Activity Report 2012

Project-Team MICMAC

Methods and engineering of multiscale computing from atom to continuum

Table of contents

Project-Team MICMAC

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Creation of the Project-Team: October 01, 2002 .

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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. Electronic structure calculations

Participants: Eric Cancès, Ismaila Dabo, Virginie Ehrlacher, David Gontier, Salma Lahbabi, Claude Le Bris, Gabriel Stoltz.

In electronic structure calculation 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 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 using a thermodynamic limit of Kohn-Sham type models. In [24], E. Cancès and G. Stoltz have 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 collaboration with M. Lewin, E. Cancès and S. Lahbabi have introduced in [54] a functional setting for mean-field electronic structure models of Hartree-Fock or Kohn-Sham types for disordered quantum systems, and used these tools to study the reduced Hartree-Fock model for a disordered crystal where the nuclei are classical particles whose positions and charges are random.

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 [22], 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 [23]. In [53], they have introduced a general theoretical framework to analyze non-consistent approximations of the discrete eigenmodes of a self-adjoint operator, focusing in particular on the discrete eigenvalues laying in spectral gaps. Applying this analysis to the supercell method for perturbed periodic Schrödinger operators, they derive optimal convergence rates for the planewave discretization method, taking numerical integration errors into account. These results, along with earlier work on greedy algorithms for nonlinear convex problems and the study of local defects in the Thomas-Fermi-von Weiszacker theory, are collected in [7].

In the work [38], Claude Le Bris, in collaboration with Pierre Rouchon (Ecole des Mines de Paris), has introduced a new efficient numerical approach, based on a model reduction technique, to simulate high dimensional Lindblad type equations at play in the modelling of open quantum systems. The specific case under consideration is that of oscillation revivals of a set of atoms interacting resonantly with a slightly damped coherent quantized field of photons. The approach may be employed for other similar equations. Current work is directed towards other numerical challenges for this type of problems.

5.2. Computational Statistical Physics

Participants: Matthew Dobson, Claude Le Bris, Frédéric Legoll, Tony Lelièvre, Francis Nier, Grigorios Pavliotis, Mathias Rousset, 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 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. One of the main difficulty is related to the metastable features of the generated trajectories: the system remains trapped over very long times in metastable

states, which means that very long trajectories need to be generated in order to obtain macroscopically relevant quantities. This is related to the fact that the timescale at the microscopic level is much smaller than the timescale at the macroscopic level. In [66], we propose a summary of the mathematical approaches to quantify metastability, and which appear to be useful to analyze the numerical methods used in molecular dynamics.

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 [42], 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).

One interest of free energy computation techniques is that they appear to be useful in other fields, like in computational statistics where multimodal measures are also frequently encountered, so that standard Markov Chain Monte Carlo appraoches also suffer from metastability.

For example, in [25], Nicolas Chopin (CREST, ENSAE), T. Lelièvre and G. Stoltz explore the application of the Adaptive Biasing Force method to Bayesian inference. This sampling method belongs to the general class of adaptive importance sampling strategies which use the free energy along a chosen reaction coordinate as a bias. Such algorithms are very helpful to enhance the sampling properties of Markov Chain Monte Carlo algorithms, when the dynamic is metastable.

In [58], G. Fort (Telecom Paris), B. Jourdain (CERMICS), E. Kuhn (INRA), T. Lelièvre and G. Stoltz have considered the Wang-Landau algorithm. The authorshave proved that the Wang-Landau algorithm converges with an associated central limit theorem, and have provided an analysis of the efficiency of the algorithm in a metastable situation.

5.2.2. Convergence to equilibrium

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

In [65], F. Nier, T. Lelièvre and G. Pavliotis study the interest of using non-reversible stochastic dynamics to enhance the rate of convergence to equilibrium, compared to reversible dynamics. A well posed optimization problem is obtained and solved in the case of a linear drift for the overdamped Langevin dynamics.

5.2.3. Metropolis Hastings algorithms

A classical sampling tool used in molecular dynamics and in computational statistics is the Metropolis-Hastings algorithm. There has been a lot of work (see G. Roberts et al.) to study how the variance of the proposal should scale with the dimension of the problem, in order to optimize the sampling procedure. Most of these works assume that (i) the target probability is the product of n one dimensional laws and that (ii) the Markov chain starts at equilibrium.

In the two works [60], [59], T. Lelièvre and his co-authors have generalized these results when the initial distribution is not the target probability. The diffusive limit in the latte case is solution to a stochastic differential equation nonlinear in the sense of McKean. They have discussed practical counterparts in order to optimize the variance of the proposal distribution to accelerate convergence to equilibrium. The analysis confirms the interest of the constant acceptance rate strategy (with acceptance rate between $1/4$ and $1/3$) first suggested in the works of G. Roberts et al., at least for the Random Walk Metropolis algorithm.

5.2.4. Thermodynamic limit

The quasicontinuum method is an approach to couple an atomistic model with a coarse-grained approximation in order to compute the states of a crystalline lattice at a reduced computational cost compared to a full atomistic simulation.

In that framework, the team has 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. We refer to [47] for a recent review. In collaboration with X. Blanc (Université Pierre et Marie Curie), F. Legoll has extended this strategy to the so-called membrane setting in [16].

When the temperature is small, a perturbation approach can be used to compute the canonical averages of these observables depending only on a few variables, at first order with respect to temperature. In collaboration with E. Tadmor, W. K. Kim, L. Dupuy and R. Miller, F. Legoll has analyzed such an approach in [46]. The numerical tests reported there show the efficiency of the approach, as long as the temperature is indeed small.

5.2.5. *Sampling trajectories*

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

Following a numerical observation in a previous work on the sampling of reactive trajectories by a multilevel splitting algorithm, F. Cérou (Inria Rennes), A. Guyader (Inria Rennes), T. Lelièvre and F. Malrieu (Université de Rennes) study theoretically in [56] the distribution of the lengths of these trajectories, using large deviation techniques.

In [37], C. Le Bris and T. Lelièvre together with M. Luskin and D. Perez from Los Alamos National Laboratoy provide a mathematical analysis of the parallel replica algorithm, which has been proposed by A. Voter in 1997 to simulate very efficiently metastable trajectories. This work opens a lot of perspectives, by using a generic tool (the quasi stationary distribution) to make a link between a continuous state space dynamics (Langevin dynamics) and a discrete state space dynamics (kinetic Monte Carlo models).

In a work in progress, T. Lelièvre and F. Nier have studied the quasi-stationnary distribution in relation for an overdamped Langevin process in a bounded domain. In the small temperature limit and by making the connection with boundary Witten Laplacians, they are able to compute accurately the spatial exit law along the boundary and non perturbative accurate formulas when the potential is changed inside the domain.

5.2.6. *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 introduced and analyzed some years ago a strategy to define 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). We refer to [47] for a recent review. The aim was to get a coarse-grained description giving access to some *dynamical* quantities (and not only *equilibrium* quantities). Together with G. Samaey (KU Leuven), they have recently studied how to use this coarse-grained description, accurate when the time scale separation is asymptotically large, to somewhat precondition the dynamics of the actual system in cases when the time scale separation is not large. For that purpose, they have used the parareal framework, to iteratively correct the sequential coarse-grained trajectory by fine scale trajectories performed in parallel. The main difficulty is that the two models (the reference one and the coarse-grained one) do not act on the same variable: the reference model evolves all the variables, whereas the coarse-grained model only evolves the slow variables. As shown in [63] in a simplified context (that of singularly perturbed ODEs), the precise coupling between both models should be done carefully.

The above study is concerned with models with continuous state spaces. S. Lahbabi and F. Legoll have studied in [61] a related question in the framework of kinetic Monte Carlo models, where the state space is discrete. For some models involving some slow and some fast variables, the effective dynamics of the slow component has been identified, and a complete proof of convergence proposed.

5.2.7. 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 [29], M. Dobson, C. Le Bris, and F. Legoll have 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 [28]. These variants, compatible with the geometric structure of the exact dynamics, are better adapted to the Hamiltonian context.

5.2.8. 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 molecular dynamics of the project-team.

Nonequilibrium molecular dynamics simulations can 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. Lelièvre, and G. Stoltz have derived a Langevin-type dynamics for a heavy particle in a non-zero background flow [57]. 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.

Let us also mention that the article on the computation of the viscosity of fluids using steady state nonequilibrium dynamics with an external nongradient bulk forcing, in the framework of the PhD of Rémi Joubaud, has also been published [34]. In addition, the study by G. Stoltz and C. Bernardin on thermal transport in one-dimensional chains of oscillators whose kinetic and potential energy functions are the same, has been accepted and is now published [13].

5.3. Complex fluids

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

In [41], Claude Le Bris and Tony Lelièvre review the state-of-the-art of numerical and mathematical results on micro-macro models for viscoelastic fluids.

Following previous works, in [32], Claude Le Bris and Tony Lelièvre together with Lingbing He analyze the longtime behaviour of nematic polymeric fluids (liquid crystals). The longtime asymptotic for such models is much richer than for flexible polymers, that were considered in a previous analysis. Indeed, for these models, periodic in time behaviours are observed.

In his PhD under the supervision of Claude Le Bris and Tony Lelièvre, David Benoît 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 in studying on the one hand the mathematical well-posedness of some macroscopic models, see [51] 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.

Related to the mathematical modelling of free-surface complex flows under gravity, a new reduced model for thin layers of a viscoelastic upper-convected Maxwell fluid was derived by S. Boyaval in collaboration with François Bouchut, and possibly discontinuous solutions were numerically simulated with a new finite-volume scheme of relaxation type that satisfies a discrete counterpart of the natural dissipation [20]. This work is being pursued for other models.

Finally, in [31], Alexandre Ern (CERMICS), Rémi Joubaud (CERMICS) and Tony Lelièvre analyze a model describing equilibrium binary electrolytes surrounded by charged solid walls. This work is done in collaboration with physicists from the group PECSA at Université Pierre et Marie Curie. Applications include the modelization of clays for the burying of nuclear waste.

5.4. Application of greedy algorithms

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

Greedy algorithms are used in many contexts for the approximation of high-dimensional functions: Proper Generalized Decomposition, Reduced Basis techniques, etc.

Various greedy algorithms for high-dimensional non-symmetric problems, and inherent theoretical and practical difficulties have been analyzed in [52]. Current research now aims at extending these techniques to the approximation of high-dimensional spectral problems. Prototypical applications include electronic structure calculations or the computation of buckling modes in mechanics.

In probabilistic methods for uncertainty quantification in mechanics, S. Boyaval has used a greedy algorithm to construct control variates for accelerating Monte-Carlo simuation in the cases where an expectation has to be computed many times [21]. The work is being applied to the uncertainty quantification in numerical models for hydraulic engineering.

Finally, in [55], Fabien Casenave (CERMICS), Alexandre Ern (CERMICS) and Tony Lelièvre study the influence of round-off errors on the evaluation of the a posteriori estimators in the reduced basis approach. In practice, the evaluation of the error estimator can become very sensitive to round-off errors. An explanation of this fact is proposed, as well as efficient remedies.

5.5. Mathematical Physics

Participant: Francis Nier.

In [10], A. Aftalion and F. Nier answer questions asked by J. Dalibard about the feasibility of artificial gauge potentials. This analysis provides the range of small parameters within which the linear adiabatic argument used by the physicists is certainly not destroyed by the non linear effects.

In [43], D. Le Peutrec, F. Nier and C. Viterbo give an accurate Arrhenius law for Witten Laplacian acting on p-forms. In the case of functions the exponentially small eigenvalues are given by exponentiated differences of enegy levels between local minima and saddle points (Arrhenius law). In the case of p-forms the association of critical points with index p and critical points with index p+1 or p-1, is more subtle and is provided by Barannikov's presentation of Morse theory.

In [11], Z. Ammari and F. Nier have proved the mean field dynamics of general bosonic systems in the presence of singular pair interaction potentials, including the important 3 dimensional Coulombic case. As compared with their previous works, they developed a slightly new strategy relying on measure transportation techniques and results presented by Ambrosio-Gigli-Savaré in their book "Gradient Flows: In Metric Spaces And In The Space Of Probability Measures" (2005).

5.6. Homogenization and related topics

Participants: Ronan Costaouec, Claude Le Bris, Frédéric Legoll, William Minvielle, Mathias Rousset, Florian Thomines.

The homogenization of (deterministic) non periodic systems is a well known topic. Although well explored theoretically by many authors, it has been less investigated from the standpoint of numerical approaches (except in the random setting). In collaboration with X. Blanc and P.-L. Lions, C. Le Bris has introduced in [17] a possible theory, giving rise to a numerical approach, for the simulation of multiscale nonperiodic systems. The theoretical considerations are based on earlier works by the same authors (derivation of an algebra of functions appropriate to formalize a theory of homogenization). The numerical endeavour is completely new. Promising results have been obtained on a simple case of a periodic system perturbed by a localized defect. Ongoing works consider other configurations, such as for instance an interface between two different crystalline phases.

A theme closely related to homogenization theory and on which several members of the project team have worked a lot in the past few years is the passage from discrete (atomistic) mechanics to continuum mechanics. In this direction, C. Le Bris, in collaboration with X. Blanc and P.-L. Lions, has established in [18] the rigorous continuum limit of the Newton equations of motion for some simple cases of one-dimensional atomistic system.

The project-team also has pursued its efforts in the field of stochastic homogenization of elliptic equations, aiming at designing numerical approaches that both are pratically relevant and keep the computational workload limited.

An interesting case in that context is when the randomness comes as a *small* perturbation of the deterministic case. As previously shown by earlier 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. A final component of the work completed by Florian Thomines during his PhD thesis has concerned the application of Reduced Basis techniques to that specific context of weakly stochastic homogenization problems. In particular, the approach has been adapted in [39] to efficiently compute the terms of the expansion previously developed by A. Anantharaman and C. Le Bris to approximate a certain category of weakly random homogenization problems. It has been demonstrated that the reduced basis technique is very helpful in this particular context and indeed allows for a speed up of the computation. Another application of the same technique, for a slightly different category of models (still in the framework of weakly random homogenization problems) originally derived by X. Blanc, P.-L. Lions and C. Le Bris, has also been explored. The difficulty, there, is to compute the various corrector equations that parametrically depend on the macroscopic location of the microstructure and the particular realization of that microstructure. The problem is definitely amenable to reduced basis techniques, as demonstrated by some preliminary tests, but definite conclusions on the general validity of the approach are yet to be obtained.

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 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 $\mathbb{R}^d$, the team has shown in [14] that the variance of this matrix can be reduced using the technique of antithetic variables. F. Legoll and W. Minvielle are currently extending this technique to nonlinear, convex homogenization problems.

In addition, C. Le Bris, F. Legoll, W. Minvielle and M. Rousset are currently investigating the possibility to use other variance reduction approaches, such as control variate techniques. A promising idea is to use the weakly stochastic model previously introduced by A. Anantharaman and C. Le Bris (in which a periodic model is perturbed by a *rare* stochastic perturbation) to build a control variate model. The preliminary results that have already been obtained are very encouraging.

Another contribution in stochastic homogenization is the following. C. Le Bris, in collaboration with X. Blanc and P.-L. Lions, has recently introduced a variant of the classical random homogenization. For that variant, as often in random homogenization, the homogenized matrix is again defined from a so-called corrector function, which is the solution to a problem set on the entire space. F. Legoll and F. Thomines have described and proved the almost sure convergence of an approximation strategy based on truncated versions of the corrector problem in [64]. F. Legoll and F. Thomines have also established, in the one-dimensional case, a convergence result on the residual process, defined as the difference between the solution to the highly oscillatory problem and the solution to the homogenized problem.

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 difficult 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 approximation). 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 [36]. 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 [36] also provides a complete analysis of the approach, extending that available for the deterministic setting. Such analysis often rely 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. Such a 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. C. Le Bris, F. Legoll and F. Thomines have established in [40] such a result for *weakly stochastic homogenization*, using 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), established by F. Legoll in collaboration with X. Blanc and A. Anantharaman [15].

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 eigenvalue problem. In [30], Y. Efendiev, J. Galvis and F. Thomines have considered the case when the problem depends on an additional parameter, and have shown how to use the Reduced Basis approach to more efficiently compute the eigenfunctions mentioned above.

Even in simple deterministic cases, there is actually still room for improvement in many different directions for the MsFEM approach. In collaboration with A. Lozinski (University of Toulouse and now at the University of Besançon) who visited the team-project repeatedly during the year, F. Legoll and C. Le Bris have introduced and studied a variant of MsFEM that considers Crouzeix-Raviart type elements on each mesh element. The continuity across edges (or facets) of the (multiscale) finite element basis set functions is enforced only weakly, using fluxes rather than point values. The approach has been analyzed (combining classical arguments from homogenization theory and finite element theory) and tested on simple, but highly convincing cases [35]. In particular, an elliptic problem set on a domain with a huge number of perforations has been considered in [62]. The variant developed outperforms all existing variants of MsFEM. A follow up on this work, in collaboration with U. Hetmaniuk (University of Washington in Seattle, two-week visitor in the project-team in the Spring of 2012), consists in the study of multiscale advection-diffusion problems. Such problems are possibly advection dominated and a stabilization procedure is therefore required. How stabilization interferes with the multiscale character of the equation is an unsolved mathematical question worth considering for numerical purposes.

Still another question related to homogenization theory that is investigated in the group is the following. Consider an elliptic equation, say in divergence form, with a highly oscillatory matrix coefficient. Is it possible to approximate the boundary value problem for different right hand sides using a similar problem with a *constant* matrix coefficient? How can this "best" constant matrix approximating the oscillatory problem be

constructed in an efficient manner? How is this matrix related to the homogenized matrix, in the limit of infinitely rapidly oscillatory coefficients? Current work is directed towards solving such issues.

5.7. Asymptotic variance reduction

Participant: Mathias Rousset.

Recently, M. Rousset has initiated a research topic on variance reduction techniques (called "asymptotic") for the simulation of stochastic models of particles. The point is to use a macroscopic (or model reduced) equation as a control variate; or in other words, to use the information of a macroscopic description to decrease the statistical error of the simulated microscopic evolution.

A first step in this program has been achieved for a microscopic model describing the individual motion of bacteriae with a Markovian velocity-jump process. The macroscopic equation is an advection-diffusion equation called the chemotaxis equation. In [44], the pobabilistic derivation of the chemotaxis equation from the individual motion of bacteriae have been carried out in a rigorous way. In [45], a numerical method simulating the individual evolution of bacteriae with "asymptotic" variance reduction have been proposed.

5.8. Computational materials spectroscopy in electrochemistry and optoelectronics

Participant: Ismaila Dabo.

Many advances in the understanding and design of nanomaterials have been enabled by spectroscopic techniques of increasing spatial and temporal resolution. In electrochemistry and optoelectronics, spectroscopy provides insight into the chain of processes involved in harnessing, storing, and delivering energy.

In support to experimental techniques, much progress has been achieved in simulating spectroscopic phenomena to shed light into energy conversion at the molecular scale. Such understanding is critical to the molecular design of a range of electrical devices, including but not limited to fuel cells, batteries, dye-sensitized solar cells, and optoelectronic devices.

The work of I. Dabo is dedicated to the development of quantum and semiclassical methods to simulate spectroscopies of electrochemical and optoelectronic materials. The achieved level of efficiency and accuracy fosters dialogue between experiment and theory for interpreting complex spectroscopic data. This year, these novel methods have been applied to simulate spectroscopic phenomena spanning the infrared to the visible and ultraviolet ranges.

The first application pertains to the infrared sum-frequency-generation (SFG) spectroscopy of adsorption mechanisms at the origin of the tolerance of fuel-cell catalytic electrodes to chemical poisoning. The study explains the critical influence of the electrode voltage in analyzing surface spectroscopy experiments (work done in collaboration with EPFL). [12], [26], [19]

The second application aims at understanding the sensitizing properties of organometallic dyes in dye-sensitized solar cells by simulating optical photoluminescence (PL) spectra, thereby elucidating the role of electron localization and ligand functionalization on the phosphorescence of organometallic complexes (work done in collaboration with the University of Minnesota). [33]

The third application is focused on the ultraviolet photoelectron spectroscopy (UPS) of photoactive nanomaterials of relevance to the design of organic photovoltaic junctions and photoelectrodes (work done in collaboration with the Italian Institute of Nanoscience, Seoul National University, and Xiamen University). [27]

Future challenges and opportunities are related to the time-dependent simulation of transient and cyclic spectra. These developments, which will be part of the widely used Quantum-ESPRESSO distribution (http://www.quantum-espresso.org), would pave the way for comprehensive studies of kinetic processes in tandem with time-resolved spectroscopic experiments.

6. Bilateral 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. 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 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 E. Cancès.
- I. Dabo is members of the ANR PANELS (Photovoltaics from Ab-initio Novel Electronic-structure Simulations).The PANELS initiative gathers three groups (CNRS, Institut Neel, France; Université de Lyon, LPMCN, France; Ecole des Ponts, Université Paris-Est, CERMICS, France) expert in methodology developments around many-body perturbation theory and a novel orbital-dependent density functional formalism, in order to study the electronic, optical and transport properties of second/third generation photovoltaic devices.
- E. Cancès is involved in the ANR BECASIM, which is concerned with the numerical simulation of Bose-Einstein condensates. This ANR has been accepted in June 2012, and is coordinated by I. Danaila (Université de Rouen).
- C. Le Bris participates to the ANR EMAQS. The scientist in charge is Karine Beauchard (CMLS, Ecole polytechnique).
- F. Legoll participates to the ANR Megas.
- T. Lelièvre is in charge of the ANR project "MEGAS".
- T. Lelièvre is member of the ANR-project "BIGMC" (PI: Gersende Fort, Telecom ParisTech) and of the ANR-project "STAB" (PI: I. Gentil, Université de Lyon).
- F. Nier is a member of ANR-NOSEVOL led by F. Hérau (Nantes) T. Ramond (Orsay) and S. Vu-Ngoc (Rennes), started in jan. 2012 for 4 years.
- F. Nier is a member of ANR-LODIQUAS led by F. Castella (Rennes) and N. Mauser (Wien), started in april 2012 for 4 years.

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),
- the GDR-CNRS 3274 Dynamique Quantique 2009-2012,
- the GDR-CNRS 2434 Analyse des Equations aux Dérivées Partielles.

The MICMAC team project is involved in two Labex, namely the Labex Bezout (started in 2011) and the Labex MMCD (started in 2012).

We have invited the following National researchers to visit our team:

- A. Lozinski (University of Toulouse and now at the University of Besançon): repeated visits during the year 2012.

7.3. International Initiatives

7.3.1. *Visits of International Scientists*

We have invited the following researchers to visit our team:

- U. Hetmaniuk (University of Washington in Seattle), March 5-16, 2012,
- B. Khoromskij and V. Khoromskaia, (Max-Planck-Institute for Mathematics in the Sciences Leipzig), December 17-20, 2012.
- G. Nguetseng (University of Yaoundé 1, Cameroon), March 19-30, 2012,

7.3.2. *Bilateral international relations*

E. Cancès is involved in a France-Berkeley project on the modelling of solvated molecules.

T. Lelièvre, G. Stoltz and F. Legoll participates to the Laboratoire International Associé (LIA) CNRS / University of Illinois at Urbana-Champaign on complex biological systems and their simulation by high performance computers. This LIA involves on the french side research teams from Université Nancy, Université de Lyon and Inria Rennes.

8. Dissemination

8.1. Animation of the scientific community

E. Cancès

- 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 workshop on the mathematics and numerical analysis of electronic structure models, Beijing, China, June 2012,
- a worskhop on quantum and atomistic modeling of materials defects, IPAM-UCLA, Los Angeles, USA, October 2012.

I. Dabo, V. Ehrlacher and G. Stoltz have co-organized a CFCAM meeting on numerical and mathematical problems for solar cell devices, in Paris, France, 5 september 2012.

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 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 held a position of Visiting Professor at the University of Chicago, October-November 2012.

F. Legoll is a member of the editorial board of SIAM MMS (2012-) and of ESAIM Proc (2012-).

F. Legoll has co-organized with B. Kraczek, R. Jones and K. Mandadapu a mini-symposium on "Atomistic basis of thermal processes in driven systems" at the 22nd International Workshop on Computational Mechanics of Materials (IWCMM XXII), Baltimore, Sept. 24-26 2012.

T. Lelièvre is an Ordway visiting professor at the University of Minnesota for the academic year 2012-2013.

T. Lelièvre has co-organized a CECAM workshop "Free energy calculations: From theory to applications" at the Ecole des Ponts, June 4th-8th 2012.

F. Nier is a member of the scientific committee of

- the workshop "Mathematics for semiconductor heterostructure 2012" WIAS-Berlin, September 2012,
- the CNRS-GDR "Dynamique Quantique" led by S. de Bièvre.

G. Stoltz has co-organized the workshop "Nonequilibrium Statistical Mechanics: Mathematical Understanding and Numerical Simulation" held at BIRS, Banff, Canada, November 12-16, 2012.

I. Dabo, V. Ehrlacher and G. Stoltz have co-organized a CFCAM discussion day on "Numerical methods and mathematical approaches for solar devices" in Inria Paris, September 5th, 2012.

V. Ehrlacher and T. Lelièvre have co-organized a thematic minisymposium on greedy algorithms for high-dimensional problems at AIMS 2012, Orlando, USA, July 2012.

8.2. Teaching - Supervision

The members of the team have taught the following courses:

- Licence: Analyse, 27h, L1, Université de Cergy Pontoise, France (S. Lahbabi)
- Licence: Analyse, 36h, L3, Ecole des Ponts, France (E. Cancès, F. Legoll, G. Stoltz, M. Rousset)
- Licence: Calcul Scientifique, 30h, L3, Ecole des Ponts ParisTech, France (M. Dobson, S. Boyaval, G. Stoltz)
- Licence: Formation au logiciel scientifique SCILAB, 12h, L3, Ecole des Ponts ParisTech, France (D. Benoit),
- Licence: Tutorat de Maths, 9h, L3, Ecole des Ponts ParisTech, France (D. Benoit),
- Licence: Probability, 42h, L3, Ecole des Ponts, France (M. Rousset).
- Licence: Projets de physique, 20h, L3, Ecole des Ponts, France (I. Dabo, G. Stoltz)
- Licence: Formation aux logiciels scientifiques, 12h, L3, Ecole des Ponts, France (I. Dabo)
- Master: Introduction au calcul Scientifique, 12h, M1, Ecole des Mines ParisTech, France (D. Benoit, W. Minvielle, G. Stoltz)

- Master: Analyse Numérique et Optimisation, 56h, M1, Ecole Polytechnique, France (E. Cancès)
- Master: Méthodes variationnelles en mécanique quantique, 12h, M2, University Paris 6, France (E. Cancès)
- 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: Analyse spectrale, 39h, M1, Ecole des Ponts, France (G. Stoltz)
- Master: Spectral theory of Schrodinger operators, 30h, M2, Université de Marne-la-Vallée, France (G. Stoltz)
- Master: Méthodes déterministes en mathématiques financières, 42h, M2, Ecole des Ponts ParisTech (T. Lelièvre).
- Master: Modéliser Programmer Simuler, 28 h, M1, Cours Ecole des Ponts ParisTech (T. Lelièvre).
- Master: Méthodes numériques probabilistes, 36 h, M2 Mathématiques et Applications, Université Pierre et Marie Curie (T. Lelièvre).
- Master: Mathématiques appliquées, 18h, University Lille 1, France (M. Rousset).
- Master: Simulation numérique en science des matériaux, 18h, M1, Ecole des Ponts, France (I. Dabo, M. Vandamme)
- Doctorat: Introduction à l'informatique scientifique, 24h, Université Paris-Est, France (I. Dabo)

F. Legoll has supervised the internship of William Minvielle (Paris 6, Master 2) from March 1st to July 31st, 2012.

The following PhD & Habilitation were defended:

- PhD: V. Ehrlacher, Some mathematical and numerical problems in quantum mechanics and uncertainty quantification, Université Paris-Est, Ecole des Ponts ParisTech, supervised by E. Cancès and T. Lelièvre
- HdR: G. Stoltz, Molecular Simulation: Nonequilibrium and Dynamical Problem, Université Paris-Est, June 18th, 2012,
- PhD: F. Thomines, Méthodes mathématiques et techniques numériques de changement d'échelle : application aux matériaux aléatoires, Université Paris-Est, Ecole des Ponts ParisTech, 22 nov. 2012, supervised by C. Le Bris.

The following PhDs are in progress:

- PhD in progress: H. Alrachid, Méthodes numériques en simulation moléculaire, Université Paris-Est, Ecole des Ponts ParisTech, started october 1st, 2012, supervised by T. Lelièvre
- 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: D. Gontier, started September 1st, 2012, supervised by E. Cancès
- 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: W. Minvielle, Méthodes numériques pour les matériaux, Université Paris-Est, Ecole des Ponts ParisTech, started october 1st, 2012, supervised by C. Le Bris and F. Legoll
- PhD in progress: N. Mourad, A mathematical and numerical analysis of the pseudopotential method, Université Paris-Est, Ecole des Ponts ParisTech and Lebanese CNRS, started September 1st, 2011, supervised by E. Cancès, A. Kashmar and A. Mourad

8.3. Conference participation

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

- D. Benoit, International Workshop on Numerical Methods for Non-Newtonian Flows, Blois (France), March 2012,
- D. Benoit, Congrès CANUM 2012, Superbesse (France), May 2012,
- D. Benoit, Multiscale Materials Modeling (MMM) conference 2012, Singapour (Singapour), October 2012
- D. Benoit, Colloque Modélisation numérique des mélanges grains-fluides, Montpellier (France), October 2012
- I. Dabo, Workshop on Corrective Approaches to DFT for Strongly-correlated Systems, CECAM, EPFL, Lausanne, June 2012
- I. Dabo, Young Engineers and Scientists Symposium, University of California, Berkeley, March 2012
- I. Dabo, CECAM Meeting on Electron Correlation, Ecole Polytechnique, Palaiseau, December 2012
- I. Dabo, Energy from the Sun: Computational Chemists and Physicists Take Up the Challenge, CECAM Conference, Cagliari, September 2012
- I. Dabo, PRACE F2F Workshop, CEA Saclay, June 2012
- I. Dabo, 2nd TYC Energy Materials Workshop, Thomas Young Centre, King's College, London, June 2012
- I. Dabo, American Physical Society Meeting, Boston, March 2012
- E. Cancès, Mathematics meets Chemistry workshop, Erlangen, Germany, March 2012,
- E. Cancès, AIMS 2012, Orlando, USA, July 2012,
- E. Cancès, ICMP 2012, Aalborg, Denmark, August 2012,
- E. Cancès, IPAM workshop, Los Angeles, USA, October 2012
- E. Cancès, weekly seminar of the mathematics department, Université d'Orsay, January 2012,
- E. Cancès, weekly seminar of the mathematics department, Berkeley University, USA, January 2012,
- E. Cancès, working group on numerical methods, Université Paris 6, January 2012,
- E. Cancès, weekly seminar of the mathematics department, ENSTA, March 2012,
- E. Cancès, K. Burke's group meeting, chemistry department, Irvine University, USA, October 2012,
- E. Cancès, NAS group meeting, physics department, Louvain-la-Neuve, Belgium, November 2012,
- V. Ehrlacher, SIAM Conference on Uncertainty Quantification, Raleigh, USA, April 2012.
- V. Ehrlacher, workshop on Mathematical and Numerical Analysis of Electronic Structure Models, Beijing, China, June 2012.
- V. Ehrlacher, 9th AIMS Conference on Dynamical Systems,Differential Equations and Applications, Orlando, USA, July 2012.
- V. Ehrlacher, Séminaire d'Analyse numérique - Equations aux dérivées partielles du Laboratoire Paul Painlevé, Lille, France, Mars 2012.
- V. Ehrlacher, Groupe de travail EDP et analyse numérique LAMA-CERMICS, Marne-la-Vallée, France, May 2012.
- V. Ehrlacher, Séminaire des thésards du laboratoire AGM, Cergy, France, May 2012.
- V. Ehrlacher, IPAM MD2012 Seminar Series, Los Angeles, USA, September 2012.

- V. Ehrlacher, Applied Mathematics/PDE Seminars of University of California of Santa Barbara, Santa Barbara, USA, November 2012.
- V. Ehrlacher, IPAM Workshop IV: Computational Methods for Multiscale Modeling of Materials Defects, Los Angeles, USA, December 2012.
- S. Lahbabi, Weekly seminar of the mathematics department, University of Cergy Pontoise, November 2012,
- C. Le Bris, plenary lecture, 60-th annual SIAM meeting, July 2012, Minneapolis, USA.
- C. Le Bris, Workshop Inhomogeneous Random Systems IRS2012, Institut Henri Poincaré (Paris), January 2012.
- C. Le Bris, International conference on PDEs, Shanghai, June 2012
- C. Le Bris, ICMS workshop Edinburgh, June 2012.
- C. Le Bris, ACMAC workshop on Image and waves in complex media, June 2012, Heraklion, Crete.
- C. Le Bris, Journées MMCS, Université de Lyon, September 2012.
- C. Le Bris, keynote lecturer, 2012 Woudschoten Conference, October, 2012, Zeist, The Netherlands.
- C. Le Bris, IPAM program on " Materials Defects: Mathematics, Computation, and Engineering", December 2012.
- C. Le Bris, Mathematics Seminar, Freie Universität Berlin, May 2012.
- C. Le Bris, Scientific and statistical computing seminar University of Chicago, October 2012.
- F. Legoll, workshop on "Mathematical theory and computational methods for multiscale problems", Singapore, January 2012,
- F. Legoll, American Physical Society meeting, Boston, February 2012,
- F. Legoll, Workshop "Mathematics meets Chemistry and Physics", Erlangen, March 2012,
- F. Legoll, CECAM workshop on "Free energy calculations: From theory to applications", Paris, June 2012,
- F. Legoll, AIMS conference, Orlando, July 2012,
- F. Legoll, WCCM conference, Sao Paulo, July 2012,
- F. Legoll, ECCOMAS conference, Wien, September 2012,
- F. Legoll, NumDiff 13 Conference, Halle, September 2012,
- F. Legoll, 22nd Int. Workshop on Computational Mechanics of Materials, Baltimore, September 2012,
- F. Legoll, Kickoff meeting of the "Laboratoire International Associé Nancy/UIUC", Nancy, November 2012,
- F. Legoll, Workshop on "Nonequilibrium Statistical Mechanics", Banff, November 2012,
- F. Legoll, séminaire du groupe de travail Homogénéisation et Echelles Multiples, Paris 6, November 2012,
- F. Legoll, Workshop on "Computational Methods for Multiscale Modeling of Materials Defects", IPAM Los Angeles, December 2012,
- F. Legoll, Lake Arrowhead culminating workshop, IPAM Los Angeles, December 2012,
- T. Lelièvre, Workshop on Multiscale Modeling, Simulation, Analysis and Application, Singapore, January 2012.
- T. Lelièvre, Workshop on Interplay of Analysis and Probability in Physics, Oberwolfach, January 2012.
- T.Lelièvre, Séminaire de mathématiques, Université de Marne-la-Vallée, January 2012.
- T. Lelièvre, Séminaire du MAPMO, Orléans, February 2012.

- T. Lelièvre, Workshop BEMOD12 "Beyond Molecular Dynamics: Long Time Atomic-Scale Simulations", MPIPKS, Dresden, March 2012.
- T. Lelièvre, Analysis seminar, MPI Leipzig, April 2012.
- T. Lelièvre, Arbeitsbereich Numerik Mathematisches Institut seminar, Uni Tuebingen, May 2012.
- T. Lelièvre, plenary speaker at the CANUM conference, Superbesse, May 2012.
- T. Lelièvre, Workshop "Computation of transition trajectories and rare events in non-equilibrium systems", ENS Lyon, June 2012.
- T. Lelièvre, Journées ERGONUM "Analyse probabiliste des systèmes en temps long", Inria Sophia-Antipolis, June 2012.
- T. Lelièvre, AIMS conference, Orlando, July 2012.
- T. Lelièvre, plenary speaker at the EVOLVE 2012 conference, Mexico, August 2012.
- T. Lelièvre, Workshop "Modelling the Dynamics of Complex Molecular Systems", Lorentz Center, Leiden, August 2012.
- T. Lelièvre, Tutorial "Materials Defects", IPAM, Los Angeles, September 2012,
- T. Lelièvre, Workshop "Quantum and Atomistic Modeling of Materials Defects", IPAM, Los Angeles, October 2012,
- T. Lelièvre, Workshop "Nonequilibrium Statistical Mechanics: Mathematical Understanding and numerical Simulation" BIRS, Banff, Canada, November 2012.
- F. Nier: Séminaire Univ. Nantes, January 2012.
- F. Nier: Invitation for one week in TU-Universität Braunschweig (Germany) February 2012
- F. Nier: Séminaire Univ. Bordeaux, March 2012.
- F. Nier: Analytic torsion and its applications, Conference organized by J.M. Bismut and W. Müller, Univ. Paris 11, June 2012.
- F. Nier: Invitation for three weeks in WIAS-Berlin (Germany), September 2012
- F. Nier: Workshop "Mathematics for Semiconductor Heterostructures: Modeling, Analysis, and Numerics", WIAS-Berlin (Germany), organized by K. Gaertner, A. Glitzky, H.C. Kaiser, and F. Nier, September 2012.
- F. Nier: Lectures on Semi-classical analysis, organized by S. Fujiie and T. Watanabe, Ritsumeikan University (Japan), October 2012.
- F. Nier: "Workshop on Spectral Analysis, Stability and Bifurcations in Modern Nonlinear Physical Systems", organized by O. Kirillov and Y. Fukumoto, BIRS Banff (Canada), November 2012.
- F. Nier: Séminaire de Probabilités, Univ. Rennes 1 (France), November 2012.
- F. Nier: Paris-London seminar, Inst. Henri Poincaré, Paris (FRANCE), December 2012
- M. Rousset, CECAM Workshop "Free energy calculations: From theory to applications", Marne-la-Vallée, June 2012,
- M. Rousset, Workshop "Mathematical and Numerical Analysis of Electronic Structure Models", Beijing, China, June 2012,
- M. Rousset, Evolve Conference, Mexico City, Mexico, August 2012.
- M. Rousset, BIRS Workshop "Nonequilibrium Statistical Mechanics: Mathematical Understanding and numerical Simulation", Banff, Canada, November 2012.
- G. Stoltz, Workshop "Quantum and Atomistic Modeling of Materials Defects", IPAM, Los Angeles, October 2012,
- G. Stoltz, Workshop "Mathematical and Numerical Analysis of Electronic Structure Models", Beijing, China, June 2012,
- G. Stoltz, CECAM workshop "Free energy calculations: From theory to applications", Marne-la-Vallée, June 2012,
- G. Stoltz, seminar at Collège de France, June 2012,
- G. Stoltz, seminar at University of Edinburgh, February 2012,

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

- E. Cancès, Chinese Academy of Sciences, Beijing, China, April 2012.
- E. Cancès, IPAM-UCLA, Los Angeles, USA, October 2012,
- F. Legoll, IPAM UCLA (program on "Materials Defects: Mathematics, Computation, and Engineering"), Los Angeles, USA, December, 2012.
- F. Nier: Invitation for one week in Tokyo Universtity (Japan), November, 2012.

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

- E. Cancès, Lectures (6h) on spectral theory for electronic structure modeling, Chinese Academy of Sciences, Beijing, China, April 2012,
- E. Cancès, Lectures (2h) on numerical methods for Density Functional Theory, Ecole des Houches, June 2012,
- C. Le Bris, Lectures on Stochastic homogenization, Series of 90-minute lectures, Summer course on homogenization, Chicago, June 18-29, 2012.
- C. Le Bris, Graduate course, 'Mathematical introduction to complex fluids modeling', The University of Chicago, 24 hours, October-November 2012.
- F. Nier, Lectures for phD students and researchers about "Semiclassical analysis and mean field dynamics", held in CERMICS-ENPC, 5x2 hours, April-May 2012.

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

- V. Ehrlacher, IPAM Workshop I: Quantum and Atomistic Modeling of Materials Defects, Los Angeles, USA, October 2012.
- W. Minvielle, IPAM Workshop IV: Quantum and Atomistic Modeling of Materials Defects, Los Angeles, USA, December 2012.

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

- V. Ehrlacher, IPAM Materials Defects: Tutorials, Los Angeles, USA, September 2012.
- V. Ehrlacher, IPAM Workshop II: Atomistic and Mesoscale Modeling of Materials Defects, Los Angeles, USA, September 2012.
- V. Ehrlacher, IPAM Workshop III: Mesoscale and Continuum Scale Modeling of Materials Defects, Los Angeles, USA, September 2012.
- S. Lahbabi, 4th meeting of the GDR quantum dynamics, Toulouse, France, February 2012
- S. Lahbabi, Spectral days 212, Munich, Germany, April 2012
- S. Lahbabi, Summer school: Ab inition simulations in condensed matter, Les Houches, France, June 2012
- W. Minvielle, Summer school on "Recent advances in the Theory of Homogenization", Chicago, June 2012,

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] V. EHRLACHER. *Quelques modèles mathématiques en chimie quantique et propagation d'incertitudes*, Université Paris-Est, July 2012, http://hal.inria.fr/tel-00719466.

[8] G. STOLTZ. *Molecular Simulation: Nonequilibrium and Dynamical Problems*, Université Paris-Est, 2012, Habilitation à diriger des recherches, Ph. D. Thesis.

[9] F. THOMINES. *Méthodes mathématiques et techniques numériques de changement d'échelle: application aux matériaux aléatoires*, Université Paris-Est, Ecole des Ponts ParisTech, 2012, Ph.D. Thesis supervised by Claude Le Bris.

Articles in International Peer-Reviewed Journals

[10] A. AFTALION, F. NIER. *Adiabatic approximation for a two-level atom in a light beam*, in "Ann. Fac. Sci. Toulouse Math. (6)", Jan 2013, vol. 22, n° 1, 81 pages, http://hal.inria.fr/hal-00641565.

[11] Z. AMMARI, F. NIER. *Mean field propagation of infinite dimensional Wigner measures with a singular two-body interaction potential*, in "Ann. Sc. Norm. Super. Pisa Cl. Sci. (5)", 2013, 49p, Forthcoming article, http://annaliscienze.sns.it/index.php?page=ForthcomingArticles.

[12] O. ANDREUSSI, I. DABO, N. MARZARI. *Revised self-consistent continuum solvation in electronic-structure calculations*, in "Journal of Chemical Physics", 2012, vol. 136, 064102.

[13] C. BERNARDIN, G. STOLTZ. *Anomalous diffusion for a class of systems with two conserved quantities*, in "Nonlinearity", 2012, vol. 25, p. 1099-1133, http://hal.archives-ouvertes.fr/hal-00593617/fr/.

[14] X. BLANC, R. COSTAOUEC, C. LE BRIS, F. LEGOLL. *Variance reduction in stochastic homogenization using antithetic variables*, in "Markov Processes and Related Fields", 2012, vol. 18, p. 31-66.

[15] X. Blanc, F. Legoll, A. Anantharaman. *Asymptotic behaviour of Green functions of divergence form operators with periodic coefficients*, in "Applied Mathematics Research eXpress", 2012, in press, http://hal.archives-ouvertes.fr/hal-00637489.

[16] X. Blanc, F. Legoll. *A numerical strategy for coarse-graining two-dimensional atomistic models at finite temperature: the membrane case*, in "Computational Materials Science", 2012, vol. 66, p. 84–95, http://hal.archives-ouvertes.fr/hal-00627294.

[17] X. Blanc, C. Le Bris, P.-L. Lions. *A possible homogenization approach for the numerical simulation of periodic microstructures with defects*, in "Milan Journal of Mathematics", 2012, vol. 80, p. 351-367.

[18] X. Blanc, C. Le Bris, P.-L. Lions. *From the Newton equation to the wave equation in some simple cases*, in "Networks and Heterogeneous Media", 2012, vol. 7, n° 1, p. 1-41.

[19] M. Blanchard, G. Morin, M. Lazzeri, E. Balan, I. Dabo. *First-principles simulation of arsenate adsorption on the surface of hematite*, in "Geochimica et Cosmochimica Acta", 2012, vol. 86, 182.

[20] F. Bouchut, S. Boyaval. *A new model for shallow elastic fluids*, in "M3AS", 2012, in press.

[21] S. Boyaval. *A fast Monte-Carlo method with a Reduced Basis of Control Variatesc applied to Uncertainty Propagation and Bayesian Estimation*, in "Comput. Methods Appl. Mech. Engrg.", Octobre 2012, vol. 241–244, p. 190–205 [*DOI :* 10.1016/j.cma.2012.05.003], http://www.sciencedirect.com/science/article/pii/S004578251200151X.

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[27] I. Dabo, A. Ferretti, C.-H. Park, N. Poilvert, Y. Li, M. Cococcioni, N. Marzari. *Donor and acceptor levels of organic photovoltaic compounds from first principles*, in "Physical Chemistry Chemical Physics", 2013, vol. 15, 685.

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[30] Y. EFENDIEV, J. GALVIS, F. THOMINES. *A systematic coarse-scale model reduction technique for parameter-dependent flows in highly heterogeneous media and its applications*, in "SIAM MMS", 2012, vol. 10, p. 1317-1343.

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Scientific Books (or Scientific Book chapters)

[47] F. Legoll, T. Lelièvre. *Some remarks on free energy and coarse-graining*, B. Engquist, P. Lötstedt, O. Runborg (editors), Lecture Notes in Computational Science and Engineering, Springer, 2012, vol. 82, p. 279–329, http://hal.inria.fr/hal-00511221.

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Other Publications

[51] D. Benoit, L. He, C. Le Bris, T. Lelièvre. *Mathematical analysis of a one-dimensional model for an aging fluid*, 2012, http://hal-enpc.archives-ouvertes.fr/hal-00676678.

[52] E. Cancès, V. Ehrlacher, T. Lelièvre. *Greedy algorithms for high-dimensional non-symmetric linear problems*, 2012, http://hal.inria.fr/hal-00745611.

[53] E. Cancès, V. Ehrlacher, Y. Maday. *Non-consistent approximations of self-adjoint eigenproblems: Application to the supercell method*, 2012, 29 pages, 5 figures, http://hal.inria.fr/hal-00694017.

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