INRIA

INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Project-Team Micmac

Methods and Engineering of Multiscale Computing from Atom to Continuum

Rocquencourt

THEME 4B

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2. 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

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 106 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 104 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 is 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 inert part of a protein) is coarse grained, and more crudely modeled by classical mechanics.

The coupling of different scales can even go up to the macroscopic scale, with methods that couple a microscopic description of matter, or at least a mesoscopic one, with the equations of continuum mechanics at the macroscopic level.

4.2. Laser control

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

Whatever the strategy, the success of these numerous experiments not only 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 even 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 Schrodinger equation, one then state 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 features 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 10^{-15} s (the femtosecond) 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 data base ?).

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.

6. New Results

6.1. Electronic structure calculations

Participants: Maxime Barrault, Eric Cancès, Hervé Galicher, Claude LeBris, François Lodier, Gabriel Turinici.

We have continued our studies on the algorithms used for electronic structure calculations. The different tracks followed are

- improvements of the so-called SCF approaches, in collaboration with the group of Gustavo Scuseria at Rice [14]
- acceleration techniques for the linear subproblem based in particular on deflation techniques [30]
- introduction of reduced basis approaches in the framework of quantum chemistry; some exploratory works have been conducted in close collaboration with the group of Antony Patera at MIT.

Apart from this main stream, two numerical works, of different nature have been conducted.

First, we have developed in [13] techniques 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.

Second, numerical schemes have been developed for the simulation of a nonlinear Schrödinger equation close to the one encountered in time dependent electronic structure calculations and modeling Bose-Einstein condensates[12].

All of these new developments and methods are meant to be inserted in the long term inside the software platform 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 these numerical works, we have pursued in our enterprise to put the models on a safe mathematical ground. We have studied the optimized effective potential approach from the theoretical viewpoint in [3].

A survey of all these new developments together with a precise and comprehensive state of the art of the mathematical knowledge in the field of quantum computational chemistry has been published in a book[1]. An abridged version of some of the main contributions of our team can be found in [5].

6.2. Molecular dynamics

Participants: Eric Cancès, Claude LeBris, Frédéric Legoll, Antonin Orriols, Gabriel Turinici.

Molecular dynamics is often used in statistical physics as an alternative to Monte Carlo methods for computing ensemble averages. Based on a theoretical result concerning the convergence of the numerical averages toward the exact result, we were able to propose in [37][9] a new method to accelerate this convergence. This has been performed in collaboration with Francois Castella, Philippe Chartier and Erwan Faou from INRIA Rennes (work supported by ARC PRESTISSIMO).

6.3. Laser control

Participants: Samir Belgacem, Adel BenHajYedder, Eric Cancès, Fabrice Cohen, Claude Dion, Claude LeBris, Mazyar Mirrahimi, Gabriel Turinici.

Following a series of works devoted to the optimal control of the alignment of a molecule by laser field and population inversion algorithms[35][33][22], our interest now focuses on the very practical issues of the laboratory implementations of closed loop optimal control. This is done in close collaboration with the group of H. Rabitz (Princeton University). We have introduced direct search algorithms into this field and assessed

their efficiency versus more commonly used algorithms such as Genetic-like algorithms [26]. A practical implementation of these ad-hoc developed algorithm is under progress in an experimental setting at Princeton University.

We also intend to address in the near future and in collaboration with Pierre Rouchon (Ecole des Mines, Paris) questions related to the inversion paradigm: use the laser field as a tool to obtain additional information on the molecular system. A related topic was already the subject of a recent work [28] focused on the discrimination of similar quantum systems.

In addition to this, and on the level of numerical analysis, we have published some mathematical results on what are the most commonly used optimization algorithms in the field of optimal control for this type of laser-matter interaction problems, namely the genetic algorithms. In [36][29], we have studied the convergence of a representative class of these algorithms.

6.4. Multiscale simulation of solids

Participants: Claude LeBris, Frédéric Legoll.

This research program divides into a theoretical part and a more numerical one.

On the theoretical side, following a series of works, in collaboration with Xavier Blanc (Laboratoire Jacques-Louis Lions, Paris), Isabelle Catto (University Paris 9), and Pierre-Louis Lions Collège de France, Paris), we have addressed the question of how to define ground state energies for systems composed of an infinite number of particles. The framework is that of quantum chemistry, where the state of matter is modelled though 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), a prototypical example being the Thomas-Fermi-von Weizsäcker model, we pass 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). But one can ask the question : is the minimal energy configuration periodic or not, a problem which is indeed known in the physics literature as the crystal problem. For such quantum problems, only one-dimensional results can be proven so far. Alternatively, one may ask whether it is possible to pass to the N goes to infinity limit when the nuclei are not arranged periodically. A construction is developed in [6][7] that allows one to properly define the energy of this infinite system, under very weak and natural conditions on the geometric arrangement of the nuclei.

In addition, we have continued our program consisting in passing from the microscale to the macroscale on the basis of quantum models at the microscale. This program has been initiated in [8] and is being continued with current work in progress that aims at enlarging the results obtained in this first publication.

On a more numerical level, Claude Le Bris and Frédéric Legoll, in collaboration with Xavier Blanc, have begun the mathematical and numerical analysis of models used in simulations for material science where an atomistic description of the sample is coupled with a macroscopic continuum description.

6.5. Multiscale simulation of complex fluids

Participants: Eric Cancès, Yousra Gati, Claude LeBris, Tony Lelièvre.

The subject of this activity covers two different applications and settings.

The first one is that of the modeling of polymeric fluid flows. We have continued our endeavor to mathematically study the models commonly used in numerical simulations by experts at nonnewtonian fluid dynamics [17][20][32]. More numerical issues, such as variance reduction techniques have been addressed in [18]. In parallel, a theoretical study of the stochastic partial differential equations that may arise in this context has been conducted in [19].

The second topic of interest deals with concentrated suspensions, and is done in collaboration with Isabelle Catto (University Paris 9). So far, the study is mainly of theoretical nature, with a view to tackle in a near

future more numerical and practical aspects. We have established the well-posedness of the Cauchy problem for the equations modeling the suspension [10].

6.6. Magnetohydrodynamics flows

Participants: Claude LeBris, Tony Lelièvre, Antonin Orriols.

In collaboration with Jean-Frédéric Gerbeau (Inria, BANG), and in association with Aluminium Péchiney, we have pursued our efforts for the numerical simulation of electrolytic cells for the industrial production of Aluminium. The results obtained so far have been detailed in [16][15]. The next steps that we envision consist in addressing the problem of optimization and control: how can we design the electromagnetic boundary conditions on the cell, or some geometrical features of the cell, in order to make the cell as efficient as possible and keep it as stable and robust as possible with respect to external perturbations.

6.7. Mathematical models for models issued from biology

Participant: Gabriel Turinici.

In the context of a collaboration with A.Danchin (Pasteur Institute) and Ng. Tuen (Hong-Kong University) we studied the impact of a biological hypothesis on the SARS virus propagation data [24]. This study is to be followed by an additional analysis that takes into account stochastic elements of the epidemic propagation.

7. Contracts and Grants with Industry

Many research activities of the team are indeed conducted in close collaboration with private companies: Pechiney for the modeling of electrolytic cells, Electricité de France for computational chemistry, molecular dynamics and multiscale simulation of solids, and companies from the elastomer industry for the multiscale simulation of rubber-like materials.

8. Other Grants and Activities

8.1. Regional activities

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

8.2. National activities

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

8.3. European Community financed activities

Some members of the team participate into the european project IHP “HYKE” (Hyperbolic and kinetic equations: Asymptotis, numerics, Applications) whose Scientist in charge is Benoît Perthame (BANG), on theoretical aspects related to the resolution of the Schrödinger equation for large systems and long times.

8.4. Bilateral international relations

8.4.1. 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 Unversity 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.

9. Dissemination

9.1. Animation of the scientific community

Claude Le Bris is VP of the SMAI (french SIAM), more particularly in charge of relation with the industrial companies.

9.2. Teaching activities

- Simulation moléculaire: aspects théoriques et numériques, cours de DEA, université Paris 6 (C. LeBris).
- Simulation moléculaire, cours de DEA, université Paris 9 (E. Cancès).
- Systèmes multiéchelles, cours de la majeure SEISM, Ecole Polytechnique (C. LeBris).
- 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. LeBris).

9.3. Conference participation

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

- AMAM conference, Nice, February 2003 (M. Barrault, E. Cancès, C. LeBris, T. Lelièvre, G. Turinici)
- IFAC Workshop on Lagrangian and Hamiltonian Methods for Nonlinear Control, Sevilla, April 2003 (C. LeBris, G.Turinici)
- "Spitalfields Day" of the London Mathematical Society and the Isaac Newton Institute, Cambridge, May 2003 (C. LeBris)
- Rigorous Ab-Initio Studies of Periodic Systems: Approaches to Electron Correlation, CECAM Workshop, May 2003, Lyon (E. Cancès, C. LeBris)
- XIIIth International Workshop on Numerical Methods for non-Newtonian Flows, June 2003, Lausanne (C. LeBris)
- PCAM Seminar of the Applied Mathematics department, Princeton University, June 2003 (C. LeBris)
- Calais, June 2003 (M. Barrault)
- Bonn University Mathematics department seminar, June 2003, (C. LeBris)
- Gerone, July 2003 (F. Lodier)
- SIAM Annual meeting, Montréal, June 2003 (E. Cancès, C. LeBris)
- International congress of quantum chemistry, Bonn, july 2003 (E. Cancès)
- London, September 2003 (T. Lelièvre)
- Oberwolfach Workshop PDE and Materials, September 2003, (C. LeBris)
- Warwick University Mathematics department seminar, October 2003, (C. LeBris)
- Oberwolfach Workshop Classical and Quantum Mechanical Models of Many-Particle Systems, November 2003 (C. LeBris)
- Workshop Discrete atomistic models and their continuum limit, Berlin, December 2003 (C. LeBris)
- Workshop Multiscale problems in quantum mechanics and averaging techniques, Leipzig, December 2003 (C. LeBris)
- PRESTISSIMO workshop, Institut Henri Poincaré, December 2003 (E. Cancès)

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