INRIA

Project-Team SIMPAF

SImulations and Modeling for PArticles and Fluids

Lille - Nord Europe

Theme : Computational models and simulation

Activity Report

2010

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The SIMPAF project mainly emanates from the PDE team of the department Paul Painlevé (UMR 8524 of CNRS) of the University of Sciences and Technologies of Lille (USTL); it has also strong interaction with other math departments in the North area (Amiens, Valenciennes) and in Paris.

1. Team

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2. Overall Objectives

2.1. Overall Objectives

The project aims at

- Studying models that describe the evolution of a fluid and/or of a large number of particles;
- Discussing the relevance and the range of validity of these models;
- Analyzing connections between different levels of modelling;
- Developing efficient numerical methods to compute the solutions of such models.

3. Scientific Foundations

3.1. PDEs for Particles and Fluids

The scientific activity of the project is concerned with PDEs arising from the physical description of particles and fluids. It covers various viewpoints:

- At first, the words "particles and fluids" could simply mean that we are interested independently in models for particles, which can either be considered as individuals (which leads to "N-particle models", N ranging from 1 to many) or through a statistical description (which leads to kinetic equations) as well as in models for fluids like Euler and Navier-Stokes equations or plasma physics.

- However, many particle systems can also be viewed as a fluid, via a passage from microscopic to macroscopic viewpoint, that is, a hydrodynamic limit.

- Conversely, a fruitful idea to build numerical solvers for hyperbolic conservation laws consists in coming back to a kinetic formulation. This approach has recently motivated the introduction of the so-called kinetic schemes.

- Eventually, one of the main topics of the project is to deal with models of particles interacting with a fluid.

By nature these problems describe multi-scale phenomena and one of the major difficulties when studying them lies in the interactions between the various scales: number of particles, size, different time and length scales, coupling...

The originality of the project is to consider a wide spectrum of potential applications. In particular, the word "particles" covers various and very different physical situations, like for instance:
- charged particles: description of semi-conductor devices or plasmas;
- photons, as arising in radiative transfer theory and astrophysics;
- neutrons, as arising in nuclear engineering;
- bacteria, individuals or genes as in models motivated by biology or population dynamics;
- planets or stars as in astrophysics;
- vehicles in traffic flow modelling;
- droplets and bubbles, as in Fluid/Particles Interaction models which arise in the description of sprays and aerosols, smoke and dust, combustion phenomena (aeronautics or engine design), industrial process in metallurgy...
We aim at focusing on all the aspects of the problem:

- Modelling mathematically complex physics requires a deep discussion of the leading phenomena and the role of the physical parameters. With this respect, the asymptotic analysis is a crucial issue, the goal being to derive reduced models which can be solved with a reduced numerical cost but still provide accurate results in the physical situations that are considered.

- The mathematical analysis of the equations provides important qualitative properties of the solutions: well-posedness, stability, smoothness of the solutions, large time behavior... which in turn can motivate the design of numerical methods.

- Eventually, we aim at developing specific numerical methods and performing numerical simulations for these models, in order to validate the theoretical results and shed some light on the physics.

The team has been composed in order to study these various aspects simultaneously. In particular, we wish to keep a balance between modelling, analysis, development of original codes and simulations.

3.2. Interactions of Micro- and Macroscopic Scales, Modelling and Simulations

3.2.1. Reduced Models; Hydrodynamic Limits

In the study of kinetic equations, it is a very usual strategy to perform a hydrodynamic limit, and then to get rid of the velocity variable and replace the kinetic equation by a convection-diffusion model. This kind of derivation is well established, under various forms, and in several fields of applications: neutron transport, semiconductor theory, SHE[1] models... However, several questions of great interest have not yet been solved:
- The computation of the convection-diffusion coefficients of the limit equation, a question which leads to additional difficulties when the small mean free path asymptotics are combined with a homogeneization limit. This problem is motivated by applications in nuclear engineering. In this case, the effective coefficients are defined through auxiliary equations and suitable averages of the oscillatory coefficients.
- Some recent works have revealed the formation of singularities in the solutions of some limit convection-diffusion equations, while the original kinetic equation has globally defined solutions. This is due to a coupling in the definition of the convective term with the macroscopic density. This singularity formation is typical of aggregation dynamics. It occurs in models with gravitational forces in astrophysics, and chemotaxis models in biology. Therefore, the natural problems are either to provide a sharp analysis (theoretical and/or based on numerics) of the singularity formation, or to complete the model to avoid such trouble.
- A crucial question for applications is to write models for intermediate regimes, for small but non zero values of the mean free path. Such models are required to remain solvable with a moderate computational cost, and to preserve more features from the kinetic level (as for instance finite speeds of propagation, which is lost with a diffusion equation). An example of such an intermediate model is the moment system obtained by using a closure by Entropy Minimization. We have proved that this model is indeed consistent with the diffusion approximation, and we propose an original scheme to treat these equations numerically. We introduce a relaxation strategy which in turn is naturally amenable to the use of asymptotic preserving splitting methods and anti-diffusive schemes for transport equations that are developed in the team. Therefore, we can compare various limited flux models and discuss on numerics their properties and advantages.

3.2.2. Radiative Transfer Theory

We are interested in the equations of the radiative transfer theory which are motivated by the description of high temperature combustion processes (spacecraft propulsion, reentry problems), space observation, nuclear weapons engineering, or inertial confinement fusion. Such problems can be described by a coupling between kinetic and macroscopic equations that comes from the "collision term", through energy, or energy-impulsion, exchanges. The hydrodynamic limit yields coupled macroscopic equations, with possibly two distinct temperatures: the temperature of the radiations and the temperature of the material. Taking into account Doppler and relativistic effects adds convective terms, which in turn might give rise to the formation of specific singularities.

The interesting points can be summarized as follows:

- The derivation of the reduced models, based on modeling arguments, is an issue, bearing in mind to describe a complete hierarchy of models;

- The coupling induces non trivial effects on the structure of the hydrodynamics system, which can modify strongly the qualitative properties of the solutions. In particular, the radiative transfer equations might exhibit non standard shocks profiles, with possible discontinuities. The computation of such discontinuous shock profiles requires a very accurate and non-diffusive numerical scheme for the convective terms. This also leads to the delicate question of the stability of travelling waves solutions.

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[1] referring to the standard vocabulary in Physics for Spherical Harmonics Expansion

These topics are the object of a very intense research activity e.g. at the Department of Computational Physics of the Los Alamos National Laboratory as well as at the French Atomic Energy Agency (CEA). We develop alternative numerical methods, based on tricky splitting approaches. When dealing with kinetic models, such methods have to be specifically designed to preserve the asymptotic properties of the model. In this approach, one computes on a time step the evolution of the unknown due the convective terms, which will be handled by anti-diffusive schemes (see the paragraph Conservation Laws below), and on the next time step, we treat source and interaction terms, that can be nonlocal and/or stiff. This leads to a fully explicit scheme which provides accurate results for a cheap numerical cost and which does not require a tedious inversion step as the implicit methods usually do. We are able to treat numerically the full coupling of radiation with hydrodynamics (Euler equations) in the non equilibrium diffusion regime.

3.2.3. *Fluid/Particles Interactions*

These models arise in the modelling of disperse suspensions in fluids, say droplet or bubble motion. Their study is motivated by applications to combustion, rocket propulsor engineering, biology, aerosols engineering, or for certain industrial processes. The main effect to take into account is the Stokes drag force, which is proportional to the relative velocity between the particle and the surrounding fluid $F(t, x, v) = \gamma(u(t, x) - v)$. However, modelling remains a major issue in this field; in particular, here are some important questions :

- Complementary effects can be taken into account: the so-called Basset force, or the added mass effect, etc. For instance, when particles flow in a pipe, a phenomenological lift force, proportional to $v \times (v - u)$, has been proposed to mimic the tendency of particles to concentrate at the center of the pipe. Even though it is moderate in strength, such a force can have crucial effects on blood flows, or on industrial processes of steel production.

- Up to now, there are only a few contributions on the description of size variations, by coagulation or fragmentation and break-up. However, in practical situations, as for combustion or biology applications, these phenomena cannot be neglected.

- Of course, the coupling with the evolution of the surrounding fluid is a crucial question that leads naturally to problems of asymptotics. Effects of "turbulence", which roughly means high and fast variations of u on the behavior of the particles, have been analyzed in some simplified situations.

The coupling with the Navier-Stokes or the Euler equations is a privileged subject for SIMPAF. Some asymptotics lead to two-phase flows models, that we are interested in investigating both from a theoretical and numerical point of view. In particular, the effect of an external force (gravitational or centrifugal) can lead to sedimentation profiles that are suspected to be stable; we would like to confirm these heuristics by a thorough numerical and theoretical study. Of course, such investigations require efficient numerical schemes to solve the fluid equations with source terms, which will be detailed in the next sections. To this end, we adapt to this framework the numerical schemes we develop for radiative transfer problems, based on splitting methods and a suitable use of the asymptotic expansion.

3.2.4. *Homogenization methods*

Homogenization methods aim at replacing a PDE with highly oscillatory coefficients by an effective PDE with smoother coefficients, whose solution still captures the "mean-field" behavior of the true oscillatory solution. The effective determination of the homogenized PDE is however not trivial (especially in the nonlinear or/and stochastic cases). Numerical approximations of the solution of the homogenized PDE is the heart of numerical homogenization.

Homogenization methods are used in many application fields. The two applications we are specifically interested in are material sciences (in particular the determination of macroscopic constitutive laws for rubber starting from polymer-chain networks) and in nuclear waste storage (in particular the evolution of nuclear wastes in complex storage devices). People involved are primarily A. Gloria, T. Goudon, and S. Krell.

The first application raises questions related to discrete stochastic homogenization of nonlinear systems, namely convergence results [8], the development of efficient numerical methods to approximate homogenized quantities [33], [23] and their analysis [24], [41], [34]. An extensive numerical study with a comparison to mechanical experiments is under progress within the ARC project DISCO. A further direction of research (initiated with the post-doc of M. de Buhan starting in December 2010 in the MACS project-team) is the analytical reconstruction of constitutive laws from in silico experiments, taking into account the specific form and properties of the expected homogenized energy density (as proved in [8]). This general strategy also applies to the homogenization of nonlinear elliptic PDEs.

The second application is in collaboration with the French agency for nuclear waste storage (ANDRA), and has started with the post-doc of S. Krell in October 2010. ANDRA is particularly interested in a system of nonlinearly coupled PDEs displaying a periodic structure at a rather small scale, and modeling the solute transfer of radioactive wastes in saturated porous media. The first question consists in determining the form of the effective coupled system of PDEs, as well as formulas for its coefficients. The second objective is to develop efficient numerical methods to approximate the solution of this system.

3.3. Charged Particles

3.3.1. *Modeling of Plasma Confinement*

Plasmas, the fourth state of the matter, play an important role in many branches of physics, such as thermonuclear fusion research, astrophysics and space physics. A plasma is a (partially) ionized gas where charged particles interact via electromagnetic fields. Since the announcement of the creation of the experimental fusion reactor ITER, and with the progress on the ICF[2] program, plasmas and their modelling got a renewed interest.

The nuclear fusion mechanisms result from the strong confinement of charged particles, either by inertial confinement (nuclear fusion reactions are initiated by heating and compressing a target - a pellet that most often contains deuterium and tritium - by the use of intense laser or ion beams) or by the - more promising - magnetic fusion confinement. The tokamaks are experimental devices which produce a toroidal magnetic field for confining a plasma.

The description of these phenomena is extremely complex and leads to delicate problems in mathematical analysis and numerical simulation. Actually, plasmas may be described with various levels of detail. The simplest possibility is to treat the plasma as a single fluid governed by the Navier Stokes Equations. A more general description is the two-fluid picture, where the ions and electrons are considered to be distinct. If electric or magnetic fields are present, then the Maxwell equations will be needed to describe them. The coupling of the description of a conductive fluid to electromagnetic fields is known generally as magnetohydrodynamics, or simply MHD.

For some cases the fluid description is not sufficient. Then, the kinetic models may become useful. Kinetic models include information on distortions of the velocity distribution functions with respect to a Maxwell-Boltzmann distribution. This may be important when currents flow, when waves are involved, or when gradients are very steep.

The main mathematical difficulties are therefore linked to the conjunction of the following elements

- these two types of models are strongly nonlinear,
- the unknowns depend on the time and space variables and, in the case of kinetic models, also on the velocity variables. Therefore, we can be led to work with variables of $1 + 3 + 3$ dimensions,
- there exist many very different scales (time scale, characteristic length ...)

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[2]Inertial Confinement Fusion

The numerical resolution of a complete system of equations, with meshes adapted to the lower scales, leads to prohibitive computational costs both in terms of memory and time. The derivation of new reduced models, corresponding to relevant asymptotic regimes (high magnetic field for example), is therefore a crucial issue. Moreover, very serious efforts must be done on the numerical methods that are used in order to reproduce the typical phenomena. This work depends on the one hand on seriously thinking over the models, the physical parameters, their typical respective scales, and on the other hand over some arguments of asymptotic analysis, which can particularly call on deterministic or random homogeneization.

3.3.2. *Spacecraft Environment*

Satellites in geostationary and low Earth orbits naturally evolve in a plasma. This ionized environment induces some perturbations which may lead to many kind of faults and to the partial or complete loss of a mission. The satellites are covered by dielectric coatings in order to protect them against thermal radiations. Electrons and ions species of the space plasma interact with the external surfaces of the satellite and modify their electrostatic charges. This effect produces potential differences between the satellite surfaces and its electric mass. When the electric field exceeds a certain level, an electrostatic discharge appears. This electric current pulse is able to disrupt the equipments, to damage the external surfaces and even to destroy some electronic components. The plasma may also be created by an other source : the electric thrusters. This new propulsion device uses the electric energy supplied by solar arrays to speed up charged species. It is more and more used in satellite industry and has preference over the classical chemical propulsion. Indeed, the latter needs a very large amount of propellant inducing an expensive rocket launch. On the one hand, the electric thrusters allow to significantly reduce the satellite weight. On the other hand, it is necessary to understand their potential impacts on the other systems of the satellite.

This line of research, which continues former works of the team CAIMAN at Sophia Antipolis, is the object of a strong collaboration with the Department Research and Technology of the company Thales Alenia Space. In this context, the PhD of S. Borghol aims at deriving models specifically adapted to the LEO or PEO altitudes[3] instead of the standard GEO[4] framework. Analysis of the models and design of numerical schemes is also discussed. N. Vauchelet proposed several evolutions for the SPARCS code, including parallel procedures. A comparizon of different numerical schemes (Finite Volume, Semi-Lagrangian, Back Trajectory) to treat the Vlasov equations of spacecraft charging has been discussed in details.

3.3.3. *Effective Energy Dissipation Models for Charged Particles*

In models of charge transport, say transport of electrons, a phenomenological friction force is generally introduced, which is proportional to the velocity v. Our idea is to go back to a more microscopic framework, with a description of the energy exchanges between the electrons and the surrounding medium. In turn, the dissipation of energy by the medium will lead to an effective friction force. The first contributions only model the transport of a unique particle, and we aim at considering now a plasma, through a statistical description. This yields a Vlasov-Poisson-like model. (More precisely, the kinetic equation is coupled to a finite, or infinite, set of oscillators.) This program requires efforts in modelling and analysis, but the questions are also really challenging for numerics, due, on the one hand, to the large number of degrees of freedom involved in the equation, and on the other hand, to the presence of stiff terms. In this way, we expect to be able to shed light on the range of validity of the Ohm law. Similar considerations also apply for heat transport and the derivation of the Fourier law.

3.4. Simulations of Complex Fluid Flows

3.4.1. *Conservation Laws*

A major issue in the numerical approximation of systems of conservation laws is the preservation of singularities (shocks, contact discontinuities...). Indeed, the derivatives of the solutions usually blow-up in finite time. The numerical scheme should be able to reproduce this phenomenon with accuracy, i.e. with a

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[3]Low Earth Orbit and Polar Earth Orbit respectively
[4]Geostationary orbit

minimum number of points, by capturing the profile of the singularity (discontinuity), and by propagating it with the correct velocity. The scheme should also be able to give some insight on the interactions between the possible singularities. Quite recently, new anti-diffusive strategies have been introduced, and successfully used on fluid mechanics problems. We focus on multidimensional situations, as well as on boundary value problems. Since a complete theory is not yet available, the numerical analysis of some prototype systems of conservation laws is a good starting point to understand multi-dimensional problems. In particular, a good understanding of the linear case is necessary. This is not achieved yet on the numerical point of view on general meshes. This question is particularly relevant in industrial codes, where one has to solve coupled systems of PDEs involving a complex coupling of different numerical methods, which implies we will have to deal with unstructured meshes. Thus, deriving non-dissipative numerical schemes for transport equations on general meshes is an important issue. Furthermore, transport phenomena are the major reason why a numerical diffusion appears in the simulation of nonlinear hyperbolic conservation laws and contact discontinuities are more subject to this than shocks because of the compressivity of shock waves (this is another reason why we focus at first on linear models).

The next step is to combine non-dissipation with nonlinear stability. An example of such a combination of preservation of sharp shocks and entropy inequalities has been recently proposed for scalar equations and is still at study. It has also been partially done in dimension one for Euler equations.

Of course, there are plenty of applications for the development of such explicit methods for conservation laws. We are particularly interested in simulation of macroscopic models of radiative hydrodynamics, as mentioned above. Another field of application is concerned with polyphasic flows and it is worth specifying that certain numerical methods designed by F. Lagoutière are already used in codes at the CEA for that purpose. We also wish to apply these methods for coagulation-fragmentation problems and for PDEs modelling the growth of tumoral cells; concerning these applications, the capture of the large time state is a particularly important question.

3.4.2. *Control in Fluid Mechanics*

Flow control techniques are widely used to improve the performances of planes or vehicles, or to drive some internal flows arising for example in combustion chambers. Indeed, they can sensibly reduce energy consumption, noise disturbances, or prevent the flow from undesirable behaviors.

Recently, open and closed active flow control was carried out in order to study the flow behavior over a backward-facing step in a transitional regime. It was done either by a global frequency destabilization at the entry of the domain, or by a local blowing or suction through the lower and upper parts of the step by the use of small jets ([60], E. Creusé, A. Giovannini (IMFT Toulouse) and I. Mortazavi (MC2 INRIA EPI, Bordeaux)). The numerical computations were based on a vortex-in-cell method. Such controls were shown to be efficient in reducing the average recirculation length value, the global flow energy, as well as the global flow enstrophy. Our objective is now to apply such a strategy on cavity flows, in order to study the effect of passive and/or active control on the average emptying time of the cavity, having in mind a lot of possible industrial or health applications (combustion, blood circulation in arteries,...).

Passive as well as active control was also performed on the "Ahmed body geometry", which can be considered as a first approximation of a vehicle profile. This work was performed in collaboration with the EPI INRIA MC2 team in Bordeaux, in the context of the research and innovation program on terrestrial transports supported by the ANR and the ADEME, leaded by Renault and PSA and managed by Jean-Luc Aider (ESPCI Paris). Here, we had in mind to combine active and passive control strategies in order to reach efficient results, especially concerning the drag coefficient, on two and three dimensional simulations [14]. Now, we are interested in the same kind of study, but for a 25° rear-window configuration, for which the 3D-effects are very important and have to be considered in the numerical simulations.

3.4.3. Numerical Methods for Viscous Flows

In the large scale computations of fluid flows, several different numerical quantities appear that are associated to different eddies, structures or scales (in space as well as in time). An important challenge in the modelling of turbulence and of the energy transfer for dissipative equations (such as Navier-Stokes equations, reaction-diffusion equations) is to describe or to model, for the long time behavior, the interaction between large and small scales. They are associated to slow and fast wavelengths respectively. The multi-scale method consists in modelling this interaction on numerical grounds for dissipative evolution equations. In Finite Elements and Finite Differences discretizations the scales do not appear naturally as in spectral approximations, their construction is obtained by using a recursive change of variables operating on nested grids; the nodal unknowns (Y) of the coarse grids are unchanged (they are of the order of magnitude of the physical solution) and those of the fine grids are replaced by proper error interpolation, namely the incremental unknowns (Z); the magnitude of the Zs is then "small". This allows to make a separation of the eddies in space (presence of nodal and incremental quantities) but also in frequency since the incremental unknowns are supported by the fine grids which capture the high frequencies while the nodal unknowns are defined on coarse grids which can represent only slow modes. Note that this approach differs from the LES model that proposes to split the flow into a mean value and a fluctuation component, the latter having small moments but not necessarily a small magnitude. This change of variable defines also a hierarchical pre-conditioner. It is well known that the (semi)explicit time marching schemes have their stability region limited by the high modes, so a way to enhance the stability is to tread numerically the scales (Y and Z) in a different manner. The inconsistency carried by the new scheme acts only on small quantities allowing for efficient and accurate schemes for the long time integration of the equations. We develop and apply this approach to the numerical simulation of Navier-Stokes equations in highly non stationary regimes. In this framework of numerical methods, we focus on the domain decomposition method together with multi-scale method for solving incompressible bidimensional NSE; the stabilized explicit time marching schemes are also studied.

The already written code can be used to treat certain low Mach number models arising in combustion theory, as well as models describing mixing of compressible fluids arising for instance when describing the transport of pollutants. The interesting thing is that this kind of model can be derived by a completely different approach through a kinetic model. Besides, this model presents interesting features, since it is not clear at all whether solutions can be globally defined without smallness assumptions on the data. Then, a numerical investigation is very useful to check what the actual behavior of the system is. Accordingly, our program is two-fold. On the one hand, we will develop a density dependent Navier-Stokes code, in 2D, the incompressibility condition being replaced by a non standard condition on the velocity field. The numerical strategy we use mixes a Finite Element method for computing the velocity field to a Finite Volume approach to evaluate the density. As a by-product, the code should be able to compute a solution of the 2D incompressible Navier-Stokes system, with variable density. On the other hand, we wish to extend our kinetic asymptotic-based schemes to such problems.

3.4.4. A posteriori error estimators for finite element methods

E. Creusé works on a posteriori error estimators for finite element methods, applied to the resolution of several partial differential equations.
A recent paper, in collaboration with S. Nicaise (LAMAV, Valenciennes), was devoted to the derivation of some so-called "reconstruction estimators" based on gradient averaging, in order to provide lower and upper bounds of the error arising from a discontinuous Galerkin approximation of a diffusion problem [20]. Now, we are interested in the full convection-reaction-diffusion case and are looking for estimations as robust as possible, in which the dependance of the constant in the data are explicitly given.
At the same time, some equilibrated-type estimators are being developed for the Reissner-Mindlin system arising in solid mechanics applications, for conforming and locking-free approximations (E. Verhille PhD). The goal is, ideally, to obtain some "asymptotic exact estimators", in order to provide an accurate bound of the error, while keeping a reasonable computational cost.

At last, a collaboration with the "Laboratoire d'électrotechnique et d'électronique de puissance de Lille (L2EP)" began one year ago, to derive a residual-based a posteriori error estimator for the Maxwell system in its vectorial and scalar potential formulation A/Φ (Z. Tang PhD). Here, the key-point is to obtain a mathematical rigorous error indicator, in order to couple it with the automatic mesh generator used by EDF for very practical issues.

4. Software

4.1. DDNS2

Participants: Caterina Calgaro [correspondant], Jacques Laminie.

The DDNS2 code is a parallel solver for unsteady incompressible Navier-Stokes flows in 2D geometries and primitive variables written in Fortran 95 with MPI as a message-passage library. Mixed finite element methods, with hierarchical basis, are used to discretize the equations and a non overlapping domain decomposition approach leads to an interface problem which involves a Lagrange multiplier corresponding to the velocity (the FETI approach). A dynamical multilevel method is developed locally on each subdomain. Several numerical estimates on the evolution of linear and nonlinear terms allow to construct the multilevel strategy which produces auto-adaptive cycles in time during which different mesh sizes, one for each subdomain, can be considered.

4.2. NS3ED

Participants: Caterina Calgaro [correspondant], Delphine Jennequin.

The NS3ED code is a solver for steady incompressible Navier-Stokes flows in three-dimensional exterior domains, written in C++. The truncated problem is discretized using an exponential mesh and an equal-order velocity-pressure finite element method, with additional stabilization terms. A bloc-triangular pre-conditioner is performed for the generalized saddle-point problem.

4.3. ns2ddv

Participants: Caterina Calgaro [correspondant], Emmanuel Creusé, Thierry Goudon, Emile Chane-Kane.

The ns2ddv code is based on a hybrid method coupling FV and FE approaches for solving the variable density Navier-Stokes equation in dimension 2. This original approach for variable density flows is described in [53]. The current version of the ns2ddv code is being developed around the GetFem++ and the Bamg softwares. It allows in particular mesh refinement strategies so that very relevant simulations can be reached (As the falling droplet with very high density ratios, see for example [25]).

4.4. RTcodes

Participants: Pauline Lafitte [correspondant], Jean-François Coulombel, Christophe Besse, Thierry Goudon.

We have developed a set of numerical codes, written in Scilab, to compute the solutions of the system coupling the Euler equations to the radiation through energy exchanges, in the non equilibrium regime. This covers several situations in the hierarchy of asymptotic problems. The code treats the one-dimensional framework. In particular the code can be used to investigate radiative shocks profiles. The main advantage of our numerical codes is that they do not require any refinement near the singularities. The numerical tests show a very good agreement with the theoretical predictions.

4.5. FPcodes

Participants: Pauline Lafitte [correspondant], Thierry Goudon.

We have developed a numerical code, written in Scilab, to compute the solutions of the two-phase flows equations describing particles interacting with a fluid through friction forces. The code treats one-dimensional situation and is well adapted to describe gravity driven flows in either bubbling or flowing regimes. In particular, it can be used to describe the evolution of pollutants in the atmosphere. The numerical strategy, based on a asymptotic-based scheme, is described in details in [54].

4.6. CLAToolBox

Participants: Christophe Besse [correspondant], Pauline Klein.

As a byproduct of the review paper [46], a user-friendly interface is offered[5] to trial and compare various numerical methods to solve the 1D Schrödinger equation with absorbant boundary conditions. We also mention [49] for a numerical investigation of blow-up phenomena in the nonlinear Schrödinger equation.

4.7. NLWcodes

Participants: Caterina Calgaro [correspondant], Jean-Paul Chehab.

We have developed a set of numerical codes, written in Matlab, to solve various 1D nonlinear wave equations (Korteweg-de-Vries, Benjamin-Ono, nonlinear Schrödinger),with or without damping term. These equations are discretized by pseudo-spectral or finite difference methods (compact schemes); a part of the corresponding study can be found in [52]. We compare the long time stability of various numerical methods and their capability to reproduce some physical invariants. These codes are still in development in order to simulate blow-up phenomena.

4.8. SPARCS

Participants: Christophe Besse, Thierry Goudon [correspondant], Nicolas Vauchelet, Ingrid Lacroix-Violet, Saja Borghol.

SPARCS is the code developed by Thales Alenia Space for the simulation of the charge phenomena the space-crafts are subject to. The current version of the code, according to the PhD thesis of O. Chanrion and M. Chane-Yook performed in collaboration with the team Caiman at Sophia Antipolis, is specialized to geostationary atmospheres. The model consists in the stationary Vlasov-Poisson system, but where instationary effects are taken into account with the boundary condition for the electric field. We participate, in particular through the post doc of N. Vauchelet, to the elaboration of an improved version of the code which includes parallelization optimized procedures, the modeling of the natural difference of potential between different dielectric surfaces of the spacecraft, as well as the possible presence of devices emitting charged particles. We aim at developing new versions designed for LEO and PEO atmospheres.

5. New Results

5.1. Statistical Physics

The analysis of multi-scale phenomena and asymptotic problems aiming at identifying the influence of microscopic scales on the macroscopic observations is a hot topic in the team. Results have been obtained concerning the derivation of effective law describing the behavior of a particle interacting with a thermal bath or a set of oscillators. This work, which combines modeling efforts, analysis and large computations, is the object of a longstanding collaboration with P. Parris (Missouri-Rolla) and is the heart of the PhD thesis of B. Aguer. Some long time effective behavior of related models has been obtained in [64].

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[5]http://math.univ-lille1.fr/~besse/site/recherche/logiciels/index.html

At the same time, M. Rousset is working on the numerical simulation of stochastically perturbed Molecular Dynamics. The main goal is to handle in the same simulation the fastest time scales (the oscillations of molecular bindings), and the slowest time scales (the so-called reaction coordinates). Recently, a monograph [31] has been published which summarized standard and state-of-the-art free energy calculations, that are used to accelerate slow variables in MD simulations. In [44] analysis of constrained dynamics is proposed, with associated numerical schemes. In [66], a new method has been proposed which drastically slows down the fast frequencies with a penalty and accelerates simulations, while conserving the statistical behavior of molecular systems.

Recently, in [67] M. Rousset has initiated some new research on variance reduction in hybrid methods, where a "fine-grained" model, typically a kinetic model, is simulated with particle/Monte-Carlo method, and the variance of the latter is reduced using the information of a "coarse-grained" model, a PDE computed with a grid method.

5.2. Hyperbolic Problems, Conservation laws and Gas Dynamics

The convergence analysis of numerical schemes for conservation laws with unstructured meshes with an original proof based on probabilistic argument is a striking result due to F. Lagoutière with F. Delarue, [21]. More generally, we refer to [65] for an overview of F. Lagoutière's works.

J.-F. Coulombel has studied the stability of finite difference approximations of hyperbolic systems with boundary conditions. This series of works, part of which is a collaboration with A. Gloria, generalizes and simplifies previous results by Gustafsson, Kreiss, Tadmor, Wu and others. In collaboration with O. Guès and M. Williams, J.-F. Coulombel has also studied the justification of geometric optics for hyperbolic boundary value problems. The results describe the reflection of highly oscillating wave trains on a boundary. Eventually, J.-F. Coulombel has studied with S. Benzoni and N. Tzvetkov well-posedness issues for some nonlocal versions of Burgers equation.

5.3. Computational Fluid Dynamics

We develop an original hybrid FV/FE[6] method to compute (2D) variable density viscous flows. The code allows to simulate complex phenomena like e. g. Rayleigh-Taylor instabilities or falling droplet with a very high density ratio [53], [25]. We are also interested in the control of flows by active devices on the backward facing step as well as on the Ahmed body configuration [60], [14]. These questions naturally lead to investigate tools of numerical analysis like e.g. *a posteriori* estimators [61], [20] or linear algebra problems [59]. In [15] C. Calgaro *et al.* address the problem of computing pre-conditioners for solving linear systems of equations with a sequence of slowly varying matrices. This problem arises in many important applications, for example in computational fluid dynamics, when the equations change only slightly possibly in some parts of the domain. In such situations, the papers discusses a number of techniques for computing incremental ILU factorizations.

5.4. Fluid/Particles Flows

We are interested in two-phase flows involving a dense and a disperse phase. These models lead to interesting mathematical questions, [9]. We develop new asymptotic preserving methods for fluid/particles flows [54]. This approach follows the scheme we developed for radiative transfer equations [55].

5.5. Plasma Physics

We obtained several results of asymptotic analysis concerning either kinetic or macroscopic models for charge transport, see [51], [50] and [57] (and we also refer to the related work [58]). Through the collaboration with Thales we participate to the development of Sparcs, a code of simulation for spacecraft electrical charge [12]. We also proposed numerical boundary conditions for the Euler system, derived from microscopic models [36]. This work extends to the derivation of fluid/kinetic matching condition.

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[6]Finite Volume/Finite Element

5.6. Analysis and numerical simulation of the Schrödinger equation

The linear or nonlinear Schrödinger equation with potential is one of the basic equations of quantum mechanics and it arises in many areas of physical and technological interest, e.g. in quantum semiconductors, in electromagnetic wave propagation, and in seismic migration. The Schrödinger equation is the lowest order one-way approximation (paraxial wave equation) to the Helmholtz equation and is called Fresnel equation in optics, or standard parabolic equation in underwater acoustics. The solution of the equation is defined on an unbounded domain. If one wants to solve such a whole space evolution problem numerically, one has to restrict the computational domain by introducing artificial boundary conditions. So, the objective is to approximate the exact solution of the whole-space problem, restricted to a finite computational domain. A review article [46] was written this year to describe and compare the different current approaches of constructing and discretizing the transparent boundary conditions in one and two dimensions. However, these approaches are limited to the linear case (or nonlinear with the classical cubic nonlinearity: an article written was dedicated to this case this year [48]) and constant potentials. Therefore, in collaboration with X. Antoine (IECN Nancy and INRIA Lorraine), we proposed to P. Klein to study, in her PhD thesis, the case of the Schrödinger equation with variable potentials. The study of the non-stationary one-dimensional case has already led to one publication [47] and some preliminary results in the stationary case are really promising. These cases are relevant since for example the equations appear in the Bose Einstein condensate with a quadratic potential.

This problem is obviously not limited to the Schrödinger equation and new developments are in progress on the Korteweg de Vries equation with M. Ehrhardt. This equation is more difficult to study due to its third order derivative in space.

The publications of Guillaume Dujardin for the last two years deal with the long time analysis of exact and numerical solutions of Schrodinger equations. In [63], G.D. shows that a class of high order exponential integrators that are of common use for parabolic equations performs well in finite time for linear and nonlinear Schrodinger equations in periodic d-dimensional domains. In particular, G.D. provides sufficient conditions to achieve high orders with such methods applied to Schrodinger equations. In [56], G.D. shows with F. Castella that the Lie-Trotter splitting method for the computation of numerical solutions of linear Schrodinger equations in a fully discrete setting preserves the regularity of the numerical solution over long times. In particular, the bounds on the regularity of the numerical solutions do not depend on the spatial discretization parameter. This completes a previous result obtained by G.D and E. Faou in a semi-discrete setting. In [62], G.D. studies the long time asymptotics of the solutions of linear Schrodinger equations considered as initial-boundary value problems on the half-line and on bounded intervals when the boundary data are periodic functions of time. G.D. obtains theoretical results using a transformation method introduced by T. Fokas and provides several numerical experiments to support them.

The Diffusion Monte-Carlo method is a powerful strategy used by chemists to estimate the groundstate energy of a N-body Schrödinger Hamiltonian with high accuracy. However, the method suffers from two major limitations :

- The quantity of physical interest is more the energy variation with respect to a parameter than the energy itself.
- The case of Fermions (as electrons of atoms) relies on constraining the random walkers in some nodal pocket (which imposes skew-symmetry on the distribution of walkers) which is only approximately known (the Fixed Node Approximation).

In the article [29], Mathias Rousset proposed a new strategy for the case of Fermions to compute the energy variation with respect to a variation of the nodal pocket. The ultimate goal is to design a Monte-Carlo strategy able to optimize the Fixed Node Approximation.

5.7. Discrete and continuous homogenization

In collaboration with R. Alicandro (Cassino) and M. Cicalese (Naples), A. Gloria has studied the derivation of continuum rubber elasticity theory from a discrete model of interacting polymer chains in [8]. The numerical study of this model is currently under investigation within the ARC project DISCO.

In collaboration with F. Otto (MPI Leipzig) [24], A. Gloria has obtained important results in stochastic homogenization, namely the first optimal variance estimate of the energy density of the corrector field for stochastic discrete elliptic equations. The proof makes extensive use of a spectral gap estimate and of deep elliptic regularity theory, bringing in fact the probabilistic arguments to a minimum. This has allowed them in [41] and A. Gloria in [33], [23] to propose and fully analyze new numerical methods to approximate homogenized coefficients at an optimal convergence rate. These results have been generalized to high dimension and further extended by A. Gloria and J.-C. Mourrat (EPFL) in [34].

5.8. Radiative Transfert

The interest of the team in developing efficient numerical methods preserving the asymptotic behavior of kinetic equations modelling the radiative transfer phenomena in the diffusive regime has recently brought two new innovative schemes. On the one hand, the moment closure equations proposed in [13] involve non local terms that lead to the introduction of specific numerical approximations. On the other hand, a new scheme [43] based on the projective integration procedure due to Gear and Kevrekidis was proved very efficient theoretically and numerically.

5.9. Complex fluid flows

A numerical treatment [42] of phase transitions arising in the modelling of the behavior of polymers near glass transition by a non linear diffusion equation was conducted in the continuation of the theoretical results by Evans and Portilheiro and Mascia, Terracina and Tesei.

6. Contracts and Grants with Industry

6.1. THALES

Participants: Christophe Besse, Thierry Goudon, Nicolas Vauchelet, Saja Borghol.

We started a new collaboration with Thales concerning the modelling and simulation of spacecraft/plasma interaction. The collaboration is the continuation of previous works performed in the project CAIMAN, at Sophia Antipolis (with S. Piperno, F. Poupaud, O. Chanrion, M. Chane-Yook). The goal is to develop the Thales code SPARCS which is designed to compute the electric potential on the spacecraft and around it. Of course, the motivation is to prevent possible failure of the spacecraft due to violent electric discharges. The current version of SPARCS, based on a back-trajectory method, is very efficient and provides an accurate computation of the potential and the distribution of charged particles on the surface. On the one hand, we try to fasten the computation by optimizing some procedures of the code and by proposing a parallel version. On the other hand, the current version of the code is specifically designed for GEO flights and our goal is to propose models and methods for treating different plasmas environments (LEO, PEO).

6.2. CEA

Participants: Thierry Goudon, Martin Parisot.

We are starting a collaborative program with the CEA (Direction des Applications Militaires) devoted to the modeling and simulation of plasmas arising in Inertial Confinement Fusion devices. We are concerned with the derivation of the so-called nonlocal models, which are variations around the standard diffusion models.

6.3. ANDRA

Participants: Thierry Goudon, Antoine Gloria, Stella Krell.

The goal of the program relies on the determination of effective coefficients for models of transfer of solutes in porous media. The problem appeals to the homogenization of convection-diffusion equations. We wish to participate to the research efforts for the numerical simulation of the disposal of radioactive waste. This work is the object of a collaboration with S. Krell and A. Gloria.

7. Other Grants and Activities

7.1. International Initiatives

7.1.1. *ANR MICROWAVE*

Participants: Christophe Besse, Ingrid Lacroix-Violet.

Ch. Besse and I. Lacroix-Violet are members of the new 4-years ANR "blanche" project MICROWAVE. Ch. Besse is the North node coordinator. The scientific subjects deal with artificial boundary conditions for dispersive equations, electromagnetism and high frequency regimes in acoustic simulations. This ANR project concerns the development of new numerical methods for wave propagation problems using tools from microlocal analysis. It focuses on microlocal analysis and numerical methods for acoustic and electromagnetic wave scattering and microlocal analysis and numerical methods for Schrödinger-type equations.

7.1.2. *ANR IODISSEE*

Participants: Christophe Besse, Pauline Lafitte, Chang Yang.

Ch. Besse has obtained a 4-years ANR grant, from the Cosinus proposal, for the project IODISSEE. P. Lafitte and C. Yang, also members of the EPI Simpaf, are involved in this project. The project IODISSEE also involves a team of mathematicians from Toulouse, a physicist team from Versailles and the Thales group. It deals with the elaboration of a physical model for helping the industrial partner for the new generation of Galileo satellites. For the last decade, satellite positioning devices became one of the most interesting means of navigation for the displacement of the goods and the people. The only current solution is based on the constellation of satellites Navstar GPS American system. Originally developed for military applications, its use was released under the Clinton administration. However, in order to guarantee its autonomy, Europe decided to launch a competitor program known as Galileo. Galileo system differs from the GPS thanks to its capability to provide real time integrity information to the user. In order to guarantee the stability of this system, it is fundamental to take into account the various problems which can affect the mission and to identify all the potential sources of system unavailability. One of the main source of data unavailability that has been identified is the phenomena of ionospheric scintillations. Indeed scintillation causes radio frequency signal amplitude fades and phase variations as satellite signals pass through the ionosphere. Such effects may induce loss of lock or cycle slips on ranging signals broadcast by Galileo satellites making them totally useless for accurate integrity information determination. Scintillations are clearly identified like a source of disturbances. They appear as the turbulent aspect of a larger disturbance of the ionospheric plasma density which have the shape of a plasma bubble. The difficulty of their modeling is due to the lacks of in situ measurements with regard to them. However, some measurements recently acquired during the mission of satellite DEMETER make possible on the one hand the validation of the models existing but also, using techniques of data-models coupling, to reinforce them. The object of this proposal is therefore to provide a physical model making it possible to anticipate the attenuation of the signals during their propagation within the disturbed Earth ionosphere.

7.1.3. *ANR MEGAS*

Participant: Mathias Rousset.

M. Rousset is involved in the ANR MEGAS. The main scientific subject is numerical methods in Molecular Dynamics simulation.

7.1.4. ANR INTOCS

Participants: Pauline Lafitte, Jean-François Coulombel, Frédéric Lagoutière.

J.-F. Coulombel has obtained a 4-years ANR grant "young researcher", for the project INTOCS. In addition to the coordinator, two other members of the EPI SIMPAF are involved in this project: P. Lafitte et F. Lagoutière. The main scientific subject of the project is the interaction of compressible waves, and more precisely the propagation of high frequency oscillations in hyperbolic boundary value problems. One of the physical motivations is the "Mach stems" formation in reacting gas flows.

7.1.5. ARC HYBRID

Participant: Mathias Rousset.

M. Rousset is involved in the ARC HYBRID. The main scientific subject is hybrid (stochastic+deterministic) numerical methods in Molecular Dynamics simulation.

7.1.6. AEN Fusion

Participants: Christophe Besse, Thierry Goudon.

SIMPAF is involved in the project led by E. Sonnendrucker from EPI Calvi, which aims at fostering the national research effort in mathematics and computer science towards the simulation of large magnetic confinement devices, like ITER. The project Fusion is currently under evaluation.

7.1.7. COADVISE European Project PEOPLE/IRSES

Participants: Christophe Besse, Caterina Calgaro, Olivier Goubet, Thierry Goudon, Jean-Paul Chehab.

In 2006, under an initiative of J.-P. Chehab, the SIMPAF team has initiated a collaborating program "3+3 Méditerranée" funded by INRIA. This program, devoted to Modelling, Analysis and Simulation of Hydrodynamic Waves, is the continuation of the MASOH project. To be more specific, the project focuses on water waves modelled by dispersive PDEs (Korteweg-De Vries, Benjamin-Ono, KP and Nonlinear Schrödinger equations). The goal is to elaborate efficient multilevel numerical schemes that will be able to help in the understanding of finite time blow up or the asymptotic smoothing effects due to damping.
As a consequence, four PhD theses were started co-advised by SIMPAF's members.

Emna Ezzoug, from Monastir, advised by E. Zahrouni, J. Laminie and O. Goubet, started in July 2006;

Ibtissem Damergi, from Monastir, by advised E. Zahrouni, Ch. Besse and O. Goubet, started in July 2006;

Salim Amr Salim Djabir, from Marrakesh, advised by M. Abounouh and J.-P. Chehab, started in January 2007;

Maithem Trabelsi, from Tunis advised by E. E. Zahrouni and J.-P. Chehab, started in September 2007.

7.1.8. ARC DISCO

Participant: Antoine Gloria.

A. Gloria is the leader of the ARC project DISCO. The main objective is the design, mathematical analysis, numerical analysis, and numerical simulation of discrete models for rubber. The participants are F. Lequeux (polymer physics, ESPCI), P. Le Tallec (mechanics, Ecole polytechnique), F. Otto (mathematics, MPI Leipzig), and M. Vidrascu (scientific computing, INRIA Paris-Rocquencourt). M. de Buhan will join the group as a post-doc for one year in December.

7.1.9. ANR AMAM

Participant: Antoine Gloria.

A.Gloria is involved in the 4-year ANR project "young researcher" AMAM, led by V. Millot (Paris 7). The aim of the project is to develop mathematical tools for the analysis of multi-scale problems in material sciences (PDEs and variational methods). The fields of interest are primarily micromagnetics, dislocations, fatigue in nonlinear elasticity, and homogenization.

7.1.10. Project CNRS-DGRSRT N° 22640

Participant: Caterina Calgaro.

The main objective of the project is the mathematical analysis and the simulation of miscible or immiscible fluids. In this context, C. Calgaro visited the University of Monastir (Tunisia). As a consequence, one PhD thesis started in october 2010 : Meriem Ezzoug, from Tunis, advised by E. Zahrouni and C. Calgaro.

8. Dissemination

8.1. Animation of the scientific community

C. Calgaro is in charge of the communication of the Math. Department and she is in charge of the relation between the University of Lille and high schools. Accordingly, she organizes various events like "Les Métiers des maths", "Stage de maths en seconde" and "Demain l'université".

8.2. Teaching

- T. Goudon and P. Lafitte are members of the jury of the national hiring committee of the "Agrégation de mathématiques".
- S. De Bièvre is a member of the jury of the national hirring committee of the "CAPES de mathématiques".
- S. De Bièvre is in charge of the Doctoral formation in Applied Mathematics at the University of Lille.
- C. Besse and E. Creusé are involved in the project of a new International Master degree at the University of Lille devoted to Scientific Computing.
- Members of the team are involved in MSc degrees at USTL (C. Calgaro, S. De Bièvre, G. Dujardin, A. Gloria, P. Lafitte, M. Rousset).
- A. Gloria gives a mini-course in the CEA-EDF-INRIA school on homogenization in December 2010.

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