INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Project-Team Micmac

Methods and Engineering of Multiscale Computing from Atom to Continuum

Rocquencourt

THEME NUM

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1. Team

Scientific leader
Claude Le Bris [Civil engineer in chief, ENPC, HdR]

Staff members (Ministère de l'Education Nationale)
Gabriel Turinici [Professor at University Paris IX Dauphine, HdR]

Administrative assistant
Laurence Bourcier [TR]

Staff members (Ministère de l'Equipement)
Eric Cancès [Civil engineer, ENPC, HdR]
Frédéric Legoll [Civil engineer, ENPC]
Tony Lelièvre [Civil engineer, ENPC]

Post-doctoral fellows
Mathias Rousset [Scholarship ENPC, from September 2006]
Anthony Scemama [Scholarship ACI simulation moléculaire, until August 2006]
Perola Milman [Scholarship ACI simulation moléculaire until April 2006]

PhD students
Guy Bencteux [Engineer at EDF]
Sebastien Boyaval [Civil engineer, ENPC]
Amélie Deleurence [Scholarship Ile de France, from October 2005]
Mohamed El Makrini [Scholarship Univ. Paris IX Dauphine]
Hervé Galicher [Schorlarship Ecole Doctorale Paris Centre]
Antoine Gloria [Civil engineer, ENPC]
Antonin Orriols [Financed by ENPC, until December 2006]
Carsten Patz [Visiting graduate student from the University of Stuttgart, until June 2006]
Gabriel Stoltz [Civil engineer, ENPC]

Collaborating scientists
Mathieu Lewin [CR, Cergy University]
Yvon Maday [Professor, University Paris VI, HdR]

Internship students
Andreea Grigoriu [student, Paris IX Dauphine University]
Serge Rehbinder [M1 Orsay University]
Moncef Elacheche [M1 Orsay University]

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.

Our activity in computational chemistry touches various aspects of the domain, theoretical aspects as well as numerical aspects. See [41] for a recent review article by C. Le Bris.

On a theoretical level, several actions are in progress. G. Stoltz has tried and improved the understanding, from a mathematical perspective, of some models used in quantum chemistry, especially non-standard models such as methods relying on second order reduced density matrix formulations, Variational Monte Carlo techniques, Optimized Effective Potentials.

E. Cancès has begun addressing issues related to the existence 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 for performing such calculations, 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 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 propose 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 thermodynamical limit on the so-called supercell model.

Both endeavours should have numerical consequences soon.

On the numerical side, one problem addressed was that of the localization of electrons in molecular systems has also been addressed. Anthony Scemama has worked in collaboration with Michel Caffarel (CNRS, IRSAMC, Toulouse) and Andreas Savin (CNRS, Laboratoire de Chimie Théorique, Paris 6) on the localization of electrons in molecular systems. Although it would be tempting to associate the Lewis structures to the maxima of the squared modulus of the wave function, the choice is to use the domains of the three-dimensional space that maximize the probability of containing opposite-spin electron pairs. They find for simple systems (CH4, H2O, Ne, N2, C2H2) domains comparable to those obtained with the Electron Localization Function (ELF) or by localizing molecular orbitals. The different domains they obtain can overlap, and this gives an interesting physical picture of the floppiness of CH5+ and of the symmetric hydrogen bond in FHF-. The presence of multiple solutions has an analogy with resonant structures, as shown in the trans-bent structure of Si2H2. Correlated wave functions were used (MCSCF or Slater-Jastrow) in the Variational Quantum Monte Carlo framework.

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. The development of the domain decomposition algorithm for the linear subproblem have been continued. Some algorithmic improvements of the most consuming part of the algorithm have resulted in significant decreases in memory and CPU demands (up to a factor 10 for alkane molecules CPU). A first version of a multiprocessor implementation has succeeded solving the linear subproblem for a polyethylen chain of 53,000 carbon atoms (more than 370,000 basis functions) in about 1 h 30 min elapsed time with 16 processors. The performance of the parallel version confirms that a high scalability can be aimed with additional implementation effort : this will be part of a future collaboration with EDF in the frame of the project "ParMat", which obtained the financial support of National Research Agency. Two articles [5], [37] have been written on the subject.

Also, in collaboration with Y.Maday (Paris 6) and N. C. Nguyen, A. T. Patera, G. Pau (MIT), we have continued our efforts to apply the reduced-basis technology to the context of computational chemistry: see [38].

Also from a numerical perspective, a number of actions concern the application of probabilistic methods (Monte-Carlo type methods) to the context of computational chemistry.

A first action regards the Quantum Monte Carlo methods. The diffusion Monte Carlo (DMC) method is a powerful strategy to estimate the ground state energy E_0 of a Schrödinger hamiltonian. It consists in writing E_0 as the long-time limit of the mean of a functional of a drift-diffusion process, with source term. Numerically, this is simulated by means of a collection of interacting random walkers, with a birth-death mechanism. As for a number of stochastic methods, a DMC calculation makes use of an importance sampling function. In the fermionic case, it has been observed that the DMC method is biased, except when the nodes of the importance sampling function exactly coincides with some ground state of the hamiltonian. This is the fixed node approximation. A mathematical analysis of this approximation is proposed in [12]. From a numerical point of view, the method is very difficult to analyse. We focussed in [43] on the analysis of the selection mechanism. In [34], we compare the efficiency of various sampling methods for DMC.

Another work on quantum Monte Carlo methods has been done by A. Scemama, in collaboration with Roland Assaraf and Michel Caffarel. It concerns the calculation of the electronic density of a molecular system by means of Monte Carlo methods. An alternative Monte Carlo estimator for the electronic density is proposed. This estimator has a simple form and can be readily used in any type of Monte Carlo simulation. Comparisons with the standard delta-function estimator show that the statistical errors are greatly reduced. Furthermore, this new estimator allows for accurate calculations of the density at any point of the physical space, even in the regions never visited during the Monte Carlo simulation.

5.2. Molecular dynamics and related problems

Participants: Eric Cancès, Claude Le Bris, Frédéric Legoll, Tony Lelièvre, Mathias Rousset, 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 efforts in the very recent years.

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

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. 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 there 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. Preliminary results have been obtained for the integration of a class of highly oscillating Hamiltonian systems [22], and more general results should follow 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).

Another instance is the development by Frédéric Legoll, in collaboration with Ben Leimkuhler (University of Edinburgh) and Yvon Maday (University Paris 6), of an algorithm able to generate a constant energy trajectory at a given kinetic temperature. Such a method is useful for systems that are too sensitive to perturbations to be thermalized, and that need to be simulated at an energy that corresponds to a given average kinetic temperature.

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, Frédéric Legoll and Tony Lelière are currently studying several methods to coarse-grain the system, in order to develop a model more suited to long time simulation.

In collaboration with E. Vanden-Eijnden, E. Faou, F. Otto, T. Lelièvre has studied a number of topics.

Stochastic differential equations with constraints naturally appear in molecular dynamics and kinetic models. The constraints may be imposed for modelling (rigid bonds) or for computational purposes (computation at a fixed reaction coordinate). We proposed a mathematical study of various discretizations of SDEs with constraints in [16], together with a discussion on the effectiveness of such methods to compute free energy differences by thermodynamic integration. The generalization to non-equilibrium dynamics is done in [26] (Jarzynski equality). We currently work on the ergodic properties of projected dynamics, and the sampling of the NVE ensemble by such SDEs (in collaboration with E. Faou).

Stochastic dynamics to compute free energy differences are widely used in computational chemistry and biology. Many recent methods rely on non-linear Markov processes, like the adaptive techniques. A unifying presentation of adaptive methods is proposed in [44], together with an efficient implementation of adaptive dynamics using an interacting particle system with birth death processes. We are currently working on a proof of convergence of a certain class of adaptive methods (in collaboration with F. Otto).

5.3. Laser control

Participants: Claude Le Bris, Andreea Grigoriu, 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) and made possible by a PICS CNRS-NSF grant.

We have addressed in [24] 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 [24] is purely theoretical. Some extension regarding the introduction of noise are discussed with our chemists parteners at Princeton and some techniques were already tested in different works [17].

We have also pursued our works in the field of numerical algorithms used to compute optimal control fields. We established the necessary adaptations [27] of the so-called “monotonic algorithms” required to switch from a continuous time setting to a (more realistic) numerical discrete time simulation.

Another contribution came from the understanding of the inner working of those algorithms: we showed that a framework can be introduced to connect them to the Lyapounov methods [32]. We pursue this research direction with new applications for more general control (and optimization) problems.

5.4. Atomistic to continuum methods

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

The team project has continued his theoretical and numerical efforts on the geral 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.

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. With a view to treating geometries of sets of particules much more general than periodic geometries, the current focus is on the case when nuclei are located at random positions. As a follow-up to the previous studies, in particular [8], [10], an effort has been placed on developping the connection between the questions examined for this passage 'atomistic to the continuum' and some more generic questions of homogenization theory. It has been shown that the objects manipulated in the two apparently uncorrelated topics can indeed be connected. This is the purpose of an ongoing series of works: [9], and publications in preparation. A review article [7] has been written on the subject.

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 (University of Stuttgart, now in Berlin).

Also on the numerical front, Frédéric Legoll has initiated with Mouhamad Hammoud, a PhD student at LAMI, ENPC, a study of 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.

5.5. Homogeneization

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

Antoine Gloria has addressed the analysis of some numerical homogenization methods, in the context of elliptic operators and nonlinear elasticity. This approach consists in introducing a kind of averaged energy that describes the effective behaviour of heterogeneous materials. This work has given rise to two INRIA research reports (RR-5625 and RR-5791) and two articles [19], [18]. Some numerical tests have completed the analysis and have been performed within the FE library Modulef.

In the continuation of the characterization of effective behaviours of heterogeneous materials, A. Gloria has studied a problem of G-closure: the determination of the set of all the effective conductivity matrices that can be obtained by the homogenization of a discrete conducting polycrystal. This work has been done in collaboration with Andrea Braides (university of Rome) and has been submitted for publication (preprint available at CVGMT).

Besides the analysis of continuous to continuous homogenization (at the micro scale the material is already considered as continuous), A. Gloria has begun to work on the derivation of effective energies for spin interactions, starting from a discrete description of the interaction and deriving a continuous limit when the characteristic length of the system goes to zero. This work is in collaboration with Roberto Alicandro (university of Cassino, Italy) and Marco Cicalese (university of Naples, Italy).

In close collaboration with A.T. Patera (MIT) and Y. Maday (CNRS/UPMC/Brown), S. Boyaval, who is beginning his PhD studies under the supervision of C. Le Bris, has tested the feasability of a reduced-basis approaches for multiscale problems. The results now allow for a fast and rigorous numerical homogenization of heterogenous material. The context is that of the homogenization of scalar elliptic equations.

5.6. Magnetohydrodynamics

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

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.

The book [4], now published, focuses on mathematical and numerical techniques for the simulation of magnetohydrodynamic phenomena, with an emphasis laid on the magnetohydrodynamics of liquid metals, on two-fluid flows and on a prototypical industrial application. Aimed at research mathematicians, engineers, and physicists, as well as those working in industry, and starting from a good understanding of the physics at play, the approach is a highly mathematical one, based on the rigorous analysis of the equations at hand, and a solid numerical analysis to found the simulations. At each stage of the exposition, examples of numerical simulations are provided, first on academic test cases to illustrate the approach, next on benchmarks well documented in the professional literature, and finally, whenever possible, on real industrial cases.

In his PhD thesis, Antonin Orriols has worked on the control of the interface in two-fluid flows. The intended application is the control of aluminium electrolysis cells, and of the free interface which separates the aluminium and the bath of aluminium oxyde in the cell. Two models can be used : a simple linear model, or a more complex non-linear model. The predictions of these two models for the stability of the cell have been compared in [42], [40]. In the case of the simple linear model, we have been able to find appropriate actuators to control the motion of the free interface (see A. Orriols Phd thesis). We are currently working on the control problem for the non-linear model.

Related to these MHD simulations, some numerical problems of a more general relevance are investigated. Such a particular problem has been the topic of some efforts in 2006. A general problem for two-fluid flows in a box is the modelling of the moving contact line, namely the boundary of the free interface between the two fluids. An adequate boundary condition between no-slip and pure slip should be derived to appropriately model the motion of the free surface. Recently, the Generalized Navier Boundary Condition have been introduced by T.Z. Qian et al. In [39], an Arbitrary Lagrangian Eulerian (ALE) formulation of the Generalized Navier Boundary Condition is proposed. The stability of the numerical scheme is analyzed, in energy norm and the validity of the approach is demonstrated by numerical experiments on two-fluid flows in narrow channels. The stability of new numerical schemes is the subject of ongoing research.

5.7. Fluid Structure Interactions

Participant: Antoine Gloria.

A. Gloria, in collaboration with Miguel Fernandez, Jean-Frédéric Gerbeau (project-team REO) and Marina Vidrascu (project-team MACS) 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 has been submitted to ESAIM proceedings, and a more substantial article is in preparation.

5.8. Complex fluids

Participants: Sebastien Boyaval, 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 the first context, the study by Claude Le Bris and Tony Lelièvre, in collaboration with Benjamin Jourdain (CERMICS) and Félix Otto (University of Bonn), of the long-time behaviour of such flows has appeared in [21]. Entropy methods are used to show an exponential decay to equilibrium. When the system is forced (non-zero boundary condition on the velocity), the exponential convergence to a stationary state can be obtained only in particular cases. On the other hand, for suspensions, as a follow up to the study of well posedness of the problem, the long time limit has been investigated by Claude Le Bris and Eric Cancès in [15].

A completely new topic is now starting, in collaboration with Philippe Coussot (LCPC), Francois Lequeux (ESPCI), Isabelle Catto (University Paris Dauphine). E. Cancès, S. Boyaval and C. Le Bris are going to perform some numerical simulations of some highly non newtonian fluids. Some issues related to thixotropic fluids, and related topics, will be under investigation.

The above very applied topics, related to the modelling of complex fluids, have motivated a series of genuinely 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 have devoted a series of (ongoing) works on the subject. See [23].

5.9. Shock Waves

Participant: Gabriel Stoltz.

G. Stoltz has investigated various aspects of the multiscale simulation of shock waves. 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. A reduced model for a description of shock waves at the microscopic level is proposed in [35]. This model relies on a dissipative particle dynamics with conserved energy, and extends a previous unidimensional model. The reactive case is currently examinated, with a view to modelling detonation processes.

5.10. Mathematical models for models issued from biology

Participant: Gabriel Turinici.

Continuing previous works in epidemiology, a review paper [36] on the SARS epidemic was delivered and is scheduled for publication in 2007. A numerical investigation concerning a hypothesis on the propagation of the TSE epidemics has also been proposed [28].

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, Ecole Nationale des Ponts et Chaussées and Paris IX Dauphine.

7.2. National activities

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 four 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 last one the team is involved in is the ANR Parmat, managed by Guy Bencteux (EDF and MICMAC).

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. Antoine Gloria has been hired for 3 months as a young stage researcher by the team of Padova, to work with Andrea Braides.

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 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

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.

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 for the following institutions and funding agencies: National Science Foundation, Banff International Research Station, DFG Excellence Initiative programme *Condensed Matter Sciences*.

C. Le Bris has organized, or co-organized, the following workshops in 2006:

-Workshop CIRM, Luminy, 22-27 january 2006.

- (with P. Bochev, R Lehoucq, G. Wagner (SNL), J. Fish (RPI)), Workshop Atomistic To Continuum coupling methods, Sandia National Laboratories, March 20-21, 2006, Albuquerque.

- (with M. Esteban(Univ. Paris Dauphine) and G. Scuseria(Rice Univ.)), Workshop *Mathematical and numerical aspects of quantum chemistry problems*, Oberwolfach, 22-26 october 2006.

8.2. Teaching activities

- Simulation moléculaire: aspects théoriques et numériques, cours de M2, université Paris 6 (E. Cancès).
- 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).
- 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, (E. Cancès, A. Gloria, G. Stoltz).
- 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, (T. Lelièvre).
- 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).
- Algèbre linéaire 3 cours à l'Université de Paris IX Dauphine (G. Turinici).
- Optimisation numérique cours à l'Université de Paris IX Dauphine (G. Turinici).
- Calcul et analyse numérique: évolution cours à l'Université de Paris IX Dauphine (G. Turinici).
- Analyse numérique des EDP cours à l'Université de Paris IX Dauphine (G. Turinici).
- Finances numériques 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, Multilevel domain decomposition for electronic structure calculations, 4th International Workshop on Parallel Matrix Algorithms and Applications (PMAA'06, Rennes), September 2006.

E. Cancès, Approximation and numerical simulation of the N-body Schrodinger equation, January 2006, laboratoire J.-L. Lions (Paris).

E. Cancès, Molecular and multiscale simulation of materialsJanuary 2006, 4-hour lecture in the framework of GdR Chant, Institut Joseph Fourier (Grenoble).

E. Cancès, A new approach of the optimized effective potential, May 2006, ICQC 2006 (Kyoto).

E. Cancès, A multiscale model for concentrated suspensions, July 2006, Peking University (Peking)

E. Cancès, Numerical analysis for electronic structure calculations: an overview, October 2006, Oberwolfach workshop.

A. Deleurence, Modelling of crystals with defects, Octobre 2006, Institut Henri Poincaré.

A. Gloria, University of Rome 3, may 2006 ;

A. Gloria, University of Bonn, November 2006 ;

A. Gloria, Annual meeting of the Italian applied mathematics society (SIMAI), Ragusa, may 2006 ;

A. Gloria, MULTIMAT midterm meeting, Antwerp, November 2006.

C. Le Bris, "Mathematical and numerical analysis for molecular simulation: accomplishments and challenges", 45 minutes invited sectional speaker, International Congress of Mathematicians, ICM Madrid 2006.

C. Le Bris, *Some mathematical issues in molecular dynamics*, Workshop "Coarse-grained Multiscale Models: Mathematical analysis and applications", Warwick University, April 24-26, 2006.

C. Le Bris, *Mathematical issues in molecular modelling*, Workshop City University of Hong-Kong, 10-11 May, 2006.

C. Le Bris, *Some mathematical issues in molecular dynamics*, **Keynote lecture** "New trends in Scientific Computing", 8th SIMAI Conference (Italian Society of Applied and Industrial Mathematics), Sicile, 22-26 May, 2006. [The other lecturers are Alfio Quarteroni, Endre Süli and Peter Deuflhard]

C. Le Bris, *On some microscopic stochastic lattices and their macroscopic limits*, International workshop Atomistic and Stochastic Aspects of Elasticity, Max Planck Institute for Mathematics in the Sciences, Berlin, May 25-27, 2006.

C. Le Bris, *Generalized solutions of SDEs with irregular coefficients and applications*, Workshop on multiscale modelling of complex fluids, Peking University, June 16-17, 2006.

C. Le Bris, **Keynote lecture**, *Recent mathematical contributions in some computational materials science problems involving the atomic scale*, Minisymposium "Atomistic-to-continuum coupling and novel methods for quantum mechanics", Seventh World Congress on Computational Mechanics, July 16 - 22, 2006, Los Angeles.

C. Le Bris, *Some mathematical issues arising in complex fluid flows*, 4th international Workshop on nonequilibrium thermodynamics and complex fluids, Rhodes, Greece, 3-7 september 2006.

C. Le Bris, *On some microscopic stochastic models of materials and their macroscopic limits*, mini-symposium "Bridging Scales for the Strength of Materials", Third International Conference on Multiscale Materials Modeling (MMM-III), Freiburg, Germany, September 18-22, 2006.

C. Le Bris, *Existence and uniqueness of solutions to Fokker-Planck type equations with irregular coefficients*, Variational methods in materials science, Scuola Normale Superiore Pisa, 2006.

C. Le Bris, Weekly seminar, Université de Cergy (2006),

C. Le Bris, Weekly seminar, Séminaire Pierre-Louis Lions du Collège de France (2006),

C. Le Bris, Weekly seminar, Université Paris Sud Orsay (2006),

C. Le Bris, Weekly seminar, Université Paris-Dauphine (2006)

C. Le Bris, Weekly seminar, University of Minnesota (2006),

C. Le Bris, Weekly seminar, Materials Modelling Laboratory Oxford University (2006)

C. Le Bris, Exposé au Séminaire inaugural de la Chaire Lafarge - X - ENPC (2006)

F. Legoll, Rencontres du GdR Chant, Grenoble, january 2006.

F. Legoll, Groupe de travail Méthodes numériques, laboratoire Jacques-Louis Lions, Paris, february 2006.

F. Legoll, Atomistic to Continuum Coupling Methods workshop, Albuquerque, march 2006.

F. Legoll, Aerospace Engineering and Mechanics department, University of Minnesota, Minneapolis, april 2006.

F. Legoll, Mini-symposium Dynamique Moléculaire du Congrès d'Analyse Numérique 2006, Guidel, may 2006.

F. Legoll, Mathematics department, Warwick University, Warwick, june 2006. Launching meeting of "Networks and Heterogeneous Media", Maiori, june 2006.

F. Legoll, 7th World Congress on Computational Mechanics, Los Angeles, july 2006.

F. Legoll, Rencontres du GdR Chant, Lyon, november 2006.

F. Legoll, Maxwell Institute Colloquium, Edinburgh, november 2006.

F. Legoll, Weierstrass Institute, Berlin, december 2006.

T. Lelièvre, Workshop on Numerics for SDEs with applications, Florida State University, Fvrier 2006.

T. Lelièvre, CANUM 2006, Guidel, Juin 2006.

T. Lelièvre, AIMS conference, Poitiers, Juin 2006.

T. Lelièvre, ECCOMAS conference, Hollande, Septembre 2006.

T. Lelièvre, SimBioMa Conference, Paris, Novembre 2006.

T. Lelièvre, Séminaire Laboratoire Jacques-Louis Lions, Janvier 2006.

T. Lelièvre, Séminaire équipe OMEGA, INRIA Sophia-Antipolis, Mai 2006.

T. Lelièvre, Séminaire KTH/SU Mathematics Colloquium, Stockholm, Mai 2006.

T. Lelièvre, Workshop CERMICS / PKU, Pekin, Juillet 2006.

T. Lelièvre, Séminaire CEMRACS, Marseille, Août 2006.

T. Lelièvre, Workshop calcul d'nergies libres, CERMICS, Paris, Octobre 2006.

T. Lelièvre, Séminaire ADAP'MC, Paris, Octobre 2006.

T. Lelièvre, Séminaire de calcul scientifique, Kiel, Novembre 2006.

A. Orriols, Seminar, RICAM, Linz, Austria, 28th November 2006.

M. Rousset, Workshop "Mathematical and numerical methods in Quantum Chemistery", Oberwolfach, October 2006.

M. Rousset, Workshop "Sequential Monte-Carlo methods", St-Anne's college, Oxford, July 2006.

M. Rousset, Workshop "Coarse-grained multiscale models: mathematical analysis and applications", Warwick University, April 2006.

M. Rousset, Séminaire, Mathematisches Institut, Universitat Bonn, November 2006.

A. Scemama, Probabilistic description of the chemical bond, July 2006, 10th RCTF (Nancy).

G. Stoltz, A simplified dual formulation of the electronic problem in terms of the second order reduced density matrix, Poster presented at the International Congress on Quantum Chemistry, Kyoto (may 2006)

G. Stoltz, Computing macroscopic properties using microscopic models, rencontre GdR CHANT (Grenoble, 12 january 2006)

G. Stoltz, (Non)equilibrium computation of equilibrium properties, ACI meeting - CIRM (Marseille, 26 january 2006)

G. Stoltz, Echantillonnage hors-équilibre, Meeting "Scientific computation" at université de Cergy (03/04/2006)

G. Stoltz, (Non)equilibrium computation of free energy differences, Seminar of the Computational Chemistry group at university of Amsterdam (2006)

G. Stoltz, Path sampling with stochastic dynamics, Poster presented at the workshp Sampling paths in molecular simulation: algorithms for phase transitions, reactivity and kinetics, Orsay (november 2006)

G. Stoltz, A simplified one-dimensional model of shock and detonation waves, Sixth Biennal International Conference on New models and hydrocodes for shock waves processes in condensed matter (Dijon, 9-14 april 2006)

G. Stoltz, Mathematical and multiscale aspects of molecular simulations - Application to shock waves, Presentation given at the PhD students' day at the CEA/DAM, Bruyères le Châtel (november 2006)

G. Turinici "Quantum control: theoretical, numerical and experimental results", in workshop *Mathematical and numerical aspects of quantum chemistry problems* Oberwolfach, Germany, Oct. 2006

G. Turinici "Theoretical approaches and numerical implementations of quantum control", in *International conference on applied analysis and differential equations*, Iasi, Romania, Sept. 2006

G. Turinici "Parallel in time control for quantum systems", at the 17th International Conference on Domain Decomposition Methods, Strobl, Austria, July 2006

G. Turinici "Exponentially convergent discretizations for PDEs: reduced basis approaches" *Mathematics and its applications : joint meeting of the SIMAI, SMAI and SMF* Torino, Italy, July 2006

G. Turinici "Experimental inversion algorithms for quantum control" *PICOF*,Nice, France, April 2006

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

A. Deleurence, ACI (CIRM), January 2006.

A. Deleurence, Advances in the atomic-scale understanding of nanostructures, Institut d'Electronique, Microélectronique et Nanotechnologie, Université Lille I, April 2006.

A. Deleurence, Ab Initio Molecular Dynamics Simulation Methods in Chemistry, University of Illinois, Urbana Champaign, August 2006.

A. Deleurence, Randomness modelling and uncertainty management, CIRM, Marseille,Cemracs 2006 ,August 2006:.

A. Deleurence, International Congress of Mathematicians, Madrid, August 2006.

A. Deleurence, GdR Chant, Equations Cinétiques et Hyperboliques: Aspects numériques, Théoriques et de Modédlisation, ENS Lyon, November 2006.

A. Deleurence, Sampling paths in molecular simulation : algorithms for phase transitions, reactivity and kinetics, Laboratoire de Chimie Physique CNRS and Université de Paris-Sud, Orsay,November 2006.

A. Gloria, Workshop on phase transitions, Centro Ennio de Giorgi, Pisa, February 2006 ;

A. Gloria, Workshop on Variational methods in Material Science, Centro Ennio de Giorgi, October 2006 ;

A. Gloria, Matematica nei materiali, Workshop internazionale presso Istituto Nazionale di Alta Matematica "Francesco Severi" Roma, 3-7 aprile 2006 ;

A. Gloria, Third Summer School in Analysis and Applied Mathematics, Rome June 5-9, 2006.

A. Orriols, spring school "Optimisation et contrôle des écoulements et transferts", March 2006, Aussois, France.

A. Orriols, CEA-EDF-INRIA summer school "Calcul haute performance", July 2006.

A. Scemama, January 2006: ACI (CIRM)

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

A. Gloria, University of Rome 3, April-June 2006 :

A. Gloria, Centro Ennio de Giorgi, Pisa, October 2006, "Variational methods in Material Science" ;

A. Gloria, University of Bonn, from October 30th to November 3rd.

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Books and Monographs

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[4] J.-F. GERBEAU, C. LE BRIS, T. LELIÈVRE. *Mathematical methods for the Magnetohydrodynamics of liquid metals*, Oxford University Press, 2006.

Articles in refereed journals and book chapters

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[6] X. BLANC, C. LE BRIS, F. LEGOLL. *Analysis of a prototypical multiscale method coupling atomistic and continuum mechanics: the convex case*, in "Acta Mathematicae Applicatae Sinica", to appear.

[7] X. BLANC, C. LE BRIS, P.-L. LIONS. *Atomistic to Continuum limits for computational materials science*, in "Mathematical Modelling and Numerical Analysis", to appear.

[8] X. BLANC, C. LE BRIS, P.-L. LIONS. *The energy of some microscopic stochastic lattices*, in "Archive for Rational Mechanics and Analysis", to appear.

[9] X. BLANC, C. LE BRIS, P.-L. LIONS. *Une variante de la théorie de l'homogénéisation stochastique des opérateurs elliptiques*, in "Note aux Comptes Rendus de l'Académie des Sciences", in press.

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[14] E. CANCÈS, M. LEWIN, G. STOLTZ. *The Electronic Ground State Energy Problem: a New Reduced Density Matrix Approach*, in "Journal of Chemical Physics", vol. 125, 2006, 064101.

[15] E. CANCÈS, C. LE BRIS. *Convergence to equilibrium for a multiscale model for suspensions*, in "Discrete and Continuous dynamical Systems B", vol. 6, n^{o} 3, 2006, p. 449-470.

[16] G. CICCOTTI, T. LELIÈVRE, E. VANDEN-EIJNDEN. *Sampling Boltzmann-Gibbs distributions restricted on a manifold with diffusions: application to free energy calculations*, in "Communications on Pure and Applied Mathematics", to appear, 2006.

[17] X.-J. FENG, C. LE BRIS, H. RABITZ, G. TURINICI. *A Closed-Loop Identification Protocol (CLIP) for Nonlinear Dynamical Systems*, in "Journal of Physical Chemistry A", vol. 110, 2006, p. 7755–7762.

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[27] Y. MADAY, SALOMON, G. TURINICI. *Monotonic time-discretized schemes in quantum control*, in "Numerische Mathematik", 2006.

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[44] T. LELIÈVRE, M. ROUSSET, G. STOLTZ. *Computation of free energy profiles with adaptive parallel dynamics*, arXiv:cond-mat/0611276.

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