

# CERMICS

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mathématiques – informatique

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## CERMICS

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

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### UNIVERSITÉ PARIS-EST

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

#### CERMICS

**École des Ponts ParisTech**

6/8 avenue Blaise-Pascal  
 Cité Descartes – Champs-sur-Marne  
 77455 Marne-la-Vallée cedex 2

Tel: 01 64 15 35 72

Fax: 01 64 15 35 86

<http://cermics.enpc.fr/>

**Director: Jean-François Delmas**

**Vice-Director: Alexandre Ern**

#### STAFF

**14 Researchers**

**4 Associate researchers**

**22 External collaborators**

**25 PhD students**

**8 Starting PhD students**

**2 Administrative assistants**

**10 Post-docs**

**15 Invited researchers**

**7 Internship students**

## QUALITATIVE RESULTS

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CERMICS is a laboratory of École des Ponts ParisTech, hosting joint research teams with INRIA and University Paris-Est of Marne-la-Vallée (UPEMLV). It is located at École des Ponts ParisTech in Champs-sur-Marne. The scientific activity of CERMICS covers several domains in scientific computing, applied probability, modelling, and optimization. It has been evaluated A+ in 2008 by the AERES. Since 2011, the three laboratories: CERMICS, LAMA (mathematic department of UPEMLV and University Paris-Est of Créteil (UPEC)) and LIGM (informatic department of UPEMLV, ENPC and ESIEE), constitute the LabEx Bézout from the French "Programme d'Investissements d'Avenir".

Three teams deal with modelling and scientific computing: the "Fluid Dynamics" team (leader: Alexandre Ern), which develops advanced numerical methods (finite elements, a posteriori error estimates, uncertainty propagation) applied to environmental flows and fluid/solid interaction, the "Molecular and Multiscale Simulations" team (leader: Tony Lelièvre), which covers several connected fields such as electronic structure calculations, numerical statistical physics, multiscale simulation of materials, etc., and the "PDE and Materials" team (leader: Régis Monneau) devoted to the mathematical modelling of material behavior at the crystalline level. Two other teams cover several important domains of applied mathematics: the "Optimization and Systems" team (leader: Michel De Lara) involved in research about optimization (mostly in a stochastic setting), system simulation, and control, and the "Applied Probability" team (leader: Benjamin Jourdain) with applications of probability theory to modelling and numerical methods. All teams have their own research domains, and collaborate on specific topics, like, for example, Quantum Monte Carlo methods for the computation of the ground state energy of a Schrödinger Hamiltonian or domain decomposition and uncertainty propagation. It can be pointed out that two teams are joint project-teams with INRIA: the "Molecular and Multiscale Simulations" team hosts the INRIA Rocquencourt project-team MICMAC (leader: Claude Le Bris), and the "Applied Probability" team takes part to the UPEMLV-INRIA Rocquencourt project-team MATHFI (leader: Agnès Sulem).

des Ponts ParisTech.

## **KEY FACTS**

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### **Staff changes, missions, visits**

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Frédéric Meunier joined CERMICS as a researcher since January 1st, 2011. In July 2006, Frédéric Meunier completed his PhD in combinatorial optimization at Université Joseph Fourier, Grenoble, under the supervision of Andras Sebö. After having spent one year in the Algo Project of Inria, until September 2007, he got a position as a researcher at the Transportation Laboratory (LVMT) of the Ecole des Ponts, where he began to be interested in transportation, logistics and operations research questions.

A. Ern delivered during a one-month invited Professorship in the Mathematics Department of University of Udine, Italy, a course on Finite volume and Finite element methods.

J.-F. Delmas has been invited one month in Tsinghua University (Beijing) to participate in a teaching program.

### **Publications and prizes**

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The CERMICS laboratory has sustained a high scientific activity: one book, more than forty five articles in international refereed journals and five chapters of books have been published. Also about eighty presentations in conferences have been made and seventeen conferences or workshops have been organized by members of CERMICS.

Tony Lelièvre was awarded the 2011 iXCore foundation prize.

### **Industrial impact**

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The activities of industrial transfer in the laboratory are strongly linked to research activities. Scientific results are mostly obtained in collaboration with Research and Development Departments of large industrial firms through research contracts (ANDRA, CNES, CEA, Creditnext, EADS, EDF, IFPEN, Société Générale, Thalès-Alenia Space, US Air Force, US Navy, etc). Nine programs, which represent a significant part of our financial support, are granted by the «Agence Nationale de la Recherche» (ANR). The level of research contracts was very high in 2011, about 500 k€ for contracts signed by École

### **Teaching**

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The members of CERMICS are strongly involved in teaching at École des Ponts ParisTech, École Polytechnique, École des Mines, ENSTA and in Masters in collaboration with Universities. Among them, École des Ponts Paristech has a strong partnership with the 2nd year Master program on Applied Mathematics and Mathematical Finance of UPEMLV, and the 2nd year Master program on Numerical Analysis and PDES of University Pierre and Marie Curie (Paris VI).

## RESEARCH TEAMS

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### 1. Applied probability

### 2. Fluid dynamics

### 3. Molecular and multiscale simulations

### 4. Optimization and systems

### 5. PDE and materials

#### 1. Applied probability

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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.

With the end of the lifetime of the project Mathfi structuring the research in mathematical finance with researchers from the UPEMLV and the INRIA, the first steps toward the creation of a new INRIA project team called MathRisk have been taken in 2011. In the same time, the chair "Measure of Financial Risks" of the Risk Fundation will soon be renewed for a five year period with the arrival of the university Paris 6 as a new partner in addition to École des Ponts, École Polytechnique and Société Générale.

The ANR program BigMC started in 2009 permits collaborations with the statisticians from the ENST and the University Paris Dauphine to enhance Monte Carlo methods especially with adaptive variance reduction techniques.

The team hosts the ANR program A3 on Random Trees and Applications (in collaboration with Universities of Orléans, Bordeaux and Nancy) which focuses on branching processes and random maps. This activity is also connected to applications in biology.

In 2011, Abdelkoddousse Ahdida has defended his PhD financed by Credinext and two students, Charline Smadi and Julien Reygnier have started new PhDs. Two postdocs Stéfano De Marco and Gilles-Edouard Espinosa have been financed by the Eurostars program. The team received the

visit of Alexander Schied, professor at Mannheim.

#### 2. Fluid dynamics

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The Fluid Dynamics team develops advanced numerical methods for environmental flows and fluid/solid interaction. The main applications are underground waste storage, interaction of shock waves with solids, runoff and erosion in hydrosystems, thin gravitational flows, and acoustics. Scientific activities are concerned with modelling, numerical analysis, and simulation. The developed numerical methods include discontinuous Galerkin, a posteriori error estimates, and finite volumes. Uncertainty quantification is an important topic, in particular stochastic Galerkin methods. Most activities are developed in partnership and involve a PhD thesis. Two new theses started in 2011, one with CEA on three-dimensional interactions of shock waves and solids and one with EDF on mimetic discrete operators with application to Navier-Stokes equations.

#### 3. Molecular and multiscale simulations

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The scientific focus of the team (which is also part of the INRIA project-team MicMac) is to analyze and improve the numerical schemes used in the simulation of materials at the microscopic level (computational chemistry, molecular dynamics), and in simulations coupling this microscopic scale with larger macroscopic scales (solid mechanics, fluid mechanics). The main domains of application are: quantum chemistry, material science and molecular dynamics. Our work pursues a twofold goal: giving the models a sound mathematical grounding, and improving the numerical approaches.

More precisely, the main topics covered by the team are the following:

- computational quantum chemistry and approximation of the Schrödinger problem
- molecular dynamics and computational statistical physics
- free surface flow
- micro-macro models for fluids
- micro-macro models for solids and stochastic homogenization
- quantum models for electrochemistry.

Let us also mention an emerging activity on uncertainty propagation and applications of greedy algorithms.

Over the years, the team has accumulated an increasingly solid expertise on such topics, which are traditionally not well known by the community in applied mathematics and scientific computing. One of the major achievements of the team is to have created a corpus of literature, authoring books and research monographs on the subject that other scientists may consult in order to enter the field. Last year, the book "Free energy computation: a mathematical perspective" (Imperial College Press) just appeared. It covers a new topic we addressed over the past five years.

Among the main achievements in 2011, let us mention the following:

- Concerning electronic structure theory, the team addressed issues related to the modeling and simulation of local defects in periodic crystals. On the numerical side, various results have been obtained concerning eigenvalue calculation problems, in particular for the computation of eigenvalues in spectral gaps of locally perturbed periodic Schrödinger operators. In addition, numerical techniques have been designed to predict the electronic spectra and electrical response of molecular and polymer compounds for organic photovoltaic semiconductors.

- Concerning molecular dynamics, new results have been obtained on efficient sampling algorithms, in particular concerning the sampling of trajectories (multilevel splitting techniques, and analysis of the parallel replica dynamics). In addition, we have been working on non-equilibrium systems (shock and detonation waves and thermal conductivity of one-dimensional chains). Finally, some integrators for Hamiltonian systems with high frequencies have been proposed. We are continuously discussing the practical counterparts of these methodological and theoretical results with practitioners (chemists and molecular biologists).

- Various results have been obtained in the field of multiscale modelling for solid materials and for fluids. In particular, many results have been obtained some models aging fluids. The activity of the team on stochastic homogenization for random materials is still growing. Many results have been obtained, in particular concerning efficient numerical strategies to compute effective properties of random materials.

In 2011, R. Costouec has defended his PhD on Numerical techniques for homogenizations with applications to random materials.

The article by I. Dabo and coworkers has been awarded the label "Editors' Suggestion" by the journal Physical Review B.

#### 4. Optimization and systems

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After the retirement of Guy Cohen, the Optimization and systems team comprises three full time researchers in 2011 -- Jean-Philippe Chancelier, Michel De Lara, Frédéric Meunier - six PhD students – Daniel Chemla, Pierre Girardeau, Vincent Leclère, Djamal Mohia, Lilian Sepulveda – two post-doc students – Bernat Gacias and Houssame Yahiaoui (till end of May)-- and four associated researchers -- Pierre Carpentier (ENSTA), Laetitia Andrieu (EDF), Kengy Barty (EDF), Anes Dallagi (EDF).

- \* Numerical methods in stochastic control. Risk Management and Probability Constraints

These themes form the core of our team research, and are developed in collaboration with EDF R&D. We have put emphasis on the implementation of price decomposition for specially structured large-scale problems under stochasticity, with the launching of Vincent Leclère doctorate. Our main application is dams management, but our perspective is the expansion of so-called smart power systems. Jean-Christophe Alais continues his doctorate on risk and optimization for the management of energies, in CIFRE convention with EDF. The application bears on dam management, where expected revenue is maximized under the probability constraint that the water level is sufficiently high in summer.

- \* Mathematical methods for sustainable management of natural resources

Michel De Lara obtained in 2011 a new international STIC-AmSud project OVIMINE, Optimization and viability in mining, with Peru and Chile. Michel De Lara co-supervises, with Olga Vasileva of Universidad del Valle (Cali, Colombia) the doctorate of Lilian Sepulveda on viability methods for the control of dengue epidemics. Michel De Lara co-supervises, with Katheline Schubert of University Paris 1, Esther Régnier's thesis on Fishery economics, a key science for improving the management of halieutic resources

#### \* Scientific software NSP

This theme is driven by J.-P. Chancelier. NSP has evolved during the present year in many aspects by adding primitives and toolboxes in collaboration with Bruno Pinçon. The cooperation with the Premia team is going on. A version of scicos 4.4 is available and work to enable compilation of a subset of the language has been started.

#### \* Transport

The study of optimization problems arising with the operations of self-service transport systems has led to various results. With R. Wolfler Calvo from University Paris 13, F. Meunier and D. Chemla have proposed algorithms for computing optimal routes for the trucks involved in the repositioning of the vehicles (say, bikes). Efficient real-time strategies with trucks or through dynamic pricings have been also designed, and experimented on the OADLIB simulator implemented by H. Yahiaoui.

F. Meunier and B. Gacias have designed an operational framework for managing a fleet of electric taxis (the charging task being crucial). This framework has been experimented through simulations and proven its efficiency.

### **5. PDE and materials**

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The main subject studied by the PDE and Materials team is the dynamics of dislocation (PhD of A. Le Guilcher, M. Al Haj, and L. Paszkowski). This work concerns different scales, from microscopic scales (simplified atomic models, like the Frenkel-Kontorova model), models of dislocation dynamics (curves of defects moving in crystals, and responsible of elasto-visco-plastic properties of metals), up to the macroscopic scale with dislocation densities. Simultaneously, we also work on different topics: models of nanotubes (PhD of D. El Kass), models of traffic (PhD of G. Costeseque with IFSTTAR laboratory), seawater intrusion (PhD of G. Chmaycem) and we also have collaboration projects with the LAMA laboratory.

## STAFF

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### Researchers (14)

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ALFONSI Aurélien, Applied Probability team, Ecole des Ponts ParisTech, research scientist  
 CANCES Eric, Molecular and Multiscale Simulations team, Ecole des Ponts ParisTech, research scientist, HdR  
 CHANCELIER Jean-Philippe, Optimization and Systems team, Ecole des Ponts ParisTech, research scientist, HdR  
 DABO Ismaila, Molecular and Multiscale Simulations team, research scientist,  
 DE LARA Michel, Optimization and Systems team, Ecole des Ponts ParisTech, research scientist, HdR  
 DELMAS Jean-François, Applied Probability team, Ecole des Ponts ParisTech, research scientist, HdR  
 ERN Alexandre, Fluid Dynamics team, Ecole des Ponts ParisTech, research scientist, HdR  
 JOURDAIN Benjamin, Applied Probability team, Ecole des Ponts ParisTech, research scientist, HdR  
 LAPEYRE Bernard, Applied Probability team, Ecole des Ponts ParisTech, research scientist, HdR  
 LE BRIS Claude, Molecular and Multiscale Simulations team, Ecole des Ponts ParisTech, research scientist, HdR  
 LELIEVRE Tony, Molecular and Multiscale Simulations team, Ecole des Ponts ParisTech, research scientist, HdR  
 MEUNIER Frédéric, Optimization and Systems team, Ecole des Ponts ParisTech, research scientist,  
 MONNEAU Régis, PDE and Materials team, Ecole des Ponts ParisTech, research scientist, HdR  
 STOLTZ Gabriel, Molecular and Multiscale Simulations team, Ecole des Ponts ParisTech, research scientist

### Associated researchers (4)

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BOULEAU Nicolas, Applied Probability team, Ecole des Ponts ParisTech, research scientist, HdR  
 EL HAJJ Ahmad (Univ. Compiègne), PDE and Materials team  
 IMBERT Cyril (Univ. Dauphine), PDE and Materials team  
 FORCADEL Nicolas (Univ. Dauphine), PDE and Materials team

### External collaborators (22)

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ANDRIEU Laetitia, Optimization and systems, EDF, Research Scientist  
 BARLES Guy, PDE and Materials, University of Tours, Research Scientist, HdR  
 BARTY Kengy, Optimization and systems, Research, EDF  
 BOUCHUT François, Fluid dynamics, UPEMLV, CNRS, Research Scientist, HdR  
 BRIANI Ariela, PDE and Materials, University of Pise, Italia, Research Scientist,  
 CANNONE Marco, PDE and Materials, UPEMLV, Professor, HdR  
 CARDALIAGUET Pierre, PDE and Materials, University of Brest, Professor, HdR  
 CARLINI Elisabetta, PDE and Materials, University La Sapienza, Italia, Research  
 CARPENTIER Pierre, Optimization and systems, ENSTA, Research Scientist  
 DALLAGI Anes, Optimization and systems, EDF, Research Scientist  
 DA LIO Francesca, PDE and Materials, University of Padoue, Italia  
 BRIANI Ariela, PDE and Materials, University of Pise, Italia, Research Scientist  
 FALCONE Maurizio, PDE and Materials, University La Sapienza, Italia, Professor  
 FOREST Samuel, PDE and Materials, ENSMP, Research director, HdR  
 FINEL Alphonse, PDE and Materials, ONERA, Research Scientist  
 HOCH Philippe, PDE and Materials, CEA, Research Scientist  
 LE BOUAR Yann, PDE and Materials, ONERA, Research Scientist  
 LE MAITRE Olivier, Fluid dynamics, LIMSI-CNRS, University of Orsay  
 LEY Olivier, PDE and Materials, University Tours, Professor, HdR  
 ROUY Elisabeth, PDE and Materials, Ecole Centrale Lyon, Research Scientist, HdR  
 VOHRALIK Martin, Fluid dynamics, LJLL, UPMC-CNRS, HdR

### Invited Researchers (15)

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CAFFARELLI Luis  
 EFENDIEV Yalchin (6 June - 6 July 2011)  
 GUERMOND Jean-Luc  
 HARTMANN Carsten (15-20 Nov 2011)  
 KUDRYAVTSEV OLEG  
 LUSKIN Mitchell (17-21 Jan 2011)  
 NIER Francis (Prof., INRIA Délégation since Sept 2011)  
 OETTINGER Hans-Christian (21-25 Mar 2011)  
 OLLA Stefano (Prof., INRIA délégation. Jan-July 2011)  
 PAVLOTIS Grigorios (Sept 2011-Dec 2011)  
 SAMAEY Giovanni (Jan 2011- July 2011)  
 SCHIED Alexander



YANNACOPOULOS Athanasios (14-18 Nov 2011)  
 ZANETTE  
 ZEITOUNI Ofer (7-12 Feb 2011)

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### Post-doctoral students (10)

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ARAKELYAN Avetik, PDE and Materials team  
 DOBSON Matthew, Molecular and Multiscale Simulations team  
 DE MARCO, Stefano, Applied Probability team  
 ESPINOSA, Gilles-Edouard, Applied Probability team  
 FRANCISCO Juliano, Molecular and Multiscale Simulations team  
 GACIAS Bernat, Optimization and System team  
 HOUSSAME Yahiaoui, Optimization and System team  
 LAYEC Alan, Optimization and Systems team  
 LI Kun, Molecular and Multiscale Simulations team  
 MIASOJEDOW Blazej, Applied Probability team

### Ph. D Students (25)

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AHDIDA Abdelkoddousse, Applied Probability team, PhD student, ENPC fellowship, ED MSTIC  
 ALAIS Jean-Christophe, Optimization and Systems team ENPC, PhD student, ED MSTIC, CIFRE EDF  
 AL HAJ Mohammad, PDE and Materials team, PhD student, CNRS fellowship, ED MSTIC ENPC and Libanon CNRS  
 BENOIT David, Molecular and Multiscale Simulations team, UPE Fellowship, PhD student,  
 CASENAVE Fabien, Fluid Dynamics team, PhD, Student, ED MSTIC, IPEF  
 CHALHOUB Nancy, Fluid Dynamics team, PhD student, ENPC and CNRS Libanon fellowship, ED MSTIC  
 CHEMLA Daniel, Optimization and Systems team ENPC, PhD student, ENPC fellowship  
 CHMAYCEM Ghada, PDE and Materials team, PhD student, ENPC and CNRS-Lebanese fellowship, ED MSTIC  
 COSTAOUEC Ronan, Molecular and Multiscale Simulations team, PhD student, ENPC fellowship, ED MSTIC  
 EL KASS Danny, PDE and Materials team, PhD student, MESR fellowship, ED MSTIC  
 EHRLACHER Virginie, Molecular and Multiscale Simulations team, PhD student, IPEF, ED MSTIC  
 HENARD Olivier, Applied Probability team, PhD student, ENPC fellowship, ED MSTIC,  
 HOSCHEIT Patrick, Applied Probability team, PhD student, ENS fellowship, ED MSTIC,  
 INFANTE ACEVEDO, José Arturo, Applied Probability team, PhD student, AXA Foundation

fellowship, ED MSTIC  
 JEUNESSE Maxence, Applied Probability team, PhD student, Chair "Measue of financial risks" fondation du risque, fellowship, ED MSTIC  
 JOUBAUD Rémi, Fluid dynamics team, PhD student, ANDRA fellowship, ED MISTIC  
 LAHBABI Salma Molecular and Multiscale Simulations team, PhD student CNRS, fellowship ED EM2C,  
 LE GUILCHER Arnaud, PDE and Materials team, PhD student, IPEF, ED MSTIC  
 LUSSO Christelle, Fluid Dynamics team, PhD student, ED MSTIC, ENPC fellowship  
 MINT MOUSTAPHA Jyda, Applied Probability team, PhD student, IFSTTAR fellowship  
 MOHIA Djamel, Optimization and Systems team ENPC, PhD student, ENPC fellowship + ED MSTIC  
 MONASSE Laurent, Fluid Dynamics team, PhD student, IPEF, ED MSTIC,  
 ROUSSEAU Marie, Fluid Dynamics team, PhD student, ENPC fellowship, ED MSTIC  
 THOMINES Florian, Molecular and Multiscale Simulations team, PhD student, IPEF, ED MSITC  
 TRYOEN Julie, Fluid Dynamics team, PhD student, ENPC fellowship, ED MSTIC

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### Starting PhD students (8)

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BONELLE Jérôme, Fluid Dynamics team, PhD student, EDF fellowship, ED MSTIC  
 COSTESEQUE Guillaume, PDE and Materials team, PhD student, ITPE, ED MSTIC  
 LECLERE Vincent, Optimization and Systems team, IPEF, ED MSTIC  
 PRADEAU Thomas, Optimization and Systems team, ENS fellowship, ED MSTIC  
 PASKOWSKI Łukasz, PDE and Materials team, polish PhD student of Wrocław University  
 PUSCAS Adela, Fluid Dynamics team, PhD student, CEA fellowship, ED MSTIC  
 REYGNIER Julien, Applied Probability team, PhD student, IPEF, Paris 6  
 SEPULVEDA Lilian, Optimization and systems Team, Colombian professor, ED MSTIC  
 SMADI Charline, Applied Probability team, PhD student, IPEF, ED MSTIC

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### Internship students (7)

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ALTMANN Robert  
 BEEKER Nathanael  
 DA SILVA Laura  
 ESTANISLAO Alejandra  
 GERMAIN Etienne  
 KRONSBELN Cornelia  
 SARRABEZOLLES Pauline

## Administrative Assistants (2)

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BACCAERT Catherine, Ecole des Ponts ParisTech  
 QUELLEU Nathalie, Ecole des Ponts ParisTech

Andreussi O., Dabo I., Marzari N., «Revised self-consistent continuum solvation in electronic-structure calculations», *Journal of Chemical Physics*, (2012) 136 064102 20 p. 10.1063/1.3676407

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## QUANTITATIVE RESULTS

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Andrieu L., Cohen G., Vázquez-Abad F., «Gradient-based simulation optimization under probability constraints», *European Journal of Operational Research*, (2011) 212 2 345-351 10.1016/j.ejor.2011.01.049

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## KNOWLEDGE PRODUCTION

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Bally V., De Marco S., «Some estimates in extended stochastic volatility models of Heston type», *Risk and Decision Analysis*, (2011) 2 4 195-206 10.3233/RDA-2011-0046

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## PUBLICATIONS

### Scientific books

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T. Lelièvre, M. Rousset and G. Stoltz  
 Free energy computations: a mathematical perspective, Imperial College Press, 2010, ISBN 978-1-84816-247-1.

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Bansaye V., Delmas J.-F., Marsalle L., Tran V. C., «Limit theorems for Markov processes indexed by continuous time Galton-Watson trees», *Annals of Applied Probability*, (2011) 21 6 2263-2314 10.1214/10-AAP757

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### Publications in a international journals Journals with review committee

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Alibaud N., Briani A., Monneau R., «Diffusion as a singular homogenization of the Frenkel-Kontorova model», *Journal of Differential Equations*, (2011) 251 4-5 785-815 10.1016/j.jde.2011.05.020

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Barrett J. W., Boyaval S., «Existence and approximation of a (regularized) Oldroyd-B model», *Mathematical Models and Methods in Applied Sciences*, (2011) 21 9 1783-1837 10.1142/S0218202511005581

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Anantharaman A., Le Bris C., «A numerical approach related to defect-type theories for some weakly random problems in homogenization», *Multiscale Modeling and Simulation: A SIAM Interdisciplinary Journal: A SIAM Interdisciplinary Journal*, (2011) 9 2 513-544 10.1137/10079639X

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Benchimol M., Benchimol P., Chappert B., De La Taille A., Laroche F., Meunier F., Robinet L., «Balancing the stations of a self-service bike hire system», *RAIRO-Operations Research*, (2011) 45 1 37-61 10.1051/ro/2011102

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Bourasseau E., Maillet J.-B., Desbiens N., Stoltz G., «Microscopic calculations of Hugoniot curves of neat TATB and of its

detonation products», *Journal of Physical Chemistry A*, (2011) 115 39 10729-10737  
10.1021/jp2047739

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Cacace S., Chambolle A., Monneau R., «A posteriori error estimates for the effective Hamiltonian of dislocation dynamics», *Numerische Mathematik*, (2011) 55 p.  
10.1007/s00211-011-0430-z

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Cancès E., Ehrlicher V., «Local defects are always neutral in the Thomas-Fermi-von Weizsäcker theory of crystals», *Archive for Rational Mechanics and Analysis*, (2011) 202 3 933-973 10.1007/s00205-011-0440-0

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Cances E., Ehrlicher V., Lelievre T., «Convergence of a greedy algorithm for high-dimensional convex nonlinear problems», *Mathematical Models and Methods in Applied Sciences*, (2011) 21 12 2433-2467  
10.1142/S0218202511005799

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Carlini E., Forcadel N., Monneau R., «A Generalized Fast Marching Method for dislocation dynamics», *SIAM Journal on Numerical Analysis*, (2011) 49 6 2470-2500  
10.1137/090770862

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Carpentier P., Chancelier J.-P., Cohen G., De Lara M., Girardeau P., «Dynamic consistency for Stochastic Optimal Control problems», *Annals of Operations Research*, (2011) 17 p.  
10.1007/s10479-011-1027-8

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Cérou F., Guyader A., Lelièvre T., Pommier D., «A multiple replica approach to simulate reactive trajectories», *Journal of Chemical Physics*, (2011) 134 5 054108 (16 pages)  
10.1063/1.3518708

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Chipot C., Lelièvre T., «Enhanced sampling of multidimensional free-energy landscapes using adaptive biasing forces», *SIAM Journal on Applied Mathematics*, (2011) 71 5 1673-1695 10.1137/10080600X

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Chopin N., Lelievre T., Stoltz G., «Free Energy Methods for Bayesian Inference: Efficient Exploration of Univariate Gaussian Mixture Posteriors», *Statistics and Computing*, (2011) 20 p. 10.1007/s11222-011-9257-9

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Dabo I., Kozinsky B., Singh-Miller N. E., Marzari N., «Erratum: Electrostatics in periodic boundary conditions and real-space corrections [Phys. Rev. B 77, 115139 (2008)]», *Physical Review B*, (2011) 84 15 2 p. 10.1103/PhysRevB.84.159910

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De Lara M., Gajardo P., Ramirez Cabrera H., «Viable harvest of monotone bioeconomic models», *Systems and Control Letters*, (2011) 60 3 192-197  
10.1016/j.sysconle.2010.12.004

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De Palma A., Kilani M., De Lara M., Piperno S., «Cordon pricing in the Monocentric city model: Theory and application to Ile-de-France», *Recherches Economiques de Louvain*, (2011) 77 2-3 105-124  
10.3917/rel.772.0105

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Di Pietro D. A., Ern A., «Analysis of a discontinuous Galerkin method for heterogeneous diffusion problems with low-regularity solutions», *Numerical Methods for Partial Differential Equations*, (2011) 17 p.  
10.1002/num.20675

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Dobson M., Luskin M., Ortner C., «Iterative methods for the force-based quasicontinuum approximation: Analysis of a 1D model problem», *Computer Methods in Applied Mechanics and Engineering*, (2011) 200 37-40 2697-2709 10.1016/j.cma.2010.07.008

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Doyen D., Ern A., «Analysis of the modified mass method for the dynamic Signorini problem with Coulomb friction», *SIAM Journal on Numerical Analysis*, (2011) 49 5 2039-2056 10.1137/100804711

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Doyen D., Ern A., Piperno S., «Time-integration schemes for the finite element dynamic Signorini problem», *SIAM Journal on Scientific Computing*, (2011) 33 1 223-249 10.1137/100791440

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Jourdain B., Roux R., «Convergence of a stochastic particle approximation for fractional scalar conservation laws», *Stochastic Processes and their Applications*, (2011) 121 5 957-988 10.1016/j.spa.2011.01.012

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Jourdain B., Lapeyre B., Sabino P., «Convenient Multiple Directions of Stratification», *International Journal of Theoretical and Applied Finance*, (2011) 14 6 867-897 10.1142/S0219024911006772

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Jourdain B., Vellekoop M., «[Regularity of the Exercise Boundary for American Put Options on Assets with Discrete Dividends](#)», *SIAM Journal on Financial Mathematics*, (2011) 2 538-561, DOI: 10.1137/100800889

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Pommaret J.-F., «Macaulay inverse systems revisited», *Journal of Symbolic Computation*, (2011) 46 9 1049-1069  
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Lelievre T., Minoukadeh K., «Long-time convergence of an Adaptive Biasing Force method: the bi-channel case», *Archive for Rational Mechanics and Analysis*, (2011) 202 1 1-34 10.1007/s00205-011-0426-y

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Samaey G., Lelievre T., Legat V., «A numerical closure approach for kinetic models of polymeric fluids: Exploring closure relations for FENE dumbbells», *Computers and Fluids*, (2011) 43 1 119-133  
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Li Y., Dabo I., «Electronic levels and electrical response of periodic molecular structures from plane-wave orbital-dependent calculations», *Physical Review B*, (2011) 84 15 11 p. 10.1103/PhysRevB.84.155127

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### Publications in other journal

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Jourdain B., Kohatsu-Higa A., «[A review of recent results on approximation of solutions of stochastic differential equations](#)», proceedings of WSAF09, Progress in Probability, (2011) 65, 141-165.

Maillet J.-B., Bourasseau E., Desbiens N., Vallverdu G., Stoltz G., «Mesoscopic simulations of shock-to-detonation transition in reactive liquid high explosive», *EPL (Europhysics Letters)*, (2011) 96 6 68007  
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### Article to appear

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A. ANANTHARAMAN, C. LE BRIS, Elements of mathematical foundations for a numerical approach for weakly random homogenization problems, in "Communications in Computational Physics", 2011, in press.

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Meunier F., «The chromatic number of almost stable Kneser hypergraphs», *Journal of Combinatorial Theory, Series A*, (2011) 118 6 1820-1828 10.1016/j.jcta.2011.02.010

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G. BENAROUS, Y. HU, S. OLLA, O. ZEITOUNI Einstein relation for biased random walk on Galton-Watson trees, in "Ann. I. H. Poincaré", 2011, to appear.

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Oberhuber T., Suzuki A., Žabka V., «The

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C. BERNARDIN, S. OLLA. Transport Properties of a Chain of Anharmonic Oscillators with random flip of velocities, in "J. Stat. Phys.", 2011, to appear

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A. CHAMBOLLE, E. LINDGREN, R. MONNEAU, The Holder infinite Laplacian and Holder extensions, accepted for publication in ESAIM-COCV.

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N. CHOPIN, T. LELIÈVRE , G. STOLTZ. Free energy methods for Bayesian inference: efficient exploration of univariate Gaussian mixture posteriors, in "Statist. Comput.", 2011, To appear, <http://hal.archives-ouvertes.fr/hal-00460914/fr/>.

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R. COSTAOUEC . Asymptotic expansion of the homogenized matrix in two weakly stochastic homogenization settings, in "Applied Math. Research Express", 2011, in press, <http://arxiv.org/abs/1102.3804>.

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N. FORCADEL, C. IMBERT, R. MONNEAU,

Homogenization of accelerated Frenkel-Kontorova models with n types of particles, accepted to Transactions of the AMS.

---

C. IMBERT, R. MONNEAU, H. ZIDANI, A Hamilton-Jacobi approach to junction problems and application to traffic flows, accepted to ESAIM-COCV.

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JOURDAIN B., SBAI M., High order discretization schemes for stochastic volatility models, accepté dans Journal of Computational Finance

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T. LELIÈVRE , M. ROUSSET, G. STOLTZ. Langevin dynamics with constraints and computation of free energy differences, in "Math. Comput.", 2011, in press, <http://hal.archives-ouvertes.fr/hal-00495517/fr/>.

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C. LIVERANI , S. OLLA. Toward the Fourier law for a weakly interacting anharmonic crystal, in "JAMS", 2011, to appear.

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R. MONNEAU, Introduction to the Fast Marching Method, accepted for publication in the proceedings of the summer school CIMPA 2010, Tripoli, Lebanon.

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R. MONNEAU, S. PATRIZI, Derivation of Orwan's law from the Peierls-Nabarro model, accepted to CPDE.

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### Book chapters

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A. ANANTHARAMAN, R. COSTAOUE C , C. LE BRIS , F. LE GOLL , F. THOMINES. Introduction to numerical stochastic homogenization and the related computational challenges: some recent

developments, Lecture Notes Series, Institute for Mathematical Sciences, National University of Singapore, 2011, vol. 22, 197.

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E. CANCE`S, M. LEWIN, G. STOLTZ. The microscopic origin of the macroscopic dielectric permittivity of crystals: A mathematical viewpoint, Lecture Notes in Computational Sciences and Engineering, Springer, 2011, vol. 82, p. 87-125.

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C. LEBRIS, F. THOMINES. A Reduced Basis approach for some weakly stochastic multiscale problems, Series in Contemporary Applied Mathematics, Higher Education Press and World Scientific publishing, 2011, submitted.

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F. LEGOLL, T. LELI`VRE. Some remarks on free energy and coarse-graining, Lecture Notes in Computational Sciences and Engineering, Springer, 2011, vol. 82, p. 279-329, <http://hal.inria.fr/hal-00511221>.

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### **Written communications in International conferences**

---

F. Casenave, N. Balin, G. Sylvand, "3D coupled resolution of acoustic waves between a potential and a uniform flow", WAVES 2011, Vancouver, Canada, July 2011

---

N. Chalhoub, A. Ern, T. Sayah, and M. Vohralik, "A posteriori error estimates for the convection-diffusion-reaction equation and the finite volume method", FVCA 2011, Prague, Czech Republic, June 2011

---

A. Ern, M. Vohralik,

"A unified framework for a posteriori error estimation in elliptic and parabolic problems with application to finite volumes", FVCA 2011, Prague, Czech Republic, June 2011

---

L. Monasse, V. Daru, C. Mariotti and S. Piperno, "A conservative coupling method for fluid-structure interaction in the compressible case", Proceedings of the sixth international conference on Computational Fluid Dynamics, ICCFD6, Saint Petersburg, Russia, July 2010

### **Invited talk in international conference**

---

M. De Lara :  
VII SEMBIOMAT, Universidad Nacional Mayor de San Marcos, Lima, Perú.

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M. De Lara :  
Congreso Latinoamericano de Biología Matemática, Armenia, Quindío, Colombia.

---

A. Ern, M. Vohralik :  
"A unified framework for a posteriori error estimation in elliptic and parabolic problems with application to finite volumes", FVCA 2011, Prague, Czech Republic, June 2011

---

A. Ern :  
"Implicit-explicit Runge-Kutta methods with stabilized finite elements for advection-diffusion equations", La Serena Numerica, Chili, Décembre 2011.

---

A. Ern :  
"Discontinuous Galerkin approximation of two-component miscible liquid-gas porous media flows", Linz, RICAM Special Semester conference, Septembre 2011.

---

R. Monneau,  
Free Boundary Problems, Theory and Applications, MSRI, Berkeley, USA, March 2011

---

R. Monneau,  
2 mini-courses in "Three days in PDE's", Univ. Roma Tor Vergata, Italy, April 2011

---

R. Monneau,  
2 mini-courses in the Spring School "Image Processing", Martel, France, April 2011

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R. Monneau,  
4 lectures during the conference "Weak KAM Theory in Italy", Cortona, Italy, September 2011

---

R. Monneau,  
Dynamical Optimization in PDE and Geometry Applications to Hamilton-Jacobi Ergodic Optimization, Weak KAM, Bordeaux, December 2011

#### **Invited talk in national conference**

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A. Ern,  
"Discontinuous Galerkin methods", Spring School on Computational Fluid Mechanics, June, Roscoff, France

#### **Platform presentation/presentation in international conference**

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I. Dabo, American Physical Society Meeting, March 2011, Dallas, United States

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I. Dabo, Electrochemical Society Meeting, May 2011, Montreal, Canada

#### **Platform presentation/presentation in national conference**

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I. Dabo, GDR coDFT, June 2011, Obernai

#### **Poster in international conference**

---

C. Lusso  
Roscoff, France, September 2011

---

M. Rousseau, O. Cerdan, A. Ern, O. Le Maître, P. Sochala,

RICAM Special Semester, Workshop 4, December 2011, Linz, Austria.

---

J. Tryoen,  
SAMHYP2011, Zurich, Switzerland, February 2011.

#### **Poster in national conference**

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D. Benoit, L. He, C. Le Bris, T. Lelièvre, SMAI 2011, May 2011, Guidel, France

---

N. Chalhoub, A. Ern, T. Sayah, M. Vohralik, SMAI 2011, May 2011, Guidel, France

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#### **Preprint-hal**

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Abbas-Turki L., Lapeyre B., «AMERICAN OPTIONS BASED ON MALLIAVIN CALCULUS AND NONPARAMETRIC VARIANCE REDUCTION METHODS», arXiv:1104.5131 hal-00589081, version 2

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Abraham R., Delmas J.-F., «Record process on the Continuum Random Tree», arXiv:1107.3657 hal-00609467, version 1

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A. Aftalion, F. Nier . Adiabatic approximation for a two-level atom in a light beam, in "Annales de la Faculté des Sciences de Toulouse: Mathématiques", 2011, submitted, <http://hal.archives-ouvertes.fr/hal-00641565/>.

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Cancès E., Stoltz G., «A mathematical formulation of the random phase approximation for crystals», arXiv:1109.2416 hal-00622929, version 1

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Casenave F., Ghattassi M., Joubaud R., «A Multiscale problem in thermal science», hal-00657838, version 1

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Chancelier J.-P., «Extensions and applications of ACF mappings», arXiv:1111.3464 hal-00640756, version 1

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I. Dabo. Resilience of gas-phase anharmonicity in the vibrational response of adsorbed carbon monoxide: limit to the reliability of surface electric-field models, in "J. Chem. Phys.", 2011, submitted.

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X. Dai , C. Le Bris , F. Le Goll , Y. Maday. Symmetric parareal algorithms for Hamiltonian systems, in "Mathematical Modelling and Numerical Analysis", 2011, submitted, <http://hal.archives-ouvertes.fr/hal-00541166/fr/>.

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De Lara M., Ocana Anaya E., Oliveros--Ramos R., Tam J., «Ecosystem Viable Yields», arXiv:1104.4266 hal-00587663, version 2

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Delmas J.-F., Hénard O., «A William's decomposition for spatially dependent superprocesses», arXiv:1106.3710 hal-00601539, version 1

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Dobson M., «There is no pointwise consistent quasicontinuum energy», arXiv:1109.1897 hal-00620875, version 1

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Dobson M., Le Bris C., Le Goll F.. Symplectic schemes for highly oscillatory Hamiltonian systems: the homogenization approach beyond the constant frequency case, in "IMA

Journal of Numerical Analysis", 2011, submitted, <http://hal.archives-ouvertes.fr/hal-00524814>.

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Ferretti A., Dabo I., Cococcioni , Marzari N.. Bridging density-functional and many-body perturbation theory: orbital-density dependence in electronic-structure functional, in "Phys. Rev. Lett.", 2011, submitted.

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He L., Le Bris C., Lelièvre T., «Periodic long-time behaviour for an approximate model of nematic polymers», arXiv:1107.3592 inria-00609763, version 1

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Imbert C., Monneau R., Zidani H., «A Hamilton-Jacobi approach to junction problems and application to traffic flows», arXiv:1107.3250 hal-00569010, version 3

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Jazar M., Monneau R., «Formal derivation of seawater intrusion models», hal-00572241, version 3

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Jeunesse M., Jourdain B., «Regularity of the American put option in the Black-Scholes model with general discrete dividends», hal-00633199, version 1

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Joubaud R., Stoltz G., «Nonequilibrium shear viscosity computations with Langevin dynamics», arXiv:1106.0633 hal-00598257, version 1

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Le Bris C. L., Lelièvre T., «Micro-macro models for viscoelastic fluids: modelling, mathematics and numerics», arXiv:1102.0325 hal-00562325, version 1

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Le Bris C., Legoll F., Thomines F., «Rate of convergence of a two-scale expansion for some "weakly" stochastic homogenization problems», arXiv:1110.5206 hal-00637493, version 1

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Le Bris C., Lelièvre T., Luskin M., Perez D., «A mathematical formalization of the parallel replica dynamics», arXiv:1105.4636 hal-00596161, version 1

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Y. LI , J . C. ZHENG, I . DABO. First-principles study of the magnetic, half-metal, and thermoelectric transport properties of inorganic-organic hybrid compounds [C<sub>4</sub>N<sub>2</sub>H<sub>12</sub>][Fe<sub>4</sub>(HPO<sub>3</sub>)<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>)<sub>3</sub>], in "The Journal of Chemical Physics", 2011, submitted.

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Leger R., «Couplage pour l'aéroacoustique de schémas aux différences finies en maillage structuré avec des schémas de type éléments finis discontinus en maillage non structuré», (2011-12-05) Serge Piperno École doctorale Mathématiques, Sciences et Technologies de l'Information et de la Communication (Paris-Est) pastel-00679119, version 1

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Lindgren E., Monneau R., «Pointwise estimates for the heat equation. Application to the free boundary of the obstacle problem with Dini coefficients», arXiv:1108.3161 hal-00614700, version 1

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Maillet J.-B., Vallverdu G., Desbiens N., Stoltz G., Bourasseau E., «Molecular Simulations of Shock to Detonation Transition in Nitromethane», arXiv:1107.3453 hal-00609415, version 1

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Martinet V., Gajardo P., De Lara M. and Ramírez Cabrera H., [Bargaining with intertemporal maximin payoffs](#), No 2011-7, EconomiX Working Papers from University of Paris West - Nanterre la Défense, EconomiX, 2011

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Meunier F., Neveu B., «Computing solutions of the paintshop necklace problem», hal-00601446, version 2

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Monneau R., Roquejoffre J.-M., Roussier-Michon V., «Travelling graphs for the forced mean curvature motion in an arbitrary space dimension», arXiv:1107.0896 hal-00606214, version 1

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Olla S., Sasada M., "Macroscopic energy diffusion for a chain of anharmonic oscillator", arXiv:1109.5297.

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Park C.-H., Ferretti A., Dabo I., Poilvert N., Marzari N., «Variational Minimization of Orbital-dependent Density Functionals», arXiv:1108.5726 hal-00617719, version 1

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## EDITORIAL BOARDS/ACTIVITY

---

Cancès E. is :

- co-Editor in chief (with P. Del Moral and J.-F. Gerbeau) (2005-) of ESAIM Proc.
  - a member of the editorial boards of Mathematical Modelling and Numerical Analysis (2006-) and of SIAM Journal of Scientific Computing (2008-). and of Communications in Mathematical Sciences (2011-).
- 

De Lara M. is :

- Environmental Modeling and Assessment (Springer), associate editor (2007-)
- 

Delmas J-F. is :

- Member of the editorial board of Applied Mathematics research express (2010-)
- 

Ern A. is :

- a member of the editorial board of SIAM Journal of Scientific Computing (2011-).
- 

Le Bris C. is :

- co-Editor-in-chief (with A.T. Patera, MIT) (2005-) of Mathematical Modeling and Numerical Analysis
- Editor-in-chief of Applied Mathematics Research Express (2003-)
- a member of the editorial boards of Archive for Rational Mechanics and Analysis (2004-), COCV (Control, Optimization and Calculus of Variations) (2003-), Mathematics in Action (2008-), Mathematics Applied in Science and Technology (2006-), Networks and Heterogeneous Media (2005-), Nonlinearity (2005-), Review of Mathematical Science (2006-), Journal de Mathématiques Pures et Appliquées (2009-).

- a member of the editorial board of the monograph series *Mathématiques et Applications, Series*, Springer (2008-), and *Modeling, Simulations and Applications, Series*, Springer (2009-).

---

Olla S. is :  
a member of the editorial boards of *Annals of Probability* and of *Probability theory and related fields*.

#### MEMBERS OF SCIENTIFIC COMMITTEES

---

Cancès E. is :  
a member of the executive committee of the CEA-EDF-INRIA schools in applied mathematics and computer science, and of the scientific committee of the GDR co-DFT.

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De Lara M. is :  
Outside member invited in the jury of the competitive entrance examination of the researchers (CR2) of INRIA Saclay

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Ern A. is :  
Member of the Scientific Committee of ANDRA (2005-).

---

Jourdain B., is :  
Member of the scientific committee of the conference *Modeling and managing financial risks*, Paris 10-13 January 2011

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Le Bris C. is :  
a member of :  
- the Scientific Program Committee of ICIAM 2011, Vancouver, Canada,  
- the scientific board of ENPC, 2008- (nominated as representative of the research scholars),

- the Comité d'experts for the *Fondation de Recherche pour l'Aéronautique et l'Espace*,  
- the Comité d'animation du domaine thématique *Mathématiques appliquées, calcul et simulation* at INRIA,  
- the International Scientific Advisory Committee of the Centre de Recherche *Mathématique*, Université de Montréal,  
- the Advisory Board of the DFG Cluster of Excellence *Engineering of Advanced Materials*, Erlangen,  
- the International Scientific Advisory Board of the DFG research center *Matheon*, Berlin.  
- Conseil de perfectionnement du Master de *Mathématiques* de l'Université Pierre et Marie Curie.

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Nier F. is :  
a member of the scientific committee of  
- the workshop "Spectral Analysis of Non-Selfadjoint operators", ANR NONAa, CIRM, December 2011,  
- the workshop "Mathematics for semiconductor heterostructure 2012" WIAS-Berlin, September 2012,  
- the CNRS-GDR "Dynamique Quantique" led by S. de Bièvre.

#### CONFERENCES/SEMINARS/MISSIONS/VISITS

---

E. Cancès, Lectures (6h) on molecular modelling, Université de Versailles-St Quentin, March 2011

---

C. Le Bris, Lectures on Stochastic homogenization, Series of 4 one-hour lectures, Colloque "Marches aléatoires, Milieux aléatoires", Roscoff, June 2011

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C. Le Bris, Lectures on Stochastic homogenization, Series of 3 one-hour lectures, Third International Riemann International School of Mathematics, "Free Surface, Multiphase and Multiphysics Problems", Verbania on the Lago Maggiore, September 2011

---

C. Le Bris, Lectures on Stochastic homogenization, Series of 3 one-hour lectures, National University of Singapore, December 2011,

---

Monneau R.  
4 Lectures in Wroclaw University (Poland)

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Monneau R.  
3 Lectures in the "Institut of Applied Physics and Computational Mathematics", Beijing, China

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Monneau R.:  
Lebanese University, invited one week in January, one week in February, one week in November

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### **Conferences/participation**

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### **International conferences Communications**

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A. Alfonsi : Modeling and managing financial risks Paris, 10-13 January 2011  
<http://www.cmap.polytechnique.fr/financialrisks/conference2011/organizing.html>

---

A. Alfonsi, Vancouver, ICIAM 2011, High Frequency Modeling & Algorithmic Trading minisymposium. <http://www.iciam2011.com/>

---

A. Alfonsi, Vancouver, ICIAM 2011, Session MS368: Computational Methods in Finance. <http://www.iciam2011.com/>

---

A. Alfonsi , Leicester, ENUMATH 2011.  
<http://www2.le.ac.uk/departments/mathematics/research/enumath2011>

---

A. Alfonsi , Annual Financial Market Liquidity Conference Budapest, Hungary.

[http://www.uni-corvinus.hu/index.php?id=liquidity\\_ws&no\\_cache=1](http://www.uni-corvinus.hu/index.php?id=liquidity_ws&no_cache=1)

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S. Boyaval, workshop on Reduced basis methods in high dimensions, Paris, June 2011,

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S. Boyaval, ICIAM, minisymposium Reduced-Basis methods, Vancouver, Canada, July 2011,

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S. Boyaval, CEMRACS, SimTech Workshop on Current Trends in Computational Fluid Mechanics, Marseille, August 2011,

---

S. Boyaval, workshop Numerical Analysis of Multiscale Problems and Stochastic Modelling, RICAM Linz, Austria, December 2011,

---

E. Cancès, workshop on computational challenges in partial differential equations, Swansea, United Kingdom, April 2011,

---

E. Cancès, workshop Polaritons 2011, CIRM, Marseille, April 2011,

---

E. Cancès, summer program on electronic structure analysis, Shanghai, China, June 2011,

---

E. Cancès, MFO workshop on mathematical methods in quantum chemistry, Oberwolfach, Germany, June 2011,

---

E. Cancès, ICIAM 2011, Vancouver, Canada, July 2011,

---

E. Cancès, Minisymposium on mathematics in materials science, Beijing, China, September 2011,

---

E. Cancès, distinguished professor lecture, Chinese Academy of Sciences, Beijing, China, September 2011,

---

P. Carpentier, J.-Ph. Chancelier, G. Cohen, M De Lara, P. Girardeau. Dynamic consistency for stochastic optimal control problems with risk constraints. COPI 2011. Paris 23-25 Nov 2011

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P. Carpentier, J.-Ph. Chancelier, G. Cohen. Optimal control under probability constraint. COPI 2011. Paris 23-25 Nov 2011.

---

P. Carpentier, J.-Ph. Chancelier, G. Cohen. Optimal control under probability constraint. SADCO Workshop Ensta ParisTech.

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N. Chalhoub : Finite volume for complex applications conference 2011, Czech Republic Prague

---

D. Chemla, F. Meunier, T. Pradeau, R. Wolfler Calvo, H. Yahiaoui: 2011 INFORMS Annual Meeting, Charlotte, USA.

---

R. Costeaouec, ICIAM 2011 conference, Vancouver, July 2011,

---

R. Costeaouec, Workshop Random Media: Homogenization and Beyond, IPAM, Los Angeles, January 2011,

---

I. Dabo, First-principles surface chemistry under applied voltage (contributed oral presentation), Electrochemical Society Meeting, Montreal, May 2011,

---

I. Dabo, American Physical Society Meeting, Dallas, March 2011,

---

M. De Lara : "Control Theory and Viability Methods for the Sustainable Management of Natural Resources", Minisymposium Optimization in economics, Austrian-French-German conference on Optimization AFG'11, Toulouse, France.

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M. Dobson, RSME2011 conference, Avila,

February 2011,

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M. Dobson, ICIAM 2011 conference, Vancouver, July 2011,

---

M. Dobson, 11th USNCCM conference, Minneapolis, July 2011,

---

M. Dobson, AMS von Neumann Symposium on Multimodel and Multialgorithm Coupling for Multiscale Problems, Snowbird, July 2011.

---

M. Dobson, workshop Nonequilibrium Processes, Obergurgl, Austria, August 2011,

---

V. Ehrlacher, ICIAM 2011, Vancouver, Canada, July 2011,

---

V. Ehrlacher, ENUMATH 2011, Leicester, United Kingdom, September 2011,

---

V. Ehrlacher, BIRS workshop on Density Functional Theory: fundamentals and applications in condensed matter physics", Banff, Canada, January 2011,

---

V. Ehrlacher, IMA workshop on Large-scale Inverse Problems and Quantification of Uncertainty, Minneapolis, United States, June 2011,

---

V. Ehrlacher, MFO workshop on mathematical methods in quantum chemistry, Oberwolfach, Germany, June-July, 2011,

---

A. Ern, 16<sup>th</sup> International Conference on Finite Elements in Flow Problems, Munich, Allemagne, Mars 2011.

---

A. Ern, ICIAM Conference, Mini-symposium on Discontinuous Galerkin methods, Vancouver, Canada, Juillet 2011.

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A. Ern, ICIAM Conference, Mini-symposium on A posteriori error analysis and mesh adaptation, Vancouver, Canada, Juillet 2011.

---

A. Ern : Enumath Conference, Mini-symposium on Advanced finite element

techniques for nonlinear evolution problems, Leicester, September 2011.

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A. Ern : Enumath Conference, Minisymposium on Stabilization Mechanisms for Convection-Dominated Problems, Leicester, September 2011.

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J. Infante Acevedo: 4<sup>th</sup> Workshop on High-Dimensional Approximation, 2011, Bonn, Germany, [http://hda2011.ins.uni-bonn.de/talks/abstract.php?a=Infante\\_Acevedo](http://hda2011.ins.uni-bonn.de/talks/abstract.php?a=Infante_Acevedo)

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R. Joubaud : Enumath Conference 2011, Leicester, Mini-symposium: Numerical Methods for Molecular Dynamics, September 2011

---

B. Jourdain : Conference Modeling and Managing Financial Risks, Paris, 10-13 January,

---

B. Jourdain : Seventh Seminar on Stochastic Analysis, Random Fields and Applications, Ascona, 23-27 May

---

C. Le Bris, plenary lecture, International conference on "Frontiers of Computational and Applied Mathematics", Peking University, Beijing China, October 2011,

---

C. Le Bris, keynote lecturer, joint MIT (CCE) - Politecnico di Milano (MOX) workshop, "Reduction Strategies for the Simulation of Complex Problems", Milano, January 2011,

---

C. Le Bris, INI/WIMCS Joint Follow-Up Meeting on Computational challenges in partial differential equations, Swansea University, April 2011,

---

C. Le Bris, "The ACMAC workshop on Stochastic Partial Differential Equations", Heraklion, Crete, June 2011,

---

C. Le Bris, Sino-French Workshop on Contemporary Applied Mathematics, Fudan University, Shanghai, July 2011,

---

C. Le Bris, ICIAM conference, Minisymposium on Reduced basis methods and their applications, Vancouver, Canada, July 2011,

---

C. Le Bris, ICIAM conference, Minisymposium on Coupling Atomistic and Continuum Simulations: Coping with Length and Time Scales, Vancouver, Canada, July 2011,

---

C. Le Bris, ICIAM conference, Minisymposium on multiscale interaction between microscopic and continuum scales, Vancouver, Canada, July 2011,

---

C. Le Bris, Workshop on Partial Differential Equations in Mathematical Physics and their Numerical Approximation, Levico Terme (Trento, Italy), September 2011,

---

C. Le Bris, Workshop Modern Techniques in the Numerical Solution of Partial Differential Equations, Heraklion, Crete, September 2011.

---

C. Le Bris, Minisymposium on mathematics in materials science, Beijing, September 2011,

---

C. Le Bris, Modern Trends in PDE's, Geometric Analysis and Mathematical Physics, University of Cergy-Pontoise, September 2011,

---

C. Le Bris, Workshop on Control and Optimization of PDEs, Graz, October 2011,

---

C. Le Bris, Workshop Modeling of defects, Singapore, December 2011,

---

C. Le Bris, Penn State University Math Colloquium, 2011,

---

C. Le Bris, NCMIS Distinguished Lecture Series National Center for Mathematics and Interdisciplinary Science, Chinese Academy of Sciences, 2011,

---

T. Lelièvre, Meeting on Computational Challenges in Partial Differential Equations, Swansea University, April 2011,

---

T. Lelièvre, Workshop on complexity and computational methods in statistics, Sante

Fe, April 2011,

---

T. Lelièvre, Workshop on Macroscopic Modeling of Materials with Fine Structure, Carnegie Mellon University, Pittsburgh, May 2011,

---

T. Lelièvre, Workshop Coarse-graining of many-body systems: analysis, computations and applications, University of Crete, Greece, June 2011,

---

T. Lelièvre, ICIAM 2011, Vancouver, July 2011,

---

T. Lelièvre, Plenary speaker at the ENUMATH conference, University of Leicester, September 2011,

---

T. Lelièvre, Minisymposium on Mathematics in Materials Science, Pekin, September 2011,

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T. Lelièvre, Workshop on Nucleation and Rare Events, Pekin, September 2011,

---

T. Lelièvre, Workshop Reduced Basis, POD or PGD-Based Model Reduction Techniques, Cachan, November 2011,

---

T. Lelièvre, Workshop on Multiscale Systems: Theory and Applications, Warwick, December 2011,

---

M. Rousseau, O. Cerdan, A. Ern, O. Le Maître, P. Sochala SIAM Conference on Mathematical & Computational Issues in the Geosciences, March 2011, Long Beach, California USA.

---

G. Samaey, SIAM Conference on Applications of Dynamical Systems, Snowbird, Utah, May 2011,

---

G. Samaey, Making it Real Seminar, Bristol University, May 2011,

---

G. Samaey, von Neumann Symposium, Snowbird, Utah, July 2011,

---

G. Stoltz, Summer school on Electronic Structure Analysis and Computation,

Shanghai Jiao Tong University, China, June 2011

---

G. Stoltz, ICIAM, Vancouver, Canada, July 2011,

---

G. Stoltz, Molecular Kinetics, Berlin, Germany, September 2011,

---

G. Stoltz, Minisymposium on mathematics in materials science, Beijing, China, September 2011,

---

G. Stoltz, journée CECAM on modeling of matter, Paris, December 2011,

---

G. Stoltz, Workshop on Multiscale Systems: Theory and Applications, Warwick, December 2011,

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### **National conferences communications**

D. Benoit, Congrès SMAI 2011, Guidel, France, May 2010,

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D. Chemla, F. Meunier, R. Wolfler Calvo: ROADEF Conference, March 2011.

---

R. Costauouec, Congrès SMAI 2011, Guidel, May 2011,

---

A. Ern, "Weighted discontinuous Galerkin methods", Workshop on advanced numerical methods for Flow problems, Marseille, September 2011.

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R. Joubaud Congrès SMAI, 5e Biennale Française des Mathématiques Appliquées, Guidel, Mini-symposium: Méthodes



numériques pour la simulation moléculaire,  
May 2011

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T. Lelièvre, Journées scientifiques MoMaS,  
Marseille, November 2011,

---

T. Lelièvre, Workshop Interactions  
EDPs/Probas, GDR CHANT, Grenoble,  
November 2011,

---

L. Monasse, V. Daru, C. Mariotti, S. Piperno,  
C. Tenaud,  
SMAI 2011, May 2011, Guidel, France

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F. Nier, Journée de la Fédération CNRS  
Amiens-Reims-Compiègne", November 2011 ,

---

F. Nier, Mathematics-Physics meeting around  
Bose-Einstein Condensates, ANR Volquan,  
Versailles, December 2011,

### Conference organization

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E. Cancès has organized or co-organized :  
- a BIRS workshop on Density Functional  
Theory: fundamentals and applications in  
condensed matter  
physics, Banff, Canada, January 2011,  
- a thematic minisymposium on electronic  
structure calculation at ICIAM 2011,  
Vancouver, Canada,  
July 2011,  
- a minisymposium on mathematics in  
materials science, Beijing, China, September  
2011.

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E. Cancès and G. Stoltz have co-organized  
the workshop "Interactions between PDEs  
and probability theory", held in Grenoble,  
France, 23-25 november 2011, in the frame-  
work of the GdR CHANT.

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M. De Lara has co-organized the École de  
printemps of the interdisciplinary network  
M3D (Porquerolles, April 2011).

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A. Ern has co-organized the Indo-European  
Winter School on Advances in Computational  
Partial Differential Equations (Goa, India,  
February 2011).

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C. Le Bris has co-organized, with M.P. Calvo  
(University of Valladolid, Spain) the minisym-  
posium "Numerical integrators of Hamiltonian  
systems and related problems", Centennial  
congress of the Spanish Royal  
Mathematical Society, February 1-5, 2011,  
Avila.

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T. Lelièvre co-organized a minisymposium on  
"Numerical Methods for Molecular Dynamics"  
at the ENUMATH 2011 conference (Septem-  
ber 2011), and a workshop on "Metastability  
and stochastic processes" at Ecole des Ponts  
(September 2011).

---

F. Meunier has organized the Annual meeting  
of the "Groupe transport et logistique" of the  
GDR RO (Institut Henri Poincaré, June 2011).

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R. Monneau:

- has co-organized the conference "Gestion  
des ressources en eau sur les côtes  
libanaises, une approche mathématique",  
(Tripoli, Lebanon, May 2011)
- has co-organized the conference  
"Ginzburg-Landau equations, Dislocations and  
Homogenization", (Ile de Ré, France, May  
2011)
- has co-organized the conference "Fronts  
and Nonlinear PDEs; A tribute to Henri  
Berestycki", (Paris, France, June 2011)

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S. Olla organized with Carlangelo Liverani a  
workshop on "Fourier's Law" at the Field In-  
stitute, Toronto in April 2011.

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G. Stoltz co-organized a minisymposium on  
"Numerical methods in molecular simulation"  
at the SMAI 2011 meeting, in Guidel, France  
(may 2011).

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## **International seminar**

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A. Alfonsi,  
"Exact and High order discretization schemes for Wishart processes and their affine extensions", Mannheim University seminar.

---

E. Cancès, "weekly seminar of the chemistry department", University of Pisa, Italy, October 2011,

---

M. De Lara :  
"El Medio Ambiente: Problemáticas, Desafíos y Perspectivas", Coloquio Internacional Embajada de Francia, Bucaramanga, Colombia.

---

M. De Lara :  
"Métodos de viabilidad para el manejo sustentable de recursos renovables", Catedra Europa 2011, Universidad del Norte, Barranquilla, Colombia.

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M. De Lara :  
"Optimización dinámica para el problema de extracción de minas en tajo abierto", Catedra Europa 2011, Universidad del Norte, Barranquilla, Colombia.

---

M. De Lara :  
"Métodos de viabilidad para el manejo sustentable de recursos renovables", Universidad de Medellin, Colombia.

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M. De Lara :  
"Métodos de viabilidad para el manejo sustentable de recursos renovables", Universidad de la Salle, Bogota, Colombia.

---

M. De Lara :  
"Control Theory and Viability Methods for the Sustainable Management of Natural Resources", Bren School of Environmental Science and Management, University of California Santa Barbara, USA.

---

M. De Lara :  
"When biases under risk are optimal under uncertainty and learning:

overestimation of low probabilities and status quo bias", Center for Evolutionary Psychology, University of California Santa Barbara, USA.

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M. De Lara :  
Dias de la Ciencia Aplicada-EAFIT, Medellin, Colombia.

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A. Ern :  
« Discontinuous Galerkin methods for problems with contrasted coefficients », University of Magdeburg, Germany, October 2011.

---

A. Ern,  
« Mathematical issues in radioactive waste storage », University of Udine, Italy, April 2011.

---

A. Ern,  
"Adaptive spectral stochastic methods for uncertain hyperbolic systems", University of Muenster, Germany, March 2011.

---

G. Samaey,  
Applied Mathematics and Mathematical Physics Seminar, Imperial College, London, June 2011,

## **National seminar**

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A. Alfonsi :  
"Exact and High order discretization schemes for Wishart processes and their affine extensions", Université d'Evry.

---

A. Alfonsi :  
"Efficient simulation schemes for some multidimensional stochastic volatility models", Petits déjeuners de la Finance, ILB.

---

N. Balin, F. Casenave :  
"Advanced methods in computational acoustics", Workshop Airbus Sound & Vibration, Toulouse, November 2011

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S. Boyaval, séminaire Université de Lille, January 2011,

---

E. Cancès, weekly seminar of the mathematics department, University of Grenoble, February 2011,

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E. Cancès, weekly seminar of the mathematics department, University of Nice, March 2011,

---

E. Cancès, weekly seminar of the mathematics department, University of Créteil, May 2011,

---

E. Cancès, weekly seminar of the chemistry department, University of Lille, November 2011,

---

F. Casenave, M. Ghattassi, R. Joubaud : "A multiscale problem in thermal science", CEMRACS 2011, Marseille, August 2011

---

I. Dabo, CEA Seminar, CEA, Saclay, September 2011,

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I. Dabo, CEA Seminar, CEA, Grenoble, September 2011,

---

I. Dabo, LPICM Seminar, Ecole Polytechnique, Palaiseau, April 2011,

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I. Dabo, GDR coDFT, Obernai, June 2011,

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I. Dabo, "Charge-carrier levels in materials from first principles", Ecole Polytechnique, Palaiseau.

---

I. Dabo, "Koopmans' theorem and orbital-dependent density functionals", CEA, Grenoble.

---

I. Dabo, "Computational electronic-structure description of periodic molecular structures: reconciling Gaussians with plane waves", CEA, Saclay

---

M. De Lara, "Théorie du contrôle et viabilité pour la gestion durable des ressources naturelles", CMAP Seminar, Ecole Polytechnique.

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M. De Lara, "Théorie du contrôle et viabilité pour la gestion durable des ressources naturelles", Probabilités-Statistiques-Contrôle Seminar, ENSTA.

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M. De Lara, "Théorie du contrôle et viabilité pour la gestion durable des ressources naturelles", Chaire Optimisation et développement durable, Ecole Polytechnique.

---

M. De Lara, "Théorie du contrôle et viabilité pour la gestion durable des ressources naturelles", INRIA Rhône-Alpes.

---

M. De Lara, "Viabilité stochastique", Réseau M3D  
École de printemps, Porquerolles.

---

M. De Lara, "When biases under risk are optimal under uncertainty and learning: overestimation of low probabilities and status quo bias", Economic Theory Workshop, Paris School of Economics.

---

A. Ern, "Implicit-explicit Runge--Kutta methods with stabilized finite elements for advection-diffusion equations", Marseille, April 2011.

---

A. Ern, "Méthodes de Galerkin discontinues pour des problèmes hétérogènes", Pau, Octobre 2011.

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R. Joubaud, Colloque final ANR METHODE, Orléans, Juin 2011;

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R. Joubaud, Modélisation en électrocinétique et milieux poreux, Lyon, Juin 2011;

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R. Joubaud, Meeting of CFCAM, Modeling of Matter, December 2011;

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B. Jourdain, Applied mathematics seminar of the collège de France

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B. Jourdain, Probability theory, Statistics and control seminar at ENSTA

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B. Jourdain, "Mathematical Finance, Numerical probability and Statistics of random processes working group"

---

T. Lelièvre, Séminaire du CMAP, Ecole Polytechnique, May 2011,

---

R. Monneau, "Hamilton-Jacobi equations on a junction and application to traffic", Groupe de travail "Calcul des variations", CMAP, Ecole Polytechnique, November 2011

---

R. Monneau, "Hamilton-Jacobi equations on a junction and application to traffic", Séminaire Univ. Lyon, November 2011

---

F. Nier, weekly seminar of the mathematics department, University of Créteil, December 2011,

---

G. Samaey, Séminaire de mathématiques appliquées, Collège de France, Paris, May 2011,

---

G. Stoltz, weekly seminar of the mathematical physics group, Université de Cergy, November 2011,

---

J. Tryoen, "Adaptive stochastic spectral method for uncertain hyperbolic systems, PRECISE Seminar, CEA/DAM, Bruyères le Châtel"

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J. Tryoen, "Adaptive stochastic spectral method for uncertain hyperbolic systems, LCR MANON Seminar, LJLL, UPMC, Paris"

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### **Seminar organization**

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A. Alfonsi is co-organizing the seminar on "Stochastic methods and finance" which is

common with UPEMLV and INRIA Mathfi project-team.

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A. Le Guilcher is co-organizing the CERMICS seminar of scientific computing, bi-monthly generalist seminar

<http://cermics.enpc.fr/seminaires/cs/seminaire.html>

### **Other scientific animation**

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#### **Scientific expertise**

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M. De Lara : invited to participate to the Centre d'analyse stratégique Commission headed by C. Gollier on "risks calculus in Public investments".

### **EDUCATION ACTIVITIES**

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#### **SUPERVISION ACTIVITY**

#### **HdR defended**

---

Chancelier J.-Ph. Contributions to optimal control of dynamical systems numerical aspects and applications.

#### **Theses defended**

---

Ahdida A., « Matrix valued processes : simulation and dependence modelling in finance », (2011-12-1) Aurélien Alfonsi, ED MSTIC, pastel-00674813, version 1

---

Costaouec R., « Numerical techniques for homogenization : application to random materials », (2011-11-23) Claude Le Bris, ED MSTIC, pastel-00674957, version 1

---

---

Monasse L., « Analysis of a discrete element method and coupling with a compressible fluid flow method », (2011-10-10) Serge Piperno ED MSTIC, pastel-00672342, version 1

---

Tryoen J. "Adaptive stochastic Galerkin methods for parametric uncertainty propagation in hyperbolic systems", (2011-11-21) Alexandre Ern and Olivier Le Maitre, ED MSTIC

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### Ongoing theses

---

J-C. Alais,  
Risk and optimization for the management of energies, PhD advisor: M. De Lara. ED MSTIC

---

M. Al Haj,  
Analysis of elasto-visco-plastic models including dislocation dynamics modeling, advisors: R. Talhouk, H. Ibrahim and R. Monneau. ED MSTIC

---

D. Benoit,  
Numerical methods for the simulation of non-newtonian fluids with applications to debris flows. PhD advisors: C. Le Bris and T. Lelièvre. ED MSTIC

---

F. Casenave,  
Non-parametric uncertainties in aeroacoustics and vibroacoustics problems, dir A. Ern and T.Lelièvre. ED MSTIC

---

N. Chalhoub,  
A posteriori error analysis for finite volume approximations of unsteady transport problems, dir. A. Ern and T. Sayah, ED MSTIC

---

D. Chemla, Algorithms for an optimized management of self-service transport, dir. F. Meunier, UPE, ED MSTIC.

---

G. Chmaycem,  
Analysis and simulation of a model for seawater intrusion, advisors: M. Jazar and R. Monneau, ED MSTIC

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G. Costeseque,  
Traffic modeling: from microscopic to macroscopic, advisors: J.-P. Lebacque and R. Monneau, ED MSTIC

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V. Ehrlacher ,  
Modelisation and simulation of photo-electrical phenomena and Uncertainty quantification in contact problems. PhD advisors: E. Cancès and T. Lelièvre. ED MSTIC

---

D. El Kass,  
Micro-macro analysis of nanotubes and dislocations, PhD advisors M. Jazar and R. Monneau. ED MSTIC

---

O. Henard,  
Multitype trees, PhD advisor J-F Delmas. ED MSTIC

---

J. Infante Acevedo, « Numerical methods for liquidity risk and pricing »  
PhD advisors: A. Alfonsi and T. Lelièvre. ED MSTIC

---

R. Joubaud,  
Multiscale modeling of clays, dir A. Ern and T. Lelièvre, ED MSTIC

---

S. Lahbabi,  
Mathematical study of quantum material with random defaults,  
PhD advisors: E. Cancès and M. Lewin. ED EM2C

---

V. Leclere,  
Risk, optimization, large systems, ED MSTIC.  
PhD advisor: M. De Lara. ED MSTIC

---

A. Le Guilcher,  
Front propagation methods and applications, advisors: A. Chambolle and R. Monneau. ED MSTIC

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C. Lusso,  
Effective vertical velocity profiles  
in gravitational flows, dir. F. Bouchut and A.  
Ern, ED MSTIC

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J. Mint Moustapha,  
Study and characterization of vehicles pla-  
toon on heavy traffic roads, B. Jourdain and  
D. Daucher. ED MSTIC

---

D. Mohia,  
Exact algorithms for multidimensional loading  
problems with order constraints, dir. F.  
Meunier, ED MSTIC

---

L. Paszkowski,  
Analytic and numerical study of dislocation  
dynamics,  
advisors: P. Biler and R. Monneau

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M. Rousseau,  
Uncertainties in overland flow and erosion  
modeling,  
dir. A. Ern, ED MSTIC

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L. Sepulveda,  
Mathematical viability methods for supervi-  
sion and control of  
endemic diseases of south-west Colombia.  
PhD advisors: M. De Lara and O. Vasilieva  
(Univ. del Valle, Cali, Colombia). ED MSTIC

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F. Thomines,  
Multi-scale numerical approaches :  
Application to homogenization of random  
materials and discrete-to-continuum coupling  
methods. PhD advisors: C. Le Bris and F.  
Legoll. ED MSTIC

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J. Reygner  
Large deviations of the current in some  
aerogel models, PhD advisors: L. Zambotti  
and B. Jourdain. ED MSTIC

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## TEACHING ACTIVITIES

### Courses at ENPC

---

A. Ahdida , O. Hénard, M. Jeunesse, B.  
Jourdain (professor in charge) , J. Reygnier,  
Probability theory and statistics, first year

---

A. Alfonsi, T. Lelièvre : Modelling, Program-  
ming and simulating, second year.

---

E. Cancès professor in charge, V. Ehracher, L.  
Monasse, R. Monneau,  
Analysis, first year.

---

F. Casenave, A. Ern professor in charge, G.  
Stoltz, M. Dobson,  
Scientific Computing, first year

---

J-P. Chancelier, course manager  
Optimization and control, 2<sup>nd</sup> year

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J-P. Chancelier, course manager  
Hazard Modelling, 2<sup>nd</sup> year

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J-P. Chancelier, M. De Lara, (professor in  
charge)  
Training in Scientific software Scicoslab.

---

I. Dabo, R. Joubaud, C. Lusso,  
Linux / Emacs / Scilab / Latex (First Year)

---

I. Dabo,  
Statistical and quantum physics projects

---

M. De Lara, professor,  
Modelling for the Sustainable Management of  
Natural Resources

---

M. De Lara, professor,  
Economics of Risk, Climate Change and Biod-  
iversity

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J.-F. Delmas, B. Jourdain,  
Jump processes with applications to energy  
markets, 3rd year ENPC and Master  
Recherche Mathématiques et Application,  
university Paris-Est Marne-la-Vallée

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B. Jourdain, B. Lapeyre,  
Monte-Carlo methods in finance, 3rd year  
ENPC and Master Recherche Mathématiques  
et Application, university Paris-Est Marne-la-  
Vallée

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T. Lelievre, professor  
Deterministic methods in mathematical  
finance.

---

F. Meunier, professor  
Operational research.

---

G. Stoltz,  
Spectral analysis

---

G. Stoltz,  
Computational statistical physics

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### Courses at UPE

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A. Alfonsi,  
Data analysis in finance : statistical  
approach, calibration, Master MAF.

---

A. Alfonsi,  
Risk measure in finance, ENPC, Master MAF,  
Master finance UPMC.

---

I. Dabo,  
Introduction to scientific computing,  
ED MSTIC, Université Paris-Est

---

G. Stoltz,  
Computational Statistical Physics, Master  
SMCD, Ecole des Ponts ParisTech

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### Courses at Paris Tech

---

A. Alfonsi,  
ENSTA: Calibration, stochastic and local  
volatility.

---

D. Benoit,  
Practical course teaching for "Introduction to  
Scientific computing", ENSMP C1003, MINES  
ParisTech

---

D. Benoit, M. Dobson, G. Stoltz, C. Lusso  
Scientific Computing, ENSMP C1003, MINES  
ParisTech

---

D. Benoit, M. Dobson, G. Stoltz  
Introduction to scientific computation, M1,  
Ecole des Mines ParisTech.

---

E. Cancès,  
Professeur chargé de cours at l'École  
Polytechnique (Numerical analysis and  
optimization)

---

M. De Lara :  
Network Optimization Renewable

---

J.-F. Delmas,  
Professeur chargé de cours at l'École  
Polytechnique  
(Random walk, Introduction to probability  
and simulation)

---

J.-F. Delmas,  
Introduction to Probability and Statistics  
(ENSTA, 1A)

---

A. Ern,  
Professeur chargé de cours at l'Ecole  
Polytechnique (Numerical analysis and  
optimization)

---

B. Jourdain,  
Professeur chargé de cours at l'Ecole  
Polytechnique (Introduction to probability  
theory, Stochastic numerical methods,  
projects in finance)

---

C. Le Bris  
Professeur chargé de cours at l'École  
Polytechnique (Numerical analysis and  
optimization)

---

C. Lusso, J. Tryoen,  
Practical course teaching for « Introduction to  
Scientific Computing », ENSMP, C1003, Mines  
Paris Tech

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J. Tryoen,  
Supervisor for FreeFem++ projects for the  
"Finite Element" course, ENSMP S3733/5,  
MINES ParisTech

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### **Other courses**

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D. Benoit et I. Dabo,  
Informatique, 50h, L2, CPGE Jean-Baptiste  
Say.

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E. Cancès, Mathematical methods in quantum  
chemistry, M2, University Paris 6.

---

R. Costaouec,  
Linear optimization and convexity, L3,  
Université Paris 6.

---

M. De Lara,  
"Mathematical Models for the Sustainable  
Management of Natural Resources", [Master  
EDDEE](#) (Economie du Développement  
Durable, de l'Environnement et de l'Energie)

---

M. De Lara,  
"Mathematical Models for the Sustainable  
Management of Natural Resources", [Master  
Mathématiques, Informatique et Applications](#)

---

M. De Lara,  
"Mathematics, Economics and Risk  
Psychology", [Master Ingénierie du Risque :  
Finance et Assurances \(IRFA\)](#)

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A. Ern,  
Discontinuous Galerkin methods, 10 hours,  
BIRS Institute, Goa, India.

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A. Ern,  
Discontinuous Galerkin methods, 4 hours,  
University of Magdeburg, Germany.

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A. Ern,  
Finite volume and finite element methods, 6  
hours, University of Udine, Italy.

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R. Joubaud,  
Vector analysis(Paris 6, L2)

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S. Lahbabi,  
Mathematics for biologists, L2, University of  
Cergy Pontoise.

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S. Lahbabi,  
Formation "C2i" (Certificat Informatique et  
Internet), L2, University of Cergy Pon-  
toise, France

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T. Lelièvre,



Stochastic numerical methods, M2  
Mathématiques et Applications, Master  
Université Pierre et Marie Curie.

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C. Lusso,  
Vector calculus, L1 Maths-Info, Université  
Paris 6

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C. Lusso,  
Numerical analysis and optimizatio, 3A,  
ESIEE-Engineering

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F. Meunier,  
Master MPRO: Optimization in graphs

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## INDUSTRIAL PARTNERSHIPS

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### CONTRACTS

#### New public contracts

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Michel De Lara,  
OVIMINE, Optimization and viability in min-  
ing, STIC-AmSud project (CNRS, INRIA,  
ministère des Affaires étrangères) with Peru  
and Chile.

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- the ANR MANIF has been accepted in June  
2011. It focuses on the mathematical and  
numerical analysis of electronic structure  
models, such as, in particular, the Kohn-  
Sham model. It includes two research teams:  
researchers from the JL Lions Laboratory  
(Paris 6) and the Micmac team.  
Head : E. Cancès.

#### Ongoing public contracts

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ANR-08-BLAN-0190 A3 (Random trees and  
applications), Partenars: Univ. Nancy, Univ. Orléans  
and Univ. Bordeaux. Head: J.-F. Delmas.

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ANR MEGAS (methods for numerical  
simulation, with an emphasis on sampling  
methods). Partenars : the INRIA project IPSO  
in Rennes, the INRIA project SIMPAF in Lille,  
the eDAM team in Nancy (chemistry).  
Head :T. Lelièvre.

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The ANR BIGMC Monte-Carlo methods for  
high-dimensional problems, with typical  
applications in financial mathematics,  
Bayesian statistics, and computational  
statistical physics.

Partners : TELECOM, University Paris  
Dauphine, and University Paris Est  
Head : G. Fort (TELECOM).

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C. Le Bris participates to the ANR EMAQS.  
The scientist in charge is K. Beauchard  
(CMLS, Ecole polytechnique).

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I. Dabo participates to the ANR CriMin  
(Crystal-chemistry of iron-bearing minerals  
and implications in the geochemical cycling of  
metal pollutants). This ANR is coordinated by  
M. Blanchard, Institut de Minéralogie de  
Physique des Milieux Condensés, Université  
Paris 6.

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S. Olla is the local coordinator of the project  
ANR LHMSHE (program ANR blanc 2007,  
renewed 2010), Hydrodynamics limit and  
statistical mechanics.

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S. Olla has been awarded an ERC advanced  
grant No 246953, Malady (Microscopic Laws  
and Dynamical System, 2010-2015). He is  
the CoPI with C. Liverani.

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F. Nier is a member of the ANR projects  
QUATRAIN (2007-2011), VOLQUAN (2007-  
2011), and NONAa (2008-2011).

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GdR Quantum dynamics: This  
interdisciplinary research network is focused  
on physical and mathematical problems  
related to the time evolution of quantum  
systems (transport problems, nonequilibrium  
systems, etc)

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GdR CoDFT,

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GdR Maths et entreprise.

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GdR correl (correlated methods in electronic  
structure computations).

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ANR METHODE on Hydrological modeling (Head : S. Cordier (Université d'Orléans)).

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ANR MODUM: this project aims to mutualise urban logistics. But instead of facilitating the matching between demand and offer, the project studies the opportunity of introducing a unique operator, whose mission would be the management of urban logistics.

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ANR POSAMU: This project aims to optimize the location and the dispatching of emergency vehicles (SAMU-SMUR in the french terminology) in Val-de-Marne. It concerns strategic as well as real-time decisions.

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CENTRAL OO project (direct financing by the IdF region): This project aims to develop tools for operating a fleet of electric taxis optimally. The main difficulty in the real-time management is to deal with the recharge. The locations of the recharge terminals or the right size of the fleet are also addressed.

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R2DS OADLIB: This project aims to study the algorithmic questions arising when trying to operate self service transport systems optimally. These questions concern the strategic level of decision as well as the real-time one.

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FUI LUMD: This project is based on the following observation: in an urban context, many trips are made with almost empty vehicles, many warehouses have not fully exploited storage capacities and intermodal exchanges are rare. The project aims to exploit these real opportunities for optimizing and mutualizing urban logistics. It will facilitate the matching between demand and logistic offer. The spin-offs will be economic, ecological and urbanistic.

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ANR Parmat (scientist in charge Guy Bencteux (EDF)).

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ANR "High performance computing and cloud computing" LN3M (scientist in charge F. Jollet, CEA-DAM) aims at developping new

numerical methods and softwares for multiscale modeling of materials.

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ANR "SIMulation of chemical REactivity at interfaces", SIRE, scientist in charge Ph. Sautet, ENS Lyon for the simulation of chemical reactivity at interfaces.

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ARC Hybrid: this collaborative research action involves INRIA teams from Rennes (IPSO), Lille (SIMPAF), Sofia-Antiopolis (TOSCA) and our project-team. The purpose of the action is to study theoretical models and numerical methods mixing deterministic and stochastic aspects in the context of molecular simulation.

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M. De Lara :  
Viable control of discrete time systems and applications,  
French-Chilean action supported by the program ECOS,  
French Ministry of Foreign Affairs.

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Partial PhD fellowship from BRGM on infiltration and erosion stochastic modeling, A. Ern.

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GNR MOMAS on Mathematical modeling for radioactive waste storage, Head: A. Ern.

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ANR LANDQUAKE 2011-2015 "Modelling of LANDslides and generated earthquakes for detection and understanding of gravitational instabilities"

### **ongoing industrial contracts**

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A. Alfonsi, B. Lapeyre: Credinext project (2009-2011) funded by "Pôle de compétitivité finance". Participants: ENPC, Ecole Polytechnique, UPEMLV, INRIA MATHFI, Pricing Partners, Thomson Reuters, Lunalogic.

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A. Alfonsi, B. Lapeyre: OSEO-Eurostars grant (2011-2012). In collaboration with Pricing Partners.

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M. De Lara : J.-C. Alais PhD thesis supervision, Electricité de France R&D

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A. Ern and T. Lelièvre,  
Non-parametric uncertainties in aeroacoustics and vibroacoustics problems, EADS

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A. Ern, T. Lelièvre and G. Stoltz,  
Multiscale modeling of clays, ANDRA

### **New industrial contracts**

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E. Cancès, V. Ehrlacher and T. Lelièvre  
Greedy algorithms and uncertainty propagation in mechanics, Michelin

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A. Ern, L. Monasse, R. Monneau,  
Shock wave/solid interaction in 3D, CEA

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A. Ern,  
Mimetic discrete operators, EDF

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### **Ongoing industrial contracts**

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A. Anantharaman, E. Cancès and C. Le Bris  
Numerical methods for random materials, EADS

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C. Le Bris,  
multiscale simulations of random materials,  
Office of Naval Research and European Office  
of Aerospace Research and Development

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### **VALORIZATION**

### **Software**

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SCCS  
(<http://qe-forge.org/projects/electroemb/>).  
The objective of the project is to develop computational tools for the description of quantum systems in aqueous environments..

Participants  
O. Andreussi, I. Dabo, N. Bonnet, N. Marzari

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- ODDFT  
(<http://qe-forge.org/projects/nkc/>).  
This project is aimed to the development and testing of novel electronic structure methods.

Participants  
I. Dabo and A. Ferretti

- Quantum-Espresso

P. GIANNOZZI, S. BARONI, N. BONINI, M. CALANDRA, R. CAR, C. CAVAZZONI, D. CERESOLI, G. L. CHIAROTTI; M. COCCIONI, I. DABO, A. DAL CORSO, S. FABRIS, G. FRATESI, S. DE CIRONCOLI, R. GEBAUER, U. GOUGOUSSIS, A. KOKALI, M. LAZZERI, L. MARTIN-SAMOS, N. MARZARI, F. MAURI, R. MAZZARELLO, S. PAOLINI, A. PASQUARELLO, L. PAULATTO, C. SBRACCIA, S. SCANDOLO, G. SCLAUZERO, A. P. SEITSONEN, A. SMOGUNOV, P. UMARI, R. M. WENTZCOVITCH

Software for quantum simulations of materials  
Personal contributions: development of electrostatic solvers, development of solvation models, development of quantum-mechanical calculation methods.

Contact: [q-e-developers@qe-forge.org](mailto:q-e-developers@qe-forge.org)

- OADLIB;  
[http://cermics.enpc.fr/~meuniefr/OADLIBSim\\_Site/](http://cermics.enpc.fr/~meuniefr/OADLIBSim_Site/); a simulator for self-service transport system, allowing easy implementation of new operation strategies.

Participants:  
D. Chemla  
F. Meunier

H. Yahiaoui

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Nsp, J-PH . CHANCELIER, B. PINCON

<http://cermics.enpc.fr/~jpc/nsp-tiddly/mine.html>

Scicoslab version 4.4.1

<http://cermics.enpc.fr/~jpc/scilab-gtk-tiddly/mine.html>

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PREMIA (13<sup>th</sup> version); Premia is a software designed for option pricing, hedging and financial model calibration. The development of increasingly complex financial products requires the use of advanced stochastic and numerical analysis techniques. A consortium of banks have been using Premia since its beginning in 1999 and have brought important contributions to the project. <https://www.rocq.inria.fr/mathfi/Premia/index.html>

**ACRONYMS****MODélisation  
MATHématique**

<b>AERES</b>	<b>Agence d'évaluation de la recherche et de l'enseignement supérieur</b>	<b>IFP</b>	<b>Institut Français du Pétrole</b>
<b>ANDRA</b>	<b>Agence Nationale pour la gestion des Déchets Radioactifs</b>	<b>INRIA</b>	<b>Institut National de Recherche en Informatique et Automatique</b>
<b>ANR</b>	<b>Agence Nationale de la Recherche</b>	<b>INSERM</b>	<b>Institut Nationale de la Santé et de la Recherche Médicale</b>
<b>BRGM</b>	<b>Bureau des Recherches Géologiques et Minières</b>	<b>IRSN</b>	<b>Institut de Radioprotection et de Sûreté Nucléaire</b>
<b>CEA</b>	<b>Commissariat à l'Energie Atomique</b>	<b>LCPC</b>	<b>Laboratoire Central des Ponts et Chaussées</b>
<b>CETMEF</b>	<b>Centre d'Etudes Techniques Maritimes et Fluviales</b>	<b>LIMSI</b>	<b>Laboratoire d'Informatique pour la Mécanique et les Sciences de l'Ingénieur</b>
<b>CNES</b>	<b>Centre National des Etudes Spatiales</b>	<b>MOMAS</b>	<b>et les Simulations numériques liées à la gestion des déchets nucléaires</b>
<b>CNRS</b>	<b>Centre National de la Recherche Scientifique</b>	<b>ONERA</b>	<b>Office National d'Etudes et Recherches Aérospatiales</b>
<b>CIFRE</b>	<b>Convention Industrielle de Formation par la Recherche</b>	<b>SMAI</b>	<b>Société de Mathématiques Appliquées et Industrielles</b>
<b>DRAST</b>	<b>Direction de la Recherche et des Affaires scientifiques et Techniques</b>	<b>UPEMLV</b>	<b>Université Paris-Est Marne-La-Vallée</b>
<b>EADS</b>	<b>European Aeronautic Defense and Space Company</b>		
<b>EDF</b>	<b>Electricité de France</b>		
<b>ED MSTIC</b>	<b>L'École Doctorale Mathématiques et Sciences et Technologies de l'Information et de la Communication</b>		
<b>ENSTA</b>	<b>Ecole Normale Supérieure de Techniques Avancées</b>		
<b>ESPCI</b>	<b>École Supérieure de Physique et Chimie Industrielles</b>		
<b>GNR</b>	<b>Groupement National de Recherches sur la</b>		