CERMICS

Centre for teaching and research in mathematics and scientific computing

École des ponts laboratory hosting joint project-teams with INRIA

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Staff
14 researchers
11 associate researchers (4 researchers of INRIA, 3 of Université Paris-Est Marne-la-Vallée, 2 of Université Nice Sophia Antipolis, 1 of Université Paris Dauphine, 1 of UR Navier – LAMI)
14 external collaborators
26 PhD students
2 administrative assistants
6 post-doc
8 invited researchers
8 internship students

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

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

It can be pointed out that two teams are, or take part to, joint project-teams with INRIA: the team "Molecular and multiscale simulations" hosts the INRIA Rocquencourt project-team MICMAC (leader: C. Le Bris), and the team "Applied Probability" hosts the UPEMLV-INRIA Rocquencourt project-team MATHFI (leader: A. Sulem).

QUALITATIVE RESULTS

KEY FACTS

Staff changes, missions, visits

A. Alfonsi was recruited in the "Applied Probability" team, after completing his post doctoral fellowship at the Technical University of Berlin (supervised by A. Schied). X. Blanc (University Pierre & Marie Curie (Paris VI) and I. Dabo (post-doctorate) joined the INRIA project-team MICMAC (respectively via "délégation" and "détachement" procedures) for one year. The INRIA project-team "CAIMAN" was closed in July. It is partly followed by the new project-team Nachos, a joint INRIA and Nice-Sophia Antipolis University team, hosting the research of N. Glinsky-Olivier.

The scientific department "Environment and Sustainable Development" of CNRS, together with the departments "Mathematics, Physics, Planet and Universe", "Social and Human Sciences", have officially launched an interdisciplinary network "Mathematics and decision for sustainable development" with biologists, economists and mathematicians, headed by M. De Lara.
J.-F. Delmas took the leadership of the group MAS (Modélisation Aléatoire et Statistique) on random models and statistics. The group MAS is one of the four thematic groups of the French society in applied mathematics SMAI (Société de Mathématiques Appliquées & Industrielles). Serge Piperno was elected as a member of the board of SMAI and took over the role of general secretary.
A. Ern is the current Director of the GDR MOMAS, 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. As such, A. Ern reported on the advances in this national programme in front of the National Advisory Committee to the Parliament (CNE) on radioactive waste management issues in October.

Professor K. Yasutomi from Ritsumeikan University in Kyoto (Japan) has joined the "Applied Probability" team for a sabbatical year (starting in September). He is interested in random numbers generation and mathematical finance. I. Mozolevski (Mathematics Department, Federal University of Santa Catarina, Brazil) has visited the "Fluid Dynamics" team for four months in 2007 in the framework of the Invited Professor scheme funded by École des ponts. He has taught in the Scientific Computing course at École des ponts.

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). More, above seventy presentations in conferences have been made. Finally, the book "Introduction to Stochastic Calculus Applied to Finance" by D. Lamberton and B. Lapeyre has been reedited.
Let us finally mention that Julien Guyon, a former student of the "Applied Probability" team, was awarded the 2006 best École des ponts PhD thesis.

Industrial impact

The activities of industrial transfer in the laboratory are strongly linked to research activities. Scientific results are partly obtained in collaboration with Research and Development Departments of large industrial firms through research contracts (Alcan, Calyon, CEA, EDF, ONERA, IFP, 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 remained very high in 2007, not far from 540k€ for École des ponts (120 k€ *via* INRIA). In addition, the research and teaching chair "Measure of financial risks" involving the École Polytechnique, the École des ponts and the Société Générale has been signed in early 2007.

RESEARCH TEAMS

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

1. Applied probability

(A. Alfonsi, M. Ben Alaya, N. Bouleau, J.-F. Delmas, J. Foki, B. Jourdain, B. Lapeyre, J. Lelong, R. Roux, M. Sbai, S. Scotti, K. Yasutomi; associate researchers: V. Bally, M.-C. Kammerer-Quenez, D. Lamberton, A. Sulem; external collaborators: A. Abbas-Turki, A. Kebaier, A. Zanette)

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

1.1. Mathematical finance

As far as mathematical finance is concerned, the team is involved in the research and teaching chair "Measure of financial risks" with the École Polytechnique and the Société Générale. It is also part of the Mathfi project together with researchers from the University Paris-Est Marne-la-Vallée and INRIA. A specificity of this project is the development of a pricing, hedging and calibration library of numerical routines called PREMIA with the financial support of a consortium of banks (Société Générale, Calyon, Natixis, CDC, etc). This is done with the contribution of A. Zanette, J. Lelong and A. Kebaier. The version V9 has been released in February 2007. The new contributions to the next version developed since include pricing algorithms for inflation-indexed options, CDOs (collateralized debt obligations) and squared CDOs, a pricing and calibration algorithm for a jump-diffusion LIBOR interest rates model, implementation of recent algorithms devoted to options written on equity particularly in high-dimensional settings or in the presence of jumps.
During his post-doctoral fellowship at TU Berlin, A. Alfonsi went on working in the continuation of his PhD thesis on the discretization of the CIR (Cox-Ingersoll-Ross) model and the Call-Put duality for American options. He also initiated collaboration with A. Schied and his team on the modelling of the liquidity risk in financial markets, which is a new hot topic in mathematical finance. Also, Peter Bank (now scientific leader of the Quantitative Products Laboratory, TU Berlin, visited the team in the framework of the X-École des ponts - SG chair "Measure of financial risks".
Julien Guyon, a former student of the team now working at the Société Générale got the 2006 PhD prize from the École des ponts foundation, which rewards the best PhD defended at École des ponts. J. Lelong defended his PhD entitled "Stochastic algorithms and Parisian options". As a one year post-doctoral fellow at INRIA Rocquencourt, he continues his collaboration with the team. A. Kebaier works two days per week at CERMICS. He was ATER at University Paris-Dauphine before being appointed assistant professor at the University of Villetaneuse in September. Finally, the thesis of S. Scotti on error calculus in finance is in progress.

1.2. Monte Carlo methods

The research in Monte Carlo methods is structured by the ANR programme ADAPtive Monte Carlo. This permits very interesting discussions with the statisticians from the ENST, École Polytechnique, INRIA and University Paris-Dauphine. During his one year post-doctorate financed by this programme, P. Etoré has developed with B. Jourdain an algorithm aimed at adaptively estimating the optimal allocation of the drawings between the strata when computing the stratified Monte Carlo estimator of an expectation of interest. With G. Fort and E. Moulines (ENST), they are currently trying to develop a stochastic algorithm able to optimize dynamically the boundaries between the strata when these boundaries are hyperplanes orthogonal to a given direction. In June, the team took part in the workshop "New directions in Monte Carlo methods" where interesting scientific contacts were made. In view of financial applications, Monte Carlo methods are coupled with time discretization schemes for the Stochastic Differential Equations governing the evolution of the asset prices. In this domain, A. Alfonsi has proposed a new discretization scheme for the CIR process which is still feasible and efficient for large volatility parameters. And the thesis of M. Sbai is in progress under the supervision of B. Jourdain. They have adapted exact simulation schemes recently developed for one-dimensional SDEs to the pricing of arithmetic average Asian options in

the Black-Scholes model.
B. Lapeyre is also the head of the ANR programme GRID (calculus grids in finance) devoted to financial computations distributed on large computer networks which also implies researchers from the CERTIS.
Applications of Monte Carlo methods in physics and chemistry are still investigated. J.-F. Delmas and B. Jourdain have refined their analysis of the waste recycling Monte Carlo algorithm proposed by physicists to improve the efficiency of the Metropolis Hastings algorithm. The collaboration of B. Jourdain with the "Molecular and multiscale simulations" team goes on with the beginning of the thesis of R. Roux who is co-advised by T. Lelièvre. This thesis is dedicated to mathematical analysis of the Adaptive Biasing Force algorithm which is used for free energy computations in molecular dynamics. Since September 2007, possible collaborations are investigated between the "Applied Probability" and the "Optimization and Systems" teams with a series of talks given by researchers from both teams.

1.3. Biology

Concerning biology, in the programme PILE, J. Foki carries on his PhD thesis on detection of language for babies in collaboration with the Necker hospital and the University of Orléans.
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. J.-F. Delmas also participates to the ANR MAEV (Modèles Aléatoires de l'Evolution et du Vivant) on random models for population evolution, random trees and coalescents.

1.4. Nonlinear PDEs

Last, in the domain of probabilistic interpretation of nonlinear PDEs, J.-F. Delmas works with R. Abraham on fragmentation and branching models. In December, J.-F. Delmas visited Academia Sinica (Taipei). B. Jourdain collaborates with S. Méléard and W. Woyczynsky on nonlinear stochastic differential equations driven by Levy processes and related particle discretizations.

2. Fluid dynamics

(M. Benjemaa, A. Bouquet, D. Di Pietro, A. Ern, N. Glinsky-Olivier, S. Meunier, S. Piperno, A. F. Stephansen, P. Sochala; associate researchers: V. Dolean, L. Fezoui, S. Lanteri, F. Rapetti; external collaborators: E. Burman, C. Dedeban, J. Virieux)

The "Fluid Dynamics" 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. Until July 2007, it hosted a part of the project-team "Caiman", joint with INRIA, CNRS and the Nice-Sophia Antipolis University (NSAU), through the Dieudonné Laboratory. The project-team Caiman, which closed in July, aimed at proposing new, efficient solutions for the numerical simulation of physical phenomena related to wave propagation (electromagnetism, acoustics, aero-acoustics, seismics, etc.). The activity of N. Glinsky-Olivier will be hosted by INRIA project-team Nachos in the future. Both PhD students advised by S. Piperno, M. Benjemaa and A. Bouquet, defended their thesis respectively in November and December. Other changes in team members during 2007 are as follows: D. Di Pietro completed his post-doctoral research project in April and joined IFP as a permanent staff member, S. Meunier defended his PhD thesis in November and joined EDF as a permanent staff member, and A. Stephansen defended her PhD thesis in December and joined the University of Bergen as a post-doctoral fellow. P. Tassi started his post-doctoral project in May and D. Doyen started his PhD in October. Professor I. Mozolevski (Mathematics Department, Federal University of Santa Catarina, Brazil) was hosted by the team for four months (February to May) in the framework of the Invited Professor scheme funded by École des ponts.

2.1. Discontinuous Galerkin (DG) and Finite Element Methods

The research on DG methods has been pursued along several directions. Following up the unified analysis of DG methods for Friedrichs' systems derived by A. Ern and J.-L. Guermond since 2005, D. Di Pietro has dealt with DG methods to approximate advection-diffusion problems with anisotropies (tensor-valued diffusivity) and singularities due to semi-definiteness of the diffusivity. After completing the mathematical and numerical analysis, D. Di Pietro set on to

develop a wide-scope DG-C++ platform able to handle diffusion problems in a broad context of applications. This software has served as a basis for the implementation of A. Stephansen's work and P. Tassi's work described below. In a spirit close to the work of D. Di Pietro, A. Stephansen has proposed and analyzed a weighted interior penalty DG method (the SWIP method) able to handle heterogeneous and anisotropic diffusion satisfactorily. The key idea is to use diffusion-dependent weights to formulate the consistency terms in the DG method, whereby the penalty parameter correctly scales as the harmonic means of normal diffusivity at mesh interfaces. Furthermore, in a joint work with E. Burman and B. Stamm (EPFL), A. Ern and I. Mozolevski have shown that the Symmetric DG method does not need stabilization in 1D for polynomials orders larger than or equal to 2. This striking fact results from the construction of a suitable interpolation of the jumps of a discrete function by means of normal derivatives at interfaces; the problem is still open in 2D. Finally, A. Ern, jointly with S. Nicaise (University of Valenciennes) and M. Vohralik (University Pierre & Marie Curie - Paris VI), have shown that it is possible to construct an accurate diffusive flux in the Raviart-Thomas-Nédélec finite element spaces for DG methods applied to elliptic problems.

2.2. Wave propagation problems

Other investigations of Discontinuous Galerkin finite element methods concern 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 refined grids...). The methods we consider are mainly developed for problems solved in the time domain with explicit (or quasi explicit, or locally implicit) time-schemes. Current applications relate to heterogeneous electromagnetism, acoustics and geophysics. Concerning electromagnetism, wave propagation problems often involve objects of very different scales. We have studied, in collaboration with France Télécom R&D, discontinuous Galerkin time domain methods for the numerical simulation of the 3D Maxwell equations on locally refined, possibly non-conforming structured meshes. The DGTD method developed on block-Cartesian grids by N. Canouet (École des ponts 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. An UPML (Unsplit Perfectly Matched Layer) region as been used to bound the computational domain. The possibility to couple DGTD methods with the fictitious domain approach has been investigated and lead to promising results on spiral antennas of mobile phones. However, further works are required to understand how to enforce a second condition on the magnetic field (which is made necessary by the non-conformity of DG approach in Hrot). 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 algorithms with local time stepping. Totally explicit algorithms have been built for two-dimensional acoustic problems, as well as locally implicit time-schemes. Although the proposed algorithm performs very well on typical 2D triangular meshes (like those produced by an automatic mesh generator around objects with small details), some instabilities may appear. A theoretical study is still open (the result was not obtained, although numerical evidence has been provided that some overlapping in CFL condition is required). Finally, DGTD-FVTD methods have been used (PhD thesis of M. Benjemaa, in collaboration with INRIA and GéoSciences Azur Unit) for the dynamic fault modelling 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). Another prototype two-dimensional software for the time-domain solution of elastodynamics with local time stepping and hp-adaptivity has been developed.

2.3. *A posteriori* error analysis and adaptive modeling

The research in this field is pursued along three directions. The main application in view in A. F. Stephansen's PhD thesis (supported by ANDRA) is the transport of radionucleides leaking from radioactive waste storage in deep geological layers. A. F. Stephansen has analyzed two a posteriori error estimates for the SWIP DG method (see above), a first one based on residual-type a posteriori error analysis which generalizes previous work on DG methods to properly handle diffusion heterogeneities, and a second one, jointly with M. Vohralik, based on flux reconstruction, which leads to even improved results. The robustness of the estimators with respect to diffusion heterogeneities and anisotropies and with respect to dominant advection has been addressed. Furthermore, all the derived estimators contain only explicitly computable constants and can thus be used for actual error control. A. F. Stephansen has implemented all the estimators in the DG-C++ platform originally developed by D. Di Pietro and has shown that the estimators can be used to generate adaptive meshes in problems exhibiting strong diffusion contrasts or strong advection. The PhD thesis of S. Meunier (supported by EDF) is concerned with the a posteriori error analysis of Euler-Galerkin approximations of poroelasticity problems. S. Meunier has derived error estimators for the pressure and the displacement, both with optimal convergence orders, and implemented them in EDF's industrial platform Code_Aster. Finally, A. Ern, in collaboration with T. Lelièvre (CERMICS), M. Braack (University of Kiel) and S. Perotto (Politecnico di Milano), has investigated adaptive modelling 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 modelling and discretization errors by solely using information retrieved from the discrete solution. 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).

2.4. Hydraulics and hydrology

The software development of a Discontinuous Galerkin based two-dimensional shallow water equations solver started in 2005 within collaboration with CETMEF has been continued in two ways. First, a Fortran77 implementation provided a robust and thoroughly-assessed tool, handling variable bathymetry, flooding and drying algorithms, and friction terms. Numerical and theoretical investigations of limiters and innovative algorithms for flooding and drying are under way. This software has been delivered to CETMEF for further extensive testing and comparison with other available software/methods. At the same time, the DG-C++ platform initiated by D. Di Pietro was extended by P. Tassi to handle the same equations. Further comparisons between the two codes are scheduled. Other directions of interest concern, in collaboration with IFP, the numerical computation of steady-state solutions for complex bathymetries and boundary conditions. Furthermore, P. Sochala has pursued his PhD thesis (currently in his third year) by developing and assessing DG-based algorithms to solve the Richards equation in unsaturated porous media. Additional numerical algorithms (in particular oscillation limiters) have been added to deal with advancing, sharp saturation fronts in challenging test cases reported in the literature. The remaining goal to achieve is the coupling of the Richards equation to surface flow propagation conditions. A contact has been initiated with the Research Unit "Hydrosystèmes et Bioprocédés" at CEMAGREF in Antony (B. Augeard, C. Kao, Y. Nédélec) to define relevant test cases.

2.5. Modelling and simulation of cohesive fracture propagation

Collaboration with EDF has been started with the PhD thesis of D. Doyen (advised by A. Ern and S. Piperno). The first steps taken concern the implementation of existing algorithms for the solution of the nonlinear problem deriving from elastostatic equations coupled with a cohesive zone model set on a geometrically prescribed fracture in a material. The nonlinear system of equations for the local displacement jumps is solved separately, following the framework of the LATIN algorithm proposed by P. Ladeveze for contact problems. It appears that this algorithm can be viewed as an augmented Lagrangian method, and conditions should be derived at the continuous level to prove well-posedness of the problem and convergence of the iterative solution procedure. At the discrete level, discrete inf-sup conditions are also investigated to prove convergence of the XFEM approach considered.

2.6. Discrete element methods for complex material dynamics

Collaboration with CEA has been started with the one-year training period of L. Monasse at

CEA. Discrete Elements Methods (DEM) have found a large field of application in granular materials, soil and rock mechanics. The handling of a set of particles interacting by means of forces and torques can lead to a wide variety of macroscopic models for the material at hand, depending on the different small-scale models chosen for the interaction forces and torques. L. Monasse, in collaboration with C. Mariotti (CEA) is working on establishing theoretical bases for and improving the models and algorithms developed in the software Mka3D, under the supervision of É. Cancès, F. Legoll (UR Navier (LAMI), École des ponts), T. Lelièvre and S. Piperno. Among several contributions, forces and torques have been slightly modified such that they derive from a discrete potential energy, reflecting the Hamiltonian structure of the continuum equations onto the discretized model. This Hamiltonian structure at the discrete level is preserved in time by using a symplectic algorithm (second-order Velocity-Verlet for translations and RATTLE for rotations). Good preservation of energy over long-time simulations has been assessed on simple but fully three-dimensional configurations.

3. Molecular & multiscale simulations

(A. Anantharaman, X. Blanc, G. Bencteux, S. Boyaval, É. Cancès, I. Dabo, A. Deleurence, M. El Makrini, H. Galicher, A. Gloria, C. Le Bris, T. Lelièvre, C. Mangoubi, K. Minoukadeh, M. Rousset, G. Stoltz, J. Saur; associate researchers: X. Blanc, F. Legoll, G. Turinici ; external collaborators : 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, and magnetohydrodynamics.

3.1. Electronic structure calculations

In computational quantum chemistry as in most of our scientific endeavors, we pursue a twofold goal: placing the models on a sound mathematical grounding, and improving the numerical approaches.

On the theoretical front, É. Cancès and G. Stoltz, in collaboration with E. Davidson (Washington State University), G. Scuseria (Rice University) and V. Staroverov (University of Western Ontario), have studied the mathematical foundations of some systematic constructions of local exchange potentials in density functional theory, including the Slater potential, the optimized effective potential (OEP), the Krieger-Li-Iafrate (KLI) approximation and the common-energy denominator approximation (CEDA) to the OEP, and the effective local potential (ELP). In particular, they showed how to reformulate these constructions in terms of variational problems, and they provided a rigorous derivation of the so-called OEP integral equation. They have also established an existence result for a coupled system of nonlinear partial differential equations, introduced by Slater to approximate the Hartree-Fock equations.

É. Cancès and A. Deleurence have addressed issues related to the modelling and simulation of local defects in periodic crystals. Computing the energies of local defects in crystals is a major issue in quantum chemistry, materials science and nano-electronics. Although several approaches have been proposed, a mathematically consistent quantum model for crystalline materials with local defects is still missing. In collaboration with Mathieu Lewin (CNRS, Cergy), É. Cancès and A. Deleurence have

proposed a new model based on formal analogies between the Fermi sea of a perturbed crystal and the Dirac sea in Quantum Electrodynamics (QED) in the presence of an external electrostatic field. Using and adapting recent mathematical tools used in QED, they suggest 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 thermodynamic limit on the so-called supercell model. They have also introduced a variational method for computing the perturbation in a basis of precomputed maximally localized Wannier functions of the reference perfect crystal. Some preliminary, promising numerical results have been obtained on a one-dimensional nonlinear model with Yukawa interaction potential.

On the numerical front, in collaboration with W. Hager (University of Florida), the domain decomposition approach, designed by M. Barrault (now at EDF), G. Bencteux, É. Cancès, and C. Le Bris for electronic structure calculations has been improved. The development of the domain decomposition algorithm for the linear subproblem has been continued. Some algorithmic improvements of the most time consuming part of the algorithm have resulted in a significant decrease in memory and CPU demands (up to a factor 10 for alkane molecules). A parallel implementation on the Blue Gene computer has allowed solving the linear subproblem for a polyethylene chain of 5 million atoms (17.5 million basis functions) in about 60 minutes on 1024 processors. The performance of the parallel version confirms that a high scalability will be reached with an additional implementation effort: this will be part of the collaboration with EDF in the frame of the project ParMat, financially supported by the ANR (National Research Agency). From a numerical analysis viewpoint, the convergence properties of the MDD algorithm have been studied, and the convergence established in a simplified setting.

3.2. Molecular dynamics and numerical statistical physics

The extremely broad field of Molecular dynamics is a field where the MICMAC project, originally more involved in the quantum chemistry side, has invested a lot of efforts in the recent years. These efforts both deal with the deterministic techniques and the probabilistic techniques used in the field.

Molecular dynamics is often employed 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 averaged long time limits of integrals calculated along a 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 and F. Legoll have initiated a study along this aim. Some results have been obtained for the integration of a class of highly oscillating Hamiltonian systems. The authors should follow up on this 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 [École des ponts – UR Navier (LAMI)] and P. Plechac (Warwick University).
In addition to the difficulty arising from the highly oscillatory character of the dynamics addressed so far, a second difficulty arises from the extremely long time frame over which the system needs to be simulated. 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. É. Cancès, A. Deleurence and F. Legoll are currently studying several methods to coarse-grain the system, in order to develop a model better suited to long time simulation.

Stochastic dynamics to compute free energy differences are widely used in computational chemistry and biology. These free energy differences can be computed using the Jarzynski equality, which can be extended to account for transitions between two submanifolds of the state space. In some cases, path sampling techniques can be used to this end, and some new algorithms to sample paths have been proposed. However, many recent methods rely on nonlinear Markov processes, like the adaptive techniques. A unifying presentation of adaptive methods has been 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 convergence result for this nonlinear dynamics has also been proved in some limiting regime, using entropy methods and a decomposition of the total entropy of the system into a microscopic part (associated with conditioned measures) and a macroscopic part (related to some global features of the system).
A related problem is the following. Molecular systems are composed of a large number of atoms. Hence, describing the state of a molecular system requires in principle a lot of degrees of freedom. However, in practice, only a few of them, the so called reaction coordinates, are actually relevant (for they describe the change of conformations, or metastable states). The statistics of these reaction coordinates is described by the free energy. T. Lelièvre is currently working with F. Legoll on how to define a closed dynamics on these reaction coordinates. The problem hence amounts to reducing the dimension of a set of SDEs, from the full set of degrees of freedom to only a few of them. Promising results have been obtained.

In addition to the above, R. Roux has started his PhD work under the supervision of B. Jourdain and T. Lelièvre on particle methods in molecular dynamics. He is currently working on the convergence of a discretization of the Adaptive Biasing Force method based on a particle method.

3.3. Atom-continuum model for electrified metal-solution interfaces

Modeling the electrical response of fuel cells at the molecular level represents a persistent challenge characterized by length scales that are orders of magnitude greater than the sizes accessible to quantum chemistry simulations. In order to overcome this limitation, a comprehensive atom-continuum model has been developed, based on a quantum molecular description of the interfacial region with a polarizable-continuum representation of the electrolyte. This approach has been applied to interpret electrochemical spectroscopy experiments. As part of the post-doc scientific programme of I. Dabo, this atom-continuum model will be complemented, by incorporating pressure, surface-tension, and acidity effects.

3.4. 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 (Mines ParisTech), H. Rabitz and G. Turinici (University of Paris Dauphine), and also in close connection with P. Rouchon, Mines ParisTech), 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.

3.5. Atomistic to continuum methods

A. Gloria has addressed with R. Alicandro (University of Cassino, Italy) and M. Cicalese (University of Naples, Italy) the variational derivation of a continuum energy starting from a discrete system of spins in interaction. This work is available as a CVGMT preprint and has been submitted for publication.

Besides, they have begun to address the derivation of rubber elasticity models from a discrete system of points in interaction, the system being described by a stochastic lattice, as introduced by X. Blanc, C. Le Bris and P.-L. Lions. An article is in preparation. As an application, it has allowed to prove the asymptotic convergence of a finite element modelling of rubber introduced by Böl and Reese.

In collaboration with P.-L. Lions (Collège de France), X. Blanc and C. Le Bris have continued to address the question of passing from the microscopic scale to the macroscopic scale. A study on the passage to continuum for stochastic lattices and the relation of this question with homogenization

theory has been published.

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, X. Blanc, F. Legoll and C. Patz (Berlin University).

3.6. Homogenization

A. Gloria has continued his work on numerical homogenization methods, addressing now the analysis of oversampling methods in the context of elliptic operators and nonlinear elasticity.
The adopted approach consists in introducing an averaged energy that describes the effective behavior of heterogeneous materials and analyze its convergence properties in terms of Gamma-convergence. The analysis of oversampling methods has been completed and some numerical tests, performed with FreeFEM++, have complemented the analysis.

Besides, A. Gloria has followed up on the work by X. Blanc, C. Le Bris and P.-L. Lions on a variant of stochastic homogenization for the case of multiple integrals in the INRIA research report RR-6316. The work is submitted for publication. The work by A. Braides (University of Rome) and A. Gloria on a problem of G-closure for a discrete polycrystal has been accepted for publication.

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

3.7. Free surface flow and magneto-hydrodynamics

In collaboration with J.-F. Gerbeau (INRIA, REO team), and in association with Alcan (formerly Aluminium Péchiney), C. Le Bris and T. Lelièvre have pursued their efforts for the numerical simulation of electrolytic cells for the industrial production of aluminum. In addition, J.-F. Gerbeau and T. Lelièvre are currently working on the stability of numerical schemes for free surface flows. The focus of this research if how to implement forces such as gravity and surface tension in Arbitrary Lagrangian Euler schemes, in such a way that the energy conservation laws holding at the continuous level are also satisfied at the discrete level.

3.8. Fluid Structure Interactions

With M. Fernandez, J.-F. Gerbeau (project-team REO), M. Vidrascu (project-team MACS), A. Gloria has introduced an alternative method to solve numerically fluid-structure interaction problems using domain decomposition algorithms and the three-dimensional shell elements developed by the project-team MACS. A preliminary version has been published. More extensive numerical tests are in progress.

3.9. Complex fluids

The subject of this activity covers two different applications and settings. The first one is the modelling of polymeric fluid flows; the second is that of suspensions.

In the first context, A. Ern and T. Lelièvre have proposed a coupled micro-macro and macro-macro numerical scheme to efficiently discretize micro-macro models for polymeric flows. The idea is to use the fine but expensive (micro-macro) model only where it is really needed, in order to reduce the computational cost. This is based on a posteriori error estimates. D. Hu and T. Lelièvre have shown how new "entropy-like" estimates can be derived for macro-macro models for viscoelastic fluids. These estimates can be used as a guideline to enhance the stability of numerical schemes, building discretization schemes that satisfy these new estimates. C. Le Bris and T. Lelièvre have written a long and didactic review of micro-macro models for complex fluids, and polymeric fluids. The paper is a rather elementary and pedagogical introduction to such models. A dedicated, final section addresses the mathematical challenges on the front of research.

In collaboration with P. Coussot (LCPC), F. Lequeux (ESPCI), I. Catto (University Paris Dauphine), another topic has started that focuses on highly non Newtonian fluids. E. Cancès, S. Boyaval and C. Le Bris are going to perform numerical simulations of new constitutive equations for viscoelastic fluids subject to thixotropic effects. This has motivated S. Boyaval, T. Lelièvre and C. Mangoubi to work on well-known numerical

stability issues related to the simulation of macroscopic constitutive equations for viscoelastic fluids. The study shows how some discretizations of the Oldroyd-B model allow for the correct free energy dissipation. Computations are being performed that take into account the results of the previous study.

Besides, a new topic is starting in collaboration with Y. Maday (UPMC-Brown) and A.T. Patera (MIT). C. Le Bris and S. Boyaval are developing new computational methods to solve high-dimensional Fokker-Planck equations parameterized by transient macroscopic quantities. The approach follows the Reduced Basis paradigm. Several variants are under study. Some of them deal with the Fokker-Planck equation itself. Some others consist in approaching the stochastic differential equation associated with the Fokker-Planck equation.

The above much applied topics, related to the modelling of complex fluids, have motivated a series of theoretical works by C. Le Bris and P.-L. Lions on the well-posedness of the mathematical equations manipulated in the modelling. Indeed, as the flow velocities in such non Newtonian flows have no particular reason to be regular, the fact that such velocities impact as parameters on the kinetic description of the microstructures motivates 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 are pursuing a series of studies on Fokker-Planck type equations, and stochastic differential equations with Sobolev regular coefficients. Interestingly, the context of complex fluids, and the lack of regularity of the coefficients in the equations in that context, have also triggered a new series of works on the renormalized solutions of ordinary differential equations.

3.10. 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. After investigating various aspects of the multiscale simulation of shock waves, G. Stoltz turned to the case of detonation. He extended a previous model based on dissipative particle dynamics and describing shock waves at the microscopic level to the case of shock waves triggering chemical reactions as they move along.

4. Optimization and systems

(J.-P. Chancelier, G. Cohen, M. De Lara, E. Lioris, B. Seck ; external collaborators: L. Andrieu, P. Carpentier)

4.1. Numerical methods in stochastic control

A. Dallagi defended his thesis in January and one of the main conclusions of this work has been that the technology of scenario trees is a rather poor tool to provide solutions of stochastic optimal control problems in terms of feedbacks. New methods (called particle methods) have been proposed in this work which proved to perform much better as revealed by numerical experiments. The results have been presented at EURO XXII in Prag last July. They were also part of the 12 hour course given by G. Cohen at the University of Melbourne, Australia, in March-April 2007 during a one month visit.

In order to explain the weakness of the scenario tree approach, we have attempted to obtain theoretical results about the convergence rate of the approximation provided by the scenario tree approach towards the exact feedback solution, as a function of the Monte Carlo sample size. This was only possible in very simple cases, but the results are already interesting in that they reveal the dramatic effect of the horizon length of the optimal control problem over this convergence rate. Those new results have been presented at SPXI in Vienna last August (G. Cohen was a member of the scientific committee of this triennial meeting of the worldwide Stochastic Programming community and he organized an invited session).

For the comparison between stochastic tree and particle approaches to be complete, the corresponding convergence rate results should also be provided for the latter approach: this is one of the objectives of P. Girardeau's starting thesis (CIFRE contract with EDF).

4.2. Systems of collective taxis

In the last year report, the beginning of a new project was announced (E. Lioris's thesis co-funded by the IMARA project of INRIA). The topic is the simulation and evaluation of

systems of collective taxis. After the first year of this project, a complete analysis of the mechanical part of the simulation (the one which describes the system dynamics: making taxis and customers meet and move in the network) is completed and analyzed as a collection of elementary events coordinated by an event stack which makes time evolve by jumping from one event to the next. This part is coded in an object-oriented language (Python). Once this mechanical part is available, we will concentrate on the various decision making algorithms which are required to operate the system in real time and react to random events. That part is the one where optimization of various trade-offs between conflicting objectives must be handled, with service quality and operation cost considerations in mind. The simulation tool will then be intensively used to tune the various parameters involved. This technology can then be used in case studies in order to grasp and delineate the range of application of such transportation systems in cities or suburban areas. A first account of this project was given at a conference in Lisbon (Portugal) in September.

4.3. THALES-CNES Contract

By the end of the year, a new cooperation has been initiated with Thales and CNES. The framework is the planning of spatial missions in order to achieve interplanetary rendez-vous. Until now, such plannings were achieved in a deterministic setting by optimizing an objective function (minimal time, minimal fuel consumption, etc.). However, various failures (e.g. momentary stops of the vessel engine) cause deviations from the ideal trajectory which may preclude the final achievement of the rendez-vous. Therefore, it may be safer to give up with optimal performance by modifying the planned trajectory in order to increase the chance of achieving the rendez-vous despite some failures occurring during the mission. The purpose of the study is thus to devise a mathematical tool which would help quantifying the trade-off of robustness vs. performance. The formulation will be based upon stochastic optimization under constraint inprobability.

4.4. Scientific computing software

J.-P. Chancelier has participated to the group animated by the Chairman of Scilab Consortium scientific board. The aim was to clarify the specification of a language for scientific computing and to evaluate the Nsp software developed at École des ponts according to the proposed specifications. The conclusions of the group were presented at the Scilab steering committee in September. In spite of our efforts, it has lead to a clear separation between the Scilab consortium project and the Nsp project.

Nsp has evolved during the present year in many aspects. As an important point, we should cite that Sedumi and SDPT3 (Matlab toolbox used in order to solve optimization over symmetric cones) are now available as Nsp contributions. Improvements in cells and sparse implementations, mexlib emulation and semantic changes in matrix functions, especially nx0 empty matrices, were hardly necessary to achieve this goal. We can also cite a rewriting and improvements in random number sample generations (B. Pinçon) and a native Windows version which should be online in January 2008. Other toolboxes like ipopt (Optimization), cholmod (Cholevsky decomposition for sparse matrices) etc., are also available. Collaboration with the Premia project was carried on to provide a better GUI for Premia in Nsp (J. Lelong).

4.5. Mathematical methods for sustainable management of renewable resources and biodiversity

This theme is driven by M. De Lara, in cooperation with different institutions and researchers.
The main activity in 2007 has been the scientific animation of the network MIFIMA (Mathematics, Informatics and Fisheries Management), a Stic-AmSud project launched in 2006 between Chile, France and Peru. A meeting took place in Chile in January, and a second one in Peru in October. M. De Lara also gave lessons at the Universidad Del Pacifico en Lima. Joint works with Chilean and Peruvian researchers focus on estimation and qualitative properties for viability domains in sustainable management models.
The scientific department Environment and Sustainable Development of CNRS, together with the departments Mathematics, Physics, Planet and Universe, Social and Human Sciences, have officially launched an interdisciplinary network "Mathematics and decision for sustainable development" with biologists, economists and mathematicians, headed by M. De Lara.

5. PDE and materials

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

The PDE and Materials team is interested in the modelling of the physics of materials, and in the theoretical and numerical analysis of these models and their simulations. At the present time, the 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 of the macroscopic plastic behavior of metals, and the understanding of plasticity at a microscopic level is one of the main motivations in this direction of research.

The activity of the team has been developed as a part of a contract ACI "jeunes chercheuses et jeunes chercheurs" of the French Ministry of Research (2003-2007), called "Modelling and mathematical analysis of dislocation dynamics". The team collaborates in particular with the laboratory of the study of microstructure LEM at the ONERA. This part of our activity mainly focuses on the complicated dynamics of interacting dislocations lines. Also, this team is part of an ANR MICA project (2006-2009, coordinator: A. Chambolle) in collaboration with three other teams (CMAP, Tours Univ. and Brest Univ.). This financial support will help substantially our team to develop our research in the following years and allow some new interactions. Finally, the team also got a grant from the Galileo project to develop our collaborations with the Italian group of M. Falcone (Univ. "La Sapienza") on some generalizations of the Fast Marching Method, with applications to dislocations dynamics.
Research was also extended 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 Paris-Est Marne-la-Vallée. In this framework, let us cite the PhD thesis of A. El Hajj, co-directed with M. Cannone. On the other hand, H. Ibrahim (PhD student, 3rd year) studies dislocations density models with scale effects. He is co-directed by M. Jazar (University of Beyrouth).

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). As another illustration of such problems, we are also working with A. Briani on the homogenization of the behavior of a material under cyclic loading.

This year has been rich in activities. We have had three PhD and one HDR defended in the team. A. Ghorbel defended his PhD in January, entitled "Numerical analysis of dislocations dynamics and applications to homogenization". His main result is an error estimate for a scheme describing the dynamics of dislocations particles in interactions. He also got some nice simulations which are a striking illustration of recent non-linear homogenization results for dislocations dynamics. A. El Hajj defended his PhD in December, entitled "Theoretical and numerical analysis of the dynamics of dislocations densities". One of his major contributions is a result of long time existence of solutions to a two-dimensional non-local transport model of Groma-Balogh describing the motion of dislocations densities. His second main contribution is a result of existence of solutions to a certain class of hyperbolic systems which is not included in the recent theory of Bianchini-Bressan. N. Forcadel obtained his PhD in July, entitled "Contribution to the analysis of partial differential equations describing the motion of fronts with applications to the dynamics of dislocations". His major contributions are the discovery of the link between dislocation dynamics and mean curvature motion and as a consequence some error estimates for a numerical scheme for mean curvature motion, the proposition of a generalized Fast Marching method for the eikonal equation with general velocity, which he has proven to be convergent, the existence of a solution to dislocations dynamics with mean curvature terms with an Almgren-Taylor Wang approach and a result of homogenization (with C. Imbert and R. Monneau) of dislocations dynamics, which contains in particular the homogenization of particles in interactions.

C. Imbert defended his "Habilitation à diriger les recherches" (HDR) in December. He has been working in our team for three years, with a strong participation both as a researcher and as an adviser for our students. In collaboration with the team, he got several important results on homogenization. His HDR covers a large number of other subjects, in particular in the framework of viscosity solutions and also for entropy solutions to hyperbolic equations.

Several meetings have been also organized. The main meeting that we have organized this year was an autumn school in Paris entitled "Introduction to numerical methods for moving boundaries". There were more than 80 participants and this was a nice opportunity to diffuse our recent numerical methods motivated by dislocations dynamics. In particular N. Forcadel gave a mini-course at this occasion. In the same spirit, and in order to develop our numerical methods, a contract has been obtained this year with the CEA to find a numerical scheme for the transport of interfaces and a working group has been created to work on this subject.

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

TEACHING- SUPERVISING

Teaching is an important activity of CERMICS members, both at École des ponts and other first rank engineering schools (École Polytechique, ENSTA) and in graduate courses (M2R) around Paris. At École des ponts, the members of CERMICS are strongly contributing to the " Applied Mathematics and Computer Science" department, in the first year (A. Ern chairs the First Year Department which supervises the whole course program for the first year studies at École des ponts; members of CERMICS are in charge of lectures on scientific computing, probabilities, analysis) as well as in the second year (Applied (the) mathematics and computer science department key-lecture "MOPSI" (modelling – implementation – simulation), frequency analysis, non-linear analysis, statistics, mathematical finance, etc.). Moreover, a third year in mathematical finance has been set up in collaboration with University Paris-Est Marne-la-Vallée: a third year student at the École des Ponts may obtain in the same time the research master degree from the university by attending a few more courses there. For the academic year 2007-2008, the success of this program is confirmed with twenty registered students from École des ponts.

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 twenty-five PhD students) and post-doctoral studies (six students in 2007).

INTERNATIONAL / NATIONAL 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 École des ponts or Ministère de l'Ecologie du Développement et de l'Aménagement Durable (MEDAD): the "Fluid Dynamics" team with LMSGC (L.

Dormieux) on transport in porous media and on hydraulics and hydrology with CETMEF (Ph. Sergent) and LNHE (M. Benoit). The "Molecular and multiscale simulations" team collaborates with UR Navier (LAMI) (F. Legoll) on time integration algorithms for molecular dynamics and with UR Navier (LMSGC) (Ph. Coussot) on highly non Newtonian 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 "Applied Probability" team, J.-F.Delmas collaborates with R. Abraham (University of Orléans) on fragmentation and branching models, and works 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 team takes part to the ANR programme ADAPtive Monte Carlo, allowing fruitful discussions with the statisticians from the ENST, École Polytechnique, INRIA and the university Dauphine. A. Kebaier works two days per week at CERMICS (formerly ATER at the University Dauphine, now appointed assistant professor at the University of Villetaneuse).
The "Fluid Dynamics" team works with ANDRA on transport in porous media, with EDF on poroelasticy, with IFP on shallow-water flows and on DG methods in general, with University Pierre & Marie Curie Paris VI (M. Vohralik) on a posteriori error estimation and with GéoSciences Azur (J. Virieux) and INRIA (S. Lanteri) on seismics. A. Ern is the current Director of the GDR (Groupement de Recherches) MOMAS, 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.
The "Molecular and multiscale simulations" team collaborates with M. Lewin (CNRS and University of Cergy-Pontoise) on a new model based on formal analogies between the Fermi sea of a perturbed crystal and the Dirac sea in Quantum Electrodynamics for electronic structure calculations, with X. Blanc (J.–L. Lions Laboratory, University Paris 6) and P. -L. Lions (Collège de France) on "atomistic to continuum" models. 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. It also pursued their efforts, in collaboration with J.-F. Gerbeau (INRIA, REO team), and in association with Alcan (formerly Aluminium Péchiney) for the numerical simulation of electrolytic cells for the industrial production of aluminum. With M. Fernandez, J.-F. Gerbeau (project-team REO), M. Vidrascu (project-team MACS), A. Gloria has worked on improved domain decomposition algorithms to solve numerically fluid-structure interaction problems.
The "Optimization and Systems" team collaborates 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. On stochastic optimization and numerical methods in stochastic control, the collaboration with L. Andrieu (EDF) goes on and a new CIFRE PhD thesis with EDF (P. Girardeau) was initiated. The collaboration on risk aversion and road choice with A. De Palma (laboratory Thema, University of Cergy-Pontoise) goes on and now includes numerical aspects (with S. Piperno). On the topic of mathematical methods for sustainable management of renewable resource and biodiversity, an interdisciplinary CNRS network "Mathematics and decision for sustainable development" with biologists, economists and mathematicians, headed by M. De Lara, was launched. Concerning the developments around the NSP Scientific Computing Software, J.-P. Chancelier has participated to the group animated by the Scilab Consortium scientific board, and collaborated with B. Pinçon (ESIAL, Henri Poincaré University Nancy 1) and F. Delebecque, J.–P. Quadrat, R. Nikoukhah (INRIA, Scilab project). M. de Lara represents École des ponts at the Scilab Consortium Board.
The "PDE and materials" team works in collaboration with the laboratory of the study of microstructure at ONERA (the French Aerospace Lab), with partners of a contract ACI "jeunes chercheuses et jeunes chercheurs" of the French Ministry of Research (2003-2007), called "Modelling and mathematical analysis of dislocation dynamics" and of the MICA ANR project (2006-2009) in collaboration with three other teams (CMAP, Tours Univ. and Brest University. In the framework of the "Pluriformations Program" with the University Paris-Est Marne-la-Vallée, the team worked with M. Cannone on dislocations density models in connection with elasto-visco-plasticity of metals.

Concerning international collaborations, the "Applied Probability" team collaborates with A. Schied (Technical University of Berlin), who hosted A. Alfonsi in postdoctoral stay. A. Alfonsi started collaboration with the team of A. Schied (TU Berlin) on the modelling of the

liquidity risk in financial markets, which is a new hot topic in mathematical finance. In December, J.-F. Delmas visited Academia Sinica (Taipei). B. Jourdain collaborates with S. Méléard (University Pierre & Marie - Paris VI) and W. Woyczynsky on nonlinear stochastic differential equations driven by Levy processes and related particle discretizations. 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 "Fluid Dynamics" team has collaboration links with E. Burman (EPFL, Switzerland and University of Sussex, UK), J.-L. Guermond (University of Texas A&M, USA), B. Achchab (University Hassan I, Morocco) and A. Souissi (University Mohammed V, Morocco) on finite element methods, with M. Braack (University of Kiel, Germany) and S. Perotto (Politecnico di Milano, Italy) on adaptive modelling.

The "Molecular and multiscale simulations" team works on the mathematical foundations of some systematic constructions of local exchange potentials in density functional theory in collaboration with E. Davidson (Washington State University), G. Scuseria (Rice University) and V. Staroverov (University of Western Ontario). They improved a domain decomposition approach in collaboration with W. Hager (University of Florida). 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). Concerning laser control of molecular processes, the collaboration with the group of H. Rabitz (Princeton University), M. Mirrahimi and P. Rouchon (Mines ParisTech) and G. Turinici (University of Paris Dauphine) is going on and made possible by a PICS CNRS-NSF grant. Concerning atomistic to continuum methods, A. Gloria worked with R. Alicandro (University of Cassino, Italy) and M. Cicalese (University of Naples, Italy) on the variational derivation of a continuum energy starting from a discrete system of spins in interaction. In close collaboration with A.T. Patera (MIT) and Y. Maday (CNRS/UPMC/Brown), S. Boyaval has tested the feasibility of a reduced-basis approach for multiscale problems. On the modelling of complex fluids, a new collaboration with Y. Maday (UPMC-Brown) and A.T. Patera (MIT) has started on developing new computational methods to solve high-dimensional Fokker-Planck equations parameterized by transient macroscopic quantities. C. Le Bris and P-L. Lions (University of Paris Dauphine) are pursuing a series of studies on related Fokker-Planck type equations, and stochastic differential equations with Sobolev regular coefficients.

The "Optimization and Systems" team cooperates with F. Vazquez–Abad (G. Cohen made a one-month visit at the University of Melbourne, Australia, in March-April). On mathematical methods for sustainable management of renewable resources and biodiversity, the team is in charge of the scientific animation of the network MIFIMA (Mathematics, Informatics and Fisheries Management), a Stic-AmSud project launched in 2006 between Chile, France and Peru. Two meetings took place in Chile and Peru. M. De Lara also gave lessons at the Universidad Del Pacifico en Lima. Joint works with Chilean and Peruvian researchers focus on estimation and qualitative properties for viability domains in sustainable management models.

The "PDE and materials" team got a grant (Galileo project) to develop their collaborations with the Italian group of M. Falcone (Univ. "La Sapienza") on some generalizations of the Fast Marching Method, with applications to dislocations dynamics. Also, H. Ibrahim (PhD student, 3rd year) studies dislocations density models with scale effects. He is co-directed by M. Jazar (University of Beyrouth). Other various collaborations can be mentioned, with the universities of Santiago (Chile) and Tokyo (Japan).

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QUANTITATIVE RESULTS

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Articles in Web of science

Alicandro R., Cicalese M., Gloria A.
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Particle methods in stochastic optimal control, an alternative to Stochastic Programming and Dynamic Programming, 22nd European Conference on Operational Research, July 8-11, 2007, Prag

De Lara M.
- Does information obey the Law of Diminishing Returns? Sensors, support functions and marginal value of information at the null, SMAI Conference on *"l'Optimisation et la Décision",* April 18-20, Paris, France, 2007

- Gittins index heuristic algorithm for open-pit mine scheduling, *VIII Seminario Internacional de Optimización y Areas Afines*, October 1-5, 2007

Deleurence A.
Modelling of local defects in crystals (poster), IMA Summer Program Classical and Quantum Approaches in Molecular Modelling, July 23rd - August 3rd, 2007, Minneapolis (US)

Ern A.
- Discontinuous Galerkin Methods for Anisotropic and Semi-Definite Diffusion with Advection, VMS Workshop, February 2007 EPFL, Lausanne, Switzerland

- Discontinuous Galerkin Methods for Anisotropic and Semi-Definite Diffusion with Advection, July 2007, ICIAM, Zurich, Switzerland

- *A posteriori* error analysis of Euler-Galerkin approximations to elliptic-parabolic problems, July 2007, RMMM, St Petersburg, Russia

- *A posteriori* error estimates based on flux reconstruction for Discontinuous Galerkin methods, ENUMATH, Graz, Austria, September 2007

Etoré P.

Workshop "New directions in Monte Carlo methods", Fleurance, France, June 25-29th

Forcadel N.

- Workshop "Mathematical models for dislocations", December 2007, Rome
- Workshop "Phase-field models for the evolution of complex structures", June 4-6th, 2007, Paris
- Workshop "Multivariate Approximation: Theory and Applications", April 26th – May 1st 2007, Cancun

Gloria A.

- ICIAM 07 (International Conference in Industrial and Applied Mathematics), July 2007, Zurich
- CMDS 11 (11th International Symposium on Continuum Models and Discrete Systems), July 2007, Paris
- Workshop on Calculus of Variations and Geometric Measure Theory, Levico, February 2007, Italy

Jourdain B.

- Workshop "New directions in Monte Carlo methods", Fleurance, June 25-29: 3h30 invited lecture on Monte Carlo methods for molecular simulation
- Workshop and Mid Term Conference on Advanced Mathematical Methods for Finance, September 18-21th, Vienna

Lapeyre B.

Adaptive Monte Carlo Methods in Finance, Department of mathematics and statistics, Boston University, Boston, April 27th

Le Bris C.

- MIT-France workshop on cement science, 2007, Cambridge (US)
- Workshop ''Numerical Analysis of Multiscale Computations'', January 28th - February 2nd, 200, Banff International Research Station for Mathematical Innovation and Discovery (BIRS)
- Workshop "Multiscale and Variational problems in Material Science and Quantum Theory of Solids", February 11 – 17th, 2007, Oberwolfach
- Workshop "Multiscale Modelling and Simulation of Complex Fluids", April 16-20th, 2007, University of Maryland, College Park
- Workshop 'Multiscale Problems', May 25-26th, 2007, Princeton University
- Workshop-Summer school "Multiscale Modelling", Stockholm, Sweden, June 4-8th, 2007.
- Effective Computational Methods for Highly Oscillatory Problems: The Interplay between Mathematical Theory and Applications, 2-6 July, 2007, Cambridge, UK
- Computational chemistry workshop, July 16-20th 2007, Warwick, UK
- IMA Summer Program, July 2007
- Workshop Mathematical Issues in Complex Fluids, October 15-19th, 2007, Beijing University
- Workshop "Multiscale Analysis for quantum systems and applications", Istituto Nazionale di Alta Matematica, Universita di Roma, October 24-26th, 2007
- Workshop "Nonlinear and Adaptive Approximation in High Dimensions", December 10-15th, 2007, Bad Honnef, Germany

Lelièvre T.

- Workshop New directions in Monte Carlo methods, June 2007, Fleurance
- SciCADE 2007, July 2007, Saint-Malo
- ICIAM07, July 2007, Zurich
- IMA summer programme on Classical and Quantum Approaches in Molecular Modelling, July 2007, Minneapolis
- Workshop Complex fluids, October 2007, Beijing,
- Workshop Particle systems, nonlinear diffusions, and equilibration, November 2007, Bonn

Lioris E., Cohen G., de la Fortelle A.

Evaluation of collective taxi systems by event-driven simulations, International Colloquium on Taxis, September 20-21th, 2007, Lisbon, Portugal

Mozolevski I.

Discontinuous Galerkin method for interface problem of coupling different order elliptic equations, May 2007, EFEF05, Marseille

Seck B., De Lara M., Andrieu L.

Electrical portfolio management under risk constraint, SMAI Conference on "*l'Optimisation et la Décision*", April 18-20th, Paris, France, 2007

Seck B., De Lara M., Andrieu L.
Optimization under risk constraint: an economic interpretation, 22nd European Conference on Operational Research, EURO XXII, July 8-11th, Prag (Czech Republic), 2007

Sochala P.
Approximation of the Richards equation by Discontinuous Galerkin methods, March 2007 SIAM GS, Santa Fe

Stephansen A. F.
A posteriori error analysis of Discontinuous Galerkin schemes for reactive transport in porous media, March 2007, SIAM GS, Santa Fe

Stoltz G.
- (Non) equilibrium computation of free energy differences, February 2007, University of Warwick

- A reduced stochastic model for shock waves, IMA Summer Program Classical and quantum approaches in molecular modelling, July 2007, Minneapolis

National conferences communications

Bencteux G.
Décomposition de domaine pour les calculs de structure électronique, 3e congrès national de mathématiques appliquées et industrielles (SMAI 2007, Praz-sur-Arly), June 2007

Bouleau N.
Finance et calcul stochastique, *Festival des sciences*, May 2007, Chamonix

Bouquet A., Dedeban C., Piperno S.
Méthode de Galerkin Discontinu appliquée à l'analyse de structures planaires, XVèmes Journées Nationales Microondes, May 23-25th, 2007, Toulouse, France

Boyaval S.
SMAI 2007 (annual meeting of the French Society of Applied and Industrial Mathematics), June 2007, Praz-sur-Arly

Delmas J.-F.
- Does waste-recycling really improve Metropolis-Hastings Monte Carlo algorithm? ANR ADAP'MC, June 2007, Fleurance (France)
- Length of coalescing trees, Journées de probabilités, September 2007, Toulon (France)

Ern A.
A posteriori error estimates based on flux reconstruction for Discontinuous Galerkin methods, November 2007, MOMAS National Workshop

Imbert C.
Invited at congress "*Intégralités fonctionnelles et EDP*'', June 2007, Nanterre

Lelièvre T.
Workshop Polymer models and related topics, Nice, February 2007, SMAI 2007, June 2007

Monneau R.
Conference for the birthday of François Murat (60 years), October 2007

Piperno S.
Méthodes de type Galerkine Discontinu pour la propagation d'ondes en domaine temporel, November 2007, general meeting GDR Ondes, (Bordeaux)

Seminars/visits given

Conference/seminar organization

International seminars given

Alfonsi A.
A Call-Put Duality for Perpetual American Options, Forschungsseminar Stochastische Analysis und Stochastik der Finanzmärkte, TU Berlin

Bouleau N.
- On the propagation of small errors, Mittag-Leffler Institute, Stockholm

- The variational Euler equation for the error calculus, international meeting in honor of Prof. Fukushima of Swansea University, October 2007
-

Briani A.
Un primo risultato di omogenizzazione in tempo per densita di dislocazioni, Workshop "Giornate di Lavoro su questioni di teoria geometrica della misura e di Calcolo delle Variazioni'', Levico Terme, Italy, February 4-9th

De Lara M.
- *Métodos de viabilidad para el manejo*

sustentable de pesquerías, January 20th, Workshop IFOP, Valparaiso, Chile

- Gittins index heuristic algorithm for open pit mine scheduling, August 22th, CMM, Santiago de Chile

- *Métodos de viabilidad para el manejo sustentable de pesquerías*, August 24th, Universidad Técnica Federico Santa María, Valparaiso, Chile

Delmas J.-F.
Prunning and immigration for continuous branching process. December 2007, Academic Sinica (Taipei)

Di Pietro D.
Introduzione ai metodi di Galerkin discontinui, March 2007, Bergamo University, Italy

Ern A.
Discontinuous Galerkin methods for Friedrichs' systems, June 2007, ETH Zurich, Switzerland

Gloria A.
October 2007, University of Bonn

Imbert Cyril
Analysis Seminar at University of Texas at Austin, September 2007

Ibrahim H.
- Nonlinear evolution equations and dynamical systems. NEEDS school and workshop, June 2007, Ametlla de Mar, Barcelona, Spain, summer school

- Introduction to dynamical systems and PDEs. JISD 2007, June 2007, Universitat Politècnica de Catalunya, Barcelona, Spain, summer school

Jourdain B.
- *Berliner Kolloquium Wahrscheinlichkeitstheorie,* Long-time behavior of particle systems interacting through their cumulative distribution functions, May 23th

- Research Seminar on Stochastic Analysis and Mathematical Finance, Stochastic flows approach to Dupire's formula, May 24th, Berlin

Le Bris C.
Weekly Seminar Penn State University, 2007

Lelièvre T.
Seminar der Partielle Differentialgleichungen und Numerik, June 2007, Universitat Zurich

Monneau R.
- Minisymposium: ICIAM 2007, July 2007 Zürich, Switzerland

- Viscosity solutions of PDE: recent advances and applications

- Meeting "Mathematical models for dislocations", December 2007, Roma

- Seminar, April 2007, University of Texas at Austin, USA

National seminars given

Alfonsi A.
A second-order discretization scheme for the CIR process: application to the Heston model', Working Group *"Methodes stochastiques et finance"*

Alfonsi A., Jourdain B.
Co-organization with M.-C. Kammerer-Quenez and A. Gloter of the MATHFI team seminar "stochastic methods and finance", Marne-la-Vallée

Briani A.
Un résultat d'homogénéisation en temps long de densités de dislocations, Groupe de travail Calcul des Variations, CEREMADE, University Paris-Dauphine, April 2nd 2007, Paris

Cancès É.
- *Simuler la matière aux différentes échelles*, Colloquium, April 2007, INRIA

- Numerical analysis for electronic structure calculations: an overview, January 2007, CEA

- Electronic structure of crystals with local defects, January 2007, Cergy

De Lara M.
- From Risk Constraints in Stochastic Optimization Problems to Utility Functions, First RiskAttitude Conference, May 10-11th, University of Montpellier

- *Propriétés de monotonicité pour le contrôle viable de systèmes dynamiques en temps discret. Application à la gestion soutenable de la pêche. Séminaire Probabilités Optimisation Contrôle*, June 13, INRIA Rocquencourt

- *Contrôle viable de systèmes dynamiques en temps discret et gestion durable des*

pêches, March 29th, Rencontre MATH-INDUSTRIE *organisée par la* SMAI, l*a* SMF *et le* CNRS

Delmas J.-F.

- Simultaneous extinction probability for the Eve-population and mutants population, ANR MAEV, Paris (France), January 2007
- Length of coalescing trees. November 2007, École Polytechnique France

Di Pietro D.

Discontinuous Galerkin methods for diffusion-advection problems, February 2007, Strasbourg

Ern A.

- *Analyse d'erreur a posteriori pour les méthodes de* Galerkine discontinues, November 28th 2007, Orsay
- *Analyse d'erreur a posteriori pour les méthodes de* Galerkine discontinues, November 30th 2007, Valenciennes

Etoré P.

- Approximation of diffusion processes with discontinuous coefficients in dimension one and applications, January 26th, University of Paris-Est Marne-la-Vallée
- Approximation of diffusion processes with discontinuous coefficients in dimension one and applications, ADAP'MC seminar
- Adaptive methods in stratified sampling, December, ADAP'MC seminar

Forcadel N.

- *Séminaire d'analyse appliquée A3*, November 26th 2007, University of Amiens
- *Groupe de travail d'homogénéisation*, November 19th 2007, University Pierre & Marie Curie - Paris VI
- *Groupe de travail Mécanique des fluides*, October 25th 2007, University of Toulouse
- *Séminaire du LMRS*, March 15th 2007, University of Rouen
- Groupe de travail du CMAP, February 9th 2007

Imbert C.

- Day "PDE methods in Finance'', University of Paris-Est Marne-la-Vallée, October 2007
- *Séminaire d'analyse numérique*, February 2007, Rennes
- *Séminaire d'Analyse et probabilités*, June 2007, University of Evry
- *Séminaire de mathématiques appliquées* du Collège de France, June 2007
- *Séminaire au groupe de travail "Analyse non linéaire''*, November 2007, laboratoire Jacques-Louis Lions, University Pierre & Marie Curie - Paris VI

Le Bris C.

- Weekly Seminar, 2007, University of Nice - Sophia-Antipolis
- *Journées EDP-Probas*, 2007

Lelièvre T.

- Seminar at UR Navier (LMSGC) École des ponts, January 2007, Paris
- Seminar *Analyse Numerique et EDP* of University Paris-Sud, May 2007

Monneau R.

- Meeting "Hamilton-Jacobi", March 2007, (Paris VI and Paris VII)
- CEA Gif-sur-Yvette, February 2007
- University of Clermont-Ferrand, May 2007

Piperno S.

Méthodes DGTD avec pas de temps adaptatif, conseil scientifique du PRF MAHPSO, December (ONERA, Châtillon)

Rousset M.

- Seminar, Institut Henri Cartan, University Poincaré, Nancy
- Seminar, Institut Galilée, University Paris XIII
- Seminar, Laboratoire Painlevé, USTL Lille 1

Missions and visits

Alfonsi A.

Second general AMAMEF conference and Banach center Conference, April 30th- May 5th 2007 Bedlewo, Poland

Lelong J.

Invited by Denis Talay, INRIA Sophia Antipolis, June 2007 (3 days).

Monneau R.
- University of Austin (Texas, USA), April 2007 (2 weeks)

- Course of the summer school "Global School on PDEs: "layers and dislocations'"; June 2007, University of Barcelona (Spain), (1 week)

Roux R.
Workshop on particle systems, non linear diffusions and equilibration, Bonn, November 12-16th

Organization

Hosted MATHFI team seminars

Alfonsi A., CERMICS
Un schéma de discrétisation d'ordre 2 pour le processus CIR: application au modèle de Heston

Arisawa M., Tohoku University, Japan
Le problème ergodique des équations intégro-différentielles avec l'opérateur de Lévy

Bally V., UPEMLV
- *Formule d'intégration par parties et application à l'étude de la densité pour des diffusions à sauts*

- *Schémas d'approximation d'ordre supérieur selon Victoir et Nynomiya*

Elie R., CREST- CEREMADE
Gestion de portefeuille sous contrainte "drawdown"

Etoré P., CERMICS
- *Méthodes adaptatives pour la stratification*

- *Approximation de processus de diffusion à coefficients discontinus en dimension un et applications*

Jourdain B., CERMICS
Le recyclage des déchets améliore-t-il l'algorithme de Metropolis-Hasting ?

Jottreau B., UML
Formation des prix pour des options binaires et application aux paris

Kazuhiro Y., Osaka University
Estimating Multidimensional Density Functions through the Malliavin-Thalmaier Formula and its Application to Finance

Kobylanski M., UPEMLV
Introduction aux équations différentielles stochastiques rétrogrades

Labart C., INRIA
An adaptive Monte Carlo algorithm for solving BSDEs

Ly Vath V., University Paris VII
*Modèle de gouvernance d'entreprise: un problème couplé de contrôle singulier/*switching

Meziou A., CMAP Polytechnique
Décomposition Max-Plus des surmartingales et application aux options Américaines et à l'assurance de portefeuille

Pagès G., University Pierre & Marie Curie - Paris VI
Multi-step Richardson-Romberg Extrapolation: Remarks on Variance Control and Complexity

Pironneau O., University Paris VI
Généralisation de l'approche Dupire à toutes les options dont l'équation aux dérivées partielles de Itô est linéaire

Rousset M., CERMICS
Enjeux numériques en dynamique moléculaire

Royer M., University Claude-Bernard Lyon 1,
Equations Différentielles Stochastiques Rétrogrades à Sauts et martingales non linéaires

Sbai M., CERMICS
- *Méthodes de Monte Carlo exactes et application au pricing d'options Asiatiques*

- *Présentation de l'article de Cruzeiro, Malliavin et Thalmaier* : "Geometrization of Monte-Carlo numerical analysis of an elliptic operator: strong approximation"

Scotti S., University of Turin & CERMICS
Approche par perturbation sur les marchés financiers

Sulem A., INRIA
Risk indifference pricing in jump diffusion markets

Tankov P., University Paris VII
Computing risk measures for CPPI-insured portfolios

Yasutomi K., Ritsumeikan University
A dependence vanishing theorem for sequence generated by Weyl transformation

Ying J., CMAP Polytechnique
L'approximation normale et Poissonnienne pour l'evaluation des CDOs

Hosted 'calcul scientifique' seminars

James F., University of Orléans
Un problème inverse en chromatographie

Dalibard A.-L., CEREMADE, University Paris-Dauphine
Homogénéisation d'une loi de conservation scalaire avec viscosité évanescente

Buttazzo G., Dipartimento di Matematica, Università di Pisa
Asymptotics for a compliance-location problem

Mangoubi C., CERMICS and Institute of Mathematics, Hebrew University of Jerusalem
Un critère de Beale-Kato-Majda pour un fluide Oldroyd-B dans un écoulement rampant

Cicalese M., Università di Napoli, Italy
Discrete systems with continuous symmetry: a variational approach to the ground states of the XY model

Pillet N., CEA/DAM, Bruyères-le-Châtel
Calculs de type multiconfiguration en physique nucléaire

Delfour M., CRM, University of Montréal, Canada
Formes et géométries comme variables de modélisation ou de contrôle

Faou E., IRISA/INRIA Rennes
Analyse des méthodes de splitting pour les équations de réaction-diffusion par le calcul stochastique

Pellenq R., Centre de recherche en matière condensée et nanosciences, Marseille
Modélisation des phénomènes liés au confinement dans les solides poreux : vers une approche multi-échelle

Mozolevski I., Federal University of Santa Catarina, Mathematical Department
Discontinuous Galerkin finite element methods for heterogeneous coupling of elliptic equations

Tassi P., CERMICS
Numerical modelling of river processes: flow, sediment transport and riverbed deformation

Assaraf R., Laboratoire de Chimie théorique, Paris VI
Calcul de derivées et de petites differences en Monte Carlo quantique

Mousseau N., Département de physique and Regroupement québécois sur les matériaux de pointe, University of Montréal
Une histoire de l'ART vue par un physicien ou Récents développements et applications aux défauts dans les semiconducteurs de la technique d'activation et de relaxation (ART)

Patera T., Department of Mechanical Engineering, MIT
Reliable Real-Time Solution of Parameterized Partial Differential Equations

Trashorras J., CEREMADE, University Paris Dauphine
Sur deux aspects du coarse-graining

Lehoucq R. B., Sandia National Laboratories
Dynamical systems and non-hermitian iterative eigensolvers

Blanchet A., Laboratoire Paul Painlevé, University of Lille I
Convergence of the mass-transport steepest descent scheme for the Keller-Segel model

Mavrantzas V., University of Patras, Greece
Modelling polymer melt rheology and dynamics: How one can benefit from atomistic simulations

Lewin M., CNRS and Laboratoire de Mathématiques "Analyse, Géométrie, Modélisation", University of Cergy-Pontoise
La limite thermodynamique des systèmes quantiques Coulombiens

Conference/seminar organized

Alfonsi A., Jourdain B.
co-organization with M.-C. Kammerer-Quenez and A. Gloter of the MATHFI team seminar "stochastic methods and finance", Marne-la-Vallée

Cancès É.
Minisymposium on "Applications to Chemistry" at the Scicade conference, Saint-Malo, July 9-13th, 2007

Ern A.
- Organization of a three-day workshop on Mathematical Methods and Simulation for Radioactive Waste Storage in Fréjus, November 14-16th 2007, 75 participants

- Co–organization (with J.–P. Croisille, R. Luce, F. Dubois and J.–F. Maitre) of a one day workshop on Numerical Methods for Fluids at the «Conservatoire National des Arts et Métiers» in Paris, December 18th 2007

Forcadel N.
Co-organization of « Ecole Introduction to numerical methods for moving boundaries' », November 12-14th 2007, ENSTA

Lapeyre B.
Coordination of the ANR program Grid Computation for Mathematical Finance (Calyon, Centrale, EDF, École des ponts, INRIA, Ixis, Paris VI, Pricing Partner, Summit, Supelec), February 2006-February 2009.

Monneau R.
- Co-organization of the workshop "Evolution of interfaces and applications", May 2007, Roscoff, France

- Co-organization of two minisymposium "Recent advances in front propagation modelling and applications", ICIAM 2007, July 2007, Zurich, Switzerland

- Co-organization of a workshop "PDE methods in finance", October 2007, Université Paris-Est Marne-la-Vallée, France

- Co-organization of the autumn school "Introduction to numerical methods for moving boundaries", November 2007, ENSTA, Paris

- Co-organization of a one-day meeting on « Mathematical models for dislocations », December 2007, Roma

Stoltz G., Gloria A., Deleurence A., Tassi P.
Co-organization of the seminar "*Calcul Scientifique*" at CERMICS.

EDUCATION ACTIVITIES

SUPERVISION ACTIVITY

Ongoing theses

Anantharaman A.
Analyse mathématique et simulation numérique de quelques modèles moléculaires et multi-échelles présentant une structure périodique, École des ponts

Bencteux G.
Méthode de décomposition de domaine pour les calculs ab initio en sciences des matériaux, École des ponts

Boyaval S.
Modélisation et simulation multi-échelle de *fluides complexes pour le génie civil*, École des ponts

Deleurence A.
Analyse mathématique et numérique de quelques modèles de simulation multi-échelle en sciences des matériaux, École des ponts

Doyen D.
Mathematical and numerical investigation of cohesive fracture propagation, École des ponts

El Makrini M.
Simulation de défaut dans les cristaux, University Paris Dauphine

Foki J.
Fidelity test, Analysis of correlation between different signals, École des ponts

Galicher H.
Couplage de modèles classiques et quantiques pour la simulation des matériaux à l'échelle moléculaire, University Paris 6

Girardeau P.
Optimisation stochastique de grands systèmes, École des ponts

Ibrahim H.
Mathematical analysis of dislocations density dynamics with scale effets, École des ponts and Univ. libanaise (co-direction R. Monneau and M. Jazar)

Lioris E.
Simulation and evaluation of collective taxi systems, École des ponts

Minoukadeh K.
Méthodes d'optimisation déterministes et stochastiques pour la simulation moléculaire, École des ponts

Roux R.
Probabilistic study of interacting particle systems: applications to molecular simulation, Ecole Nationale Supérieure de Cachan

Scotti S.
Dirichlet forms methods in finance, (co-supervisor: Prof. Pratelli M.)

Seck B.
From risk constraints in stochastic optimization problems to utility functions, École des ponts

Sbai M.
Simulation of stochastic differential equations in finance, École des ponts

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

Sochala P.
Numerical methods for coupling subsurface and surface flows, École des ponts

Theses defended

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

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

Dallagi A.
Méthodes particulaires en commande optimale stochastique, University of Paris i

El Hajj A.
Analyse théorique et numérique de la dynamique de densités de dislocations, UPEMLV

Forcadel N.
Contribution à l'analyse d'équations aux dérivées partielles décrivant le mouvement de fronts avec applications à la dynamique des dislocations, École des ponts

Gloria A.
Méthodes numériques multiéchelles en élasticité non linéaire, École des ponts

Ghorbel A.
Numerical analysis of dislocations dynamics and applications to homogeneization, École des ponts

Lelong J.
Asymptotic properties of stochastic algorithms and pricing of Parisian options, École des ponts

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

Stephansen A.
A posteriori error analysis applied to reactive transport in porous media, École des ponts

Stoltz G.
Problèmes de transfert d'échelle en simulation des matériaux, École des ponts

HDR

Imbert C.
Équations intégro-différentielles non-linéaires: questions d'existence, de régularité et d'homogénéisation, University Paris-Dauphine

TEACHING ACTIVITIES

Lectures

École des ponts

- **Analysis, 1st year**

Cancès É. (prof. in charge), Ern A., Monneau R.

- **Analyse en fréquences**

Cancès É.

- **Computational Mechanics**

Ern A. (prof. in charge)

- **Epistemology**

Bouleau N., Chatzis K, Walliser B.

- **Introduction to the scientific software Scilab, 1st year**

Chancelier J.-P. (prof. in charge), De Lara M. (prof. in charge), Deleurence A., Galicher H., Jarry R., Roux R., Sbai M., Sochala P., Tartar M.

- ***Introduction à la physique statistique et la physique quantique***
Stoltz G.

- **Mathematical finance, 2nd year**
Jourdain B. (professor in charge), Lapeyre B., Sbai M.

- **Mathematical modelling for the sustainable management of natural resource, Master EDDEE (Économie du développement durable, de l'environnement et de l'énergie)**
De Lara M.

- ***Méthodes déterministes en mathématiques financières***
Lelièvre T.

- **Modeling, Programming and Simulating, 2nd year**
Alfonsi A, Lapeyre B., Lelièvre T.

- **Modeling for the sustainable management of natural resource**
De Lara M.

- **Probability and statistics, 1st year**
Jourdain B. (prof. in charge), Alfonsi A., De Lara M , Lelièvre T., Sbai M.

- **Probabilistic Tools for Finance**
De Lara M.

- ***Remise à niveau en analyse et calcul scientifique pour les maîtres es sciences***
Deleurence A.

- **Scientific Computing**
Ern A. (prof. in charge), Gloria A, Mozolevski I., Piperno S., Sportisse B., Stoltz G.

- **Statistics, 2nd year**
Delmas J.-F. (prof. in charge), Rousset M., Roux R.

École Polytechnique

- ***Analyse numérique et optimisation, PC du cours de G. Allaire et P.-L. Lions***
Cancès É., Le Bris C.

- **Introduction to Probability Theory and simulation, 1st year**
Delmas J.-F., Jourdain B.

- **Monte Carlo methods in Finance, formation cycle of the College of Polytechnique**
Jourdain B., Lelong J.

- Delmas J.-F., Professeur chargé de cours

- **Projects and courses in Finance, Applied mathematics specialization, 3rd year**
Jourdain B.

École de printemps MFN, Roscoff, June 2007
Éléments finis : méthodes de Galerkine discontinues
Ern A.

ENSAI
Numerical Methods in Finance, third year course
Lelong J.

Mines ParisTech

- **Automatic control, Scilab tutorial**
Chancelier J.-P., Petit N., Rouchon P.

- **Acoustics, computer science and music**
Chancelier J.-P., D'Andrea B.

- **Differentiable optimization**
Carpentier P.

ENSTA

- **Differentiable optimization**
Carpentier P.

- **Introduction to probability and statistics, 1st year**
Delmas J.-F. (professor in charge), Sbai M., Lelong J.

- **Lectures on Numerical Methods in Finance, 2nd year course**
Lelong J.

- **Optimization of large systems**
Carpentier P.

- **Practicals on Numerical simulation in C++, second year course**
Lelong J.

- **Practicals on Markov Chains, second year course**
Lelong J.

ESIEE

- **Analyse et algèbre linéaire**
Bencteux G.

- **Analyse numérique et Optimisation**
Deleurence A.

- **Probability and statistics, 3rd year,**
Roux R. (assistant professor)

Université Paris I

- **Mathématiques, TD au niveau L1**
Deleurence A.

- **Numerical methods for stochastic optimization, Master MMMEF**
Carpentier P.

- **Risk measures and risk constraints, Master MMMEF**
De Lara M.

- **Stochastic Control: continuous time, numerical methods and application to Finance, Master MMMEF**
Chancelier J.-P.

- **Sensitivity and error calculus, application to finance, Master2**
Bouleau N., Chorro Ch.

Université Paris VI

- **Méthodes de Galerkin discontinues et applications, M2R Maths, S4, Parcours ANEDP**
Ern A., Girault V., Piperno S.

- **Méthodes probabilistes, M2 Mathématiques et Applications**
Lelièvre T.

- **Simulation moléculaire : aspects théoriques et numériques, cours de M2**
Blanc X., Cancès É.

- **Systèmes multiéchelles, cours de M2**
Le Bris C.

University Paris VI, University of Paris-Est
Risk measure in finance, M2 course
Delmas J.-F.

University of Paris-Est Marne-la-Vallée

- **Stochastic models, M2 course**
Delmas J.-F.

University of Paris-Est Marne-la-Vallée et École des ponts
Course on "Monte Carlo methods for finance", Master programme in Random analysis and systems
Jourdain B., Lapeyre B.

University of Melbourne, Australia,
Stochastic Optimal Control: variational approaches, sampling and information, numerical resolution,
Cohen G.

Halmstad University, Sweden
Master in Financial Mathematics Lectures on Numerical Methods in Finance 2006-2007
Chancelier J.-P., Lapeyre B., Sulem A.

Universidad del Pacifico, Lima, Peru
Matemática e Informática para el Manejo Sustentable de Recursos Naturales
De Lara M.

Columbia University
Stochastic algorithms and applications to Monte Carlo methods in finance, March-April 2007, PHD course.
Lapeyre B.

Halmstad University, Sweeden
Numerical methods for Finance: Monte Carlo methods, January 2007, Master's Programme in Financial Mathematics
Lapeyre B.

Textbooks for teaching activities

Cancès É., Ern A.
Analysis
École des ponts

Chateau X., Dormieux L., Ern A.
Computational mechanics
École des ponts

De Lara M.
Sustainable Management of Natural Resource : Mathematical Models and Methods
École des ponts

Ern A.
- Scientific computing

École des ponts

- La méthode de Galerkine discontinue

Ecole de printemps MFN, Roscoff, June 2007

Delmas J.-F.
- Statistique (Statistics), 2nd year

École des ponts

- Introduction to probability and statistics, 1st year

ENSTA

Jourdain B.
- Probability and statistics

1st year École des ponts

- Monte Carlo methods for financial m^odels,

3rd year École des ponts

Lelong J.
Numérical Methods in Finance
3rd year, ENSAI

INDUSTRIAL PARTNERSHIPS

CONTRACTS AND GRANTS

Alcan-Pechiney
Le Bris C., Lelièvre T.
Numerical simulation of aluminum electrolysis

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

CEA
Cancès É., Stoltz G.
Study on scale transfer in materials simulations

CETMEF
Ern A., Piperno S., Tassi P.
Discontinuous Galerkin methods for Saint-Venant equations

EADS Foundation
Foki J., Chauveau D., Delmas J.-F.
Modelisation and statistical study for the program PILE

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

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

EDF
Ern A., Piperno S.
Modelling and simulation of dynamic crack propagation

EDF LNHE
Ern A., Piperno S.
Dynamics and propagation of waves near shorelines. Selection of a mathematical model and a numerical method for a 2DH simulation software

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

IFP
Ern A., Piperno S., Tassi P.
Hydrological transport of sediments; steady-state solution of Shallow Water Equations with Discontinuous Galerkin finite element methods

ONERA
Piperno S.
Time domain Discontinuous Galerkin finite element methods with local order of accuracy and time-stepping for wave propagation problems

PREMIA consortium
Alfonsi A., Etoré P., B. Jourdain, Lapeyre B., Lelong J., Sbai M.
Pricing and hedging procedures library financed by a consortium of banks

Thales-Alenia and CNES
Carpentier P., Chancelier J.-P., Cohen G., De Lara M.
Optimal planning of spatial missions in order to achieve interplanetary rendez-vous, with trade-off between performance and robustness to failures.

X- École des ponts -Société Générale
Alfonsi A., Delmas J.-F., Jourdain B., Lapeyre B.
Research and teaching chair "Measure of financial risks"

COLLABORATIONS WITH CIFRE

EDF
CIFRE of D. Doyen
Mathematical and numerical investigation of cohesive fracture propagation, École des ponts

EDF
CIFRE of P. Girardeau
Optimisation stochastique de grands systèmes, École des ponts

SOFTWARE

Di Pietro D.
Development of a general Discontinuous Galerkin solver for elliptic problems (10k line, C++ software); further developments by A. F. Stephansen for *a posteriori* error estimates.

Lelong J., Chancelier J.-P.
Development of an Nsp interface for Premia (integration of the American Monte Carlo module in the core of Premia, making it available both to the Nsp and Excel interfaces). Implementation of a C API for matrices and hypermatrices to ease future developments in Premia.

Piperno S.
Development of a Discontinuous Galerkin Time-Domain solver of wave equations in two space dimensions (acoustics, elastodynamics), on unstructured triangulations, with adaptive local time step and polynomial accuracy (10k line Fortran 77 software)

Piperno S., Ern A.
Development of a Discontinuous Galerkin Time-Domain solver of two-dimensional shallow water equations on unstructured triangular meshes, with variable bathymetry and flooding/drying, with variable polynomial accuracy (8k line Fortran 77 software).

Sochala P.
Development of a Discontinuous Galerkin solver for two-dimensional flows in variably saturated soils (8k line, C software)

Tassi P.
Development of a Discontinuous Galerkin Time-Domain solver of two-dimensional shallow water equations on unstructured triangular meshes, with variable bathymetry and flooding/drying, with variable polynomial accuracy (5k line, C++ software)

ACRONYMS

ACI Action Concertée Incitative

ANDRA Agence Nationale pour la Gestion des Déchets Radioactifs

ANR Agence Nationale de la Recherche

ATER Attaché Temporaire d'Enseignement et de Recherche

BRGM Bureau de Recherches Géologiques et Minières

CEA Commissariat à l'Energie Atomique

CEMAGREF Centre National du Machinisme Agricole, du Génie Rural, des Eaux et Forêts

CERTIS Centre d'Enseignement et de Recherche en Technologies de l'Information et Systèmes (École des ponts)

CETMEF Centre d'Etudes Maritimes et Fluviales

CIFRE Convention Industrielle de Formation par la Recherche

CMAPX Centre de Mathématiques Appliquées de l'Ecole Polytechnique

CNRS Centre National de la Recherche Scientifique

EDF Electricité de France

École des ponts École Nationale des Ponts et Chaussées

ENST École Nationale Supérieure des Télécommunications

ENSTA École Nationale Supérieure de Techniques Avancées

ESIAL École Supérieure d'Informatique et Applications de Lorraine

EPFL École Polytechnique Fédérale de Lausanne

ESPCI École Supérieure de Physique et Chimie Industrielles

GDR MOMAS Groupement de Recherche Modélisations Mathématiques et Simulations

HDR Habilitation à Diriger des Recherches

IFP Institut Français du Pétrole

INRIA Institut National de Recherche en Informatique et en Automatique

IRSN Institut de radioprotection et de sûreté nucléaire

LAMI Laboratoire Analyse des Matériaux et Identification (UR Navier -École des ponts)

LMSGC Laboratoire des Matériaux et des Structures du Génie Civil (UR Navier - École des ponts)

LNHE Laboratoire National d'Hydraulique et Environnement

MIT Massachusetts Institute of Technology

ONERA Office National d'Etudes et Recherches Aérospatiales

UPEMLV University Paris-Est Marne-la-Vallée

UPMC University Pierre & Marie Curie, Paris VI