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Project-Team MICMAC

Methods and engineering of multiscale computing from atom to continuum

IN COLLABORATION WITH: Centre d'Enseignement et de Recherche en Mathématiques et Calcul Scientifique (CERMICS)

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THEME
Computational models and simulation

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Project-Team MICMAC

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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. Computational quantum chemistry

Participants: Eric Cancès, Ismaila Dabo, Virginie Ehrlacher, Salma Lahbabi, Francis Nier, 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, V. Ehrlacher, S. Lahbabi and G. Stoltz have addressed issues related to the modeling and simulation of local defects in periodic crystals (see [61] for a pedagogical introduction).

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 using a thermodynamic limit of Kohn-Sham type models. In [29], E. Cancès and G. Stoltz studied the time evolution of defects within this model, in the context of linear response, which allowed them to give a rigorous meaning to the Adler-Wiser formula for the frequency-dependent dielectric permittivity of crystals. In [27] 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 like metals. In collaboration with M. Lewin, E. Cancès and S. Lahbabi are working on the extension of Kohn-Sham like models to disordered systems.

On the numerical side, E. Cancès has worked with Y. Maday and R. Chakir (University Paris 6) on the numerical analysis of the electronic structure models. In [26], they have obtained optimal *a priori* error bounds for the the planewave approximation of the Thomas-Fermi-von Weizsäcker and the Kohn-Sham LDA models. Together with Y. Maday, E. Cancès and V. Ehrlacher have analyzed the computation of eigenvalues in spectral gaps of locally perturbed periodic Schrödinger operators [28].

Photovoltaic cells based upon organic photovoltaic (OPV) semiconductors are cost-effective, light-weight alternatives to conventional silicon and thin-film technologies. This year, in collaboration with A. Ferretti, N. Poilvert, N. Marzari (MIT and University of Oxford), M. Cococcioni (University of Minnesota), and Y. L. Li (Xiamen University), I. Dabo has worked on the prediction of the electronic spectra and electrical response of molecular and polymer compounds for OPV applications. Specifically, Y. L. Li and I. Dabo have implemented an efficient computational method for studying the electrical response of semiconducting polymers, in close agreement with more expensive local basis-set algorithms [52]. In parallel, A. Ferretti, I. Dabo, M. Cococcioni, and N. Marzari have applied recently developed electronic-structure theories, namely, orbital-dependent density-functional theories (OD-DFTs), to describe donor and acceptor levels in semiconducting organic materials, demonstrating that OD-DFT is apt at describing donor and acceptor levels within 0.1-0.4 and 0.2-0.6 eV of experiment [41]. Future work includes the prediction of the band structure of semiconductor alloys and the simulation of molecular heterojunctions.

The current works by F. Nier related to electronic structure calculations concern the mean field limit of the quantum dynamics in the bosonic setting; and the non linear modelling of Bose-Einstein condensates. A few years ago, Z. Ammari and F. Nier initiated a program about the Hamilton mean field dynamics of a large numbers of bosons. Their approach reconsiders the old idea that the mean field limit in the bosonic setting is actually a semiclassical limit in infinite dimension. In previous works, they proved results which are general with respect to the initial data but hold for bounded interactions. They also proved that the dynamics of the

BBGKY hierarchy, often used within the mean field theory, is actually a projected picture of the dynamics of Wigner measures in the infinite dimensional phase-space. Recently in [10], they obtained such results for singular pair interaction potentials, which include the Coulombic (attractive or repulsive) case in dimension $d = 3$. Regarding the modelling of Bose-Einstein condensates, F. Nier and collaborators have developed in [9] complete analysis of the nonlinear adiabatic ansatz proposed by physicists for the simulation of rotating Bose-Einstein condensates.

5.2. Computational Statistical Physics

Participants: Matthew Dobson, Claude Le Bris, Frédéric Legoll, Tony Lelièvre, Francis Nier, Stefano Olla, Grigorios Pavliotis, Giovanni Samaey, Gabriel Stoltz.

The extremely broad field of Molecular dynamics (MD) is a domain where the MICMAC project-team, originally more involved in the quantum chemistry side, has invested a lot of efforts 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.

5.2.1. Free Energy calculations

For large molecular systems, the information of the whole configuration space may be summarized in a few coordinates of interest, called reaction coordinates. An important problem in chemistry or biology is to compute the effective energy felt by those reaction coordinates, called free energy.

In the article [51], Tony Lelièvre, Mathias Rousset and Gabriel Stoltz study the application of constrained Langevin dynamics to the computation of free energy differences, by thermodynamic integration techniques and fluctuation relation (à la Jarzynski).

The work by T. Lelièvre and K. Minoukadeh on the longtime convergence of the ABF method in a particular bi-channel scenario (which was already mentioned in last year's activity report) has been accepted for publication [50]. Likewise, the work by Nicolas Chopin (CREST, ENSAE), T. Lelièvre and G. Stoltz on application of the ABF method to Bayesian inference is about to appear, see [30].

5.2.2. Sampling trajectories

There exist a lot of methods to sample efficiently Boltzmann-Gibbs distributions. The situation is much more intricate as far as the sampling of trajectories (and especially metastable trajectories) is concerned.

In [32], 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 obtained results are very interesting. Current research aims at testing the technique on practical cases.

In [49], C. Le Bris and T. Lelièvre together with M. Luskin and D. Perez have proposed a mathematical analysis of the parallel replica algorithm,introduced by A. Voter in 1997 to efficiently simulate metastable trajectories. This work opens a lot of perspectives using a generic tool (the quasi stationary distribution) to relate continuous state space dynamics (Langevin type dynamics) to discrete state space dynamics (kinetic Monte Carlo type models). A follow-up work consists in theoretically investigating another related approach, the hyperdynamics method.

5.2.3. Nonequilibrium systems

The efficient simulation of molecular systems is known to be a much more complicated problem when the system is subjected to a non-conservative external forcing than when the system experiences conservative forces. Together with the sampling of metastable dynamics mentioned above, these are the two major research focus in MD of the project-team.

On this topic, G. Stoltz continued his long lasting collaboration with physicists at CEA/DAM on reduced models for shock and detonation waves. More precisely, he published two works applying some simulation techniques he devised to actual energetic materials of interest to physicists, namely (i) a technique to sample constraints in average and allowing to compute the Hugoniot curve efficiently, which was applied to reacting TATB [24]; and (ii) a reduced stochastic dynamics to model detonation waves, applied to a material with properties close to nitromethane and allowing an atomistic simulation of the shock-to-detonation transition [55].

F. Legoll and G. Stoltz pursued their studies of the anomalous thermal conductivity of one dimensional chains. They have investigated the case of a chain of rotors subjected to a mechanical forcing. In collaboration with A. Iacobucci and S. Olla (CEREMADE, Paris Dauphine) they have shown in [44] that the mechanical forcing can have a counter-intuitive effect and reduce the thermal current. Besides this numerical study, G. Stoltz, in collaboration with C. Bernardin (ENS Lyon) considered in [18] the issue of thermal transport in one of the simplest possible one dimensional model, a chain of oscillators whose kinetic and potential energy functions are the same, and which are subjected to a stochastic noise exchanging all the variables. The system therefore has only two conservation laws, the energy and the total length. A hydrodynamic limit consisting of a system of conservation laws can be obtained before the onset of shocks. However, the thermal transport is anomalous: this can be proved by analytical computations for harmonic interactions, or demonstrated numerically in the general case.

G. Stoltz also studied techniques to compute the viscosity of fluids using steady state nonequilibrium dynamics with an external nongradient bulk forcing, in the framework of the context of the PhD of Rémi Joubaud, see [45]. The two authors have proved a linear response result, and obtained asymptotic scalings of the viscosity in terms of the friction coefficients of the underlying Langevin dynamics. G. Stoltz and G. Pavliotis are now extending the results to the case of time dependent nongradient external forcings.

Nonequilibrium molecular dynamics simulations can also be used to compute the constitutive relation between the strain rate and stress tensor in complex fluids. This is fulfilled simulating molecular systems subject to a steady, non-zero macroscopic flow at a given temperature. Starting from a bath model, M. Dobson, F. Legoll, T. Lelievre, and G. Stoltz have derived a Langevin-type dynamics for a heavy particle in a non-zero background flow.The resulting dynamics, which is theoretically obtained when a *unique* large particle is considered, is numerically observed to also perform well when a *system* of many interacting particles within shear flow is considered.

5.2.4. 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. On the other hand, obtaining a correct description of the dynamics along ξ is complicated.

F. Legoll and T. Lelièvre have continued their work on the definition and the analysis 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 to get a coarse-grained description giving access to some *dynamical* quantities, such as residence times in metastable basins. These basins are usually assumed to be completely described by ξ. They have proposed an effective dynamics, which is derived using conditional expectations. The first accuracy result, obtained in 2010, is phrased in terms of an estimate on the relative entropy between the law of $\xi(X_t)$ and the law of its approximation, at any time t (see [63] for a description of the results in a simple case). If an appropriate time-scale separation is present in the system, then the effective dynamics is accurate in the sense of time-marginals. The obtained numerical results showed that this dynamics can also be used to accurately compute residence times in potential energy wells, and thus seem to be accurate in a much stronger sense. Together with S. Olla, they have started to analyze the pathwise accuracy of the proposed coarse-grained dynamics.

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

5.2.5. Convergence to equilibrium

An important question for the analysis of sampling techniques is the rate of convergence to equilibrium for stochastic trajectories.

F. Nier continues to investigate the spectral properties of Witten Laplacians and Kramers-Fokker-Planck operators. In a recent collaboration with D. Le Peutrec and C. Viterbo, the Arrhenius law for metastable states, in its refined version also known as Eyring-Kramers law, was extended to p-forms. Very accurate analytical results have been provided for the exponentially small eigenvalues of Witten Laplacians acting on p-forms.

F. Nier has started a collaboration with T. Lelièvre about accurate exit laws for Smoluchowski processes, via a Witten complex approach. Investigations with G. Pavliotis and T. Lelièvre have started about non gradient diffusion systems.

5.2.6. Hamiltonian dynamics

Constant energy averages are often computed as long time limits of time averages along a typical trajectory of the Hamiltonian dynamics. One difficulty of such a computation is the presence of several time scales in the dynamics: the frequencies of some motions are very high (e.g. for the atomistic bond vibrations), while those of other motions are much smaller. This problem has been addressed in a two-fold manner.

Fast phenomena are often 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 [38], 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 extends previous works of the team. The proposed algorithms can now handle the case when the (unique) fast frequency depends on the slow degrees of freedom, or when there are several fast constant frequencies.

Another track to simulate the system for longer times is to resort to parallel computations. An algorithm in that vein is the parareal in time algorithm. It is based on a decomposition of the time interval into subintervals, and on a predictor-corrector strategy, where the propagations over each subinterval for the corrector stage are concurrently performed on the processors. Using a symmetrization procedure and/or a (possibly also symmetric) projection step, C. Le Bris and F. Legoll, in collaboration with X. Dai and Y. Maday, have introduced several variants of the original plain parareal in time algorithm [35]. These variants, compatible with the geometric structure of the exact dynamics, are better adapted to the Hamiltonian context.

5.3. Complex fluids

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

In [48], Claude Le Bris and Tony Lelièvre have reviewed the state-of-the-art of numerical and mathematical results on micro-macro models for viscoelastic fluids.

Following previous works, Claude Le Bris and Tony Lelièvre together with Lingbing He have analyzed in [43] the longtime behaviour of nematic polymeric fluids (liquid crystals). The longtime asymptotics for such models is much richer than for flexible polymers, which were considered in previous analysis. Indeed, for these models, periodic in time behaviours are expected.

In his PhD under the supervision of Claude Le Bris and Tony Lelièvre, David Benoit studies models of aging fluids developed at the ESPCI (Ecole supérieure de physique et de chimie industrielles) and designed to take into account phenomena such as shear thinning, aging and shear banding in falling sphere experiments. The work consists on the one hand in studying the mathematical well-posedness of some macroscopic models and on the other hand in trying to understand the link between such macroscopic models and microscopic models which have been proposed to describe such fluids.

In the line of his former work [15], Sébastien Boyaval has pursued his work about the mathematical modelling of viscoelastic fluid flows. A new reduced model for thin layers of elastic gravity flows with a free surface was derived in collaboration with François Bouchut, following similar hydrostatic assumptions to those which lead to the Saint-Venant equations as a usual reduced model for shallow water flows. The model is naturally endowed with an energy but the conservative part is non-standard: the energy is not convex with respect to the conservative variables. It is convex with respect to other (more physical) variables. For the numerical simulation of possibly discontinuous solutions, a relaxation scheme is proposed in order to ensure that the numerical approximation mimicks the natural energy dissipation.

In [58], Tony Lelièvre together with Giovanni Samaey and Vincent Legat explored some numerical techniques to get closed macroscopic equations from microscopic models. The proposed method can be seen as a way to justify and extend techniques based on the so-called quasi-equilibirium approximation.

In [40], the effect of a topography on a free surface flow is studied using the free-surface Navier Stokes equations and ALE method for discretization.

5.4. Application of greedy algorithms

Participants: Sébastien Boyaval, Eric Cancès, Virginie Ehrlacher, Tony Lelièvre.

The manuscript [25] where E. Cancès, V. Ehrlacher and T. Lelièvre study the convergence of greedy algorithms to nonlinear convex problems has been accepted for publication. Current research now aims at extending such techniques to non-symmetric problems.

S. Boyaval has continued his study of a new variance reduction method introduced with T. Lelièvre. It makes an innovative use of a greedy algorithm in order to construct control variates for a parameterized family of Monte-Carlo estimator. New successful applications are typical problems in uncertainty quantification.

5.5. Homogenization

Participants: Ronan Costaouec, Claude Le Bris, Frédéric Legoll, Francis Nier, Florian Thomines.

The project-team has pursued its efforts in the field of stochastic homogenization of elliptic equations. The various contributions of the team, which aim at designing numerical approaches that both are pratically relevant and keep the computational workload limited, have been presented from a unified perspective in [59].

An interesting case in that context is when the randomness comes as a *small* perturbation of the deterministic case. As previously shown by former works of the project-team, 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. This previous analysis was performed manipulating the exact correctors, solutions to PDEs posed on $\mathbb{R}^d$. In practice, one can only consider a truncated version of these corrector problems, which is next discretized using e.g. a Finite Element method. The previous analysis has been extended to this practical situation by R. Costaouec [31].

In the work mentioned above, the perturbation to the deterministic case is supposed to be small in the L^∞ norm (that is, almost surely small). The team has also considered 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 covered by that framework). The approach proves to be very efficient from a computational viewpoint, in comparison to the standard approach of stochastic homogenization, as shown in [13], [12]. In that setting, the computation of the homogenized matrix requires repeatedly solving a corrector-like equation for various configurations of the material. For this purpose, C. Le Bris and F. Thomines have shown how to adapt the Reduced Basis approach to the specific context, to even further reduce the computational cost [62].

The team has also proceeded 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 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 [60], [19]. R. Costaouec, C. Le Bris and F. Legoll are currently investigating the possibility to use other variance reduction approaches, such as control variate techniques.

From a numerical perspective, the Multiscale Finite Element Method is a classical strategy to address the situation when the homogenized problem is not known, or when the scale of the heterogeneities, although small, is not considered to be zero (and hence the homogenized problem cannot be considered as a sufficiently accurate 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 [46]. 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. The work [46] also provides a complete analysis of the approach, extending that available for the deterministic setting. Such an analysis often relies on the rate of convergence of the two scale expansion (in the sense of homogenization theory) of the solution to the highly oscillatory elliptic partial differential equation. The result is classic for periodic homogenization. In generic stochastic homogenization, the rate can be arbitrary small, depending on the rate with which the correlations of the random coefficient vanish. In [47], such a result has been established for *weakly stochastic homogenization*. This result is a key ingredient for the numerical analysis of the MsFEM approach proposed in [46].

Still in the framework of the Multiscale Finite Element approach, F. Thomines has further investigated, in collaboration with Y. Efendiev and J. Galvis (Texas A&M University), the use of Reduced Basis methods. They have considered an extension of the MsFEM approach, well suited to the high contrast case, i.e. the case when the ratio between the maximum and the minimum values of the heterogeneous coefficient is large. The main idea of this extension is to complement the standard MsFEM basis functions with the eigenfunctions (associated to the first small eigenvalues) of a local eigenproblem. In [39], Y. Efendiev, J. Galvis and F. Thomines have considered the case when the problem depends on an additional parameter, and shown how to use the Reduced Basis approach to more efficiently compute the eigenfunctions mentioned above.

The theoretical results obtained by the team on variance reduction [19] and on the rate of convergence of the two scale expansion of the solution to a highly oscillatory, weakly random PDE [47], both rely on asymptotic properties of the Green function of the elliptic operator $Lu = -\text{div}\ (A\nabla u)$, where A is a periodic, coercive and bounded matrix. In collaboration with X. Blanc (CEA) and A. Anantharaman, F. Legoll has established some results of this question [11]. This contribution presents in a unified manner and complements several results already given in the literature.

All the works previously mentioned are concerned with elliptic PDEs. F. Nier has studied various problems in the context of wave propagation in random heterogeneous media. In collaboration with S. Breteaux (PhD student in Rennes), he has derived a Boltzmann type equation from first principles of quantum mechanics, using the bosonic QFT presentation of Gaussian random fields. Various extensions of this result are currently under investigation.

5.6. 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.

The quasicontinuum method couples an atomistic model to a continuum approximation in order to compute deformed states of a crystalline lattice at a reduced computational cost compared to a full atomistic simulation. In collaboration with M. Luskin (University of Minnesota) and C. Ortner (Warwick), M. Dobson analyzed the use of numerical solvers for approximating solutions to the equilibrium equations of the force-based quasicontinuum method [37]. In particular, it was shown that a previously-proposed modified conjugate gradient algorithm has unstable modes since the linearized operator is generally not positive-definite. Based on observed properties of the spectrum, convergence rates are given for the GMRES method applied to the operator.

Still in the framework of quasicontinuum methods, several consistent couplings have been proposed in the literature in the past years. M. Dobson showed the impossibility of constructing higher-order consistent couplings for quasicontinuum energies [36]. The analysis is performed in the one-dimensional situation, and is based on the fact that the truncation error gives lower bounds on the global error on the deformation gradient. A consequence of this result is that the so-called quasi-nonlocal energy (which is one of the coupling schemes proposed earlier) has asymptotically optimal error bounds.

The team has also 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. In the one-dimensional setting, an efficient strategy that bypasses the simulation of the whole system had been proposed in 2010. In collaboration with X. Blanc (CEA), F. Legoll has extended this strategy to the so-called membrane setting [20]: the system is composed of atoms that lie on a two-dimensional lattice, and have a unique degree of freedom, representing their height. The strategy can also be used 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 [63].

5.7. Surface chemistry and electrochemistry

Participant: Ismaila Dabo.

Rising energy imperatives have revived strong interest in electrochemical cells (e.g., fuel cells) and photoelectrochemical cells (e.g., dye-sensitized solar cells). Understanding and improving the electrical performance of such systems entails the accurate description of electrode-electrolyte interfaces at the microscopic level. Despite recent advances in the application of computational methods to study realistic electrode-electrolyte interfaces, capturing the effect of the applied electrical voltage and solvent electrical response remains a central challenge in computational electrochemistry. In order to address this difficulty, a comprehensive model for chemical systems embedded in ionic media has been developed. The model couples a quantum description of the electrode with a continuum representation of the electrolyte.

This year, in collaboration with O. Andreussi (MIT) and N. Marzari (University of Oxford), I. Dabo has worked on improving the predictive accuracy and numerical implementation of the continuum solvation model to describe molecular systems and metallic surfaces in interaction with a solvent [14]. The revised model overcomes some of the numerical limitations encountered in existing solvation models and extends their range of applicability. The approach proceeds by recasting the problem in terms of induced polarization charges that act as a direct mapping of the continuum dielectric solvent. The model is defined in a self-consistent manner in terms of the first-principles electronic density of the solute, thereby limiting the number of numerical parameters involved in existing solvation methods. The model accounts for additional pressure and cavitation contributions. The resulting self-consistent continuum solvation (SCCS) model provides an effective, compact fit of computational and experimental data, with solvation energies in error of 0.3-0.4 kcal/mol. The model is implemented in the widely used open-source program QUANTUM-ESPRESSO, exploiting a numerical approach that is intrinsically parallel, robust, and straightforward to adapt to most electronic-structure codes.

In terms of practical applications in surface science and electrochemistry, the adsorption of arsenate (a severe contaminant in drinking water) at the surface of biogeochemical minerals has been studied in collaboration with M. Blanchard and G. Morin (Université Paris 6) [22]. The simulation of infrared spectroscopic experiments for carbon monoxide (a severe catalytic poison) at catalytic surfaces has also been addressed in [33]. Future work includes the generalization of the SCCS model to surfaces in contact with a reservoir of electrons, and molecular dynamics simulations of electrode surfaces.

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. A recent exemple is a contract with Michelin for greedy algorithms and uncertainty propagation in mechanics. 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. Partnerships and Cooperations

7.1. Regional activities

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

7.2. National Initiatives

The project-team is involved in several ANR projects:

- 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. It is coordinated by Eric Cancès.
- F. Legoll, T. Lelièvre and G. Stoltz participate to the ANR MEGAS. 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.
- T. Lelièvre and G. Stoltz participate to the ANR Big MC, which 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).
- C. Le Bris participates to the ANR EMAQS. The scientist in charge is Karine Beauchard (CMLS, Ecole polytechnique).
- F. Nier is a member of the ANR projects QUATRAIN (2007-2011), VOLQUAN (2007-2011), and NONAa (2008-2011).
- 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.

In addition, the team is participating in

- 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,
- the GdR correl (correlated methods in electronic structure computations).

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.

7.4. International Initiatives

7.4.1. Visits of International Scientists

We invited the following researchers to visit our team:

- O. Zeitouni (University of Minnesota and Technion), February 7-12, 2011,
- H. C. Öttinger (ETH Zürich), March 21-25, 2011,
- Y. Efendiev (Texas A & M University), June 6 - July 6, 2011,
- A. Yannacopoulos (Athens University), November 14-18, 2011,
- C. Hartmann (Freie Universität Berlin), November 15-20, 2011.

7.4.2. Bilateral international relations

E. Cancès and V. Ehrlacher are involved in a France-Berkeley project on the modelling of solvated molecules.

8. Dissemination

8.1. Animation of the scientific community

E. Cancès

- 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-), of SIAM Journal of Scientific Computing (2008-), and of Communications in Mathematical Sciences (2011-),
- is a member of the executive committee of the CEA-EDF-INRIA schools in applied mathematics and computer science,
- is a member of the scientific committee of the GDR co-DFT.

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.

Eric 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 framework of the GdR CHANT.

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-), COCV (Control, Optimization and Calculus of Variations) (2003-), Mathematics in Action (2008-), 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 a member of the Scientific Program Committee of ICIAM 2011, Vancouver, Canada.

C. Le Bris is a member of

- 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.

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

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

F. Nier 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.

S. Olla is a member of the editorial boards of Annals of Probability and of Probability theory and related fields. He has organized with Carlangelo Liverani a workshop on “Fourier’s Law” at the Field Institute, Toronto in April 2011.

Gabriel Stoltz co-organized a mini-symposium on “Numerical methods in molecular simulation” at the SMAI 2011 meeting, in Guidel, France (may 2011).

8.2. Teaching

The members of the team have taught the following lectures:

- Licence: Formation au logiciel scientifique SCILAB, 12h, L3, Ecole des Ponts, France (D. Benoit, I. Dabo)
- Licence: Informatique, 50h, L2, CPGE Jean-Baptiste Say, France (D. Benoit, I. Dabo)

- Licence: Analyse, 36h, L3, Ecole des Ponts, France (E. Cancès, V. Ehrlacher, F. Legoll, F. Thomines)
- Licence: Optimisation linéaire et convexité, 36h, L3, Université Paris 6, France (R. Costaouec)
- Licence: Calcul Scientifique, 30h, L3, Ecole des Ponts ParisTech, France (M. Dobson, G. Stoltz)
- Licence: Mathématiques pour biologistes, 36h, L2, University of Cergy Pontoise, France (S. Lahbabi)
- Licence: Formation "C2i" (Certificat Informatique et Internet), 30h, L2, University of Cergy Pontoise, France (S. Lahbabi)
- Master: Introduction au calcul Scientifique, 12h, M1, Ecole des Mines ParisTech, France (D. Benoit, M. Dobson, G. Stoltz)
- Master: Analyse, 40h, M1, EPFL, Switzerland (S. Boyaval)
- Master: Analyse Numérique et Optimisation, 56h, M1, Ecole Polytechnique, France (E. Cancès, C. Le Bris)
- Master: Méthodes mathématiques en chimie quantique, 12h, M2, University Paris 6, France (E. Cancès)
- Master: Introduction à la physique quantique et statistique, 20h, M1, Ecole des Ponts, France (I. Dabo)
- Master: Mathématiques des modèles multiéchelles, 39h, M1, Ecole des Ponts ParisTech, France (F. Legoll)
- Master: Problèmes multi-échelles, 24h, M2, Université Paris 6, France (F. Legoll)
- Master: Méthodes numériques probabilistes, 36 h, M2 Mathématiques et Applications, Université Pierre et Marie Curie, France (T. Lelièvre)
- Master: Modéliser Programmer Simuler, 28 h, M1, Cours Ecole des Ponts ParisTech, France (T. Lelièvre)
- Master: Méthodes déterministes en mathématiques financières, 42h, M2, Ecole des Ponts ParisTech, France (T. Lelièvre)
- Master: Analyse spectrale, 39h, M1, Ecole des Ponts, France (G. Stoltz)
- Master: Computational Statistical Physics, 18h, M2, Ecole des Ponts, France (G. Stoltz)
- Doctorat: Introduction à l'informatique scientifique, 16h, D, Université Paris-Est, France (I. Dabo)

G. Stoltz supervised the internships of Laura Da Silva (Paris 7, Master 1 in biology (AIV)) from March, 1st to April 30th, 2011, and the internship of Etienne Germain (Ecole des Ponts, first year of training), from April 15th to July 15th.

The following PhD & Habilitation were defended:

- HdR: F. Legoll, Contributions à l'étude mathématique et numérique de quelques modèles en simulation multi-échelle des matériaux, Université Paris 6 Pierre et Marie Curie, 17 oct. 2011,
- PhD: R. Costaouec, Techniques numériques d'homogénéisation: application aux matériaux aléatoires, Université Paris-Est, Ecole des Ponts ParisTech, 23 nov. 2011, supervised by C. Le Bris.

The following PhDs are in progress:

- PhD in progress: D. Benoit, Méthodes numériques pour la simulation des fluides non-Newtoniens, Université Paris-Est, Ecole des Ponts ParisTech, started october 1st, 2010, supervised by C. Le Bris and T. Lelièvre
- PhD in progress: V. Ehrlacher, Some mathematical and numerical problems in quantum mechanics and uncertainty quantification", Université Paris-Est, Ecole des Ponts ParisTech, started october 1st 2009, supervised by E. Cancès and T. Lelièvre
- PhD in progress: S. Lahbabi, Mathematical study of quantum crystals with random defects, University of Cergy-Pontoise, started september 1st 2010, supervised by E. Cancès and M. Lewin
- PhD in progress: F. Thomines, Méthodes numériques multi-échelles: application á l'homogénéisation des matériaux aléatoires, Université Paris-Est, Ecole des Ponts ParisTech, started on Sept. 1st, 2009, supervised by C. Le Bris

8.3. Conference participation

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

- D. Benoit, Congrès SMAI 2011, Guidel, France, May 2010,
- S. Boyaval, séminaire Université de Lille, January 2011,
- S. Boyaval, workshop on Reduced basis methods in high dimensions, Paris, June 2011,
- S. Boyaval, ICIAM, minisymposium Reduced-Basis methods, Vancouver, Canada, July 2011,
- 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,
- E. Cancès, weekly seminar of the mathematics department, University of Grenoble, February 2011,
- 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 Pisa, Italy, October 2011,
- E. Cancès, weekly seminar of the chemistry department, University of Lille, November 2011,
- R. Costaouec, Congrès SMAI 2011, Guidel, May 2011,
- R. Costaouec, ICIAM 2011 conference, Vancouver, July 2011,
- I. Dabo, CEA Seminar, CEA, Saclay, September 2011,
- I. Dabo, CEA Seminar, CEA, Grenoble, September 2011,
- I. Dabo, LPICM Seminar, Ecole Polytechnique, Palaiseau, April 2011,
- I. Dabo, GDR coDFT, Obernai, June 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. Dobson, RSME2011 conference, Avila, February 2011,
- M. Dobson, ICIAM 2011 conference, Vancouver, July 2011,
- M. Dobson, 11th USNCCM conference, Minneapolis, 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,
- 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, Modern Trends in PDE's, Geometric Analysis and Mathematical Physics, University of Cergy-Pontoise, September 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, 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,
- F. Legoll, workshop on "Multiscale simulation of heterogeneous materials and coupling of thermodynamic models", Louvain, January 2011,
- F. Legoll, workshop on "Mathematical Analysis for Peridynamics", Oberwolfach, January 2011,
- F. Legoll, Workshop "Random Media: Homogenization and Beyond", IPAM, Los Angeles, January 2011,
- F. Legoll, RSME2011 conference, Avila, February 2011,
- F. Legoll, seminar of the POEMS team-project, Paris, February 2011,
- F. Legoll, Fraunhofer Institute seminar, Kaiserslautern, March 2011,
- F. Legoll, workshop on Stochastic Multiscale Methods, Banff, March 2011,
- F. Legoll, Applied Mathematics Colloquium, Caltech, April 2011,

- F. Legoll, 10ième Colloque National en Calcul des Structures, Giens, May 2011,
- F. Legoll, workshop on “Ginzburg-Landau equations, Dislocations and Homogenization”, Ile de Ré, May 2011,
- F. Legoll, Workshop on “Coarse-graining of many-body systems”, Heraklion, June 2011,
- F. Legoll, AMS von Neumann Symposium on Multimodel and Multialgorithm Coupling for Multiscale Problems, Snowbird, July 2011,
- F. Legoll, ICIAM 2011 conference, Vancouver, July 2011,
- F. Legoll, 11th USNCCM conference, Minneapolis, July 2011,
- F. Legoll, Enumath conference, Leicester, September 2011,
- F. Legoll, Mini-symposium on Mathematics in Materials Science, September 2011,
- F. Legoll, 3rd Summer School of the Large Scale Initiative "FUSION", Paris, September 2011,
- F. Legoll, Numerical analysis seminar, Department of Mathematics, Texas A & M University, September 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, Séminaire du CMAP, Ecole Polytechnique, May 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,
- T. Lelièvre, Workshop on Nucleation and Rare Events, Pekin, September 2011,
- T. Lelièvre, Journées scientifiques MoMaS, Marseille, November 2011,
- T. Lelièvre, Workshop Reduced Basis, POD or PGD-Based Model Reduction Techniques, Cachan, November 2011,
- T. Lelièvre, Workshop Interactions EDPs/Probas, GDR CHANT, Grenoble, November 2011,
- T. Lelièvre, Workshop on Multiscale Systems: Theory and Applications, Warwick, December 2011,
- 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,
- 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. Samaey, SIAM Conference on Applications of Dynamical Systems, Snowbird, Utah, May 2011,
- G. Samaey, Making it Real Seminar, Bristol University, May 2011,
- G. Samaey, Applied Mathematics and Mathematical Physics Seminar, Imperial College, London, June 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, weekly seminar of the mathematical physics group, Université de Cergy, November 2011,
- G. Stoltz, journée CECAM on modeling of matter, Paris, December 2011,
- G. Stoltz, Workshop on Multiscale Systems: Theory and Applications, Warwick, December 2011,
- F. Thomines, workshop on “Multiscale simulation of heterogeneous materials and coupling of thermodynamic models”, Louvain, January 2011,
- F. Thomines, ICIAM 2011 conference, Vancouver, July 2011,
- F. Thomines, Enumath conference, Leicester, September 2011,
- F. Thomines, Numerical analysis seminar, Department of Mathematics, Texas A & M University, September 2011,

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

- F. Legoll, Texas A & M University, College Station, USA, 30 Nov - 9 Dec 2011,
- F. Thomines, Texas A & M University, College Station, USA, September 2011,

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

- 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,
- 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 Maggioren, September 2011,
- C. Le Bris, Lectures on Stochastic homogenization, Series of 3 one-hour lectures, National University of Singapore, December 2011,
- F. Legoll, Lectures (5h) on "Some recent numerical approaches for random multiscale materials", EMS School and Workshop on Mathematics for Multiscale Phenomena, Bedlewo, October 2011,
- F. Legoll, Lectures (3h) on "Energie libre et dynamique réduite en dynamique moléculaire", GdR CHANT workshop on “Interactions EDPs/Probas: modèles probabilistes pour la simulation moléculaire”, Grenoble, November 2011.

Members of the project-team have presented posters in the following events:

- R. Costaouec, Workshop Random Media: Homogenization and Beyond, IPAM, Los Angeles, January 2011,
- M. Dobson, AMS von Neumann Symposium on Multimodel and Multialgorithm Coupling for Multiscale Problems, Snowbird, July 2011,
- M. Dobson, Metastability and stochastic processes, Ecole des Ponts ParisTech, September 2011,
- F. Thomines, Workshop “Random Media: Homogenization and Beyond”, IPAM, Los Angeles, January 2011.

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

- S. Lahbabi, BIRS workshop on Density Functional Theory: fundamentals and applications in condensed matter physics", Banff, Canada, January 2011,
- S. Lahbabi, MFO workshop on mathematical methods in quantum chemistry, Oberwolfach, Germany, June-July 2011,
- S. Lahbabi, Modern Trends in PDE's, Geometric Analysis and mathematical physics, Cergy, September 2011,
- S. Lahbabi, Frontiers in Mathematical Physics, Cergy, May 2011,
- S. Lahbabi, Summer school on current topics in Mathematical Physics, Vienna, Austria, August 2011,

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] R. COSTAOUEC. *Techniques numériques d'homogénéisation: application aux matériaux aléatoires*, Université Paris-Est, Ecole des Ponts ParisTech, 2011, Ph.D. Thesis supervised by Claude Le Bris.

[8] F. LEGOLL. *Contributions à l'étude mathématique et numérique de quelques modèles en simulation multi-échelle des matériaux*, Université Paris 6 Pierre et Marie Curie, 2011, Habilitation à diriger des recherches, Ph. D. Thesis.

Articles in International Peer-Reviewed Journal

[9] 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/.

[10] Z. AMMARI, F. NIER. *Mean field propagation of Wigner measures and BBGKY hierarchies for general bosonic states.*, in "HAM preprint", 2011, http://hal.archives-ouvertes.fr/hal-00644656/.

[11] A. ANANTHARAMAN, X. BLANC, F. LEGOLL. *Asymptotic behaviour of Green functions of divergence form operators with periodic coefficients*, in "Applied Math. Research Express", 2011, submitted, http://hal.archives-ouvertes.fr/hal-00637489.

[12] A. ANANTHARAMAN, C. LE BRIS. *A numerical approach related to defect-type theories for some weakly random problems in homogenization*, in "Multiscale Model. Sim.", 2011, vol. 9, n^{o} 2, p. 513-544.

[13] 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.

[14] O. ANDREUSSI, I. DABO, N. MARZARI. *Revised self-consistent continuum solvation in electronic-structure calculations*, in "J. Chem. Phys.", 2011, submitted.

[15] J. W. BARRETT, S. BOYAVAL. *Existence and approximation of a (regularized) Oldroyd-B model*, in "M3AS", 2011, vol. 21, n^{o} 9, p. 1783–1837, http://hal.archives-ouvertes.fr/hal-00409594/fr/.

[16] G. BENAROUS, Y. HU, S. OLLA, O. ZEITOUNI. *Einstein relation for biased random walk on Galton–Watson trees*, in "Ann. I. H. Poincare", 2011, to appear.

[17] 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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[19] X. BLANC, R. COSTAOUEC, C. LE BRIS, F. LEGOLL. *Variance reduction in stochastic homogenization using antithetic variables*, in "Markov Processes and Related Fields", 2011, in press.

[20] X. BLANC, F. LEGOLL. *A numerical strategy for coarse-graining two-dimensional atomistic models at finite temperature: the membrane case*, in "Computational Materials Science", 2011, submitted, http://hal-enpc.archives-ouvertes.fr/hal-00627294/fr/.

[21] X. BLANC, C. LE BRIS, P.-L. LIONS. *From the Newton equation to the wave equation in some simple cases*, in "NHM", 2011, submitted.

[22] M. BLANCHARD, G. MORIN, M. LAZZERI, E. BALAN, I. DABO. *First-principles simulation of arsenate adsorption on the (112) surface of hematite*, in "Geochemica Cosmochimica Acta", 2011, submitted.

[23] F. BOUCHUT, S. BOYAVAL. *A new model for shallow elastic fluids*, in "JNNFM", 2011, submitted, http://hal-enpc.archives-ouvertes.fr/hal-00628651.

[24] E. BOURASSEAU, J.-B. MAILLET, N. DESBIENS, G. STOLTZ. *Microscopic calculations of Hugoniot curves of neat TATB and of its detonation products*, in "J. Phys. Chem. A", 2011, vol. 115, n^{o} 39, p. 10729-10737, http://hal.archives-ouvertes.fr/hal-00595191/fr/.

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[60] X. BLANC, R. COSTAOUEC, C. LE BRIS, F. LEGOLL. *Variance reduction in stochastic homogenization: the technique of antithetic variables*, Lecture Notes in Computational Sciences and Engineering, Springer, 2011, vol. 82, p. 47-70.

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