CERMICS

Centre d'Enseignement et de Recherche en Mathématiques et Calcul Scientifique

ENPC laboratory hosting joint project-teams with INRIA

Laboratoire de l'ENPC participant à des projets communs avec l'INRIA

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Director: Serge PIPERNO
Vice-Director: Jean-François DELMAS

Staff

13 researchers
11 associate researchers (4 researchers of INRIA, 3 of University of Marne-la-Vallée, 2 of University Nice - Sophia Antipolis, 1 of University Paris Dauphine, 1 of LAMI)
15 external collaborators
29 PhD students
2 administrative assistants
6 post-docs,
2 invited researchers
11 internship students

CERMICS is a laboratory of ENPC, formerly joint with INRIA, and hosting INRIA project-teams. It is located mainly at ENPC in Champs-sur-Marne and for a small part at INRIA Sophia Antipolis. The scientific activity of CERMICS covers several domains in scientific computing, modeling, and optimization.

Two teams deal with modeling and scientific computing: «Fluid Mechanics» (leader: A. Ern) and «Molecular and multiscale simulations» (leader: E. Cancès). Three other teams cover several important domains of applied mathematics: «Optimization and Systems» (leader: G. Cohen), «Applied Probabilities» (leader: B. Jourdain) with applications of probability theory to numerical models and methods, and «PDE and materials» (leader: R. Monneau) devoted to mathematical modeling of material behavior at the crystalline level. All teams have their own research domains, which does not exclude collaborations: for example, the teams «Applied Probabilities» and «Molecular and multiscale simulations» have a last collaboration on multi-scale simulations on Quantum Monte Carlo methods for Schrödinger Hamiltonian, etc...

It can be pointed out that three teams are or take part to joint project-teams with INRIA: the team «Molecular and multi-scale simulations» hosts INRIA Rocquencourt project-team MICMAC (leader: C. Le Bris), the team «Applied Probabilities» hosts INRIA Rocquencourt project-team MATHFI (leader: A. Sulem) and «Fluid Mechanics» hosts a part of INRIA Sophia Antipolis project-team CAIMAN (leader: S. Piperno till 1/9/2006, S. Lanteri later on)

Staff changes, missions, visits
J.F. Pommaret retired mid 2006 (team «Optimization and Systems», topic: formal study of systems of partial differential equations). He has been nominated as an emeritus researcher of ENPC. During the summer 2006, A. Alfonsi and J. Guyon, both civil servants from the «corps des Ponts», defended their PhD theses: J. Guyon joined the quantitative research team on equity at the Société Générale, and A. Alfonsi will join back the team «Applied Probabilities» in summer 2007 (as permanent staff) after spending the current academic year as a postdoc at Technical University of Berlin, supervised by A. Schied. Finally, the scientific leadership of INRIA project-team «CAIMAN» was transferred from S. Piperno to S. Lanteri on September, 1st 2006. Concerning visits, A. Schied was invited by J.–F. Delmas and made a one-month stay at CERMICS. A. Schied gave a postgraduate course on model uncertainty and risk measures in the seminar of the Mathfi project. J.–F. Delmas has held a visiting professor position at the University of California at San Diego, during spring 2006.

Publications and prizes
The CERMICS laboratory has sustained a high scientific activity: over forty articles have been published in international refereed journals (and over thirty have been accepted for publications). Also above fifty presentations in conferences have been made. Last but not least, three books have been published by researchers of CERMICS: two volumes of Springer's «Mathématiques et applications» series «Méthodes mathématiques en Chimie Quantique : une introduction» by E. Cancès, C. Le Bris, and Y. Maday, and «Modèles aléatoires : applications aux sciences de l'ingénieur et du vivant», by J.–F. Delmas and B. Jourdain) and the comprehensive «Mathematical methods for the Magnetohydrodynamics of liquid metals» (Oxford University Press), by J.–F. Gerbeau, C. Le Bris, T. Lelièvre.
Let us finally mention that Serge Piperno was awarded the Blaise Pascal 2006 prize (Gamni-Smai). This prize rewards each year one or more researchers (aged under 40) for their contribution (obtained in France) in the fields of scientific computing, statistics or applied mathematics in engineering domains.

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 (Alcan, Calyon, CEA, EADS, EDF, Suez, etc). An emerging part of our financial supports is granted by the «Agence Nationale de la Recherche» (ANR), the French equivalent of the American NSF, which proposes several scientific program calls and grants (the laboratory is mainly funded through «High-performance computing and Simulation» and «Non thematic» programs of the ANR). The overall research contracts have reached a record in 2006, not far from 550k€ for ENPC (100k€ via INRIA). In addition, a research and teaching chair «Measure of financial risks» involving the École Polytechnique, the École des Ponts and the Société Générale is in preparation and its agreement should be signed in early 2007.
A. Ern has been appointed as of 01 January 2006 Director of the Groupement de Recherches MOMAS. MOMAS is a research project federation supported by ANDRA, BRGM, CEA, CNRS, IRSN and EDF aiming at improving mathematical models and simulation tools for safety assessment of nuclear waste repositories.

Teaching and supervising
Teaching is an important activity of CERMICS members, both at ENPC and other first rank engineering schools (Ecole Polytechique) and in graduate courses (M2R) around Paris. At ENPC, the members of CERMICS are strongly contributing to the mathematical and computer engineering department, in the first year (chair of the department, lectures on scientific computing, probabilities, analysis) as well as in the second year (the mathematics and computer science department key-lecture “modeling-implementation-simulation”, frequency analysis, non-linear analysis, statistics, etc). Moreover, a third year in mathematical finance has been set up in collaboration with University of Marne-la-Vallée. In addition to organizing and giving courses, the global activity of the laboratory also includes accompanying and supervising students throughout their education, for their projects, internships, as well as PhD theses (approximately thirty PhD students) and post-doctoral studies (six students in 2006).

National / International collaborations
The different teams in CERMICS have many national and international collaborations with other scientific centers and institutions meeting the highest standards. The main national and international relations are listed in the following.
Several teams collaborate with other research centers of ENPC or «Ministère de l'Equipement»: the «Fluid Mechanics» team with LMSGC (L. Dormieux) on transport in porous media and on hydraulics and hydrology with CETMEF (Ph. Sergent). The «Molecular and multiscale simulations» team collaborates with LAMI (F. Legoll) on time integration algorithms for molecular dynamics and with LMSGC (Ph. Coussot) on multi-scale simulation of fluids (also with F. Lequeux of ESPCI and I. Catto of University Paris Dauphine). B. Lapeyre collaborates with CERTIS on the ANR GRID project. G. Cohen collaborates with LVMT on collective taxis system optimization.

Other national collaborations are the following.
The «Fluid Mechanics» works with ANDRA on transport equations in media with strong heterogeneities and anisotropies, and with J. Virieux (GeoSciences Azur) and S. Lanteri (INRIA) on seismics.
The «Applied Probabilities» team collaborates with R. Abraham (University of Orléans) on fragmentation and branching models, M. Ben Alaya (University Paris 13) on nonlinear models in rheology, F. Malrieu (University Rennes 1) on the long-time behavior of particle systems and PDEs, on detection of language for babies with the Necker hospital

and the University of Orléans, and with L. Marsalle (University Lille 1) on detection of aging in cells.
The «Molecular and multiscale simulations» team collaborates with M. Lewin (CNRS and University of Cergy-Pontoise) on second order reduced density matrix formulations for quantum chemistry and on the modeling of defects in crystalline materials, with M. Caffarel (IRSAMC at Toulouse) and A. Savin, R. Assaraf (LCT, University Paris 6) on the localization of electrons in molecular systems and quantum Monte Carlo methods. Concerning numerical statistical physics, the team collaborates with (F. Castella, Ph Chartier, E. Faou (INRIA Rennes) on the numerical integration of a class of highly oscillating Hamiltonian systems. The team also collaborates with X. Blanc (J.–L. Lions Laboratory, University Paris 6) and P. -L. Lions (Collège de France) on questions around the definition of ground state energies for some microscopic systems composed of an infinite number of particles on one hand, and on the other hand on the well-posedness of some non Newtonian flow models. Finally, the team pursues its efforts for the numerical simulation of electrolytic cells for the industrial production of aluminum in collaboration with J.–F. Gerbeau (project-team REO, INRIA).
The «Optimization and Systems» team started a collaboration with A. de La Fortelle (project-team IMARA, INRIA) on the simulation and the optimal control of systems of collective taxis operating in large cities. They are involved in various activities in stochastic optimization with L. Andrieu (EDF) and A. de Palma (University of Cergy-Pontoise), and development around the NSP–Scilab Scientific Computing Software with B. Pinçon (ESIAL, Henri Poincaré University Nancy 1) and F. Delebecque, J.–P. Quadrat, R. Nikoukhah (INRIA, Scilab project). On the topic of mathematical methods for sustainable management of renewable resource and biodiversity, the team develops many collaborations on various themes, such as fisheries management (ACI Moorea), risk aversion and road choice (with the laboratory Thema of University of Cergy-Pontoise).
The «PDE and materials» team works in collaboration with the laboratory of the study of microstructure at ONERA (the French Aerospace Lab), with partners a newly launched ANR project on (CMAP Ecole Polytechnique, University of Tours and University of Brest), and with M. Cannone, (LAMA, University of Marne-la-Vallée), C. Imbert (University Montpellier 2) and E. Rouy (MAPLY, University Lyon 1) on dislocations density models in connection with elasto-visco-plasticity of metals.

Concerning international collaborations, the «Fluid Mechanics» team has collaboration links with J.-L. Guermond (University of Texas A&M), P. Zunino (Politecnico di Milano) and E. Burman (EPFL) on DG methods, with M. Braack (University of Heidelberg) and S. Perotto (Politecnico di Milano) on adaptive modeling and meshing techniques.
The «Molecular and multiscale simulations» team works on some non-standard models used in quantum chemistry, like Effective Local Potentials in collaboration with E.R. Davidson (University of Washington), G.E. Scuseria and V.N. Staroverov (Rice University), on domain decomposition approaches for electronic structure calculations with W.W. Hager (University of Florida) and reduced-basis methods applied to chemistry with Y. Maday (University Paris 6, J.–L. Lions Laboratory), and N. C. Nguyen, A. T. Patera, and G. Pau (MIT). The team also works on numerical statistical physics (computation of canonical averages associated with potential energies that include stiff terms) with P. Plechac (Warwick University) and stochastic differential equations and stochastic dynamics in collaboration with E. Vanden–Eijnden (Courant Institute), E. Faou (INRIA), F. Otto (University of Bonn). Concerning laser control of molecular processes, the collaboration with the group of H. Rabitz (Princeton University) goes on. In collaboration with M. Mirrahimi and P. Rouchon (Ecole des Mines de Paris), H. Rabitz (Princeton University), and G. Turinici (University Paris Dauphine), the team addresses some questions related to the use of the laser field as a tool to obtain additional information on the molecular system. Concerning the multi-scale simulation of solids, works with A. Braides (University of Rome) on numerical homogenization methods are in progress, as well as on the analysis of “continuous to continuous” homogenization with R. Alicandro (University of Cassino) and M. Cicalese (University of Naples), and on the feasibility of reduced-basis approaches for multiscale problems with A.T. Patera (MIT) and Y. Maday (University Paris 6, J.–L. Lions Laboratory). Finally, different aspects of multi-scale simulations of fluids are investigated, like the modeling of polymeric fluid flows with F. Otto (University of Bonn)
The «Optimization and Systems» team cooperates with F. Vazquez–Abad (formerly at the University of Montreal, Canada, now at the University of Melbourne, Australia) and with R. Henrion (Weierstrass Institute, Berlin), on stochastic optimization and decision making in a stochastic environment. On mathematical methods for sustainable management of renewable resources and biodiversity, the team has started a cooperation with Chile and Peru (MIFIMA: Mathematics, Informatics and Fisheries Management) for which M. de Lara is the principal investigator (action supported by the regional cooperation program STIC–

AmSud, 2006-2008)
The «Applied Probabilities» team collaborates with A. Schied (Technical University of Berlin) which visited us during one month and is the advisor of the postdoctoral stay of A. Alfonsi. The team collaborates with A. Zanette (University of Udine) on the software Premia. Finally, N. Bouleau studies Dirichlet Forms in collaboration with M. Röckner (University of Bielefeld) and I. Shigekawa (University of Kyoto.

The «PDE and materials» team develops collaborations with the group of M. Falcone (University La Sapienza) on some generalizations of the Fast Marching Method, with applications to dislocations dynamics. Let us also mention the collaboration on dislocations density models with scale effects (PhD of I. Hassan) with M. Jazar (Beyrouth University) and various international collaborations with Chile and Japan.

RESEARCH TEAMS

Applied probabilities

(A. Alfonsi, J.–F. Delmas, J. Foki, J. Guyon, B. Jourdain, B. Lapeyre, R. Laviollette, J. Lelong, V. Lemaire, M. Sbai, S. Scotti, A. Zanette; external associate researchers: R. Abraham, M. Ben Alaya, N. Bouleau)

The team is mainly interested in the study of probabilistic numerical algorithms with applications going from mathematical finance to biology and quantum chemistry. The other important research field is the probabilistic interpretation of PDEs, especially nonlinear ones.
During the summer 2006, A. Alfonsi and J. Guyon, both civil servants from the «corps des Ponts», defended their PhD theses respectively entitled «Modelisation of credit risk. Calibration and discretization of financial models» and «Probabilistic models in finance and biology. Limit theorems and applications». And, concerning staff, the main evolution in 2006 is the recruiting of A. Alfonsi who will join back the team in summer 2007 after spending the current academic year as a postdoc in the Technical University of Berlin, supervised by A. Schied. This postdoc is a continuation of the collaboration initiated during the visit in March 2006 of A. Schied who was invited by J.–F. Delmas. A. Schied then gave a postgraduate course on model uncertainty and risk measures in the seminar of the Mathfi project. J.–F. Delmas has held a visiting professor position at the University of California at San Diego, during spring 2006. After his thesis, J. Guyon has joined the quantitative research team on equity at the Société Générale. Further collaboration with him should be eased by the most noticeable fact concerning scientific partnerships: the preparation of the research and teaching chair «Measure of financial risks» involving the École Polytechnique, the École des Ponts and the Société Générale. The agreement should be signed in early 2007.

Mathematical finance
As far as mathematical finance is concerned, the team is still part of the Mathfi project together with researchers from the University of Marne-la-Vallée and INRIA. 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, EDF, Natexis, CDC). This is done with the contribution of A. Zanette, J. Lelong and V. Lemaire. The version 8 has been released in February 2006. The new contributions to the next version developed since include a CDO pricer dealing with various copula models, calibration and pricing algorithms for interest rates models, implementation of recent algorithms devoted to options written on equity and a pricing algorithm for swing options on electricity. The theses of J. Lelong on stochastic algorithms in finance and of S. Scotti on error calculus in finance are in progress. Mohamed Sbai is starting his PhD on the discretization of financial models.
The research in Monte Carlo methods is structured by the ANR program ADAPtive Monte Carlo. This permits very interesting discussions with the statisticians from the ENST, École Polytechnique, INRIA and the University Paris Dauphine. P. Etoré starts a postdoc on adaptive stratified sampling methods financed by this program. B. Lapeyre is also the head of the ANR program GRID (calculus grids in finance) devoted to financial computations distributed on large computer networks which also implies researchers from CERTIS, the computer science research laboratory of ENPC.

Monte Carlo methods
Applications of Monte Carlo methods in physics and chemistry are still investigated. J.-F. Delmas and B. Jourdain have analyzed the waste recycling Monte Carlo algorithm proposed by physicists to improve the efficiency of the Metropolis Hastings algorithm.

Physics and chemistry
The collaboration of B. Jourdain on Molecular simulations with the “Molecular and multi-scale simulations” team goes on with the postdoc of M. Rousset and the Master training period of R. Roux. In the domain of probabilistic interpretation of nonlinear PDEs,

J.-F. Delmas works with R. Abraham on fragmentation and branching models. B. Jourdain collaborates with M. Ben Alaya on a nonlinear model in rheology and with F. Malrieu on the long-time behavior of particle systems and PDEs.

Biology
Concerning biology, in the program 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. This research is supervised by J.-F. Delmas, who also collaborates with L. Marsalle on models for the detection of aging in cells, in the continuation of the study initiated by J. Guyon in his thesis. The thesis of A. Siri-Jégousse co-supervised by J.-S. Dhersin on the study of non-binary branching models is also in progress.

Dirichlet Forms
For several years, N. Bouleau has been participating to the international conferences and seminars organized by Japan and Germany on «Dirichlet Forms and Stochastic Analysis», whose main correspondents are M. Röckner (University of Bielefeld) and I. Shigekawa (University of Kyoto) and attempt to enlarge the participation to French teams.

Fluid dynamics

(M. Benjemaa, A. Bouquet, D. Di Pietro, K. Djadel, A. Ern, N. Glinsky-Olivier, S. Meunier, S. Piperno, A. Stephansen, P. Sochala, P. Tardif; external associate researchers: M. Braack, R. Burman, C. Dedeban, J.-L. Guermond, J. Virieux)

The "Mécanique des fluides" team of CERMICS develops advanced numerical methods based on finite elements and a posteriori error estimates applied to transport problems in porous media, hydraulics, and wave propagation. Since 2006, it hosts a part of the project-team "caiman", joint with INRIA, CNRS and the Nice-Sophia Antipolis University (NSAU), through the Dieudonné Laboratory. The caiman team aims at proposing new, efficient solutions for the numerical simulation of physical phenomena related to wave propagation (electromagnetism, acoustics, aero-acoustics, seismics, etc). Scientific activities sweep a large range from physical modeling 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 2006 are as follows: the post-doctoral research project of K. Djadel was completed in August while that of D. Di Pietro started on February. The PhD thesis of P. Tardif was defended in December. The scientific leadership of INRIA project-team caiman was transferred from S. Piperno to S. Lanteri in September.

Finite Element Methods
The team research in finite element methods deals with Discontinuous Galerkin (DG) methods and, marginally, with stabilized continuous finite element methods. The research on DG methods has been pursued along two directions. Firstly, following up the unified analysis of DG methods for Friedrichs' systems derived by A. Ern and J.-L. Guermond (Texas A&M University) since 2005, D. Di Pietro has dealt during the first part of his post-doctoral project with DG methods to approximate advection-diffusion problems with anisotropies (tensor-valued diffusivity) and singularities due to semi-definiteness of the diffusivity. Broadly speaking, these problems fall into the class of mixed elliptic-hyperbolic problems and their mathematical analysis is by no means standard. D. Di Pietro has proposed a suitable framework based on proper interface conditions to ensure well-posedness at the continuous level. Then, he designed, analyzed and implemented a DG approximation that leads to optimal (with respect to mesh-size) and robust (with respect to diffusivity anisotropies and singularities) error estimates. Secondly, further investigations of Discontinuous Galerkin finite element methods deal with linear wave propagation problems. The discontinuous approaches (finite volumes, DG) allow great modularity and can achieve high-accuracy with many kinds of meshes (unstructured grids, non-conforming grids, locally refine grids...). Our methods are mainly developed for problems solved in the time domain with explicit time-schemes. We are also considering extensions towards locally implicit time schemes. Current applications relate to heterogeneous electromagnetics, acoustics, propagation of acoustic waves in a non-uniform steady compressible flow (aeroacoustics) and geophysics. Concerning electromagnetics, wave propagation problems often involve objects of very different scales.
The second topic concerning finite elements is the stabilization of continuous finite element methods by penalizing the jumps of the gradient of the discrete solution. A. Ern and E. Burman (EPFL) have derived a general error analysis for the approximation of Friedrichs' systems by such methods. The advantage of stabilized continuous finite element methods with respect to DG methods is that on a given mesh, the former require less memory than the latter.

Wave propagation problems
We have studied, in collaboration with France Telecom R&D, discontinuous Galerkin time

domain methods for the numerical simulation of the three-dimensional Maxwell equations on locally refined, possibly non-conforming structured meshes. The DGTD method developed on block-Cartesian grids by N. Canouet (ENPC PhD thesis, 2003) with divergence-free basis functions with varying accuracy, second-order leap-frog scheme, and centered fluxes has been re-implemented in a Cartesian grid setting in the context of PhD thesis subject of Antoine Bouquet. We consider investigating the possibility to couple DGTD methods with the fictitious domain approach. We have also been developing symplectic local time-stepping schemes for wave propagation problems. Using a DG spatial discretization with totally centered numerical fluxes (non dissipative approach), the stability limit of the methods, related to the smallest elements in the mesh, calls for the construction of local-time stepping algorithms. These schemes have already been developed for N-body mechanical problems and are known as symplectic schemes. Totally explicit algorithms have been built for two-dimensional acoustic problems, as well as locally implicit time-schemes. Although the proposed algorithm perform very well on real-life two-dimensional unstructured meshes (like those produced by an automatic mesh generator around objects with small details), some instabilities may appear. A theoretical study is under way, which aims at giving a sufficient stability condition on the time step involving the mesh size distribution. Finally, DGTD-FVTD methods have been used (PhD thesis of M. Benjemaa, in collaboration with INRIA and GeoSciences Azur Unit) for the dynamic fault modeling in seismic activity (2D P-SV wave propagation in a vertical, linear, isotropic, and heterogeneous medium or 3D linear elastodynamics). The finite volumes are the elements of the simplicial mesh: this allows for an easy inclusion of the physical heterogeneities and meshing around faults (or the free surface). The fault, whose location is prescribed (with a prescribed or dynamic transient behavior), is modeled as infinitely thin simplex interfaces and numerical fluxes take into account dynamically evolving boundary conditions. Arbitrary non-planar faults (following element edges) can be explicitly included in the mesh as well as several models for the propagation of the rupture (especially a slip-weakening friction law).

Transport in porous media

Concerning transport in porous media, the main application in view is the transport of radionucleides leaking from radioactive waste storage in deep geological layers. In our research group, two research topics are investigated. The goal of A. Stephansen's PhD thesis (supported by ANDRA) is to develop and analyze DG methods to approximate transport equations in media with strong heterogeneities and anisotropies and then to design robust error indicators to adapt the mesh in transient problems. Part of her work is carried in collaboration with P. Zunino (Politecnico di Milano). Her main result in 2006 is the design, analysis and implementation of a specific variant of a DG method, the so-called Symmetric Weighted Interior Penalty (SWIP) method that properly handles vanishing diffusion and anisotropies. Secondly, the goal of S. Meunier's PhD thesis (supported by EDF) is to derive space-time a posteriori error indicators for coupled thermo-hydro-mechanics problems and to implement them in EDF software (Code_Aster). Such couplings are important in near-field calculations near waste repositories and may affect the amount of pollutants released into the environment. The main result in 2006 is the completion of the space-time a posteriori error analysis including global upper bounds and local lower bounds for the error. Finally, P. Tardif has completed his PhD thesis supervised by A. Ern jointly with L. Dormieux (LMSGC Laboratory at ENPC). P. Tardif has extended his work on single-phase transport to two-phase transport in which a component diluted in a carrier gas is transported while the liquid phase consists of disconnected menisci localized at the pore level. His main results are finite element simulations to evaluate diffusion and dispersion tensors in 3D sphere networks. The software he developed provides a tool to assess quantitatively the impact of pore morphology and advection velocity on these tensors.

Hydraulics and hydrology

Concerning hydraulics and hydrology, the collaboration with CETMEF which started in 2005 has been continued. The goal of K. Djadel's post-doctorate research has been to design and analyze DG methods to approximate the shallow-water equations. Targeted applications include waves propagating on dry beds to simulate floods or dam breaks. Furthermore, P. Sochala's has pursued his PhD thesis (currently in his second year) by developing and assessing DG-based algorithms to solve the Richards equation in unsaturated porous media.

Adaptive modeling and adaptive mesh simulations

A. Ern, in collaboration with M. Braack (Heidelberg University) and S. Perotto (Politecnico di Milano), has investigated adaptive modeling techniques (coupled to adaptive meshing techniques) driven by a posteriori error analysis. Given (say) two models, an inaccurate one and an accurate one, the goal is to equilibrate modeling and discretization errors by solely using information retrieved from the discrete

solution and that of a suitable discrete dual problem. Two applications are explored: polymeric fluid flows (with T. Lelièvre and M. Braack) and changing the space dimension to improve or coarsen the model (with S. Perotto).

Molecular and multi-scale simulations

(E. Cancès, G. Bencteux, S. Boyaval, A. Deleurence, M. El Makrini, H. Galicher, A. Gloria, C. Le Bris, T. Lelièvre, A. Orriols, C. Patz, M. Rousset, A. Scemama, G. Stoltz; external associate researcher: M. Lewin)

The scientific activity of the molecular and multiscale simulation team covers several fields: electronic structure calculations, numerical statistical physics, laser control of molecular processes, multiscale simulation of materials (solids and fluids), and magneto-hydrodynamics.

Electronic structure calculations
On a theoretical level, several actions are in progress. E. Cancès and G. Stoltz have tried and improved the understanding, from a mathematical perspective, of some models used in quantum chemistry, especially non-standard models such as methods relying on second order reduced density matrix formulations (in collaboration with M. Lewin, CNRS, Cergy) and Effective Local Potentials (in collaboration with E.R. Davidson – University of Washington -, and with G.E. Scuseria and V.N. Staroverov – Rice University).
E. Cancès and A. Deleurence have begun addressing issues related to the existence 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 for performing such calculations, a mathematically consistent quantum model for crystalline materials with local defects is still missing. In collaboration with M. Lewin, E. 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 propose 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 through a thermodynamical limit on the so-called supercell model.

On the numerical side, one problem addressed was that of the localization of electrons in molecular systems. A. Scemama has worked in collaboration with M. Caffarel (CNRS, IRSAMC, Toulouse) and A. Savin (CNRS, LCT, Theoretical Chemistry Laboratory, Paris 6) on the localization of electrons in molecular systems. Although it would be tempting to associate the Lewis structures to the maxima of the squared modulus of the wave function, the choice is to use the domains of the three-dimensional space that maximize the probability of containing opposite-spin electron pairs. They find for simple systems (CH4, H2O, Ne, N2, C2H2) domains comparable to those obtained with the Electron Localization Function (ELF) or by localizing molecular orbitals. The different domains they obtain can overlap, and this gives an interesting physical picture of the floppiness of CH5+ and of the symmetric hydrogen bond in FHF-. The presence of multiple solutions has an analogy with resonant structures, as shown in the trans-bent structure of Si2H2. Correlated wave functions were used (MCSCF or Slater-Jastrow) in the Variational Quantum Monte Carlo framework.
In collaboration with W.W. Hager (University of Florida), the domain decomposition approach, designed by M. Barrault (now at EDF), G. Bencteux, E. 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. Some algorithmic improvements of the most consuming part of the algorithm have resulted in significant decreases in memory and CPU demands (up to a factor 10 for alkane molecules). A first version of a multiprocessor implementation has succeeded solving the linear subproblem for a polyethylen chain of 106,000 atoms (more than 370,000 basis functions) in about 90 minute elapsed time with 16 processors. The performance of the parallel version confirms that a high scalability can be aimed with additional implementation effort: this will be part of a future collaboration with EDF in the frame of the project «ParMat», which obtained the financial support of National Research Agency.
Also, in collaboration with Y. Maday (J.L Lions Laboratory, Paris 6), and N. C. Nguyen, A. T. Patera, G. Pau (MIT), we have continued our efforts to apply the reduced-basis technology to the context of computational chemistry.
From a numerical perspective, a number of actions concern the application of probabilistic methods (Monte-Carlo type methods) to the context of computational chemistry.
A first action regards the Quantum Monte Carlo methods. The diffusion Monte Carlo (DMC) method is a powerful strategy to

estimate the ground state energy E0 of a Schrödinger Hamiltonian. It consists in writing E0 as the long-time limit of the mean of a functional of a drift-diffusion process, with source term. Numerically, this is simulated by means of a collection of interacting random walkers, with a birth-death mechanism. As for a number of stochastic methods, a DMC calculation makes use of an importance sampling function. In the fermionic case, it has been observed that the DMC method is biased, except when the nodes of the importance sampling function exactly coincide with some ground state of the Hamiltonian. This is the fixed node approximation. A mathematical analysis of this approximation has been proposed by E. Cancès, B. Jourdain and T. Lelièvre. From a numerical point of view, the method is very difficult to analyze. Besides, M. El Makrini, B. Jourdain and T. Lelièvre have worked on the analysis of some selection mechanism.
In collaboration with M. Caffarel, E. Cancès, T. Lelièvre, A. Scemama and G. Stoltz have proposed a new numerical scheme for VMC calculations based on the discretization of a Langevin equation in the phase space, complemented by a Metropolis acceptance-rejection step.
Another work on quantum Monte Carlo methods has been done by A. Scemama, in collaboration with R. Assaraf (CNRS, LCT, Theoretical Chemistry Laboratory, University Paris 6) and M. Caffarel. It concerns the calculation of the electronic density of a molecular system by means of Monte Carlo methods. An alternative Monte Carlo estimator for the electronic density is proposed. This estimator has a simple form and can be readily used in any type of Monte Carlo simulation. Comparisons with the standard delta-function estimator show that the statistical errors are greatly reduced. Furthermore, this new estimator allows for accurate calculations of the density at any point of the physical space, even in the regions never visited during the Monte Carlo simulation.

Numerical statistical physics
The extremely broad field of Molecular dynamics is a field where the team, originally more involved in the quantum chemistry side, has invested a lot of efforts in the very recent years. These efforts both deal with the deterministic techniques and the probabilistic techniques used in the field.
Molecular dynamics is often used in statistical physics for computing ensemble averages. The bottom line for this is the assumed ergodicity of the Hamiltonian dynamics in the microcanonical ensemble. Ensemble averages are thus expressed as long time limits of averaged along trajectory. One difficulty of such a computation is the presence of several time scales in the dynamics: the frequencies of some movements are very high (e.g. for the atomistic bond vibrations), while they are much smaller for some other movements. Actually, these fast phenomena are relevant only through their mean effect on the slow phenomena, and a precise description of them 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 has initiated, in collaboration with F. Legoll (LAMI) a study along this aim. Preliminary results have been obtained for the integration of a class of highly oscillating Hamiltonian systems, and more general results should follow soon. The different methods to address this problem are discussed with F. Castella, P. Chartier and E. Faou from INRIA Rennes, with the funding of ANR Ingemol ("Intégration numérique géométrique des équations hamiltoniennes").
A similar problem appears when one wants to compute canonical averages associated to potential energies that include stiff terms. This subject is studied by C. Le Bris and M. Rousset in collaboration with F. Legoll and P. Plechac (Warwick University).
The dynamics of a molecular system usually consists of two different phases: oscillations of the system around a local minimum of the potential energy (that is, in a metastable state), and rare hoppings from a metastable basin to another one. In order to perform an efficient exploration of the phase space, it is important to simulate the system long enough such that several metastable basins have been visited. However, it is extremely difficult to achieve such a goal when using a full atomistic description of the system, again because of the presence of several time scales in the dynamics. In collaboration with F. Legoll, E. Cancès, A. Deleurence and T. Lelièvre are currently studying several methods to coarse-grain the system, in order to develop a model more suited to long time simulation.
In collaboration with E. Vanden-Eijnden (Courant Institute), E. Faou, F. Otto (University of Bonn), T. Lelièvre has studied a number of topics related to Stochastic Differential Equations (SDEs) and Stochastic Dynamics. SDEs with constraints naturally appear in molecular dynamics and kinetic models. The constraints may be imposed for modeling (rigid bonds) or for computational purposes (computation at a fixed reaction coordinate). A mathematical study of various discretizations of SDEs with constraints has been proposed, together with a discussion on the effectiveness of such methods to compute free energy differences by thermodynamic integration. The generalization to non-equilibrium dynamics (Jarzynski equality) has also been performed.

A current work on the ergodic properties of projected dynamics, and the sampling of the NVE ensemble (ensemble with fixed particle Number, Volume and Energy) by such SDEs, is in progress.
Stochastic dynamics to compute free energy differences are widely used in computational chemistry and biology. Many recent methods rely on nonlinear Markov processes, like the adaptive techniques. A unifying presentation of adaptive methods is proposed by T. Lelièvre, M. Rousset and G. Stoltz, together with an efficient implementation of adaptive dynamics using an interacting particle system with birth/death processes. A current work on a proof of convergence of a certain class of adaptive methods (in collaboration with F. Otto) is in progress.

Laser control of molecular processes
Our interest closely follows the recent prospects opened by the laboratory implementations of closed loop optimal control. This is done in collaboration with the group of H. Rabitz (Princeton University) and made possible by a PICS CNRS-NSF grant.
In collaboration with M. Mirrahimi (Ecole des Mines de Paris), H. Rabitz and G. Turinici (University Paris Dauphine), and also in close connection with P. Rouchon (Ecole des Mines des Paris), C. Le Bris has addressed some questions related to the inversion paradigm: use the laser field as a tool to obtain additional information on the molecular system. Some extensions regarding the introduction of noise are discussed with our chemists partners at Princeton and some techniques have also been tested.

Multi-scale simulation of solids
On the theoretical side, in collaboration with X. Blanc (J.-L. Lions Laboratory, University Paris 6) and P.L. Lions (Collège de France), C. Le Bris has continued to address the question of how to define ground state energies for some microscopic systems composed of an infinite number of particles. With a view to treating geometries of sets of particles much more general than periodic geometries, the current focus is on the case when nuclei are located at random positions. As a follow-up to the previous studies, an effort has been placed on developing the connection between the questions examined for this passage 'atomistic to the continuum' and some more generic questions of homogenization theory. It has been shown that the objects manipulated in the two apparently uncorrelated topics can indeed be connected.
An independently investigated track is the possibility to perform thermodynamic limits (used in the past for defining the energy per unit volume of an infinite sample of matter) this time on the free energy, i.e. in the presence of temperature effects. Some preliminary steps have been performed by C. Le Bris, in collaboration with X. Blanc, F. Legoll and C. Patz (University of Stuttgart, now in Berlin).
A. Gloria has addressed the analysis of some numerical homogenization methods, in the context of elliptic operators and nonlinear elasticity. Some numerical tests have completed the analysis and have been performed within the Finite Element library Modulef.
In the continuation of the characterization of effective behaviors of heterogeneous materials, A. Gloria has studied a problem of G-closure: the determination of the set of all the effective conductivity matrices that can be obtained by the homogenization of a discrete conducting polycrystal. This work has been done in collaboration with A. Braides (University of Roma).
Besides the analysis of “continuous to continuous” homogenization (at the micro scale the material is already considered as continuous), A. Gloria has begun to work on the derivation of effective energies for spin interactions, starting from a discrete description of the interaction and deriving a continuous limit when the characteristic length of the system goes to zero. This work is in collaboration with R. Alicandro (University of Cassino, Italy) and M. Cicalese (University of Naples, Italy).
In close collaboration with A.T. Patera and Y. Maday, S. Boyaval, who is beginning his PhD studies under the supervision of C. Le Bris, has tested the feasibility of reduced-basis approaches for multiscale problems. The results now allow for a fast and rigorous numerical homogenization of heterogeneous materials. The context is that of the homogenization of scalar elliptic equations.

Multi-scale simulation of fluids
The subject of this activity covers two different applications and settings.
The first one is the modeling of polymeric fluid flows, the second is that of suspensions. In the first context, the study by C. Le Bris and T. Lelièvre, in collaboration with B. Jourdain and F. Otto (University of Bonn), of the long-time behavior of such flows has been published. Entropy methods are used to show an exponential decay to equilibrium. When the system is forced (non-zero boundary condition on the velocity), the exponential convergence to a stationary state can be obtained only in particular cases. On the other hand, for suspensions, as a follow up to the study of well posedness of the problem, the long time limit has been investigated by C. Le Bris and E. Cancès.
A completely new topic is now starting, in collaboration with Ph. Coussot (LCPC), F. Lequeux (ESPCI), I. Catto (University Paris Dauphine). E. Cancès, S. Boyaval and C. Le Bris are going to perform some numerical simulations of some highly non Newtonian

fluids. Some issues related to thixotropic fluids, and related topics, will be under investigation.
The above much applied topics, related to the modeling of complex fluids, have motivated a series of genuinely theoretical works by C. Le Bris and P-L. Lions (College de France) on the well-posedness of the mathematical equations manipulated in the modeling. Indeed, as the flow velocities in such non Newtonian flows have no particular reason to be regular, the fact that such velocities have an influence as parameters on the kinetic description of the microstructures motivate a number of theoretical questions. The well-posedness of Fokker-Planck type equations, and the related stochastic differential equations, is a topic of great mathematical relevance and interest. Indeed, such equations with potentially irregular coefficients and parameters arise in a number of fields. C. Le Bris and P-L. Lions have devoted a series of (ongoing) works on the subject.
G. Stoltz has investigated various aspects of the multiscale simulation of shock waves. Shock and detonation waves are truly multiscale phenomena, involving very small time and length scales at the shock front. It is therefore very interesting to propose coarser models to simulate them. A reduced model for a description of shock waves at the microscopic level has been proposed. This model relies on a dissipative particle dynamics with conserved energy, and extends a previous one-dimensional model. The reactive case is currently investigated, with a view to modeling detonation processes.

Magneto-hydrodynamics
In collaboration with J.F. Gerbeau (INRIA, REO), and in association with Alcan (formerly Aluminium Péchiney), C. Le Bris, T. Lelièvre and A. Orriols have pursued their efforts for the numerical simulation of electrolytic cells for the industrial production of Aluminum.
A book by J.–F. Gerbeau, C. Le Bris and T. Lelièvre, focusing on mathematical and numerical techniques for the simulation of magnetohydrodynamic phenomena has been published, with an emphasis laid on the magnetohydrodynamics of liquid metals, on two-fluid flows and on a prototypical industrial application. Aimed at research mathematicians, engineers, and physicists, as well as those working in industry, and starting from a good understanding of the physics at play, the approach is a highly mathematical one, based on the rigorous analysis of the equations at hand, and a solid numerical analysis to found the simulations. At each stage of the exposition, examples of numerical simulations are provided, first on academic test cases to illustrate the approach, next on benchmarks well documented in the professional literature, and finally, whenever possible, on real industrial cases.
In his PhD thesis, A. Orriols has worked on the control of the interface in two-fluid flows. The intended application is the control of aluminum electrolysis cells, and of the free interface which separates the aluminum and the bath of aluminum oxide in the cell. Two models can be used: a simple linear model, or a more complex non-linear model. The predictions of these two models for the stability of the cell have been compared (cf. T. Tomasino et al., Proceeding of the 2006 TMS Annual Meeting and Exhibition, J.–F. Gerbeau et al, Proceedings of the ECCOMAS 2006 Conference). In the case of the simple linear model, we have been able to find appropriate actuators to control the motion of the free interface (see A. Orriols PhD thesis). We are currently working on the control problem for the non-linear model.
Related to these MHD simulations, some numerical problems of a more general relevance are investigated. Such a particular problem has been the topic of some efforts in 2006. A general problem for two-fluid flows in a box is the modeling 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 to appropriately model the motion of the free surface. Recently, the Generalized Navier Boundary Condition has been introduced by T.Z. Qian et al. An Arbitrary Lagrangian Eulerian (ALE) formulation of the Generalized Navier Boundary Condition has proposed by J.–F. Gerbeau 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. The stability of new numerical schemes is the subject of ongoing research.

Optimization and systems

(J.P. Chancelier, G. Cohen, M. de Lara, A. Dallagi, E. Lioris, J.F. Pommaret, B. Seck, C. Strugarek; external associate researchers: L. Andrieu, P. Carpentier)

The activity report of last year gave a fairly complete view of the main research topics of the team. The following is an update of that description.

Max-plus algebra and algebraic analysis of PDE systems
First of all, J.–F. Pommaret retired in mid 2006 and the topic on formal study of systems of partial differential equations, and its

application to various domains of engineering science, will probably cease to be active in the group with this retirement, although J.F. Pommaret has been nominated as an emeritus researcher of ENPC. Also, the cooperation of G. Cohen with INRIA on Max-Plus has been stopped at the end of 2005, so that those two events altogether mean a certain slowing down of the system theoretical component in the activities of the team.

Simulation and optimal control

On the other hand, a new topic emerged in 2006 with the beginning of the thesis of E. Lioris which represents a new theme of collaboration with INRIA (IMARA project) and also with LVMT (F. Leurent). The purpose is to study systems of collective taxis operating in large cities. The first step is to devise a discrete event simulation tool which would allow us to optimize the numerous design and operation parameters of such a complex system. Various operating policies (ranging from purely decentralized to completely centralized) can be considered and we aim at conducting a cost/effectiveness comparison of those variants with the help of the simulation tool. Ultimately, this analysis will try to define the range of application of such systems in cities according to the level of demand such a system can attract, to evaluate performances (as compared with individual taxis in particular) and fares that can make the system economically viable, etc. A first communication on this topic has been submitted to the International Workshop on Taxis, Lisbon, Portugal, September 2007.

Stochastic optimization

In the more traditional activity of the team on stochastic optimization and control, C. Strugarek's thesis has been defended in May 2006 and A. Dallagi's thesis will come to an end in January 2007. Both theses owe much to the permanent financial support and scientific interest of EDF. As described in previous reports, our approach of such problems from the point of view of numerical resolution methods moved away rather radically from the widespread technique of «scenario trees» to evolve towards more subtle techniques based on a thorough analysis of the various ways of writing optimality conditions for such problems. The present devised techniques bring a clear improvement over scenario trees on numerical experiments conducted so far, but admittedly, further theoretical analysis is required to sustain those experimental evidences.

A 24 hour course on deterministic and stochastic optimization and control, together with related probabilistic topics, has been given for EDF engineers in May and June 2006, with contributions of most members of our team, plus B. Lapeyre and B. Jourdain from the Applied Probabilities team.

Another aspect of decision making in a stochastic environment the so-called «risk attitude». This topic was initiated in the team several years ago by L. Andrieu's thesis on the treatment of probabilistic constraints in stochastic optimization. This was the opportunity for cooperation with Prof. F. Vazquez-Abad (formerly at the University of Montreal, Canada, now with the University of Melbourne, Australia) who visited our team several times since the beginning of this research, including a new two week visit in October 2006. A paper is in preparation on that work. In addition, C. Strugarek renewed collaboration with R. Henrion (Weierstrass Institute, Berlin) on the same topic with a resulting publication. Also related to this theme is the thesis of B. Seck which is at the end of its first year under the joint supervision of M. de Lara and L. Andrieu (EDF). The purpose of this work (mainly supported by EDF) is to study how the standard cost-benefit analysis should be modified in order to take risk (and uncertainty) into account. Different approaches are used in finance (Value-at-Risk, Conditional Value-at-Risk, Downside Risk Measures and Efficiency Ratio) to model the impact of risk in project evaluation. Another approach, rather popular in Economics, is based on the use of utility functions. One objective of our research is to compare and relate those various approaches. Finally, applications of the risk management in decision making are considered in the context of transportation (investments and road choice). This involves L. Andrieu, M. de Lara, J.-P. Chancelier in cooperation with A. de Palma (University of Cergy-Pontoise).

Scilab Scientific Computing Software

The NSP project development, initiated by J.–P. Chancelier, was carried on in 2006 by adding and improving data types and primitives to the language (for example addition of Matlab cell data structure). A set of Scilab toolboxes has been ported to NSP, as for example UMFPACK (sparse linear algebra), GLPK, LPSOLVE (Linear Programming and Mixed Linear Programming), OPTIM (Scilab optimization toolboxes). The Scicos toolbox (block-diagram graphical editor) is almost totally ported to NSP. Premia, a large toolbox for Numerical Finance (Mathfi project Inria/Enpc) was also ported to NSP. B. Pinçon at ESIAL (Ecole Supérieure d' Informatique et Applications de Lorraine, Henri Poincaré University Nancy 1) is now deeply involved, and the NSP project still maintains collaborations with F. Delebecque and J.-P. Quadrat (INRIA) for NSP development and with R. Nikoukhah (INRIA) for Scicos port to NSP. The Chairman of Scilab Consortium scientific board, E. Ledinot

(Dassault Aviation), is in charge of the animation of a group which was created in order to evaluate NSP and discuss its possible integration in the current Scilab code. The group mainly started by trying to specify what should be a scientific software interpretor in order to prepare an evaluation grid for Scilab and NSP. All the people involved in NSP development participate to that group.

Mathematical methods for sustainable management of renewable resources and biodiversity.
M. de Lara is developing many collaborations on various themes, such as mathematical methods for fisheries management (ACI Moorea, MIFIMA), risk aversion and road choice (with the laboratory THEMA, "Théorie économique, modélisation et applications", UMR CNRS University of Cergy-Pontoise), economic interpretation of sustainable development, invariance and environmental preferences, or sustainable management of biodiversity under uncertainty and global dynamics. He is also the coordinator of the project MOOREA (Methods and Optimization Tools in Applied Ecology) and organized two meetings in 2006. Finally, M. de Lara participated to the project «Economic Interpretation of Sustainable Development, Invariance and Environmental Preferences» (ACI action of MENESR) and to the project «Marine Reserves, Models for a Sustainable Management of Biodiversity under Uncertainty and Global Dynamics». Two new research actions were launched in 2006: a cooperation with Chile and Peru was initiated (MIFIMA: Mathematics, Informatics and Fisheries Management) for which M. de Lara is the principal investigator (action supported by the regional cooperation program STIC-AmSud, [2006—2008]) and a cooperation on risk aversion and road choice with the THEMA group (participation to ANR RiskAttitude).

PDE and materials

(A. El Hajj, M. El Rhabi, N. Forcadel, H. Ibrahim, A. Ghorbel, R. Monneau; external associate researchers: A. Briani, M. Cannone, P. Hoch, C. Imbert)

The PDE and Materials team is interested in the modeling 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.

Dislocation dynamics
Our main activity is a part of a contract ACI «Jeunes chercheuses et jeunes chercheurs» of the French Ministry of Research (2003-2007), called «Modeling and mathematical analysis of dislocation dynamics». We work in particular in collaboration with the laboratory of the study of microstructure (LEM, ONERA). This part of our activity mainly focuses on the complicated dynamics of interacting dislocation lines. Let us cite in particular the works in progress of N. Forcadel (PhD student, 3rd year) on the link between dislocation dynamics and mean curvature motion, and A. Ghorbel (PhD defense in early 2007) about the study of a one-dimensional model of interacting dislocations and homogenization.
Let us mention that this year, our team got an ANR project (2006-2009) in collaboration with three other teams (CMAP, Tours University and Brest University; coordinator: A. Chambolle). This financial support will help substantially our team to develop our research in the following years and allow some new interactions.
We also got a grant from the Galileo project to develop our collaborations with the Italian group of M. Falcone (University La Sapienza) on some generalizations of the Fast Marching Method, with applications to dislocations dynamics.
At the same time, we have extended our research to the study of dislocations density models in connection with elasto-visco-plasticity of metals. This project is a part of the «Pluriformations Program» with the University of Marne-la-Vallée. In this framework, let us cite the PhD thesis of A. El Hajj (2nd year), co-directed with M. Cannone. On the other hand, H. Ibrahim (PhD student, 2nd year) studies dislocations density models with scale effects. He is co-directed by M. Jazar (Beyrouth University). We also welcomed M. El Rhabi on a post-doctoral position working on the link between these models and the mechanics, in connection with S. Forest of the Center of Materials (ENSMP).
Part of our objectives is to establish the connection between the dynamics of a finite number of dislocations lines and the dynamics of dislocations densities, based on non-linear homogenization tools. We have done significant progress in this direction with C. Imbert (at partial time in CERMICS) and E. Rouy (Lyon University). A. Ghorbel in his PhD (to be defended in 2007) investigates the «Numerical analysis of dislocations dynamics and applications to homogenization». He has obtained some long time existence and uniqueness results for non-local Hamilton-Jacobi equations describing the dynamics of

dislocations particles in interactions and some error estimates have been presented for corresponding schemes. Numerical simulations have also been done and give a striking illustration of recent non-linear homogenization results for dislocations dynamics.

Free boundary problems
Even if it is not the main activity of the team, let us underline that R. Monneau continued his activity in the framework of the contract ACI NIM on a different subject: PDE and finance. Let us more generally mention that the team continues its international collaborations, in particular with Chili, Japan and Italy. Finally, we have to stress the fact that our team is strongly involved in teaching activities, both at the ENPC and at the University, where each year we welcome several students for short research projects.

CERMICS members

Researchers
Cancès Eric
Chancelier Jean Philippe
Cohen Guy
De Lara Michel
Delmas Jean-François
Ern Alexandre
Glinsky-Olivier Nathalie
Jourdain Benjamin
Lapeyre Bernard (part-time)
Le Bris Claude
Lelièvre Tony
Monneau Régis
Piperno Serge
Pommaret Jean-François (till June 2006)

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Dolean Victorita (UNSA)
Fezoui Loula (INRIA)
Kammerer-Quenez Marie-Claire (UMLV)
Kohatsu-Higa Arturo (INRIA)
Lamberton Damien (UMLV)
Lanteri Stéphane (INRIA)
Legoll Frédéric (LAMI)
Rapetti Francesca (UNSA)
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Ben Alaya Mohamed (Univ. Paris 13)
Braack Malte (Univ. Heidelberg)
Briani Ariela (Univ. Pise)
Bouleau Nicolas (ENPC)
Burman Erik (EPFL)
Cannone Marco (UMLV)
Carpentier Pierre (ENSTA)
Dedeban Claude (FT R&D, La Turbie)
Guermond Jean-Luc (Texas …)
Hoch Philippe (CEA)
Imbert Cyril (Univ. Montpellier)
Lewin Mathieu (CNRS, Univ. Cergy-Pontoise)
Virieux Jean (Geosciences Azur, UNSA)

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Bencteux Guy
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Boyaval Sébastien
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Deleurence Amélie
El Hajj Ahmad
El Makrini Mohamed
Foki Julien
Forcadel Nicolas
Galicher Hervé
Ghorbel Amin
Gloria Antoine
Guyon Julien
Ibrahim Hassan
Laviolette Ralf
Lelong Jérôme
Lioris Eugénie
Meunier Sébastien
Orriols Antonin
Sbai Mohammed
Scotti Simone
Seck Babacar
Sochala Pierre
Stephansen Annette
Stoltz Gabriel
Strugarek Cyrille
Tardif d'Hamonville Pierre

Post-doctoral students
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Djadel Karim
El Rhabi Mohammed
Milman Perola
Rousset Mathias
Scemama Antony

Internship students
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Moreau Simon (ENPC)
Basquin Philippe (Institut Galilee)
Hanping Tong (2nd year, ENSTA)
Elacheche Moncef (M1 Orsay),
Rehbinder Serge (M1 Orsay)
Lahbabi Salma (ENPC)
Bennani Iqbal (ENPC)
Lantaume Hugo (ENPC)
Boudjerada Rachida (Univ. H. Boumedienne)
Yakhou Zouhair (Ecole Mohammadia)

Visiting Researchers
Schied Alexander (TU Berlin)
Patz Carsten (PhD student, Univ of Stuttgart)

Administrative Assistants
Berte Sylvie
Elouali Khadija (till 31/8/2006)
Ouhanna Martine (starting 15/11/2006)

TEACHING

Organization

A. Ern chairs the First Year Department at ENPC. This department supervises the whole course program for the first year studies at ENPC.

S. Piperno organized the «Mathematics and Computer Science Department opening week» at INRIA Sophia Antipolis for the students of Ecole Nationale des Ponts et Chaussées.

Lectures

Mathematical methods for finance
ENPC
A. Alfonsi, J. Guyon, B. Jourdain

Epistemology
ENPC
N. Bouleau, K. Chatzis, B. Wallliser

Sensitivity and error calculus, application to finance
Master2, universities Paris I and Paris VI
N. Bouleau, C. Chorro

Analysis
ENPC
E. Cancès (professor in charge), A. Ern, R. Monneau

Fourier analysis and spectral theory
ENPC
E. Cancès

Molecular simulation: theoretical and numerical aspects
University Paris 6
E. Cancès

Numerical analysis and optimization
Ecole Polytechnique
E. Cancès, C. Le Bris

Differentiable optimization
ENSTA
P. Carpentier

Differentiable optimization
ENSMP
P. Carpentier

Optimization of large systems
ENSTA
P. Carpentier

Numerical methods for stochastic optimization
Master Mathématiques, Informatique et Applications, PARIS 1
P. Carpentier

Stochastic Control: continuous time, numerical methods and application to Finance
Master Mathématiques, Informatique et Applications, University Paris 1
J.–P. Chancelier

Acoustics, computer science and music
ENSMP
J.–P. Chancelier, B. D'Andrea

Numerical Methods in Finance
Master in Financial Mathematics
Halmstad University, Sweden
J.–P. Chancelier, B. Lapeyre, A. Sulem

Scilab course
ENPC
J.–P. Chancelier, M. De Lara, A. Dallagi

Automatic control, Scilab tutorial
ENSMP
J.–P Chancelier, P. Rouchon

Stochastic Optimization and Control
EDF
G. Cohen, M. De Lara, J.–P. Chancelier, P. Carpentier, B. Lapeyre, B. Jourdain

Risk measure in finance
M2, University Paris 6
J.-F. Delmas

Stochastic models
M2, UMLV
J.–F. Delmas

Statistics
ENPC
J.–F. Delmas, J. Guyon, C. Strugarek

Introduction to probability and statistics ENSTA
J.–F. Delmas, J. Guyon, J. Lelong

Computational Mechanics
ENPC master
A. Ern

Scientific Computing
ENPC
A. Ern (professor in charge), A. Gloria, S. Piperno, G. Stoltz

Projects and courses in Finance
Applied mathematics specialization, Ecole

Polytechnique,
B. Jourdain, B. Lapeyre

Introduction to Probability Theory and simulation
Ecole Polytechnique,
B. Jourdain

Monte-Carlo methods in Finance
Formation cycle of College of Ecole Polytechnique,
B. Jourdain

Probability and statistics
ENPC
B. Jourdain (professor in charge), A. Alfonsi, M. De Lara, T. Lelièvre

Monte-Carlo methods in finance
ENPC and Master2 Applied Mathematics, UMLV
B. Lapeyre, B. Jourdain

Modelisation and Simulation
ENPC,
B. Lapeyre, T. Lelièvre

Mathematics for the Sustainable Management of Natural ressource
Master EDDEE (Economics of Sustainable Development, Environment and Energy)
M. De Lara

Multiscale systems
University Paris 6
C. Le Bris

Numerical Methods in Finance
ENSTA
J. Lelong

Markov Chains
ENSTA
J. Lelong

Non-probabilistic methods in mathematical finance
ENPC
T. Lelièvre

Non Linear Analysis and Applications
ENPC
R. Monneau

Fluid-structure interactions
Mastère de Mécanique Numérique, ENSMP,
S. Piperno

Introduction to scientific computation
ENSTA
C. Strugarek

Complex Analysis
ENSTA
C. Strugarek

PUBLICATIONS

Articles in press (and accepted for publication)

M. Barrault, E. Cancès, C. Le Bris, W.W. Hager
Multilevel domain decomposition for electronic structure calculations
J. Comput. Phys.

K. Barty, P. Girardeau, J.-S. Roy, C. Strugarek
A Q–Learning Algorithm with Continuous State Space
Optimization Online, October 2006

K. Barty, J.-S. Roy, C. Strugarek
Hilbert valued perturbed subgradient algorithms
Math. Oper. Res.

K. Barty, J.-S. Roy, C. Strugarek
Closed–loop stochastic gradient algorithms
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M. Bernacki, S. Piperno
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Analysis of finite element methods for coupled hydro-mechanical problems ECCOMAS CFD 2006 Conference, Egmond aan Zee, The Netherlands, September 5–8, 2006

S. Meunier, A. Ern, G. Nicolas, O. Boiteau
Analyse de méthodes éléments finis pour des problèmes couplés Hydro-Mécaniques, Congrès national d'analyse numérique, Guidel, France, May 2006

R. Monneau
Multiscale Materials Modeling Symposium «Statistical Approaches to irreversible Deformation and Failure of Materials», Freiburg, Germany, September, 2006

R. Monneau
Modeling of dislocations dynamics and link with the mean curvature motion, «Modeling and analysis of phase transitions», Pisa, Italy, January 2006

R. Monneau,
Modeling of dislocations dynamics and homogenization, «Mathematics and its applications'», Torino, Italy, July 2006

R. Monneau
Homogenization of dislocations dynamics, «New Trends in Viscosity Solutions and Nonlinear PDE's», Lisbon, Portugal, July 2006

R. Monneau
Homogenization of dislocations dynamics, Workshop «PDE and Materials», Oberwolfach, Germany, September 2006

R. Monneau
Regularity results on the free boundary for american options, «Journées Solutions de viscosité et applications en contrôle et en

finance», University Paris Dauphine, Paris, November 2006

A. Orriols
Algorithmes de contrôle d'interface libre. Implémentation sur un modèle MHD linéaire, Congrès National d'Analyse Numérique, CANUM 2006, Guidel, June 2006

S. Piperno
Symplectic local time-stepping in non-dissipative DGTD methods applied to wave propagation problems, ECCOMAS CFD 2006 Conference, Egmond aan Zee, The Netherlands, September 5–8, 2006

M. Rousset
Workshop «Mathematical and numerical methods in Quantum Chemistry», Oberwolfach, 22–26 October 2006

G. Scarella, O. Clatz, S. Lanteri, S. Oudot, J.–P. Pons, S. Piperno, J. Wiart
Modélisation numérique réaliste de l'exposition des tissus de la tête à un champ électromagnétique issue d'un téléphone mobile, CEM 2006, 13ème colloque international et exposition sur la compatibilité électromagnétique, Saint-Malo, France, April 4–6, pp. 175–177, 2006

S. Scotti
Perturbative approach in financial markets AMASES's Conference (Italian association for applied mathematics in economy and social sciences), Trieste, Italy, September 2006

S. Scotti
Perturbative approach in financial markets Conference PRIN Matematica finanziaria (National Italian research project in financial mathematics), Lecce, Italy, September 2006

B. Seck
From risk constraints to utility functions in stochastic optimization, convergence of approximations of stochastic optimization problems subject to measurability constraints, International Conference on Mathematics of Optimization and Decision Making, Pointe–à–Pitre, April 18–21, 2006

G. Stoltz
A simplified dual formulation of the electronic problem in terms of the second order reduced density matrix, Poster presented at the International Congress on Quantum Chemistry, Kyoto, May 2006

C. Strugarek, P.Carpentier, J.–P. Chancelier, G. Cohen, M. De Lara
Decomposition for Dynamic Stochastic Programs, International Conference on Mathematics of Optimization and Decision Making, Pointe–à–Pitre, April 18–21 2006

T. Tomasino, M. Le Hervet, O. Martin, T. Lelièvre
Stability analysis of simplified electrolysis cells with MISTRAL, Light Metal, Proceeding of the 2006 TMS Annual Meeting and Exhibition, pp. 335–340, 2006

Research reports

R. Abraham, J. F. Delmas
Asymptotics for the small fragments of the fragmentation at nodes, CERMICS Research report n°2006– 305

R. Abraham, J.-F. Delmas
Changing the branching mechanism of a continuous state branching process using immigration, CERMICS Research report n°2006 – 318

A. Alfonsi, B. Jourdain
A call–put duality for perpetual american options, CERMICS Research report n°2006–307

A. Alfonsi, B. Jourdain
General Duality for Perpetual American Options, CERMICS Research report n°2006–333

M. Ben Alaya, B. Jourdain
Probabilistic approximation of a nonlinear parabolic equation occurring in rheology, CERMICS Research report n°2006–314

M. Benjemaa, S. Piperno, N. Glinsky–Olivier
Etude de stabilité d'un schéma volumes finis pour les équations de l'élastodynamique en maillages non structurés, CERMICS Research report n°2006–310

N. Bouleau
When and how an error yields a Dirichlet form, CERMICS Research report n°2006–308

N. Bouleau
On some errors related to the graduation of measuring instruments, CERMICS Research report n°2006–316

N. Bouleau
On the coarsest topology preserving continuity, CERMICS Research report n°2006–317

N. Bouleau
An extension to the Wiener space of the arbitrary functions principle, CERMICS Research report n°2006–319

E. Burman, A. Ern
A continuous finite element method with face penalty to approximate Friedrichs' systems, CERMICS Research report nº2006–298

E. Carlini, M. Falcone, N. Forcadel, R. Monneau
Convergence of a Generalized Fast Marching Method for a non–convex eikonal equation, CERMICS Research report nº2006–325

J.–P. Chancelier
Epi–convergence of stochastic optimization problems involving both random variables and measurability constraints approximations, CERMICS Research report nº2006–323

J.–P. Chancelier, M. De Lara, A. De Palma
Risk aversion in one–armed bandit problems, CERMICS Research report nº2006–322

G. Ciccotti, T. Lelièvre, E. Vanden–Eijnden
Sampling Boltzmann–Gibbs distributions restricted on a manifold with diffusions: application to free energy calculations, CERMICS Research report nº2006–309

F. Da Lio, N. Forcadel, R. Monneau
Convergence of a non-local eikonal equation to anisotropic mean curvature motion. Application to dislocations dynamics, CERMICS Research report nº2006–303

M. De Lara, L. Doyen, T. Guilbaud, M.–J. Rochet
Monotonic properties for the viable control of discrete time systems, CERMICS Research report nº2006–299

J.–F. Delmas
Fragmentation at height associated to Lévy processes, CERMICS Research report nº2006–300

J.–F. Delmas
Height process for super-critical continuous state branching process, CERMICS Research report nº2006–329

J.–F. Delmas, B. Jourdain
Does waste–recycling really improve Metropolis–Hastings Monte Carlo algorithm? CERMICS Research report nº2006–331

D. A. Di Pietro, A. Ern, J.–L. Guermond
Discontinuous Galerkin methods for anisotropic semi-definite diffusion with advection, CERMICS Research report nº 2006–330

V. Dolean, H. Fol, S. Lanteri, S. Piperno
Méthodes de type Galerkin discontinu pour la résolution numérique des équations de Maxwell en régime fréquentiel, CERMICS Research report nº2006–311

A. El Hajj
Existence and uniqueness of a solution of a non-conservative Burgers type system describing the dynamics of dislocations densities, CERMICS Research report nº2006–324

A. El Hajj, N. Forcadel
A convergent scheme for a non-local coupled system modeling dislocations densities dynamics, CERMICS Research report nº2006–313

A. Ern, J.–L. Guermond
Discontinuous Galerkin methods for Friedrichs' systems. Part III. Multi-field theories with partial coercivity, CERMICS Research report nº 2006–320

A. Ern, A. Stephansen, P. Zunino
A Discontinuous Galerkin method with weighted averages for advection-diffusion equations with locally vanishing and anisotropic diffusivity, CERMICS Research report nº2006–332

N. Forcadel
An error estimate for a new scheme for mean curvature motion, CERMICS Research report nº2006–334

A. Ghorbel, P. Hoch, R. Monneau
A numerical study for the homogenization of one–dimensional models describing the motion of dislocations, CERMICS Research report nº2006–327

A. Ghorbel, R. Monneau
Well–posedness and numerical analysis of a one-dimension non–local transport equation modeling dislocations dynamics, CERMICS Research report nº2006–304

J. Guyon
Limit theorems for bifurcating Markov Chains. Application to the detection of cellular aging, CERMICS Research report nº 2006–301

C. Imbert, R. Monneau
Homogenization of first order equations with periodic Hamiltonians Part I: local equations, CERMICS Research report nº 2006–302

B. Jourdain
Stochastic flows approach to Dupire's formula, CERMICS Research report nº 2006–326

C. Labart, J. Lelong
Pricing double barrier Parisian Options using Laplace transforms, CERMICS Research report

nº 2006–328

C. Le Bris
Mathematics for molecular simulation: accomplishments and challenges, CERMICS Research report nº2006–296

T. Lelièvre, M. Rousset, G. Stoltz
Computation of free energy differences through nonequilibrium stochastic dynamics: the reaction coordinate case, CERMICS Research report nº2006–306

T. Lelièvre, M. Rousset, G. Stoltz
Computation of free energy profiles with adaptive parallel dynamics, arXiv: cond–mat/0611276 (2006)

J. Lelong
Central limit theorems for truncating and averaging stochastic algorithms: a functional approach, CERMICS Research report nº2006–312

R. Monneau
A kinetic formulation of moving fronts and application to dislocations dynamics, CERMICS Research report nº2006–315

G. Stoltz
Path sampling with stochastic dynamics: some new algorithms, arXiv preprint cond-mat (2006) 0607650.

C. Strugarek
Interchange of minimization and integration with measurability constraints, CERMICS Research report n°2006-321

P. Tardif D'Hamonville, A. Ern, L. Dormieux
Finite element evaluation of diffusion and dispersion tensors in periodic porous media with advection, CERMICS Research report nº2006–297

CONTRACTS

CONTRACTS WITH PRIVATE FUNDS

PREMIA software: pricing and hedging procedures library financed by a consortium of banks
A. Alfonsi, J.F. Delmas, J. Guyon, B. Jourdain, B. Lapeyre.

Atom-to-continuum multiscale numerical simulation of materials (EDF)
E. Cancès, C. Le Bris

Study on scale transfer in materials simulations (CEA)
E. Cancès, G. Stoltz

From Risk Constraints in Stochastic Optimization Problems to Utility Functions, EDF (Electricité de France), [2005–2008]
M. De Lara, Babacar Seck

Discontinuous Galerkin methods for Saint-Venant equations (CETMEF)
A. Ern, K. Djadel, S. Piperno

Fondation EADS: Modelisation and statistical study for the program PILE
J. Foki, D. Chauveau, J.–F. Delmas

Evaluation of MAXDGk for a coupled Vlasov/Maxwell software (CEA/CESTA)
S. Lanteri, S. Piperno, L. Fezoui (INRIA contract)

Numerical simulation of aluminum electrolysis (Alcan–Pechiney)
C. Le Bris, T. Lelièvre, A. Orriols

Space-time error indicators for thermo-hydro-mechanics in Code_Aster (EDF)
S. Meunier, A. Ern

Expertise in the parallelization of structured grid schemes on clusters (FT R&D),
S. Piperno, S. Lanteri, A. Bouquet (INRIA contract)

A posteriori error analysis applied to reactive transport in porous media (ANDRA)
A. Stephansen, A. Ern

CONTRACTS WITH PUBLIC FUNDS

ANR LN3M « Logiciels Nouvelle génération pour la Modélisation Multiéchelle des Matériaux » (coordinator: F. Jollet, CEA-DAM)
E. Cancès, A. Deleurence, G. Stoltz

ANR INGEMOL “Intégration numérique géométrique des equations Hamiltoniennes” (non-thematic maths and interactions program, coordinator: Ph. Chartier, IRISA)
E. Cancès, C. Le Bris, T. Lelièvre

ACI «Simulations moléculaires» (ACI «mathématiques et interactions» coordinator: (C. Le Bris)
E. Cancès, C. Le Bris, G. Stoltz

STIC–AmSud MIFIMA “Mathematics, Informatics and Fisheries Management, responsible”, Action supported by the regional cooperation program STIC–AmSud, [2006–2008]
M. De Lara

ANR «Environment and re-Emergence of

Infectious Deseases in the Amazonian Basin», participation, ANR Programme Santé–environnement et Santé–travail, [2005--]
M. De Lara

ANR «RiskAttitude: economy and risk», participation, ANR blanche, [2005--]
M. De Lara

ACI « Economic Interpretation of Sustainable Development, Invariance and Environmental Preferences », participation, action concertée incitative du ministère de la Recherche (ACI Modélisation économique du développement durable), [2005--]
M. De Lara

ACI «Development of Deterministic and Stochastic Methods for Theoretical Ecology and Fisheries Management», responsible, action concertée incitative du ministère de la Recherche (ACI écologie quantitative). [2002--]
M. De Lara

ANR «Adaptative Monte Carlo Methods» (CIS 2006 program)
J.–F. Delmas, B. Jourdain, B. Lapeyre

Contract with Centre des Matériaux d'Evry (ENSMP)
M. El Rhabi, R. Monneau

ANR «Quantitative Seismic Hazard Assessment » (program «Catastrophes telluriques et Tsunamis» CATATSU-2005, coordinator: J. Virieux)
N. Glinsky-Olivier, S. Lanteri, S. Piperno, M. Benjemaa

ANR «High Order Finite Element Particle-In-Cell Solvers on Unstructured Grids» (CIS 2006 program, coordinator: E. Sonnendrücker, via INRIA)
S. Lanteri, S. Piperno

ANR «Grilles de calcul pour les mathématiques financières» (CIS 2005 program)
B. Lapeyre (coordinator)

ACI «Modelisation and numerical analysis of dislocation dynamics» (ACI Jeunes chercheurs, MENRT)
R. Monneau

ACI «EDP method in market finance» (ACI Nouvelles Interfaces des Mathematiques)
R. Monneau

ECOS-CONYCIT Collaboration contract France–Chile (ECOS-CONYCIT C02E06, ENPC)
R. Monneau

ANR «Mouvement d'Interfaces, Calcul et Applications» (ANR 2006-2009)
R. Monneau

DISSEMINATION

Editorial activity

E. Cancès is co-Editor in chief (with P. Del Moral and J.–F. Gerbeau) of ESAIM Proc. He is a member of the editorial board of Mathematical Modelling and Numerical Analysis.

C. Le Bris is a member of the board of directors of the SMAI (french SIAM). He is co-Editor-in-chief (with A. T. Patera, MIT) of Mathematical Modelling and Numerical Analysis. He is a member of the editorial boards of Applied Mathematics Research Express, Archive for Rational Mechanics and Analysis, COCV (Control, Optimization and Calculus of Variations), Mathematics Applied in Science and Technology, Networks and Heterogeneous Media, Nonlinearity, Review of Mathematical Science.

S. Piperno is member of the editing committee of «Progress in computational fluid dynamics» (Inderscience).

International seminars given

N. Bouleau
Arbitrary functions principle and Dirichlet forms, Kyoto University, Japan, September

E. Cancès
A multiscale model for concentrated suspensions, Peking University (Peking), July

M. De Lara
Centro de Modelamiento Matematico / UMI CNRS, Universidad de Chile, Santiago de Chile, Chile, 9 August 2006, Sustainability of Fisheries Management and Viable Control of Discrete Time Systems

M. De Lara
IMCA Instituto de Matematica y Ciencias Afines, Lima, Peru, 16 August 2006, Sustainability of Fisheries Management and Viable Control of Discrete Time Systems

M. De Lara
Instituto de Fomento Pesquero, Valparaiso, Chile, 17 August 2006, Sustainability of Fisheries Management and Viable Control of Discrete Time Systems

J.–F. Delmas
Fragmentation of continuous random trees (at height and at nodes) and asymptotics of small fragments. University of California, San Diego (U.S.A), April

J.–F. Delmas
How to detect aging for E. coli cells
University of California, San Diego (USA), May

D. Di Pietro
Discontinuous Galerkin methods for anisotropic semi-definite diffusion with advection, Math Dept., Texas A&M, USA, October

A. Ern
Discontinuous Galerkin methods for Friedrichs' systems, Math Dept., Texas A&M, USA, January

A. Ern
Discontinuous Galerkin methods for Friedrichs' systems, University of Bergamo, Italy, February

B. Lapeyre
Tokyo Institute of Technology, seminar on Financial Engineering, «Premia an experimental option pricer», November

B. Lapeyre
Osaka University, Graduate School of Engineering Sciences, a unified framework for adaptive variance reduction methods, November

C. Le Bris
University of Minnesota

C. Le Bris
Materials Modeling Laboratory Oxford University

C. Le Bris
Existence and uniqueness of solutions to Fokker-Planck type equations with irregular coefficients, Variational methods in materials science, Scuola Normale Superiore Pisa

T. Lelièvre
Stockholm, May

T. Lelièvre
Workshop CERMICS / PKU, Peking, July

R. Monneau
Introduction à la dynamique des dislocations et resultats recents, Journées «Analyse non linéaire'» (University of Sfax, Tunisie), November

R. Monneau
ETH Zurich (Suisse) April

A. Orriols
University of Linz, Austria, November

M. Rousset
University of Bonn, Germany, November

M. Rousset
Workshop «Sequential Monte-Carlo methods», St-Anne's college, Oxford, July

M. Rousset
Workshop «Coarse-grained multiscale models: mathematical analysis and applications», Warwick University, April

G. Stoltz
(Non) equilibrium computation of free energy differences, Seminar of the Computational Chemistry group at university of Amsterdam

National seminars given

K. Barty, P. Girardeau, J.–S. Roy, C. Strugarek
American Option Pricing with Functional Stochastic Algorithms, Séminaire Bachelier, Institut H. Poincaré, Paris, March

N. Bouleau
University Louis Pasteur, Strasbourg, Spécifications en analyse numérique stochastique, April

N. Bouleau
University Louis Pasteur, Strasbourg, Quelques précisions sur les erreurs, April

E. Cancès
Laboratoire J.–L. Lions (Paris).

E. Cancès
4 hours lecture in the framework of GdR Chant, Institut Joseph Fourier (Grenoble). Molecular and multiscale simulation of materials, January

J.–F. Delmas
Autour des processus de branchement continu. University of Orléans, October

J.–F. Delmas
Immigration et élagage pour les processus de branchement. Ecole Polytechnique, November

A. Deleurence
Institute Henri Poincaré, Modeling of crystals with defects, October

A. Ern
Une présentation unifiée des méthodes de Galerkin Discontinu via les systèmes de Friedrichs, University of Provence, June

A. Ern
Discontinuous Galerkin Methods for Anisotropic and Semi-Definite Diffusion with Advection, Strasbourg University, November

J. Foki
WAIMH Congress (World Association For Infant Mental Health), Paris. The Multidisciplinary Basis of the Research Program Pile (International Program for the Children's Speech), July

B. Jourdain
Introduction to the DMC method in quantum chemistry, IRMAR, University Rennes 1, April

B. Jourdain
Introduction to the DMC method in quantum chemistry, CEREMADE, University Paris Dauphine, May

B. Lapeyre
CDC Ixis bank, mini course on Adaptive Monte-Carlo methods, October

M. De Lara
ANR RiskAttitude, October, Risk aversion, road choice and the one-armed bandit problem, October

C. Le Bris
University of Cergy-Pontoise

C. Le Bris
Séminaire Pierre-Louis Lions du Collège de France

C. Le Bris
University Paris Sud Orsay

C. Le Bris
University Paris Dauphine

C. Le Bris
Exposé au Séminaire inaugural de la Chaire Lafarge – Lyon – ENPC. École Polytechnique

T. Lelièvre
J.–L. Lions Laboratory, University Paris 6, January

T. Lelièvre
INRIA Sophia-Antipolis, May

T. Lelièvre
Séminaire ADAP'MC, October

T. Lelièvre
CIRM, Marseille, August

T. Lelièvre
Workshop on Numerics for SDEs with applications, Florida State University, February

J. Lelong
Journées MAS à Lille: A Central Limit Theorem for Truncating Stochastic Algorithms, September

J. Lelong
Société Générale, Stochastic algorithm and Adaptive Variance Reduction Method, July

J. Lelong
Groupe de travail du CMAP, Ecole Polytechnique, Central Limit Theorems for Truncating and Averaging Stochastic Algorithms a functional approach, June

R. Monneau
Introduction à la dynamique des dislocations, PPF «Dynamique des systèmes complexes», La Grave, France, December

R. Monneau
ENS Cachan, Antenne de Bretagne, Rennes, May

S. Piperno
J.–L. Lions Laboratory, University Paris 6, June

S. Piperno
ONERA-Chatillon, June

S. Piperno
Collège de France (Maths and Computer Science Prizes ceremony), December

A. Scemama
Probabilistic description of the chemical bond, 10th Rencontre des Chimistes Théoriciens Francophones, Nancy, July

G. Stoltz
CEA/DAM, November

G. Stoltz
Computing macroscopic properties using microscopic models, rencontre GdR CHANT, Grenoble, January

G. Stoltz
(Non) equilibrium computation of equilibrium properties, ACI meeting - CIRM Marseille, January

G. Stoltz
Echantillonnage hors-équilibre, Meeting «Scientific computation» at University of Cergy-Pontoise, April

G. Stoltz
Path sampling with stochastic dynamics, Poster presented at the workshop Sampling paths in molecular simulation: algorithms for phase transitions, reactivity and kinetics,

Orsay, November

G. Stoltz
A simplified one-dimensional model of shock and detonation waves, Sixth Biennal International Conference on New models and hydrocodes for shock waves processes in condensed matter, Dijon, April

Missions and visits

E. Cancès
Peking University (Peking), A multiscale model for concentrated suspensions, July

M. De Lara
Curso de Matematica e Informatica para la Gestion Sostenible de Recursos Naturales / Mathematics and Informatics for Sustainable Management of Renewable Ressource, cours CIMPA, The Havana, Cuba, September

M. De Lara
Curso de Matematica e Informatica para l Gestion Sostenible de Recursos Naturales / Mathematics and Informatics for Sustainable Management of Renewable Resource, IMCA Instituto de Matematica y Ciencias Afines, Lima, Peru, November

J.F. Delmas
University of California, San Diego, spring (3 months)

J. Lelong
Invited by Professor Syoiti Ninomiya in Tokyo (Center for Research in Advanced Financial Technology, Tokyo Institute of Technology) Truncated Stochastic Algorithms and Variance Reduction: toward an automatic procedure, November

R. Monneau
ETH Zürich (Suisse), 2 days, April

SUPERVISION ACTIVITY

Ongoing PHD Theses

G. Bencteux,
Domain decomposition methods for ab initio computations in mateiral sciences, ENPC.

M. Benjemaa
Numerical simulation of dynamical rupture in seisms using finite volumes methods on unstructured meshes, University of Nice-Sophia Antipolis

A. Bouquet
Adaptation of fictitious domain methods to discontinuous Galerkin methods with subgridding, University of Nice-Sophia Antipolis

S. Boyaval
Multiscale modelisation and simulation of complex fluids for civil engineering, ENPC

A. Dallagi
Particle methods in stochastic optimal command, University Paris 1

A. Deleurence
Mathematical and numerical analysis of multiscale simulation models in material sciences, ENPC

A. El Hajj
Analysis and numerical analysis of elasto-visco-plastic models with dislocations ENPC (co-direction: R. Monneau of CERMICS and M. Cannone of UMLV)

M. El Makrini
Simulation of defects in crystals, University Paris Dauphine

J. Foki
Fidelity test, analysis of correlation between different signals, ENPC

N. Forcadel
Mathematical analysis of dislocations models with mean curvatures terms, ENPC

H. Galicher
Coupling of classical and quantum models for the molecular scale simulation of materials, University Paris 6

A. Ghorbel
Numerical analysis of dislocations dynamics, ENPC

A. Gloria
Multiscale numerical methods in nonlinear élasticity, ENPC

H. Ibrahim
Mathematical analysis of dislocations density dynamics with scale effects, ENPC (co-direction: R. Monneau and Mustapha Jazar of University libanaise)

R. Laviolette
Options pricing for energy derivatives in models with jumps, ENS Cachan

J. Lelong
Stochastic Algorithms and calibration problems in Finance, UMLV

E. Lioris
Simulation and evaluation of collective taxi systems, ENPC

S. Meunier
Space-time error indicators for thermo–hydro-mechanics in Code_Aster, ENPC

M. Sbai
Simulation of stochastic differential equations in finance, ENPC

S. Scotti
Dirichlet forms methods in finance, ENPC and University of Pisa

B. Seck
From Risk Constraints in Stochastic Optimization Problems to Utility Functions, ENPC

A. Siri-Jegousse
Whright Fisher models and non-homogeneous coalescing process, ENPC

P. Sochala
Numerical methods for coupling subsurface and surface flows, ENPC

A. Stephansen
A posteriori error analysis applied to reactive transport in porous media, ENPC

G. Stoltz
Problems of scale transfer in material simulation, ENPC

Defended PHD Theses

A. Alfonsi
Credit risk, calibration and discretization of financial models, ENPC

J. Guyon
Probabilistic modeling in finance and biology. Limit theorems and applications, ENPC

A. Orriols
Optimization and control algorithms of free surfaces. Application to the industrial production of aluminum à la production industrielle d'aluminium, ENPC

C. Strugarek
Variational approaches and other contributions to stocahstic optimization, ENPC

P. Tardif d'Hamonville
Numerical evaluation of advective and diffusive transport in multi-phase porous media, ENPC

HOSTED SEMINARS

Working group of Mathfi team

Organized by J. Guyon, B. Jourdain and M.–C. Kammerer–Quenez

N. Privault (University of la Rochelle)
Intégration par parties pour les processus ponctuels et application numérique en calcul de sensibilités

M.-P. Bavouzet (UMLV et INRIA)
Intégration par parties pour des processus de sauts et applications en Finance

D. Hernandez (CIMAT Mexico)
On the convergence of the value iteration algorithm for partially observed risk–sensitive control problems

P. Lescot (University of Picardie)
Processus de Bernstein et transformations d'Alili–Patie

F. Panloup (University Paris 6)
Estimation de la mesure invariante d'une EDS dirigée par un processus de Lévy

A. Schied (Technical University of Berlin)
Aspects of model uncertainty and robustness in finance and economics I and II. Some recent results on risk measures

E. Moulines (ENST)
Méthodes de Monte-Carlo adaptatives

V. Genon–Catalot (University Paris 5)
Filtrage explicite de diffusions discrtises

C. Chorro (ENPC)
Calcul d'erreur par formes de Dirichlet: quelques résultats asymptotiques

G. Pages (University Paris 6)
Quantification fonctionnelle, régularité trajectorielle et processus de Levy

S. Loisel (University Lyon 1)
Diffrentiation de fonctionnelles de processus de risque et allocation de réserve optimale

P. Gapeev (Russian Academy of Sciences, Institute of Control Sciences)
Optimal switching problems in jump-diffusion models

G. Di Nunno (CMA, University of Oslo)
On a version of the fundamental theorem of asset pricing and events of small but positive probability

P. Tankov (University Paris 7)
Quadratic hedging with jumps

E. Ekstrom (University of Manchester)
Properties of option prices in models with jumps

S. Levendorsk (CMA, University of Oslo)
Wiener-Hopf factorization techniques in Finance I and II

B. Ivorra (University Montpellier 2)
An hybrid optimization method for the management of a credit portfolio under constraints

S. Crepey (University of Evry)
Couverture d'obligations convertibles avec risque de défaut

J.–F. Delmas (CERMICS)
Introduction aux mesures de risque I et II

Xiao Wei (CUFE, Beijing)
Asymptotic ruin probabilities for discrete time risk models with heavy-tailed claims

S. Roland (University of Evry)
Some Issues on Utility Maximization under Partial Information

A. De La Fortelle (INRIA)
Une nouvelle classe de changement de mesure pour le mouvement brownien et application pour la réduction de variance

M. Hoffmann (UMLV)
Reconstruction de la volatilité multifractale à partir de données historiques haute fréquence I

B. Jourdain (CERMICS)
Formule de Dupire et flot stochastique

A. Gloter (UMLV)
Reconstruction de la volatilité multifractale à partir de données historiques haute fréquence II

F. Avram (University of Pau)
Problèmes de ruine en assurance

Scientific computing seminar

Organized by A. Gloria and G. Stoltz

G. Stoltz (CERMICS/ENPC)
Introduction à la dynamique moléculaire

R. Pollet (CEA/Saclay)
Profils d'énergie libre par la méthode des collines ou métadynamique

M. Athènes (CEA/Saclay)
Méthodes d'échantillonnage de chemins hors-équilibre

T. Lelièvre (ENPC/CERMICS
Calculation of free energy differences using stochastic dynamics

K. Pernal (Vrije Universiteit, Amsterdam and University of Szczecin, Poland)
One-electron reduced density matrix functional theory–functionals, and response properties

Alfio Borzi (University of Graz)
Some recent results on quantum optimal control problems: Three–level quantum dots and Bose Einstein condensates in magnetic microtraps

G. James (INSA Toulouse)
Le problème de l'existence de «breathers» dans une chaîne de particules en interaction non-linéaire

Tiziano Passerini (Politecnico di Milano)
Mathematical models for cerebral circulation

Antoine Sellier (LadHyx)
Migration thermocapillaire de bulles: une approche par équations intégrales de frontière

F. Périn
Bornes et résultats asymptotiques pour les caractéristiques électromagnétiques effectives d'un milieu diphasique ordonné

E. Darve (Stanford University)
Méthodes numériques pour le calcul d'énergies libres

SOFTWARE

J. P. Chancelier
Development of Nsp, experimental re-implementation of Scilab (Presentation to the Steering Committee of Scilab, January 18th, 2006)

Applied probability team and team Mathfi PREMIA (version 7), option pricing software.

J. Lelong
Involvement in Premia administration of the

CVS serveur used for the development of Premia implementation of a new compiling sequence using the auto-tools maintenance a new web page for Premia devoted to corrections of bugs implementation of an algorithm for the pricing of Parisian options based on Laplace transforms.

LIST OF ACRONYMS

ACI: Action Concertée Incitative
ANDRA: Agence nationale pour la gestion des déchets radioactifs
ANR: Agence nationale de la Recherche
BRGM: Bureau des recherches géologiques et minières
CEA: Commissariat à l'énergie atomique
CNRS : Centre national de la recherche scientifique
GDR MOMAS: Groupement de recherches sur la Modélisation mathématique et les simulations numériques liées à la gestion des déchets nucléaires
IRSN: Institut de radioprotection et de sûreté nucléaire
EDF: Electricité de France
CEMAGREF: Centre national du machinisme agricole, du génie rural, des eaux et forêts
CEREVE: Centre d'Enseignement et de Recherche Eau, Ville, Environnement
CETMEF: Centre d'Etudes Techniques Maritimes et Fluviales
EPFL: Ecole Polytechnique Fédérale de Lausanne
GDR: Groupement de Recherche
INERIS: Institut National de l'Environnement Industriel et des Risques
LMSGC: Laboratoire des matériaux et des structures du génie civil
MOMAS: Modélisations mathématiques et simulations numériques liées aux problèmes de gestion des déchets nucléaires
PAI: Programme d'Actions Intégrées du Ministère des Affaires Extérieures
QHAN: Qualité et fonctionnement hydrologique des systèmes aquatiques du groupement d'Antony
UMLV: Marne-la-Vallée University
UNSA: Nice – Sophia Antipolis University