INRIA

Project-Team Micmac

Methods and Engineering of Multiscale Computing from Atom to Continuum

Rocquencourt

THEME NUM

Activity Report

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1. Team

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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. Electronic structure calculations

Participants: Maxime Barrault, Guy Bencteux, Eric Cancès, Amélie Deleurence, Hervé Galicher, Claude Le Bris, Tony Lelièvre, Mathieu Lewin, François Lodier, Mohamed El Makrini, Gabriel Stoltz, Gabriel Turinici.

We have continued our studies of the existing algorithms used for electronic structure calculations, and our enterprise consisting in designing new, efficient and rigorously founded, algorithms. In designing new algorithmic techniques, three major tracks are followed .

The first track concerns domain decomposition techniques for the linear subproblem. This work by Eric Cancès and Claude Le Bris is a joint work with William Hager, University of Florida, and it is the major contribution of the PhD thesis of Maxime Barrault, defended in December 2005. The algorithm designed already outperforms most of the existing approaches, and is in any event an efficient preconditionner for the latter. The work has been submitted for publication [7]. Guy Bencteux (Engineer at Electricité de France, currently pursuing graduate studies under the supervision of Claude Le Bris) will take over for Maxime Barrault as the principal contributor. Maxime Barrault, Claude Le Bris, Eric Cancès and William Hager are currently examining various possible improvements of the method, with a view to making the algorithm the most successful one to date.

The second major track consists in adapting reduced basis approaches to the specific context of computational chemistry. This work, in collaboration with Antony Patera and his graduate student George Pau at MIT, has been continued in 2005. Promising results were obtained on test cases, notably by Ngoc Cuyong Nguyen (University of Singapore) and Maxime Barrault [5]. The setting chosen is issued from the materials science context. It is the calculation of elastic constants of crystalline materials using ab initio calculations. Real cases should be addressed soon. Methodologically, the developed technique is of generic interest. It concerns the extension of the reduced basis paradigm to nonlinear vector-valued variational problems.

The third major track is that of the Diffusion Monte Carlo (DMC) method. It is the principal work of Anthony Scemama, currently post-doctoral fellow in our group. New numerical strategies are being tested, in collaboration with Michel Caffarel (CNRS Toulouse), and also following ideas by Mathias Rousset and Gabriel Stoltz, which come from a different context (see below the question of sampling the canonical distribution).

Apart from this main stream, we have completed the development of techniques [23] for locating electrons in molecules and thereby bridging the classical chemical description in terms of covalent, ionic, ...bonds and the quantum description of the electronic structure in terms of wavefunctions. This is a joint effort with Andreas Savin, from the theoretical chemistry laboratory at University Paris 6. Eric Cancès, Hervé Galicher and Mathieu Lewin (postdoctoral fellow in the group until October, and now researcher at CNRS, University of Cergy) have also proposed a new strategy [18] to compute the first electronic excited state in the framework of multiconfiguration methods.

All these new developments and methods are meant to be inserted in the long term inside the software platform ASPIC that we are currently developing (in collaboration with Yves Achdou, University Paris 7).

The current status of this software allows us to perform electronic structure calculations on simple systems, within a C++ environment, and relying on rigorous numerical analysis tools.

In parallel with the above numerical works, we have pursued in our enterprise to put the models and the techniques on a sound mathematical grounding. Instances of such a program are:

- the study [39] by Gabriel Stoltz of a possible multiscale modelling of detonation waves in materials,
- the study [19] by Eric Cancès, Benjamin Jourdain and Tony Lelièvre of the foundation of the diffusion Monte Carlo method,
- the study [8] by Eric Cancès and Xavier Blanc of the well-posedness of some orbital-free models used in materials science simulations,
- the development, by Eric Cancès, Amélie Deleurence and Mathieu Lewin, of new theoretical models for defaults (stacks) in crystalline materials.

We have also devoted a huge effort to a pedagogic endeavour that we consider crucial. The twofold purpose is to both attract to the field of computational chemistry more mathematicians, and introduce the chemists to a growing and important mathematical literature devoted to the models and techniques they use.

Two state of the art review articles [29], [32] have been published in order to provide the community with a reliable account of all recent developments in the field both from a mathematical and a numerical viewpoint.

In addition, lecture notes [1] from a course on the mathematical and numerical analysis of the models from computational chemistry, at the DEA (M2) level, have been published.

Another book [2], which is supposed to give a comprehensive account of the past decades of mathematical effort devoted to molecular modelling, is in preparation. The authors are Claude Le Bris, Eric Cancès, Gabriel Turinici and Yvon Maday (University Paris 6).

5.2. Molecular dynamics and related problems

Participants: Eric Cancès, Amélie Deleurence, Claude Le Bris, Tony Lelièvre, Frédéric Legoll, Gabriel Stoltz, Gabriel Turinici.

Molecular dynamics is often used 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. Based on a theoretical result concerning the convergence of the numerical averages toward the exact result, we were able to propose a new method to accelerate this convergence. Two contributions, one presenting the theoretical aspects and the other dealing with an application, have been published, in [15] and [14], respectively. Some extensions of the existing results should be studied in the near future.

This scientific program, which is a collaboration with François Castella, Philippe Chartier and Erwan Faou from INRIA Rennes, has been initiated in the context of ARC PRESTISSIMO 2003-2004 and is being continued with a different funding (ACI "Nouvelles interfaces des mathématiques").

While the interest on numerical simulations over extremely long times remains the core of the collaboration, some other topics related to molecular dynamics are also explored.

One instance is the difficult problem of the efficient numerical integration of highly oscillatory differential equations (which is the case in molecular dynamics simulations because many, disproportionate, time scales are present in the system). A study by Claude Le Bris and Frédéric Legoll has been initiated, also with the collaboration of Petr Plechac (Warwick University).

Another instance is the study [34] by Frédéric Legoll, in collaboration with Mitchell Luskin and Richard Moeckel (University of Minnesota), of the Nosé-Hoover thermostatted dynamics for sampling the canonical ensemble. The concern there is to assess the ergodicity of the thermostatted system in the canonical ensemble. Such a study is a first step towards the comprehension of the full problem, which would have drastic consequences on the actual practice, as thermostatted dynamics remains a method of choice for sampling the canonical ensemble, despite the definite success of stochastic techniques, which we also considered.

Two other topics must indeed be mentioned, both related with stochastic techniques, while all the above lies on the deterministic side.

First, a systematic comparison of some sampling techniques has been performed in [20]. The comparison comprises both deterministic algorithms, such as thermostatted molecular dynamics simulations, and stochastic algorithms, such as discretizations of the Langevin dynamics. The techniques are compared in terms of accuracy, efficiency, computational cost. The results obtained could contribute to change the landscape of sampling techniques in the years to come.

Second, a work [31] has been devoted to the mathematical analysis and the design of a numerical algorithm for efficiently performing the calculation of free energies. This is an issue of paramount practical importance, which Claude Le Bris and Tony Lelièvre treat in collaboration with Eric Vanden-Eijnden (Courant Institute). Another related work [30] on the various discretization schemes used for simulating constrained stochastic differential equations should follow.

In addition to this, Gabriel Stoltz has developed in [37], in collaboration with Mathias Rousset (University of Nice), an improvement of the now standard technique by Jarzynski used for computing canonical distributions and free energy differences. The idea has also been extended in collaboration with Tony Lelièvre for the computation of free energy differences using constrained dynamics.

5.3. Laser control

Participants: Claude Le Bris, Perola Milman, Mazyar Mirrahimi, Gabriel Turinici.

Our interest focuses on the very practical issues of the laboratory implementations of closed loop optimal control. This is done in collaboration with the group of H. Rabitz (Princeton University) and made possible by a PICS CNRS-NSF grant. Of particular interest is for instance the description of the most important parameters to be used in the optimization of the laser field. This is in particular important to shed some light on the intimate physical mechanism underlying the control process. A numerical strategy for identifying these parameters has been tested. A publication of the promising results obtained should come shortly.

We have addressed in [33] in collaboration with Mazyar Mirrahimi and Herschel Rabitz (and also in close connection with Pierre Rouchon) 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 [33] is purely theoretical. Some extension regarding the introduction of noise should be addressed shortly. Computations, more extensive than the simple ones used to demonstrate feasability so far, should also be performed.

Lyapounov methods for the numerical resolution of the evolution equations have also been introduced in joint works with Mazyar Mirrahimi and Pierre Rouchon [35], [36].

All this is the material of the PhD thesis defended by Mazyar Mirrahimi.

Following previous works on the so called "monotonic algorithms" we continued this year both on the improvement of the previous results [47] and on their application to novel situations, partially in collaboration with Claude Dion from the Physics Department of the Umea University [38], [43].

An important step ahead was the illustration of a special relationship between the monotonic algorithms and the Lyapounov schemes. Two initial publications [46], [50] will be followed shortly by a journal paper currently under review.

A different approach to implement the "parareal" scheme for accelerating the simulation of quantum control was studied with Y. Maday and J. Salomon and the results are available in J. Salomon's thesis defended Fall 2005.

Finally, studies on the controllability were pursued to settle the higher order perturbation theory [45] or for different models [42].

5.4. Multiscale simulation of solids

Participants: Antoine Gloria, Claude Le Bris, Frédéric Legoll, Carsten Patz.

As was the case for many years now, our research program in the multiscale simulation of solids divides into a theoretical part and a more numerical one.

On the theoretical side, in collaboration with Xavier Blanc (Laboratoire Jacques-Louis Lions, Paris) and Pierre-Louis Lions (Collège de France), Claude Le Bris has continued to address the question of how to define ground state energies for some microscopic systems composed of an infinite number of particles. The framework is that of quantum chemistry, where the state of matter is modelled through variational problems that couple a classical description of the nuclei with a quantum description of the electrons. Starting from a model for the molecule (finite number N of nuclei-say of unit charge- and an equal finite number N of electrons), one passes to the limit when N goes to infinity. When the nuclei are enforced to sit on the sites of a periodic lattice, asymptotically filling the entire lattice $\mathbf{Z}^3$, then the problem is solved by the so-called bulk limit problem for periodic crystals (series of work by I. Catto, C. Le Bris and P.-L. Lions in the 1990s).

With a view to treating geometries of sets of particles much more general than periodic geometries, the current focus is on the case when nuclei are located at random positions. An appropriate notion of stochastic lattices is defined, along with an adequate notion of ground state energy, the latter of course depending on the model chosen for the modelling of interactions. One publication [12] describes the main results obtained so far. Further extensions are currently considered, and will also be the material for new publications.

In addition, the same authors have continued their program consisting in passing from the microscale to the macroscale on the basis of quantum models at the microscale, and adapted this program to the stochastic setting, in [41]. Again, extensions are envisioned.

Another 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, Antoine Gloria and Carsten Patz. Definite conclusions about the success of the approach are yet to be obtained.

On the numerical front, Claude Le Bris and Frédéric Legoll, in collaboration with Xavier Blanc, have published the mathematical and numerical analysis of a prototypical model for simulations in materials science. The model under study couples an atomistic description of the sample with a macroscopic continuum description. The case of a convex interaction potential is described in [9], while the physically relevant case of a nonconvex potential is the purpose of the study [10].

Again for pedagogic purposes, the state of the art on the mathematical results known to date on computational models coupling the atomistic scale with the continuum scale has been reviewed in [11].

The above studies are very much related to the usual paradigm of homogenization, although the discrete setting manipulated in our studies is somewhat unusual, and different from the purely continuous setting of standard homogenization theory. A work in preparation should shed some light on this.

The PhD work of Antoine Gloria precisely deals with the standard homogenization theory. Starting from the modelling of foams, he has focused on some theoretical questions related to the homogenization of elliptic operators. A first significant contribution has appeared in [24], while a second one [49] should be soon ready.

5.5. Multiscale simulation of complex fluids

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

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 both contexts, our focus in 2005 has been the understanding of the long-time behaviour of the flows. This is in particular in order to understand questions related to return to equilibrium, and dissipation of energy in such problems. For polymeric fluids, the study has been conducted by Claude Le Bris and Tony Lelièvre, in collaboration with Benjamin Jourdain (CERMICS) and Félix Otto (University of Bonn). The work is published in [27]. On the other hand, for suspensions, as a follow up to the study [17] of well posedness of the problem, the long time limit has been investigated by Claude Le Bris and Eric Cancès in [21].

It should also be noticed that Claude Le Bris gave in the summer 2005 a series of lectures on the modelling of complex fluids at the Peking University in Beijing, China. This could be the first step in a long term collaboration with this institution.

Various extensions of the works performed so far are on the agenda, both on the theoretical side, and on the numerical side. One could cite the construction of stable algorithms for the simulation of complex fluids, based upon the introduction of an appropriate entropy. One could also cite the development of reduced basis methods for the numerical simulation of complex fluids, and more generally for discretization schemes concurrently coupling two differents scales. The latter work will be conducted with the help of our collaborators at MIT and at University Paris 6.

5.6. Magnetohydrodynamics flows

Participants: Claude Le Bris, Tony Lelièvre, Antonin Orriols.

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

A comprehensive series of tests have been performed to validate the approach on test cases closer to the actual industrial situation. The purpose of these test cases was twofold. First, we identified pertinent cost functions and commands for a control problem aiming at optimizing the motion and position of a moving interface between two liquids. Second, we were able to compare some well known results in the literature obtained by linear stability analysis performed on simplified systems and those obtained by a fully nonlinear approach. On this particular point, a significant practical result has been presented in [44]. We intend to follow more deeply these two roads in the future.

In addition to this, Jean-Frédéric Gerbeau, Claude Le Bris and Tony Lelièvre have completed the writing of a book [3] presenting a complete account of the past decade of efforts, and comparing the approach and the simulation strategy with those of competitors. A short summary [28] of the problems and techniques for MHD has also been written by Claude Le Bris.

5.7. Mathematical models for models issued from biology

Participants: Eric Cancès, Frédéric Legoll, Gabriel Turinici.

The acceleration of simulations of the stochastic evolutions equations that appear in cell and molecular biology was the topic of a collaboration with A. Alfonsi (CERMICS / ENPC), W. Huisinga (Frei U. Berlin) and B. Di Ventura (EMBL). A sound mathematical foundation for the simulations in hybrid joint stochastic-deterministic frameworks has been introduced and tested on a system of biological interest [6].

On the other hand, continuing previous works in epidemiology, a review paper [40] on the SARS epidemic was delivered and is scheduled for publication in 2006.

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, 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 and Ecole Nationale des Ponts et Chaussées.

7.2. National activities

The team was part of the research action GDR Density Functional Theory (2002-2005) whose scientific leader used to be H. Dreysse, devoted to the development of DFT methods for the simulation of materials and complex systems. It was also a part of the research action GDR Interaction de particules (2002-2005), whose scientific leader used to be Th. Goudon, on questions related to the modeling of many particles systems.

Claude Le Bris is the scientific leader of a program initiative ACI "Nouvelles interfaces des mathématiques" devoted to various questions related to computational chemistry, molecular simulations and multiscale problems.

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 three 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.

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.

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 and that of André Bandrauk at University of Sherbrooke (Canada), respectively on questions related to laser control and to the solution of the Schrödinger equation for a large number of degrees of freedom. The collaboration with Herschel Rabitz is part of a PICS CNRS-NSF collaboration between Princeton University and the Laboratoire J.-L. Lions (Paris 6).

8. Dissemination

8.1. Animation of the scientific community

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

Claude Le Bris has been nominated co-Editor in chief of Mathematical Modelling and Numerical Analysis (together with A.T. Patera, MIT). He is also associate editor in 5 international journals.

Claude Le Bris has co-organized (with André Bandrauk (Sherbrooke University) and Michel Delfour (Université de Montréal)) an international conference on High-dimensional partial differential equations, at CRM Montréal, August 2005.

Eric Cancès is a member of the new editorial board on Mathematical Modelling and Numerical Analysis and co-Editor in chief (with P. Del Moral and J.-F. Gerbeau) of ESAIM Proc.

Frédéric Legoll has co-organized, with Benedict Leimkuhler (University of Leicester), a Focus group on Molecular dynamics and Sampling at IMA, Minneapolis, Spring 2005.

Gabriel Turinici co-organized until August 2005 a modelisation and scientific computing seminar at INRIA Rocquencourt.

8.2. Teaching activities

- Simulation moléculaire: aspects théoriques et numériques, cours de DEA, université Paris 6 (E. Cancès and G. Turinici).

- Systèmes multiéchelles, cours de DEA, université Paris 6 (C. Le Bris).

- Systèmes multiéchelles, cours de la majeure SEISM, Ecole Polytechnique (C. Le Bris).

- Analyse numérique et optimisation, PC du cours de G. Allaire et P.-L. Lions, Ecole Polytechnique (E. Cancès).

- Calcul scientifique et Analyse, cours à l'Ecole Nationale des Ponts et Chaussées, (E. Cancès).

- Analyse en fréquences, cours à l'Ecole Nationale des Ponts et Chaussées, (E. Cancès).

- Modéliser, Programmer, Simuler, cours à l'Ecole Nationale des Ponts et Chaussées, (C. Le Bris).

- 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).

- Analyse, cours à l'Ecole Nationale des Ponts et Chaussées, (F. Legoll).

- Analyse numérique ESIEE (G. Stoltz)

- Calcul scientifique cours à l'Ecole Nationale des Ponts et Chaussées, (G. Turinici).

- Algebre linéaire 3, cours à Paris-Dauphine (G. Turinici)

- Analyse numérique des EDP, cours à Paris-Dauphine (G. Turinici)

8.3. Conference participation

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

- School in Bangalore, India, February 2005 (Eric Cancès, Claude Le Bris)

- The Montreal scientific computing days, February 2005 (Tony Lelièvre)

- Séminaire de Mathématiques Appliquées du Collège de France, March 2005 (Eric Cancès)

- Multimat network conference on Multiscale numerical methods for advanced materials, Paris, March 2005 (Frédéric Legoll)

- Workshop on Atomic Motion to macroscopic models, IMA, Minneapolis, April 2005 (Claude Le Bris, Frédéric Legoll)

- SIAM Dynamical System 2005 conference, Snowbird, May 2005 (Tony Lelièvre)

- Workshop on moving interfaces, CEA, May 2005 (Tony Lelièvre)

- IMA Workshop: Effective Theories for Materials and Macromolecules, Minneapolis, June 2005 (Claude Le Bris, Antoine Gloria).

- Foundations of computational mathematics international conference, Santander (Spain), July 2005 (Claude Le Bris, two talks; Frédéric Legoll).

- Vortices in Bose-Einstein condensates, Les Treilles (France), July 2005 (Eric Cancès).

- ICMS 'Dynamical Problems in Mathematical Materials Science' conference, keynote speaker, Edinburgh (UK), July 2005 (Claude Le Bris)

- International conference on High-dimensional partial differential equations, CRM Montréal, August 2005 (Eric Cancès)

- Workshop on Meshfree Methods for Partial Differential Equations, Bonn, September 2005 (Frédéric Legoll)

- Computational stochastic differential equations, Bedlewo, September 2005 (Tony Lelièvre)

- International Conference Broad-Minded Modeling in Continuum Physics, in honor of Gianfranco Capriz on his 80th birthday, Rome, October 2005 (Claude Le Bris, could not give talk due to airlines strike in France)

- Workshop on Multiscale Analysis and Computation, IPAM-UCLA, Los Angeles, November 2005 (Claude Le Bris)

- "Multiscale Modeling in Soft Matter and Bio-Physics" sept. 2005 IPAM-UCLA (G. Stoltz)

- "Time acceleration methods in molecular dynamics" oct. 2005 IPAM-UCLA (G. Stoltz)

- IPAM-UCLA, Lake Arrowhead retreat, December 2005 (Claude Le Bris, Frédéric Legoll, Gabriel Stoltz)

- IPAM-UCLA "Bridging timescales and lengthscales in biophysics and material sciences", sept-dec 2005 (Antoine Gloria)

- SCPDE 2005 Conference, Hong Kong, December 2005 (Tony Lelièvre)

- Conference "Optimal Control of Coupled Systems of PDE" Oberwolfach, Germany, April (G. Turinici)

- MIC 2005 Conference, Innsbruck, feb. 2005 (G. Turinici)

- Conference CDC-ECC 2005, Seville Spain, dec. 2005

- Seminar of the Mathematics department (Claude Le Bris): Universitè di Pavia, Peking University, University of California San Diego, Ecole Polytechnique Fédérale de Lausanne

- Seminar of the Mathematics department (Tony Lelièvre): Courant Institute (New York), Penn State University, Massachusetts University, Freie Universität (Berlin), ENS Rennes
- Seminar of the Mathematics department (Eric Cancès): IMA (Minneapolis), IPAM-UCLA (Los Angeles), Tuebingen University
- Seminar of the Mathematics department (Frédéric Legoll): IMA (Minneapolis), University of Minnesota (Minneapolis).
- Seminar of the Chemistry department (Eric Cancès): IRSAMC (Toulouse), Pisa University
- Interdisciplinary seminar of Sandia National Labs, Albuquerque, USA (Eric Cancès, Claude Le Bris, Frédéric Legoll)
- Seminar CEA/DAM/DPTA/PMC 11/06/ 2005 (G. Stoltz)
- Seminar IPAM-UCLA du 23/09/2005 (G. Stoltz)
- Seminar "Materials and Simulation Process Center" (Caltech, 29/11/2005) (G. Stoltz)
- Seminar of the Mathematics department (Gabriel Turinici): IMA (Minneapolis), University of Minnesota (Minneapolis).
- Seminar IMATI-CNR Pavia, may 2005 (G. Turinici)
- Séminaire de Mathématiques Appliquées du Collège de France, Nov. 2005 (G. Turinici)
- Seminar SUPELEC, april 2005 (G. Turinici)

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