

CERMICS

mathématiques – informatique

CERMICS

Laboratory of applied mathematics and scientific computing
(*Centre d'Enseignement et de Recherche en Mathématiques et Calcul Scientifique*)

Université Paris-Est

École des Ponts ParisTech laboratory hosting joint project-teams with INRIA

CERMICS

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Director: Serge Piperno

Vice-Director: Jean-François Delmas

Staff (83)

15 Researchers

4 Associate researchers

23 External collaborators

22 PhD students

2 Administrative assistants

6 Post-docs

5 Invited researchers

6 Internship students

QUALITATIVE RESULTS

CERMICS is a laboratory of École des Ponts ParisTech, hosting joint research teams with INRIA and University Paris-Est of Marne-la-Vallée (UPEMLV). It is located at École des Ponts ParisTech in Champs-sur-Marne. The scientific activity of CERMICS covers several domains in scientific computing, modelling, and optimization.

Three teams deal with modelling and scientific computing: the “Fluid Dynamics” team (leader: Alexandre Ern), which develops advanced numerical finite element methods applied to transport in porous media, hydraulics, and wave propagation, the “Molecular and Multiscale Simulations” team (leader: Éric Cancès), which covers several connected fields such as electronic structure calculations, numerical statistical physics, multiscale simulation of materials, etc., and the “PDE and Materials” team (leader: Régis Monneau) devoted to the mathematical modelling of material behavior at the crystalline level. Two other teams cover several important domains of applied mathematics: the “Optimization and Systems” team (leader: Michel de Lara) involved in research about optimization (mostly in a stochastic setting), system simulation, and control, and the “Applied Probability” team (leader: Benjamin Jourdain) with applications of probability theory to numerical models and methods. All teams have their own research domains, and collaborate on specific topics, like, for example, multiscale simulations on Quantum Monte Carlo methods for the computation of the ground state energy of a Schrödinger Hamiltonian.

It can be pointed out that two teams are, or take part to, joint project-teams with INRIA: the team “Molecular and Multiscale Simulations” hosts the INRIA Rocquencourt project-team MICMAC (leader: Claude Le Bris), and the team “Applied Probability” hosts the UPEMLV-INRIA Rocquencourt project-team MATHFI (leader: Agnès Sulem).

Key facts

Staff changes, missions, visits

Gabriel Stoltz joined CERMICS as a researcher since 1st September, 2008. He completed his PhD at CERMICS, under the supervision of Éric Cancès, and defended it in June 2007. He then did a post-doc at IMPMC (University Paris VI and VII) with Francesco Mauri. His scientific activities concentrate on the mathematical and numerical study of models for molecular simulation (quantum physics, statistical physics).

Serge Piperno took the head of the École des Ponts ParisTech Research departement at the end of 2008. He has been replaced at the head of CERMICS by Jean-François Delmas. Éric Cancès and Claude Le Bris, the latter as distinguished Ordway visitor, have honored a long-term invitation from the University of Minnesota (School of Mathematics and IMA).

The Applied Probability team hosted Professor Francesco Russo (part-time with INRIA) and his PhD students during his sabbatical year in the MathFi project. Professor Kenji Yasutomi ended his sabbatical year in the Applied Probability team. Professor Igor

Mozolevski from Federal University of Santa Catarina (Brasil) has joined the Fluid Dynamics team for a sabbatical year. He is investigating the modelling and simulation of two-phase water-air flows in porous media. A FAST programme with Feliza Vazquez-Abad (Melbourne University, Austria) has been launched by the Optimization and Systems team, and an ECOS Sud action was started between Chile and France on estimation and qualitative properties for viability domains in sustainable management models. Professor Mustapha Jazar (Beyrouth University Lebanon) visited the PDE and Materials team for one month.

In 2008, CERMICS received six post-doctoral students and had twenty two PhD students, among them six defended their PhD in 2008.

Serge Piperno was the General Secretary of the French Society in applied mathematics (*Société de Mathématiques Appliquées et Industrielles*). Jean-François Delmas was in charge of the group MAS (« *Modélisation Aléatoires et Statistiques* ») on random models and statistics, one of the four thematic groups of SMAI.

Alexandre Ern is the Director of the Groupement MOMAS, a national research programme supported by ANDRA, BRGM, CEA, CNRS, EDF and IRSN which involves twenty laboratories and which aims at improving mathematical models and simulation tools for safety assessment of nuclear waste repositories.

Publications and prizes

The CERMICS laboratory has sustained a high scientific activity: about forty articles have been published in international refereed journals (and over twenty have been accepted for publications). Also above fifty presentations in conferences have been made and twelve conferences or workshop have been organized by members of CERMICS.

The book “Sustainable management of natural resources” from Michel De Lara and Luc Doyen has been published. The prize of the best École des Ponts ParisTech PhD defended in 2007 has been awarded *ex aequo* to Nicolas Forcadel (PDE and Materials team) and Gabriel Stoltz (Molecular and Multiscale Simulation team).

Industrial impact

The activities of industrial transfer in the laboratory are strongly linked to research activities. Scientific results are mostly obtained in collaboration with Research and Development Departments of large industrial firms through research contracts [(CNES, CEA, EADS, EDF, ONERA, IFP, Rio Tinto (formerly Pechiney and then Alcan), Thalès-Alenia Space, etc)]. Ten programmes, which represent a significant part of our financial supports, are granted by the « *Agence Nationale de la Recherche* » (ANR), the French equivalent of the American NSF, which proposes several scientific programme calls and grants.

The programme CREDINEXT from the « *pôle de compétitivité* » finance innovation involving industrial partners and the CERMICS among other academic partners started in 2008. The overall research contracts remained very high in 2008, about 444 k€ for École des Ponts ParisTech.

Teaching

The members of CERMICS are strongly involved in teaching at École des Ponts ParisTech, École Polytechnique, Mines ParisTech, ENSTA) and in Masters in collaboration with Universities.

Among them, École des Ponts ParisTech has convention with Master 2nd year Applied Mathematics and Mathematical finance with UPEMLV, Master 2nd year Numerical analysis and PDE with University Pierre and Marie Curie (Paris VI).

Research teams

1. Applied probability
2. Fluid dynamics
3. Molecular and multiscale simulations
4. Optimization and systems
5. PDE and materials

1. Applied probability

Abdelkoddousse Ahdida, Aurélien Alfonsi, Jean-François Delmas, Julien Foki, Benjamin Jourdain, Bernard Lapeyre, Raphaël Roux, Mohamed Sbai, Simone Scotti, Arnaud Siri-Jégousse, Kenji Yasutomi, Antonino Zanette

The team is mainly interested in the study of probabilistic numerical algorithms with applications going from mathematical finance to biology, quantum chemistry and molecular simulation. The other important research field is the probabilistic interpretation of PDEs, especially nonlinear ones.

1.1 Mathematical finance

The team is involved in the research and teaching chair “Measure of financial risks” with the École Polytechnique and the Société Générale. The team is also part of the Mathfi project together with researchers from the UPEMLV and the INRIA. In september, Francesco Russo (University Paris 13) has joined the Mathfi project for one year and he spends half time at CERMICS together with his PhD students: Nadia Belaribi and Cristina Di Girolami. One specificity of this project is the development of a pricing, hedging and calibration library of numerical routines called PREMIA with the financial support of a consortium of banks (Société Générale, CaLyon, Natixis, CDC). This is done with the contribution of A. Zanette, J. Lelong and A. Kebaier. The version 10 has been released in February 2008. The new contributions to the next version developed since include pricing algorithms for path-dependent options written on stocks or on interest rates in Lévy driven models, pricing algorithms for variance swaps, discretization schemes for the Heston model, pricing and calibration algorithms for CDOs in credit risk.

A. Alfonsi continues his collaboration with A. Schied on the modeling of the liquidity risk in financial markets. A. Ahdida has started his PhD on low-discrepancy sequences in finance under the supervision of B. Lapeyre. He also works with A. Alfonsi on loss models for credit risk. This PhD is financed by the Credinext Project of the « *pôle de compétitivité* » Finance Innovation. During the second year of his PhD, M. Sbai has worked under the supervision of B. Jourdain on the joint modelling of indexes and their composing stocks: by studying the asymptotics of a large number of stocks, they have addressed the calibration of a model where the index influences the dynamics of its composing stocks. In October, S. Scotti has defended his thesis on error calculus in finance.

1.2 Monte Carlo methods

The ANR programme AdapMC permits very interesting discussions with the statisticians from the ENST and the University Paris Dauphine. A new programme called BigMC involving the same partners for the period 2009-2012 has been selected by the ANR. For stratified sampling estimators with strata boundaries given by hyperplanes orthogonal to a given direction, P. Étoré, G. Fort, B. Jourdain and E. Moulines have developed a stochastic algorithm able to optimize dynamically this direction and proved that optimization of the abscissae of the strata boundaries along this direction is not useful. For the expectation of a function of a normal random vector, B. Jourdain and J. Lelong have proposed and studied an importance sampling estimator in which the importance sampling parameter is computed by minimizing the empirical approximation of the variance.

In view of financial applications, Monte Carlo methods are coupled with time discretization schemes for the stochastic differential equations governing the evolution of the asset prices. In this domain, A. Alfonsi is working on schemes with high order of weak convergence: he has completed a paper on the discretization of CIR processes and studies the approximation of the maximum in time of the solution of a one-dimensional SDE, the discretization of SDEs driven by the fractional Brownian motion and the discretization of Wishart processes respectively with A. Kohatsu Higa, A. Kebaier and A. Ahdida.

Applications of Monte Carlo methods in physics and chemistry are still investigated. The collaboration of B. Jourdain with the team Molecular and Multiscale Simulations goes on with the thesis of R. Roux who is co-advised by T. Lelièvre. This thesis is dedicated to the mathematical analysis of the Adaptive Biasing Force algorithm which is used for free energy computations in molecular dynamics.

1.3 Biology

In the programme PILE, J. Foki carries on his PhD thesis on detection of language for babies in collaboration with the Necker hospital and the University of Orléans.

J.-F. Delmas and L. Marsalle study the detection of aging in cells using models developed previously in collaboration with F. Taddéi (INSERM at Necker) and integrating dying cells. This work is now extended to continuous time with the collaboration of V. Bansaye and V.-C. Tran.

The thesis of A. Siri-Jégousse co-supervised by J.-F. Delmas and J.-S. Dhersin on the study of non-binary branching models is also in progress. J.-F. Delmas also participates to the ANR project MAEV (*Modèles Aléatoires de l'Évolution du Vivant*) on random models for population evolution, random trees and coalescent.

1.4 Random trees and nonlinear PDEs

In the domain of branching processes and random trees, J.-F. Delmas works with R. Abraham and G. Voisin on general pruning procedures. The project “A3” on random trees and applications, headed by J.-F. Delmas and involving the Universities of Bordeaux, Orléans, Paris-Sud, Paris VI, Nancy and UPEMLV for the period 2009-2012 has been selected by the ANR.

Finally, in the domain of probabilistic interpretation of nonlinear PDEs, B. Jourdain collaborates with J. Fontbona on the long time

behaviour of systems of stochastic vortices associated with the 2nd incompressible Navier-Stokes equation.

2. Fluid dynamics

Nancy Chalhoub, Florent Chazel, David Doyen, Alexandre Ern, Nathalie Glinsky-Olivier, Laurent Monasse, Igor Mozolevski, Serge Piperno, Pierre Sochala, Pablo Tassi, Julie Tryoen

The Fluid Dynamics team develops advanced numerical methods for the simulation of environmental flows (in soils, on their surface, and along the coast), wave propagation (electro-magnetism, acoustics, aero-acoustics, seismics), crack propagation in elastic solids, and complex flows in interaction (fluid-structure interactions, real gases). Scientific activities sweep a large range from physical modelling to design and analysis of numerical methods. A particular emphasis is put on their validation on realistic configurations and their algorithmic - possibly parallel - implementation.

Changes in team members during 2008 are as follows: N. Chalhoub, L. Monasse, and J. Tryoen started their PhD in October 2008, P. Sochala defended his PhD thesis on December 3rd 2008, and Professor I. Mozolevski from Federal University of Santa Catarina (Brasil) has joined the team for a sabbatical year (starting in February 2008).

One of the core expertises of the team concerns Discontinuous Galerkin (DG) methods. Such methods can be viewed as Finite Element methods employing discontinuous (local) basis functions and also as Finite Volume methods allowing for higher polynomial degrees within mesh cells. DG methods offer a high flexibility in dealing with non-conforming meshes, spatially varying polynomial approximations, local time-stepping, and more generally are particularly well suited to multi-physics, multi-domain approaches coupling different models within subdomains.

The contribution of the team concerns:

- the theoretical foundations of the method, in particular the newly introduced concept of weakly converging discrete gradients for piecewise polynomial functions along with new discrete Sobolev embeddings in discrete DG spaces;
- the *a posteriori* analysis of the method for convection-diffusion-reaction problems with heterogeneous data;
- the application of the method in hydraulics and hydrology, to approximate the Richards' equation and the Saint-Venant (shallow-water) equations;
- the analysis of (local) time-stepping schemes for linear wave propagation.

Applications to fluid flow modelling and simulation are fourfold. Firstly, within the PhD thesis of P. Sochala, the coupling of sub-surface, variably saturated, flows with overland flows has been investigated, leading in particular to mass-conservative coupling time-stepping algorithms. Secondly, within the post-doc of P. Tassi and in partnership with the Project ANR « *METHODE* », CETMEF, and IFP, a DG-C++ software is developed to simulate the shallow-water equations possibly coupled to a sediment transport equation. Thirdly, Professor I. Mozolevski has investigated during his sabbatical year in the team the modelling and simulation of two-phase water-air flows in porous media. Finally, F. Chazel has derived during his post-doc, in partnership with the

Saint-Venant Laboratory of École des Ponts ParisTech, new Boussinesq-type models for nonlinear and dispersive wave propagation in coastal and harbour areas.

Applications to solid mechanics have followed two paths. On the one hand, within the PhD thesis of D. Doyen in partnership with EDF R&D, a three-field augmented Lagrangian formulation has been derived and analyzed to approximate static unilateral contact problems with cohesive forces. Numerical tests have also been undertaken to explore the dynamic case where inertia effects play a role. On the other hand, within the PhD thesis of L. Monasse, in collaboration with Ch. Mariotti, *Commissariat à l'Énergie Atomique – Direction des Applications Militaires (CEA/DAM)* and V. Daru and Ch. Tenaud *Laboratoire d'Informatique pour la Mécanique et les Sciences de l'Ingénieur (LIMSI)*, a Lagrangian discrete element method proposed by CEA has been optimized and partly analyzed, leading now to accurate and stable solutions to structural dynamics problems with large deformations, and the analysis of the coupling of these discrete elements with Eulerian formulations for fluids has been started.

Finally, with the PhD thesis of J. Tryoen in collaboration with O. Le Maître (LIMSI), a new topic has been launched since the summer 2008, namely the quantification of uncertainty propagation in hyperbolic equations using polynomial chaos expansions and Galerkin projections. The first application, uncertainties in the initial condition and on the wave speed for 1D inviscid shock tubes, has yielded promising results.

3. Molecular and multiscale simulations

Hanan Amor, Arnaud Anantharaman, Xavier Blanc, Guy Benteux, Sébastien Boyaval, Éric Cancès, Ronan Costouec, Ismaila Dabo, Claude Le Bris, Tony Lelièvre, Kimiya Minoukadeh, Gabriel Stoltz

The scientific activity of the Molecular and Multiscale Simulation team covers several fields: electronic structure calculations, numerical statistical physics, atomistic to continuum methods, homogenization methods, free surface flows and magnetohydrodynamics, and complex fluids.

3.1 Electronic structure calculations

É. Cancès and A. Deleurence have addressed issues related to the modelling and simulation of local defects in periodic crystals. Computing the energies of local defects in crystals is a major issue in quantum chemistry, materials science and nano-electronics. Although several approaches have been proposed, a mathematically consistent quantum model for crystalline materials with local defects was still missing. In collaboration with M. Lewin (CNRS, Cergy), É. Cancès and A. Deleurence have proposed a new model based on formal analogies between the Fermi sea of a perturbed crystal and the Dirac sea in Quantum Electrodynamics (QED) in the presence of an external electrostatic field. Using and adapting recent mathematical tools used in QED, they have suggested a new mathematical approach for the self-consistent description of a crystal in the presence of a defect. The justification of this model is obtained using a thermodynamic limit on the so-called supercell model. They have also introduced a variational

method for computing the perturbation in a basis of precomputed maximally localized Wannier functions of the reference perfect crystal. Some preliminary, promising numerical results have been obtained on a one-dimensional nonlinear model with Yukawa interaction potentials.

Besides, existence results for the extended Kohn-Sham LDA (local density approximation) model as well as for the two-electron Kohn-Sham GGA (generalized gradient approximation) model have been obtained by A. Anantharaman and É. Cancès, using the concentration-compactness method.

On the numerical front, new numerical schemes for solving the constrained optimization problems arising in Density Matrix Functional Theory have been proposed by É. Cancès, in a joint work with K. Pernal (University of Szczecin, Poland). These numerical schemes have better convergence properties than the pre-existing ones.

In collaboration with W. Hager (University of Florida), the domain decomposition approach, designed by M. Barrault (now at EDF), G. Bencteux, É. Cancès, and C. Le Bris for electronic structure calculations has been improved. The development of the domain decomposition algorithm for the linear subproblem has been continued. Further algorithmic improvements of the most time consuming part of the algorithm have resulted in a significant decrease in memory and CPU demands (up to a factor 10 for alkane molecules) and of the overall accuracy of the resulting domain decomposition algorithm.

A parallel implementation on the Blue Gene computer has allowed to solve the linear subproblem for a polyethylen chain of five million atoms (17.5 million basis functions) in about sixty minutes on 1 024 processors, confirming the high scalability of the method. The current version of the code allows to simulate elongated systems such as linear polymers or nanotubes. A new version of the code, designed for the simulation of more complex systems, is currently in development, notably by H. Amor in the context of her post-doc, and in the framework of a collaboration with EDF supported by the ANR project « *Parallélisation pour la simulation des matériaux* » (PARMAT). From a numerical analysis viewpoint, the convergence properties of the MDD algorithm have been studied, and the convergence established in a simplified setting.

Quantum mechanical calculations are frequently used in computational surface science for predicting catalytic activities, for elucidating chemical processes, and for interpreting spectroscopic experiments. In recent years, several methods have been developed to extend the application of first-principles DFT methods to surface electrochemistry.

Nevertheless, computational approaches to treat electrochemical systems (*e.g.*, fuel cells and batteries) as a function of the applied voltage have been lacking. In collaboration with N. Marzari, B. Kozinsky and N. Singh-Miller (MIT), I. Dabo, Y. Li and É. Cancès have developed an atom-continuum model for the first-principles simulation of catalytic systems under electrochemical conditions. They have implemented and validated an efficient algorithm to solve the nonlinear partial differential equations underlying the model. In addition, they have developed a method to perform electronic-structure optimizations at fixed applied potential, eliminating inherent numerical instabilities.

This seems to be the first implementation of electronic-structure calculations under realistic electrochemical conditions at constant applied potential. They are currently focusing on the parallelization of these algorithms for their final incorporation in the Quantum-Espresso computational toolkit. In the near future, they plan to apply this electrochemical model to the determination of reaction pathways under applied potential.

In collaboration with physicists from *Institut de Minéralogie et de Physique des Milieux Condensés* (IMPMC) Paris VI, G. Stoltz has studied the thermal conductivity of carbon nanotubes using methods from quantum statistical physics. Carbon nanotubes are very interesting materials from a theoretical viewpoint (they are “real” materials for which Fourier’s law does not hold, as predicted by the theoretical predictions for one dimensional systems), but also for industrial applications since they have outstanding mechanical, electronic and thermal properties. This work has focused on the reduction of the thermal conductance generated by the presence of isotope disorder.

In collaboration with C. Brouder (IMPMC, Paris VI) and G. Panati (University La Sapienza, Roma), G. Stoltz has also studied the validity of the Gell’Mann and Low formula on a simple finite dimensional example. The Gell’Mann and Low formula is an important formula in many-body perturbation theory, and is at the basis of almost all approximation schemes in this field. Loosely speaking, it says that the eigenstate of a Schrödinger type operator, associated with a non-degenerate eigenvalue, can be transformed into the eigenstate of a perturbed Schrödinger operator, upon some renormalization procedure. However, when the eigenstate is degenerate, it is unclear how to perform such a renormalization. Work is on progress to generalize in an abstract setting the results found in the simple finite dimensional case.

3.2 Numerical statistical physics

Sampling of constrained dynamics. In many cases, the dynamics of the system under study is restrained to some submanifold of the whole accessible space. A famous instance is the Hamiltonian dynamics, for which the energy of the system is constant. Hamiltonian dynamics is useful for computing average properties assuming ergodicity. However, constant energy sampling may be achieved with stochastic dynamics as well; such a scheme has been analyzed by E. Faou (INRIA Rennes) and T. Lelièvre; rates of convergence have been provided. Constrained SDEs also appear for the sampling of measures defined on submanifolds, which is useful for thermodynamics integration. C. Le Bris, T. Lelièvre and E. Vanden-Eijnden (Courant Institute) have proved the consistency of various numerical schemes (predictor-corrector schemes).

Highly-oscillatory dynamics. Constant energy averages are often computed as long time limits of time averages along a typical trajectory of the Hamiltonian dynamics. One difficulty of such a computation is the presence of several time scales in the dynamics: the frequencies of some motions are very high (*e.g.* for the atomistic bond vibrations), while those of other motions are much smaller. Actually, fast phenomena are only relevant through their mean effect on the slow phenomena, and their precise description is not needed. Consequently, there is a need for time integration algorithms that take into account these fast phenomena only in an averaged way, and for which the time step is not restricted by the

highest frequencies. C. Le Bris and F. Legoll (UR Navier/Structures Team) have initiated a study along this line, and obtained encouraging results that have been reported. The authors currently follow up on this subject, in collaboration with F. Castella, P. Chartier and E. Faou from INRIA Rennes.

Adaptive sampling methods. For large molecular systems, the information of the whole configuration space may be summarized in a few coordinates of interest, called reaction coordinates. An important problem in chemistry or biology is to compute the effective energy felt by those reaction coordinates, called free energy. The Adaptive Biasing Force method is a stochastic algorithm used to compute this free energy. It is based upon a nonlinear dynamics, which uses the reaction coordinate to prevent the system from being trapped in metastable regions. The nonlinearity in the dynamics comes from a conditional expectation computed with respect to the solution. A convergence result for this nonlinear dynamics has been obtained by T. Lelièvre, M. Rousset (INRIA Lille) and G. Stoltz, in some limiting regime, using entropy methods and a decomposition of the total entropy of the system into a microscopic part (associated with conditioned measures) and a macroscopic part (related to some global features of the system). In addition, B. Jourdain, T. Lelièvre and R. Roux have studied a particle approximation of this dynamics, relying on Nadaraya-Watson estimators for the conditional expectation. They have obtained a result of convergence to a solution of the Adaptive Biasing Force dynamics, and subsequently an existence result for this dynamics. As a by-product of the work, T. Lelièvre has obtained a new result for proving a logarithmic Sobolev inequality on a measure m defined on \mathbb{R}^n , assuming that a logarithmic Sobolev inequality holds for the marginals f^*m and the conditional measures $m(\cdot|f)$ associated to some function $f: \mathbb{R}^n \rightarrow \mathbb{R}^m$ (with $m \llcorner \mathbb{R}^n$). This theoretical result has practical interest in molecular dynamics, where f is the reaction coordinate, and where the above assumptions are often met in practice.

Entropy methods have also been employed by J.-B. Maillet and G. Stoltz for proving the convergence of a dynamics to sample a system with constraints fixed in average. The proposed sampling strategy was used to compute the Hugoniot curve of Argon (*i.e.* all the states that can be reached by a shock compression from a given state).

The free energy completely describes the statistics of the reaction coordinates. F. Legoll and T. Lelièvre are currently working on the definition of a dynamics closed in these reaction coordinates. The problem hence amounts to reducing the dimension of a set of SDEs, from the full set of degrees of freedom to only a small subset of them. Encouraging numerical results have been obtained, along with estimates on the accuracy on the proposed effective dynamics (again using entropy techniques).

Search for reaction paths. The microscopic dynamics used to sample the configurations of the system are often trapped in metastable states. A major numerical issue is therefore the search for transition paths connecting metastable states. É. Cancès, F. Legoll, K. Minoukadeh and two of their collaborators at CEA Saclay have proposed an improvement to an existing eigenvector following method, the Activation-Relaxation Technique nouveau (ARTn), for searches of saddle points and transition pathways on a given potential energy surface. Local convergence and robustness of the algorithm have been established, and the new method

has been successfully tested on point defects in body centered cubic iron.

3.3 Atomistic to continuum methods

The project-team has continued its theoretical and numerical efforts on the general topic of “passage from the atomistic to the continuum”. This concerns theoretical issues arising in this passage but also the development and the improvement of numerical simulations coupling the two scales.

In collaboration with C. Patz (WIAS, Berlin) and F. Legoll (UR Navier/Structures Team), X. Blanc and C. Le Bris have recently addressed questions related to finite temperature modelling of atomistic systems, and derivation of coarse-grained descriptions. The starting observation is that, for atomistic systems at constant temperature, relevant quantities are statistical averages of some functions (called observables in that context) with respect to the Gibbs measure. One particular case of interest is when the observable at hand does not depend on all the variables, but only on some of them (gathered in a region of interest, where some defects appear, for instance). In that case, a relevant quantity to compute is the free energy associated to these few degrees of freedom. In the one-dimensional setting, an efficient strategy, that bypasses the simulation of the whole system, has been proposed to compute this free energy, as well as averages of such observables. This strategy is based on a rigorous thermodynamical procedure. Current efforts aim at extending the strategy to more complex cases.

3.4 Homogenization methods

X. Blanc and C. Le Bris have studied, for homogenization of elliptic partial differential equations, the applicability of ideas based on filtering. The bottom line is to modify the corrector problem by introducing a filtering function, in order to improve the efficiency of the method. Some popular methods, such as the oversampling method, can indeed be considered as special instances of such a general strategy. Encouraging numerical results, supported by a rigorous theoretical analysis, have been reported in the case of periodic and quasi-periodic settings.

Efforts in the field of stochastic homogenization of elliptic equations have also been pursued. An interesting case in that context is when the randomness comes as a small perturbation of the deterministic case. This case has been studied by X. Blanc and C. Le Bris, in collaboration with P.-L. Lions (*Collège de France*). This analysis naturally gives rise to a numerical strategy, which is currently implemented by R. Costouec, as the first stage of his PhD thesis.

In the work mentioned above, the perturbation to the deterministic case is supposed to be small. A. Anantharaman and C. Le Bris are currently working on extending this study to the case when the perturbation is small in a weaker norm, typically the L_1 norm (that is, only the expectation of the perturbation is assumed to be small).

In the context of parabolic homogenization, A. Anantharaman has addressed the question of boundary layers in time (close to the initial time $t=0$) and space (close to the domain boundaries), in collaboration with G. Allaire (CMAP). The idea is to add boundary layer terms to the usual approximate solution (which is computed by solving the homogenized problem and the corrector

problems), so that the difference between the exact solution and the approximate solution can be estimated, and more precisely controlled in interesting functional spaces. Some interesting preliminary steps have been performed, but definite conclusions on this problem have yet to be obtained.

Also at the numerical level, S. Boyaval has tested the feasibility of a reduced-basis approach for multiscale problems in the context of (deterministic) homogenization of scalar elliptic equations. The project is a close collaboration with A.-T. Patera (MIT) and Y. Maday (CNRS/UPMC/Brown). The results allow for a fast and rigorous numerical homogenization of heterogeneous materials.

Furthermore, in collaboration with Y. Maday (CNRS/UPMC/Brown), N.C. Nguyen and A.-T. Patera (MIT), S. Boyaval and C. Le Bris have studied the applicability of reduced-basis ideas to variational problems with stochastic parameters. The motivation stems from the need of taking into account many different random microstructures in the context of stochastic homogenization. One of the bottlenecks is that the solutions, for different stochastic parameters, to a given partial differential equation, form a high-dimensional space. To address this difficulty, different approaches have been recently suggested in the literature on uncertainty quantification for stochastic partial differential equations. The combination of these approaches with the reduced-basis method has been tested and analyzed for a scalar (linear) elliptic problem with stochastic boundary conditions.

3.5 Free surface flows and magneto-hydrodynamics

The project-team is since many years a long-term collaborator of RioTinto (formerly Pechiney, and Alcan) on the modelling of aluminium electrolysis cells. Several theoretical and numerical topics of research are issued from this collaboration. The subsequent problem is one instance of those.

A general difficulty for two-fluid flows in a box is the modelling of the moving contact line, namely the boundary of the free interface between the two fluids. An adequate boundary condition between no-slip and pure slip should be derived in order to appropriately model the motion of the free surface. Recently, the Generalized Navier Boundary Condition have been introduced by T.-Z. Qian *et al.* An Arbitrary Lagrangian Eulerian (ALE) formulation of the Generalized Navier Boundary Condition has been proposed by J.-F. Gerbeau (INRIA, project-team REO) and T. Lelièvre. The stability of the numerical scheme is analyzed in energy norm and the validity of the approach is demonstrated by numerical experiments on two-fluid flows in narrow channels.

3.6 Complex fluids

In this field, two subjects related to the discretization of models for complex flows have been addressed: (1) free energy dissipative schemes for macroscopic models (like Oldroyd-B model) and (2) analysis of a numerical method to solve high-dimensional PDEs, with application to the Fokker-Planck equation involved in micro-macro models (like FENE model).

In collaboration with C. Mangoubi (The Hebrew University of Jerusalem), S. Boyaval and T. Lelièvre have analyzed the stability

of various finite element schemes, regarding free energy. More precisely, it is known that the Oldroyd-B model is dissipative when considering a free energy rather than the usual energy considered by many authors. A natural question is then: do the numerical schemes used in practice satisfy similar free energy dissipative properties? Some criteria to be satisfied in order for the finite element scheme to enjoy such a property have been identified. The log-formulation recently introduced by Fattal *et al.* is also analyzed and it is proved that the associated numerical scheme is unconditionally stable (with respect to the timestep) which may explain the rather good results obtained in practice with this formulation.

As a follow-up, S. Boyaval and J.-W. Barrett (Imperial College, London, UK) are currently completing a study on the convergence of free-energy-dissipative finite element approximations to regularized Oldroyd-B models. Using a particular discretization of the advection term, they show that it is possible to use continuous finite element spaces to obtain a discrete analogue of the free energy bound for a regularized Oldroyd-B model. Moreover, convergence (up to a subsequence), as the mesh parameters tend to zero, of such a scheme is proved, which yields existence of global-in-time solutions to this modified Oldroyd-B system.

In collaboration with Ph. Coussot (LCPC) and F. Lequeux (ESPCI), É. Cancès, S. Boyaval and C. Le Bris are working on numerical simulations of constitutive equations for viscoelastic fluids subject to thixotropic effects. The combination of such developments with the free-energy-dissipative finite element schemes mentioned above is currently under study, as well as benchmark simulations that can be compared to actual experiments.

Moreover, equations for thixotropic viscoelastic fluids that involve a high-dimensional stochastic modelling (Fokker-Planck equation) also exist which have motivated the further study of a reduction method (the reduced-basis method) and its application to stochastic models, in collaboration with Y. Maday (University Paris 6 and Brown University) and A.-T. Patera (MIT).

A numerical method for high dimensional PDEs

In collaboration with Y. Maday (University Paris 6 and Brown University), C. Le Bris and T. Lelièvre have analyzed a numerical method recently proposed by Ammar *and al.* to solve the Fokker-Planck equation for micro-macro models for complex fluids. This method is based on a representation of the solution as a sum of tensor products of one-dimensional functions, and a greedy algorithm to compute sequentially the terms of the sum. Using known results from approximation theory, a variational formulation of the numerical method (arising from the minimization of some functional) is proved to actually converge to the solution. Many questions remain open concerning the original algorithms proposed (based on the Euler-Lagrange equations associated to the minimization problem), in particular in the case of non self-adjoint operators.

Finally, in collaboration with P.-L. Lions, C. Le Bris has shown existence and uniqueness of solutions to Fokker-Planck type equations with irregular coefficients. This theoretical question originates from the analysis of micro-macro models for polymeric fluids.

4. Optimization and systems

Jean-Philippe Chancelier, Guy Cohen, Michel De Lara, Luc Doyen, Pierre Girardeau, Moez Kilani, Eugénie Lioris, Babacar Seck

External collaborators : Laetitia Andrieu, Kengy Barty, Pierre Carpentier, Anes Dallagi

4.1 Numerical methods in stochastic control

This theme is the core of our team. One of the goals of P. Girardeau's thesis (CIFRE contract with EDF, under the supervision of G. Cohen and P. Carpentier) is to analyze the rate of convergence of the various numerical methods considered so far in previous theses issued from our group in the past ten years. In practically all those methods, Monte-Carlo sampling is used to approximate expectations (or conditional expectations), but since "solutions" are expected in terms of feedback laws, there is also the necessity of some sort of functional approximation. The latter is a source of bias which can be asymptotically reduced by increasing the number of "elements" or "coefficients" to be estimated, but the variance of those estimates is likely to blow up with the number of such elements if the number of Monte Carlo samples is not increased correlatively. Therefore, the true problem is to find the right balance and fine tuning between the number of elements used in the functional approximation and the number of Monte Carlo samples so as to get the best asymptotic rate of convergence of the mean quadratic error as a function of the size of the numerical problem to be solved (this problem size involves both numbers). This approach is probably the most objective way of comparing all those methods.

Another direction of development of P. Girardeau's thesis is the study of some decomposition techniques (akin to "price" decomposition) in a particular stochastic and dynamic framework. Using a model which is frequently encountered in EDF problems (with independent subsystems coupled by static equilibrium constraints), the attempt is to formulate subproblems based on the individual subsystems in which, for each particular subsystem, the "rest of the world" is summarized by some dual information to be adjusted at a second "coordination" level. The benefit of such an approach can be assessed by using the results on the previous topic about the rate of convergence of numerical methods.

4.2 Risk Management and Probability Constraints

Taking risk into account in optimization problems is gaining importance in our team. In 2008, a FAST programme with F. Vazquez-Abad (Melbourne University, Australia) has been launched. B. Seck defended his thesis "From Risk Constraints in Stochastic Optimization Problems to Utility Functions", financed by EDF, under the supervision of M. De Lara and with the participation of L. Andrieu (EDF). We exhibited connections between a loss aversion coefficient and Conditional Value-at-Risk constraints, a specific result among the more general study of maximin economic formulations of how to maximize profit under risk constraints.

The first year of the collaboration with Thalès-Alenia-Space and CNES was devoted to experimenting with an approach based on a previous work of the group (L. Andrieu's thesis and collabora-

tion with F. Vázquez-Abad of Melbourne University) on academic examples of increasing complexity. The main goal is to solve an optimal control problem in which the control may be randomly and temporarily shut down; a constraint upon reaching the final target with a certain probability is imposed to account for this possible failure. Using duality, our approach consists in converting this problem into one of finding a saddle point of some Lagrangian expressed as an expectation, and to compute this saddle point by a stochastic Arrow-Hurwicz algorithm. Successful numerical results have been obtained with simple problems having some common features with the "true" problem. The next year will be devoted to raising the level of complexity and realism of the problems addressed.

4.3 Transport

In 2008, the Region Île-de-France financed the post-doctorate of Moez Kilani on the monocentric urban model with congestion faring. Supervised by M. De Lara, A. de Palma and S. Piperno, this work yielded an efficient algorithm and an interesting application to the Île-de-France case.

The Systems of collective taxis project is driven by G. Cohen and is made of two parts: one is to set up a discrete event simulation tool (written in Python) which is a virtual system in which customers, taxis, dispatchers, etc., mechanically evolve as they would do in the real life; the other part is the "intelligent" part made up of all the on-line and off-line management decisions and algorithms.

The final purpose is to study and fine tune the algorithms by experimenting with the mechanical simulation part as long as the set-up of a mathematical model is impossible because of the complexity of such a system. At this stage, the mechanical simulation part is operational, the post-treatment methods of the data base which is build up during the simulation in order to evaluate performances is almost complete, and the study of some on-line management algorithms has started.

Joint seminars with *Laboratoire Ville Mobilité Transport* have been initiated.

4.4 Mathematical methods for sustainable management of renewable resources and biodiversity

This theme is driven by M. De Lara, in cooperation with different institutions and researchers, national or international.

The main activity in 2008 has been the scientific animation of the network MIFIMA (Mathematics, Informatics and Fisheries Management), a Stic-AmSud project launched in 2006 between Chile, France and Peru.

An ECOSud action also started in 2008 between Chile and France on estimation and qualitative properties for viability domains in sustainable management models. L. Doyen and M. De Lara published in 2008 a book "Sustainable Management of Natural Resources Mathematical Models and Methods" (Springer).

4.5 Scientific software NSP

This theme is driven by J.-P. Chancelier. NSP has evolved during the present year in many aspects by adding primitives and tool-boxes in collaboration with Bruno Pinçon.

For example an interface was added with the parallel toolbox MPI. It gives the possibility to make full parallel tests of the Premia project. An important task was to add the lacking features which were needed in order to facilitate the port of the current version of scicos. This should be achieved during the first semester of 2009 and should lead to an official release of NSP. We have set up a newsgroup, a bug report tool and a wiki site (through google code) in order to prepare the release.

We have also participated to the last release (4.3) of ScilabGtk renamed ScicosLab.

5. PDE and materials

Houda Faour, Ahmad El Hajj, Nicolas Forcadel, Hassan Ibrahim, Cyril Imbert, Régis Monneau

The PDE and Materials team is interested in the modelling of the physics of materials, and in the theoretical and numerical analysis of these models and their simulations.

At the present time, our group concentrates its efforts on the study of the dynamics of line defects in crystals, called dislocations.

The typical length of these defects is the micron. These dislocations are responsible for the macroscopic plastic behavior of metals, and the understanding of plasticity at a microscopic level is one of our main motivations in this direction of research.

Our activity has been developed in the past few years in collaboration with the Laboratory for Microstructure Studies (LEM) at the ONERA. This part of our activity mainly focuses on the complicated dynamics of interacting dislocation lines.

Our team is part of an ANR project (2006-2009) in collaboration with three other teams (CMAP, Tours Univ. and Brest Univ.), whose responsible is A. Chambolle. This financial support helps substantially our team to develop our research and will allow some new interactions. We will in particular welcome S. Cacace on a post-doc position in 2009.

In the same spirit, and in order to develop our numerical methods, we have obtained a contract with the CEA to find a numerical scheme for the transport of interfaces and a working group has been created to work on this subject. We also organized several conferences. Let us mention in particular a Summer School CEA-EDF-INRIA entitled: Numerical methods for Hamilton-Jacobi equations and hyperbolic conservation laws.

We have also extended our research to the study of dislocations density models in connection with elasto-visco-plasticity of metals. This project has been carried out in the PhD thesis of H. Ibrahim, who studied dislocations density models with scale effects.

H. Ibrahim defended his PhD in June 2008 with greatest honors. He was co-directed by Prof. M. Jazar (from Beyrouth University) who was awarded one month invited position at École des Ponts ParisTech.

Part of our objectives is to establish the connection between the dynamics of a finite number of dislocation lines and the dynamics of dislocation densities, based on non-linear homogenization tools. We have accomplished significant progress in this direction with C. Imbert and N. Forcadel (at partial time in CERMICS).

On dislocation dynamic, N. Forcadel obtained a permanent position at Dauphine University.

As another interesting fact, we can mention that a former PhD student of our team, Adrien Blanchet obtained a permanent position at Toulouse University.

Finally, we have to stress on the fact that our team is strongly involved in teaching activities, both at the École des Ponts ParisTech and at the University, where each year we welcome several students for short research projects.

Staff

Researchers (15)

ALFONSI Aurélien
 CANCÈS Éric
 CHANCELIER Jean-Philippe
 COHEN Guy
 DE LARA Michel
 DELMAS Jean-François
 ERN Alexandre
 GLINSKY-OLIVIER Nathalie
 JOURDAIN Benjamin
 LAPEYRE Bernard
 LE BRIS Claude
 LELIÈVRE Tony
 MONNEAU Régis
 PIPERNO Serge
 STOLTZ Gabriel

Researchers in joint research teams (5)

BALLY Vlad	UPEMLV
LAMBERTON Damien	UPEMLV
LELONG Jérôme	INRIA
RUSSO Francesco	INRIA
SULEM Agnès	INRIA

Associated researchers (4)

EL HAJJ Ahmad	Univ. Orléans
FORCADEL Nicolas	Univ. Dauphine
IBRAHIM Hassan	Univ. Dauphine
IMBERT Cyril	Univ. Dauphine

External collaborators (23)

ANDRIEU Laetitia	EDF
BARLES Guy	Univ. Tours
BARTY Kengy	EDF
BLANC Xavier	INRIA
BRIANI Ariela	Univ. Pise
CARDALIAGUET Pierre	Univ. Brest
CARLINI Elisabetta	Univ. La Sapienza
CANNONE Marco	UPLMV
CARPENTIER Philippe	ENSTA
DA LIO Francesca	Univ. Padoue
DALLAGI Anes	EDF
FALCONE Maurizio	Univ. La Sapienza
FINEL Alphonse	ONERA
FOREST Samuel	ENSMP
HOCH Philippe	CEA
LE BOUAR Yann	ONERA
LEY Olivier	Univ. Tours
ROUY Élisabeth	Centrale Lyon
ZANETTE Antonino	Univ. of Udine

Visiting Researchers (6)

ALIBAUD Nathael (one week)
 DEL MAR GONZALEZ Maria (January)
 JAZAR Mustapha (mid June – mid July)
 MOZOLEVSKI Igor (one year)
 YASUTOMI Kenji (one year)

Post-doctoral students (6)

AMOR Hanen
 CHAZEL Florent
 DABO Ismaila
 KILANI Moez
 LI Yanli
 TASSI Pablo

Ph. D Students (22)

AHDIDA Abdelkoddousse
 ANANTHARAMAN Arnaud
 BENCTEUX Guy (defended in December)
 BOYAVAL Sébastien
 CHALHOUB Nancy
 COSTAOUEC Ronan
 DELEURENCE Amélie (defended in December)
 DOYEN David
 FAOUR Houda
 FOKI Julien
 GIRARDEAU Pierre
 IBRAHIM Hassan (defended in June)
 MINOUKADEH Kimiya
 LIORIS Eugénie
 MONASSE Laurent
 ROUX Raphaël
 SBAI Mohamed
 SCOTTI Simone (defended in October)
 SECK Babacar (defended in September)
 SOCHALA Pierre (defended in December)
 SIRI-JEGOUSSE Arnaud (Univ. Paris Descartes)
 TRYOEN Julie

Internship students (6)

AMINATA NIELE Coulibaly
 BELLEKRID Amine
 BOUDGERADA Rachida (Univ. Boumediene, Algeria)
 DE MAAK Alexis
 LESOUHAITIER Pierre
 PATRIZI Stefania (mid March and April)

Administrative Assistants (2)

BACCAERT Catherine (since June)
 BERTE Sylvie (until July)
 OUHANNA Martine

QUANTITATIVE RESULTS

Knowledge production

PUBLICATIONS¹

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ERN Alexandre, MOZOLEVSKI Igor, SCHUH Luciane

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ETORÉ Pierre, JOURDAIN Benjamin

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FAOU Erwan, LELIÈVRE Tony

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MONNEAU Régis, FORCADEL Nicolas

“Existence of solutions for a model describing the dynamics of junctions between dislocations”. *SIAM (Society for Industrial and Applied Mathematics), Journal on Mathematical Analysis* (accepted)

MONNEAU Régis, FORCADEL Nicolas, IMBERT Cyril

“Homogenization of the dislocation dynamics and of some particle systems with two-body interactions”. *Discrete and Continuous Dynamical Systems - A*, March 2009, vol. 23 (3) pp. 785 - 826

MONNEAU Régis, FORCADEL Nicolas, IMBERT Cyril

“Homogenization of fully overdamped Frenkel-Kontorova models”. *Journal of Differential Equations*, 1st February 2009, 246 (3) 0, pp. 1057-1097
doi:[10.1016/j.jde.2008.06.034](https://doi.org/10.1016/j.jde.2008.06.034)

MONNEAU Régis, BENGURIA Raphaël, DOLBEAULT Jean

“Harnack inequalities and discrete-continuum error estimates for a chain of atoms with two-body interactions”. *Journal Statistical Physics* (accepted)
doi:[10.1007/s10955-008-9662-4](https://doi.org/10.1007/s10955-008-9662-4)

MONNEAU Régis, WEISS Georg

“Pulsating traveling waves in the singular limit of a reaction-diffusion system in solid combustion”. *Annales de l'Institut Henri Poincaré, Non Linear Analysis*, Available online, 27th September 2008 (in press)
doi:[10.1016/j.anihpc.2008.09.002](https://doi.org/10.1016/j.anihpc.2008.09.002)

Article in press in other “A-ranked” publications**CHANCELIER Jean-Philippe, DE LARA Michel, DE PALMA André**

“Risk aversion in expected intertemporal discounted utilities bandit problems”. *Theory and Decision*, 2008 (in press)
doi:[10.1007/s11238-008-9105-3](https://doi.org/10.1007/s11238-008-9105-3)

MAILLET Jean-Bernard, STOLTZ Gabriel

“Sampling constraints in average: the example of Hugoniot curves”. *Applied Mathematics Research Express* (to appear)

MONNEAU Régis, FORCADEL Nicolas, IMBERT Cyril

“Viscosity solutions for particle systems and homogenization of dislocation dynamics”. Contribution to the collective book “On the notions of solutions to nonlinear elliptic problems: results and developments”. *Quaderni di Matematica* 23, publication of the Department of Mathematics of the Seconda Università di Napoli, Caserta, 2008. Editors: A. Alvino, A. Mercaldo, F. Murat, I. Peral. (accepted, to appear in summer 2009)

Other publications**BOULEAU Nicolas**

Crise financière et mathématiques. Le Figaro.fr, Friday, 31st October, 2008

MONNEAU Régis

A new numerical method for the computation of dislocation dynamics. *Dossier de recherche de l'École des Ponts*, n° 18

Scientific Books**DE LARA Michel, DOYEN Luc**

Sustainable Management of Natural Resources. In: *Mathematical Models and Methods, Berlin: Springer-Verlag*, 2008, 266 p.
ISBN: 978-3-540-79073-0

Book chapters**ALFONSI Aurélien**

Cox-Ingersoll-Ross (CIR) model. In: *Encyclopedia in Finance*. Wiley, (to appear in 2009)

BARRAULT Maxime, BENCTEUX Guy, CANCÈS Éric, William W. HAGER, LE BRIS Claude

Domain decomposition and electronic structure computations: a promising approach. In: *Partial Differential Equations: Modelling and Numerical Simulation*. Springer Series in scientific computation, 2008, vol. 41, pp. 147-166

LAPEYRE Bernard

Chapter on variance reduction methods for financial models. In: *Encyclopedia of Quantitative Finance*, 2008 (accepted, to appear)

Research reports

ABRAHAM Romain,
DELMAS Jean-François,
VOISIN Guillaume

Pruning a Lévy continuum random tree
CERMICS Research Report 374

ANANTHARAMAN Arnaud, CANCÈS Éric

On Kohn-Sham models with LDA and GGA exchange-correlation functional
Preprint INRIA-00325660, 2008

BLANC Xavier, LE BRIS Claude,
LEGOLL Frédéric, PATZ Carsten

Finite-temperature coarse-graining of one-dimensional models: mathematical analysis and computational approaches
Preprint INRIA-00282107, 2008

BOUQUET Antoine, DEDEBAN Claude,
PIPERNO Serge

Discontinuous Galerkin Time-Domain solution of Maxwell's equations on locally-refined grids with fictitious domains
CERMICS Research Report 380

BOYAVAL Sébastien, LE BRIS Claude,
MADAY Yvon, NGUYEN Ngoc Cuong,
PATERA Antony

A reduced basis approach for variational problems with stochastic parameters: Application to Heat Conduction with Variable Robin Coefficient
CERMICS Research Report 385
Preprint INRIA-00311463

CANCÈS Éric, LEGOLL Frédéric,
MARINICA Mihai-Cosmin,
MINOUKADEH Kimiya, WILLAIME F.

Some improvements of the ART method for finding transition pathways on potential energy surfaces
Preprint arXiv:0806.4354, 2008

DELMAS Jean-François,
MARSALLE Laurence

Detection of cellular aging in a Galton-Watson process
CERMICS Research Report 391

DESJARDIN Valérie, FOKI Julien,
CHAUVEAU Didier, DELMAS Jean-François

Analyse statistique de la communication par le système perceptif d'un bébé (de 3 à 9 mois) avec sa mère
hal-00324170

DI PIETRO Daniele A., ERN Alexandre

Discrete functional analysis tools for Discontinuous Galerkin methods with application to the incompressible Navier-Stokes equations
CERMICS Research Report 381

ERN Alexandre, STEPHANSEN Annette F., VOHRALIK Martin

Guaranteed and robust discontinuous Galerkin *a posteriori* error estimates for convection-diffusion-reaction problems
CERMICS Research Report 370

ÉTORÉ Pierre, FORT Gersende,
JOURDAIN Benjamin, MOULINES Éric

On Adaptive Stratification
CERMICS Research Report 386

JOURDAIN Benjamin, LELIÈVRE Tony,
ROUX Raphaël

Existence, uniqueness and convergence of a particle approximation for the Adaptive Biasing Force process
doi:[hal.archives-ouvertes.fr:hal-00370821_v1](https://hal.archives-ouvertes.fr/hal-00370821_v1)

JOURDAIN Benjamin, LELONG Jérôme

Robust Adaptive Importance Sampling for Normal Random Vectors
CERMICS Research Report 389

JOURDAIN Benjamin, SBAI Mohamed

Coupling index and stocks
CERMICS Research Report 392

LE BRIS Claude, LEGOLL Frédéric

Integrators for highly oscillatory Hamiltonian systems: an homogenization approach
Preprint INRIA-00165293

LE BRIS Claude, LELIÈVRE Tony,
MADAY Yvon

Results and questions on a nonlinear approximation approach for solving high-dimensional partial differential equations.
CERMICS Research Report 390

LE BRIS Claude, LEGOLL Frédéric

Integrators for highly oscillatory Hamiltonian systems: an homogenization approach
Preprint INRIA-00165293

SOCHALA Pierre, ERN Alexandre,
PIPERNO Serge

Mass conservative BDF-discontinuous Galerkin/explicit finite volume schemes for coupling subsurface and overland flows
CERMICS Research Report 387

STOLTZ Gabriel, LAZZERI Michele,
MAURI Francesco

Thermal transport in isotopically disordered carbon nanotubes
Preprint arXiv:0810.1830, 2008

Written conference communications

DI PIETRO Daniele A, ERN Alexandre

A Discontinuous Galerkin flux for anisotropic heterogeneous second-order elliptic problems.

Finite Volumes for Complex Applications V, 2008, pp. 777-794, R. Eymard and J.-M. Hérard (Eds.), John Wiley & Sons, London, UK

ERN Alexandre, PEROTTO Simona,
VENEZIANI Alessandro

Hierarchical model reduction for advection-diffusion-reaction problems. In: *Numerical Mathematics and Advanced Applications*, K. Kunisch, G. Of and O. Steinbach (Eds.), Springer, Berlin, 2008, pp. 703-710
doi:[10.1007/978-3-540-69777-0](https://doi.org/10.1007/978-3-540-69777-0)

ERN Alexandre, PIPERNO Serge,
TASSI Pablo

A well-balanced Runge-Kutta Discontinuous Galerkin method for the shallow-water equations with flooding and drying. In: *Finite Volumes for Complex Applications V*, R. Eymard and J.-M. Hérard (Eds.), J. Wiley & Sons, London, UK, 2008, pp. 367-374

MONNEAU Régis, EL HAJJ Ahmad,
IBRAHIM Hassan

Derivation and study of dynamical models of dislocation densities (Accepted to proceedings of CANUM 2008)

Contracts/grants for academic research

Obtained

ALFONSI Aurélien, DELMAS Jean-François,
JOURDAIN Benjamin, LAPEYRE Bernard,
LELIÈVRE Tony

ANR BigMC
Monte Carlo methods in large dimension

ALFONSI Aurélien, LAPEYRE Bernard
CréditNext

Project financed by the “*pôle de compétitivité finance*” In Paris that involves Ecole Polytechnique, École des Ponts ParisTech, UPEMLV and INRIA on the Academic side and Euronext, Pricing Partners and Lunalogic on the professional side)

DELMAS Jean-François
ANR A3

Random trees and applications
« *Arbres aléatoires et applications* »

LELIÈVRE Tony, SAUTET Philippe (ENS Lyon)

ANR « SIRE »

« *Calcul intensif et grilles de calcul* »

Ongoing**ALFONSI Aurélien, DELMAS Jean-François, JOURDAIN Benjamin, LAPEYRE Bernard**
Fondation du risque

X-Ponts-Société Générale chair “Financial risks”

ALFONSI Aurélien, JOURDAIN Benjamin, LAPEYRE Bernard, SBAI Mohamed
Premia consortium

Pricing and hedging procedures library financed by a consortium of banks

CANCÈS Éric
ANR LN3M CEA-DAM

Scientific computation and computational grids « *Calcul intensif et grilles de calcul* » (lead by JOLLET F.)

CANCÈS Éric
ANR Parmat - EDF

Scientific computation and computational grids « *Calcul intensif et grilles de calcul* » (lead by BENCTEUX Guy)

DELMAS Jean-François
ANR MAEV

Stochastic modelling for the evolution of population (*Modélisation aléatoire et évolution du vivant*)

DELMAS Jean-François, FOKI Julien
EADS Foundation

Programme PILE on the apparition of the langage fo babies

DELMAS Jean-François, JOURDAIN Benjamin, LAPEYRE Bernard
ANR ADAP’MC

Adaptative Monte Carlo methods

DE LARA Michel
Programme ECOS Sud

Viable control of discrete time systems and applications

DE LARA Michel
Regional cooperation programme
STIC - Amérique du Sud (CNRS-INRIA-Affaires étrangères)
MIFIMA (Mathematics, Informatics and Fisheries Management)**DE LARA Michel**
Réseau thématique pluridisciplinaire
CNRS RTP M3D
Mathematics and management for sustainable resources**DE LARA Michel**
R2DS Île-de-France
TARIFU - *Effets des politiques de tarification de la congestion sur les formes urbaines***ERN Alexandre, PIPERNO Serge, TASSI Pablo**
ANR METHODE
*Modélisation de l’écoulement sur une topographie avec des hétérogénéités orientées et des différences d’échelles***ERN Alexandre**
GNR MOMAS
*A posteriori error estimation, uncertainty quantification and discontinuous Galerkin methods***LAPEYRE Bernard**
Coordination of the ANR programme Grid Computation for Mathematical Finance (Calyon, Centrale, EDF, École des Ponts ParisTech, INRIA, Ixis, Paris VI, Pricing Partner, Summit, Supelec), February 2006-June 2009**LAPEYRE Bernard**
ANR GCPMF
*Grilles de calcul appliquées à des problèmes de mathématiques financière***LELIÈVRE Tony**
ANR INGEMOL « *non-thématique* »
(lead by Philippe Chartier, INRIA Rennes)**MONNEAU Régis**
CEA/DAM IDF, signé en 2007
Space-time analysis of interfaces between different type of materials for the numerical simulation of inertial confinement fusion**MONNEAU Régis**
ANR MICA 2006-2009
« *Mouvement d’interfaces, calcul et applications* »**EDITORIAL BOARDS/ACTIVITY****DE LARA Michel**
Environmental modeling & assessment**PIPERNO Serge**
Member of the editorial board of the journal “Progress in computational fluid dynamics”**CANCÈS Éric,**
ESAIM Proceedings
(co-editor-in-chief with P. Del Moral and J.-F. Gerbeau)**CANCÈS Éric**
Mathematical modeling and numerical analysis**CANCÈS Éric**
SIAM Journal of Scientific Computing**LE BRIS Claude**
Mathematical modeling and numerical analysis
(co-editor-in-chief with Tony Patera)**LE BRIS Claude**
Applied mathematics research express
(Editor-in-chief)**LE BRIS Claude**
Archive for rational mechanics and analysis**LE BRIS Claude**
Control, optimization and calculus of variations**LE BRIS Claude**
Mathematics applied in science and technology**LE BRIS Claude**
Networks and heterogeneous media**LE BRIS Claude**
Nonlinearity

LE BRIS Claude

Review of mathematical science

LE BRIS Claude

Mathématiques et applications, series, Springer

LE BRIS Claude

Modeling, simulations and applications, series, Springer

MEMBERS OF SCIENTIFIC COMMITTEES**ERN Alexandre**

Scientific committee of ANDRA

ERN Alexandre

Scientific committee for MOMAS

ERN Alexandre

Benchmark on reactive transport (completed November 2008)

LAPEYRE Bernard

Member of the program committee of the “Conference on optimization and practices in industry”, 26-28th November, 2008

LAPEYRE Bernard

Member of the scientific committee of the “Conference on numerical methods in finance”, Udine (Italy), 25-27th June, 2008

LAPEYRE Bernard

Member of the programme committee of the “Parallel and distributed computing in finance”, Rome (Italy), 25-29th May, 2009

LE BRIS Claude

Scientific program committee of *Conference franco-canadienne de Mathématiques* 2008, Montreal (Canada)

LE BRIS Claude

Scientific program committee of ICIAM 2011, Vancouver (Canada)

LE BRIS Claude

Board of directors of SMAI (French SIAM)

LE BRIS Claude

Scientific board of École des Ponts ParisTech, 2008 (nominated as representative of the research scholars)

LE BRIS Claude

Evaluation panels for the DFG-Priority (Extraction of Quantifiable Information from Complex Systems), 2008

AWARDS/GRANTS**FORCADEL Nicolas**

Thesis prize of École des Ponts ParisTech, June

STOLTZ Gabriel

Thesis prize of École des Ponts ParisTech, June

CONFERENCES/SEMINARS/ MISSIONS/VISITS**Conferences/participation****International conferences communications****ALFONSI Aurélien**

High order discretization schemes for the CIR process: application to Heston and Affine models. In: Bachelier Conference 2008, 15-19th July, 2008, London (UK)

ALFONSI Aurélien

High order discretization schemes for the CIR process: application to Heston and Affine models. In: *Financial Seminar*, September 2008, Osaka University

ALFONSI Aurélien

High order discretization schemes for the CIR process: application to Heston and affine models. In: *Financial Seminar*, November 2008, Cornell University, Ithaca New York (USA)

BENCTEUX Guy

Multilevel domain decomposition for electronic structure calculations. In: *Workshop on numerical methods in density functional theory*, 23-25th June, 2008, Berlin (Germany)

BENCTEUX Guy

Domain decomposition linear-scaling approach for density computation in electronic structure calculations. In: *Working group on modeling and numerical analysis*, Institute for Mathematics, 3rd June, 2008, TU Berlin

BLANC Xavier

Second Canada-France Congress, UQAM, June 2008, Montreal (Canada)

BOULEAU Nicolas

Dirichlet forms generated by the arbitrary functions principle. Technic University, January 2008, Vienne (Autriche)

BOYAVAL Sébastien

Global solutions to modified Oldroyd-B models. In: *Workshop on multiscale modeling of complex fluids 2007-2008, thematic programme on multiscale modelling of complex fluids* (organized by Beijing University, Beijing international center for mathematical research), May 2008, Beijing (China)

CANCÈS Éric

Density functional theory for materials science: a mathematical perspective (Invited plenary lecture). In: SIAM conference on mathematical aspects of materials science, 11-14th May 2008, Philadelphia (USA)

CANCÈS Éric

Mathematical modelling of electronic structures. In: IMA tutorial on mathematical and computational approaches to quantum chemistry, 26-27th September 2008, Minneapolis (USA)

CANCÈS Éric

Toward multiscale simulation of fuel cells. In: Fourth international conference on Multiscale Materials Modelling (MMM-08), October 2008, Tallahassee (USA)

CANCÈS Éric

Density functional theory for defective crystals. In: *Weekly seminar of the applied mathematics department*, November 2008, University of Minnesota, Minneapolis (USA)

COHEN Guy

Optimal Control is a matter of trade-off...just as in real life. In: *Workshop on the occasion of the retirement of Prof. Geert Jan Olsder*, 12-14th November, 2008, Delft (the Netherlands)

DABO Ismaila

Real-space correction scheme for computing the electrostatic potential of electronic systems. In: *Numerical methods in density-functional theory workshop*, July 2008, TU Berlin

DABO Ismaila

First-principles simulation of electrochemical systems under applied voltage: vibrational Stark effect for CO on platinum electrodes. In: *DFT meets experiment workshop, IFW*, August 2008, Dresden

DE LARA Michel

Explicit construction of viability kernels and management of ecosystems. In: *Colloque CLAIO 2008*, 9-12th September, 2008, Cartagena (Colombia)

DE LARA Michel

Discrete-time viability methods for sustainable management. In: *Second workshop on game theory in energy, resources and environment*, 20-21st November, 2008, GERAD - HEC Montréal (Canada)

DE LARA Michel

Managing conflict economic and ecological objectives in dynamic ecosystem models by viability methods: application to the Hake-Anchovy Peruvian Fisheries, Dept of biology, 26th August, 2008, Mc Gill, Montreal (Canada)

DE LARA Michel

Explicit construction of viability kernels for sustainable management of ecosystems with an application to the Hake-Anchovy Peruvian Fisheries. In: *Séminaire du GERAD conjoint avec la Chaire de théorie des jeux et gestion*, 27th August, 2008, Montreal (Canada)

DE LARA Michel

Mathematics for sustainable management. Departamento de matemáticas Universidad nacional de Colombia, 15th September, 2008, Medellín (Colombia)

DELMAS Jean-François

Immigration and pruning for continuum random trees; In: *Second Canada France Congress*, June 2008, Montréal (Canada)

DELMAS Jean-François

How to detect aging for E. coli cells? National Chiao Tung University, January 2008, Taiwan

DELMAS Jean-François

Length of coalescent trees. National Tsing Hua University, January 2008, Taiwan

ERN Alexandre

Improved energy norm *a posteriori* error estimation based on flux reconstruction for discontinuous Galerkin methods. In: *GAMM Conference*, 1st April 2008, Bremen (Germany)

ERN Alexandre

Convergence of discontinuous Galerkin methods by compactness. In: EFEF, 31th May 2008, Gotteborg (Sweden)

ERN Alexandre

Convergence of discontinuous Galerkin methods by compactness with application to Navier-Stokes equations. In: *VMS Conference*, 24th June 2008, Saarbrücken (Germany)

ERN Alexandre

Improved energy norm *a posteriori* error estimation based on flux reconstruction for discontinuous Galerkin methods. 15th April, 2008, University of Milan (Italy)

ERN Alexandre

Convergence of discontinuous Galerkin methods by compactness, 24th April, 2008, University of Sussex (UK)

JOURDAIN Benjamin

Numerical analysis of the QMC method in a simple case. In: *Workshop on numerical methods in molecular simulation*, 7-11th April, 2008 Bonn (Germany)

JOURDAIN Benjamin

SDEs nonlinear in the sense of McKean driven by Levy processes and related PDEs. In: *Workshop on Nonlocal operators and Applications*, 28th April – 2nd May, 2008, Banff (Canada)

JOURDAIN Benjamin

Adaptive optimal allocation in stratified sampling methods. In: *Conference on numerical methods in finance*, 25-27th June, 2008, Udine (Italy)

JOURDAIN Benjamin

Robust adaptive variance reduction for normal random vectors. In: *Workshop on computational methods with applications in finance, insurance and the life sciences*, RICAM special semester, 17-21st November, 2008, Linz (Autriche)

KILANI Moez, DE LARA Michel, DE PALMA André, PIPERNO Serge

Cost/benefit analysis in a simple monocentric city model with congestion pricing. In: *48th Congress of the European Regional Science Association*, August 2008, Liverpool (UK)

LAPEYRE Bernard

Méthodes Monte Carlo et quasi-Monte Carlo en calcul scientifique, Montréal (Canada), 6-11th July, 2008

LAPEYRE Bernard

Conference on “Numerical methods in finance”. Udine (Italy), 25-27th June, 2008

LE BRIS Claude

Domain decomposition and electronic structure calculations: a new approach (Invited plenary lecture). In: *18th International conference on domain decomposition methods*, 12-15th January, 2008, Jerusalem

LE BRIS Claude

On Fokker-Planck equations with Sobolev regular coefficients and their relation to polymer science. In: Workshop “EDP and applications”, 26th-29th March, 2008, Hammamet (Tunisia)

LE BRIS Claude

Numerical analysis of a method for high-dimensional Fokker-Planck equations in polymer science. In: *Workshop “Multiscale problems in complex fluids”*, 26-30th May, 2008, Beijing (China)

LE BRIS Claude

Domain decomposition and electronic structure calculations: a new approach Minisymposium on Electronic structure calculations. In: *SIAM Conference on Mathematical Aspects of Materials Science*, 11-14th May, 2008, Philadelphia (USA)

LE BRIS Claude

From stochastic lattices to continuum elasticity. Minisymposium on discrete to continuum. In: *SIAM Conference on mathematical aspects of materials science*, 11-14th May, 2008, Philadelphia (USA)

LE BRIS Claude

Mathematics: decades behind chemistry IMA Workshop on Mathematical and numerical aspects of electronic structure calculations, September 2008, Minneapolis (USA)

LE BRIS Claude

Fokker-Planck and stochastic differential equations with Sobolev regular coefficients. In: *DqF workshop on stochastic differential equations: models and numerics*, 20-22nd October, 2008, KTH Stockholm (Sweden)

LE BRIS Claude

Recent progress in stochastic homogenization. Invited keynote speaker in the minisymposium “Mathematical issues in multiscale materials modelling”. In: *Fourth international conference on multiscale materials modelling* (MMM-08), Florida State University, 27-31st October, 2008, Tallahassee (USA)

LE BRIS Claude

Coarse-graining of one-dimensional models at positive temperature. In: IMA Workshop on “Development and analysis of multiscale methods”, 3-7th November, 2008, Minneapolis (USA)

LE BRIS Claude

Weekly seminar of institute of computational mathematics of the Chinese Academy of sciences, February and May 2008 (China)

LE BRIS Claude

Weekly seminar of institute of applied physics. Technische Universität, June 2008, Berlin (Germany)

LE BRIS Claude

Weekly seminar of Freie Universität Berlin, June 2008 (Germany)

LE BRIS Claude

School of mathematics colloquium. University of Minnesota, September 2008 (USA)

LE BRIS Claude

Series of lectures “Computational statistical mechanics” and “Stochastic modelling of materials”, graduate level, 20 hours, Winter 2008, Beijing University

LE BRIS Claude

Series of 5 one-hour lectures “From molecular theories to continuum elasticity: a possible track”. ICMA Summer School Carnegie Mellon, June 2008

LE BRIS Claude

Series of 5 one-hour lectures “Concurrent models. Atomistic to continuum (AtC) modelling”, May 2008, Santiago de Compostela (Chili)

LE BRIS Claude

Series of lectures “Molecular simulation: a mathematical initiation”, 20 hours, fall 2008, University of Minnesota

LELIÈVRE Tony

Workshop on adaptive Markov chain Monte Carlo methods. In: ADAPSKI, January 2008, Bormio (Italy)

LELIÈVRE Tony

Workshop BIRS mathematical and numerical methods for free energy calculations in molecular systems, June 2008, Banff (Canada)

LELIÈVRE Tony

Workshop DqF stochastic differential equations: models and numerics, October 2008, Stockholm (Sweden)

LELIÈVRE Tony

Workshop molecular dynamics thermostats and convergence to equilibrium, November 2008, Edinburgh (UK)

MONNEAU Régis

Giornata INdAM, Padova, June 2008 (Italia)

MONNEAU Régis

Symposium on trends in applications of mathematics to mechanics, September 2008, Levico (Italia)

MONNEAU Régis

Dislocations 2008, October 2008, Hong-Kong (China)

MONNEAU Régis

University of Wroclaw, February 2008 (Poland)

STOLTZ Gabriel

Oberwolfach meeting “Atomistic models of materials”, April 2008 (Germany)

STOLTZ Gabriel

Meeting on “Numerical methods for free energy computations” June 2008, Banff (Canada)

TASSI Pablo

A discontinuous Galerkin method for free surface flows with topography and dry lands WCCM8/ECCOMAS 2008, Venice (Italy)

TASSI Pablo

Discontinuous Galerkin methods for morphodynamic modelling WCCM8/ECCOMAS 2008, Venice (Italy)

National conferences communications**ALFONSI Aurélien**

Optimal execution strategies in limit order books with general shape functions Journées MAS, 27-29th August 2008, Rennes

ALFONSI Aurélien

Optimal execution strategies in limit order books with general shape functions Seminar Bachelier, 1st February, Paris

ALFONSI Aurélien

Optimal execution strategies in limit order books with general shape functions, *GT Méthodes stochastiques et finance*, 18th April, Champs-sur-Marne

ALFONSI Aurélien

High order discretization schemes for the CIR process: application to Heston and Affine models. In : *Seminar Bachelier*, 10th October, Paris

BOULEAU Nicolas

Méthode de la particule prêtée et applications aux processus de Lévy. July 2008, Orléans University

BOULEAU Nicolas

La méthode de la particule prêtée, comment et pourquoi ça marche ? October 2008, UPEMLV

BOYAVAL Sébastien

From free-energy-dissipative schemes for the Oldroyd-B equation to global-in-time (regularized) solutions. In: Centre International de Rencontres Mathématiques (CIRM), CEMRACS 08 “Modélisation et Simulation de Fluides Complexes”, August 2008, Marseille

BOYAVAL Sébastien

Reduced-Basis approach for variational problems with stochastic parameters. In: *GDR MOMAS*, November 2008, IHP, Paris

CANCÈS Éric

Thermodynamic limits for defective crystals. In: *Journées analyse et physique mathématique*, June 2008, IHP, Paris

CANCÈS Éric

Structure électronique de cristaux présentant des défauts locaux. In: *POEMs seminar*, ENSTA, June 2008, Paris

CARPENTIER Pierre,

CHANCELIER Jean-Philippe, COHEN Guy
Robust approach for aerospace optimal control problems. In: *COP1'08 EDF Conference on Optimization and Practices in Industry*, 26-28th November, 2008, Paris

CARPENTIER Pierre,

CHANCELIER Jean-Philippe, COHEN Guy
Robust approach for aerospace optimal control problems aerospace dynamics and optimal control workshop, 23th May, 2008, ENSTA, Paris

CARPENTIER Pierre, GIRARDEAU Pierre

Decomposition techniques for stochastic optimal control problems. In: *COP1'08 EDF Conference on Optimization and Practices in Industry*, 26-28th November, 2008, Paris

DE LARA Michel

Aversion au risque, choix d'itinéraires, et le problème du bandit manchot
Séminaire Modélisation des Réseaux de Transport, 11th December, 2008, École des Ponts ParisTech

DELEURENCE Amélie

Modélisation de cristaux périodiques avec ou sans défauts. In : *CANUM*, May 2008, Saint-Jean-de-Monts

DELMAS Jean-François

Elagage et immigration pour les processus de branchement continus. January 2008, Orsay University

DELMAS Jean-François

Elagage et immigration pour les processus de branchement continus. May 2008, Lille University

DOYEN David, ERN Alexandre, PIPERNO Serge

Analyse d'une méthode d'éléments finis pour la propagation quasi-statique des fissures. In : National congress "Analyse Numérique", May 2008, Saint-Jean-de-Monts

ERN Alexandre

Improved energy norm a posteriori error estimation based on flux reconstruction for discontinuous Galerkin methods. In: National congress "Analyse Numérique" May 2008, Saint-Jean-de-Monts

ERN Alexandre

Discontinuous Galerkin Methods. CEA-EDF-INRIA School on Hamilton-Jacobi equations, 15-19th September, 2008, Rocquencourt

ERN Alexandre

Estimations d'erreur a posteriori robustes et garanties pour les méthodes de Galerkin discontinues, March 2008, University of Cergy

ERN Alexandre

Méthode de Galerkin discontinue et estimation d'erreur a posteriori. In : *Groupe de travail EDF*, May 2008, EDF R&D, Clamart

ERN Alexandre

Estimations d'erreur a posteriori par flux équilibrés pour les méthodes de Galerkin discontinues. September 2008, University of Valenciennes

ERN Alexandre

Quelques résultats d'analyse fonctionnelle discrète et application aux méthodes de Galerkin discontinu, 21th November 2008, University of Paris XIII, Villetaneuse

JOURDAIN Benjamin

Large portfolio losses, a dynamic contagion model by Dai Pra, Runggaldier, Sartori, Tolotti, Credit risk seminar, 7th February, 2008, Évry University

KILANI Moez, DE LARA Michel, DE PALMA André, PIPERNO Serge

Congestion pricing and long term urban form: an application to Île-de-France. In: *Third International Conference on Funding Transportation Infrastructure*, 19-20th June, 2008, Paris

LE BRIS Claude

Seminar at *Laboratoire d'analyse numérique (JLL)*
December 2008, Paris VI

LELIÈVRE Tony

Stochastic dynamics and probability Workshop GREFI-MEFI 2008, March 2008, Marseille

LELIÈVRE Tony

Seminar at ENS Lyon, January 2008

LELIÈVRE Tony

Seminar at University Paris Dauphine, February 2008

LELIÈVRE Tony

Seminar *Équations aux dérivées partielles et applications*. Collège de France, April 2008

LELIÈVRE Tony

Seminar MODANT, April 2008, Grenoble

LELIÈVRE Tony

Seminar *Équations aux dérivées partielles*, September 2008, Chambéry

LELIÈVRE Tony

Seminar *Équations aux dérivées partielles et analyse numérique*, October 2008, Lille

LELIÈVRE Tony

CEMRACS 2008, course (3 hours) on "Multiscale modelling of complex fluids: a mathematical initiation", July 2008, Marseille

LELIÈVRE Tony

École Doctorale ECODOQUI, course (3 hours) on "Méthodes stochastiques en dynamique moléculaire", November 2008, Paris

MONNEAU Régis

Working group "Homogenization", January 2008, Paris 6 University

MONNEAU Régis

Laboratory of Mechanics and Acoustics (LMA), February 2008, Marseille

MONNEAU Régis

Seminar of Jacques-Louis Lions Laboratory, June 2008, Paris 6 University

PIPERNO Serge

A well-balanced Runge-Kutta Discontinuous Galerkin method for the Shallow-Water Equations with flooding and drying. 26th June 2008, *Université Technologique de Compiègne*

PIPERNO Serge

A well-balanced Runge-Kutta Discontinuous Galerkin method for the Shallow-Water Equations with flooding and drying. In: Seminar « *Calcul Scientifique* », 26th March 2008, INRIA Rocquencourt

PIPERNO Serge

Méthodes DGTD avec pas de temps et ordre adaptatifs. In : Seminar, IRMA, 12th February 2008, Strasbourg

ROUX Raphaël

Approximation particulière d'une méthode adaptative de calcul d'énergie libre. In : *Journée MAS de la SMAI*, 29th August 2008, Rennes

ROUX Raphaël

« *Approximation particulière d'une méthode adaptative de calcul d'énergie libre* ». In : Seminar « *processus stochastiques* », 17th November, 2008, Rennes

ROUX Raphaël

« *Calculs d'énergie libre et systèmes de particules en interaction* ». In : *Séminaire des doctorants de l'université Lille 1*, 4th December, 2008, Lille

STOLTZ Gabriel

Seminar at université de Strasbourg, February 2008

TASSI Pablo

Discontinuous Galerkin methods for flow and transport: environmental applications. Université Paris 6, Laboratoire Jacques-Louis Lions, 29th September 2008, Paris

TASSI Pablo

« *La méthode de Galerkin discontinue appliquée aux équations de Saint-Venant et à la géomorphologie fluvial* », Université Blaise Pascal, Laboratoire de Mathématiques, 4th December 2008, Clermont-Ferrand

VAZQUEZ-ABAD Félisa, CARPENTIER Pierre, COHEN Guy

Optimisation under probability constraints: an approach via quantiles. In: COPI'o8 EDF Conference on Optimization and Practices in Industry, 26-28th November, 2008, Paris

Conference/seminar organized**International seminars****CANCÈS Éric (with W. E and M. ORTIZ)**

Minisymposium on Electronic structure calculations. In: *SIAM Conference on Mathematical Aspects of Materials Sciences*, 11-14th May, 2008 Philadelphia (USA)

CANCÈS Éric (with L. BRONSARD and M. ESTEBAN)

Session on Variational and numerical methods in geometry, physics and chemistry. In: *2nd Canada-France congress*, 1-5th June, 2008, Montreal (Canada)

CANCÈS Éric (with J. MEZA)

IMA Tutorial on Mathematical and computational approaches to quantum chemistry, 26-27th September, 2008, Minneapolis (USA)

CANCÈS Éric (with A. KRYLOV, J. MEZA and J. PERDEW)

IMA workshop on “Mathematical and numerical aspects of electronic structure calculations”, 29th September - 3th October, 2008, Minneapolis (USA)

LE BRIS Claude (with WEINAN E, Chun LIU, An-Chang SHI, Qi Wang, Pingwen ZHANG)

The Organizing Committee (only non Chinese national) of the thematic year “Multiscale modeling of complex fluids”, Beijing University, 2007-2008 (China)

LE BRIS Claude (with Michael ORTIZ, Stefan MUELLER)

The organizing committee of the SIAM Conference on Mathematical Aspects of Materials Science, 11-14th May, 2008, Philadelphia (USA)

LE BRIS Claude (with Anna CHAKA, Bill HASE, Michael HOLST, Yousef SAAD, Tamar SCHLICK, Donald G. TRUHLAR, E. WEINAN)

The organizing committee (only non American national) of the IMA thematic year “Mathematics and Chemistry”, 2008-2009, Minneapolis (USA)

MONNEAU Régis

Co-organization of the workshop “Nonlocal operators and applications”, April 2008, BANFF (Canada)

MONNEAU Régis

Organization of a minisymposium “Dislocations”, CANUM 2008, May 2008 Summer School CEA-EDF-INRIA

National seminars**DE LARA Michel**

Comité de programme du COPI'o8 EDF Conference on Optimization and Practices in Industry, 26-28th November, 2008, Paris

JOURDAIN Benjamin

Session on Simulation of stochastic differential equations
Journée MAS, 27-29th August, Rennes

LELIÈVRE Tony

Has been a co-organizer of a mini-symposium on hybrid methods at CANUM, May 2008, Saint-Jean-de-Monts

MONNEAU Régis

Numerical methods for Hamilton-Jacobi equations and hyperbolic conservation laws, September 2008, Rocquencourt

Missions and visits**ALFONSI Aurélien**

Invitation at the Osaka University by Prof. Arturo Kohatsu-Higa, 23rd September-2nd October

ALFONSI Aurélien

Invitation at Ithaca (Cornell) by Prof. Alexander Schied, 17-21st November

CANCÈS Éric

Has honored long term invitations from the following institutions:
Brown University, July-August 2008, Providence, USA
University of Minnesota, IMA, September-December 2008, Minneapolis (USA)

DE LARA Michel

Several missions in Peru, Chile, Colombia related to international programs Stic-AmSud and Ecos Sud

DELMAS Jean-François

Journées MAS, August 2008, Rennes

DELMAS Jean-François

Journées ANR MAEV, September 2008

ERN Alexandre

University of Sussex (3 days in April and 2 days in November 2008)

ERN Alexandre

University of Milan (3 days in April 2008)

ERN Alexandre

Federal University of Santa Catarina, Brasil (1 week in February 2008)

LE BRIS Claude

Has honored long term invitations from the following institutions: University of Minnesota (Distinguished Ordway Visitor, School of Mathematics and IMA), Minneapolis (USA)

LE BRIS Claude

Academic year 2008-2009 Beijing University, Winter term 2008

MONNEAU Régis

University of Wroclaw, Poland, 2 weeks

MONNEAU Régis

February 2008 and 2 weeks April 2008

MONNEAU Régis

Lebanese University, 3 weeks, August 2008

VEESER A. (Professor at University of Milan)

Visited the Fluid Mechanics Team in July 2008

Education activities

SUPERVISION ACTIVITY

Ongoing theses

ANANTHARAMAN Arnaud

Mathematical analysis and numerical simulations for some periodic molecular and multiscale models
École des Ponts ParisTech

AHDIDA Abdelkoddousse

Pricing and hedging credit derivatives, Credit risk derivatives and Numerical aspects
École des Ponts ParisTech

BELLABAS B.

Error calculus for positioning systems (DLR Munich)

BOYAVAL Sébastien

Modelling and simulations for complex fluids
École des Ponts ParisTech

CHALHOUB Nancy

Finite volume methods and *a posteriori* error estimets for unstrody transport problems
École des Ponts ParisTech

COSTAQUEC Ronan

Numerical methods for homogeneization
École des Ponts ParisTech

DOYEN David

Dynamic crack propagation with cohesive forces
École des Ponts ParisTech

FAOUR Houda

Analysis of new models for elasto-viscoplastic materials, taking into account dislocation dynamics
École des Ponts ParisTech and University of Liban

FOKI Julien

Statistical analysis of speech precursors for babies
École des Ponts ParisTech

GIRARDEAU Pierre

High dimensional problems in stochastic dynamical systems

LIORIS Eugénie

Simulations for shared taxis
École des Ponts ParisTech

MINOUKADEH Kimiya

Deterministic and stochastic optimisation methods for molecular simulations
École des Ponts ParisTech

MONASSE Laurent

Discrete finite element methods for structural dynamics and coupling with fluid mechanics
École des Ponts ParisTech

ROUX Raphaël

Probabilistic study of interacting particle systems: applications to molecular simulation
École des Ponts ParisTech

SBAI Mohamed

Simulation of stochastic differential equations in finance
École des Ponts ParisTech

SIRI-JEGOUSSE Arnaud

Whright Fisher models and non-homogeneous coalescing process
Study of coalescent trees

TRYOEN Julie

Uncertainty quantification for hyperbolic problems
École des Ponts ParisTech

Theses defended

BENCTEUX Guy

Improvement of a domain decomposition method for electronic structure computations
École des Ponts ParisTech

DELEURENCE Amélie

Mathematical analysis and numerical simulations of multi-scale models for materials
École des Ponts ParisTech /Bourse Île-de-France

IBRAHIM Hassan

Analysis of parabolic/Hamilton-Jacobi systems modelizing the dynamics of dislocation densities in a bounded domain
École des Ponts ParisTech and University of Liban

SECK Babacar

From Risk Constraints in Stochastic Optimization Problems to Utility Functions
École des Ponts ParisTech

SCOTTI Simone

Dirichlet forms methods in finance I
Scuola Normale Superiore di Pisa and
École des Ponts ParisTech

SOCHALA Pierre

Numerical methods for subsurface flows
confed with overland flows
École des Ponts ParisTech

TEACHING ACTIVITIES**Lectures****École des Mines ParisTech****Automatic control, Scilab tutorial**

CHANCELIER Jean-Philippe, PETIT Nicolas,
ROUCHON Pierre

Acoustics, computer science and music

CHANCELIER Jean-Philippe, D'ANDREA
NOVEL Brigitte

École Polytechnique**Analyse numérique et optimisation**

CANCÈS Éric, LE BRIS Claude

Introduction to probability, 1st year

DELMAS Jean-François

Projects in finance, 3rd year

JOURDAIN Benjamin

Random walks, 2nd year

DELMAS Jean-François

Stochastic numerical methods, 3rd year

JOURDAIN Benjamin

École des Ponts ParisTech**Analysis 1st year**

CANCÈS Éric: Professor in charge,
ANANTHARAMAN Arnaud, BOYVAL
Sébastien, ERN Alexandre, MONNEAU
Régis

Frequence Analysis, 2nd year

CANCÈS Éric, STOLTZ Gabriel

Scientific computing, 1st year

ERN Alexandre: Professor in charge,
PIPERNO Serge, STOLTZ Gabriel

Epistemology

BOULEAU Nicolas, CHATZIS Kostas,
WALLISER bernard

Introduction to mathematical methods for finance, 2nd year

LAPEYRE Bernard

Introduction to statistical physics, 2nd year

DABO Ismaila

Linux / Emacs / Scilab / LaTeX course 1st year

Professors: DE LARA Michel, CHANCELIER
Jean-Philippe,
Assistant professors :BOYVAL Sébastien,
DABO Ismaila, MINOUKADEH Kimiya,
SOCHALA Pierre, TASSI Pablo

Mathematics and applications, Major: Finance, TD, M2R

AHDIDA Abdelkoddousse, SBAI Mohamed

Deterministic methods in financial mathematics, 3rd year

LELIÈVRE Tony

Modeling programming and simulations, 2nd year

ALFONSI Aurélien, KERIVEN Renaud,
LELIÈVRE Tony, MONASSE Pascal

Modelling for the sustainable management of natural resource 1A

DE LARA Michel, Professor

Monte-Carlo methods in finance, 3rd year

JOURDAIN Benjamin, LAPEYRE Bernard

Probabilistic Tools for Finance, 2A

DE LARA Michel, Professor

Probability theory and statistics, 1st year

Professor in charge: JOURDAIN Benjamin,
Assistant professors : ALFONSI Aurélien,
DE LARA Michel, SBAI Mohamed,
TOUBOL Alain

Numerical simulations and multi-scale methods, Master SMCD

Chaire Lafarge
STOLTZ Gabriel

ENSTA**Calibration, local volatility and stochastic, 3rd year, Master MMMEF (Paris I)**

ALFONSI Aurélien

Introduction to probability and statistics, 1st year

DELMAS Jean-François (Prof.), SBAI
Mohamed, ROUX Raphaël

ESIEE**Numerical analysis and optimization, TD L3**

DELEURENCE Amélie

Department of Matematics, University del Valle, Cali (Colombia)**Manejo sostenible de recursos naturales: modelos y métodos matematicos 16-19th September 2008**

DE LARA Michel

Doctoral school ICMS**Levy processes in finance**

DELMAS Jean-François, JOURDAIN
Benjamin, LAPEYRE Bernard

ISBS**Numerical analysis, TP de MATLAB**

MINOUKADEH Kimiya

University Paris I**Mathematical modelling for the sustainable management of natural resource**

DE LARA Michel

Master MMMEF, Paris**Mathematical modelling for the sustainable management of natural resource**

DE LARA Michel

Numerical methods in stochastic optimization, Master MMMEF

CARPENTIER Pierre

Stochastic control, numerical methods and Finance applications, Master MMEF

CHANCELIER Jean-Philippe

University Paris-Est-Marne-La-Vallée

Monte-Carlo methods for finance

JOURDAIN Benjamin, LAPEYRE Bernard

Risk measures in finance, M2

DELMAS Jean-François

Stochastic models, M2

DELMAS Jean-François

University of Paris VI

Probabilistic numerical methods M2

LELIÈVRE Tony

Discontinuous Galerkin methods with applications, M2

ERN Alexandre, PIPERNO Serge

Risk measures in finance, M2

DELMAS Jean-François

Molecular simulations numerical and theoretical aspects, M2

CANCÈS ÉRIC

Multi-scale systems, M2

LE BRIS Claude

Textbooks for teaching activities

DELMAS Jean-François

Introduction to probability and statistics

ERN Alexandre

Scientific computing
École des Ponts ParisTech

JOURDAIN Benjamin

Probability and statistics, 1st year
École des Ponts ParisTech

JOURDAIN Benjamin

Monte Carlo methods for financial models, 3rd year
École des Ponts ParisTech

Industrial partnerships

CONTRACTS

RioTinto (formerly Pechiney and Alcan)

LE BRIS Claude, LELIÈVRE Tony
Modeling of electrolytic cells

EADS

ANANTHARAMAN Arnaud, CANCÈS Éric
Multiscale models for composite materials

EDF

BENCTEUX Guy, CANCÈS Éric, LE BRIS Claude
Electronic structure calculations

Thalès-Alenia Space France and CNES

COHEN Guy, CARPENTIER Pierre,
CHANCELIER Jean-Philippe
Interplanetary robust trajectories

EDF

DE LARA Michel
From risk constraint for stochastic optimisation to utility fonctions

EDF

DOYEN David, ERN Alexandre, PIPERNO Serge
Dynamic crack propagation with cohesive forces

EDF

HAZEL Florent, ERN Alexandre, PIPERNO Serge
Wave propagation in sea and harbourn areas

IFP

ERN Alexandre, PIPERNO Serge, TASSI Pablo
Steady state flow computations for stratigraphy applications

COLLABORATIONS WITH “CIFRE”

(Convention Industrielle de Formation par la Recherche)

EDF R&D OSIRIS

GIRARDEAU Pierre
High dimension problems in stochastic dynamical optimisations
Theses financed through contract

EDF

DOYEN David
Dynamic crack propagation with cohesive forces
Theses financed through contract

VALORIZATION

Software (ongoing)

ALFONSI Aurélien, JOURDAIN Benjamin, LAPEYRE Bernard, SBAI Mohamed

Participation in the development of the PREMIA software

Public programmes support

CONTRACTS REPORTS

ANR (three projects)

DE LARA Michel

ANR (one project)

DELMAS Jean-François

Agropolis Fondation (RTRA Montpellier Agronomie et Développement Durable)

DELMAS Jean-François

Participation to public policies

TALK IN THE NATIONAL CONFERENCE

Avenir de l'enseignement des mathématiques, « Finance and mathematics », 26-27th November

LAPEYRE Bernard, *ministère de l'Éducation nationale*