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Project-Team micmac

Methods and engineering of multiscale computing from atom to continuum

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Theme : Computational models and simulation

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1. Team

Research Scientists

Sébastien Boyaval [Research scientist, Civil engineer, ENPC]
Eric Cancès [Research scientist, Civil engineer in chief, ENPC, HdR]
Ismaila Dabo [Research scientist, temporary position, INRIA, then Civil Engineer, ENPC]
Claude Le Bris [Team leader, Civil engineer in chief, ENPC, HdR]
Frédéric Legoll [Research scientist, Civil engineer, ENPC]
Tony Lelièvre [Research scientist, Civil engineer, ENPC, HdR]
Gabriel Stoltz [Research scientist, Civil engineer, ENPC]
Mathieu Lewin [External collaborator, CR, CNRS Cergy University, HdR]

Faculty Members

Gabriel Turinici [External collaborator, Faculty member, Professor at University Paris IX Dauphine, HdR]
Atsushi Suzuki [Invited Professor, INRIA, until September 2010, HdR]
Stefano Olla [Professor 'en délégation', Université Paris Dauphine, HdR]

PhD Students

Arnaud Anantharaman [PhD student, Civil Engineer, ENPC, until August 2010]
David Benoit [PhD student, Scholarship ENPC]
Ronan Costaouec [PhD student, Scholarship ENPC]
Virginie Ehrlacher [PhD student, Civil engineer, ENPC]
Andreea Grigoriu [PhD student, Scholarship Paris IX Dauphine University, until September 2010]
Salma Lahbabi [PhD student, Financed by ENPC and CNRS, from September 2010 on]
Kimiya Minoukadeh [PhD student, Financed by ENPC and ANR CIS LN3M]
Raphaël Roux [PhD student, Financed by Ecole Normale Supérieure]
Florian Thomines [PhD student, Civil engineer, ENPC]

Post-Doctoral Fellows

Bradley Dickson [Post doctoral fellow, Financed by ANR, until February 2010]
Matthew Dobson [Post doctoral fellow, Financed by NSF]
Juliano Francisco [Post doctoral fellow, Financed by the Brazilian government, from February 2010 on]
Mustapha Hamdi [Post doctoral fellow, Financed by INRIA, until September 2010]
Francois Huveneers [Post doctoral fellow, Financed by ERC, from September 2010 on]
Yanli Li [Post doctoral fellow, Financed by ANR, until January 2010]
David Pommier [Post doctoral fellow, Financed by ANR, until July 2010]

Administrative Assistant

Laurence Bourcier [Administrative assistant, TR]

2. Overall Objectives

2.1. Overall Objectives

The MICMAC project-team has been created jointly by the Ecole des Ponts ParisTech (ENPC) and INRIA in October 2002. It is hosted by the CERMICS laboratory (Centre d'Enseignement et de Recherches en MathématIques et Calcul Scientifique) at ENPC. The permanent research scientists of the project-team have positions at CERMICS and at two other laboratories of Ecole des Ponts: Institut Navier and Laboratoire Saint-Venant. The scientific focus of the project-team is to analyze and improve the numerical schemes used in the simulation of computational chemistry at the microscopic level and to create simulations coupling this microscopic scale with meso- or macroscopic scales (possibly using parallel algorithms). Over the years, the project-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 project-team is to have created a corpus of literature, authoring books and research monographs on the subject [1], [2], [3], [5], [6] that other scientists may consult in order to enter the field.

3. Scientific Foundations

3.1. Scientific Foundations

Quantum Chemistry aims at understanding the properties of matter through the modeling of its behavior at a subatomic scale, where matter is described as an assembly of nuclei and electrons. At this scale, the equation that rules the interactions between these constitutive elements is the Schrödinger equation. It can be considered (except in few special cases notably those involving relativistic phenomena or nuclear reactions) as a universal model for at least three reasons. First it contains all the physical information of the system under consideration so that any of the properties of this system can in theory be deduced from the Schrödinger equation associated to it. Second, the Schrödinger equation does not involve any empirical parameters, except some fundamental constants of Physics (the Planck constant, the mass and charge of the electron, ...); it can thus be written for any kind of molecular system provided its chemical composition, in terms of natures of nuclei and number of electrons, is known. Third, this model enjoys remarkable predictive capabilities, as confirmed by comparisons with a large amount of experimental data of various types. On the other hand, using this high quality model requires working with space and time scales which are both very tiny: the typical size of the electronic cloud of an isolated atom is the Angström (10^{-10} meters), and the size of the nucleus embedded in it is 10^{-15} meters; the typical vibration period of a molecular bond is the femtosecond (10^{-15} seconds), and the characteristic relaxation time for an electron is 10^{-18} seconds. Consequently, Quantum Chemistry calculations concern very short time (say 10^{-12} seconds) behaviors of very small size (say 10^{-27} m^3) systems. The underlying question is therefore whether information on phenomena at these scales is useful in understanding or, better, predicting macroscopic properties of matter. It is certainly not true that *all* macroscopic properties can be simply upscaled from the consideration of the short time behavior of a tiny sample of matter. Many of them derive from ensemble or bulk effects, that are far from being easy to understand and to model. Striking examples are found in solid state materials or biological systems. Cleavage, the ability minerals have to naturally split along crystal surfaces (e.g. mica yields to thin flakes) is an ensemble effect. Protein folding is also an ensemble effect that originates from the presence of the surrounding medium; it is responsible for peculiar properties (e.g. unexpected acidity of some reactive site enhanced by special interactions) upon which vital processes are based. However, it is undoubtedly true that *many* macroscopic phenomena originate from elementary processes which take place at the atomic scale. Let us mention for instance the fact that the elastic constants of a perfect crystal or the color of a chemical compound (which is related to the wavelengths absorbed or emitted during optic transitions between electronic levels) can be evaluated by atomic scale calculations. In the same fashion, the lubricative properties of graphite are essentially due to a phenomenon which can be entirely modeled at the atomic scale. It is therefore reasonable to simulate the behavior of matter at the atomic scale in order to understand what is going on at the macroscopic one. The journey is however a long one. Starting from the basic principles of Quantum Mechanics to model the matter at the subatomic scale, one finally uses statistical mechanics to reach the macroscopic scale. It is often necessary to rely on intermediate steps to deal with phenomena which take place on various *mesoscales*. It may then be possible to couple one description of the system with some others within the so-called *multiscale* models. The sequel indicates how this journey can be completed focusing on the first smallest scales (the subatomic one), rather than on the larger ones. It has already been mentioned that at the subatomic scale, the behavior of nuclei and electrons is governed by the Schrödinger equation, either in its time dependent form or in its time independent form. Let us only mention at this point that

- both equations involve the quantum Hamiltonian of the molecular system under consideration; from a mathematical viewpoint, it is a self-adjoint operator on some Hilbert space; *both* the Hilbert space and the Hamiltonian operator depend on the nature of the system;
- also present into these equations is the wavefunction of the system; it completely describes its state; its L^2 norm is set to one.

The time dependent equation is a first order linear evolution equation, whereas the time-independent equation is a linear eigenvalue equation. For the reader more familiar with numerical analysis than with quantum

mechanics, the linear nature of the problems stated above may look auspicious. What makes the numerical simulation of these equations extremely difficult is essentially the huge size of the Hilbert space: indeed, this space is roughly some symmetry-constrained subspace of $L^2(\mathbb{R}^d)$, with $d = 3(M + N)$, M and N respectively denoting the number of nuclei and the number of electrons the system is made of. The parameter d is already 39 for a single water molecule and rapidly reaches 10^6 for polymers or biological molecules. In addition, a consequence of the universality of the model is that one has to deal at the same time with several energy scales. In molecular systems, the basic elementary interaction between nuclei and electrons (the two-body Coulomb interaction) appears in various complex physical and chemical phenomena whose characteristic energies cover several orders of magnitude: the binding energy of core electrons in heavy atoms is 10^4 times as large as a typical covalent bond energy, which is itself around 20 times as large as the energy of a hydrogen bond. High precision or at least controlled error cancellations are thus required to reach chemical accuracy when starting from the Schrödinger equation. Clever approximations of the Schrödinger problems are therefore needed. The main two approximation strategies, namely the Born-Oppenheimer-Hartree-Fock and the Born-Oppenheimer-Kohn-Sham strategies, end up with large systems of coupled *nonlinear* partial differential equations, each of these equations being posed on $L^2(\mathbb{R}^3)$. The size of the underlying functional space is thus reduced at the cost of a dramatic increase of the mathematical complexity of the problem: nonlinearity. The mathematical and numerical analysis of the resulting models has been the major concern of the project-team for a long time. In the recent years, while part of the activity still follows this path, the focus has progressively shifted to problems at other scales. Such problems are described in the following sections.

4. Application Domains

4.1. Electronic structure of large systems

As the size of the systems one wants to study increases, more efficient numerical techniques need to be resorted to. In computational chemistry, the typical scaling law for the complexity of computations with respect to the size of the system under study is N^3, N being for instance the number of electrons. The Holy Grail in this respect is to reach a linear scaling, so as to make possible simulations of systems of practical interest in biology or material science. Efforts in this direction must address a large variety of questions such as

- how can one improve the nonlinear iterations that are the basis of any *ab initio* models for computational chemistry?
- how can one more efficiently solve the inner loop which most often consists in the solution procedure for the linear problem (with frozen nonlinearity)?
- how can one design a sufficiently small variational space, whose dimension is kept limited while the size of the system increases?

An alternative strategy to reduce the complexity of *ab initio* computations is to try to couple different models at different scales. Such a mixed strategy can be either a sequential one or a parallel one, in the sense that

- in the former, the results of the model at the lower scale are simply used to evaluate some parameters that are inserted in the model for the larger scale: one example is the parameterized classical molecular dynamics, which makes use of force fields that are fitted to calculations at the quantum level;
- while in the latter, the model at the lower scale is concurrently coupled to the model at the larger scale: an instance of such a strategy is the so called QM/MM coupling (standing for Quantum Mechanics/Molecular Mechanics coupling) where some part of the system (typically the reactive site of a protein) is modeled with quantum models, that therefore accounts for the change in the electronic structure and for the modification of chemical bonds, while the rest of the system (typically the inert part of a protein) is coarse grained and more crudely modeled by classical mechanics.

The coupling of different scales can even go up to the macroscopic scale, with methods that couple a microscopic description of matter, or at least a mesoscopic one, with the equations of continuum mechanics at the macroscopic level.

4.2. Computational Statistical Mechanics

The orders of magnitude used in the microscopic description of matter are far from the orders of magnitude of the macroscopic quantities we are used to: The number of particles under consideration in a macroscopic sample of material is of the order of the Avogadro number $\mathcal{N}_A \sim 10^{23}$, the typical distances are expressed in Å (10^{-10} m), the energies are of the order of $k_{\mathrm{B}}T \simeq 4 \times 10^{-21}$ J at room temperature, and the typical times are of the order of 10^{-15} s when the proton mass is the reference mass.

To give some insight into such a large number of particles contained in a macroscopic sample, it is helpful to compute the number of moles of water on earth. Recall that one mole of water corresponds to 18 mL, so that a standard glass of water contains roughly 10 moles, and a typical bathtub contains 10^5 mol. On the other hand, there are approximately 1.3×10^{18} m^3 of water in the oceans, *i.e.* 7.2×10^{22} mol, a number comparable to the Avogadro number. This means that inferring the macroscopic behavior of physical systems described at the microscopic level by the dynamics of several millions of particles only is like inferring the ocean's dynamics from hydrodynamics in a bathtub...

For practical numerical computations of matter at the microscopic level, following the dynamics of every atom would require simulating $\mathcal{N}_A$ atoms and performing $\mathrm{O}(10^{15})$ time integration steps, which is of course impossible! These numbers should be compared with the current orders of magnitude of the problems that can be tackled with classical molecular simulation, where several millions of atoms only can be followed over time scales of the order of 0.1 μs.

Describing the macroscopic behavior of matter knowing its microscopic description therefore seems out of reach. Statistical physics allows us to bridge the gap between microscopic and macroscopic descriptions of matter, at least on a conceptual level. The question is whether the estimated quantities for a system of N particles correctly approximate the macroscopic property, formally obtained in the thermodynamic limit $N \to +\infty$ (the density being kept fixed). In some cases, in particular for simple homogeneous systems, the macroscopic behavior is well approximated from small-scale simulations. However, the convergence of the estimated quantities as a function of the number of particles involved in the simulation should be checked in all cases.

Despite its intrinsic limitations on spatial and timescales, molecular simulation has been used and developed over the past 50 years, and its number of users keeps increasing. As we understand it, it has two major aims nowadays.

First, it can be used as a *numerical microscope*, which allows us to perform "computer" experiments. This was the initial motivation for simulations at the microscopic level: physical theories were tested on computers. This use of molecular simulation is particularly clear in its historic development, which was triggered and sustained by the physics of simple liquids. Indeed, there was no good analytical theory for these systems, and the observation of computer trajectories was very helpful to guide the physicists' intuition about what was happening in the system, for instance the mechanisms leading to molecular diffusion. In particular, the pioneering works on Monte-Carlo methods by Metropolis et al, and the first molecular dynamics simulation of Alder and Wainwright were performed because of such motivations. Today, understanding the behavior of matter at the microscopic level can still be difficult from an experimental viewpoint (because of the high resolution required, both in time and in space), or because we simply do not know what to look for! Numerical simulations are then a valuable tool to test some ideas or obtain some data to process and analyze in order to help assessing experimental setups. This is particularly true for current nanoscale systems.

Another major aim of molecular simulation, maybe even more important than the previous one, is to compute macroscopic quantities or thermodynamic properties, typically through averages of some functionals of the system. In this case, molecular simulation is a way to obtain *quantitative* information on a system, instead of resorting to approximate theories, constructed for simplified models, and giving only qualitative

answers. Sometimes, these properties are accessible through experiments, but in some cases only numerical computations are possible since experiments may be unfeasible or too costly (for instance, when high pressure or large temperature regimes are considered, or when studying materials not yet synthesized). More generally, molecular simulation is a tool to explore the links between the microscopic and macroscopic properties of a material, allowing one to address modelling questions such as "Which microscopic ingredients are necessary (and which are not) to observe a given macroscopic behavior?"

4.3. Homogenization and related problems

Over the years, the project-team has developed an increasing expertise on how to couple models written at the atomistic scale, with more macroscopic models, and, more generally, an expertise in multiscale modelling for materials science.

The following observation motivates the idea of coupling atomistic and continuum description of materials. In many situations of interest (crack propagation, presence of defects in the atomistic lattice, ...), using a model based on continuum mechanics is difficult. Indeed, such a model is based on a macroscopic constitutive law, the derivation of which requires a deep qualitative and quantitative understanding of the physical and mechanical properties of the solid under consideration. For many solids, reaching such an understanding is a challenge, as loads they are submitted to become larger and more diverse, and as experimental observations helping designing such models are not always possible (think of materials used in the nuclear industry). Using an atomistic model in the whole domain is not possible either, due to its prohibitive computational cost. Recall indeed that a macroscopic sample of matter contains a number of atoms on the order of 10^{23}. However, it turns out that, in many situations of interest, the deformation that we are after is not smooth in *only a small part* of the solid. So, a natural idea is to try to take advantage of both models, the continuum mechanics one and the atomistic one, and to couple them, in a domain decomposition spirit. In most of the domain, the deformation is expected to be smooth, and reliable continuum mechanics models are then available. In the rest of the domain, the expected deformation is singular, one needs an atomistic model to describe it properly, the cost of which remains however limited as this region is small.

From a mathematical viewpoint, the question is to couple a discrete model with a model described by PDEs. This raises many questions, both from the theoretical and numerical viewpoints:

- first, one needs to derive, from an atomistic model, continuum mechanics models, under some regularity assumptions that encode the fact that the situation is smooth enough for such a macroscopic model to be a good description of the materials;
- second, couple these two models, e.g. in a domain decomposition spirit, with the specificity that models in both domains are written in a different language, that there is no natural way to write boundary conditions coupling these two models, and that one would like the decomposition to be self-adaptive.

More generally, the presence of numerous length-scales in material science problems represents a challenge for numerical simulation, especially when some *randomness* is assumed on the materials. It can take various forms, and includes defects in crystals, thermal fluctuations, and impurities or heterogeneities in continuous media. Standard methods available in the literature to handle such problems often lead to very costly computations. Our goal is to develop numerical methods that are more affordable. Because we cannot embrace all difficulties at once, we focus on a simple case, where the fine scale and the coarse-scale models can be written similarly, in the form of a simple elliptic partial differential equation in divergence form. The fine scale model includes heterogeneities at a small scale, a situation which is formalized by the fact that the coefficients in the fine scale model vary on a small length scale. After homogenization, this model yields an effective, macroscopic model, which includes no small scale. In many cases, a sound theoretical groundwork exists for such homogenization results. We consider mostly the setting of stochastic homogenization of linear, scalar, second order elliptic PDEs, where analytical formulas for the effective properties are known. The difficulty stems from the fact that they generally lead to prohibitively costly computations. For such a case, simple

from the theoretical viewpoint, our aim is to focus on different practical computational approaches to speed-up the computations. One possibility, among others, is to look for specific random materials, relevant from the practical viewpoint, and for which a dedicated approach can be proposed, that is less expensive than the general approach.

5. New Results

5.1. Electronic structure theory

Participants: Eric Cancès, Ismaila Dabo, Virginie Ehrlacher, Juliano Francisco, Salma Lahbabi, Claude Le Bris, Yanli Li, Gabriel Stoltz.

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

E. Cancès, G. Stoltz and V. Ehrlacher have addressed issues related to the modeling and simulation of local defects in periodic crystals. Computing the energies of local defects in crystals is a major issue in quantum chemistry, materials science and nano-electronics. In collaboration with M. Lewin (CNRS, Cergy), E. Cancès and A. Deleurence have proposed in 2008 a new model for describing the electronic structure of a crystal in the presence of a local defect. This model is based on formal analogies between the Fermi sea of a perturbed crystal and the Dirac sea in Quantum Electrodynamics (QED) in the presence of an external electrostatic field. The justification of this model is obtained through a thermodynamic limit of Kohn-Sham type models. They have also introduced a variational method for computing the perturbation in a basis of precomputed maximally localized Wannier functions of the reference perfect crystal. In [27], E. Cancès and M. Lewin have pushed forward the analysis of this model and have used it to construct a rigorous mathematical derivation of the Adler-Wiser formula for the dielectric permittivity of crystals. A pedagogical introduction to all these contributions is given in the proceedings paper [53], where some elements on a work in progress by E. Cancès and G. Stoltz about the time-dependent version of the Hartree model (known as the random-phase approximation) are provided. In [26] E. Cancès et V. Ehrlacher have proved that local defects are always neutral in the Thomas-Fermi-von Weisäcker (TFW) theory. In this respect, all TFW crystals behave as metals.

E. Cancès has also worked with Y. Maday and R. Chakir (University of Paris 6) on the numerical analysis of variational approximations of nonlinear elliptic eigenvalue problems. In [24], they provide *a priori* error estimates for variational approximations of the ground state energy, eigenvalue and eigenvector of problems of the form $-\mathrm{div}(A\nabla u) + Vu + f(u^2)u = \lambda u$, $\|u\|_{L^2} = 1$. They focus in particular on the Fourier spectral and pseudospectral approximation (for periodic problems) and on the $\mathbb{P}_1$ and $\mathbb{P}_2$ finite-element discretizations. In [25], they obtain optimal *a priori* error bounds for the the planewave approximation of the Thomas-Fermi-von Weizsäcker and the Kohn-Sham LDA model.

E. Cancès has also proposed, in collaboration with F. Lipparini and B. Mennucci (University of Pisa), and with M. Caricato, M.J. Frish and G. Scalmani (Gaussian Inc.), a variational formulation of the polarizable continuum model for the modelling of solvated molecules [46]. This new formulation allows for simultaneous optimization of the molecular geometry, the electronic density and the apparent surface charge representing the polarization of the solvent.

The numerical analysis of a simplified version the domain decomposition method proposed by M. Barrault (now at EDF), E. Cancès, W. Hager (University of Florida), and C. Le Bris, designed to solve the linear subproblem in electronic structure calculations, has been carried out in the past few years and recently published in [15].

In collaboration with C. Brouder (IMPMC, Paris 6 and 7) and G. Panati (University La Sapienza, Roma), G. Stoltz has also proved the Gell-Mann and Low formula for systems with degenerate ground states in [22]. This formula relates an eigenstate of an initial reference Hamiltonian to a perturbed one, using some adiabatic switching. The key point of the work has been to identify the directions within the initial degenerate space in which the switching can be performed.

In collaboration with A. Ferretti, N. Poilvert, N. Marzari (MIT and University of Oxford) and M. Cococcioni (University of Minnesota), I. Dabo and Y. L. Li have worked on the prediction of the photo-electric properties of organic molecules and nano-particles [34]. One important practical outcome of this collaborative effort is the derivation of an efficient computational scheme to predict photo-emission energies (i.e., the quantized energies at which a photon can eject an electron from a sample of material) in close agreement with spectroscopy experiments. This level of performance is achieved by imposing a non-convexity condition to conventional density-functional theory (DFT) approximations. This computational model finds potential applications in organic photovoltaics, electronics, and opto-electronics. Future extensions include the prediction of the band gap of semiconductors, the description of the linear and nonlinear electrical response of polymer compounds, and the simulation of molecular electronic junction devices.

Some works started this year. During his post-doctoral stay in our team, Juliano Francisco began studying the numerical issues encountered in the so-called LDA+U method, and also proposed new algorithms in the DIIS fashion to find local minimizers of the electronic energy. He is currently testing the methods on test cases. Besides, Salma Lahbabi started her PhD thesis, on the homogenization of defects in infinite periodic crystals.

5.2. Molecular dynamics and related problems

Participants: Matthew Dobson, Bradley Dickson, Claude Le Bris, Frédéric Legoll, Tony Lelièvre, Kimiya Minoukadeh, Stefano Olla, David Pommier, Raphaël Roux, Gabriel Stoltz.

The extremely broad field of Molecular dynamics is a domain where the MICMAC project-team, originally more involved in the quantum chemistry side, has invested a lot of effort in the recent years. Molecular dynamics may also be termed "computational statistical physics" since the main aim is to numerically estimate average properties of materials as given by the laws of statistical physics. The project-team studies both deterministic and probabilistic techniques used in the field. On these topics, we have benefited from funding from the ARC Hybrid and the ANR MEGAS ("MEthodes Géométriques et échantillonnage : Application à la Simulation moléculaire").

5.2.1. Free Energy calculations

For many large molecular systems, the information of the whole configuration space may be summarized in a few coordinates of interest, called reaction coordinates. An important problem in chemistry or biology is to compute the effective energy felt by those reaction coordinates, called free energy. T. Lelièvre and G. Stoltz, together with M. Rousset, wrote a review book on free energy computations [6], presenting the mathematical understanding of state-of-the-art numerical methods.

Besides this review work, Tony Lelièvre and Gabriel Stoltz wrote several contributions to the domain:

- with Mathias Rousset (INRIA Lille), they studied the thermodynamic integration method, and nonequilibrium methods in the Jarzynski fashion for Langevin dynamics, see [44];
- with Nicolas Chopin (CREST, ENSAE), they used free energy techniques in the context of Bayesian statistics to sample efficiently posterior distributions arising from mixture models, see [30];
- with Frédéric Legoll, Brad Dickson and Paul Fleurat-Lessard (Département de chimie, ENS Lyon), they improved some adaptive methods where the biasing potential is updated (in contrast to the update of the derivative of this potential as for ABF), see [35].

Concerning the Adaptive Biasing Force (ABF) method, various results have been obtained in the framework of the PhD thesis of K. Minoukadeh [9] and R. Roux [10].

The Adaptive Biasing Force (ABF) method is a stochastic algorithm used to compute the free energy. It is based upon a nonlinear dynamics, which uses the mean force as a biasing force to prevent the system from being trapped in metastable regions. The nonlinearity in the dynamics comes from a conditional expectation computed with respect to the solution.

The new results on this topic are the following:

- The convergence of the algorithm can be accelerated by using multiple walkers, each following similar dynamics but driven by independent Brownian motions. The use of multiple walkers allows for further improvement via a selection mechanism, whereby the walkers are weighted according to a given fitness function and resampled at fixed time intervals. T. Lelièvre and K. Minoukadeh, together with C. Chipot (University of Illinois, on leave from Université Henri Poincaré - Nancy 1), have shown, in [47], the applicability of the method to realistic biological systems. Their work has in particular highlighted cases in which the standard ABF method, using a single walker, fails to converge within reasonable time scales;
- In [45], T. Lelièvre and K. Minoukadeh study the longtime convergence of the ABF method in a particular bi-channel scenario. Using entropy arguments and logarithmic Sobolev inequalities, previous results have shown that the rate of convergence of the ABF method is limited by the metastable features of the canonical measures conditioned to being at fixed values of the reaction coordinate. In [45], an improvement on existing results is proposed, in the presence of metastabilities at fixed values of the reaction coordinate, which is a generic case encountered in practice. More precisely, a bi-channel case is considered, where two channels along the reaction-coordinate direction exist between an initial and final state, separated from each other by a region of low probability. With hypotheses made on 'channel-dependent' conditional measures, it is shown on a newly introduced bi-channel model, that the convergence of the ABF method is in fact not limited by metastabilities in directions orthogonal to the reaction coordinate under two crucial assumptions: (i) exchange between the two channels is possible for some values of the reaction coordinate and (ii) the free energy is a good bias in each channel.
- In [40], T. Lelièvre and R. Roux study in collaboration with B. Jourdain the convergence of a discretization method using interacting particles for the Adaptive Biasing Force method. Another work on interacting particle systems and their links to nonlinear partial differential equations is [41] where R. Roux (in collaboration with B. Jourdain) studies a probabilistic interpretation of fractional scalar conservation laws.
- In [29], T. Lelièvre, in collaboration with C. Chipot, studies a generalization of the standard ABF approach in order to deal with high-dimensional reaction coordinates. A mathematical analysis gives some insight on typical assumptions required for the method to be efficient and some numerical tests on real test cases demonstrate the interest of the approach.

5.2.2. Effective dynamics

For a given molecular system, and a given reaction coordinate $\xi : \mathbb{R}^n \mapsto \mathbb{R}$, the free energy completely describes the statistics of $\xi(X)$ when $X \in \mathbb{R}^n$ is distributed according to the Gibbs measure. This allows to compute coarse-grained *equilibrium* quantities.

F. Legoll and T. Lelièvre have worked on the definition of a coarse-grained dynamics that approximates $\xi(X_t)$, when the state of the system X_t evolves according to the overdamped Langevin equation (which is ergodic for the Gibbs measure). The aim is hence to get a coarse-grained description giving access to some *dynamical* quantities, such as residence times in metastable basins (we usually assume that these basins are completely described through ξ). They have proposed an effective dynamics, which is derived using conditional expectations, and have proved an estimate on its accuracy in terms of the relative entropy between the law of $\xi(X_t)$ and the law of its approximation, at any time t (see [43] and also [57] for a description of the results in a simpler case). If an appropriate time-scale separation is present in the system, then the effective dynamics is accurate in the above sense of time-marginals. The obtained numerical results show that this dynamics can also be used to accurately compute residence times in potential energy wells.

The extension of the numerical strategy to the case when the reference dynamics on the whole system is the Langevin dynamics is currently under study. Promising numerical results have already been obtained in collaboration with a master's student (F. Galante).

5.2.3. Sampling trajectories of metastable systems

As explained above, the free energy provides a useful description of a system's thermodynamic quantities. However, computing dynamics at equilibrium is also sometimes necessary in practice, in particular to compute reactive paths.

In [28], T. Lelièvre and D. Pommier, in collaboration with F. Cérou and A. Guyader (INRIA Rennes, ASPI) investigated the interest of an Adaptive Multilevel Splitting algorithm to compute reactive paths, and estimate transition rates. The numerical results obtained on simple cases are very promising. An ARC project between MICMAC and ASPI has been submitted in order to pursue research in this direction.

5.2.4. Nonequilibrium systems

Benefiting from the presence of S. Olla (on leave from Université Paris Dauphine), a work on the thermal conductivity of one-dimensional chains has been completed by F. Legoll and G. Stoltz, in collaboration with A. Iacobucci, see [39]. The system under study is a chain of anharmonic oscillators interacting via the nonlinear Toda potential. In the absence of any external perturbation, the thermal current across the system does not decrease with the size N of the system, leading to a thermal conductivity diverging linearly with N. Our investigations focused on the impact of stochastic perturbations of the dynamics, preserving locally the momentum and the energy. Our numerical simulations showed that these perturbations are not sufficient to achieve a finite conductivity, but nonetheless lead to a reduction of the thermal conductivity which increases asymptotically as CN^α with $0 < \alpha < 1$.

We also turned to the study of algorithms to compute the shear viscosity by nonequilibrium simulations, focusing more specifically on the so-called (p-)SLLOD method. This work in progress constitutes one of the basis of the PhD thesis of Rémi Joubaud (cosupervised by T. Lelièvre and A. Ern, involving also G. Stoltz). The aim is to understand the mathematical foundations of the method (existence and uniqueness of the invariant measure, derivation of the linear response properties, etc) and to improve the numerical methods currently available through some variance reduction technique.

M. Dobson, C. Le Bris, F. Legoll, T. Lelièvre and G. Stoltz have also started to investigate questions related to the simulation of a molecular fluid under constant stress or under constant strain rate.

5.2.5. Highly Oscillating Problems

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

In [36] and [37], M. Dobson, C. Le Bris, and F. Legoll developed integrators for Hamiltonian systems with high frequencies. The integrators were derived using homogenization techniques applied to the Hamilton-Jacobi PDE associated to the Hamiltonian ODE. This work extended previous works of C. Le Bris and F. Legoll [42] by generating preconditioned algorithms that work when there is a unique fast frequency that depends on the slow degrees of freedom, or when there are several fast constant frequencies. We have also applied our strategy to a simple non-linear pendulum. The resulting algorithm performed well compared to related algorithms in the dynamical systems literature. We collaborated on this subject with F. Castella, P. Chartier, and E. Faou from INRIA Rennes.

5.3. Surface chemistry and electrochemistry

Participants: Eric Cancès, Ismaila Dabo, Yanli Li.

Chemical reactions at metal surfaces are of central relevance to most electrochemical energy technologies (e.g., fuel cells and batteries) and emission control applications (e.g., catalytic converters and exhaust detectors), as well as to many industrial production processes (e.g., chemical deposition) and important natural phenomena (e.g., ice crystallization). Typically, in electrochemical devices, chemical reactions take place at the surface of an electrode in the presence of an electrolyte (i.e., an aqueous solution containing ions) and in the presence of an infinite reservoir of electrons that sets the value of the electrical potential.

This year, in collaboration with N. Bonnet, N. Marzari (MIT and University of Oxford), I. Dabo and Y. L. Li have addressed the numerical solution of the nonlinear modified Poisson-Boltzmann (MPB) equations obtained by coupling a quantum molecular description of the electrode with a classical continuous representation of the liquid electrolyte. This approach has been applied to the prediction of the electrical properties and surface energy of catalytic electrodes [54] and to the interpretation of experimental spectroscopic data [61]. Our current effort focuses on implementing alternative iterative techniques for the solution of the nonlinear MPB problem. Additionally, we are working on extending the grand-canonical method recently proposed by E. Cancès *et al.* [33] (for the simulation of electronic systems in contact with a reservoir of electrons) to the case of generalized electronic entropy techniques for improving the numerical sampling of electronic observables.

5.4. Atomistic to continuum methods

Participants: Matthew Dobson, Claude Le Bris, Frédéric Legoll.

The project-team has continued their theoretical and numerical efforts on the general topic of "passage from the atomistic to the continuum". This concerns theoretical issues arising in this passage but also the development and the improvement of numerical simulations coupling the two scales. As pointed out in the review article [18], this topic shares many common features with the modelling of complex fluids, another domain in which the project-team has been strongly involved for many years.

In collaboration with C. Ortner (Oxford) and A. Shapeev (EPFL, Lausanne), M. Dobson characterized the spectral properties of the 1D linearized force-based quasicontinuum method, an algorithm which reduces computational cost by coupling atomistic simulation with a continuum approximation, for the simulation of materials at zero temperature. The algorithm is based on a decomposition of the domain into two disjoint regions, one where the atomistic force-balance laws are applied and another one where the continuum force-balance laws are applied. The resulting force law, for the whole domain, does not derive from a total energy. We have shown in [62] that the linear operator is similar to an operator deriving from an energy and we characterized the eigenvalues.

In collaboration with X. Blanc (CEA) and, some years ago, with C. Patz (WIAS, Berlin), C. Le Bris and F. Legoll have addressed questions related to the finite temperature modeling of atomistic systems and derivation of coarse-grained descriptions, such as canonical averages of observables depending only on a few variables and free energies associated to these specific degrees of freedom. In the one-dimensional setting an efficient strategy that bypasses the simulation of the whole system had been proposed in [19]. This strategy is based on a rigorous thermodynamic procedure. Using these results, we have shown how to derive the stress-strain relation for one-dimensional chains of atoms, e.g. the relation between the elongation of the chain and the stress, at any given temperature [57]. Recent efforts in the project-team aim at extending the strategy to more complex cases. Promising results have been obtained in the 2D scalar case [59].

Another situation of major interest, beyond the static setting, is the dynamical case. Some preliminary work, on some simple models, has been conducted by C. Le Bris, in collaboration with X. Blanc (CEA) and P.-L. Lions (Collège de France).

5.5. Homogenization

Participants: Arnaud Anantharaman, Sébastien Boyaval, Ronan Costaouec, Claude Le Bris, Frédéric Legoll, Florian Thomines.

In collaboration with X. Blanc (CEA), C. Le Bris has studied, for homogenization of elliptic partial differential equations, the applicability of ideas based on filtering. The bottom line is to modify the corrector problem by introducing a filtering function, in order to improve the efficiency of the method. Some popular methods, such as the oversampling method, can indeed be considered as special instances of such a general strategy. Encouraging numerical results, supported by a rigorous theoretical analysis, have been reported in the recently published study [17], in the case of periodic and quasi-periodic settings.

The project-team has also pursued and amplified its efforts in the field of stochastic homogenization of elliptic equations. The various contributions of the team, which aim to design numerical approaches that both are practically relevant and keep the computational workload limited, have been presented from a unified perspective in [49].

An interesting case in that context is when the randomness comes as a *small* perturbation of the deterministic case. This situation can indeed be handled with a dedicated approach, which turns out to be far more efficient than the standard approach of stochastic homogenization, as explained in [56].

This case has been studied by C. Le Bris, in collaboration with P.-L. Lions (Collège de France) and X. Blanc (CEA). The analysis naturally gives rise to a numerical strategy, which has been studied and implemented by R. Costaouec, C. Le Bris and F. Legoll [31], [60].

In the work mentioned above, the perturbation to the deterministic case is supposed to be small in the L^∞ norm (that is, it is almost surely small). In [13], A. Anantharaman and C. Le Bris have extended this study to the case when the perturbation is small in a weaker norm, typically a L^p norm with $p < \infty$ (the case when only the *expectation* of the perturbation is assumed to be small, rather than the perturbation itself, is also covered by that framework). The approach proves to be very efficient from a computational viewpoint. It is rigorously founded in a certain class of settings and has been successfully numerically tested in more general settings [12], [11].

The team has also pursued its effort to address, from a numerical viewpoint, the case when the randomness is not small. In that case, using the standard homogenization theory, one knows that the homogenized tensor, which is a deterministic matrix, depends on the solution of a stochastic equation, the so-called corrector problem, which is posed on the *whole* space $\mathbb{R}^d$. This equation is therefore delicate and expensive to solve. In practice, the space $\mathbb{R}^d$ is truncated to some bounded domain, on which the corrector problem is numerically solved. In turn, this yields a converging approximation of the homogenized tensor, which happens to be a *random* matrix. For a given truncation of $\mathbb{R}^d$, R. Costaouec, C. Le Bris and F. Legoll, in collaboration with X. Blanc (CEA), have studied how to reduce the variance of this matrix, using the technique of antithetic variables, which is a method widely used in other fields of application. Its efficiency in the context of stochastic homogenization has been extensively studied, both numerically and theoretically: encouraging numerical results have been obtained (see [32], [50]), supported by a rigorous theoretical analysis [16].

From a numerical perspective, the Multiscale Finite Element Method is a classical strategy to address the situation when the homogenized problem is not known (e.g. in nonlinear cases), or when the scale of the heterogeneities, although small, is not considered to be zero (and hence the homogenized problem cannot be considered as an accurate enough model). The extension of this strategy to the stochastic case, when the tensor describing the properties of the material is the sum of a periodic term and a small random term, has been studied by C. Le Bris, F. Legoll and F. Thomines [64]. A method with a much smaller computational cost than the original MsFEM in the stochastic setting has been proposed. Provided the stochastic perturbation is indeed small, the proposed method is as accurate as the original one.

Furthermore, still in the context of elliptic homogenization, S. Boyaval and C. Le Bris studied the applicability of reduced-basis ideas to variational problems with stochastic parameters, in collaboration with Y. Maday (University Paris 6), N.C. Nguyen and A.T. Patera (MIT). The motivation stems from the need to take into account many different random microstructures in the context of stochastic homogenization. One of the bottlenecks is that the solution field to a given partial differential equation with stochastic parameters is a high-dimensional space. To address this difficulty, different approaches have been recently suggested in the literature on uncertainty quantification for stochastic partial differential equations. A state-of-the-art review

on reduced basis techniques applied to partial differential equations with stochastic parameters can be read in [21].

In the context of parabolic homogenization, A. Anantharaman has pursued the study of boundary layers in time (close to the initial time $t = 0$) and space (close to the domain boundaries), in collaboration with G. Allaire (CMAP) and E. Cancès. The idea is to add space, time and space-time boundary layer terms to the usual approximate solution (which is computed by solving the homogenized problem and the corrector problems), so that the difference between the exact solution and the approximate solution can be estimated, and more precisely controlled in interesting functional spaces. The main difficulty is that the classical space boundary layers (usually defined in the stationary case) and the classical time boundary layers (usually defined in an infinite domain) are not compatible one with each other. Progress has been made in the understanding of this issue. For rectangular domains, some boundary layers have been proposed, the accuracy of which relies on strong regularity assumptions [7].

5.6. Free surface flows

Participants: Tony Lelièvre, Atsushi Suzuki.

We mention two current projects using the free surface flow code (Mistral) which has been developed over the past ten years with J.-F. Gerbeau.

A. Suzuki and T. Lelièvre are investigating the interest of the Generalized Navier Boundary Condition (previously studied in collaboration with J.-F. Gerbeau) for the study of the dependency of the dynamics contact angle as a function of the capillary number (Tanner's law).

T. Lelièvre, in collaboration with A. Ern and R. Joubaud and within the ANR METHODE have studied the the flow of a thin layer of fluid over a wavy surface [38] and more precisely the definition of a critical Reynolds number beyond which no stationary flow is observed.

5.7. Complex fluids

Participants: David Benoit, Sébastien Boyaval, Claude Le Bris, Tony Lelièvre.

The stability of finite element discretizations for constitutive equations describing the motion of viscoelastic fluids is still being investigated by S. Boyaval. Numerical simulations are being performed [52] and a collaboration with J.W. Barrett (Imperial College, London, UK) [14] considers extensions on a previous work.

To address the numerical simulation of micro-macro models, one can use numerous stochastic processes describing the time evolution of particles diluted in the fluid, rather than computing the probability density functional solution to a Fokker-Planck equation. Two numerical methods have been proposed in [20] to reduce the variance in the Monte-Carlo evaluation of the expected values for the stress variable. The approaches are based on the Reduced-Basis method, which is used for speeding up the computation of many solutions to a parameterized partial differential equation at many parameter values. It also has many possible extensions to other applications such as the calibration of the volatility in finance or Bayesian statistics (see the state-of-the-art review article on reduced basis techniques applied to stochastic problems [21]). Some open questions related to the relatively good numerical success of the method are still under investigation [51].

Besides, T. Lelièvre has studied in collaboration with G. Samaey (KU Leuven) and V. Legat (UC Louvain) the derivation of macroscopic constitutive laws from the microscopic FENE model, using numerical closures, see [48]. This work is the starting point of our collaboration with G. Samaey, who will join the project-team as a visitor in January 2011 to work on macroscopic constitutive laws for granular materials.

5.8. Application of greedy algorithms

Participants: Eric Cancès, Virginie Ehrlacher, Claude Le Bris, Tony Lelièvre.

C. Le Bris and T. Lelièvre, in collaboration with Y. Maday, had studied in 2009 a numerical method based on greedy algorithms to solve high-dimensional linear partial differential equations. Following this work, E. Cancès, V. Ehrlacher and T. Lelièvre have extended in [23] the method to nonlinear convex problems, and in particular to contact problems via penalization methods, with application to uncertainty propagation in solid mechanics problems or to the computation of the committor function in molecular dynamics.

5.9. Problems in Statistical Mechanics

Participant: Stefano Olla.

S. Olla continues to develop his research around hydrodynamic limits: derive macroscopic evolution equation for conserved quantities (energy, mass etc.) from microscopic dynamics (in particular classical Hamiltonian dynamics, possibly perturbed by some conservative noise).

The main result obtained this year in collaboration with Makiko Sasada (University of Tokyo) is the proof that a linearized heat equation describes the diffusion of energy in a one dimensional chain of anharmonic oscillators perturbed by a local energy conserving noise. This result is obtained under a direct diffusive space-time scale limit (article in preparation). Previous results, like the one obtained by S. Olla with C. Liverani, are obtained only through a weak coupling limit [65], [58].

S. Olla is also involved in the qualitative and quantitative study of thermal conductivity for systems of anharmonic oscillators. With C. Bernardin (ENS Lyon), they obtained upper and lower bounds on the thermal conductivity that illustrate the asymptotic behaviour of this transport coefficient as a function of the temperature and the pressure. In the same work, the entropy production properties of the corresponding non-equilibrium stationary state are studied, and the Green-Kubo representation formula for the thermal conductivity is proved rigorously (in preparation).

With an hyperbolic space-time scale S. Olla obtained (in collaboration with N. Even, University of Heidelberg) Euler equation for a system on anharmonic oscillators under the effect of an external tension [63].

The writing of the monograph *Fluctuations in Markov Processes: Time Symmetry and Martingale Approximations* [55] (in collaboration with T. Komorowski and C. Landim) has been concluded this year, and will be published by Springer in the series *Grundlehren der mathematischen Wissenschaften* in 2011. It concerns time symmetry techniques (reversibility and extensions) in the study of central limit theorems for Markov processes, with applications from hydrodynamic limits to homogenization in random environments.

S. Olla continues his investigations of the Einstein relation and linear response for random walks in random environments, in collaboration with G. Benarous and O. Zeitouni. The program is to compute effective macroscopic velocities for particles in random environment driven by an external force (gravity, electric field etc.). Partial results (exact lower bounds) have been obtained for a random walk in a random Galton-Watson tree.

5.10. Laser control

Participants: Andreea Grigoriu, Claude Le Bris, Gabriel Turinici.

The mathematical and numerical aspects of laser control (manipulation of molecular systems using laser beams) have been a major scientific topic for the project-team for a long time. In the past couple of years, the center of mass of our activity around this topic, animated and directed by Gabriel Turinici, has shifted to Paris Dauphine. In the project-team, Claude Le Bris is the only permanent researcher still involved in the activity. In 2010, the thesis [8] of Andreea Grigoriu was defended. In the next few years, the activity around laser control might see a revival in the project-team, depending on the available funding and the interactions with other research groups.

6. Contracts and Grants with Industry

6.1. Contracts and Grants with Industry

Many research activities of the project-team are conducted in close collaboration with private or public companies: EADS, Commissariat à l'Energie Atomique for computational chemistry, molecular dynamics and multiscale simulation of solids. The project-team is also supported by Office of Naval Research and European Office of Aerospace Research and Development, for multiscale simulations of random materials. All these contracts are operated at and administrated by the Ecole des Ponts.

7. Other Grants and Activities

7.1. Regional activities

The project-team is shared between INRIA and Ecole des Ponts ParisTech.

7.2. National activities

The project-team is involved in seven ANR projects.

The first one, the ANR MEGAS, has been accepted in 2009. Its aims are to study several methods for numerical simulation, with an emphasis on sampling methods. It includes four research teams: the INRIA project IPSO in Rennes, the INRIA project SIMPAF in Lille, the eDAM team in Nancy (chemistry), and our team. The scientist in charge is Tony Lelièvre.

The second one is Big MC: the project is focused on the study of Monte-Carlo methods for high-dimensional problems, with typical applications in financial mathematics, Bayesian statistics, and computational statistical physics. Three nodes participate to this project: one research team at the Institut TELECOM, another one at CEREMADE, University Paris Dauphine, and the third one at University Paris Est (including two members of our team). The coordinator is Gersende Fort (TELECOM).

The third one is the ANR METHODE on Hydrological modeling (scientist in charge S. Cordier (Université d'Orléans)).

The fourth one is the ANR Parmat (scientist in charge Guy Bencteux (EDF)).

The fifth one (ANR "Calcul intensif et grilles de calcul" LN3M, scientist in charge F. Jollet, CEA-DAM) aims at developing new numerical methods and softwares for multiscale modeling of materials.

S. Olla is the local coordinator of the sixth one, the project ANR LHMSHE (programme blanc 2007, renewed 2010), Limites hydrodynamiques et mécanique statistique hors équilibre.

The seventh one is the ANR "Calcul intensif et grilles de calcul" SIRE, scientist in charge Ph. Sautet, ENS Lyon for the simulation of chemical reactivity at interfaces.

In addition, the team is participating in

- the 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,
- the 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),
- the GdR CoDFT,
- the GdR Maths et entreprise.

7.3. European Community financed activities

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

8. Dissemination

8.1. Animation of the scientific community

E. Cancès is

- is co-Editor in chief (with P. Del Moral and J.-F. Gerbeau) (2005-) of ESAIM Proc.
- is a member of the editorial boards of Mathematical Modelling and Numerical Analysis (2006-) and of SIAM Journal of Scientific Computing (2008-),
- has co-organized the Minisymposium on electronic structure (SIAM MS10, Philadelphia, May 2010),
- has co-organized the Workshop on the numerical analysis of orbital-free and Kohn-Sham models (Paris, September 2010),
- has organized the CEA-EDF-INRIA Winter School on homogenization (Rocquencourt, December 2010).

C. Le Bris is co-Editor-in-chief (with A.T. Patera, MIT) (2005-) of Mathematical Modeling and Numerical Analysis. He is editor-in-chief of Applied Mathematics Research Express (2003-). He is a member of the editorial boards of Archive for Rational Mechanics and Analysis (2004-), Communications in Mathematical Sciences (2007-), 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-), Journal de Mathématiques Pures et Appliquées (2009-). He is a member of the editorial board of the monograph series Mathématiques & Applications, Series, Springer (2008-), and Modeling, Simulations and Applications, Series, Springer (2009-).

C. Le Bris has been

- the Charles Amick lecturer 2010 at the University of Chicago, and has delivered a series of lectures there, in October 2010.

C. Le Bris has been a member of

- the “Scientific Committee” of the Fifth European Conference on Computational Fluid Dynamics (ECCOMAS CFD 2010), Lisbon, 14-17 June 2010,
- the organizing committee of the international conference "Dynamical Analysis of Molecular Systems", Edinburgh, June 28-July 2, 2010,
- the scientific committee (as Co-chair) of the ESF-EMS international conference on "Highly Oscillatory Problems", 13–17 September 2010, Isaac Newton Institute for Mathematical Sciences, Cambridge.

C. Le Bris 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.

F. Legoll has co-organized:

- with H. Ben Dhia (Centrale Paris), F. Feyel (Onera and ENSMP) and V. Kouznetsova (TU Eindhoven), a mini-symposium on "Arlequin, FE2 and other embedded domains methods for multimodel and multiscale mechanical problems: advances, analyses and computation of challenging fine scales applications", during the 4th European Conference on Computational Mechanics (May 16-21, 2010, Paris),
- with B. Leimkuhler, a mini-symposium on Molecular Dynamics during the Dynamics Days Europe 2010 conference (September 6-10, 2010, Bristol, UK).

F. Legoll and T. Lelièvre have co-organized a mini-symposium on "Coarse-graining and effective dynamics in molecular simulation" during the Multiscale Molecular Modelling conference (June 30 - July 3, 2010, Edinburgh).

T. Lelièvre, F. Legoll and G. Stoltz have co-organized the CEA-EDF-INRIA school “Simulation of hybrid dynamical systems and applications to molecular dynamics” (IHP, Paris, 27-30 september 2010). http://cermics.enpc.fr/~stoltz/Hybrid2010/hybrid_workshop.html

T. Lelièvre has co-organized a mini-symposium on “Uncertainty propagation” at Journées MAS (Bordeaux, september 2010).

S. Olla is

- a Member of the editorial board on Annals of Probability (since 2009)
- a Member of the Scientific Board of the agreement GREFI-MEFI between CNRS and INDAM (Istituto NAzionale di Alta Matematica, Italy).

S. Olla has co-organized the workshop ’Large Scale Dynamics’ (Oberwolfach, Nov. 8-12 2010).

8.2. Honors

T. Lelièvre has been awarded, jointly with Jean-Frédéric Gerbeau (INRIA Rocquencourt) the “Grand Prix Alcan” by the French Academy of Sciences.

S. Boyaval has been awarded in 2010 the 2009 “Prix de thèse en Mathématiques et STIC” by the Université Paris Est.

The article [34], by I. Dabo and coworkers A. Ferretti, N. Poilvert, Y. L. Li, N. Marzari, M. Cococcioni, has been awarded the label "Physical Review Editor’s Suggestion".

8.3. Teaching activities

- Calcul scientifique, (30h), Cours Ecole Nationale des Ponts et Chaussées (S. Boyaval, G. Stoltz)
- Analyse, (36 h), cours Ecole Nationale des Ponts et Chaussées (E. Cancès, V. Ehrlacher, F. Legoll, F. Thomines),
- Simulation moléculaire: aspects théoriques et numériques, (24 h), cours de M2, Université Paris 6 (E. Cancès, M. Lewin),
- Analyse numérique et optimisation, (56 h), PC du cours de G. Allaire et P.-L. Lions, Ecole Polytechnique (E. Cancès, C. Le Bris),
- Introduction à l’informatique scientifique, (12h), TP à l’Université Paris-Est (I. Dabo),
- Informatique, (32h), TP en CPGE Jean-Baptiste Say (I. Dabo).
- Object Oriented Progamming: C++, (42h) cours de M1, Université Paris 1 Panthéon-Sorbonne (K. Minoukadeh),
- Object Oriented Progamming: C++, (18h) cours de M2, Université Paris 1 Panthéon-Sorbonne (K. Minoukadeh),

- Analyse Numérique et Optimisation, (12h) cours à l'ISBS (K. Minoukadeh),
- Analyse spectrale, (21h), Cours Ecole Nationale des Ponts ParisTech (G. Stoltz),
- Computational Statistical Physics, (18h), Master SMCD, Ecole des Ponts ParisTech (G. Stoltz),
- Mathématiques des modèles multiéchelles, (39h), Cours Ecole Nationale des Ponts et Chaussées (F. Legoll)
- Problèmes multi-échelles, (24h), cours de M2, Université Paris 6 (F. Legoll)
- Optimisation linéaire, (36h), Cours Université Paris 6 (R. Costaouec)
- Formation au logiciel scientifique SCILAB, (12h), Cours Ecole Nationale des Ponts et Chaussées (D. Benoit, R. Costaouec, I. Dabo, K. Minoukadeh)
- Outils mathématiques pour le génie des systèmes industriels, (72h), TD University Paris - Est (R. Roux)
- Méthodes déterministes en mathématiques financières, (42h), Cours Ecole des Ponts ParisTech (T. Lelièvre)
- Modéliser Programmer Simuler, (84 h), Cours Ecole des Ponts ParisTech (T. Lelièvre)
- Méthodes numériques probabilistes, (36 h), Cours M2 Mathématiques et Applications, Université Paris 6 (T. Leliévre)

8.4. Conference participation

Members of the project-team have delivered lectures in the following seminars, workshops and international conferences:

- A. Anantharaman, SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, May 23-26, 2010,
- S. Boyaval, Oberseminar Angewandte Mathematik, Stuttgart University, January 2010,
- S. Boyaval, ECCM 2010, Paris, May 2010,
- S. Boyaval, Uncertainty Quantification workshop at ICMS, Edinburgh, May 2010,
- S. Boyaval, Joint SIAM/RSME-SCM-SEMA Meeting DSPDEs'10, Barcelona, June 2010,
- S. Boyaval, ECCOMAS CFD 2010, Lisbon, June 2010,
- S. Boyaval, Recent Trends in Differential Equations: Analysis and Discretisation Methods at Bielefeld University, November 2010,
- S. Boyaval, Nonstandard Discretizations for Fluid Flows workshop at BIRS, Banff, November 2010,
- E. Cancès, Annual DMV meeting, Munich (Germany), March 2010,
- E. Cancès, Final symposium of the german-wide priority program 1145 "Modern and Universal First-Principles Methods for Many-Electron Systems in Chemistry and Physics" of the german science foundation (DFG), Bad Herrenalb, March 2010,
- E. Cancès, CANUM 2010 (plenary lecture), Carcans-Maubuisson, June 2010,
- E. Cancès, GDR Chant Summer School, Vienna, August 2010,
- E. Cancès, Workshop on the numerical analysis of orbital-free and Kohn-Sham models, Paris, September 2010,
- E. Cancès, New Approaches in Many-Electron Theory - NAMET workshop, Mainz, September 2010,
- E. Cancès, Fifth international conference on multiscale material modelling (MMM 2010), Freiburg, October 2010,
- E. Cancès, CWB 2010, Curitiba, August 2010,

- E. Cancès, Pacifichem 2010 international congress, Honolulu, December 2010,
- E. Cancès, weekly seminar of the mathematics department, University of Villetaneuse, April 2010,
- E. Cancès, weekly seminar of the chemistry department, University of Pisa, June 2010,
- E. Cancès, weekly seminar of the mathematics department, Princeton University, October 2010,
- R. Costaouec, SIAM Conference on Mathematical Aspects of Materials Science, Philadelphie, May 2010,
- R. Costaouec, European Conference on Computational Mechanics, Paris, May 2010,
- R. Costaouec, Congrès National d'Analyse Numérique, Carcans-Maubuisson, June 2010,
- I. Dabo, Electronic-structure Challenges in Materials Modeling and Applications Workshop, CECAM Lausanne, June 2010,
- I. Dabo, Ab Initio Electrochemistry Workshop, CECAM Lausanne, July 2010,
- I. Dabo, Psi-k Conference, FU Berlin, September 2010,
- I. Dabo, Pacifichem International Chemical Congress, Honolulu Convention Center, December 2010,
- M. Dobson, SIAM Mathematical Aspects of Materials Science, Philadelphia, May 2010,
- M. Dobson, CANUM, Carcans-Maubuisson, June 2010,
- M. Dobson, Highly Oscillatory Problems: Computation, Theory and Application, Cambridge University, September 2010,
- V. Ehrlacher, Journées Fiabilité des Matériaux et des Structures, INSA Toulouse, March 24th-26th, 2010,
- V. Ehrlacher, CECAM tutorial "Linear and non-linear responses of solids with the ABINIT software: phonons, electric fields, and other perturbations", CECAM-EPFL, Lausanne, Switzerland, April 26th-30th, 2010,
- V. Ehrlacher, 4th European Conference on Computational Mechanics, Paris, May 16th-21st, 2010,
- V. Ehrlacher, SIAM Conference on Mathematical Aspects of Materials and Science, Philadelphia, United States, May 22-27, 2010,
- V. Ehrlacher, 40e Congrès National d'Analyse Numérique, Carcans-Maubuisson, May 31st - June 4th, 2010,
- V. Ehrlacher, PhD students seminar at Laboratoire Jacques-Louis Lions, Université Paris VI, June 8th, 2010,
- V. Ehrlacher, ASME 2010 3rd Joint US-European Fluids Engineering Summer Meeting, Montreal, Canada, August 1st-5th, 2010,
- V. Ehrlacher, Gordon Research Conference: "Defects in semiconductors", New London, United States, August 8th-13th, 2010,
- V. Ehrlacher, Journées MAS, Bordeaux, August 31st - September 3rd, 2010,
- V. Ehrlacher, Journées Scientifiques de l'association calcul de structures et modélisation "Méthodes de réduction de modèle dans le calcul scientifique", Ecole Centrale de Nantes, September 2nd-3rd, 2010,
- V. Ehrlacher, Journées du GdR MoMaS, IHP, October 6th, 2010,
- C. Le Bris, (plenary lecture) Seventh International Congress of Computational Physics 7, Beijing, May 17 - 20, 2010,
- C. Le Bris, One-day workshop on Computational Chemistry, Peking University, Beijing, January 2010.

- C. Le Bris, "Stress Tensor Effects on Compressible Flows" Workshop, Morningside Institute Beijing, January 2010.
- C. Le Bris, Inhomogeneous Random Systems workshop, Institut Henri Poincaré (Paris), January 26–27, 2010.
- C. Le Bris, "Stochastic Partial Differential Equations and their Applications" Workshop, Isaac Newton Institute, Cambridge, March 29 - April 1, 2010.
- C. Le Bris, International conference "Dynamical Analysis of Molecular Systems", Edinburgh, June 28-July 3, 2010.
- C. Le Bris, International conference STAMM 2010, Berlin, September 2010,
- C. Le Bris, International Workshop on "New Theoretical Paths in Many-Electron Problems: Basic Physical Principles and Mathematical Rigor", Mainz, September 20-24, 2010,
- C. Le Bris, Second symposium on Engineering of advanced materials, Erlangen-Nurnberg University, November 16-18, 2010,
- C. Le Bris, International Workshop on Multi-Scale Methods in Computational Engineering at Technische Universität Darmstadt on December 9-10, 2010,
- C. Le Bris, Ecole Homogénéisation numérique Workshop, INRIA, December 2010.
- C. Le Bris, Institute of Computational mathematics of the Chinese Academy of Science, January 2010 and May 2010,
- C. Le Bris, Seminar of the Department of Mathematics, Université d'Orsay, September 2010,
- C. Le Bris, Probability Seminar of the University of Minnesota, February 2010,
- C. Le Bris, Colloquium Beijing University, May 2010,
- C. Le Bris, Colloquium IRM Montreal, October 2010,
- C. Le Bris, Seminar of Laboratoire de Mécanique des solides de l'Ecole Polytechnique, October 2010,
- F. Legoll, Highly oscillating problems workshop, St Malo, January 2010,
- F. Legoll, Annual DMV meeting, Munich, March 2010,
- F. Legoll, internal seminar of Navier laboratory on Discrete and molecular simulations, March 2010,
- F. Legoll, mini-symposium Theory and Applications of Computational Hybrid Models of Solids, SIAM conference Mathematical aspects of materials science, Philadelphia, May 2010,
- F. Legoll, mini-symposium Effective macroscopic descriptions of microscopic dynamics, SIAM conference Dynamical Systems and PDEs, Barcelona, June 2010,
- F. Legoll, Multiscale Molecular Modelling conference, Edinburgh, July 2010,
- F. Legoll, Dynamics Days Europe 2010 conference, Bristol, September 2010,
- F. Legoll, Highly Oscillatory Problems conference, Cambridge, September 2010,
- F. Legoll, Large scale stochastic dynamics workshop, Oberwolfach, November 2010,
- F. Legoll, seminar "Sciences Numériques pour la Mécanique", Ecole Centrale Paris, November 2010,
- T. Lelièvre, Workshop on Mathematical problems of computational chemistry, Beijing, January 2010,
- T. Lelièvre, European Conference on Computational Mechanics (ECCM 2010), Paris, May 2010
- T. Lelièvre, Workshop Multiscale Molecular Modelling, Edinburgh, June 2010,
- T. Lelièvre, Journées scientifiques CSMA, Nantes, September 2010,

- T. Lelièvre, (plenary lecture) ESF conference on Highly Oscillatory Problems: From Theory to Applications, Cambridge, September 2010,
- T. Lelièvre, Workshop on Large Scale Stochastic Dynamics, Oberwolfach, November 2010,
- T. Lelièvre, Séminaire Equations aux dérivées partielles et applications, Collège de France, January 2010,
- T. Lelièvre, Groupe de Travail Probabilités, Statistique, et applications, Université de Marne-la-Vallée, February 2010,
- T. Lelièvre, Séminaire de probabilités, Rennes, March 2010,
- T. Lelièvre, Séminaire équations aux dérivées partielles et applications, ENS Lyon, March 2010,
- T. Lelièvre, Séminaire de probabilités, Nancy, April 2010,
- T. Lelièvre, Séminaire Laboratoire Jacques-Louis Lions, June 2010,
- T. Lelièvre, Seminar at the Institute of Computational Mathematics (CAS), January 2010,
- T. Lelièvre, Seminar at Cornell University (CEE), February 2010.
- T. Lelièvre, Analysis seminar, MPI Leipzig, October 2010,
- K. Minoukadeh, PhD students seminar, CEREMADE, University Paris-Dauphine, Paris, May 20, 2010,
- K. Minoukadeh, SIAM: Emerging Topics in Dynamical Systems and PDEs, Barcelona, May 31 - June 4, 2010,
- K. Minoukadeh, Multiscale Molecular Modelling 2010, Edinburgh, June 30 - July 3, 2010,
- K. Minoukadeh, Simulation of hybrid dynamical systems, IHP, Paris, September 27-30, 2010,
- K. Minoukadeh, PhD students seminar, AGM, Université de Cergy-Pontoise, November 15, 2010,
- K. Minoukadeh, Seminar at the Department of Computer Science, K.U. Leuven, December 2010,
- S. Olla, Mathematica-Physics Seminar, IHP, Paris, 11 January 2010,
- S. Olla, WIMCS Colloquium, Swansea, UK, 26 March 2010,
- S. Olla, Pacific Rim Conference, Stanford, USA, June 28-July 2 2010,
- S. Olla, Math-Phys Seminar, Rutgers University, NJ, USA, 14 October 2010,
- S. Olla, Math-Phys Seminar, Princeton University, NJ, USA, 20 October 2010,
- S. Olla, Groupe de Travail Hors Equilibre, IHP, Paris, 4 November 2010,
- S. Olla, Probability Seminar, Technical University, Budapest, Hungary, december 2010,
- R. Roux, Groupe de Travail "Probabilités, Statistiques et Applications", University Paris-Est Marne-La-Vallée, January 2010,
- R. Roux, Séminaire "Big'MC - Méthodes de Monte Carlo en grande dimension", Institut Henri Poincaré, February 2010,
- R. Roux, Colloque "Jeunes Probabilistes et statisticiens", Le Mont-Dore, May 2010,
- R. Roux, Conference "Nonlocal operators and Partial Differential Equations", Institute of Mathematics of the Polish Academy of Sciences, June 2010,
- G. Stoltz, Multiscale Molecular Modelling workshop, Edinburgh (United-Kingdom), June 2010,
- G. Stoltz, CANUM 2010, Carcans-Maubuisson (France), May 2010,
- G. Stoltz, Workshop Large Scale Stochastic Dynamics, Oberwolfach (Germany), November 2010.

Members of the project-team have presented posters in the following seminars, workshops and international conferences:

- I. Dabo, Psi-k Conference, FU Berlin, September 2010 (2 posters)

Members of the project-team have participated (without giving talks nor presenting posters) in the following seminars, workshops and international conferences:

- M. Dobson, Highly Oscillatory Systems workshop, Dinard, February 2010,
- M. Dobson, Journées Louis Antoine - Transport optimal, Rennes, April 2010,
- M. Dobson, Simulation of hybrid dynamical systems and applications to molecular dynamics, Institut Henri Poincaré, September 2010,
- C. Le Bris, Workshop on Quantum-Classical Modeling of Chemical Phenomena, University of Maryland, March 8-11, 2010,
- C. Le Bris, Workshop on Large Scale Stochastic Dynamics, Oberwolfach, November 8-12, 2010,
- F. Thomines, European Conference on Computational Mechanics, Paris, May 2010,
- F. Thomines, SIAM Mathematical aspects of materials science conference, Philadelphia, May 2010.

Members of the project-team have delivered the following series of lectures:

- T. Lelièvre, Lectures (4h30) on Multiscale modelling of complex fluids : a mathematical initiation, in Workshop stress tensor effects on fluid mechanics, Morningside Institute, Beijing, January 2010,
- T. Lelièvre, Lectures (4h) on Free Energy Computations, Cornell University (School of Civil and Environmental Engineering), February 2010,
- T. Lelièvre, Lectures (3h) on Stochastic processes, PDEs and molecular dynamics, Université de Lille, September 2010,
- C. Le Bris, Lectures on 'Navier-Stokes type equations and related problems', i- MATH School on Coupled PDE in Multiphysics and Industrial Applications, Centro Internacional de Encuentros Matematicos, Castro Urdiales (Spain), June 14-25, 2010,
- C. Le Bris, Lectures on *Stochastic Homogenization: An introduction to some recent variants and to numerical approaches*, International workshop "Viscosity methods and nonlinear PDEs", Sapporo, Japan, 20-23 July 2010,
- C. Le Bris, Lectures on "A selection of mathematical topics in multiscale sciences", French-Spanish Jacques-Louis Lions school, La Corona (Spain), 6- 10 September 2010,
- C. Le Bris, Lectures "Charles Amick memorial Lectures", University of Chicago, October 2010.
- S. Olla, Non-equilibrium macroscopic dynamics of chains of anharmonic oscillators, CERMICS, January-February 2010.

In addition to the above, some members of the team have been invited for stays in institutions abroad:

- E. Cancès, Brown University, Providence, USA, July-August 2010.

9. Bibliography

Major publications by the team in recent years

[1] E. CANCÈS, M. DEFRANCESCHI, W. KUTZELNIGG, C. LE BRIS, Y. MADAY. *Computational Quantum Chemistry: A Primer*, 2003, Le Bris, Claude (ed.), Special Volume: Computational Chemistry. Amsterdam: North-Holland. Handb. Numer. Anal. 10, 3-270 (2003).

[2] E. CANCÈS, C. LE BRIS, Y. MADAY. *Mathematical Methods in Quantum Chemistry. An Introduction. (Méthodes mathématiques en chimie quantique. Une introduction.)*, Mathématiques et Applications (Berlin) 53. Berlin: Springer. xvi, 409 p. , 2006.

[3] I. CATTO, C. LE BRIS, P.-L. LIONS. *The Mathematical Theory of Thermodynamic Limits: Thomas-Fermi Type Models.*, Oxford Mathematical Monographs. Oxford: Clarendon Press. xiii, 277 p., 1998.

[4] J.-F. GERBEAU, C. LE BRIS, T. LELIÈVRE. *Mathematical Methods for the Magnetohydrodynamics of Liquid Metals*, Numerical Mathematics and Scientific Computation. Oxford: Oxford University Press., 324 p., 2006.

[5] C. LE BRIS. *Multi-scale Analysis. Modeling and Simulation. (Systèmes multi-échelles. Modélisation et simulation.)*, Mathématiques et Applications (Berlin) 47. Berlin: Springer. xi, 212 p., 2005.

[6] T. LELIÈVRE, M. ROUSSET, G. STOLTZ. *Free Energy Computations: A Mathematical Perspective*, Imperial College Press, 458 p., 2010.

Publications of the year

Doctoral Dissertations and Habilitation Theses

[7] A. ANANTHARAMAN. *Analyse mathématique de quelques modèles en calcul de structures électroniques et homogénéisation*, Université Paris Est, Ecole des Ponts ParisTech, 2010.

[8] A. GRIGORIU. *Approches numériques et théoriques en contrôle quantique*, Université Paris Dauphine, 2010.

[9] K. MINOUKADEH. *Méthodes déterministes et stochastiques pour la simulation moléculaire*, Université Paris-Est, Ecole des Ponts ParisTech, 2010.

[10] R. ROUX. *Étude probabiliste de systèmes de particules en interaction. Applications à la simulation moléculaire*, Université Paris-Est, Ecole des Ponts ParisTech, 2010.

Articles in International Peer-Reviewed Journal

[11] A. ANANTHARAMAN, C. LE BRIS. *A numerical approach related to defect-type theories for some weakly random problems in homogenization*, in "SIAM Multiscale Modeling & Simulation", 2010, submitted, http://hal.archives-ouvertes.fr/hal-00487759/fr/.

[12] A. ANANTHARAMAN, C. LE BRIS. *Elements of mathematical foundations for a numerical approach for weakly random homogenization problems*, in "Communications in Computational Physics", 2010, submitted, http://hal.archives-ouvertes.fr/hal-00487762/fr/.

[13] A. ANANTHARAMAN, C. LE BRIS. *Homogénéisation d'un matériau périodique faiblement perturbé aléatoirement (Homogenization of a weakly randomly perturbed periodic material)*, in "C.R. Acad. Sci. Paris, Ser. I.", 2010, vol. 348, n^{o} 9-10, p. 529-534.

[14] J. W. BARRETT, S. BOYAVAL. *Existence and approximation of a (regularized) Oldroyd-B model*, in "Mathematical Models and Methods in Applied Sciences (M3AS)", 2010, accepted for publication, http://fr.arxiv.org/abs/0907.4066.

[15] G. BENCTEUX, E. CANCÈS, W. W. HAGER, C. LE BRIS. *Analysis of a Quadratic Programming Decomposition Algorithm*, in "SIAM Journal on Numerical Analysis", 2010, vol. 47, n^{o} 8, p. 4517-4539, http://hal.inria.fr/inria-00169080/.

[16] X. BLANC, R. COSTAOUEC, C. LE BRIS, F. LEGOLL. *Variance reduction in stochastic homogenization using antithetic variables*, in "Markov Processes and Related Fields", 2010, accepted for publication.

[17] X. BLANC, C. LE BRIS. *Improving on computation of homogenized coefficients in the periodic and quasi-periodic settings*, in "Networks and Heterogeneous Media", 2010, vol. 5, n^{o} 1, p. 1–29, http://hal.archives-ouvertes.fr/inria-00387214/fr/.

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[19] X. BLANC, C. LE BRIS, F. LEGOLL, C. PATZ. *Finite-temperature coarse-graining of one-dimensional models: mathematical analysis and computational approaches*, in "Journal of Nonlinear Science", 2010, vol. 20, n^{o} 2, p. 241-275, http://hal.inria.fr/inria-00282107/en/.

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[22] C. BROUDER, G. PANATI, G. STOLTZ. *Gell-Mann and Low formula for degenerate unperturbed states*, in "Ann. I. H. Poincare-Phy", 2010, vol. 10, n^{o} 7, p. 1285-1309, http://hal.archives-ouvertes.fr/hal-00394223.

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[28] F. CEROU, A. GUYADER, T. LELIÈVRE, D. POMMIER. *A multiple replica approach to simulate reactive trajectories*, in "J. Chem. Phys.", 2010, To appear, http://hal.archives-ouvertes.fr/hal-00506047/fr/.

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Scientific Books (or Scientific Book chapters)

[49] A. ANANTHARAMAN, R. COSTAOUEC, C. LE BRIS, F. LEGOLL, 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, 2010, submitted.

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Other Publications

[59] X. BLANC, F. LEGOLL. *A numerical strategy for coarse-graining two-dimensional atomistic models at finite temperature: the membrane case*, 2010, in preparation.

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