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Team MATHERIALS

MATHematics for MatERIALS

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

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THEME
Numerical schemes and simulations

Table of contents

Team MATHERIALS

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Creation of the Team: 2014 January 01.

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2. Overall Objectives

2.1. Overall Objectives

The MATHERIALS 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 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 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 team has accumulated an increasingly solid expertise on such topics, which are traditionally not well known by the community in applied mathematics and scientific computing. One of the major achievements of the team is to have created a corpus of literature, authoring books and research monographs on the subject [1], [2], [3], [5], [6] that other scientists may consult in order to enter the field.

3. Research Program

3.1. Research Program

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 of minerals 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 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. Homogenization and related problems

Over the years, the 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.

4.2. 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.

4.3. 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?"

5. New Results

5.1. Electronic structure calculations

Participants: Eric Cancès, Virginie Ehrlacher, David Gontier, 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 and N. Mourad have mathematically analyzed the density functional perturbation theory, both in the non-degenerate case (that is, when the Fermi level is not an eigenvalue of the Kohn-Sham hamiltonian) and in the degenerate case. They have in particular proved that Wigner's 2n+1 rule holds in both cases. D. Gontier has obtained a complete, explicit, characterization of the set of spin-polarized densities for finite molecular systems. This problem was left open in the pioneering work of von Barth and Hedin setting up the Kohn-Sham density functional theory for magnetic compounds. He has also extended a previous work by Anantharaman and Cancès, and proved the existence of minimizers for the spin-polarized Kohn-Sham model in the presence of a magnetic field within the local spin density approximation.

E. Cancès has pursued his long-term collaboration with Y. Maday (UPMC) on the numerical analysis of electronic structure models. With L. He (ENPC) and R. Chakir (IFSTTAR), they have designed and analyzed a two-grid methods for nonlinear elliptic eigenvalue problems, which can be applied, in particular, to the Kohn-Sham model. Some numerical tests demonstrating the interest of the approach have been performed with the Abinit software. Together with G. Dusson (UMPC), B. Stamm (UMPC), and M. Vohralík (Inria), they have designed a new post processing method for planewave discretizations of nonlinear Schrödinger equations, and used it to compute sharp *a posteriori* error estimators for both the discretization error and the algorithmic error (convergence threshold in the iterations on the nonlinearity).

Implicit solvation models aims at computing the properties of a molecule in solution (most chemical reactions take place in the liquid phase) by replacing all the solvent molecules but the few ones strongly interacting with the solute, by an effective continuous medium accounting for long-range electrostatics. E. Cancès, Y. Maday (Paris 6), and B. Stamm (Paris 6) have recently introduced a very efficient domain decomposition method for the simulation of large molecules in the framework of the so-called COSMO implicit solvation models. In collaboration with F. Lipparini (UPMC, B. Mennucci (Department of Chemistry, University of Pisa) and J.-P. Picquemal (Paris 6), they have implemented this algorithm in widely used computational software products (Gaussian and Tinker). The extension of this method to other implicit solvation models is work in progress.

Claude Le Bris, in collaboration with Pierre Rouchon (Ecole des Mines de Paris), has pursued the study of 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: Thomas Hudson, Frédéric Legoll, Tony Lelièvre, Mathias Rousset, Gabriel Stoltz.

The work of the team in this area is concentrated on two new directions: the sampling of reactive trajectories (where rare events dictate the dynamics of the system), and the computation of average properties of nonequilibrium systems (which completes the more traditional field of expertise associated with techniques to compute free energy differences).

5.2.1. Sampling of reactive trajectories

Finding trajectories for which the system undergoes a significant change is a challenging task since the transition events are typically very rare. Several methods have been proposed in the physics and chemistry literature, and members of the team have undertaken their study in the past years.

A prominent example is the parallel replica method where several replicas of the system evolve on different processors, until one of them undergoes a transition. Several extensions and refinements to the original method were proposed by T. Lelièvre:

- together with D. Aristoff and G. Simpson, he proposed in [7] an adaptation of the Parallel Replica method for Markov chains;
- together with A. Binder and G. Simpson, he introduced in [17] a generalized parallel replica dynamics. The idea is to extend the applicability of the original algorithm by computing on the fly the so-called decorrelation time.

Another class of techniques to compute reactive trajectories is based on splitting techniques. C.E. Bréhier, T. Lelièvre and M. Rousset have performed in [21] an analysis of the Adaptive Multilevel Splitting algorithm, which is a rare event simulation method where several replicas are evolved concurrently, and selected to favor exploration in a given direction. The computational cost of the algorithm is studied in details in the limit of a large number of replicas.

5.2.2. Nonequilibrium systems

G. Stoltz, together with G. Pavliotis (Imperial College) and Rémi Joubaud, studied in [27] the response of equilibrium systems evolving according to a Langevin dynamics, to external, space-time dependent forcings. In particular, they found out that, even if the external forcing is periodic in time and space with a vanishing space-time average, the systems in general evolves with a non-zero average velocity. It may even be the case that the average velocity is in the direction opposite to the average forcing (when the latter is non-zero), which can be seen as an example of negative mobility. The behavior of the system over diffusive time scales (in the reference frame obtained by removing the average velocity) is also studied, for arbitrary forcing strengths. This work was initiated when G. Pavliotis was a visiting member of the team MATHERIALS.

A numerical analysis of the error arising in the computation of transport coefficients, with an emphasis on mobility and self-diffusion, was provided by M. Fathi, A.A Homman and G. Stoltz in [25] in the case when Metropolis-Hastings algorithms are used to stabilize straightforward discretizations of overdamped Langevin dynamics.

Together with Herbert Spohn (TU München), G. Stoltz has verified the relevance of mode-coupling predictions for the scaling of space time correlations of invariants for one dimensional systems subjected to a non-reversible deterministic dynamics perturbed by an exchange noise [32]. In particular, it has been confirmed that the equilibrium relaxation of the invariants involves two modes, a traveling sound mode and a standing heat mode (related to the energy current and height autocorrelation functions). Both modes exhibit a superdiffusive scaling, of Lévy type for the heat mode, and of KPZ type for the sound mode.

5.2.3. Free energy computations

The topic of free energy computations is still a significant research area of the team. T. Lelièvre and G. Stoltz, together with G. Fort and B. Jourdain, studied the Self-Healing Umbrella Sampling (SHUS) method in [26]. This method is an adaptive biasing method to compute free energies on the fly by appropriately penalizing already visited regions. The convergence of the method relies on a rewriting as a stochastic approximation method with random steps, and can therefore be seen as a variation of the Wang-Landau method. The efficiency of the SHUS algorithm was assessed for a model two-dimensional system in terms of exit times out of a metastable set.

Concerning practical applications, G. Stoltz, together with A.A. Homman, E. Bourasseau, P. Malfreyt, L. Strafella and A. Ghoufi have worked on the computation of surface tension in droplets [10], using alchemical transformations where the droplet volume is artificially varied.

Finally, T. Lelièvre, together with J. Comer, J.C. Gumbart, J. Hénin, A. Pohorille and C. Chipot, wrote a review article on the adaptive biasing force method [9].

5.2.4. Thermodynamic limit

Another work in progress is related to the understanding of the origin of hysteresis in rubber-made materials. When submitted to cyclic deformations, the strain-stress curve of these materials indeed shows a hysteresis behavior, which seems to be independent of the speed of loading.

Some years ago, members of the team have suggested a model, at a mesoscale, to explain this behavior. This model was written in terms of a system made of a finite number of particles. One of the aim of the post-doc of Thomas Hudson, who joined the team in Sept. 2014, is to make progress on that question, and to understand whether a thermodynamic limit of the model previously proposed can be identified.

5.2.5. Reduced models

We propose in [13] a procedure for replacing a complex, reactive potential of REBO type by a simple harmonic approximation, in regions where the system is close to equilibrium. The parameters of the harmonic approximation are chosen so that the phonon spectrum is exactly reproduced. We are currently testing the ability of the so-obtained hybrid model to predict the fracture of graphene.

5.3. Complex fluids

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

Sébastien Boyaval has pursued his research about the mathematical modelling of complex free-surface flows. On the one hand, the numerical investigation of 3D effects with a VOF approach was carried out for multiphase flows in collaboration with the CFSFlow code developers at EPFL [11]. On the other hand, the reduced modelling of viscoelastic effects within Saint-Venant framework was carried out for asymptotically thin layers above rough bottoms [8].

5.4. Application of greedy algorithms

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

Model reduction techniques are very important tools for applications. They consist in deriving from a high-dimensional problem, a low-dimensional model, which very quickly gives reliable results. In particular, the team is interested in two techniques: Proper Generalized Decomposition (greedy algorithms) and Reduced Basis techniques.

Eric Cancès, Virginie Ehrlacher and Tony Lelièvre have extended a greedy algorithm suggested for the resolution of high-dimensional eigenvalue problems in order to approximate the solution of the many-body Schrödinger electronic problem. The main technical difficulty in the extension of these algorithms lies in the antisymmetry of the wavefunction of the electrons. To deal with this difficulty, an approximation of the wavefunction is computed as a sum of Slater determinants, each Slater determinant function being computed in an iterative way.

Virginie Ehrlacher has obtained preliminary encouraging results on greedy algorithms for parametric eigenvalue problems. The method has been applied to the computation of the first buckling mode of a plate in the presence of a defect, the position of the defect playing the role of a parameter entering the eigenvalue problem defining the first buckling mode of the plate.

A new numerical method for the construction of an efficient reduced-order model for the solution of the Vlasov equation, arising in plasma physics or in the modeling of electron transport in semiconductors, has been tested by Damiano Lombardi (REO Inria team) and Virginie Ehrlacher. This method is based on the use of an analytic Lax Pair for the Vlasov equations and is inspired by previous works done on transport equations by Jean-Frederic Gerbeau, Damiano Lombardi and Elisa Schenone. Encouraging preliminary numerical results have been obtained.

5.5. Homogenization and related topics

Participants: Sébastien Brisard, Ludovic Chamoin, Virginie Ehrlacher, Claude Le Bris, Frédéric Legoll, Simon Lemaire, François Madiot, William Minvielle.

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 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. The theoretical results obtained to date are being collected in a series of manuscripts that will be available shortly.

The team 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.

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.

In [28], F. Legoll and W. Minvielle have proposed a variance reduction procedure, based on the control variate technique, to obtain estimates of the apparent homogenized tensor with a smaller statistical error (at a given computational cost) than standard Monte Carlo approaches. The control variate technique is based on using a surrogate model, somewhat in the spirit of a preconditionner. In [28], the surrogate model that is used is inspired by a weakly stochastic approach previously introduced by A. Anantharaman and C. Le Bris to describe periodic models perturbed by rare defects.

In addition, C. Le Bris, F. Legoll and W. Minvielle have investigated the possibility to use another variance reduction technique based on computing the corrector equation only for selected environments. These environments are chosen based on the fact that their statistics in the finite supercell matches the statistics of the materials in the infinite supercell. This method yields an estimator with a smaller variance that standard estimators. Preliminary encouraging numerical results have been obtained.

As pointed out above, the corrector problem is in practice solved on a large bounded domain, often complemented with periodic boundary conditions. Solving that problem can still be challenging, in particular because producing a conforming mesh of realistic heterogeneous microstructures can be a daunting task. In such situations, numerical methods formulated on cartesian grids may be more interesting. These methods can still be Finite Element Methods, or methods in the spirit of that proposed by Moulinec and Suquet in the mid-nineties. In their approach, the corrector problem (a partial differential equation) is reformulated as an equivalent integral equation. This equation can readily be discretized using a Galerkin approach. This leads to numerical schemes that can be implemented as a matrix-free method. In [18], S. Brisard and F. Legoll have reviewed the different variants that have been proposed in the literature along these ideas, and proposed a mathematical analysis of the numerical schemes. This work extends in various directions previous works by S. Brisard.

In somewhat the same vein, Eric Cancès, Virginie Ehrlacher and Frédéric Legoll (in collaboration with Benjamin Stamm, University Paris 6) have worked on alternative methods to approximate the homogenized coefficients of a random stationary material. These methods are alternative to those proposed e.g. by Bourgeat and Piatniski, and which consist in solving a corrector problem on a bounded domain. The method introduced is based on a new corrector problem. This problem is posed on the entire space. In some cases (including the case of randomly located spherical inclusions), it can be recast as an integral equation posed on the surface of the inclusions. The problem can then be efficiently solved via domain decomposition and using spherical harmonics.

We have discussed above approaches to efficiently compute the homogenized coefficient, assuming we have a complete knowledge of the microstructure of the material. We have actually also considered a related inverse problem, and more precisely a parameter fitting problem. Knowing the homogenized quantities, is it possible to recover some features of the microstructure properties? Obviously, since homogenization is an averaging procedure, not everything can be recovered from macroscopic quantities. A realistic situation is

the case when a functional form of the distribution of the microscopic properties is assumed, but with some unknown parameters to determine. In collaboration with A. Obliger and M. Simon, F. Legoll and W. Minvielle have addressed that problem in [29], showing how to determine the unknown parameters of the microscopic distribution on the basis of macroscopic (e.g. homogenized) quantities.

From a numerical perspective, the Multiscale Finite Element Method (MsFEM) 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 MsFEM has been introduced more than 10 years ago. However, even in simple deterministic cases, there is actually still room for improvement in many different directions. In collaboration with A. Lozinski (University of Besançon), 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. That approach has been analyzed and tested on an elliptic problem set on a domain with a huge number of perforations. 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) and A. Lozinski (University of Besançon), consists in the study of multiscale advection-diffusion problems. Such problems are possibly advection dominated and a stabilization procedure is therefore required. How stabilization interplays with the multiscale character of the equation is an unsolved mathematical question worth considering for numerical purposes. In that spirit, C. Le Bris, F. Legoll and F. Madiot have studied several variants of the Multiscale Finite Element Method (MsFEM), specifically designed to address multiscale advection-diffusion problems in the convection-dominated regime. Generally speaking, the idea of the MsFEM is to perform a Galerkin approximation of the problem using specific basis functions, that are precomputed (in an offline stage) and adapted to the problem considered. Several possibilities for the basis functions have been examined (for instance, they may or may not encode the convection field). The various approaches have been compared in terms of accuracy and computational costs.

Most of the numerical analysis studies of the MsFEM are focused on obtaining *a priori* error bounds. In collaboration with L. Chamoin, who is currently in delegation in our team (from ENS Cachan, since September 2014), we have started to work on *a posteriori* error analysis for MsFEM approaches, with the aim to develop error estimation and adaptation tools. We have extended to the MsFEM case an approach that is classical in the computational mechanics community for single scale problems, and which is based on the so-called Constitutive Relation Error (CRE). Once a numerical solution u_h has been obtained, the approach needs additional computations in order to determine a divergence-free field as close as possible to the exact flux $k\nabla u$. In the context of the MsFEM, it is important to be able to do all the expensive computations in an offline stage, independently of the right-hand side. The standard CRE approach thus needs to be adapted to that context, in order to keep that feature that makes it adapted to a multiscale, multi-query context. The preliminary approach that we have introduced already yields promising results.

Still another question investigated in the group is to find an alternative to standard homogenization techniques when these latter are difficult to use in practice. This is the aim of the post-doc of Simon Lemaire, which began in June 2014, and which takes over previous works of the group on the subject. Consider a linear elliptic equation, say in divergence form, with a highly oscillatory matrix coefficient, and assume that this problem is to be solved for a large number of right-hand sides. If the coefficient oscillations are infinitely rapid, the solution can be accurately approximated by the solution to the homogenized problem, where the homogenized coefficient has been evaluated beforehand by solving the corrector problem. If the oscillations are moderately rapid, one can think instead of MsFEM-type approaches to approximate the solution to the reference problem. However, in both cases, the complete knowledge of the oscillatory matrix coefficient is required, either to build the average model or to compute the multiscale basis. In many practical cases, this coefficient is often only partially known, or merely completely unavailable, and one only has access to the solution of the equation for some loadings. This observation has lead to think about alternative methods, in the following spirit. Is it possible to approximate the reference solution by the solution to a problem with a

constant matrix coefficient? How can this 'best' constant matrix approximating the oscillatory problem be constructed in an efficient manner?

A preliminary step, following discussion and interaction with A. Cohen, has been to cast the problem as a convex optimization problem. We have then shown that the 'best' constant matrix defined as the solution of that problem converges to the homogenized matrix in the limit of infinitely rapidly oscillatory coefficients. Furthermore, the optimization problem being convex, it can be efficiently solved using standard algorithms. C. Le Bris, F. Legoll and S. Lemaire are currently working on making the resolution of the optimization problem as efficient as possible.

To conclude this section, we mention a project involving V. Ehrlacher, C. Le Bris and F. Legoll, in collaboration with G. Leugering and M. Stingl (Cluster of Excellence, Erlangen-Nuremberg University). This project aims at optimizing the shape of some materials (modelled as structurally graded linear elastic materials) in order to achieve the best mechanical response at the minimal cost. As often the case in shape optimization, the solution tends to be highly oscillatory, thus the need of homogenization techniques. Materials under consideration are being thought of as microstructured materials composed of steel and void and whose microstructure patterns are constructed as the macroscopic deformation of a reference periodic microstructure. The optimal material (i.e. the best macroscopic deformation) is the deformation achieving the best mechanical response. For a given deformation, we have first chosen to compute the mechanical response using a homogenized model. We are currently aiming at computing the mechanical response at the microscale, using the highly oscillatory model. Model reduction techniques (such as MsFEM, Reduced Basis methods, ...) are then in order, in order to expedite the resolution of the oscillatory problem, which has to be solved at each loop of the optimization algorithm. Current efforts are targeted towards choosing an appropriate model reduction strategy.

5.6. Miscellaneous

Participants: Sébastien Boyaval, Tony Lelièvre, Sébastien Boyaval.

T. Lelièvre together with F. Casenave and A. Ern propose in [24] an extension of the classical reduced basis method in order to extend its range of applicability to black-box codes.

S. Boyaval started investigating new high-order methods on generalized non-conforming meshes in collaboration with Daniele di Pietro [14].

In [31], M. Rousset considers space homogenous Boltzmann kinetic equations in dimension $d \geq 3$ with Maxwell collisions (and without Grad's cut-off). An explicit Markov coupling of the associated conservative stochastic N-particle system is constructed, yielding a N-uniform α-power law trend to equilibrium.

6. Bilateral Contracts and Grants with Industry

6.1. Contracts and Grants with Industry

Many research activities of the team are conducted in close collaboration with private or public companies: CEA, SANOFI, IRDEP. The 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. National Initiatives

The 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 MATHERIALS team. It is coordinated by E. Cancès.
- 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.
- T. Lelièvre is member of the ANR-project "STAB" (PI: I. Gentil, Université de Lyon).
- The team also benefited from a NEEDS interdisciplinary funding from CNRS on numerical methods for the simulation of defects in materials

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 Shocks,
- the GdR Maths et entreprise,
- the GdR correl (correlated methods in electronic structure computations),
- the GdR CoDFT (electronic structure computations using density functional theory).

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

7.2. European Initiatives

The ERC consolidator Grant MSMATH (ERC Grant Agreement number 614492, PI T. Lelièvre) has started in June 2014.

7.3. International Initiatives

T. Lelièvre, G. Stoltz and F. Legoll participate 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 de Nancy, Université de Lyon and Inria Rennes.

7.4. International Research Visitors

7.4.1. Visits of International Scientists

J. Weare (University of Chicago) has been invited for a one month stay (February-March 2014) with the support of the Labex Bezout.

7.4.2. Visits to International Teams

F. Legoll, T. Lelièvre and G. Stoltz have visited the group of K. Schulten (Urbana-Champaign) on January 27-30, 2014

8. Dissemination

8.1. Promoting Scientific Activities

S. Brisard has co-organized the "Stochastics and Material Mechanics" mini-symposium at the 2014 "European Mechanics of Materials Conference", organized at Gothenburg (Sweden), 27-29 August 2014.

E. Cancès

- is a member of the editorial boards of Mathematical Modelling and Numerical Analysis (2006-), of SIAM Journal of Scientific Computing (2008-), 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.

He was an Ordway visiting professor at the University of Minnesota for the academic year 2013-2014.

He has organized or co-organized:

- the 2nd workshop on " Mathematical and numerical analysis of electronic structure models", Berlin, April 2014,
- the workshop " Horizon math 2014 ", Rueil Malmaison, December 2014.

C. Le Bris is editor-in-chief of Applied Mathematics Research Express (2003-). He is a managing editor of Networks and Heterogeneous Media. He is a member of the editorial boards of Annales mathématiques du Québec (2013-), Archive for Rational Mechanics and Analysis (2004-), COCV (Control, Optimization and Calculus of Variations) (2003-), Mathematics in Action (2008-), Nonlinearity (2005-), Journal de Mathématiques Pures et Appliquées (2009-).

He is a member of the editorial boards 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 Cabinet of the High Commissioner for Atomic Energy,
- 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,
- the "Conseil scientifique de la SMAI" (Scientific Council of the French Applied Maths Society)s,
- the International Mathematical Union Circle,
- the "Conseil de perfectionnement du Master de Mathématiques" of the University Pierre et Marie Curie.

C. Le Bris has held a position of Visiting Professor at the University of Chicago, February-October-November 2014.

He has been a member of the Program Committee of ICM 2014 in Seoul and is a member of

- the scientific committee of the conference Dimension reduction: mathematical methods and Applications, Pennsylvania State University, March 21-24, 2015.

He has co-organized

- with P. Souganidis and S. Weinberger, the conference *Prospects in Applied Mathematics*, Chicago, 19-20 October 2014.

He has been the Göran Gustafsson Lecturer in Mathematics 2014, KTH, Stockholm.

F. Legoll

- is a member of the editorial board of SIAM MMS (2012-) and of ESAIM Proc (2012-),
- is a member of the Scientific Committee of SciCADE 2015.

T. Lelièvre

- is editor-in-chief of ESAIM: Proceedings (with D. Chafai, P. Lafitte and C. Mouhot),
- co-organized the Workshop "Numerical methods for high-dimensional problems" at the Ecole des Ponts, April 14-18th 2014 (with Virginie Ehrlacher, Yvon Maday and Anthony Nouy),
- co-organized the Journées Inverse problems for multiscale and stochastic problems, Ecole des Ponts, October 2-3rd 2014 (with Virginie Ehrlacher, Frédéric Legoll and Karam Sab),
- co-organized the MoMaS'14 conference. CIRM, November 17-20th, 2014 (with Grégoire Allaire, Clément Cancès, Alexandre Ern and Raphaèle Herbin),
- co-organizes the Journées EDP-Probas at Institut Henri Poincaré (with F. Malrieu),
- is the head of the GDR MoMaS, a French research group on the mathematical modeling and the numerical simulations for nuclear waste management problems (Main scientific themes: multiscale models for flows in porous media, molecular simulation of clays, multiphase flows),
- is in charge of the Theme 4 (Stochastic modeling, quantification and uncertainty propagation for multiscale mechanical models of materials) of the Labex MMCD,
- is involved in the organization of the IHP trimester "Numerical Methods for PDEs", Autumn 2016 (with D. A. Di Pietro, A. Ern and L. Formaggia).

G. Stoltz has

- co-organized the workshop "Computational methods for statistical mechanics - at the interface between mathematical statistics and molecular simulation" at ICMS (Edinburgh, UK), June 2-6, 2014 (with G. Pavliotis, Imperial College London, and Ch. Hartmann, FU Berlin)
- has given a public lecture on "Computer Simulations: The third way of doing science", at ICMS (Edinburgh, UK, June 2014)

8.2. Teaching - Supervision - Juries

The members of the team have taught the following courses:

- Licence: Probabilités (18h) et calcul scientifique (18h), Ecole Centrale Paris (S. Boyaval),
- Licence: Analyse, 36h, L3, Ecole des Ponts, France (E. Cancès, D. Gontier, F. Legoll, M. Rousset, W. Minvielle, V. Ehrlacher, S. Lemaire)
- Licence: Remise à niveau en analyse de base et algèbre linéaire, 18h, L3, ESIEE (S. Lemaire)
- Licence: Calcul Scientifique, 30h, L3, Ecole des Ponts ParisTech (G. Stoltz)
- Master: Mathématiques des modèles multiéchelles, 39h, M1, Ecole des Ponts ParisTech (F. Legoll)
- Master: Problèmes multiéchelles, 24h, M2, Université Paris 6 (F. Legoll)
- Master: Coques et Structures avancées, 24h, M1, Ecole des Ponts ParisTech (S. Brisard)
- Master: Conception des Structures, 14h, M1, Ecole des Ponts ParisTech (S. Brisard)
- Master: Images et Mécanique, 6h, M2, Ecole des Ponts ParisTech (S. Brisard),
- Master: Imagerie des Milieux Désordonnés, 9h, M2, Ecole des Ponts ParisTech (S. Brisard)
- Master: Modélisation mathématique des vagues (3h00), M1, Ecole Nationale des Ponts et Chaussées (S. Boyaval),
- Master: Processus Stochastiques, 18h. M1, ESIEA (C.-E. Bréhier),
- Master: Outils Probabilistes pour la Finance, M1, Ecole des Ponts, France (M. Rousset),
- Master: Processus de Markov et temps long, 30h, M2, Université Paris-Est (M. Rousset),
- Master: Analyse spectrale, 39h, M1, Ecole des Ponts, France (G. Stoltz, V. Ehrlacher)
- 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: Analyse spectrale, 39h, M1, Ecole des Ponts, France (V. Ehrlacher, G. Stoltz)
- Master: Projets de physique, 10h, M1, Ecole des Ponts, France (V. Erhlacher, G. Stoltz)
- Master: Introduction au calcul Scientifique, 13h, M1, Ecole des Mines ParisTech, France (G. Stoltz, F. Madiot)
- Master: théorie spectrale des opérateurs de Schrödinger, 30h, M2, Université de Marne-la-Vallée, France (G. Stoltz)

The following PhD were defended by students members of the research group at the Ecole des Ponts:

- David Benoit, Méthodes numériques pour la simulation des fluides non-Newtoniens, Université Paris-Est, Université Paris Est, started October 1st, 2010, supervised by C. Le Bris and T. Lelièvre, January 22nd 2014.

The following PhDs are in progress (some of the following students conduct their research on a daily basis in other research groups, co-supervised by members of MATHERIALS) :

- François Madiot, Multiscale finite element methods for advection diffusion problems, Université Paris-Est, Ecole des Ponts ParisTech, started october 1st, 2013, supervised by C. Le Bris and F. Legoll,
- William Minvielle, Méthodes numériques pour les matériaux, Université Paris-Est, Université Paris Est, started october 1st, 2012, supervised by C. Le Bris and F. Legoll,
- David Gontier, Université Paris-Est, started September 1st, 2012, supervised by E. Cancès,
- Ahmed-Amine Homman, Multiscale methods for the simulation of shock and detonation waves, Université Paris-Est, Ecole des Ponts ParisTech and CEA/DAM, started April 1st, 2013, supervised by G. Stoltz and J.-B. Maillet,
- Zofia Trstanova, A mathematical analysis of some importance sampling strategies in molecular dynamics, Université Joseph Fourier and Inria Grenoble, started June 1st 2013, supervised by S. Redon and G. Stoltz,
- Gerome Faure, Multiscale methods for the simulation of shock and detonation waves, Université Paris-Est, Ecole des Ponts ParisTech and CEA/DAM, started November 1st 2014, supervised by G. Stoltz and J.-B. Maillet,
- Boris Nectoux, Métastabilité et distribution quasi-stationnaire, since November 2014, supervised by T. Lelièvre and E. Cancès,
- Houssam Alrachid, Méthodes numériques en dynamique moléculaire, Ecole des Ponts ParisTech, since September 2012, supervised by T. Lelièvre,
- Rémi Sainct, Modèles multi-échelles pour le trafic, IFFSTAR and Ecole des Ponts ParisTech, since September 2013, supervised by T. Lelièvre and X. Louis.

The following HDR was defended:

- Mathias Rousset, Probability in computational physics and biology: some mathematical contributions, Université Paris-Est, 27 nov. 2014.

8.3. Conference participation

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

- S. Boyaval, Séminaire mathématiques appliquées à RWTH, IGPM, 2014,
- S. Boyaval, Groupe de travail mathématiques appliquées à Université de Marne la Vallée, LAMA, 2014,
- C.-E. Bréhier, SPDEs and Applications IX, Trento, Italy, January 2014,
- C.-E. Bréhier, MCQMC 2014, Leuven, Belgium, April 2014,
- C.-E. Bréhier, Journées MAS 2014, Toulouse, August 2014,
- C.-E. Bréhier, Seminar of Numerical Analysis, Geneva, Switzerland, October 2014,
- C.-E. Bréhier, Seminar of Probability and Statistics, Bordeaux, November 2014,
- S. Brisard, Séminaire LabEx MMCD – Industrie, ENPC, July 2014,
- S. Brisard, Journées annuelles NEEDS – Milieux Poreux, Paris, December 2014,

- E. Cancès, CIRM meeting on advanced numerical methods for the simulation of Bose-Einstein condensates, February 2014,
- E. Cancès, Ki-Net Workshop on mathematical and numerical methods for complex quantum systems, Chicago, March 2014,
- E. Cancès, Mathematics colloquium, University of Minnesota, April 2014,
- E. Cancès, Weakly seminar of the chemistry department, University of Minnesota, April 2014,
- E. Cancès, Weakly seminar of the mathematics department, Bonn, May 2014,
- E. Cancès, Weakly seminar of the mathematics department, Amiens, June 2014,
- E. Cancès, IPAM workshop on materials defects, Lake Arrowhead, June 2014,
- E. Cancès, Oberwolfach workshop on computational multiscale methods, June 2014,
- E. Cancès, IPAM summer school on Electronic structure theory of materials and (bio)molecules, Los Angeles, July 2014,
- E. Cancès, International congress of mathematicians (invited lecture), Seoul, August 2014,
- E. Cancès, Workshop on Solution for solvation, on the occasion of Prof. Tomasi's 80th birthday, Pisa, September 2014,
- E. Cancès, Annual meeting of the ANR Becasim, Lille, September 2014,
- E. Cancès, BIRS workshop on multiscale models for crystal defects, Banff, September 2014,
- E. Cancès, ICERM workshop on high-dimensional approximation, integration and optimization, Providence, October 2014,
- E. Cancès, Prospects in applied mathematics, Chicago, October 2014,
- E. Cancès, Workshop on mathematics integrated to industry, Sao Jose dos Campos, November 2014,
- E. Cancès, X-IHES Laurent Schwartz seminar, November 2014,
- E. Cancès, Zurich colloquium on applied and computational mathematics, November 2014,
- E. Cancès, Horizons math 2014, Rueil Malmaison, December 2014,
- V. Ehrlacher, LJLL workshop on "Sparse tensor methods", University Paris 6, France, January 2014,
- V. Ehrlacher, Seminar of the mathematics department of Chemnitz University, Chemnitz, Germany, February 2014,
- V. Ehrlacher, GdR AMORE meeting, ENS Cachan, France, March 2014,
- V. Ehrlacher, Workshop on "Numerical methods for electronic structure calculations", Berlin, Germany, April 2014,
- V. Ehrlacher, IPAM Workshop on Materials Defects: Mathematics, Computation and Engineering, Lake Arrowhead, USA, June 2014,
- V. Ehrlacher, ICOSAHOM conference, Salt Lake City, USA, June 2014,
- V. Ehrlacher, WCCM conference, Barcelona, Spain, July 2014,
- V. Ehrlacher, Banff workshop on "Multiscale models for crystal defects", Banff, Canada, September 2014,
- V. Ehrlacher, Journée Forum CEA Incertitudes, CEA DAM Bruyères-le-Chatel, France, September 2014,
- V. Ehrlacher, LJLL workshop on "Sparse tensor methods", University Paris 6, France, December 2014,
- D. Gontier, Theoretical and numerical aspects of quantum transport, Aalborg, April 2014,
- D. Gontier, Mathematical and numerical analysis of electronic structure models, April 2014,
- D. Gontier, Solid math, Trieste, June 2014,

- C. Le Bris, Workshop 'Multiscale Problems from Physics, Biology and Materials Science', Shanghai Jiao Tong University, May 28-31, 2014,
- C. Le Bris, Workshop at the Mittag-Leffler Institute, September 2014,
- C. Le Bris, Final conference of the SPP 1324, Marburg, November 2014,
- C. Le Bris, Colloquium of the Imperial College, March 2014,
- C. Le Bris, Colloquium of the Eindhoven Multiscale Institute, March 2014,
- C. Le Bris, Outreach Conference of the Series Sciences and Society, Université de Lorraine, Region Lorraine, November 2014,
- F. Legoll, Weekly seminar, Imperial College, London, February 2014,
- F. Legoll, Workshop "From atomistic to continuum models in material science", L'Aquila (Italy), April 2014,
- F. Legoll, Workshop on Computational Aspects of Multiscale Materials Modeling, Evanston (USA), May 2014,
- F. Legoll, Weekly seminar, Augsburg University, May 2014,
- F. Legoll, Reunion Conference of the Materials Defects IPAM program, Los Angeles, June 2014,
- F. Legoll, Oberwolfach workshop "Computational Multiscale Methods", June 2014,
- F. Legoll, 8th International Workshop on Parallel Matrix Algorithms and Applications, Lugano, July 2014,
- F. Legoll, AIMS conference, Madrid, July 2014,
- F. Legoll, WCCM conference, Barcelona, July 2014,
- F. Legoll, Workshop on Multiscale Models of Crystal Defects, Banff, Sept. 2014,
- F. Legoll, MMM conference, Berkeley, October 2014,
- F. Legoll, Journées annuelles NEEDS, Nantes, October 2014,
- F. Legoll, Atelier du GdR ModMat "De l'atome au code industriel", Marseille, December 2014,
- T. Lelièvre, conference MCMSKI, Chamonix, January 2014,
- T. Lelièvre, conference on applied mathematics, MPI Lepipzig, January 2014,
- T. Lelièvre, séminaire K. Schulten group, Urbana Champaign, January 2014,
- T. Lelièvre, CECAM conference, Lugano, March 2014,
- T. Lelièvre, conférence MCQMC, Leuven, April 2014,
- T. Lelièvre, ICMS lecture, "Computational methods for statistical mechanics", Edinburgh, June 2014,
- T. Lelièvre, Numerical Analysis for Partial Differential Equations, Sussex, June 2014,
- T. Lelièvre, ICMS conference, "Multiscale Computational Methods in Materials Modelling Meeting", Edinburgh, June 2014,
- T. Lelièvre, Oberseminar Analysis, Munich, June 2014,
- T. Lelièvre, Inria TOSCA team seminar, July 2014,
- T. Lelièvre, AIMS conference, Madrid, July 2014,
- T. Lelièvre, ENS Cachan, Séminaire pour les nouveaux normaliens, September 2014,
- T. Lelièvre, ANR Stab conference, Lyon, September 2014,
- T. Lelièvre, CECAM conference, Mainz, October 2014,
- T. Lelièvre, Inria POEM team seminar, Paris, October 2014,
- T. Lelièvre, Statistics Colloquium, Chicago, October 2014,
- T. Lelièvre, Séminaire EDP non linéaires, Université Paris 13, December 2014,

- T. Lelièvre, Séminaire ENS Chimie, Paris, December 2014,
- W. Minvielle, Weekly seminar, Creteil University, April 2014,
- W. Minvielle, Summer school on Applied Analysis for Materials, Berlin, September 2014,
- W. Minvielle, Workshop on Multiscale Models of Crystal Defects, Banff, Sept. 2014,
- W. Minvielle, Workshop on "Stochastic and multiscale inverse problems", ENPC, October 2-3, 2014,
- W. Minvielle, MOMAS Conference, Marseille, November 2014,
- M. Rousset, MCQMC 2014, Leuven, Belgium, April 2014.
- M. Rousset, AIMS 2014, Madrid, Spain, July 2014.
- G. Stoltz, workshop “Mathematical and Numerical Analysis of Electronic Structure Models”, Berlin, April 2014,
- G. Stoltz, workshop “Theoretical and Numerical Aspects of Quantum Transport”, Aalborg, Denmark, April 2014,
- G. Stoltz, 10th AIMS conference on Dynamical Systems, Differential Equations and Applications, Madrid, July 2014,
- G. Stoltz, seminar of University of Lille, september 2014,
- G. Stoltz, MOMAS meeting, Marseille, November 2014,

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

- E. Cancès, one month at the University of Minnesota as an Ordway professor.

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

- C. Le Bris, Göran Gustafsson Lecturer in Mathematics 2014, KTH, Stockholm,
- C. Le Bris, Lectures on Numerical stochastic homogenization, 5 hours, RTG Summer School, The University of Chicago, July 2014,
- C. Le Bris, Lectures on Nonperiodic homogenization of elliptic equations, 6 hours, Berlin Mathematical School, TU Berlin, September 2014,
- C. Le Bris, Graduate course on ’Model reduction’, The University of Chicago, 10 hours, Fall 2014,
- T. Lelièvre, 2 hours lecture, ICMS "Computational methods for statistical mechanics", Edinburgh, June 2014,

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

- D. Gontier, IPAM summer school on Electronic structure theory of materials and (bio)molecules, Los Angeles, July 2014,
- W. Minvielle, CANUM 2014, Carry le Rouet, April 2014,

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

- S. Brisard, 8th International Workshop on Parallel Matrix Algorithms and Applications, Lugano, July 2014,
- L. Chamoin, séminaire du Collège de France, December 2014,
- S. Brisard, Journées annuelles NEEDS, Nantes, October 2014,
- S. Lemaire, Summer school on Applied Analysis for Materials, Berlin, September 2014,
- F. Madiot, CANUM 2014, Carry-le-Rouet, April 2014,
- F. Madiot, Inaugural Chicago Summer School in Analysis, Chicago, July 2014,
- F. Madiot, Summer school on Applied Analysis for Materials, Berlin, September 2014,
- W. Minvielle, Inaugural Chicago Summer School in Analysis, Chicago, July 2014.

9. Bibliography

Major publications by the team in recent years

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