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PhD Yearbook | 2010

Chair:
Prof. Paolo Biscari

DOCTORAL PROGRAM IN MATHEMATICAL MODELS AND METHODS IN ENGINEERING

Equations are everywhere! Between the atmosphere and the wing of a spaceship, in the blood flowing in an artery, on the demarcation line between ice and water at the poles, in the motion of the tides, in the charge density of a semiconductor, in the compression algorithms of a signal sending images from outer space. Such equations represent real problems. The Mathematical Engineer can see and understand the nature of these equations, and can develop models in order to understand their relevant qualities and solve real problems.
This PhD program aims at training young researchers by providing them with a strong mathematical background and with ability to apply their knowledge to the solution of real-world problems that arise in various areas of science, technology, industry, finance, management, whenever advanced methods are required in analysis, design, planning, decision and control activities. PhD students carry out their research both in the development of new mathematical methods and in the implementation and improvement of advanced techniques in connection with specific contexts and applications.
The Faculty of the PhD program is responsible for the organization of the training and research activities of the PhD students. Decisions of the Faculty comply with the requirements and standards of the Doctoral School of the Politecnico di Milano. A Chairman is elected within the Faculty, for representative and coordination activities.
Admission of students to the PhD program is decided after examination of the candidates. Students applying to our program must provide their CV, along with reference and motivation letters.
After admission, each student is assigned a tutor. The tutor is a member of the Faculty who assists the student in the early stages of his career, especially in the choice of the courses and in identifying a thesis advisor.
The overall activity of the PhD students can be quantified in 180 credits. The PhD program has a duration of three years.
Activity can be classified into:

- introductory courses (no minimum number of credits required);
- main courses (at least 40 credits);
- specialized research training, including seminars, tutoring activity, participation to workshops/conferences, and scientific publications (at least 20 credits);
- development of a doctoral thesis (at least 90 credits).

At the end of each academic year, the PhD students report to the Faculty about their activity. The students report about attendance of courses and exams (and the corresponding grades), participation in various scientific activities (seminars, conferences, summer schools etc.), planning and intermediate results on their research project and preparation of the PhD thesis, and any other relevant activity. At the annual meeting the students also receive a grade by the Faculty. A negative grade may entail repetition of the current year of doctoral study (with suspension of the grant, if any) or exclusion from the PhD program, depending on the Faculty's decision. Mobility of PhD students to other institutions is strongly encouraged and financial support is provided to this purpose.

Among others, let us mention some typical types of professional skills and possible occupations of the graduated Doctors: analytic and numerical treatment of differential models for physical and industrial problems, quantitative methods in finance and risk management, operations research and optimisation, statistical modelling and data analysis.

Placement of graduated Doctors is expected in the following positions: research and development divisions of businesses, businesses involved in innovative design activities, financial institutions such as banks or insurance companies, public or private research centres, public and/or governmental agencies for social, economical, scientific study, planning or evaluation, Universities.

Since the PhD program in Mathematical Models and Methods in Engineering (formerly, Mathematical Engineering) has been active since the year 2001, we expect that a larger number of institutions and businesses will soon become more and more aware of the professional skills and expertise of graduated doctors.

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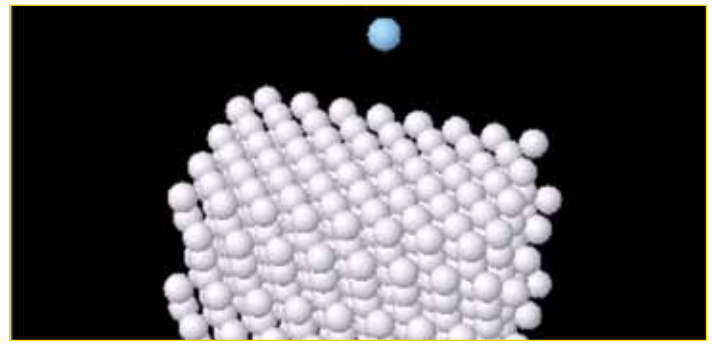
A COMPARISON OF COMPUTATIONAL MODELS OF GAS-SURFACE INTERACTION

Marco Carnini

Gas-surface interaction plays an important role in determining properties of micro and nanoflows, which are of growing interest in the last few years: due to the rapid advancement of micro machining technology over the past decades, a full range of new devices has been developed. They are commonly referred to as MEMS or NEMS (Micro and Nano Electro Mechanical Systems); the first are made of components in micrometer tange, the latter in nanometer range. Both of them integrate electronic and mechanical functionalities (micro bolometers, actuators, pumps or motors) and may thereby form physical, biological, and chemical sensors. The potential of very small machines was appreciated long before the technology existed that could make them: a common reference is a Richard Feynman's lecture, *There's Plenty of Room at the Bottom* at an American Physical Society meeting on December 29, 1959.
When small length scales gas flows are studied, the mean free path of the gas molecules is not negligibly small compared with the characteristic length of the systems. As a consequence, a microscopic approach based on kinetic gas theory is necessary. Within the framework of the kinetic theory of dilute gases, gas-surface interaction models provide boundary conditions for the distribution function of molecular velocities at locations where the gas is in contact with a solid wall. When dealing with flows of dilute gases, the characteristic space and time scales are much larger than molecular sizes and molecular interaction times which are the natural space and time scales of gas-surface interaction. Hence, it is quite natural to describe the gas-wall interaction by assuming that the solid boundary can be replaced by a smooth, structureless and impenetrable surface which acts on the gas distribution function by means of a scattering kernel, which gives the probability that a molecule impinging on the wall with velocity between v_1 and *v1+dv1* is *instantaneously* re-emitted at the *same location r* with velocity between *v* and *v1+dv1*.
In principle, the scattering kernel could be obtained if a complete mathematical description of the motion of a gas molecule interacting with the molecules of the solid lattice could be given. However, obvious mathematical difficulties force to abandon such an approach in favor of more heuristic formulations in which phenomenological scattering kernels expressions, containing a small number of adjustable parameters, are proposed.
The main drawback connected with phenomenological scattering kernels is the difficulty of establishing relationships between the kernel parameters and the fundamental physical quantities (intermolecular potentials, mass ratios) governing gas-wall interaction. In absence of such relationships, modelling a specific flow condition requires tuning the kernel parameters and repeating the tuning procedure on each change of the flow condition which involves gas-wall interaction.
The need of a deeper understanding of fluid-wall interaction has triggered a number of studies in which molecular dynamics (MD) techniques have been used to investigate atomic or molecular scattering from solid surfaces. In principle, MD allows obtaining, on the ground of fundamental physical quantities, the (numerical) desired detailed description of gas-wall interaction which cannot be obtained in analytical form. Thermal and momentum accommodation coefficients of various atomic and molecular gases in contact with metal surfaces have been obtained. Unfortunately, a full MD simulation of a dilute gas interacting with a solid wall would have prohibitive computational costs.
Attempts have been made to develop hybrid MD-DSMC simulation methods. Although feasible, hybrid simulations still remain computationally demanding since MD limits the rate of the faster Monte Carlo algorithm. In order to reduce the computational cost of gas-wall interaction while keeping an MD-like approach, a number of attempts have been made to simplify the dynamics of a gas molecule interacting with a solid lattice. The guiding idea is to reduce or eliminate the necessity of a detailed description of the motion of the lattice molecules by a sensible modelling of the forces acting on the impinging gas molecule.
The goal is achieved by adopting the formalism of Generalized Langevin Equation (GLE).
The lattice molecules are then divided into background and foreground molecules.
The effects of former group are replaced by a fluctuating force field, whereas an MD-like technique is adopted to describe the interaction between the gas molecule and the small number of molecules in the latter group.
The approach can be further simplified by eliminating the calculation of the motion of foreground molecules. A kinetic model is proposed in literature in which gas atoms interact with the solid lattice through a potential obtained from the superposition of a hard sphere potential and a soft attractive tail. Comparisons of model predictions with the results of MD simulations have shown that it is possible to adjust the model parameter to obtain good quantitative agreement with MD results. However, good or satisfactory agreement is not always obtained for a wide range of physical conditions.
Starting from the results of the kinetic gas-surface interaction model, the research work described in thesis aims at examining gas-surface interaction computational models of increasing complexity, in order to better understand the effects of the simplifications introduced into the dynamics on the model performances.
Moreover, the computational cost of the various models has been considered, in view of a possible coupling to a Boltzmann DSMC solver. The following three computational models have been considered, all of them being more complex than the kinetic model.



1. Argon molecule near a f.c.c. 111 Platinum lattice.

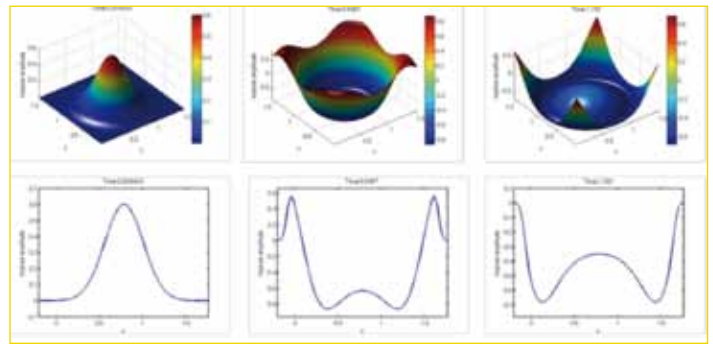
- An Einstein solid model interacting with a single gas molecule.
- A Debye solid model interacting with a single gas molecule.
- A Lennard-Jones solid interacting with a single gas molecule. This the most complete model whose results have been used as a reference to judge about the quality of the simpler ones.

In all simulations, the solid physical parameters have been tuned to simulate a Platinum surface interacting with Argon or Xenon atoms. For each gaseous species, both Lennard-Jones and Morse potentials have been used to describe gas-wall interaction, in order to assess the sensitivity of scattering patterns to potential properties. In performing comparisons, the Lennard-Jones and Morse potential parameters have been set to have *the same well depth and the same minimum position.*
In addition to the comparison of the above gas-surface model, preliminar computational experiments on the coupling of the kinetic model with a Boltzmann solver have been performed to study the effects of non-local scattering on the drag coefficients of nanosized particles.

MODELLING AND NUMERICAL SIMULATIONS OF WAVES ON UNBOUNDED DOMAIN

Paola Curci

There are many physical phenomena based on wave propagation that result interesting for engineering applications. Study of these phenomena is important to perform experiments, develop devices and recover informations in the field of electro-magnetics, optics, acoustics, seismic, oceanography and aerodynamics. Our attention is focused on electro-magnetics and seismic applications like that light propagation in optical waveguides and propagation of seismic signals for oil and gas exploring. The physical problems involved in these applications are very complex and their full understanding requires laboratory experiments or proves in loco.
Since these investigations can be often very expensive, accurate numerical simulations of wave phenomena can result an important instrument for design and development of the related engineering applications.
In the following we will enter into details of the two problems classes of our interest.
Optical communications have make possible high speed information transmission.
Progress of this recent research area requires novel photonic applications to transmit, rout and process light very fast.
In this thesis we have developed a simulation tool for modelling dielectric waveguides. Based on solving an eigenvalue problem, this method can be used to compute the modes for a wide variety of guiding structures. Waveguides are basic structures of devices and circuits in optics so it is very important to characterize them depending on signal frequency. They are electromagnetic transmission lines that constitute the interconnections between optical integrated components. We want study waveguide light propagation at the optical frequencies of interest by means of mode analysis.
We are interested to accurately compute the propagation constants and the corresponding field distributions on waveguide section of fundamental modes.
Our computational approach is based on the numerical resolution of Maxwell's eigenproblem trough a suitable implementation of the Finite Element (FE) method. The main problem whit this approach is the appearance of spurious modes: unphysical solutions that do not satisfy the solenoidality of electric and magnetic displacement. In order to overcome this difficulty, many strategies have been developed. We chose a sufficient condition which puts constraints on the FE spaces for the approximation of the field components.
In optical waveguide the region of interest extends in all practical terms to infinity. FE method is not directly applicable to unbounded domains. Since for guided modes the field decays rapidly far from the core, it is possible truncate computational domain.
To truncate the physical space, artificial boundaries and corresponding boundary conditions are introduced.
There are several classes of methods that can be used to truncate problems on unbounded or large domains.
In our case we adopt the absorbing perfectly matched layer (PML) technique.
Absorbing layer methods are based on surrounding the computational domain with a external finite width layer. In this region the governing equations are modified so that the solutions decay rapidly without reflections. PML is a particular absorbing layer method with the ideal properties to be effective independent of frequency, polarization and direction of the impinging wave. In this work we define and implement PML region as a simple anisotropic layer characterized by a real permittivity and permeability tensors.
The oil and gas industry requires imaging techniques for exploring complex sub-surface structures.
The depth image of an Earth area is usually obtained by moving ("migrating") reflection seismic events to their proper source locations. One of the most accurate migration method is Reverse-Time Migration (RTM). This method is based on the backward propagation of the recorded seismic wavefield. Seismic migration is directly related to seismic modelling. The latter describes the forward process of propagating waves from sources to receivers. It is used to obtain seismic traces by means of numerical simulations. These synthetic data are usually used to test RTM algorithms by a comparison between the migration image and the velocity field of forward model.
Thus, RTM algorithms reliability strongly depends on the accuracy of synthetic data.
In this study we focus on developing an accurate and efficient seismic modelling tool based on Finite Difference (FD) method. We approximate the acoustic wave equation in a three dimensional setting using finite difference centered operators of order 2 in time and 2M in space (M=1,2,3,4,5), on an uniform grid. We study the amplitude and dispersion error introduced by the FD schemes. In particular, we use the Von Neumann analysis to determine a set of CFL threshold values that avoid numerical instabilities. Moreover we deal with the problem of finding a suitable scheme able to minimize the dispersion error and in the meantime to contain the computational costs of the numerical simulations. Thus, we compare the different FD schemes with a varying spatial order, M=1,2,3,4,5. We find out that the scheme satisfying these requirements is the forth order scheme.
The simulation of waves in unbounded media requires suitable transparent boundary conditions.
To avoid spurious boundary reflections we choose to surround the computational domain by a perfectly matched layer (PML) designed to absorb outgoing waves.
We use the Hagstrom's PML formulation with an our original discretization. The accuracy and stability of this particular PML implementation are validated by means of 2D numerical simulations.
The simulation of a seismic impulse, performed by our modelling tool with the second order in time and space FD scheme, is shown in Fig.1.
To conclude we extend the previous stability analysis to the anisotropic acoustic wave equation for VTI media discretized with a second order in time and 2M in space FD scheme.
The CFL limits of FD schemes have been estimate both in 2D and 3D. For the anisotropic case this is, to our knowledge, an original result.



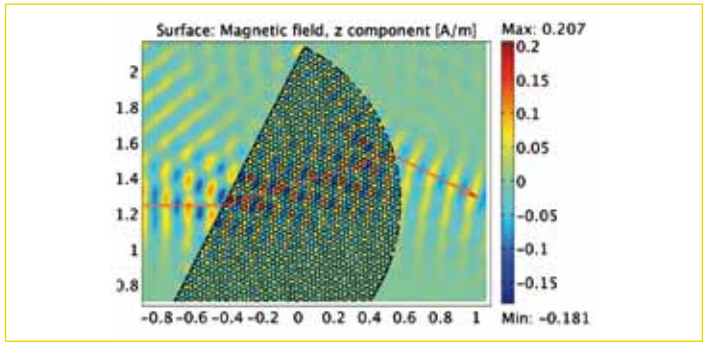
1. Numerical simulation of a seismic impulse in an isotropic medium with PML boundary conditions

MATHEMATICAL AND NUMERICAL MODELING OF WAVE PROPAGATION IN INHOMOGENEOUS AND ANISOTROPIC MEDIA

Paolo Ferrandi

In this work we study wave propagation phenomena in inhomogeneous and anisotropic media of special interest in some engineering fields. In particular, we focus on electromagnetic wave propagation in nanostructures for photonics, in hydrocarbon reservoir fractures and seismic wave propagation for deep earth imaging. In the literature, wave propagation is a well-studied phenomenon both from a mathematical as well as from a numerical modeling perspective. Nevertheless the increasing complexity of the engineering problems requires an accurate choice and tuning of the existing numerical techniques and the development of new methods.

As a first application field, we address the mathematical and numerical modeling of electromagnetic wave propagation in self-aggregating nanostructured materials for photonics. This research project involved the Mathematics, the Electronics and Information, the Chemistry Materials and Chemical Engineering departments of Politecnico di Milano and Corecom (``Consortium for Researches in Optical Processing and Switching''), a laboratory owned by Pirelli and Politecnico di Milano. The project objectives are both the design of an innovative material (self-aggregating porous alumina) for photonics applications and the design of optical devices based on it.

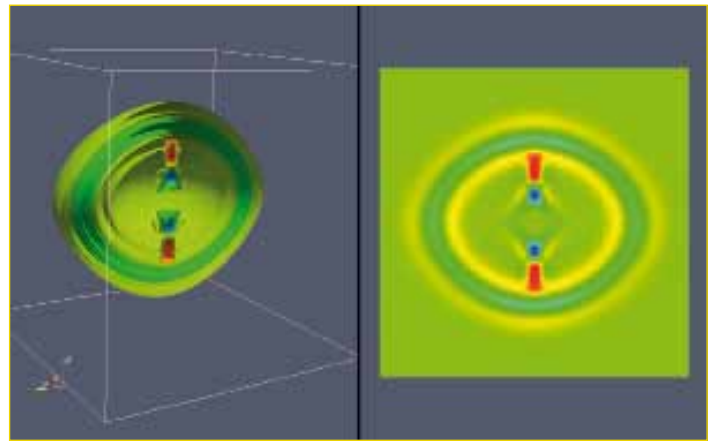


1. Superprism effect in nanostructured photonic device. Magnetic field, z component.

The optical properties of porous alumina, which depend on the manufacturing process, are strictly connected to the functional behavior required to design new photonic devices. In particular we focus on devices based on the peculiar physical phenomena allowed by the photonic band structure. Possible applications of such devices are in wavelength division multiplexing (WDM) transmission technologies, optical communications and chemical sensing. A mass production of a low cost and high refracting device is a key point for WDM applications. Alumina refractive index (around 1.7) is quite close to that of the air (about 1), hence a porous alumina nanostructure must be fine tuned to exhibit a photonic band gap behavior in air. Both a mathematical and a numerical model are essential to set up and tune the manufacturing process towards a material that exhibits such properties; moreover a functional characterization of new possible optics and photonics devices, by means of numerical simulations, is mandatory prior to the development of the electrochemical process.

We modeled the photonic band structure by solving a Maxwell eigenvalue problem in periodic domain. Hence we designed and characterized the functional behavior of a photonic device by means of a Finite Element Method (FEM). We numerically solved the electromagnetic wave propagation (Fig.1). Although the device has a very limited radial extension of only 20 lattice cells, it can exhibit anomalous refraction effects, like *superprism* effect and negative refraction. The dispersion can be positive or negative and it can be strong, even more than one order of magnitude greater than a usual plastic prism and almost constant on a wide wavelength range (e.g., 80nm around 1550nm), or alternatively it can show a very strong peak in a range of few nanometers. The attenuation is always below the engineering specifications. These effects involve the first photonic band, which allows a monomodal propagation because it is separated from the other bands by a complete band-gap. The first photonic band is also the less sensitive to the lattice defects. We also suggest investigating two new applications, for chromatic dispersion compensation and thermophotovoltaic applications. Moreover in a future simulation of an entire system, the choice of FEM allows the adoption of more complex techniques, like adaptive finite elements, discontinuous or mixed formulations etc.

We also applied three-dimensional and bidimensional Maxwell equations to model the propagation of a georadar signal in thin dissipative media, for geophysical applications. The high aspect ratio of thin media like fractures represent a challenge for any numerical method. In this work, which is still in the early stages, we modeled three-dimensional and bidimensional fractures by means of FEMs. We first dealt with the problem of determining the physical properties of the medium, then of finding a suitable discretization for the Maxwell problem. The first numerical results encourage a deeper research in novel models to treat this kind of problem.



2. Seismic wave propagating in anisotropic medium. Pressure isosurfaces (left) and pressure on the yz plane (right). Artificial non-reflecting boundaries are applied.

As a third application field, we dealt with the problem of seismic wave propagation for deep earth imaging. Deep imaging by solving the full wave equation is an up-to-date technique to discover new hydrocarbon reservoirs. From a computational point of view this is a very challenging task, because a typical test case is composed by the repetition of about 100 thousand time dependent simulation, each one characterized by ~10 billion degrees of freedom and ~10 thousand time steps. Seismic waves propagate in inhomogeneous and anisotropic media (subseafloors layers of sandstone, shale, salt and other materials). The traditional elasticity equations imply a unfeasible computational cost, hence we applied a properly modified acoustic equation to mimic the anisotropic propagation. The real problem is set in the ocean and so we needed to develop artificial non-reflecting boundaries, for isotropic and anisotropic problems, to limit the computational domain.

We developed a software to solve three-dimensional problems, with isotropic and anisotropic media, perfectly matched layers and absorbing boundary conditions, by means of FDTD centered and uncentered schemes of arbitrary order (Fig.2). We also faced the problem of avoiding the storing of the entire solution to save mass memory space. Finally we studied the well-posedness of a time-harmonic optimal control model problem based on the seismic scattering problem.

The modeling of nanostractures for photonics was partially supported by grants from the Fondazione Cariplo (Rif. 2004.1105/11.4988 - Bando Ricerca Applicata).
The modeling of a georadar signal was partially supported by the Research Contracts between RSI-TECH/Altran Italia and MOX (Modeling and Scientific Computing), Mathematics Department, Politecnico di Milano.
The research about seismic exploration was partially supported by a Research Contract between ENI S.p.A. and MOX (Modeling and Scientific Computing), Mathematics Department, Politecnico di Milano.

SPECTRAL ELEMENT DISCRETIZATION OF OPTIMAL CONTROL PROBLEMS

Loredana Gaudio

Optimal control problems arise in many applications in science, engineering and economy fields. For such problems, an accurate determination of the quantity of interest is an important asset to improve the performance of the model discretization as well as the capability to better describe the phenomena itself. The main results achieved in this thesis consist of the development, analysis and testing of hN-adaptive algorithms for the solution of optimal control problems, discretized by means of Spectral Element Methods (SEMs). Here h indicated the maximum diameter of the spectral element, while N is the maximum polynomial degree used within every element.
The goal was to achieve a suitable accuracy on the error of a given cost functional (which represents the output of physical interest), according to a criterion of minimization of the total number of degrees of freedom.

In particular, we addressed and developed the following topics:

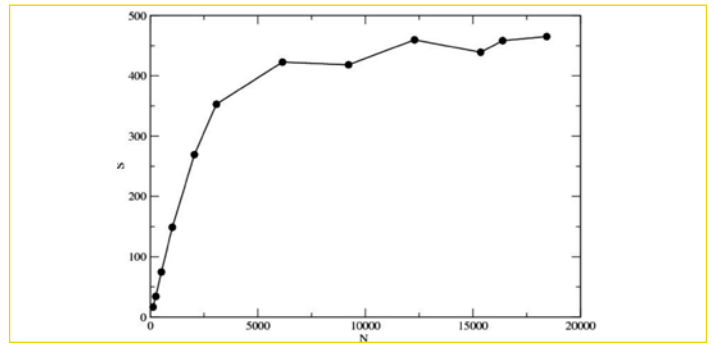
- *high order solvers for PDEs.* The main characteristic of SEMs is to combine the exponential convergence properties of global Spectral Methods with the domain discretization capability of low-order Finite Elements Methods (FEMs). Typically, the elements size of a SEM is much larger than the elements size required by a finite element discretization. Moreover, the conformity property between contiguous elements is more restrictive for quadrilateral meshes than for triangular ones. These characteristics could sometimes limit the geometric discretization flexibility of the spectral element method, and its applicability to problems of practical interest, especially when domains have geometric singularities and for solutions with low regularity. This limit might be resolved by the implementation of nonconforming formulations, e.g. the SEM with Pointwise Matching Condition (PMC) as well as the Symmetric Interior Penalty Galerkin (SIPG) methods. We have presented and numerically tested the accuracy of such high order methods on nonconforming configurations. Namely, we have addressed the question of how the convergence rate of such methods behaves for different hN-adaptive algorithms, for which an automatic refinement of h or N parameters need to be characterized;
- *a posteriori error estimate* on the cost functional. In order to evaluate the accuracy on the cost functional (employed to design an adaptive spectral element method) we have presented a posteriori error estimates on the cost functional, based on a duality argument, by which the error on the state, adjoint and control functions are related one to each other;
- *design of hN-adaptive strategies.* We have designed hN-adaptive strategies for the automatic local refinement of the mesh size as well as the polynomial approximation degree on each spectral element, associated to the optimal control problem. The error estimate on the cost functional is considered as an effective measure of the discretization error of the optimal control problem. The proposed hN-adaptive algorithms are based on the splitting of the error on the cost functional in two components: an iteration error and a discretization error. For linear optimal control problems, the iteration error is minimized in the iterative process for the optimal control solution. Instead, the discretization error is reduced via the adaptive strategy, through the use of a posteriori error estimate. The choice between h or N refinement is based on a predicted error reduction algorithm.

Numerical tests have highlighted the good convergence properties of the considered discretizations, the efficiency of the error estimate and the associated hN-adaptive strategy. In such tests, the proposed estimate for the discretization error has driven to an automatic design of either the mesh and the polynomial degrees in a configuration strictly dependent on the problem considered. More information are used where the state function change more rapidly.
Finally, we have applied the proposed hN-adaptive algorithm to environmental pollution control problems. By mathematical simulations based on atmospheric dispersion modelling, one can describe how the air pollutants disperse in the ambient atmosphere. Then, these dispersion models can be used to estimate or to predict the downwind concentration of air pollutants emitted from sources such as industrial plants. Numerical results have been carried out on different atmospheric stability classes. The same strategy here proposed can be extended to many engineering problems of practical interest.

GPU ACCELERATION OF RAREFIED GAS DYNAMIC SIMULATIONS

Gian Pietro Ghiroldi

At macroscopic length scale, the continuum description of gas flows using the Navier-Stokes equation is, in most situations, accurate enough to describe flows under usual conditions. However, when the characteristic length scale of the physical domain is comparable with the molecular mean free path (the average distance travelled by molecules between collisions) or when there is steep gradients in fluid properties (such as in the interior of a shock wave) the Navier-Stokes equation cease to be valid and the kinetic equations must be used.
Kinetic theory of gases deals with non-equilibrium gas flows which are met in several different physical situations ranging from the re-entry of spacecraft in upper atmosphere to fluid-structure interaction in small-scale device. The numerical solution of the kinetic equations for realistic flow conditions is a challenging task because the unknown function depends, in principle, on seven variables. Moreover the computation of the Boltzmann collision operator requires the approximate evaluation of a fivefold integral. Among the numerical methods of solution used in rarefied gas dynamics, the DSMC method is the most popular and widely used. However, in simulating high frequency unsteady flows, typical of microfluidic applications, the computing effort required by the DSMC becomes often so high to make numerical simulations prohibitive. In such situations using direct methods to solve the Boltzmann equation is a valid alternative. An important feature of kinetic equations for dilute gases is the locality of the collision term, hence the time consuming evaluation of the collision integral can be concurrently executed at each spatial grid point on parallel computers.
Today massively data-parallel systems such as the Graphics Processing Units (GPUs) are available for approximately two single-precision GFLOP/s per Euro, several order of magnitude less expensive than supercomputers a decade ago. Unfortunately, the level of effort and expertise required to maximize application performance on these kinds of systems has not significantly decreased during the past few years. Mainly for this reason only few applications used these relatively low-cost systems to perform work that would otherwise take a large compute clusters of traditional processors. Over the last two years using GPUs for general purpose computation is becoming easier, as different programming systems are made available on the market. In particular the system provided by NVIDIA® called CUDA™ (Compute Unified Device Architecture), used throughout this work, exposes the GPU processing power in the C programming language and can be integrated in existing applications with ease. This capability has led to many successful applications in computational physics where GPUs have been used to accelerate CPU critical applications such as molecular dynamics, computational fluid dynamics, magnetized plasma and many more. However no applications to kinetic theory of gases seem to have been considered yet.
The present work has investigated the possibility of exploiting the computational power of modern GPUs to solve kinetic equations in rarefied gas dynamics. The work progressed in three stages. In the first stage in order to make the algorithm development easier, the computations have been performed replacing the full non-linear Boltzmann collision integral with its simpler BGKW approximation. By solving two benchmark problems such as the one dimensional shock wave structure and the two dimensional driven cavity flow it has been shown that adopting a particularly simple form of the numerical scheme



1. Speed up factor S of the parallel code versus the number of cells in physical space N_s for the driven cavity flow problem. $S = T_{CPU}/T_{GPU}$ where T_{CPU} and T_{GPU} are the times used by the CPU and GPU respectively.

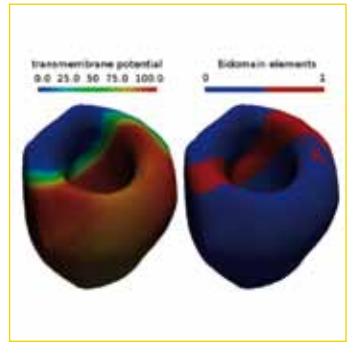
(rectangular space cells, uniform and fixed grid size) the porting of the sequential code onto GPUs allows a reduction of the computing time of two orders of magnitude with respect to the CPU implementation.

In view of this encouraging result the second stage involved the numerical solution on the GPU of the full nonlinear Boltzmann equation.
The Boltzmann equation has been solved on a regular non -uniform grid of the phase space with a Monte Carlo method with a variance reduction technique for the evaluation of the collision integral.
By solving the two dimensional driven cavity flow it has been shown a reduction of the computing time of two orders of magnitude (see Figure 1).
The test problem have also clearly shown the main obstacle toward the application of the GPU algorithms to more complex flows. The major limiting factor of the GPU implementations for the Boltzmann equation is the size of the physical memory, not the number of the crunching capability.
Thanks to the reduction of the computing time, it has been possible, to perform a quite preliminar exploration of the limits of linearized kinetic theory, in the last part of the work. Two-dimensional driven cavity subsonic flows have been computed in a wide range of the reference Mach number.
As expected, it has been found that the linearized theory can provide accurate results only within a limited range of the Mach number. The deviation from linearized theory also depends on the particular flow quantity of interest.
For example, the linearized theory can accurately predict the velocity flow field up to Mach 0.3. For other macroscopic quantities, such as the mean tangential component of the heat flux along the moving plate, the limits of applicability of the linearized theory is further reduced. The obtained results are of some interest for DSMC applications, since there seems to be overlap between the validity range of the linearized kinetic theory and the range where traditional DSMC can produce accurate results with reasonable computing effort. Such overlap might allow for rescaling DSMC solutions at relatively high Mach number (say 0.1) down to smaller values. Future research will be devoted to the GPU implementation of more accurate numerical schemes in order to reduce the memory demand of the present formulation. This is a compulsory step toward the analysis of more complex two or three dimensional flows involving also gas mixtures.

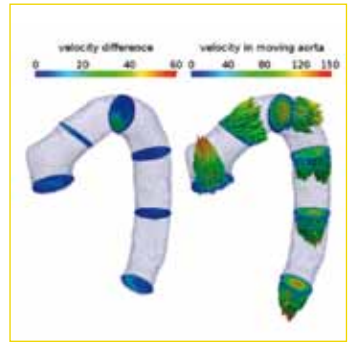
NUMERICAL METHODS FOR CARDIOVASCULAR PROBLEMS: COMPUTATIONAL ELECTROCARDIOLOGY AND FLUID DYNAMICS IN MOVING DOMAINS

Lucia Mirabella

This work addresses the mathematical modeling and numerical simulation of cardiovascular phenomena, such as the propagation of the electrical signal in the heart and the blood flow in large arteries. It is part of a research line devoted to set up a system of mathematical models, numerical techniques and software tools able to help clinicians by providing additional information to support the medical decision process, in the relevant and complex field of cardiovascular diseases. This work focuses both on the development of accurate and efficient methods for electrocardiology simulations and on the integration of medical data on the motion of biological tissues within the numerical models and simulations.
We introduce the main features of the circulatory system, describing with more details anatomy, physiology and some pathological behaviors of the heart. In particular we present the organization of the myocardial tissue and the micro- and macroscopical mechanisms that make the electrical signal propagate, since a large part of the present work concerns the effective numerical simulation of this phenomenon. We then focus on the mathematical models that are commonly used to describe the signal propagation in the tissue. More precisely, models for electrocardiology result from the coupling between a cell level model, which reproduces the sudden variation of the electrical potential across a single cell membrane, and a tissue level one, which describes how the transmembrane potential propagates in the tissue.
The transmembrane potential variation in time (called *action potential*) is due to chemical processes at microscopical level and can be modeled by exploiting equations of different complexity, according to the level of detail to be reached. Here we focus on the simple *Rogers-McCulloch* model and the more complex *Luo-Rudy phase I* model.
The most used models for the action potential propagation in the tissue are the accurate Bidomain model, which describes both the extracellular and the intracellular domain, and the Monodomain model, a simplified version of the Bidomain one. Due to its mathematical structure, the Bidomain model is expensive to be solved numerically while the Monodomain model is less expensive but does not reproduce accurately the action potential propagation in some cases. To exploit the advantages of both models, two novel numerical methods have been developed during this work and are reported in the thesis. In particular we first present an ad-hoc preconditioner for the Bidomain, based on a proper reformulation of the Monodomain problem, developed and tested in collaboration with L. Gerardo-Giorda, F. Nobile, M. Perego and A. Veneziani. This preconditioner is proven to be optimal with respect to the mesh size parameter and 3D numerical tests show that it leads to important reductions (more than 50% on fine meshes) of the CPU time required by the simulation, with respect to a standard strategy. Secondly we propose a model adaptivity strategy, which consists in solving a hybrid model called Hybridomain, corresponding to the Bidomain model in a partition of the computational domain, and to the Monodomain one in the remaining part (joint work with F. Nobile and A. Veneziani).
The choice of the partition is time dependent and is performed on the basis of a model error estimator which controls the difference between the solution of the Bidomain and the solution of the Hybridomain model.
The Bidomain is locally activated where the model error estimator is large, while the Monodomain in solved elsewhere (Fig. 1).



1. 1. Transmembrane potential (in mV) computed using the Hybridomain model (on the left) and corresponding partition of the domain (on the right) in Bidomain (red) and Monodomain elements (blue). The Bidomain activation captures the propagating front.



2. Comparison between the fluid velocity (cm/s) computed by the FD simulation and the one computed by the IB motion simulation. The picture displays the difference between these velocity fields (on the left) and the IB velocity field (on the right).

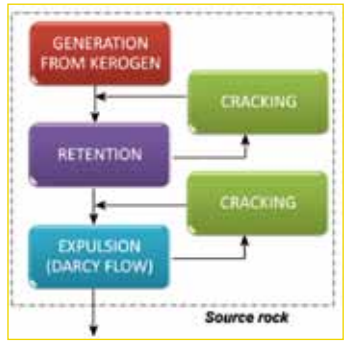
Simulations of healthy and unhealthy behaviors, on 3D heart geometries, show that this strategy, which can also be coupled to the use of the Monodomain preconditioner, allows to save computational time and to maintain a good accuracy of the results.
In the last part of the work we focus on developing and testing a pipeline to include the actual motion of biological structures in the simulation. This technique has a general validity, and it has been successfully applied in this work to the simulation of blood fluid dynamics in moving vessels. In particular from a set of medical images of a specific region acquired at different time frames during the cardiac cycle, we extract the domain of interest and we track the motion of each point in time, using a proper registration algorithm (in collaboration with M. Piccinelli). To this aim, a registration algorithm called *non-rigid viscous fluid registration* is studied and implemented, obtaining promising preliminary results. Then the problem equations are formulated in a moving domain framework. In the case of blood flow in arteries the natural choice is the *Arbitrary Lagrangian Eulerian formulation*. Finally the simulation of the interested phenomenon is performed in a moving domain. This image-based (IB) motion strategy is applied to the modeling of blood flow in a patient-specific aortic arch geometry, comparing the results with a fixed-domain (FD) simulation (in collaboration with T. Passerini) (Fig. 2).

We also propose a validation of the approach, through a comparison with the results of a more standard fluid-structure interaction (FSI) algorithm. The technique is promising since the differences between the two computed solution fields are very small and the IB motion numerical simulations require less computational effort than standard FSI strategies. The same pipeline can be applied to perform electrocardiology simulations in a moving heart, but the large displacements occurring in the heart make it necessary to devise ad hoc registration algorithms. A particular attention in the present work has been devoted to the design and implementation of algorithms in order to develop and test the numerical approaches proposed, in the framework of the LifeV software project (www.lifev.org).

A NUMERICAL MODEL FOR GENERATION, RETENTION, AND EXPULSION OF HYDROCARBONS FROM SOURCE ROCK

Anna Scotti

Oil industry is resorting more and more often to mathematical and numerical modeling to locate new oil and gas reservoirs, and to exploit the existing ones at their best. Oil exploration is indeed a very expensive and risky operation, with a chance of success ranging from 30 to 80%. The numerical simulation of generation and migration processes can support geologic analysis in tracking hydrocarbons ''from source to trap" and therefore reduce the risk in oil exploration.
The generation of hydrocarbons - oil and gas - takes place in a layer of sediments rich in organic matter called source rock in correspondence of an interval of pressure and temperature known as the ''oil window". The generated hydrocarbons then migrate to accumulate in a reservoir. Migration consists of two distinct stages, characterized by different mechanisms and time scales: during the first stage, denoted as primary migration, oil and gas are expelled from the source rock as the layer compacts, while during secondary migration the hydrocarbons move towards the reservoir through the porosity and fractures of the rocks.
We developed a mathematical model for generation and primary migration of hydrocarbons and an efficient numerical tool for their simulation. A realistic numerical simulation of these processes allows, first of all, given the thermal history of the basin and the physical characteristics of the source rock such as porosity and organic matter content, to estimate the amount of hydrocarbons generated throughout hundreds of million years. Moreover numerical simulations can provide information on the timing of expulsion supporting and completing the reconstructions made by geologists. Finally, if a detailed description of chemical reactions and retention processes is provided, it is possible to forecast the chemical composition of the products, which is typically very different from that resulting from laboratory analysis, and most of all the fraction of gas versus oil in the expelled products. This last information has obviously a major economic impact.
Primary migration is characterized by a strong coupling among chemical reactions, selective retention phenomena and the flow of water and hydrocarbons in the porosity of the rock. Most of the models proposed so far in literature either focus on retention processes, relying on a detailed reaction scheme, or model the fluid flow in the rock accounting for a simplified single-component generation. The detailed simulation of generation and retention, coupled with a multi-phase and multi-component fluid flow is indeed a challenging task.



1. Generation, retention and expulsion of hydrocarbons: a flow chart of the process

The solid organic matter, called kerogen, which is part of the source rock, at the proper temperature starts cracking into simpler molecules generating hydrocarbons. The products can in turn undergo chemical reactions, denoted as cracking reactions, and form lighter compounds. Recently the concept has been established that it is important to take into account retention processes such as the solution of hydrocarbons into the organic matter, or the trapping of molecules in nanometric pores. These phenomena depend strongly on the molecular properties, therefore some types of hydrocarbons are more likely to be retained than others and the global chemical composition of the products can change significatively. The expulsion of the ''free" products from the source rock has not been completely understood yet, mostly because it is very difficult to replicate the process in a laboratory experiment or to take direct measurements of source rocks. So far the existing models are either based on compaction or diffusion as the main driving force for expulsion. We model expulsion as a Darcy flow driven by compaction, and regard water and hydrocarbons as immiscible phases. It must be stressed that the products keep undergoing cracking reactions until they finally leave the source rock, therefore the model must simulate chemical reactions coupled with the fluids flow since the characteristic time scales of reactions and expulsion are comparable.
The algorithm for the numerical approximation of the problem relies on a sequential approach to decouple the equations. A fully coupled approach, although possible in principle, would be very expensive in presence of nonlinear and discontinuous reaction terms. The two-phase Darcy problem, cast as a parabolic equation for pressure and a degenerate parabolic equation for the oil phase saturation, is decoupled via a sequential splitting analogous to the well known IMPES (Implicit Pressure-Explicit Saturation) approach which is often employed in reservoir simulations. Mixed hybridized finite elements are employed for the approximation of the Darcy law, because of their good properties of local mass conservation and flux continuity, at the expense of a slightly higher computational cost with respect to classic methods. The equation for the oil phase saturation, which expresses a mass balance for the hydrocarbons in the source rock, is an advection-diffusion-reaction equation with degenerate diffusion. Its approximation is based on an ADR (advection-diffusion-reaction) operator splitting which allows to solve the advection part as a nonlinear conservation law via a Godunov method, and the diffusion part exploiting the expanded FEM method. As concerns the reaction part, the integration of chemical reactions must satisfy mass conservation and preserve the nonnegativity of the solution at any time. Moreover the presence of retention processes introduces jump discontinuities in the ODE system that describes the chemical reactions with additional difficulties from the analytic and numeric point of view.
The results of the simulations proved that the chemical reactions and the fluid flow strongly influence each other, therefore a correct prediction of the expelled products quality and of the expulsion time is possible only if the coupled system is considered. For instance, a different spatial distribution of the organic matter can influence the expulsion timing and thus yield a different chemical composition. Conversely, the results also showed that retention processes not only change the composition of the expelled hydrocarbons, but modify the timing of expulsion, which is slightly delayed. Both monodimensional (along the rock thickness) and bidimensional (in a vertical section) simulations showed that the diffusion due to the presence of capillary pressure not only is not negligible, but plays an important role in expulsion.
The work presented in this thesis has been sponsored by Eni S.p.A, and part of the algorithms developed has been implemented in a software for the simulation of primary migration currently in use at Eni S.p.A. They are being tested against experiments being carried out at the Eni laboratories.