterministic air hockey game (fig. 25), and a stochastic fishing experiment with a real-time physical simulator (fig. 26), we are now building the experimental setup of the fishing experiment in order to carry out the experiments with naive users.

### 6.2.3.2. Adaptive task execution for implicit human-robot coordination



*Figure 26. Illustration of SGIM-D and SGIM-IM algorithms*





*Figure 27. Illustration of SGIM-D and SGIM-IM algorithms*

**Participants:** Ievgen Perederieiev, Manuel Lopes, Freek Stulp.

We began a project which goal is to study how computational models of multi-agent systems can be applied in situations where one agent is a human. We aim at applications where robots collaborate with humans for achieving complex tasks..

A very important capability for efficient collaborative work is the mutual agreement of a task and the ability to predict the behavior of others. We address such aspect by studying methods that increase the predictability of the robot actions. An efficient motor execution becomes the one that not just optimize speed and minimizes energy but also the one that improves the reliability of the team behavior. We are studying policy gradient methods and working on policy improvement algorithms ( $PI^2$ ,  $CEM$  and  $CMAES$ ). A feasibility study will consider a simple task between a robot and a person where the goal is to coordinate the way a set of three colored buttons is pressed.

## 6.2.4. Unsupervised learning of motor primitives

### 6.2.4.1. Clustering activities

**Participants:** Manuel Lopes, Luis Montesano, Javier Almingol.

Learning behaviors from data has applications in surveillance and monitoring systems, virtual agents and robotics among others. In our approach, we assume that in a given unlabeled dataset of multiple behaviors, it is possible to find a latent representation in a controller space that allows to generate the different behaviors. Therefore, a natural way to group these behaviors is to search a common control system that generate them accurately.

Clustering behaviors in a latent controller space has two major challenges. First, it is necessary to select the control space that generate behaviors. This space will be parameterized by a set of features that will change for different behaviors. Usually, each controller will minimize a cost function with respect to several task features. The latent representation is in turn defined by the selected features and their corresponding weight. Second, an unknown number of such controllers is required to generate different behaviors and the grouping must be based on the ability of the controller to generate the demonstrations using a compact set of controllers.

We propose a Dirichlet Process based algorithm to cluster behaviors in a latent controller space which encodes the dynamical system generating the observed trajectories. The controller uses a potential function generated as a linear combination of features. To enforce sparsity and automatically select features for each cluster independently, we impose a conditional Laplace prior over the controller parameters. Based on this models, we derive a sparse Dirichlet Process Mixture Model (DPMM) algorithm that estimates the number of behaviors and a sparse latent controller for each of them based on a large set of features [38].

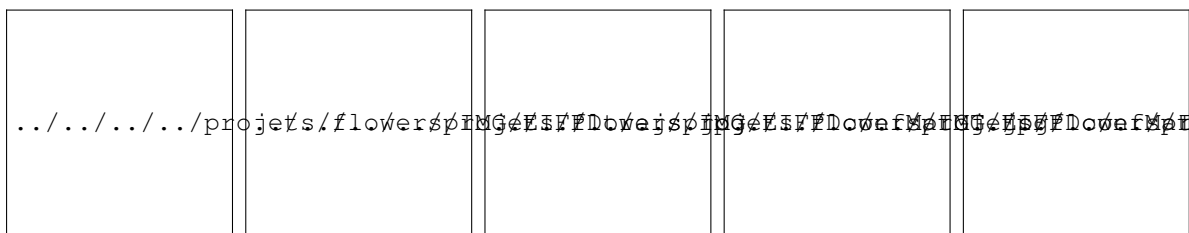


Figure 28. EIFPD dataset. (a) Trajectories of the EIFPD to be clustered (color is non-informative). (b-d) correspondence matrix for the 474 trajectories for the labeled ground truth, the KMeans in measurement space and the DPMM, respectively. (e) Reconstructed trajectories from the initial point using the estimated parameters of the DPMM algorithm. Due to the large number of clusters (37), colors are repeated for different clusters.

#### 6.2.4.2. *Learning the Combinatorial Structure of Demonstrated Behaviors with Inverse Reinforcement Control*

**Participants:** Olivier Mangin, Pierre-Yves Oudeyer.

We have elaborated and illustrated a novel approach to learning motor skills from demonstration. This approach combines ideas from inverse reinforcement learning, in which actions are assumed to solve a task, and dictionary learning. In this work we introduced a new algorithm that is able to learn behaviors by assuming that the observed complex motions can be represented in a smaller dictionary of concurrent tasks. We developed an optimization formalism and show how we can learn simultaneously the dictionary and the mixture coefficients that represent each demonstration. We presented results on a toy problem and shown that our algorithm finds an efficient set of primitive tasks where naive approaches such as PCA and using a dictionary built from random examples fail to achieve the same tasks. These results that were presented as [60], extend the ones from [103].

#### 6.2.4.3. *Interaction of Maturation and Intrinsic Motivation for Developmental Learning of Motor Skills in Robots*

**Participants:** Adrien Baranes, Pierre-Yves Oudeyer.

We have introduced an algorithmic architecture that couples adaptively models of intrinsic motivation and physiological maturation for autonomous robot learning of new motor skills. Intrinsic motivation, also called curiosity-driven learning, is a mechanism for driving exploration in active learning. Maturation denotes here mechanisms that control the evolution of certain properties of the body during development, such as the number and the spatio-temporal resolution of available sensorimotor channels. We argue that it is useful to introduce and conceptualize complex bidirectional interactions among these two mechanisms, allowing to actively control the growth of complexity in motor development in order to guide efficiently exploration and learning. We introduced a model of maturational processes, taking some functional inspiration from the myelination process in humans, and show how it can be coupled in an original and adaptive manner with the intrinsic motivation architecture SAGG-RIAC (Self-Adaptive Goal Generation - Robust Intelligent Adaptive Curiosity algorithm), creating a new system, called McSAGG-RIAC. We then conducted experiments to evaluate both qualitative and quantitative properties of these systems when applied to learning to control a high-dimensional robotic arm, as well as to learning omnidirectional locomotion in a quadruped robot equipped with motor synergies. We showed that the combination of active and maturational learning can allow to gain orders of magnitude in learning speed as well as reach better generalization performances. A journal article is currently being written.

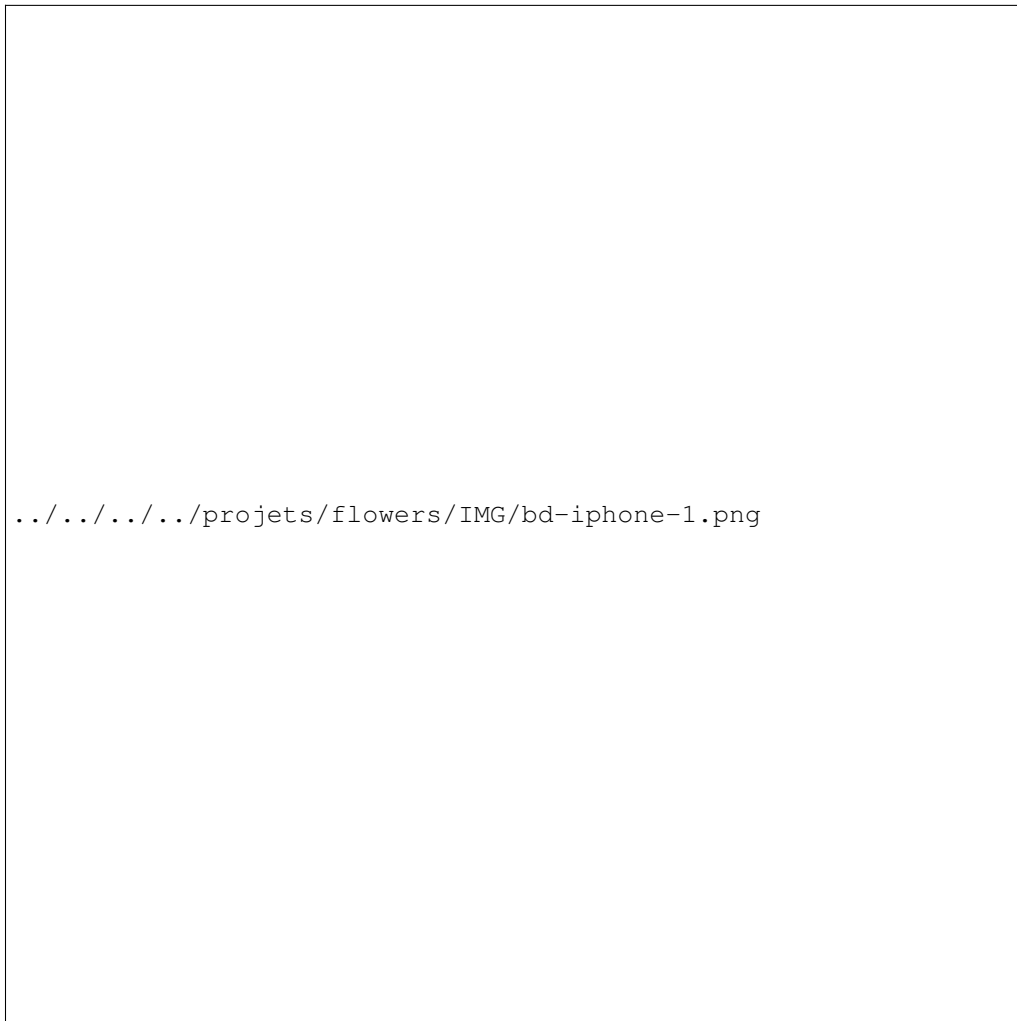
### 6.3. Autonomous and Social Perceptual Learning

#### 6.3.1. *The Impact of Human-Robot Interfaces on the Learning of Visual Objects*

**Participants:** Pierre Rouanet, Pierre-Yves Oudeyer, Fabien Danieau, David Filliat.

We have continued and finalized a large-scale study of the impact of interfaces allowing non-expert users to efficiently and intuitively teach a robot to recognize new visual objects. We identified challenges that need to be addressed for real-world deployment of robots capable of learning new visual objects in interaction with everyday users. We argue that in addition to robust machine learning and computer vision methods, well-designed interfaces are crucial for learning efficiency. In particular, we argue that interfaces can be key in helping non-expert users to collect good learning examples and thus improve the performance of the overall learning system. Then, we have designed four alternative human-robot interfaces: three are based on the use of a mediating artifact (smartphone, wiimote, wiimote and laser), and one is based on natural human gestures (with a Wizard-of-Oz recognition system). These interfaces mainly vary in the kind of feedback provided to the user, allowing him to understand more or less easily what the robot is perceiving, and thus guide his way of providing training examples differently. We then evaluated the impact of these interfaces, in terms of learning efficiency, usability and user's experience, through a real world and large scale user study. In this experiment, we asked participants to teach a robot twelve different new visual objects in the context of a robotic game. This game happens in a home-like environment and was designed to motivate and engage users in an interaction where using the system was meaningful. We then analyzed results that show significant differences among

interfaces. In particular, we showed that interfaces such as the smartphone interface allows non-expert users to intuitively provide much better training examples to the robot, almost as good as expert users who are trained for this task and aware of the different visual perception and machine learning issues. We also showed that artifact-mediated teaching is significantly more efficient for robot learning, and equally good in terms of usability and user's experience, than teaching thanks to a gesture-based human-like interaction. This work was published in the IEEE Transactions on Robotics [34].



*Figure 29. Smartphone Interface. To make the robot collect a new learning example, users have to first draw the robot's attention toward the object they want to teach through simple gestures. Once the robot sees the object, they touch the head of the robot to trigger the capture. Then, they directly encircle the area of the image that represents the object on the screen. The selected area is then used as the new learning example. The combination of the video stream and the gestures facilitate the achievement of joint attention.*

### **6.3.2. Developmental object learning through manipulation and human demonstration**

**Participants:** Natalia Lyubova, David Filliat.



*Figure 30. Wiimote + laser pointer interface. With this interface users can draw the robot's attention with a laser pointer toward an object. The laser spot is automatically tracked by the robot. They can ensure that the robot detects the spot thanks to haptic feedback on the Wiimote. Then, they can touch the head of the robot to trigger the capture of a new learning example. Finally, they encircle the object with the laser pointer to delimit its area which will be defined as the new learning example.*



*Figure 31. The real world environment designed to reproduce a typical living room. Many objects were added in the scene in order to make the environment cluttered.*



*Figure 32. iCub performing curiosity-driven exploration and active recognition of visual objects in 3D*

The goal of this work is to design a visual system for a humanoid robot. We used a developmental approach that allows a humanoid robot to continuously and incrementally learn entities through interaction with a human partner in a first stage before categorizing these entities into objects, humans or robot parts and using this knowledge to improve objects models by manipulation in a second stage. This approach does not require prior knowledge about the appearance of the robot, the human or the objects. The proposed perceptual system segments the visual space into proto-objects, analyses their appearance, and associates them with physical entities. Entities are then classified based on the mutual information with proprioception and on motion statistics. The ability to discriminate between the robot's parts and a manipulated object then allows to update the object model with newly observed object views during manipulation. We evaluate our system on an iCub robot, showing the independence of the self-identification method on the robot's hands appearances by wearing different colored gloves. The interactive object learning using self-identification shows an improvement in the objects recognition accuracy with respect to learning through observation only [52], [51].

### 6.3.3. *A Comparison of Geometric and Energy-Based Point Cloud Semantic Segmentation*

#### *Methods*

**Participants:** Mathieu Dubois, Alexander Gepperth, David Filliat.

The software we developed for object segmentation and recognition rely on a geometric segmentation of the space. We tested alternative methods for this semantic segmentation task in which the goal is to find some relevant classes for navigation such as wall, ground, objects, etc. Several effective solutions have been proposed, mainly based on the recursive decomposition of the point cloud into planes. We compare such a solution to a non-associative MRF method inspired by some recent work in computer vision.

The results [42] shows that the geometric method gives superior results for the task of semantic segmentation in particular for the object class. This can be explained by the fact that it incorporates a lot of domain knowledge (namely that indoor environments are made of planes and that objects lie on top of them). However, MRF segmentation gives interesting results and has several advantages. First most of its components can be used for other purpose or in other, less constrained, environments where domain knowledge is not available. For instance we could try to recognize more precisely the objects. Second it requires less tuning since most parameters are learned from the database. Third, it uses the appearance information which could help to identify different types of ground or wall (this was one of the goal in the CAROTTE challenge). Last but not least, as it gives a probabilistic output, it allows the robot to draw hypothesis on the environment and adapt its behavior. Therefore we think it is interesting to investigate improvements to improve the exploitation of the structure of the point clouds.

### 6.3.4. *Efficient online bootstrapping of sensory representations*

**Participant:** Alexander Gepperth.

This work [86] is a simulation-based investigation exploring a novel approach to the open-ended formation of multimodal representations in autonomous agents. In particular, we addressed here the issue of transferring (bootstrapping) features selectivities between two modalities, from a previously learned or innate reference representation to a new induced representation. We demonstrated the potential of this algorithm by several experiments with synthetic inputs modeled after a robotics scenario where multimodal object representations are bootstrapped from a (reference) representation of object affordances, focusing particularly on typical challenges in autonomous agents: absence of human supervision, changing environment statistics and limited computing power. We proposed an autonomous and local neural learning algorithm termed PROPRE (projection-prediction) that updates induced representations based on predictability: competitive advantages are given to those feature-sensitive elements that are inferable from activities in the reference representation, the key ingredient being an efficient online measure of predictability controlling learning. We verified that the proposed method is computationally efficient and stable, and that the multimodal transfer of feature selectivity is successful and robust under resource constraints. Furthermore, we successfully demonstrated robustness to noisy reference representations, non-stationary input statistics and uninformative inputs.

### 6.3.5. *Simultaneous concept formation driven by predictability*

**Participants:** Alexander Gepperth, Louis-Charles Caron.

This work [83] was conducted in the context of developmental learning in embodied agents who have multiple data sources (sensors) at their disposal. We developed an online learning method that simultaneously discovers meaningful concepts in the associated processing streams, extending methods such as PCA, SOM or sparse coding to the multimodal case. In addition to the avoidance of redundancies in the concepts derived from single modalities, we claim that meaningful concepts are those who have statistical relations across modalities. This is a reasonable claim because measurements by different sensors often have common cause in the external world and therefore carry correlated information. To capture such cross-modal relations while avoiding redundancy of concepts, we propose a set of interacting self-organization processes which are modulated by local predictability. To validate the fundamental applicability of the method, we conducted a plausible simulation experiment with synthetic data and found that those concepts which are predictable from other modalities successively "grow", i.e., become overrepresented, whereas concepts that are not predictable become systematically under-represented. We additionally explored the applicability of the developed method to real-world robotics scenarios.

### 6.3.6. *The contribution of context: a case study of object recognition in an intelligent car*

**Participants:** Alexander Gepperth, Michael Garcia Ortiz.

In this work [84], we explored the potential contribution of multimodal context information to object detection in an "intelligent car". The used car platform incorporates subsystems for the detection of objects from local visual patterns, as well as for the estimation of global scene properties (sometimes denoted scene context or just context) such as the shape of the road area or the 3D position of the ground plane. Annotated data recorded on this platform is publicly available as the "HRI RoadTraffic" vehicle video dataset, which formed the basis for the investigation. In order to quantify the contribution of context information, we investigated whether it can be used to infer object identity with little or no reference to local patterns of visual appearance. Using a challenging vehicle detection task based on the "HRI RoadTraffic" dataset, we trained selected algorithms (context models) to estimate object identity from context information alone. In the course of our performance evaluations, we also analyzed the effect of typical real-world conditions (noise, high input dimensionality, environmental variation) on context model performance. As a principal result, we showed that the learning of context models is feasible with all tested algorithms, and that object identity can be estimated from context information with similar accuracy as by relying on local pattern recognition methods. We also found that the use of basis function representations [1] (also known as "population codes" allows the simplest (and therefore most efficient) learning methods to perform best in the benchmark, suggesting that the use of context is feasible even in systems operating under strong performance constraints.

### 6.3.7. *Co-training of context models for real-time object detection*

**Participant:** Alexander Gepperth.

In this work [85], we developed a simple way to reduce the amount of required training data in context-based models of real-time object detection and demonstrated the feasibility of our approach in a very challenging vehicle detection scenario comprising multiple weather, environment and light conditions such as rain, snow and darkness (night). The investigation is based on a real-time detection system effectively composed of two trainable components: an exhaustive multiscale object detector (signal-driven detection), as well as a module for generating object-specific visual attention (context models) controlling the signal-driven detection process. Both parts of the system require a significant amount of ground-truth data which need to be generated by human annotation in a time-consuming and costly process. Assuming sufficient training examples for signal-based detection, we showed that a co-training step can eliminate the need for separate ground-truth data to train context models. This is achieved by directly training context models with the results of signal-driven detection. We demonstrated that this process is feasible for different qualities of signal-driven detection, and maintains the performance gains from context models. As it is by now widely accepted that signal-driven object detection can be significantly improved by context models, our method allows to train strongly improved detection systems without additional labor, and above all, cost.



## 6.4. Robot Multimodal Learning of Language and Action

### 6.4.1. Learning semantic components from sub-symbolic multi-modal perception

**Participants:** Olivier Mangin, Caio Tomazelli Da Silva Oliveira, Pierre-Yves Oudeyer.

Perceptual systems often include sensors from several modalities. However, existing robots do not yet sufficiently discover patterns that are spread over the flow of multimodal data they receive. In this work we establish a framework to learn multimodal components from perception. We use a nonnegative matrix factorization algorithm to learn a dictionary of components that represent meaningful elements present in the multimodal perception, without providing the system with a symbolic representation of the semantics. In [53] we illustrate this framework by showing how a learner discovers word-like components from observation of gestures made by a human together with spoken descriptions of the gestures, and how it captures the semantic association between the two. These experiments were further extended during the internship of Caio Tomazelli Da Silva Oliveira. Importantly these experiments provide an example of language grounding into perception, and feature global understanding of a linguistic task without requiring its compositional understanding. The code of the experiments from [53] as well as the motion dataset have been made publicly available to improve the reproducibility of the experiments.

### 6.4.2. Curiosity-driven exploration and interactive learning of visual objects with the ICub robot

**Participants:** Mai Nguyen, Natalia Lyubova, Damien Gerardeaux-Viret, David Filliat, Pierre-Yves Oudeyer.

We studied how various mechanisms for cognition and learning, such as curiosity, action selection, imitation, visual learning and interaction monitoring, can be integrated in a single embodied cognitive architecture. We have conducted an experiment with the iCub robot for active recognition of objects in 3D through curiosity-driven exploration, in which the robot can manipulate the robot or ask a human user to manipulate objects to gain information and recognise better objects (fig. 27). For this experiment carried out within the MACSi project, we address the problem of learning to recognise objects in a developmental robotics scenario. In a life-long learning perspective, a humanoid robot should be capable of improving its knowledge of objects with active perception. Our approach stems from the cognitive development of infants, exploiting active curiosity-driven manipulation to improve perceptual learning of objects. These functionalities are implemented as perception, control and active exploration modules as part of the Cognitive Architecture of the MACSi project. We integrated a bottom-up vision system based on swift feature points and motor-primitive based robot control with the SGIM-ACTS algorithm (Socially Guided Intrinsic Motivation with Active Choice of Task and Strategy) as the active exploration module. SGIM-ACTS is a strategic learner who actively chooses which task to concentrate on, and which strategy is better according to this task. It thus monitors the learning progress for each strategy on all kinds of tasks, and actively interacts with the human teacher. We obtained an active object recognition approach, which exploits curiosity to guide exploration and manipulation, such that the robot can improve its knowledge of objects in an autonomous and efficient way. Experimental results show the effectiveness of our approach: the humanoid iCub is now capable of deciding autonomously which actions must be performed on objects in order to improve its knowledge, requiring a minimal assistance from its caregiver. This work constitutes the base for forthcoming research in autonomous learning of affordances. This work has been published in a conference [57] and in a journal paper [28].

### 6.4.3. Imitation Learning and Language

**Participants:** Thomas Cederborg, Pierre-Yves Oudeyer.

We have studied how context-dependant imitation learning of new skills and language learning could be seen as special cases of the same mechanism. We argue that imitation learning of context-dependent skills implies complex inferences to solve what we call the "motor Gavagai problem", which can be viewed as a generalization of the so-called "language Gavagai problem". In a full symbolic framework where percepts and actions are continuous, this allows us to articulate that language may be acquired out of generic sensorimotor imitation learning mechanisms primarily dedicated at solving this motor Gavagai problem. Through the use

of a computational model, we illustrate how non-linguistic and linguistic skills can be learnt concurrently, seamlessly, and without the need for symbols. We also show that there is no need to actually represent the distinction between linguistic and non-linguistic tasks, which rather appears to be in the eye of the observer of the system. This computational model leverages advanced statistical methods for imitation learning, where closed-loop motor policies are learnt from human demonstrations of behaviours that are dynamical responses to a multimodal context. A novelty here is that the multimodal context, which defines what motor policy to achieve, includes, in addition to physical objects, a human interactant which can produce acoustic waves (speech) or hand gestures (sign language). This was published in [26].

#### **6.4.4. Learning to Interpret the Meaning of Teaching Signals in Socially Guided Robot Learning**

**Participants:** Manuel Lopes, Jonathan Grizou, Thomas Cederborg, Pierre-Yves Oudeyer.

We elaborated an algorithm to bootstrap shared understanding in a human-robot interaction scenario where the user teaches a robot a new task using teaching instructions yet unknown to it. In such cases, the robot needs to estimate simultaneously what the task is and the associated meaning of instructions received from the user. For this work, we consider a scenario where a human teacher uses initially unknown spoken words, whose associated unknown meaning is either a feedback (good/bad) or a guidance (go left, right, ...). We present computational results, within an inverse reinforcement learning framework, showing that a) it is possible to learn the meaning of unknown and noisy teaching instructions, as well as a new task at the same time, b) it is possible to reuse the acquired knowledge about instructions for learning new tasks, and c) even if the robot initially knows some of the instructions' meanings, the use of extra unknown teaching instructions improves learning efficiency. Published articles: [43], [45].

An extension to the use of brain signals has been made [44]. Do we need to explicitly calibrate Brain Machine Interfaces (BMIs)? Can we start controlling a device without telling this device how to interpret brain signals? Can we learn how to communicate with a human user through practical interaction? It sounds like an ill posed problem, how can we control a device if such device does not know what our signals mean? This paper argues and present empirical results showing that, under specific but realistic conditions, this problem can be solved. We show that a signal decoder can be learnt automatically and online by the system under the assumption that both, human and machine, share the same a priori on the possible signals' meanings and the possible tasks the user may want the device to achieve. We present results from online experiments on a Brain Computer Interface (BCI) and a Human Robot Interaction (HRI) scenario.

#### **6.4.5. Active Learning for Teaching a Robot Grounded Relational Symbols**

**Participants:** Johannes Kulick, Tobias Lang, Marc Toussaint, Manuel Lopes.

The present work investigates an interactive teaching scenario, where a human aims to teach the robot symbols that abstract geometric (relational) features of objects. There are multiple motivations for this scenario: First, state-of-the-art methods for relational Reinforcement Learning demonstrated that we can successfully learn abstracting and well-generalizing probabilistic relational models and use them for goal-directed object manipulation. However, these methods rely on given grounded action and state symbols and raise the classical question Where do the symbols come from? Second, existing research on learning from human-robot interaction has focused mostly on the motion level (e.g., imitation learning). However, if the goal of teaching is to enable the robot to autonomously solve sequential manipulation tasks in a goal-directed manner, the human should have the possibility to teach the relevant abstractions to describe the task and let the robot eventually leverage powerful relational RL methods (see Figure 33 ). We formalize human-robot teaching of grounded symbols as an Active Learning problem, where the robot actively generates geometric situations that maximize his information gain about the symbol to be learnt. We demonstrate that the learned symbols can be used in a relational RL framework for the robot to learn probabilistic relational rules and use them to solve object manipulation tasks in a goal-directed manner. [47].



Figure 33. Active learning of symbol descriptions on a real world robot.

## 6.5. Robot Design and Morphological Computation

### 6.5.1. The Poppy Humanoid Robot: Leg Design for Biped Locomotion

**Participants:** Matthieu Lapeyre, Pierre Rouanet, Pierre-Yves Oudeyer.

In this paper introduced for Poppy as a novel humanoid robotic platform designed to jointly address three central goals of humanoid robotics: 1) study the role of morphology in biped locomotion; 2) study full-body compliant physical human-robot interaction; 3) be robust while easy and fast to duplicate to facilitate experimentation. The taken approach relies on functional modeling of certain aspects of human morphology, optimizing materials and geometry, as well as on the use of 3D printing techniques. In this article, we have focused on the presentation of the design of specific morphological parts related to biped locomotion: the hip, the thigh, the limb mesh and the knee. We also presented an initial experiments showing properties of the robot when walking with the physical guidance of a human. [50].

### 6.5.2. Poppy Humanoid Platform: Experimental Evaluation of the Role of a Bio-inspired Thigh Shape

**Participants:** Matthieu Lapeyre, Pierre Rouanet, Pierre-Yves Oudeyer.

In this paper, we present an experimental evaluation of the role of the morphology in the Poppy humanoid platform. More precisely, we have investigated the impact of the bio-inspired thigh, bended of  $60^\circ$ , on the balance and biped locomotion. We compare this design with a more traditional straight thigh. We describe both the theoretical model and real experiments showing that the bio-inspired thigh allows the reduction of falling speed by almost 60% (single support phase) and the decrease of the lateral motion needed for the mass transfer from one foot to the other by 30% (double support phase). We also present an experiment where the robot walks on a treadmill thanks to the social and physical guidance of expert users and we show that the bended thigh reduces the upper body motion by about 45% indicating a more stable walk.[48].

### 6.5.3. Morphological computation and body intelligence

#### 6.5.3.1. Comparative Study of the Role of Trunk in Human and Robot Balance Control

**Participants:** Matthieu Lapeyre [correspondant], Christophe Halgand, Jean-Renã© Cazalet, Etienne Guillaud, Pierre-Yves Oudeyer.

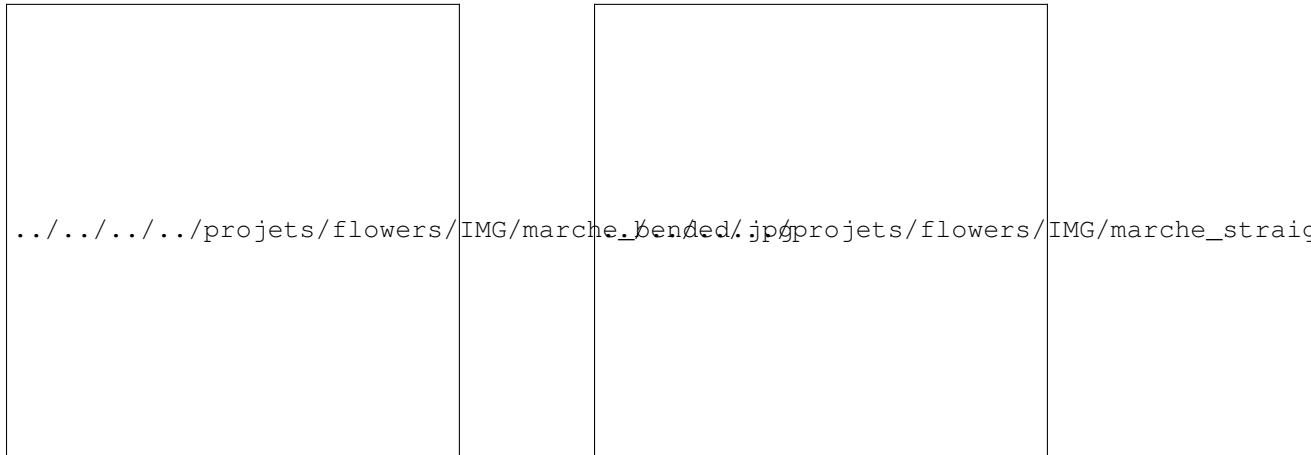


Figure 34. Five pictures have been taken while Poppy was walking and were stacked to obtain a qualitative view of the difference in the walking behavior in function of the morphology of the thigh.

Numerous studies in the field of functional motor rehabilitation were devoted to understanding the functioning of members but few are interested in the coordination of the trunk muscles and the relationship between axial and appendicular motricity which is essential in maintaining balance during travel. Acquiring new knowledge on this subject is a prerequisite in the development of new therapeutic strategies to restore motor function to the overall development of robotic orthosis that would assist the movement. Many robotic orthosis using EMG signals were unfortunately using few joints [82] and a system for controlling a multi articulated spine has not yet been developed. We propose here to use a multidisciplinary approach to define the neuro-mechanical principles where an axial system is operating in synergy with human and robot limbs.

To bring us a theoretical framework, we chose to study the reactions of the Acroban humanoid robot. Including 5 joints in the trunk, Acroban can reproduce in part the fluid movements of the human body [101] and especially to test its behavior when its trunk is held fixed or his arms are no longer used for rebalance. To disrupt postural balance in humans and robots, we have developed a low cost mobile platform (see Figure 35). This platform is made up of a broad stable support ( $0.8 \times 5m$ ) mounted on a skateboard having a power of 800W. The substitution of the initial order of skate by an embedded microcontroller allows us to generate mono-axial perturbations precise intensity and duration to ensure repeatability of the disturbance. We capture movements (Optitrack 250Hz) and record the acceleration of the platform (accelerometer embedded 2kHz), the center of pressure (WiiBalanceBoard 60Hz), and electromyography (EMG).

The experimental device (mobile platform and synchronized recordings) is operational. Preliminary experiments have allowed us to refine the profiles of disturbance on the robot Acroban. The analysis of preliminary results is in progress. Following this study, we hope to improve the modeling of the motor system in humans and robotic simulation as a basis for the development of robotic orthosis axial system. Second, the results provide a basis for improved balancing of Acroban primitives but also the development of future humanoid robots.

## 6.6. Educational Technologie

### 6.6.1. KidLearn: Adaptive Personalization of Educational Content with Machine Learning

Kidlearn is a research project studying how machine learning can be applied to intelligent tutoring systems. It aims at developing methodologies and software which adaptively personalize sequences of learning activities



Figure 35. Experimental setup for comparative study of the role of the trunk in human and robot balance control

to the particularities of each individual student. Our systems aim at proposing to the student the right activity at the right time, maximizing concurrently his learning progress and its motivation. In addition to contributing to the efficiency of learning and motivation, the approach is also made to reduce the time needed to design ITS systems.

Intelligent Tutoring System (ITS) are computer environments designed to guide students in their learning. Through the proposal of different activities, it provides teaching experience, guidance and feedback to improve learning. The FLOWERS team has developed several computational models of artificial curiosity and intrinsic motivation based on research on psychology that might have a great impact for ITS. Results showed that activities with intermediate levels of complexity, neither too easy nor too difficult but just a little more difficult than the current level, provide better teaching experiences. The system is based on the combination of three approaches. First, it leverages Flowers team's recent models of computational models of artificial curiosity and intrinsic motivation based on research in psychology and neuroscience. One overview can be found in [27]. Second, it uses state-of-the-art Multi-Arm Bandit (MAB) techniques to efficiently manage the exploration/exploitation challenge of this optimization process. Third, it leverages expert knowledge to constrain and bootstrap initial exploration of the MAB, while requiring only coarse guidance information of the expert and allowing the system to deal with didactic gaps in its knowledge. In 2013, we have run a first pilot experiment in elementary schools of Région Aquitaine, where 7-8 year old kids could learn elements of mathematics thanks to an educational software that presented the right exercises at the right time to maximize learning progress. A report is available at: <http://arxiv.org/pdf/1310.3174v1.pdf>.

## 6.7. Other applications

### 6.7.1. Real-time Reaction-Diffusion Simulation: a Machine Learning Technique

**Participants:** Thomas Degrís, Nejib Zemzemi.

Carmen is an Inria team working on modeling the electrical activity of the human heart. Their models are mainly based on reaction-diffusion equations. These methods are expensive in terms of computational costs which limits their use in practice. More specifically, some recent surgical intervention techniques on the heart (atrial ablation) requires to identify the source of the electrical wave. Finding such sources requires an optimization procedure. Using classical methods, this procedure is very heavy computationally.

In this project, our goal is to reduce the computational cost using supervised learning techniques. The idea is to replace the incremental resolution of partial differential equations by more suitable data structures for real-time running. Starting from data generated by simulating different excitations scenarios on a human atria, this data is afterwards used as a training data set for machine learning algorithms. This approach will allow a faster optimization procedure.

This work is in collaboration with Nejib Zemzemi from the Inria Carmen team. This project is in preliminary steps.

### **6.7.2. Appearance-based segmentation of indoors/outdoors sequences of spherical views**

**Participant:** David Filliat.

In collaboration with Patrick Rives and Alexandre Chapoulie from the Arobas team at Inria Sophia-Antipolis, we developed a method for environment segmentation based on spherical views [41]. Navigating in large scale, complex and dynamic environments requires reliable representations able to capture metric, topological and semantic aspects of the scene for supporting path planning and real time motion control. In a previous work, we addressed metric and topological representations thanks to a multi-cameras system which allows building of dense visual maps of large scale 3D environments. The map is a set of locally accurate spherical panoramas related by 6dof poses graph. The work presented here is a further step toward a semantic representation. We aim at detecting the changes in the structural properties of the scene during navigation. Structural properties are estimated online using a global descriptor relying on spherical harmonics which are particularly well-fitted to capture properties in spherical views. A change-point detection algorithm based on a statistical Neyman-Pearson test allows us to find optimal transitions between topological places. Results are presented and discussed both for indoors and outdoors experiments.

### **6.7.3. Modelling Stop Intersection Approaches using Gaussian Processes**

**Participant:** David Filliat.

In collaboration with Javier-Ibanez Guzman and Alexandre Armand from Renault, we developed an approach toward the development of an electronic co-pilot adapted to the driver behavior [39]. Indeed, each driver reacts differently to the same traffic conditions, however, most Advanced Driving Assistant Systems (ADAS) assume that all drivers are the same. This work proposes a method to learn and to model the velocity profile that the driver follows as the vehicle decelerates towards a stop intersection. Gaussian Processes (GP), a machine learning method for non-linear regressions are used to model the velocity profiles. It is shown that GP are well adapted for such an application, using data recorded in real traffic conditions. GP allow the generation of a normally distributed speed, given a position on the road. By comparison with generic velocity profiles, benefits of using individual driver patterns for ADAS issues are presented.

## MANAO Team

# 5. New Results

## 5.1. Axis 1: Analysis and Simulation

### 5.1.1. Second Order Analysis of Variance in Multiple Importance Sampling

**Participants:** H. Lu, R. Pacanowski, X. Granier

Monte Carlo Techniques are widely used in Computer Graphics to generate realistic images. Multiple Importance Sampling reduces the impact of choosing a dedicated strategy by balancing the number of samples between different strategies. However, an automatic choice of the optimal balancing remains a difficult problem. Without any scene characteristics knowledge, the default choice is to select the same number of samples from different strategies and to use them with heuristic techniques (e.g., balance, power or maximum). We introduced [16] a second-order approximation of variance for balance heuristic. Based on this approximation, we automatically distribute samples for direct lighting without any prior knowledge of the scene characteristics. For all our test scenes (with different types of materials, light sources and visibility complexity), our method actually reduces variance in average (see Figure 9). This approach will help developing new balancing strategies.



Low to high glossy materials with five diffuse area light sources      Glossy materials with high-frequency environment map lighting

Figure 9. Our per-pixel second-order approximation of the variance leads to a new and automatic approach for balancing the number of samples between two different sampling strategies. Except for light sources, the inset images show the sample distribution for each pixel. The yellow corresponds to the default balance heuristic strategy [101]. Compared to the balance heuristic, the variance is reduced by (**Left**) 26% and (**Right**) 20% in average (14% and 11% for the standard deviation).

### 5.1.2. Rational BRDF

**Participants:** R. Pacanowski, L. Belcour, X. Granier

Over the last two decades, much effort has been devoted to accurately measuring Bidirectional Reflectance Distribution Functions (BRDFs) of real-world materials and to use efficiently the resulting data for rendering. Because of their large size, it is difficult to use directly measured BRDFs for real-time applications, and fitting the most sophisticated analytical BRDF models is still a complex task.

We have presented Rational BRDF [21], a general-purpose and efficient representation for arbitrary BRDFs, based on Rational Functions (RFs). Using an adapted parametrization, Rational BRDFs offer 1) a more compact and efficient representation using low-degree RFs, 2) an accurate fitting of measured materials with guaranteed control of the residual error, and 3) efficient importance sampling by applying the same fitting process to determine the inverse of the Cumulative Distribution Function (CDF) generated from the BRDF for use in Monte-Carlo rendering.

### 5.1.3. *Decomposing intensity gradients into information about shape and material*

**Participants:** P. Barla, G. Guennebaud, X. Granier

Recent work has shown that the perception of 3D shapes, material properties and illumination are inter-dependent, although for practical reasons, each set of experiments has probed these three causal factors independently. Most of these studies share a common observation though: that variations in image intensity (both their magnitude and direction) play a central role in estimating the physical properties of objects and illumination. Our aim is to separate retinal image intensity gradients into contributions of different shape and material properties, through a theoretical analysis of image formation [11].

We find that gradients can be understood as the sum of three terms: variations of surface depth conveyed through surface-varying reflectance and near-field illumination effects (shadows and inter-reflections); variations of surface orientation conveyed through reflections and far-field lighting effects; and variations of surface micro-structures conveyed through anisotropic reflections. We believe our image gradient decomposition constitutes a solid and novel basis for perceptual inquiry. We first illustrate each of these terms with synthetic 3D scenes rendered with global illumination. We then show that it is possible to mimic the visual appearance of shading and reflections directly in the image, by distorting patterns in 2D. Finally, we discuss the consistency of our mathematical relations with observations drawn by recent perceptual experiments, including the perception of shape from specular reflections and texture. In particular, we show that the analysis can correctly predict certain specific illusions of both shape and material.

## 5.2. Axis 2: From Acquisition to Display

### 5.2.1. *Interactive Spatial Augmented Reality*

**Participants:** B. Ridel, P. Reuter, X. Granier

We propose the revealing flashlight [26], a new interaction and visualization technique in spatial augmented reality that helps to reveal the details of cultural heritage artifacts (see Figure 3), since they often contain details that are difficult to distinguish due to aging effects such as erosion. We locally and interactively augment a physical artifact by projecting an expressive 3D visualization that highlights its features, based on an analysis of its previously acquired geometry at multiple scales.

Our novel interaction technique simulates and improves the behavior of a flashlight: according to 6-degree-of-freedom input, we adjust the numerous parameters involved in the expressive visualization - in addition to specifying the location to be augmented. This makes advanced 3D analysis accessible to the greater public with an everyday gesture, by naturally combining the inspection of the real object and the virtual object in a co-located interaction and visualization space. The revealing flashlight can be used by archeologists, for example, to help decipher inscriptions in eroded stones, or by museums to let visitors interactively discover the geometric details and meta-information of cultural artifacts. We confirm its effectiveness, ease-of-use and ease-of-learning in an initial preliminary user study and by the feedbacks of two public exhibitions.

### 5.2.2. *High Dynamic Range, Multispectral, Polarization, and Light-Field Imaging*

**Participants:** A. Manakov, J. Restrepo, R. Hegedüs, I. Ihrke





*Figure 10. (Top) Novel optical converter module that can be placed between a camera and its lens. This module can be configured flexibly to allow for multi-spectral, polarization, high-dynamic range, or light field imaging. It works by splitting the original image into a number of copies that can be optical filtered separately (Bottom, Left). Computational post-processing allows for unprecedented flexibility in image post-processing such as post-capture control of illumination, polarization state, exposure setting or focus. (Bottom,Right) The basis of the operational principle of the aforementioned prototype is imaging in mirror systems.*

In [5] we propose a non-permanent add-on that enables plenoptic imaging with standard cameras (see also Figure 10 top and left). Our design is based on a physical copying mechanism that multiplies a sensor image into a number of identical copies that still carry the plenoptic information of interest. Via different optical filters, we can then recover the desired information. A minor modification of the design also allows for aperture sub-sampling and, hence, light-field imaging. As the filters in our design are exchangeable, a reconfiguration for different imaging purposes is possible. We show in a prototype setup that high dynamic range, multispectral, polarization, and light-field imaging can be achieved with our design.

### 5.2.3. *Structure of a Planar Mirror System from Multiple Observations of a Single Point*

**Participants:** I. Reshetouski, A. Manakov, I. Ihrke

We have investigated the problem of identifying the position of a viewer inside a room of planar mirrors with unknown geometry in conjunction with the room's shape parameters [25] (see also Figure 10 bottom right). We consider the observations to consist of angularly resolved depth measurements of a single scene point that is being observed via many multi-bounce interactions with the specular room geometry. Applications of this problem statement include areas such as calibration, acoustic echo cancelation and time-of-flight imaging. We theoretically analyze the problem and derive sufficient conditions for a combination of convex room geometry, observer, and scene point to be reconstructable. The resulting constructive algorithm is exponential in nature and, therefore, not directly applicable to practical scenarios.

To counter the situation, we propose theoretically devised geometric constraints that enable an efficient pruning of the solution space and develop a heuristic randomized search algorithm that uses these constraints to obtain an effective solution. We demonstrate the effectiveness of our algorithm on extensive simulations as well as in a challenging real-world calibration scenario.

### 5.2.4. *Mirrors in Computer Graphics, Computer Vision and Time-of-Flight Imaging*

**Participants:** I. Reshetouski, I. Ihrke

We have investigated the state of the art in dealing with the geometry of mirror systems [28].

Mirroring is one of the fundamental light/surface interactions occurring in the real world. Surfaces often cause specular reflection, making it necessary to design robust geometry recovery algorithms for many practical situations. In these applications the specular nature of the surface is a challenge. On the other side, mirrors, with their unique reflective properties, can be used to improve our sensing modalities, enabling applications such as surround, stereo and light field imaging. In these scenarios the specular interactions are highly desirable. Both of these aspects, the utilization and circumvention of mirrors are present in a significant amount of publications in different scientific areas. These publications are covering a large number of different problem statements as well as many different approaches to solutions. In this survey we focused on a collection and classification of the work in this area.

### 5.2.5. *Computational Fabrication and Display of Material Appearance*

**Participant:** I. Ihrke

We have investigated the state of the art in digital material fabrication and active display technology [22].

After decades of research on digital representations of material and object appearance, computer graphics has more recently turned to the problem of creating physical artifacts with controllable appearance characteristics.

While this work has mostly progressed in two parallel streams – display technologies as well as novel fabrication processes – we believe there is a large overlap and the potential for synergies between these two approaches. In this report, we summarize research efforts from the worlds of fabrication display, and categorize the different approaches into a common taxonomy. We believe that this report can serve as a basis for systematic exploration of the design space in future research.

## 5.3. Axis 3: Rendering, Visualization and Illustration

### 5.3.1. *Real-Time Sampling from Captured Environment Map*

**Participants:** H. Lu, R. Pacanowski, X. Granier



Figure 11. Time-varying light samples distribution for one pixel (cyan dot) on the dragon model when lit with a dynamic environment map [95]. This example runs in average at 145 fps using Multiple Importance Sampling with 50 samples for the Lafortune energy conserving Phong BRDF with a shininess exponent set to 150.

We have introduced [23] a simple and effective technique for light-based importance sampling of dynamic environment maps based on the formalism of Multiple Importance Sampling (MIS). The core idea is to balance per pixel the number of samples selected on each cube map face according to a quick and conservative evaluation of the lighting contribution: this increases the number of effective samples. In order to be suitable for dynamically generated or captured HDR environment maps, everything is computed on-line for each frame without any global preprocessing. Our MIS formalism can be easily extended to other strategies such as BRDF importance sampling.

### 5.3.2. Screen-Space Curvature for Production-Quality Rendering and Compositing

**Participants:** N. Mellado, P. Barla, G. Guennebaud, P. Reuter

Curvature is commonly employed for enhancing details in textured 3D models, or to modulate shading at the rendering or compositing stage. However, existing methods that compute curvature in object space rely on mesh-based surfaces and work at the vertex level. Consequently, they are not well adapted to production-quality models that rely on either subdivision surfaces with displacement and bump maps, or on implicit and procedural representations. In practice they would require a view-dependent scene discretization at each frame, to adapt geometry to visible details and avoid aliasing artifacts. Our approach [24] is independent of both scene complexity and the choice of surface representations since it computes mean curvature from scratch at each frame in screen-space. It works without any pre-process and provides a controllable screen-space scale parameter, which makes it ideal for production requirements, either during rendering or compositing.

### 5.3.3. Smooth Surface Contours with Accurate Topology

**Participant:** P. Bénard

Computing the visible contours of a smooth 3D surface is a surprisingly difficult problem, and previous methods are prone to topological errors, such as gaps in the outline. Our approach [13] is to generate, for each viewpoint, a new triangle mesh with contours that are topologically-equivalent and geometrically close to those of the original smooth surface. The contours of the mesh can then be rendered with exact visibility. The core of the approach is Contour-Consistency, a way to prove topological equivalence between the contours of two surfaces. Producing a surface tessellation that satisfies this property is itself challenging; to this end, we introduce a type of triangle that ensures consistency at the contour. We then introduce an iterative mesh generation procedure, based on these ideas. This procedure does not fully guarantee consistency, but errors are not noticeable in our experiments. Our algorithm can operate on any smooth input surface representation; we use Catmull-Clark subdivision surfaces in our implementation. We demonstrate results computing contours of complex 3D objects, on which our method eliminates the contour artifacts of other methods.

## 5.4. Axis 4: Editing and Modeling

### 5.4.1. Implicit Skinning and Modeling

**Participant:** G. Guennebaud

Geometric skinning techniques, such as smooth blending or dual-quaternions, are very popular in the industry for their high performances, but fail to mimic realistic deformations. Other methods make use of physical simulation or control volume to better capture the skin behavior, yet they cannot deliver real-time feedback. In collaboration with IRIT (Toulouse) and the Imagine team (Grenoble), we developed the first purely geometric method handling skin contact effects and muscular bulges in real-time. Our insight is to exploit the advanced composition mechanism of volumetric, implicit representations for correcting the results of geometric skinning techniques (cf. Figure 12 -a). The mesh is first approximated by a set of implicit surfaces. At each animation step, these surfaces are combined in real-time and used to adjust the position of mesh vertices, starting from their smooth skinning position. This deformation step is done without any loss of detail and seamlessly handles contacts between skin parts. As it acts as a post-process, our method fits well into the standard animation pipeline. Moreover, it requires no intensive computation step such as collision detection, and therefore provides real-time performances. This work has been published at Siggraph this year [20] and featured by the 3DVF website <http://www.3dvf.com/actualite-6678-siggraph-2013-methode-skinning-implicite.html>.

Still in collaboration with IRIT, we addressed the challenging problem of finding adequate bounds for implicit modeling with compact field functions. Recent advances in implicit surface modeling now provide highly controllable blending effects. These effects rely on the field functions of  $\mathbb{R}^3 \rightarrow \mathbb{R}$  in which the implicit surfaces are defined. In these fields, there is an outside part in which blending is defined and an inside part. The implicit surface is the interface between these two parts. As recent operators often focus on blending, most efforts have been made on the outer part of field functions and little attention has been paid on the inner part. Yet, the inner fields are important as soon as difference and intersection operators are used. This makes its quality as crucial as the quality of the outside.

In this work we analyzed these shortcomings, and deduced new constraints on field functions such that differences and intersections can be seamlessly applied without introducing discontinuities or field distortions. In particular, we showed how to adapt state of the art gradient-based union and blending operators to our new constraints. Our approach enables a precise control of the shape of both the inner or outer field boundaries. We also developed a new set of asymmetric operators tailored for the modeling of fine details while preserving the integrity of the resulting fields. This work has been published at Shape Modeling International 2013 [14].

### 5.4.2. Surface reconstruction

**Participants:** J. Chen, G. Guennebaud, P. Barla, X. Granier

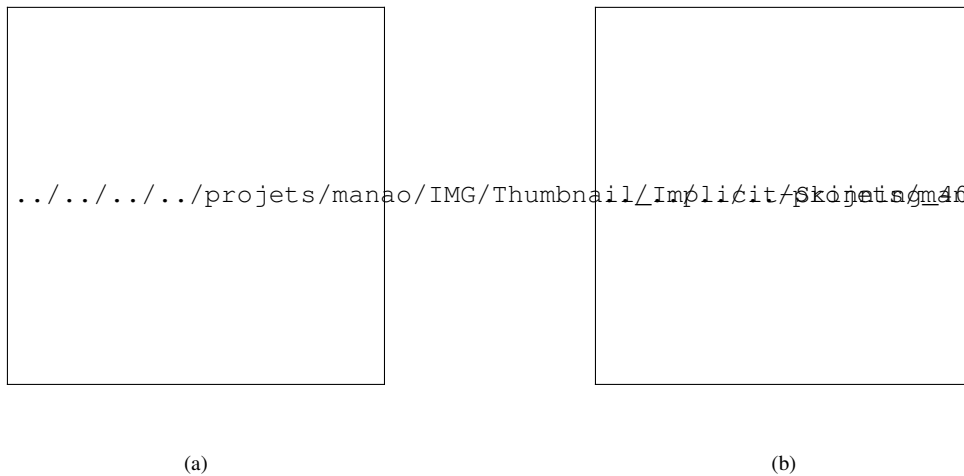


Figure 12. (a) Illustration of the implicit skinning technique. (b) Surface reconstruction from non-oriented normals

Reconstructing a smooth surface from a set of points is still a challenging problem. Most of the popular techniques assume correctly oriented points as inputs. However, in many situations, computing a consistent orientation of the normal field is as difficult as the reconstruction itself. In a recent work, we extended the Algebraic Point Set Surface method to support non oriented normals (cf. Figure 12 -b). By fitting algebraic spheres, our approach outperforms simple local methods based on non-oriented planar fit while still being fast since it involves only local computations. The core of this new technique also proved to be useful for image processing. This work as been published at Computer Graphics Forum [3].

#### 5.4.3. Manipulation of Anisotropic Highlights

**Participants:** B. Raymond, P. Barla, G. Guennebaud, X. Granier

We have developed [19] a system for the direct editing of highlights produced by anisotropic BRDFs, which we call anisotropic highlights. We first provide a comprehensive analysis of the link between the direction of anisotropy and the shape of highlight curves for arbitrary object surfaces. The gained insights provide the required ingredients to infer BRDF orientations from a prescribed highlight tangent field. This amounts to a non-linear optimization problem, which is solved at interactive framerates during manipulation. Taking inspiration from sculpting software, we provide tools that give the impression of manipulating highlight curves while actually modifying their tangents. Our solver produces desired highlight shapes for a host of lighting environments and anisotropic BRDFs.

## POTIOC Team

# 6. New Results

## 6.1. Navigation techniques in 3D digital cities on mobile touch devices

**Participants:** Jacek Jankowski, Thomas Hulin, Martin Hachet.

This study aimed at characterizing today's most common interaction techniques for street-level navigation in 3D digital cities, for mobile touch devices, in terms of their efficiency and usability. To do so, we conducted a user study, where we compared target selection (Go-To), rate control (Joystick), position control, and stroke-based control navigation metaphors (see Figure 3 ). The results suggest that users performed best with the Go-To interaction technique. The subjective comments showed a preference of novices towards Go-To and expert users towards the Joystick technique. This work has been accepted for publication at the 3DUI 2014 conference [15].



*Figure 3. Four techniques for navigating in a 3D city on a mobile touch device.*

As part of this project on Navigation in 3D digital cities, the Potioc group also built a tutorial about interaction techniques for 3D environments. It was presented at Eurographics 2013 [13] and Web3D 2013 [14]. The goal of this work is to provide an up-to-date state-of-the-art of this topic to the community.

## 6.2. Interaction with spatial augmented reality for physical drawing

**Participants:** Jérémy Laviolle, Martin Hachet.

We developed tools that enable precise interactive projection on pieces of paper. The sheets of paper are tracked by a camera while the user's inputs (e.g., touch and hovering events) are detected by a Kinect. The paper acts as a screen, its image coming from an overhead projector. The focus of this work is to use such tools to assist the creation of physical drawings and painting. In this context we propose Digital Construction Lines (DCL), in opposition with physical construction lines. Traditionally, the structure of a physical drawing can be created with construction lines which are light pencil strokes. These strokes are then erased during the drawing process. With DCL, it is not required to erase the construction lines anymore. Furthermore, it is possible to create construction lines on fragile material like a canvas for waterpainting or on fresh paint. It also enables construction lines on a dark canvas. In addition to these projection advantages, it is possible to create these DCL interactively and directly onto the support. Consequently, the DCL complement the physical ones during the creation process.

We investigated in a user study if the DCL could effectively replace the physical construction lines, and compared the performance (speed, cleanliness) between the two kinds of construction lines. In this user study we also evaluated the quality and usability of projection of thin lines in a fully controlled environment with a low-cost setup. The study showed that DCL could effectively replace physical construction lines, even though it might not be desirable. The study also showed that the drawing experience was as pleasant with projection, and with the usual tools. The feedback about the quality of tracking and projection was also positive. The only negative evaluation concerned the size of the projection area, which was limited by the resolution of the projector. This work was published as part of Jérémy Laviolle's PhD thesis [4].

PapARt was also used as part of a museum exhibition on the Lascaux caves, together with other 3D UI from Potioc. This exhibition has provided us with the opportunity to experiment with touch-based interfaces for manipulating 3D virtual objects. We targeted three tasks: observing rare objects with Cubtile, reassembling object fragments with Toucheo, and reproducing artwork with PapARt [7] (see Figure 5). These exhibitions allowed us to experiment our systems in real conditions. It led to a Living Lab, where the visitors can test our devices.

## 6.3. Rouages: Revealing the Mechanisms of Digital Musical Instruments to the Audience

**Participants:** Florent Berthaut, Martin Hachet, Pierre-Marie Plans.

We have developed Rouages [10], a mixed-reality display system associated with a 3D visualization application. Rouages reveals the mechanisms of digital musical instruments in two ways. First, by amplifying musicians' gestures with virtual extensions of the sensors. Second, by representing the sound components with 3D shapes and specific behaviors and by showing the impact of musicians' gestures on these components. In addition, we have explored new setups to enhance collaboration between musicians using our VR-based instruments. This is illustrated in Figure 6.

## 6.4. Gateway driving simulator

**Participants:** Florian Larrue, Pauline Davignon, Martin Hachet.

As part of the SIMCA FUI project, the POTIOC team focuses on the design and evaluation of a gateway driving simulator (see Figure 7), to teach drivers how to drive an airport gateway in virtual reality, i.e., in a safe and cost-effective environment. We conducted a comprehensive user study to assess the impact of various parameters on user performances. This study allowed us to provide a set of recommendations for the design of an actual simulator.



*Figure 4. Using Digital Construction Lines for spatial augmented reality-based physical drawing.*





*Figure 5. Manipulation of a 3D model and lighting conditions for drawing on a prehistoric object in a museum.*



*Figure 6. Collaborative setup for enhancing interaction between immersed musicians.*



Figure 7. Gateway simulator.

## 6.5. Training Approaches for Brain-Computer Interfaces

**Participants:** Fabien Lotte, Florian Larrue, Christian Mühl.

While recent research on Brain-Computer Interfaces (BCI) has highlighted their potential for many applications, they remain barely used outside laboratories due to a lack of robustness. Spontaneous BCI (i.e., mental imagery-based BCI) often rely on mutual learning efforts by the user and the machine, with BCI users learning to produce stable EEG patterns (spontaneous BCI control being widely acknowledged as a skill) while the computer learns to automatically recognize these EEG patterns, using signal processing. Most research so far was focused on signal processing, mostly neglecting the human in the loop. However, how well the user masters the BCI skill is also a key element explaining BCI robustness. Unfortunately, despite the importance of BCI training protocols, they have been scarcely studied so far, and used mostly unchanged for years. In our work, we advocate that current human training approaches for spontaneous BCI are most likely inappropriate. We notably studied instructional design literature in order to identify the key requirements and guidelines for a successful training procedure that promotes a good and efficient skill learning. This literature study highlighted that current spontaneous BCI user training procedures satisfy very few of these requirements and hence are likely to be suboptimal. We therefore identified the flaws in BCI training protocols according to instructional design principles. We also proposed new research directions that are theoretically expected to address some of these flaws and to help users learn the BCI skill more efficiently. This work has been published in the *Frontiers in Neuroscience* journal [9].

On a related topic, together with colleagues from Inria Rennes (A. Lécuyer and L. Bonnet, Hybrid team) we explored the design and evaluation of multiuser BCI applications, notably to see their impact on user training and performance. We created a multiuser videogame called BrainArena in which two users can play a simple football game by means of two BCIs. They can score goals on the left or right side of the screen by simply imagining left or right hand movements (see Figure 8). To add another interesting element, the gamers can play in a collaborative manner (their two mental activities are combined to score in the same goal),



Figure 8. Multiplayer BCI-based gaming and feedback [5].

or in a competitive manner (the gamers must push the ball in opposite directions). Interestingly enough, our results showed that compared to a single player version of the same BCI-game, collaborative multiplayer BCI-gaming increased the motivation and performance of the most skilled of each player pairs, while leaving the performance of the other players unchanged, hence proving a useful tool to improve BCI training. This work has been published in the IEEE Transactions on Computational Intelligence and AI in Games journal [5].

## 6.6. Inducing, measuring and estimating mental and psychosocial stress from physiological signals

**Participants:** Christian Mühl, Camille Jeunet, Fabien Lotte.

Stress is a major societal issue with negative impacts on health and economy. Physiological computing offers a continuous, direct, and unobtrusive method for stress level assessment and computer-assisted stress management. However, stress is a complex construct and its physiology can vary depending on its source, for example cognitive load or social evaluation. To study the feasibility of physiology-based load-invariant psychosocial stress-detection, we designed a stress-induction protocol able to independently vary the relevant types of psychophysiological activity: mental and psychosocial stress. In [27], [17], we validate the efficacy of our protocol to induce psychosocial and mental stress. Our participants (N=24) had to perform a cognitive task associated with two workload conditions (low/high mental stress), in two contexts (low/high psychosocial stress), during which we recorded subject's self-reports, behavior, physiology and neurophysiology. Questionnaires showed that the subjectively perceived level of anxiety varied with the psychosocial stress induction, while perceived arousal and mental effort levels vary with mental stress induction. Behavior and physiology corroborated the validity of our protocol further. Heart rate and skin conductance globally increased after psychosocial stress induction relative to the non-stressful condition. Moreover, we demonstrated that higher workload tasks (mental stress) led to decrease in performance and a marked increase of heart rate.



Figure 9. The setup of the experiment to induce and measure mental and psychosocial stress.

Based on this protocol, we also explored the effect of stress on workload estimation. Workload estimation from electroencephalographic signals (EEG) offers a highly sensitive tool to adapt the human-computer interaction to the user state. To create systems that reliably work in the complexity of the real world, a robustness against contextual changes (e.g., mood), has to be achieved. To study the resilience of state-of-the-art EEG-based workload classification against stress, we test the capability of the workload classifier to generalize across affective contexts (stress/non-stress). We show that the classifier is able to transfer between affective contexts, though performance suffers. However, cross-context training is a simple and powerful remedy allowing the extraction of features more resilient to task-unrelated variations in signal characteristics, leading to a performance comparable to within-context training and testing.

## 6.7. Exploring electroencephalography as an evaluation method for human-computer interaction

**Participants:** Jérémy Frey, Léonard Pommereau, Fabien Lotte, Christian Mühl, Martin Hachet.

Evaluating human-computer interaction is essential as a broadening population uses machines, sometimes in sensitive contexts. However, traditional evaluation methods may fail to combine real-time measures, an objective approach and data contextualization. We presented a review seeking how neuroimaging techniques can respond to such needs. We focused on electroencephalography (EEG), as it could be handled effectively during a dedicated evaluation phase. We identified workload, attention, vigilance, fatigue, error recognition, emotions, engagement, flow and immersion as being recognizable by EEG. We find that workload, attention and emotions assessments would benefit the most from EEG. Moreover, we advocate to study further error recognition through neuroimaging to enhance usability and increase user experience. This review paper was published in the proceeding of the Physiological Computing Systems (PhyCS) conference [12].



*Figure 10. Stereoscopic display studied through EEG by varying apparent depth.*

Along this line of research, we also explored whether it was possible to assess the zone of comfort in stereoscopic displays using electroencephalography. Indeed, the conflict between vergence (eye movement) and accommodation (crystalline lens deformation) occurs with every stereoscopic display. It could cause important stress outside the "zone of comfort", when stereoscopic effect is too strong. This conflict has already been studied using questionnaires, during viewing sessions of several minutes. We built an experimental protocol (see Figure 10 ) which compares two different comfort conditions using electroencephalography over short viewing sequences. Analyses showed significant differences both in event-related potentials and in frequency bands power. By extending our protocol it should be possible to study at the same time comfort and depth perception, having a better understanding of stereoscopy.