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Project-Team Micmac

Methods and Engineering of Multiscale Computing from Atom to Continuum

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THEME NUM

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2. Overall Objectives

2.1. Overall Objectives

The MICMAC project-team has been created jointly by the Ecole Nationale des Ponts et Chaussées (ENPC) and the INRIA in October 2002. It is hosted by the CERMICS laboratory (Centre d'Enseignement et de Recherches en Mathématiques, Informatique et Calcul Scientifique) at ENPC. The scientific focus of the project-team is to analyze and improve the numerical schemes used in the simulations of computational chemistry at the microscopic level, and in the simulations coupling this microscopic scale with larger, meso or macroscopic, scales.

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] 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 be deduced in theory from the Schrödinger equation associated to it. Second, the Schrödinger equation does not involve any empirical parameter, 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} meter), and the size of the nucleus embedded in it is 10^{-15} meter; the typical vibration period of a molecular bond is the femtosecond (10^{-15} second), and the characteristic relaxation time for an electron is 10^{-18} second. Consequently, Quantum Chemistry calculations concern very short time (say 10^{-12} second) behaviors of very small size (say 10^{-27} m^3) systems. The underlying question is therefore whether information on phenomena at these scales is or not of some help to understand, or better predict, 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 proceed (also) from ensemble or bulk effects, that are far from being easy to understand and to model. Striking examples are found in the solid state 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 on the other hand *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 lubrifying properties of graphite are essentially due to a phenomenon which can be entirely modeled at the atomic scale.

It is therefore founded 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*. Possibly, one approach is coupled to the others within the so-called *multiscale* models. The sequel indicates how this journey can be completed focusing rather on the first scale (the subatomic one), than on the latter 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 in fact extremely difficult the numerical simulation of

these equations 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 reaches rapidly 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 indeed, 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 is one of the major concern of the project-team.

4. Application Domains

4.1. Large systems simulation

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 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 require to address a large variety of questions such as

- how to improve the nonlinear iterations that are the basis of any ab initio models for computational chemistry?
- how to more efficiently solve the inner loop which most often consists in the solution procedure for the linear problem (with frozen nonlinearity)?
- how to 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 and 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 on 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 account 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. Laser control

The laser control of chemical reactions is today an experimental reality. Experiments, carried out by many groups of researchers and in many different contexts and settings, have demonstrated the feasibility of controlling the evolution of a quantum system using a laser field. All these experiments exploit the remarkable properties of quantum interactions (interferences) between one, or more, external interactions (e.g. lasers) and the sample of matter under study. In order to create the ad hoc interferences that will drive the system to the desired goal, one can either play with the dephasing between two beams, or conveniently choose the frequencies of the beams, or also make use of the two aspects mixed together, which amounts to allowing for "all" possible laser fields as in optimal control schemes.

Whatever the strategy, the success of these numerous experiments not only validates the idea of manipulating and controlling quantum systems with lasers, but also motivates the need for further theoretical studies in this direction, in order to further improve the results and the range of their applicability; interest in this research area has also been increasing in more applied communities. The standard modeling for the problem of the laser control of a molecular system involves the time-dependent Schrödinger equation which rules the evolution of the wavefunction describing the state of the system. On the basis of the Schrödinger equation, one then states a control problem, either in the framework of exact control or in the framework of optimal control.

The first fact to underline as a crucial feature of the problem of laser control is the orders of magnitude in time and space that are typically encountered here. The space scale is indeed that of an atom, say 10^{-10} m, but more important than that, the time scale is of the order of the femtosecond (10^{-15} s) and can even go down to the attosecond (10^{-18} s). As surprising as it may seem, the laser fields can literally be "tailored" on these tiny timescales. They can involve huge intensities (10^{12} W/cm^2 and above), and their shots can be cycled at 1 KHz. Apart from being very impressive, these orders of magnitude mean one thing for whom is not an expert: one can do several thousands of experiments in a minute. This ability changes the whole landscape of the control problem, for making an experiment is here far cheaper than running a numerical simulation. This has motivated the paradigm of closed-loop optimization when the criterion to be optimized is evaluated on-the-fly on an experimental device. One of the current challenging issue for the mathematicians taking part into the field is to understand how to take advantage of a combined experimental/numerical strategy. In this respect, it is to be noted that the experimental side can come from on-the-fly experiments (how to decide what to do?), but may also come from the tremendous amount of data that can be (and actually is) stored from the billions of experiments done to this day (how to dig into this database?).

A second point is to remark the way in which the control enters the problem: the control multiplies the state. Theoretically and numerically, this bilinear nature causes difficulties. Finally, open-loop control is dealt with, at least for two reasons: first, the timescale on which the phenomenon goes is too short for the current capabilities of electronic devices, which prevents closing the loop within one experiment; but secondly, feedback control means measuring something, which in a quantum framework means interacting with and thus perturbing the system itself. These two bottlenecks might be overcome in the future, but this will undoubtedly require a lot of theoretical and technical work.

A third peculiarity regards the choice of admissible laser fields as control : what types of $E(t)$ should be allowed when setting up the control problem? This question leads to a dichotomy : one can choose either to restrict oneself to the experimentally feasible fields, or to basically let the field free, therefore allowing for very general laser fields, even those out of reach for the contemporary technology. The two tracks may be followed. In particular, the second track, the most "imaginative" one (rather unusual in comparison to other contexts), can serve as a useful technical guide for building the lasers for tomorrow's technology.

A final key issue is robustness. It is of course a standard fact in every control problem that the control obtained needs to be robust, for obvious practical reasons. The somewhat unusual feature in the present setting is that the experiments show that they are surprisingly robust with respect to all kinds of perturbations (noise, uncertainties in the measures, ...). Clearly, there is here something to be understood at the theoretical level, e.g. by envisioning new modeling strategies that incorporate undesirable perturbations.

5. New Results

5.1. Computational quantum chemistry

Participants: Hanen Amor, Arnaud Anantharaman, Guy Bencteux, Eric Cancès, Ismaila Dabo, Amélie Deleurence, Claude Le Bris, Yanli Li, Gabriel Stoltz.

In computational quantum chemistry as in most of the project-team's scientific endeavours, a twofold goal is pursued: placing the models on a sound mathematical grounding, and improving the numerical approaches.

E. Cancès and A. Deleurence have addressed issues related to the modeling and simulation of local defects in periodic crystals. Computing the energies of local defects in crystals is a major issue in quantum chemistry, materials science and nano-electronics. Although several approaches have been proposed, a mathematically consistent quantum model for crystalline materials with local defects was still missing. In collaboration with Mathieu Lewin (CNRS, Cergy), Eric Cancès and Amélie Deleurence have proposed in [14] a new model 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. Using and adapting recent mathematical tools used in QED, they have suggested a new mathematical approach for the self-consistent description of a crystal in the presence of a defect. The justification of this model is obtained using a thermodynamic limit on the so-called supercell model. They have also introduced a variational method for computing the perturbation in a basis of precomputed maximally localized Wannier functions of the reference perfect crystal [15]. Some preliminary, promising numerical results have been obtained on a one-dimensional nonlinear model with Yukawa interaction potentials.

Besides, existence results for the extended Kohn-Sham LDA (local density approximation) model as well as for the two-electron Kohn-Sham GGA (generalized gradient approximation) model, have been obtained by A. Anantharaman and E. Cancès, using the concentration-compactness method [6].

On the numerical front, new numerical schemes for solving the constrained optimization problems arising in Density Matrix Functional Theory [17] have been proposed by E. Cancès, in a joint work with K. Pernal (University of Szczecin, Poland). These numerical schemes have better convergence properties than the pre-existing ones.

In collaboration with W. Hager (University of Florida), the domain decomposition approach, designed by M. Barrault (now at EDF), G. Bencteux, E. Cancès, and C. Le Bris for electronic structure calculations has been improved [36]. The development of the domain decomposition algorithm for the linear subproblem has been continued. Further algorithmic improvements of the most time consuming part of the algorithm have resulted in a significant decrease in memory and CPU demands (up to a factor 10 for alkane molecules) and of the overall accuracy of the resulting domain decomposition algorithm. A parallel implementation on the Blue Gene computer has allowed to solve the linear subproblem for a polyethylen chain of 5 million atoms (17.5 million basis functions) in about 60 minutes on 1024 processors, confirming the high scalability of the method. The current version of the code allows to simulate elongated systems such as linear polymers or nanotubes. A new version of the code, designed for the simulation of more complex systems, is currently in development, notably by H. Amor in the context of her post-doc, and in the framework of a collaboration with EDF supported by the ANR project "Parmat". From a numerical analysis viewpoint, the convergence properties of the MDD algorithm have been studied, and the convergence established in a simplified setting [8].

Quantum mechanical calculations are frequently used in computational surface science for predicting catalytic activities, for elucidating chemical processes, and for interpreting spectroscopic experiments. In recent years, several methods have been developed to extend the application of first-principles DFT methods to surface electrochemistry. Nevertheless, computational approaches to treat electrochemical systems (e.g., fuel cells and batteries) as a function of the applied voltage have been lacking. In collaboration with N. Marzari, B. Kozinsky and N. Singh-Miller (MIT), I. Dabo, Y. Li and E. Cancès have developed an atom-continuum model for the first-principles simulation of catalytic systems under electrochemical conditions. They have implemented and validated an efficient algorithm to solve the nonlinear partial differential equations underlying the model

[19], [18]. In addition, they have developed a method to perform electronic-structure optimizations at fixed applied potential, eliminating inherent numerical instabilities [18]. This seems to be the first implementation of electronic-structure calculations under realistic electrochemical conditions at constant applied potential. They are currently focusing on the parallelization of these algorithms for their final incorporation in the Quantum-Espresso computational toolkit. In the near future, they plan to apply this electrochemical model to the determination of reaction pathways under applied potential.

In collaboration with physicists from IMPMC (Paris 6), G. Stoltz has studied the thermal conductivity of carbon nanotubes using methods from quantum statistical physics. Carbon nanotubes are very interesting materials from a theoretical viewpoint (they are 'real' materials for which Fourier's law does not hold, as predicted by the theoretical predictions for one dimensional systems), but also for industrial applications since they have outstanding mechanical, electronic and thermal properties. This work has focused on the reduction of the thermal conductance generated by the presence of isotope disorder [35].

In collaboration with C. Brouder (IMPMC, Paris 6) and G. Panati (University La Sapienza, Roma), G. Stoltz has also studied the validity of the Gell'Mann and Low formula on a simple finite dimensional example [13]. The Gell'Mann and Low formula is an important formula in many-body perturbation theory, and is at the basis of almost all approximation schemes in this field. Loosely speaking, it says that the eigenstate of a Schrödinger type operator, associated with a non-degenerate eigenvalue, can be transformed into the eigenstate of a perturbed Schrödinger operator, upon some renormalization procedure. However, when the eigenstate is degenerate, it is unclear how to perform such a renormalization. Work is on progress to generalize in an abstract setting the results found in the simple finite dimensional case.

5.2. Molecular dynamics and related problems

Participants: Eric Cancès, Claude Le Bris, Frédéric Legoll, Tony Lelièvre, Kimiya Minoukadeh, Raphaël Roux, Gabriel Stoltz.

The extremely broad field of Molecular dynamics is a domain where the MICMAC project-team, originally more involved in the quantum chemistry side, has invested a lot of 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. The proceedings article [29] written by three researchers of the team-project, reviews some of the current challenges in this field.

5.2.1. Sampling of constrained dynamics.

In many cases, the dynamics of the system under study is restrained to some submanifold of the whole accessible space. A famous instance is the Hamiltonian dynamics, for which the energy of the system is constant. Hamiltonian dynamics is useful for computing average properties assuming ergodicity. However, constant energy sampling may be achieved with stochastic dynamics as well; such a scheme is analyzed by E. Faou (INRIA Rennes) and T. Lelièvre in [20], where rates of convergence are also provided. Constrained SDEs also appear for the sampling of measures defined on submanifolds, which is useful for themodynamics integration. In [27], C. Le Bris, T. Lelièvre and E. Vanden-Eijnden (Courant Institute) have proved the consistency of various numerical schemes (predictor-corrector schemes).

5.2.2. Highly-oscillatory 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. Actually, fast phenomena are only relevant through their mean effect on the slow phenomena, and their precise description is not needed. Consequently, there is a need for time integration algorithms that take into account these fast phenomena only in an averaged way, and for which the time step is not restricted by the highest frequencies. C. Le Bris and F. Legoll have initiated a study along this line, and obtained encouraging results that have been reported in [25]. The authors currently follow up on this

subject, in collaboration with F. Castella, P. Chartier and E. Faou from INRIA Rennes, and with the funding of ANR INGEMOL ("Intégration numérique et géométrique des équations hamiltoniennes").

5.2.3. Ergodicity of deterministic sampling methods.

Despite the success of stochastic techniques, deterministic sampling methods, such as the Nosé-Hoover dynamics, are still often used in the applied community to compute canonical averages. In collaboration with M. Luskin and R. Moeckel (University of Minnesota), F. Legoll has studied the Nosé-Hoover dynamics when applied to completely integrable systems. Using averaging and KAM techniques, it has been showed that the dynamics is actually not ergodic with respect to the Gibbs measure [30]. This extends a previous work that addressed the simple case of the harmonic oscillator.

5.2.4. Adaptive sampling methods.

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. The Adaptive Biasing Force method is a stochastic algorithm used to compute this free energy. It is based upon a nonlinear dynamics, which uses the reaction coordinate to prevent the system from being trapped in metastable regions. The nonlinearity in the dynamics comes from a conditional expectation computed with respect to the solution. A convergence result for this nonlinear dynamics has been presented by T. Lelièvre, M. Rousset and G. Stoltz in [33], in some limiting regime, using entropy methods and a decomposition of the total entropy of the system into a microscopic part (associated with conditioned measures) and a macroscopic part (related to some global features of the system).

In addition, B. Jourdain, T. Lelièvre and R. Roux have studied a particle approximation of this dynamics, relying on Nadaraya-Watson estimators for the conditional expectation. They have obtained in [23] a result of convergence to a solution of the Adaptive Biasing Force dynamics, and subsequently an existence result for this dynamics.

As a by-product of the work [33], T. Lelièvre has obtained in [32] a new result for proving a logarithmic Sobolev inequality on a measure μ defined on $\mathbb{R}^n$, assuming that a logarithmic Sobolev inequality holds for the marginals $\xi * \mu$ and the conditional measures $\mu(\cdot|\xi)$ associated to some function $\xi : \mathbb{R}^n \to \mathbb{R}^m$ (with $m < n$). This theoretical result has practical interest in molecular dynamics, where ξ is the reaction coordinate, and where the above assumptions are often met in practice.

Entropy methods have also been employed by J.B. Maillet and G. Stoltz in [34] for proving the convergence of a dynamics to sample a system with constraints fixed in average. The proposed sampling strategy was used to compute the Hugoniot curve of Argon (*i.e.* all the states that can be reached by a shock compression from a given state).

The free energy completely describes the statistics of the reaction coordinates. F. Legoll and T. Lelièvre are currently working on the definition of a dynamics closed in these reaction coordinates. The problem hence amounts to reducing the dimension of a set of SDEs, from the full set of degrees of freedom to only a small subset of them. Encouraging numerical results have been obtained [39], along with estimates on the accuracy on the proposed effective dynamics (again using entropy techniques).

Related to adaptive sampling, F. Legoll has developed a dynamical method able to generate a constant energy trajectory at a given kinetic temperature, in collaboration with B. Leimkuhler and E. Noorizadeh (University of Edinburgh). Such a method is useful for systems that need to be simulated using the Newton equations (for any other dynamics introduces too large a perturbation in the system), at an energy that corresponds to a given average kinetic temperature. Some results obtained with this method are exposed in [31].

5.2.5. Search for reaction paths.

The microscopic dynamics used to sample the configurations of the system are often trapped in metastable states. A major numerical issue is therefore the search for transition paths connecting metastable states. E. Cancès, F. Legoll, K. Minoukadeh and two of their collaborators at CEA Saclay proposed in [16] an

improvement to an existing eigenvector following method, the Activation-Relaxation Technique nouveau (ARTn), for searches of saddle points and transition pathways on a given potential energy surface. Local convergence and robustness of the algorithm have been established, and the new method has been successfully tested on point defects in body centered cubic iron.

5.3. Atom-continuum model for electrified metal-solution interfaces

Participants: Eric Cancès, Ismaila Dabo, Yanli Li.

Modeling the electrical response of fuel cells at the molecular level represents a persistent challenge characterized by length scales that are orders of magnitude greater than the sizes accessible to quantum chemistry simulations. In order to overcome this limitation, a comprehensive atom-continuum model has been developed, based on a quantum molecular description of the interfacial region with a polarizable-continuum representation of the electrolyte [19]. This approach has been applied to interpret electrochemical spectroscopy experiments [40]. As part of the post-doc scientific program of Ismaila Dabo, this atom-continuum model is being complemented, by incorporating pressure, surface-tension, and acidity effects.

5.4. Laser control

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

The project-team's interest closely follows the recent prospects opened by the laboratory implementations of closed loop optimal control. This is done in collaboration with the group of H. Rabitz (Princeton University).

5.4.1. Toolkit discretization

Recently the "toolkit" discretization introduced to accelerate the numerical resolution of the time-dependent Schrödinger equation arising in quantum optimal control problems demonstrated good results on a variety of models. However, when coupling this class of methods with the so-called monotonically convergent algorithms, numerical instabilities affect the convergence of the discretized scheme. An adaptation of the "toolkit" method has been proposed, which preserves the monotonicity of the procedure. The theoretical properties of the new algorithm are illustrated by numerical simulations [7].

5.4.2. Beyond bi-linear control

The control of quantum dynamics induced by an intense laser field continues to be a challenge to both experiment and theory. In this context, optimal control theory is an efficient tool for designing laser pulses able to control quantum processes. Different methods have been developed to solve the optimal equations among which the monotonically convergent iterative schemes. For these algorithms, the increase of the cost functional is guaranteed at each iteration.

A vast majority of works have considered a linear interaction between the quantum system and the electromagnetic field. This linear interaction corresponds, for molecular systems, to the first-order dipolar approximation of the permanent dipole moment. Due to the intensity of the field or to the particular structure of the problem, some systems need to go beyond this approximation e.g., for the control of molecular orientation and alignment of a linear molecule by non-resonant laser pulses. The natural question arises of whether one can apply monotonically convergent algorithms to such systems interacting nonlinearly with the field. This question has been answered by proposing monotonic algorithms when an arbitrary nonlinearity is considered.

A key ingredient to ensure the monotonic convergence of the algorithms is to consider a nonstandard cost functional that instead of penalizing the intensity of the field, i.e., the square of the electric field, penalizes a higher exponent depending on the order of the nonlinearity. A family of algorithms has been developed; the efficiency of these algorithms has been tested on the orientation dynamics of a linear molecule with nonlinearity of order 3 [24].

5.4.3. Propagator space methods

Traditionally, the numerical simulations consider some description of the interaction of the laser and the system, of which the most used is the *dipole approximation*, and perform optimizations considering the laser intensity as the main variable. A different view of the problem has been taken: the evolution semigroup of unitary propagators is considered and it is asked that the resulting Hamiltonian be consistent with the chosen approximation type. The specific optimization algorithm is now implemented and the first encouraging numerical results are presented in a submitted work [22].

5.5. Atomistic to continuum methods

Participants: Xavier Blanc, Claude Le Bris, Frédéric Legoll.

The project-team has continued their theoretical and numerical efforts on the general topic of "passage from the atomistic to the continuum". This concerns theoretical issues arising in this passage but also the development and the improvement of numerical simulations coupling the two scales. The lecture notes [37] review some of the numerical methods used in this context, along with some numerical analysis results.

In collaboration with C. Patz (WIAS, Berlin), X. Blanc, C. Le Bris and F. Legoll have recently addressed questions related to finite temperature modeling of atomistic systems, and derivation of coarse-grained descriptions. The starting observation is that, for atomistic systems at constant temperature, relevant quantities are statistical averages of some functions (called observables in that context) with respect to the Gibbs measure. One particular case of interest is when the observable at hand does not depend on all the variables, but only on some of them (gathered in a region of interest, where some defects appear, for instance). In that case, a relevant quantity to compute is the free energy associated to these few degrees of freedom. In the one-dimensional setting, an efficient strategy, that bypasses the simulation of the whole system, has been proposed to compute this free energy, as well as averages of such observables. This strategy is based on a rigorous thermodynamical procedure. Encouraging results have been reported in [9]. Current efforts in the project-team aim at extending the strategy to more complex cases.

5.6. Homogenization

Participants: Arnaud Anantharaman, Xavier Blanc, Sébastien Boyaval, Ronan Costaouec, Claude Le Bris, Frédéric Legoll.

X. Blanc and C. Le Bris have studied, for homogenization of elliptic partial differential equations, the applicability of ideas based on filtering. The bottom line is to modify the corrector problem by introducing a filtering function, in order to improve the efficiency of the method. Some popular methods, such as the oversampling method, can indeed be considered as special instances of such a general strategy. Encouraging numerical results, supported by a rigorous theoretical analysis, have been reported in the ongoing work [38], in the case of periodic and quasi-periodic settings.

The project-team has also pursued its efforts in the field of stochastic homogenization of elliptic equations. An interesting case in that context is when the randomness comes as a *small* perturbation of the deterministic case. This case has been studied by X. Blanc and C. Le Bris, in collaboration with P.-L. Lions (Collège de France). This analysis naturally gives rise to a numerical strategy, which is currently implemented by R. Costaouec, as the first stage of his PhD thesis.

In the work mentioned above, the perturbation to the deterministic case is supposed to be small in the L^∞ norm (that is, it is almost surely small). A. Anantharaman and C. Le Bris are currently working on extending this study to the case when the perturbation is small in a weaker norm, typically the L^1 norm (that is, only the *expectation* of the perturbation is assumed to be small).

In the context of parabolic homogenization, A. Anantharaman has addressed the question of boundary layers in time (close to the initial time $t = 0$) and space (close to the domain boundaries), in collaboration with G. Allaire (CMAP). The idea is to add boundary layer terms to the usual approximate solution (which is computed by solving the homogenized problem and the corrector problems), so that the difference between the exact solution and the approximate solution can be estimated, and more precisely controlled in interesting functional spaces. Some interesting preliminary steps have been performed, but definite conclusions on this problem have yet to be obtained.

Also at the numerical level, S. Boyaval has tested the feasibility of a reduced-basis approach for multiscale problems in the context of (deterministic) homogenization of scalar elliptic equations. The project is a close collaboration with A.T. Patera (MIT) and Y. Maday (CNRS/UPMC/Brown). The results allow for a fast and rigorous numerical homogenization of heterogeneous materials [10].

Furthermore, in collaboration with Y. Maday (CNRS/UPMC/Brown), N.C. Nguyen and A.T. Patera (MIT), S. Boyaval and C. Le Bris have studied the applicability of reduced-basis ideas to variational problems with stochastic parameters. The motivation stems from the need of taking into account many different random microstructures in the context of stochastic homogenization. One of the bottlenecks is that the solutions, for different stochastic parameters, to a given partial differential equation, form a high-dimensional space. To address this difficulty, different approaches have been recently suggested in the literature on uncertainty quantification for stochastic partial differential equations. The combination of these approaches with the reduced-basis method has been tested and analyzed for a scalar (linear) elliptic problem with stochastic boundary conditions [11].

5.7. Free surface flow and magnetohydrodynamics

Participants: Claude Le Bris, Tony Lelièvre.

The project-team is since many years a long-term collaborator of RioTinto (formerly Pechiney, and Alcan) on the modeling of aluminium electrolysis cells. An overview of the work performed over the years is presented in [4]. Several theoretical and numerical topics of research are issued from this collaboration. The subsequent problem is one instance of those.

A general difficulty for two-fluid flows in a box is the modeling of the moving contact line, namely the boundary of the free interface between the two fluids. An adequate boundary condition between no-slip and pure slip should be derived in order to appropriately model the motion of the free surface. Recently, the Generalized Navier Boundary Condition have been introduced by T.Z. Qian et al. In [21], an Arbitrary Lagrangian Eulerian (ALE) formulation of the Generalized Navier Boundary Condition is proposed. The stability of the numerical scheme is analyzed in energy norm and the validity of the approach is demonstrated by numerical experiments on two-fluid flows in narrow channels. This work is in collaboration with J.-F. Gerbeau (INRIA REO).

5.8. Complex fluids

Participants: Sebastien Boyaval, Eric Cancès, Claude Le Bris, Tony Lelièvre.

In this field, two subjects related to the discretization of models for complex flows have been addressed: (i) free energy dissipative schemes for macroscopic models (like Oldroyd-B model) and (ii) analysis of a numerical method to solve high-dimensional PDEs, with application to the Fokker-Planck equation involved in micro-macro models (like FENE model).

(i) Free energy dissipative schemes

In [12], the stability of various finite element schemes is analyzed regarding free energy. More precisely, it is known from a previous work that the Oldroyd-B model is dissipative when considering a free energy rather than the usual energy considered by many authors. A natural question is then: do the numerical schemes used in practice satisfy similar free energy dissipative properties ? Some criteria to be satisfied in order for the finite element scheme to enjoy such a property have been identified. The log-formulation recently introduced by Fattal et al. is also analyzed and it is proved that the associated numerical scheme is unconditionally stable (with respect to the timestep) which may explain the rather good results obtained in practice with this formulation. This work is in collaboration with C. Mangoubi (The Hebrew University of Jerusalem).

As a follow-up, S. Boyaval and J.W. Barrett (Imperial College, London, UK) are currently completing a study about the convergence of free-energy-dissipative finite element approximations to regularized Oldroyd-B models. Using a particular discretization of the advection term, they show that it is possible to use continuous finite element spaces to obtain a discrete analogue of the free energy bound for a regularized Oldroyd-B model. Moreover, convergence (up to a subsequence), as the mesh parameters tend to zero, of such a scheme is proved, which yields existence of global-in-time solutions to this modified Oldroyd-B system.

In collaboration with Philippe Coussot (LCPC) and Francois Lequeux (ESPCI), E. Cancès, S. Boyaval and C. Le Bris are working on numerical simulations of constitutive equations for viscoelastic fluids subject to thixotropic effects. The combination of such developments with the free-energy-dissipative finite element schemes developped in [12] is currently under study, as well as benchmark simulations that can be compared to actual experiments.

Moreover, equations for – thixotropic – viscoelastic fluids that involve a high-dimensional stochastic modeling (Fokker-Planck equation) also exist which have motivated the further study of a reduction method (the reduced-basis method) and its application to stochastic models, in collaboration with Y. Maday (University Paris 6 and Brown University) and A.T.Patera (MIT).

(ii) A numerical method for high dimensional PDEs

The work [26] analyzes a numerical method recently proposed by Ammar et al. to solve the Fokker-Planck equation for micro-macro models for complex fluids. This method is based on a representation of the solution as a sum of tensor products of one-dimensional functions, and a greedy algorithm to compute sequentially the terms of the sum. Using known results from approximation theory, a variational formulation of the numerical method (arising from the minimization of some functional) is proved to actually converge to the solution. Many questions remain open concerning the original algorithms proposed (based on the Euler-Lagrange equations associated to the minimization problem), in particular in the case of non self-adjoint operators. The work is joint work with Y. Maday (University Paris 6 and Brown University).

Finally, the work [28] by C. Le Bris in collaboration with P.-L. Lions shows existence and uniqueness of solutions to Fokker-Planck type equations with irregular coefficients is studied. This theoretical question originates from the analysis of micro-macro models for polymeric fluids.

6. Contracts and Grants with Industry

6.1. Contracts and Grants with Industry

Many research activities of the project-team are indeed conducted in close collaboration with private or public companies: RioTinto (formerly Pechiney and Alcan) for the modeling of electrolytic cells, EADS, Electricité de France and Commissariat à l'Energie Atomique for computational chemistry, molecular dynamics and multiscale simulation of solids. Industrialists interested by the production and transformation of elastomeric materials are also partners of the project-team.

7. Other Grants and Activities

7.1. Regional activities

The project-team is shared between INRIA, Ecole Nationale des Ponts et Chaussées and Paris Dauphine.

7.2. National activities

The project-team is part of the program initiative “Infrastructure et Outils Logiciels pour la Simulation (IOLS)”, itself part of the “Pole Systematic Paris-Region”.

The project-team is now involved in seven ANR projects.

The first one, the ANR “non-thématique” INGEMOL, animated by Philippe Chartier (INRIA Rennes), focuses on geometric numerical methods for Hamiltonian equations with applications to molecular simulation and laser beam propagation.

The second one (ANR “Calcul intensif et grilles de calcul” LN3M, lead by F. Jollet, CEA-DAM) aims at developping new numerical methods and softwares for multiscale modeling of materials.

The third one (ANR “non thématique” ACCQUAREL, lead by G. Turinici and with teams from Dauphine, Paris VI and Cergy Universities) is focusing on relativistic quantum theory.

The fourth one concerns G. Turinici, leader of the Paris Dauphine team of the C-QUID ANR project (animated by J.M. Coron).

The fifth one the project-team is involved in is the ANR Parmat, managed by Guy Bencteux (EDF and MICMAC).

The sixth one (ANR “Calcul intensif et grilles de calcul” SIRE, lead by Ph. Sautet, ENS Lyon) focuses the simulation of chemical reactivity at the interfaces.

The seventh one is the ANR METHODE (Hydrological modeling), S. Cordier (Université d’Orléans).

7.3. European Community financed activities

Some members of the project-team have participated in the european project (Marie Curie Research Training Networks) “MULTIMAT" devoted to the multiscale modeling of materials (scientist in charge Nick Schryvers), which has concluded in 2008. The project-team is again part of new application for a similar network.

T. Lelièvre, G. Stoltz and F. Legoll have participated in the HIM program on Computational Mathematics Hausdorff Center for Mathematics, More specifically, they have co-organized a Junior Hausdorff Trimester program in Bonn (March 24th – May 4th, 2008), on “Numerical methods in molecular simulation” (see http://www.hausdorff-research-institute.uni-bonn.de/numerical-methods). This program included a one week workshop (April 7th – April 11th, 2008).

G. Turinici is associate member of the "Optimization with PDE Constraints (OPTPDE)" project of the ESF.

7.4. Bilateral international relations

7.4.1. Americas

Continuous and permanent cooperations have been established with the group of Gustavo Scuseria at Rice University on questions related to electronic structure calculations for large systems, that of Herschel Rabitz at Princeton University on questions related to laser control. The project-team obtained a PICS CNRS-NSF grant for a collaboration between Princeton University and the Laboratoire CEREMADE (Paris Dauphine).

8. Dissemination

8.1. Animation of the scientific community

E. Cancès is a member of the editorial board of Mathematical Modeling and Numerical Analysis (2006-) and of SIAM Journal of Scientific Computing (2008-).

E. Cancès is co-Editor in chief (with P. Del Moral and J.-F. Gerbeau) (2005-) of ESAIM Proc.

E. Cancès has co-organized the following events in 2008:

- (with W. E and M. Ortiz) Minisymposium on Electronic structure calculations, SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, May 11-14, 2008.

- (with L. Bronsard and M. Esteban) Session on Variational and numerical methods in geometry, physics and chemistry, 2nd Canada-France congress, Montreal, June 1-5, 2008.

- (with J. Meza) IMA Tutorial on Mathematical and computational approaches to quantum chemistry, Minneapolis, September 26-27, 2008.

- (with A. Krylov, J. Meza and J. Perdew), IMA workshop on Mathematical and numerical aspects of electronic structure calculations, Minneapolis, September 29 - October 3, 2008.

E. Cancès has honored long term invitations from the following institutions: Brown University, Providence, USA, July-August 2008; University of Minnesota, IMA, Minneapolis, USA, September-December 2008.

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 Applied in Science and Technology (2006-), Networks and Heterogeneous Media (2005-), Nonlinearity (2005-), Review of Mathematical Science (2006-). He is a member of the editorial board of the monograph series Mathématiques et Applications, Series, Springer (2008-), and Modeling, Simulations and Applications, Series, Springer (2009-).

C. Le Bris has served as a member of

- the evaluation panels for the DFG-Priority *Extraction of Quantifiable Information from Complex Systems*, 2008,

- the scientific program committee of Conférence franco-canadienne de Mathématiques 2008, Montréal,

- the organizing committee (only non Chinese national) (with Weinan E, Chun Liu, An-Chang Shi, Qi Wang, Pingwen Zhang) of the thematic year *Multiscale modeling of complex fluids*, Beijing University, Beijing 2007-2008,

- the organizing committee (with Michael Ortiz, Stefan Mueller, ...) of the SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, May 11-14, 2008.

C. Le Bris is a member of

- the organizing committee (only non American national) (with Anna Chaka, Weinan E, Bill Hase, Michael Holst, Yousef Saad, Tamar Schlick, Donald G. Truhlar) of the IMA thematic year *Mathematics and Chemistry*, Minneapolis 2008-2009,

- the Scientific Program Committee of ICIAM 2011, Vancouver, Canada,

- the board of directors of SMAI (French SIAM),

- the scientific board of ENPC, 2008- (nominated as representative of the research scholars).

C. Le Bris is a Distinguished Ordway Visitor 2008-2009, School of Mathematics, University of Minnesota.

C. Le Bris has honored long term invitations from the following institutions: University of Minnesota, IMA, Minneapolis, USA, academic year 2008-09; Beijing university, Winter term 2008.

C. Le Bris and T. Lelièvre are co-organizers of a workshop on numerical methods in rheology, Ecole des Ponts, January 2009.

F. Legoll has honored a short term invitation from Technische Universität Berlin, July 2008.

F. Legoll, T. Lelièvre and G. Stoltz have honored a short term invitation from HIM program on Computational Mathematics Hausdorff Center for Mathematics, Bonn.

T. Lelièvre has been a co-organizer of a mini-symposium on hybrid methods at CANUM 2008, May 2008.

G. Turinici is a member of

-the organizing committee of the workshop "Quantum control and coherence" to be held in March 2009 within the thematic year *Mathematics and Chemistry*, Minneapolis 2008-2009,

- the organizing committee of the workshop "Mathematical approaches in optimization, modellisation and control" April, 11, 2008, Iasi, Romania.

8.2. Teaching activities

- Analyse, cours à l'Ecole Nationale des Ponts et Chaussées (A. Anantharaman, S. Boyaval, E. Cancès, F. Legoll),
- Analyse en fréquences, cours à l'Ecole Nationale des Ponts et Chaussées (E. Cancès, G. Stoltz),
- Simulation moléculaire: aspects théoriques et numériques, cours de M2, Université Paris 6 (E. Cancès, M. Lewin).
- Analyse numérique et optimisation, PC du cours de G. Allaire et P.-L. Lions, Ecole Polytechnique (E. Cancès, C. Le Bris),
- Introduction à la physique statistique et à la physique quantique, cours à l'Ecole Nationale des Ponts et Chaussées (I. Dabo, F. Legoll),
- Analyse numérique et Optimisation, TD ESIEE (L3) (A. Deleurence),
- Analyse 1, cours à l'Université Paris Dauphine (A. Grigoriu) (TD 40H, L1)
- Mathématiques des modèles multi-échelles, cours à l'Ecole Nationale des Ponts et Chaussées (F. Legoll, M. Lewin).
- Systèmes multiéchelles, cours de M2, Université Paris 6 (C. Le Bris),
- Probabilités et applications, (42h), Cours ENPC (T. Lelièvre),
- Méthodes déterministes en mathématiques financières, (42h), Cours ENPC (T. Lelièvre),
- Modéliser Programmer Simuler, (27h), Cours ENPC (T. Lelièvre),
- Analyse Numérique, TP de MATLAB à l'ISBS (K. Minoukadeh),
- Introduction à Scilab, cours à l'Ecole Nationale des Ponts et Chaussées (K. Minoukadeh),
- Statistiques, cours à l'ENPC (R. Roux),
- Probabilités et Statistiques, TD à l'ESIEE (R. Roux),
- Introduction aux probabilités et aux statistiques, TD à l'ENSTA (R. Roux),
- Simulation numérique et méthodes de changement d'échelles, (12h) Mastère SMCD, Chaire Lafarge, ENPC (G. Stoltz),
- Algèbre linéaire 3, cours à l'Université Paris Dauphine (G. Turinici) (21H, L2),
- Analyse numérique: évolution, cours à l'Université Paris Dauphine (G. Turinici) (20H cours, 40H TD, M1)
- Introduction à l'analyse numérique des EDP, cours à l'Université Paris Dauphine (G. Turinici) (30H, M2),
- Méthodes numériques en finance, cours à l'Université Paris Dauphine (G. Turinici) (9H, M2),
- Approches quantitatives et numériques des stratégies financières, cours à l'Université Paris Dauphine (G. Turinici) (21H, M2).

8.3. Conference participation

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

- G. Bencteux, Workshop on Numerical Methods in Density Functional Theory, Berlin, June 23-25, 2008.
- G. Bencteux, Institute for Mathematics, TU Berlin, June 3, 2008.
- X. Blanc, Second Canada-France Congress, UQAM, Montréal, June 2008
- S. Boyaval, Hilton Phoenix East/Mesa AZ (December 07), at SIAM Conference on Analysis of Partial Differential Equations (PD07).
- S. Boyaval, Beijing International Center for Mathematical Research (May 08), at Workshop "Multiscale Modeling of Complex Fluids", 2007-2008 Thematic Program on Multiscale Modeling of Complex Fluids organized by Beijing University.
- S. Boyaval, Centre International de Rencontres Mathématiques (CIRM, August 08), at CEMRACS 08 "Modélisation et Simulation de Fluides Complexes"
- S. Boyaval, GDR MOMAS, IHP Paris, novembre 2008.
- E. Cancès, Invited plenary lecture, SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, May 11-14, 2008.
- E. Cancès, Journées analyse et physique mathématique, IHP, June 2008.
- E. Cancès, POEMs seminar, ENSTA, June 2008.
- E. Cancès, IMA Tutorial on Mathematical and computational approaches to quantum chemistry, Minneapolis, September 26-27, 2008.
- E. Cancès, Fourth International Conference on Multiscale Materials Modeling (MMM-08), Tallahassee, October 2008.
- E. Cancès, weekly seminar of the Applied Mathematics Department, University of Minnesota, Minneapolis, November 2008.
- I. Dabo, Numerical Methods in Density-functional Theory Workshop, TU Berlin, July 2008.
- I. Dabo, DFT meets Experiment Workshop, IFW, Dresden, August 2008.
- A. Deleurence, CANUM, Saint-Jean de Monts, May 2008.
- A. Grigoriu "Mathematical approaches in optimization, modellisation and control" April, 11, 2008, Iasi, Romania
- A. Grigoriu, participated and obtained the poster prize at the "Congrès National d'Analyse Numérique", May 2008.
- C. Le Bris, Invited plenary lecture, 18th International Conference on Domain Decomposition Methods, Jerusalem, January 12th – 15th, 2008
- C. Le Bris, weekly seminar of Institute of computational mathematics of the Chinese Academy of Sciences, February and May 2008
- C. Le Bris, Workshop "EDP and applications", Hammamet, Tunisia, March 26th –29th, 2008
- C. Le Bris, Workshop "Multiscale problems in complex fluids", Beijing, May 26th – 30th, 2008
- C. Le Bris, Minisymposium on Electronic structure calculations, SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, May 11th – 14th, 2008
- C. Le Bris, Minisymposium on Discrete to Continuum, SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, May 11th – 14th, 2008
- C. Le Bris, weekly seminar of Institute of Applied Physics, Technische Universität Berlin, June 2008
- C. Le Bris, weekly seminar of Freie Universität Berlin, June 2008
- C. Le Bris, IMA Workshop on Mathematical and numerical aspects of electronic structure calculations, Minneapolis, September 2008

- C. Le Bris, DqF workshop on Stochastic Differential Equations: Models and Numerics, KTH Stockholm, October 20th – 22nd, 2008
- C. Le Bris, Invited keynote speaker in the minisymposium "Mathematical issues in multiscale materials modeling", Fourth International Conference on Multiscale Materials Modeling (MMM-08), Florida State University, Tallahassee, October 27th – 31st, 2008
- C. Le Bris, IMA Workshop on "Development and Analysis of Multiscale Methods", Minneapolis, November 3rd – 7th, 2008
- C. Le Bris, séminaire du Laboratoire d'analyse numérique (JLL) Paris VI, December 2008
- C. Le Bris, School of Mathematics Colloquium, University of Minnesota (2008)
- C. Le Bris, Series of lectures "Computational statistical mechanics" and "Stochastic modeling of materials", graduate level, Beijing University, 20 hours, winter 2008.
- C. Le Bris, Series of 5 one-hour lectures "From molecular theories to continuum elasticity: a possible track", CMA Summer school Carnegie Mellon, June 2008
- C. Le Bris, Series of 5 one-hour lectures "Concurrent models. Atomistic to continuum (AtC) modeling", Santiago de Compostela, May 2008.
- C. Le Bris, Series of lectures "Molecular simulation: a mathematical initiation", University of Minnesota, 20 hours, fall 2008.
- F. Legoll, Series of 3 two-hours lectures on "Multiscale methods coupling atomistic and continuum mechanics", Technische Universität Berlin, July 2008.
- F. Legoll, IAM seminar, Bonn University, April 24th, 2008
- F. Legoll, Minisymposium "Atomistic to Continuum Coupling Methods for Solids", SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, May 11th – 14th, 2008
- F. Legoll, workshop "ITER: aspects plasmas et matériaux", Paris, May 22nd – 23rd, 2008
- F. Legoll, workshop "Gradient models and elasticity", Warwick, June 9th – 12th, 2008
- F. Legoll, workshop "Free Energy Calculations", Banff, June 16th – 20th, 2008
- F. Legoll, Kolloquium der Arbeitsgruppe Modellierung, Numerik, Differentialgleichungen, Technische Universität Berlin, July 8th, 2008
- F. Legoll, Max Planck Institute Oberseminar, Leipzig, July 15th, 2008
- F. Legoll, Minisymposium "Mathematical issues in multiscale materials modeling", Fourth International Conference on Multiscale Materials Modeling (MMM-08), Florida State University, Tallahassee, October 27th – 31st, 2008
- F. Legoll, workshop "Development and analysis of multiscale methods", IMA, Minneapolis, November 3rd – 7th, 2008
- F. Legoll, EDF LAMSID weekly seminar, Paris, November 27th, 2008
- F. Legoll, workshop "Interplay of Analysis and Probability in Physics", Oberwolfach, November 30th – December 6th, 2008
- F. Legoll, weekly seminar, Zentrum Mathematik, Technische Universität München, December 2008
- T. Lelièvre, Workshop on adaptive Markov chain Monte Carlo methods, ADAPSKI, Bormio, January 2008.
- T. Lelièvre, Workshop GREFI-MEFI 2008, Stochastic dynamics and probability, Marseille, March 2008.
- T. Lelièvre, Workshop BIRS Mathematical and Numerical Methods for Free Energy Calculations in Molecular Systems, Banff, June 2008.
- T. Lelièvre, Workshop DqF Stochastic Differential Equations: Models and Numerics, Stockholm, October 2008.

- T. Lelièvre, Workshop Molecular Dynamics, Thermostats and Convergence to Equilibrium, Edinburgh, November 2008.
- T. Lelièvre, Séminaire ENS Lyon, January 2008.
- T. Lelièvre, Séminaire Université Paris Dauphine, February 2008.
- T. Lelièvre, Séminaire Equations aux dérivées partielles et applications, Collège de France, April 2008.
- T. Lelièvre, Séminaire MODANT, Grenoble, april 2008.
- T. Lelièvre, Séminaire Equations aux dérivées partielles, Chambéry, September 2008.
- T. Lelièvre, Séminaire Equations aux dérivées partielles et analyse numérique, Lille, October 2008.
- T. Lelièvre, CEMRACS 2008, cours (3h) sur le thème "Multiscale modeling of complex fluids: a mathematical initiation", Marseille, July 2008.
- T. Lelièvre, Ecole Doctorale ECODOQUI, cours (3h) sur le thème "Méthodes stochastiques en dynamique moléculaire", Paris, November 2008.
- R. Roux, Journées MAS de la SMAI, Rennes (France, August 2008)
- R. Roux, Seminar “Probability and stochastic processes” at Université de Rennes 1 (France, November 2008)
- R. Roux, PhD students seminar at Université Lille 1 (France, December 2008)
- G. Stoltz, seminar at Université de Strasbourg (February 2008)
- G. Stoltz, Oberwolfach meeting "Atomistic models of materials" (Germany, April 2008)
- G. Stoltz, Banff meeting on “Numerical methods for free energy computations” (Canada, June 2008)
- G. Turinici "Mathematical approaches in optimization, modellisation and control" April, 11, 2008, Iasi, Romania
- G. Turinici, invited conference at the workshop "Control of quantum and spacial phenomena", Dijon, June 2008, Université de Bourgogne
- G. Turinici, seminar Dijon, April 2008, Université de Bourgogne
- G. Turinici, invited conference at the "9-ème Colloque Franco-Roumain de Math. Appl.", Brasov, Sept 2008, Romania
- G. Turinici, invited conference at the workshop "Mathematics and applications", Bucarest, Sept 2008, Romanian Academy of Science
- G. Turinici, invited conference at the workshop " Optimization with PDE Constraints" Warsaw, Dec. 11-13, 2008.

Members of the project-team have participated (without giving talks) in the following seminars, workshops and international conferences:

- A. Anantharaman, Colloque du Groupement de Recherche Européen "Mathematics and Quantum Physics", Université de Cergy-Pontoise (January/February 2008)
- A. Anantharaman, SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, May 11th – 14th, 2008
- K. Minoukadeh and R. Roux, Numerical methods in molecular simulation, Bonn (Germany, April 2008)
- K. Minoukadeh and R. Roux, "Mathematics of Multiscale Phenomena", Berlin Mathematical School (Germany, September 2008)
- K. Minoukadeh, Second Canada-France Congress, UQAM, Montréal (Canada, June 2008)
- R. Roux, GREFI-MEFI 2008, Marseille (France, March 2008)

9. Bibliography

Major publications by the team in recent years

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[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., 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.

Year Publications

Articles in International Peer-Reviewed Journal

[6] A. ANANTHARAMAN, E. CANCÈS. *On Kohn-Sham models with LDA and GGA exchange-correlation functionals*, in "Annales de l'IHP, Analyse non linéaire", submitted, Preprint INRIA-00325660, 2008.

[7] M. BELJHAJ, S. SALOMON, G. TURINICI. *A stable toolkit method for quantum control problems*, in "J. Phys. A: Math. Theor.", vol. 41, 2008, 362001.

[8] G. BENCTEUX, E. CANCÈS, W. HAGER, C. LE BRIS. *Analysis of a quadratic programming decomposition algorithm*, in "SIAM J. on Numerical Analysis", submitted, https://hal.inria.fr/inria-00169080.

[9] X. BLANC, C. LE BRIS, F. LEGOLL, C. PATZ. *Finite-temperature coarse-graining of one-dimensional models: mathematical analysis and computational approaches*, in "Journal of Nonlinear Science", submitted, http://hal.inria.fr/inria-00282107/en/.

[10] S. BOYAVAL. *Reduced-Basis Approach for Homogenization beyond the Periodic Setting*, in "SIAM Multiscale Modeling & Simulation", vol. 7, n^{o} 1, 2008, p. 466-494.

[11] S. BOYAVAL, C. LE BRIS, Y. MADAY, N. NGUYEN, A. PATERA. *A Reduced Basis Approach for Variational Problems with Stochastic Parameters: Application to Heat Conduction with Variable Robin Coefficient*, in "Comput. Methods Appl. Mech. Engrg.", submitted, http://hal.inria.fr/inria-00311463/fr/.

[12] S. BOYAVAL, T. LELIÈVRE, C. MANGOUBI. *Free-energy-dissipative schemes for the Oldroyd-B model*, in "M2AN", accepted, 2008, http://fr.arxiv.org/abs/0801.2248.

[13] C. BROUDER, G. STOLTZ, G. PANATI. *Adiabatic approximation, Gell-Mann and Low theorem and degeneracies: A pedagogical example*, in "Phys. Rev. A", vol. 78, 2008.

[14] E. CANCÈS, A. DELEURENCE, M. LEWIN. *Local defects in periodic crystals: the reduced Hartree-Fock case*, in "Comm. Math. Phys.", vol. 281, 2008, p. 129-177.

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