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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 team has been created jointly by the Ecole Nationale des Ponts et Chaussées (ENPC) and the INRIA in October 2002. It is hosted in the CERMICS laboratory (Centre d'Enseignement et de Recherches en Mathématiques, Informatique et Calcul Scientifique) at ENPC. The scientific focus of the 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.

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 which originates in the presence of the surrounding medium; it is responsible of peculiar properties (e.g. unexpected acidity of some reactive site enhanced by special interactions) on which rely vital processes.

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 modelled 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 couples one approach to the others within the so-called *multiscale* models. In the following we shall indicate how this journey can be done, 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) shows itself 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 our work.

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 small enough variational space, whose dimension is kept limited while the size of the system increases?

An alternative strategy to diminishing 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 therefore for the modification of chemical bonds, while the rest of the system (typically the innert 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 validate the idea of manipulating and controlling quantum systems with lasers, but also motivate 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, we deal here with open-loop control, 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 we allow 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 on the theoretical level, e.g. by envisioning new modeling strategies that incorporate undesirable perturbations.

5. New Results

5.1. Computational quantum chemistry

Participants: Guy Bencteux, Eric Cancès, Amélie Deleurence, Hervé Galicher, Claude Le Bris, Tony Lelièvre, Mohamed El Makrini, Mathias Rousset, Gabriel Stoltz, Gabriel Turinici.

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

On the theoretical front, E. Cancès and G. Stoltz, in collaboration with E. Davidson (Washington State University), G. Scuseria (Rice University) and V. Staroverov (University of Western Ontario), have studied the mathematical foundations of some systematic constructions of local exchange potentials in density functional theory, including the Slater potential, the optimized effective potential (OEP), the Krieger-Li-Iafrate (KLI) approximation and the common-energy denominator approximation (CEDA) to the OEP, and the effective local potential [22] (ELP). In particular, they showed in [47] how to reformulate these constructions in terms of variational problems, and they provided a rigorous derivation of the so-called OEP integral equation. They have also established an existence result for a coupled system of nonlinear partial differential equations, introduced by Slater to approximate the Hartree-Fock equations.

E. Cancès and A. Deleurence have addressed issues related to the modelling 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 is still missing. In collaboration with Mathieu Lewin (CNRS, Cergy), Eric Cancès and Amélie Deleurence have proposed in [46] 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 suggest 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 through 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 [45]. Some preliminary, promising numerical results have been obtained on a one-dimensional nonlinear model with Yukawa interaction potential.

On the numerical front, 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 [6], [39]. The development of the domain decomposition algorithm for the linear subproblem has been continued. Some 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). 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 [5]. The performance of the parallel version confirms that a high scalability will be reached with an additional implementation effort : this will be part of the collaboration with EDF in the frame

of the project "ParMat", financially supported by the ANR (National Research Agency). From a numerical analysis viewpoint, the convergence properties of the MDD algorithm have been studied, and the convergence established in a simplified setting [43].

5.2. Molecular dynamics and related problems

Participants: Eric Cancès, Claude Le Bris, Frédéric Legoll, Tony Lelièvre, Mathias Rousset, Rafaël Roux, Gabriel Stoltz.

The extremely broad field of Molecular dynamics is a field where the MICMAC project, originally more involved in the quantum chemistry side, has invested a lot of efforts in the recent years.

These efforts both deal with the deterministic techniques and the probabilistic techniques used in the field.

Molecular dynamics is often employed in statistical physics for computing ensemble averages. The bottom line for this is the assumed ergodicity of the Hamiltonian dynamics in the microcanonical ensemble. Ensemble averages are thus expressed as averaged long time limits of integrals calculated along the actual trajectory.

One difficulty of such a computation is the presence of several time scales in the dynamics: the frequencies of some movements are very high (e.g. for the atomistic bond vibrations), while they are much smaller for some other movements. Actually, these fast phenomena are relevant only through their mean effect on the slow phenomena, and a precise description of them 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. Claude Le Bris and Frédéric Legoll have initiated a study along this aim. Some results have been obtained for the integration of a class of highly oscillating Hamiltonian systems [23], [24]. The authors should follow up on this soon. The different methods to address this problem are discussed with François Castella, Philippe Chartier and Erwan Faou from INRIA Rennes, with the funding of ANR Ingemol (“Intégration numérique géométrique des équations hamiltoniennes”).

A similar problem appears when one wants to compute canonical averages associated to potential energies that include stiff terms. This subject is studied by Claude Le Bris, Frédéric Legoll and Mathias Rousset in collaboration with Petr Plechac (Warwick University).

In collaboration with Ben Leimkuhler and Emad Noorizadeh (University of Edinburgh), Frédéric Legoll has developed a dynamical method able to generate a constant energy trajectory at a given kinetic temperature. Such a method is useful for systems that need to be simulated according to Newton equations (for any other dynamics introduces too much perturbation in the system), at an energy that corresponds to a given average kinetic temperature. Some preliminary results are exposed in [28].

In addition to the difficulty arising from the highly oscillatory character of the dynamics addressed so far, a second difficulty arises from the extremely long time frame over which the system needs to be simulated. The dynamics of a molecular system usually consists of two different phases: oscillations of the system around a local minimum of the potential energy (that is, in a metastable state), and rare hoppings from a metastable basin to another one. In order to perform an efficient exploration of the phase space, it is important to simulate the system long enough such that several metastable basins have been visited. However, it is extremely difficult to achieve such a goal when using a full atomistic description of the system, again because of the presence of several time scales in the dynamics. Eric Cancès, Amélie Deleurence and Frédéric Legoll are currently studying several methods to coarse-grain the system, in order to develop a model better suited to long time simulation.

Stochastic dynamics to compute free energy differences are widely used in computational chemistry and biology. These free energy differences can be computed using the Jarzynski equality, which can be extended to account for transitions between two submanifolds of the state space [30]. In some cases, path sampling techniques can be used to this end, and some new algorithms to sample paths are presented in [35]. However, many recent methods rely on non-linear Markov processes, like the adaptive techniques. A unifying presentation of adaptive methods is proposed in [31] together with an efficient implementation of adaptive dynamics using an interacting particle system with birth-death processes. A convergence result for this

nonlinear dynamics has also been proved in [50], 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).

A related problem is the following. Molecular systems are composed of a large number of atoms. Hence, describing the state of a molecular system requires in principle a lot of degrees of freedom. However, in practice, only a few of them, the so called *reaction coordinates*, are actually relevant (for they describe the change of conformations, or metastable states). The statistics of these reaction coordinates is described by the free energy. Frédéric Legoll and Tony Lelièvre are currently working on how to define a closed dynamics on 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 few of them. Promising results have been obtained in [49].

In addition to the above, Rafaël Roux has started his PhD work under the supervision of B. Jourdain and T. Lelièvre on particle methods in molecular dynamics. He is currently working on the convergence of a discretization of the Adaptive Biasing Force method based on a particle method.

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

Participants: Eric Cancès, Ismaila Dabo.

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 [12], [13]. This approach has been applied to interpret electrochemical spectroscopy experiments [15], [14]. As part of the post-doc scientific program of Ismaila Dabo, this atom-continuum model will be complemented, by incorporating pressure, surface-tension, and acidity effects.

5.4. Laser control

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

Our 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).

We have addressed in [27] in collaboration with Mazyar Mirrahimi (INRIA Rocquencourt) and Herschel Rabitz, and in close connection with Pierre Rouchon (Ecole des Mines de Paris) some questions related to the inversion paradigm: use the laser field as a tool to obtain additional information on the molecular system. The focus of [27] is purely theoretical. Following recent works by Mazyar Mirrahimi and Pierre Rouchon where dipole moment entries are recovered from measures, Andreea Grigoriu studied during her internship the effects of limitations on the number of measures (and the possibility to use extrapolation for the missing data).

Another direction of research involves the possibility to simultaneously control several systems with the same external field. In order to be able to treat systems whose coupling structure is bipartite we revisited and extended a previous result (see [36]).

We have also pursued our works in the field of numerical algorithms used to compute optimal control fields. We proposed algorithms and documented their performance for the situation when some form of dissipation is included in the model [37].

Another numerical contribution [32] came from the adaptation of the monotonic algorithms in the "parareal" setting. A re-thinking of the whole framework was necessary and the monotonicity was found to be written as an optimisation problem with intermediary targets.

5.5. Atomistic to continuum methods

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

The team project has continued his 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.

A. Gloria has addressed with R. Alicandro (University of Cassino, Italy) and M. Cicalese (University of Naples, Italy) the variational derivation of a continuum energy starting from a discrete system of spins in interaction. This work is available as a CVGMT preprint [3] and has been submitted for publication. Besides, they have begun to address the derivation of rubber elasticity models from a discrete system of points in interaction, the system being described by a stochastic lattice, as introduced by X. Blanc, C. Le Bris and P.-L. Lions. An article is in preparation. The main result has been announced in [4]. As an application, it has allowed to prove in [38] the asymptotic convergence of a finite element modeling of rubber introduced by Böl and Reese.

In collaboration with Pierre-Louis Lions (Collège de France), Xavier Blanc and Claude Le Bris have continued to address the question of passing from the microscopic scale to the macroscopic scale. A study on the passage to continuum for stochastic lattices and the relation of this question with homogenization theory has been published, [8].

An independently investigated track is the possibility to perform thermodynamic limits (used in the past for defining the energy per unit volume of an infinite sample of matter) this time on the free energy, i.e. in the presence of temperature effects. Some preliminary steps have been performed by Claude Le Bris, Xavier Blanc, Frédéric Legoll and Carsten Patz (Berlin University).

On the numerical front, Frédéric Legoll studies with Mouhamad Hammoud, PhD student at LAMI (ENPC), methods for coupling a discrete model with a continuous one, in a dynamical setting. The aim is to coarse-grain the system (e.g. make use of a continous model) only in regions where the deformation is small, that is where a quadratic approximation for the potential energy can be used.

5.6. Homogenization

Participants: Xavier Blanc, Sebastien Boyaval, Antoine Gloria, Claude Le Bris, Frédéric Legoll.

A. Gloria has continued his work on numerical homogenization methods, addressing now the analysis of oversampling methods in the context of elliptic operators and nonlinear elasticity. The approach adopted consists in introducing an averaged energy that describes the effective behaviour of heterogeneous materials and analyze its convergence properties in terms of Γ-convergence. The analysis of oversampling methods has given rise to the INRIA research report RR-6127 and to the article [18]. Some numerical tests, performed with FreeFEM++, have complemented the analysis.

Besides, A. Gloria has followed up on the work by X. Blanc, C. Le Bris and P.-L. Lions on a variant of stochastic homogenization for the case of multiple integrals in the INRIA research report RR-6316. The work is submitted for publication.

The work by A. Braides (University of Rome) and A. Gloria on a problem of G-closure for a discrete polycrystal has been accepted for publication [10].

In close collaboration with A.T. Patera (MIT) and Y. Maday (CNRS/UPMC/Brown), S. Boyaval has tested the feasability of a reduced-basis approach for multiscale problems. The context is that of the homogenization of scalar elliptic equations. The results allow for a fast and rigorous numerical homogenization of heterogenous material. They will appear in [9].

5.7. Free surface flow and magnetohydrodynamics*

Participants: Claude Le Bris, Tony Lelièvre.

In collaboration with Jean-Frédéric Gerbeau (Inria, REO), and in association with Alcan (formerly Aluminium Péchiney), Claude Le Bris and Tony Lelièvre have pursued their efforts for the numerical simulation of electrolytic cells for the industrial production of Aluminium.

In addition, J.F. Gerbeau and T. Lelièvre are currently working on the stability of numerical schemes for free surface flows [48]. The focus of this research if how to implement forces such as gravity and surface tension in Arbitrary Lagrangian Euler schemes, in such a way that the energy conservation laws holding at the continuous level are also satisfied at the discrete level.

5.8. Fluid Structure Interactions

Participant: Antoine Gloria.

M. Fernandez, J.-F. Gerbeau (project-team REO), M. Vidrascu (project-team MACS) and A. Gloria have introduced an alternative method to solve numerically fluid-structure interaction problems using domain decomposition algorithms and the three-dimensional shell elements developed by the project-team MACS. A preliminary version is available in [41]. More extensive numerical tests are in progress.

5.9. Complex fluids

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

The subject of this activity covers two different applications and settings. The first one is the modeling of polymeric fluid flows, the second is that of suspensions.

In the first context, A. Ern and T. Lelièvre have proposed a coupled micro-macro and macro-macro numerical scheme to efficiently discretize micro-macro models for polymeric flows [17]. The idea is to use the fine but expensive (micro-macro) model only where it is really needed, in order to reduce the computational cost. This is based on a posteriori error estimates. D. Hu and T. Lelièvre have shown in [21] how new "entropy-like" estimates can be derived for macro-macro models for viscoelastic fluids. These estimates can be used as a guideline to enhance the stability of numerical schemes, building discretization schemes that satisfy these new estimates. C. Le Bris and T. Lelièvre have written a long and didactic review of micro-macro models for complex fluids, and polymeric fluids in particular [25]. The paper is a rather elementary and pedagogical introduction to such models. A dedicated, final section addresses the mathematical challenges on the front of research.

In collaboration with Philippe Coussot (LCPC), Francois Lequeux (ESPCI), Isabelle Catto (University Paris Dauphine), another topic has started that focuses on highly non newtonian fluids. E. Cancès, S. Boyaval and C. Le Bris are going to perform numerical simulations of new constitutive equations for viscoelastic fluids subject to thixotropic effects.

This has motivated S. Boyaval, T. Lelièvre and C. Mangoubi to work on well-known numerical stability issues related to the simulation of macroscopic consitutive equations for viscoelastic fluids. The study shows how some discretizations of the Oldroyd-B model allow for the correct free energy dissipation.

Computations are being performed that take into account the results of the previous study.

Besides, a new topic is starting in collaboration with Y. Maday (UPMC-Brown) and A.T.Patera (MIT). C. Le Bris and S. Boyaval are developing new computational methods to solve high-dimensional Fokker-Planck equations parameterized by transient macroscopic quantities. The approach follows the Reduced Basis paradigm. Several variants are under study. Some of them deal with the Fokker-Planck equation itself. Some others consist in approaching the stochastic differential equation associated with the Fokker-Planck equation.

The above very applied topics, related to the modelling of complex fluids, have motivated a series of theoretical works by C. Le Bris and P-L. Lions on the well-posedness of the mathematical equations manipulated in the modelling. Indeed, as the flow velocities in such non newtonian flows have no particular reason to be regular, the fact that such velocities impact as parameters on the kinetic description of the microstructures motivate a number of theoretical questions. The well-posedness of Fokker-Planck type equations, and the related stochastic differential equations, is a topic of great mathematical relevance and interest. Indeed, such equations with potentially irregular coefficients and parameters arise in a number of fields. C. Le Bris and P-L. Lions are pursuing a series of studies on Fokker-Planck type equations, and stochastic differential equations with Sobolev regular coefficients, see [26]. Interestingly, the context of complex fluids, and the lack of

regularity of the coefficients in the equations in that context, have also triggered a new series of works on the renormalized solutions of ordinary differential equations. The Note [20] and the work [19] are instances of this new theoretical endeavour.

5.10. Shock Waves

Participant: Gabriel Stoltz.

Shock and detonation waves are truly multiscale phenomena, involving very small time and length scales at the shock front. It is therefore very interesting to propose coarser models to simulate them. After investigating various aspects of the multiscale simulation of shock waves, G. Stoltz turned to the case of detonation. He extended a previous model based on dissipative particle dynamics and describing shock waves at the microscopic level to the case of shock waves triggering chemical reactions as they move along [33].

6. Contracts and Grants with Industry

6.1. Contracts and Grants with Industry

Many research activities of the team are indeed conducted in close collaboration with private or public companies: Alcan (formerly Pechiney) 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 partner of our team.

7. Other Grants and Activities

7.1. Regional activities

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

7.2. National activities

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

The team is now involved in six ANR projects. The first one (ANR "non thématique" INGEMOL, leaded by Ph. Chartier, IRISA) focuses on geometric numerical methods for Hamilton 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 modelling 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. G. Turinici is also responsible at the Paris Dauphine team of the C-QUID GIP-ANR project. The fourth one the team is involved in is the ANR Parmat, managed by Guy Bencteux (EDF and MICMAC). The fifth one (ANR "Calcul intensif et grilles de calcul" SIRE, led by Ph. Sautet, ENS Lyon) concerns the simulation of chemical reactivity at the interfaces. The sixth one is the ANR METHODE (Hydrological modelling), S. Cordier (Université d'Orléans).

7.3. European Community financed activities

Some members of the team participate into the european project (Marie Curie Research Training Networks) "MULTIMAT" devoted to the multiscale modelling of materials, scientist in charge Nick Schryvers.

T. Lelièvre, G. Stoltz and F. Legoll participate in the HIM program on Computational Mathematics Hausdorff Center for Mathematics, Bonn.

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 team has applied for a renewed PICS CNRS-NSF collaboration between Princeton University and the Laboratoire CEREMADE (Paris Dauphine).

8. Dissemination

8.1. Animation of the scientific community

G. Bencteux and C. Le Bris have co-organized (with G. Zérah (CEA)) the summer school : "Multiscale methods in materials", Saint-Lambert des Bois, June 25-July 6, 2007.

E. Cancès is a member of the editorial board of Mathematical Modelling and Numerical Analysis (2006-).

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

E. Cancès has organized, or co-organized, the following events in 2007:

- Minisymposium on “Applications to Chemistry” at the Scicade conference, July 9-13, 2007, Saint-Malo

- (with N. Marzari, Y. Saad and G. Scuseria), IMA Summer program on quantum molecular simulations, July 30-August 3, 2007, Minneapolis

F. Legoll has co-organized with Eric Darve the mini-symposium “Molecular Dynamics” at SciCade 07 conference (9-13 July 2007, St Malo, France).

F. Legoll has organized a workshop at the Ecole Nationale des Ponts et Chaussées on “Models and numerical methods for granular materials” (19-21 november 2007).

C. Le Bris is a member of the board of directors of the SMAI (french SIAM).

C. Le Bris is co-Editor-in-chief (with A. T. Patera, MIT) (2005-) of Mathematical Modelling and Numerical Analysis. He is a member of the editorial boards of Applied Mathematics Research Express (2003-), 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-).

C. Le Bris has acted as referee, or evaluation committee member, for the following institutions and funding agencies: Banff International Research Station (Canada), DFG Excellence Initiative programme *Scientific Computing* (Germany), Lisbon University (Portugal).

C. Le Bris is a member of the organizing committee (with Weinan E, Chun Liu, An-Chang Shi, Qi Wang, Pingwen Zhang) of the thematic year *Multiscale modelling of complex fluids* , Beijing University,China 2007-2008.

G. Stoltz and A. Gloria have co-organized the seminar "Scientific computing" at CERMICS (2006- September 2007). From September 2007 on, A. Deleurence is one of the two co-organizers.

G. Turinici co-organized with M. Lewin the "Computational issues in relativistic quantum chemistry" workshop at the ICIAM 2007 congress (Zurich).

8.2. Teaching activities

- Analyse et algèbre linéaire, ESIEE (G. Bencteux).
- Simulation moléculaire: aspects théoriques et numériques, cours de M2, université Paris 6 (X. Blanc, E. Cancès).
- Analyse, cours à l'Ecole Nationale des Ponts et Chaussées, (E. Cancès, F. Legoll).
- Calcul scientifique, cours à l'Ecole Nationale des Ponts et Chaussées, (A. Gloria, G. Stoltz).
- Analyse en fréquences, cours à l'Ecole Nationale des Ponts et Chaussées, (E. Cancès).
- Introduction à la physique statistique et à la physique quantique, cours à l'Ecole Nationale des Ponts et Chaussées, (G. Stoltz).
- Analyse numérique et Optimisation, TD à l'ESIEE (L3) (A. Deleurence),
- Remise à niveau en analyse et calcul scientifique pour les maîtres ès sciences, cours ENPC (M1) (A. Deleurence),
- Mathématiques, TD à l'Université de Paris I (L1) (A. Deleurence),
- Initiation à Scilab, TP à l'ENPC (A. Deleurence).
- 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).
- Analyse numérique et optimisation, PC du cours de G. Allaire et P.-L. Lions, Ecole Polytechnique (E. Cancès, C. Le Bris).
- Modéliser, Programmer, Simuler, cours à l'Ecole Nationale des Ponts et Chaussées, (T. Lelièvre, with A. Alfonsi and J.-P. Pons).
- Probabilités et Applications, cours à l'Ecole Nationale des Ponts et Chaussées, (T. Lelièvre).
- Méthodes déterministes en mathématiques financières, cours à l'Ecole Nationale des Ponts et Chaussées, (T. Lelièvre, with O. Bokanowski).
- Méthodes probabilistes, M2 Mathématiques et Applications, Université Pierre et Marie Curie (T. Lelièvre).
- Statistique et analyse de données, cours à l'Ecole Nationale des Ponts et Chaussées, (M. Rousset).
- Algèbre linéaire 3 / L2 cours à l'Université de Paris IX Dauphine (G. Turinici).
- Aspects quantitatives et numériques des stratégies financières / M2 cours à l'Université de Paris IX Dauphine (G. Turinici).
- Calcul et analyse numérique: évolution / M1 cours à l'Université de Paris IX Dauphine (G. Turinici).
- Analyse numérique des EDP / M2 cours à l'Université de Paris IX Dauphine (G. Turinici).
- Finances numériques / M2 cours à l'Université de Paris IX Dauphine (G. Turinici).

8.3. Conference participation

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

G. Bencteux, 3ème congrès national de mathématiques appliquées et industrielles (SMAI 2007, Praz sur Arly) June 2007

G. Bencteux, Parallel Computing 2007, Jülich, September 2007

X. Blanc, XX congreso de ecuaciones diferenciales y aplicaciones, X congreso de matematica aplicada Universidad de Sevilla, 24-28 septembre 2007.

S. Boyaval, SMAI 2007 (annual meeting of the french Society of Applied and Industrial Mathematics), Praz-sur-Arly (June 07)

S. Boyaval, Workshop on Mathematical Issues in Complex Fluids organized by Beijing University;

S. Boyaval, SIAM Conference on Analysis of Partial Differential Equations (PD07), Phoenix Arizona (December 2007)

E. Cancès, CEA, January 2007

E. Cancès, MIT-France workshop on cement science, Cambridge (US), January 2007

E. Cancès, Cergy, January 2007

E. Cancès, Colloquium INRIA, April 2007

E. Cancès, Berkeley, May 2007

E. Cancès, IMA, July 2007

E. Cancès, Demon developers, Paris, August 2007

E. Cancès, CECAM workshop, Lyon, September 2007

E. Cancès, Tromso, September 2007

E. Cancès, Rouen, December 2007

I. Dabo, American Physical Society Meeting, Denver, March 2007

I. Dabo, Institute for Mathematics and its Applications Summer Program, Minneapolis, July 2007

I. Dabo, Annual Fuel-cell Program Review, Boston, August 2007

I. Dabo, American Chemical Society Meeting, Boston, August 2007

A. Deleurence, IMA Summer Program Classical and Quantum Approaches in Molecular Modeling, Minneapolis, July 23rd - August 3rd, 2007

F. Legoll, Second Atomistic to Continuum Coupling Methods workshop, Austin, April 2007

F. Legoll, Daily seminar of the Highly Oscillating Problems program, Newton Institute, Cambridge (UK), April 2007

F. Legoll, Applying Geometric Integrators workshop, Edinburgh, April 2007

F. Legoll, Internal seminar of LAMI laboratory, Montpellier, May 2007

F. Legoll, 8ième Colloque National en Calcul des Structures, Giens, May 2007

F. Legoll, Multiple time scale problems and foundation of Molecular Dynamics workshop, Princeton, May 2007

F. Legoll, SciCade 07 conference, Saint-Malo, July 2007.

F. Legoll, IMA summer program on Classical and Quantum approaches in Molecular Modeling, Minneapolis, July 23-August 3, 2007

A. Gloria, ICIAM 07 (International Conference in Industrial and Applied Mathematics), Zurich, July 2007

A. Gloria, CMDS 11 (11th International Symposium on Continuum Models and Discrete Systems), Paris, July 2007.

A. Gloria, Workshop on Calculus of Variations and Geometric Measure Theory, Levico, Italy, February 2007.

A. Gloria, University of Bonn, October 2007.

C. Le Bris, MIT-France workshop on cement science, Cambridge (US), 2007.

C. Le Bris, Workshop "Numerical Analysis of Multiscale Computations", Banff International Research Station for Mathematical Innovation and Discovery (BIRS), Jan. 28 - Feb. 2, 2007.

C. Le Bris, Workshop 'Multiscale and Variational problems in Material Science and Quantum Theory of Solids', Oberwolfach, Feb. 11 - Feb. 17, 2007.

C. Le Bris, Workshop 'Multiscale Modeling and Simulation of Complex Fluids', University of Maryland, College Park, April 16-20, 2007.

C. Le Bris, Workshop 'Multiscale Problems', Princeton University May 25-26, 2007.

C. Le Bris, Workshop-Summer school 'Multiscale Modeling', Stockholm, Sweden, June 4-8, 2007.

C. Le Bris, Effective Computational Methods for Highly Oscillatory Problems: The Interplay Between Mathematical Theory and Applications, Cambridge, UK, 2-6 July, 2007.

C. Le Bris, Computational chemistry workshop, Warwick, UK, 16-20 July 2007.

C. Le Bris, IMA Summer Program, July 2007.

C. Le Bris, Workshop Mathematical Issues in Complex Fluids, Beijing University, October 15-19, 2007.

C. Le Bris, Workshop "Multiscale Analysis for quantum systems and applications", Istituto Nazionale di Alta Matematica, Universita di Roma, October 24-26, 2007.

C. Le Bris, Workshop 'DFT and related problems', Princeton University, October 27-28, 2007. [Could not give talk due to air transport strike in France]

C. Le Bris, Workshop 'Nonlinear and Adaptive Approximation in High Dimensions' , Bad Honnef, Germany, December 10-15, 2007.

C. Le Bris, Weekly Seminar, Université de Nice, 2007.

C. Le Bris, Journées EDP-Probas, 2007.

C. Le Bris, Weekly Seminar Penn State University, 2007.

T. Lelièvre, Workshop Polymer models and related topics, Nice, February 2007. SMAI 2007, June 2007.

T. Lelièvre, Workshop New directions in Monte Carlo methods, Fleurance, June 2007

T. Lelièvre, SciCADE 2007, Saint-Malo, July 2007.

T. Lelièvre, ICIAM07, Zurich, July 2007.

T. Lelièvre, IMA summer program on Classical and Quantum Approaches in Molecular Modeling, Minneapolis, July 2007.

T. Lelièvre, Workshop Complex fluids, Beijing, October 2007.

T. Lelièvre, Workshop Particle systems, nonlinear diffusions, and equilibration, Bonn November 2007.

T. Lelièvre, Seminar at LMSGC (ENPC), Paris, January 2007.

T. Lelièvre, Seminar Analyse Numerique et EDP of Université Paris-Sud, May 2007.

T. Lelièvre, Seminar ber Partielle Differentialgleichungen und Numerik, Universitat Zurich, June 2007.

M. Rousset, Seminar, Institut Henri Cartan, Université Poincaré, Nancy.

M. Rousset, Seminar, Institut Galilée, Université Paris XIII.

M. Rousset, Seminar, Laboratoire Painlevé, USTL Lille 1.

G. Stoltz, University of Warwick, February 2007

G. Stoltz, IMA Summer Program Classical and quantum approaches in molecular modeling, Minneapolis, July 2007.

G. Turinici ICIAM 2007, Zurich

G. Turinici Applied Mathematics group seminar, Toulouse juin 2007

G. Turinici : invited speaker "Mathematical Sciences Foundation", Paris sept 2007

Members of the team (G. Bencteux, A. Deleurence, A. Gloria, F. Legoll, G. Stoltz) have given courses and animated hands-on sessions at the CEA EDF INRIA school on “Multiscale Methods in Materials” (Saint-Lambert, June 2007).

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

G. Bencteux, "Classical and Quantum Approaches in Molecular Modeling", IMA Summer Program, Minneapolis, July 23 - August 3, 2007.

G. Bencteux, "Use of the O(N) ab initio code CONQUEST", Tutorial CECAM, September 2007.

S. Boyaval, Centre de Physique des Houches, Flow in glassy systems, European Rheology School, 5-9 February 2007

S. Boyaval, IMA 2007 Summer Program, Classical and Quantum Approaches in Molecular Modeling, July 23-August 3, 2007

E. Cancès, Maximally Localized Wannier Functions: Concepts, Applications, and Beyond, CECAM workshop, June 2007

M. Rousset, Scicade, St Malo, July 9-13, 2007

G. Stoltz, Scicade, St Malo, July 9-13, 2007

G. Stoltz, "Statistical physics out of equilibrium", IHP Program, Paris, September-December 2007

G. Stoltz, MRS fall meeting, Boston, November 2007

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