INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Project-Team Simpaf

SImulation and Modelling for PArticles and Fluids

Futurs

THEME NUM

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1. Team

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.

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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

Keywords: *Asymptotic analysis*, *Computational Fluid Dynamics*, *Conservation Laws*, *Fluid Mechanics*, *Hyperbolic Systems*, *Kinetic Equations*, *PDEs*, *Parabolic Systems*, *Plasma Physics*.

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 multiscale 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

Keywords: *Asymptotic Preserving Schemes*, *Fluid-Particles Flows*, *Hydrodynamic Limit*, *Radiative Transfer*, *Statistical Physics*.

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 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 recently 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 nondiffusive numerical scheme for the convective terms. This also leads to the delicate question of the stability of travelling waves solutions.
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 the convective terms, which will be handled by antidiffusive 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 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.

3.3. Charged Particles

Keywords: *Euler-Maxwell equations*, *Euler-Poisson equations*, *Magnetized plasmas*, *Ohm's law*, *Plasma Physics*, *Spacecraft charge modeling*, *Vlasov-Maxwell equations*, *Vlasov-Poisson equations*.

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 FIC 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 ...)

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, this last 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 and the PhD of S. Borghol is essentially devoted to this subject.

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

Keywords: *Anti-Diffusive Schemes*, *Conservation Laws*, *Control*, *Finite elements methods*, *Finite volume methods*, *Turbulence*, *Viscous Flows*.

3.4.1. Conservation Laws

A major issue in the numerical analysis 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 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 non-linear 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 non-linear 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

Nowadays, passive control techniques are widely used to improve the performances of planes or vehicles. In particular these devices can sensibly reduce energy consumption or noise disturbances. However, new improvements can be obtained through an active control of the flow, which means by activating mechanical devices. This is a very promising theme.

The first results are concerned with the control of the 2D compressible Navier-Stokes equations over a dihedral plane. The technical device consists in a small hole which allows to suck or to inject some fluid in the flow, depending on the pressure measured at another point. This improves the aerodynamics performance of the dihedral. Variants are possible, for instance by considering several such devices and taking into account the local properties of the flow.

Another work is concerned with simulation of the control of low Reynolds number flows (laminar regimes) over a backward facing step by imposing pulsed inlet velocities. Such a flow can be considered as a toy-model for the modelling of combustion phenomena. The goal is to understand and control vortex formations, by making the frequency and amplitude of the incoming fluid vary.

Recently, previous results on the step were generalized to the transitional regime, with a work of E. Creusé, A. Giovannini (IMFT Toulouse) and I. Mortazavi (EPI Inria MC2, Bordeaux). The nonstationarity property of the uncontrolled flow allows to use some closed-loop control strategies. The control process is either a global one, by imposing a pulsed inlet velocity like for the laminar case, or a local one by the use of two horizontal jets located on the vertical side of the step.

Our current objective is now to apply such techniques on the "Ahmed body geometry", which can be considered as a first approximation of a vehicle profile. This work is performed in collaboration between E. Creusé and C.H. Bruneau (EPI Inria MC2, 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). One of the main points is now to understand and to make use of the correlation law between the actions imposed on the wall and the drag coefficient of the profile. Significant energy saving could then be obtained.

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 multiscale 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 and a fluctuation component, this last one having small moments but not necessarily a small magnitude. This change of variable defines also a hierarchical preconditioner. 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 multiscale 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.

4. Software

4.1. Simula+

Keywords: *A posteriori Estimators*, *Finite Elements Methods*, *Linear Systems*, *Mesh Generation*.

Participant: Emmanuel Creusé [correspondant].

See the web page http://www.univ-valenciennes.fr/lamav/Simula+

The project Simula+ involves the LAMAV laboratory of the Valenciennes and Hainaut-Cambrésis University (UVHC) and LPMM laboratory from University and engineering schools ENSAM and ENIM of Metz. The project Simula+ aims at constructing C++ libraries devoted to scientific computing.

The motivation of this project is to organize the sharing and development of numerical routines. The final goal is to reduce significantly the time that is necessary to write scientific codes, and instead use more time to develop original methods and simulate applied problems. More precisely, the library contains three kinds of routines :

- The MOL++ library. This library is composed of some basic procedures of numerical linear algebra (direct and iterative methods for large space linear systems). These routines are developed both by the LAMAV and the LPMM. The goal is not to develop a wide range of solvers (a lot of commercial and free codes already exist to do it), but to have the only needed "material" for the following applications we are interested in.
- The FEMOL++ library. This library is composed of some procedures related to mesh refinement, finite element calculations, and a posteriori error estimators. It is developed by the LAMAV. Once again, the goal is not to do the same as well-known commercial codes, but to develop a specific work. The partial differential equations to be solved come mainly from fluid mechanics problems. They are rather standard (Laplacian, Stokes, $p-$Laplacian), and the geometries of the domains are academic. The originality of this work relies on the a posteriori error estimators derivation, for conform as well as for non conform finite element methods, and for isotropic as well as for anisotropic meshes. This topic is a large part of the research made by E. Creusé and S. Nicaise. These estimators are proved to be efficient and reliable from the theoretical point of view. The FEMOL++ library allows to illustrate and to validate these theoretical results by numerical computations.
- The MateriOL++ library. This library is composed of some procedures relative to the modelling of the multi-physics behaviour of some intelligent materials. It is developed by the LPMM.

Because of the recent leaving of several PhD students of the LAMAV laboratory previously involved in the development of Simula+, a posteriori error estimates functionalities should be from now developed in the GetFem++ software in collaboration with Yves Renard (INSA Lyon), author of the code (see http://home.gna.org/getfem/). GetFem++ is, like Simula+, a C++ library. It allows the use of a vast choice of finite elements for 2D and 3D simulations. It is based on a complete linear algebra library (GMM++). Finally, It follows objectives very closed to the Simula+ ones. Consequently, we would like to federate the numerical capabilities of both teams on the same code for a more efficient development strategy. The connection of this code to the SIMPAF project relies on the fact that it will allow to develop several a posteriori error estimators related to fluid-mechanics problems. Moreover, finite element and mesh functionalities will naturally be used in the codes developed by the project. It is already the case for the C++ code developed for the simulation of the low-Mach number flows (see section 3.4.3).

4.2. DDNS2

Keywords: *2D geometry*, *Domain Decomposition Methods*, *Dynamical Multi-Level Methods*, *Finite Elements Methods*, *Navier-Stokes*, *incompressible*.

Participants: Caterina Calgaro [correspondant], Jacques Laminie [projetsimpaf].

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.

4.3. NS3ED

Keywords: *Exponential Mesh*, *Exterior Domains*, *Navier-Stokes*, *Preconditioning*, *Saddle-point Problems*.

Participants: Caterina Calgaro [correspondant], Delphine Jennequin [projetsimpaf].

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 preconditioner is performed for the generalized saddle-point problem.

4.4. NSVarDens

Keywords: *Incompressible Navier-Stokes*, *Rayleigh-Taylor Instability*, *Variable Density*.

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

The NSVarDens 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 [12]. The code, with a current version in Matlab, is still in a development phase, but simulations of the Rayleigh-Taylor instabilities prove the efficiency of the code. An optimized version will be produced soon and it will be completed by mesh refinements strategy.

4.5. RTcodes

Keywords: *AP schemes*, *Radiative Transfer*, *Radiative shocks*.

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

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, as in e. g. [38]. 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.

4.6. FPcodes

Keywords: *AP schemes*, *Fluid-Particles flows*, *Gravity driven flows*.
Participants: Pauline Lafitte [correspondant], Thierry Goudon [projetsimpaf].

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 [33].

4.7. CLAToolBox

Keywords: *Absorbant boundary conditions*, *Schrödinger equation*.
Participants: Christophe Besse [correspondant], Pauline Klein [projetsimpaf].

As a byproduct of the review paper [30], a user-friendly interface is offered[1] to trial and compare various numerical methods to solve the 1D Schrödinger equation with absorbant boundary conditions.

4.8. NLWcodes

Keywords: *Benjamin-Ono*, *Korteweg-de-Vries*, *non linear Schrödinger equations*.
Participants: Caterina Calgaro [correspondant], Jean-Paul Chehab [projetsimpaf].

We have developed a set of numerical codes, written in Matlab, to solve various 1D non linear wave equations (Korteweg-de-Vries, Benjamin-Ono, non linear 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 [32]. 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.

5. New Results

5.1. Analysis and Simulation for Fluid Mechanics

5.1.1. Hybrid Methods for Density-Dependent Viscous Flows.

We develop a density dependent Navier-Stokes code in 2D, cite ccg. The first goal is to design a performing code for incompressible flows, but we wish to extend the scheme to deal with situation where the incompressibility condition being replaced by a relation on the velocity field and the gradient of the density. The numerical strategy we use mixes a Finite Element method for computing the velocity and the pressure to a Finite Volume approach to evaluate the density. The cornerstone of our contribution relies on the definition of suitable compatibility condition between the two methods and a clever way to define the velocity to be used at the interface of the control volumes. The current version of the code computes solutions of the 2D incompressible Navier-Stokes system with variable density. and can be applied to the difficult test of Rayleigh-Taylor instabilities, with high density ratio and high Reynolds number. Reinforced by the arrival of E. Chane-Kane on this project, we wish to write a more involved version of the code able to deal with heavier simulations. We also plan to include other functionalities such as adaptive local mesh refinements.

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

5.1.2. Estimators and Control.

On this topics, the breakthrough we obtained are the following:

- With M. Farhloul (University of Moncton, Canada) and L. Paquet, E. Creusé has obtained new estimators of residual type for the finite element methods solving the $p-$laplacian by hybridization [17].

- In the same field, with S. Nicaise, E. Creusé has obtained new estimators of residual type for the finite element methods solving a second order problem [18]. The originality of the analysis consists in combining two different finite element methods in both the subdomains into which the computational domain splits.

- With A. Giovannini (Toulouse) and I. Mortazavi (Bordeaux 1), E. Creusé brings out the effects of a control based on pulsed entry velocity for a flow in transient regime over a step, [40].

5.1.3. Conservation Laws.

F. Lagoutière develops anti-diffusive numerical strategies for conservation laws. A crucial requirement for the applications is that the method should work on non structured meshes. In particular he is interested in multiphase flows [23]. Another important question relies on the large time behavior of numerical schemes: Indeed, the usual error estimates are proportional to the final time of the computation so that the relevant information disappears as time goes to infinity; having sharp estimates is crucial when one wants to investigate numerically the asymptotic trend of the model, like e.g. for applications in biology, see e.g. [4]. New schemes for conservation laws are currently under study that satisfy error estimates independent of the final time.
Ch. Chalons and J.-F. Coulombel are able to justify the convergence of the so called "pressure relaxation" model to the Euler equations [35]. This result is interesting in view of the development of new numerical schemes since the model under consideration can be solved with a low numerical cost.
J.-F. Coulombel studies the stability of finite difference schemes for the approximation of hyperbolic problems with boundary conditions. The point relies on the extension to the discrete framework of the "block structure" known for the continuous case. Then, the stability results of Gustaffson-Kreiss-Sundström and the ones that followed can be generalized to a broader class of schemes, not restricted to dissipative schemes.

5.1.4. Artificial boundary conditions for the Schrödinger equations.

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 [30] was written this year to describe and compare the different actual 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) 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 (see preliminary results in [5]. These cases are relevant since for example the equations appear in the Bose Einstein condensate with a quadratic potential. The new results (based on a pseudo differential approach) are promising.

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 are more difficult to study due to its third order derivative in space.

5.2. Models and Methods for Many Particles Systems

5.2.1. Diffusion Approximation: Reduced Models and Numerical Analysis.

A challenge that has motivated a lot of works consists in discussing intermediate models in-between the full kinetic equation – too complicated for numerical simulations – and the diffusion equation that misses most of the properties of the original model (finite speed of propagation for instance). We have proposed in [13] new numerical schemes based on splitting techniques specifically adapted to diffusion regimes. The main idea behind this strategy is the separation between the hydrodynamic quantities and the fluctuations. Hence, the method we design is explicit, asymptotic preserving, well balanced and mass preserving thanks to a suitable treatment of the numerical boundary conditions. This approach applies equally well to the original kinetic equation and to the macroscopic models coming from closure approximations. The numerical experiments demonstrate the abilities of the scheme to give accurate quantitative estimates of the errors made by the approximations to the kinetic equation. The first order closure based on an Entropy Minimization Principle is shown to provide a quite accurate approximation for the kinetic equation in the diffusive limit.

5.2.2. Radiative Transfer.

Th. Goudon and P. Lafitte have introduced the splitting method described above for treating coupled models for radiation and hydrodynamics which involve a kinetic equation describing the specific intensity of radiation coupled to the Euler system for the surrounding material. The coupling arises from energy and impulsion exchanges, and more complex phenomena are due to the Doppler effects. Different asymptotic systems can be obtained depending on leading effects of scattering or absorption. Doppler effects introduce also corrective terms in the limit equations. We wish to investigate numerically the solutions of the full system of radiative hydrodynamics.

Besides, the coupling with radiation changes the structure of the hydrodynamics equations and the qualitative properties of the solutions. The modification of the shock profiles is an important question for applications and leads to numerical difficulties due to the possible apparition of discontinuities. A first study of these phenomena appears in the PhD thesis of Ch. Lin [7] where we describe small amplitude radiative shocks: the existence of smooth profiles is justified for radiative hydrodynamics in non equilibrium regimes, the smaller the shocks, the smoother the profile. This analysis is completed by stability results, [28] and derivation of asymptotic models illustrated by numerical experiments [20]. This work is continued by J.-F. Coulombel and C. Mascia. J.-F. Coulombel and P. Lafitte have constructed a numerical scheme designed for computing the shocks profiles of the radiative transfer equations [38]. The simulations allows to verify the theoretical results and to investigate profiles with large amplitude.

5.2.3. Fluid-Particles Flows.

With J. A. Carrillo, Th. Goudon and P. Lafitte have adapted the AP method designed for diffusive regimes to the context of fluid-particles flows [33]. The basic model couples the Euler system describing the density and velocity of the fluid to a Vlasov-Fokker-Planck for the density of particles. The difficulty consists in deriving a convenient approximation of the semi-group associated to the Fokker-Planck operator. The method allows to investigate both the bubbling and the flowing regime. It is particularly adapted to deal with gravity driven flows and we show the formation of sedimentation profiles.

Besides, with T. Takahashi (EPI Corida, Nancy) and N. Seguin (Univ. Paris-VI), F. Lagoutière analysed a inviscid fluid-particle interaction model. Such models are intended to mimic fluid-particle interactions and are classical: see the works of Domelevo, Domelevo and Roquejoffre, Goudon, Vazquez and Zuazua for example. The originality in this new study is to consider the *inviscid* Burgers equation and its *weak* solutions, taking into account *shocks*. The difficulty is to understand the interaction between the particle and the "fluid" when the particle is moving within a shock of the Burgers equation. It is shown that the Riemann problem has a global solution. Numerical results with more than one particle show interesting behaviors involving collisions, which do not appear in the diffusive model of Vazquez and Zuazua for instance.

5.2.4. Charged Particles.

F. Castella, P. Degond and Th. Goudon are part of a program intended to understand the effect of high oscillations of the force field on particles systems, see [15]. Such a question arises when describing electrons in a crystal subject to laser solicitation or in certain models of tokamaks. The aim is to study the influence of deterministic or random variations of the perturbation for classical models – Liouville type equations for the distribution function of electrons in phase space – or quantum models – Bloch like equations for the density matrix of the electrons. These results are in the spirit of the method developed for the homogenization of transport(-diffusion) equations, see e.g. [22]. A classical version of the Bloch equation with a relaxation term intended to mimic the models well established in quantum theory has been introduced. A unified description of both classical and quantum models, for deterministic or random perturbations is now available, see [14].
Furthermore, M. Bostan (Univ. Besançon and EPI Calvi) and Th. Goudon justify the asymptotic analysis of Fokker-Planck models coupled to the Maxwell system [31], [11]. The arguments rely on entropy estimates. A relaxation regime has been investigated by Th. Goudon, V. Miljanovic and C. Schmeiser for a model of charge transport in semconductors in [21] In her PhD thesis, I. Violet analyses asymptotic regimes for the stationary Euler-Poisson system (small electrons mass, quasi neutral regimes,...) with a specific attention to the boundary layers [29]. The analysis is completed by numerical simulations based on modern finite-volume approaches [34] She is also interested in evolution models taking into account quantum corrections [25], [24].

5.2.5. Diffusion and Hamiltonian Models.

S. De Bièvre and P. Parris, together with A. Silvius have started an analytical and numerical study of Hamiltonian models for transport of particles moving through deformable media containing many spatially localized environmental degrees of freedom. In these first papers, the accent was on the equilibrium properties of the system, and a detailed study of the temperature dependence of the diffusion constant was made. This study exhibited two very different mechanisms for diffusion at low and high temperatures, leading to two different power laws for the temperature dependence. In collaboration with P. Lafitte, S. De Bièvre and P. Parris are now extending this work to stationary non-equilibrium situations [41], [42], which are the object of much study lately. In this context they explore various issues in transport theory when an external driving field is present. They investigate in particular the validity of linear response theory for the current and the applicability of fluctuation-dissipation relations such as the Einstein relation linking the mobility to the diffusion constant. Their study shows that, in spite of the conventional wisdom on this issue, a monochromatic environmental heat bath is capable of producing a linear or Ohmic response for the transport properties of a particle moving through it : the current is indeed proportional to the applied field. This work requires a huge computational effort, using a lot of CPU and data treatment time.

The result is based on the simulation of the behavior of particles that interact with a chain of 10^5 oscillators such that there is a free zone in between two successive oscillators. The whole system is subject to an external constant force field and the goal is to check the validity of the linear response theory and of the Einstein relation, which relates the diffusion constant to the mobility. To that end, first the diffusion constant is computed in the absence of a force field, as a function of the temperature of the system, the strength of the particle/oscillator coupling and the relative length of the oscillator/free zone. These first computations already require a very large number of operations, since we need to simulate enough particle trajectories ($\simeq 10^4$) to have good statistics and on a large enough time interval ($T \simeq 10^6 - 10^7$) to ensure the asymptotic regime is reached. Secondly, the mobility is obtained as a mean value of mobilities computed for several values of the force field for given system parameters. As a result, the number of computations increases significantly, and so does the analysis time needed to determine a good trade-off between the runtime and the number of trajectories. In the end, a typical data point in the final graph takes an average of a week of CPU time and we computed 54 such data points. In order to obtain these results, we used the computational resources of the laboratory Paul Painlevé, of the GDS MATHRICE (CNRS 2754), as well as the resources provided by GRID 5000, using up to 200 nodes at the same time. Comparisons of their results to experimental data for charge transport in appropriate physical systems such as organic molecular crystals are envisaged.

5.2.6. Molecular Dynamics.

This was the research topics of M. Rousset during his PhD and more precisely during his post doc at the EPI MicMac. He obtained results in the following directions:

- The computation of free energy profiles from non equilibrium dynamics with parallel interacting dynamics is presented in a previous work. By selecting the dynamics (using a Jarzynski-like equality) the closest to equilibrium, we compute the free energy without sampling useless trajectories. The generalization to dynamics with constraints (like rigid bonds) that evolves in time is done in [26]

- Stochastic dynamics to compute free energy differences are widely used in computational chemistry and biology. Many recent methods rely on non-linear Markov processes, like the adaptive techniques. A unifying presentation of adaptive methods is proposed in [27], together with an efficient implementation of adaptive dynamics using an interacting particle system with birth death processes. A new proof of convergence of a certain class of adaptive methods has been recently obtained in [45]

-A cornerstone in molecular dynamics is to carry out numerical schemes that can deal with fast forces that induce highly oscillatory behaviors. This difficulty can be relaxed when one only needs to compute canonical averages by slowing down fast degrees of freedom. This leads to some new numerical strategies currently studied with Claude Le Bris and Frédéric Legoll in collaboration with Petr Plechac (Warwick University).

6. Contracts and Grants with Industry

6.1. THALES

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

We started a new collaboration with Thalés 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 the SPARCS code, 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 make the computations faster by optimizing certain 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. Our goal is to propose models and methods for treating different plasmas environments (LEO, PEO).

6.2. INRETS

Participants: Emmanuel Creusé, Maurice Largen.

The research unit LEOST of INRETS (institut National de Recherche sur les Transports et leur Sécurité) develops experimental devices to trial the electromagnetic compatibilities of various devices embarked in vehicles. The objective of the present collaboration is to write a model and to propose a corresponding numerical code to evaluate the capacitance of the TEM chamber used for the tests at INRETS [6]. M. Largen made a training period in the SIMPAF team, completed by a temporary contract of engineer at INRETS on this topics. This work will give rise to a research publication.

7. Other Grants and Activities

7.1. ARC “Magnetized Plasmas”

Participants: Christophe Besse, Thierry Goudon, Caterina Calgaro.

SIMPAF is an active member of a specific INRIA Research Program, ARC, that is focused on Mathematical Models and Numerical Simulations for Magnetized Plasmas. This project, led by E. Sonnendrücker, aims at fostering the leader teams in the French applied mathematics community interested in these topics. The ARC is composed of the INRIA projects CALVI, MC2, SCALAPPLIX, SIMPAF, the laboratory MIP in Toulouse and the researchers of the Atomic Energy Agency in Cadarache.
Ch. Besse worked recently on the modelling of ionospheric plasma [10]. He derived new models of fluid nature (macroscopic level), based on Euler equations for electrons and ions, and coupled to the Maxwell equations. He investigated the limits of several physical parameters and built a new hierarchy of models to describe some ionospheric instabilities. The mathematical analysis was performed and showed the instability of the limit model. The effects of turbulence were taken into account in order to restore the stability of the solutions. In parallel, an intensive numerical work was done and simulations were performed and compared to some real phenomena. The geometry of the magnetic field was also taken into account and the curvature effects, always neglected in previous ionospheric plasma model, were shown to be very important. This expertise can combine with the study performed within the team on the effects of the microscopic properties onto macroscopic scales and the derivation of low and high field regimes for Vlasov-Poisson or Vlasov-Maxwell models. Coming back to the modelling questions around ITER this would lead to the derivation and the study of Vlasov or Euler-type models, in which the self-consistent force field satisfies a complex equation, linked to the gyrokinetic effects.
While clearly SIMPAF has at hand all the material necessary to deal with the kinetic models describing tokamaks, and to propose derivation of reduced models and suitable numerical procedures, we have been involved also in some problems related to the visualization of the results. Indeed, the Gysela code used at the CEA produces a huge amount of data whose treatment could be particularly tough for obtaining a relevant picture of the motion of the charged particles. Ch. Besse proposed various solutions to the CEA team for handling the visualisation of the results.

7.2. Project 3+3 "Méditerranée" MASOH

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

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 is devoted to Modelling, Analysis and Simulation of Hydrodynamic Waves. 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. The project[2] brings together various collaborations the node of which is SIMPAF; the involved teams are

- France: SIMPAF, Amiens, Paris-Sud,

- Morocco : Marrakesh,

- Tunisia: Monastir,

- Spain: Granada.

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.

[2] described at the URL:http://math.univ-lille1.fr/~chehab/MASOH/masoh.html

In the context of the MASOH program, for research and teaching at the doctoral level, Th. Goudon visited Granada; C. Calgaro, M. Abounouh, L. Di Menza, J.-P. Chehab visited the University of Monastir; while C. Calgaro, J.-P. Chehab, E. Zahrouni went to Marrakech. Besides, the PhD students spend a while in Amiens. The publications [43], [8], [32] are directly related to interactions organized within this network.

7.3. Visits and invitation abroad

Th. Goudon has been invited at ICES Austin, Texas and at the Math. Dept. of Texas A & M, College Station.

P. Lafitte has been invited at the CRM, Barcelona twice and at the University of Roma I.

S. De Bièvre is invited for a two weeks stay at McGill University (december 2007) during which time he will speak at the workshop "Ergodicity in realistic Hamiltonian systems".

8. Dissemination

8.1. Animation of the Scientific Community

• S. De Bièvre is member of the scientific committee of the GDRE network "Mathematics and Quantum Physics" of the CNRS.
• Th. Goudon is member of the scientific committee of the CNRS European network GREFI-MEFI.
• C. Calgaro, J.-F. Coulombel and Th. Goudon are editors of the book "Analysis and Simulation of Fluid Dynamics" [1] appeared in the series Advances in Mathematical Fluid Mechanics, Birkhaüser.
• C. Calgaro is responsible for the Communication in the Department of Mathematics of the University of Lille. She organizes a annual colloquium addressed to the undergraduate students, on "Les métiers des Mathématiques". She is also strongly involved in the organization of various events aimed at offering a picture of the research activity in mathematics towards a broad audience of non-specialists and schools.
• C. Calgaro and P. Lafitte organize a annual workshop "Rencontres Numériques en mécanique des fluides".
• J.F. Coulombel and P. Lafitte organized a session of the CNRS network MOAD (MOdélisation, Asymptotique, Dynamique non-linéaire, GDR 2948), Lille, March 21-23, 2007.
• Th. Goudon and P. Lafitte organized a session of the Société Mathématique de France devoted to "Mathematical Models and Numerical Methods in Radiative Transfer", Labo. J. A. Dieudonné UMR 621, Univ. Nice, August 2007.
• M. Rousset is involved in the organization of a HIM (Hausdorff Research Institute for Mathematics) Junior Trimester Program on Numerical methods in molecular simulation to be held in Bonn, February-April 2008.
• S. De Bièvre is invited to organize a session on "Quantum chaos" at the Mathematical Horizons for Quantum Physics programme of the Institute for Mathematical Sciences of the National University of Singapore in august 2008.
• The mathematics departments in the North area of France (namely from the Universities of Lille, Valenciennes, Calais, Amiens) decided some time ago to merge their efforts every year on specific topics and to organize jointly several events; 2008 will be specifically devoted to PDE and Numerical Analysis and our team will be involved in several scientific events:

- Workshop "Open Dynamical Systems III", organized by J.-M. Bouclet, S. De Bièvre and M. Rousset

- Workshop "9th IMACS International Symposium on Iterative Methods in Scientific Computing" organized by M. Bellalij, C. Calgaro, J.-P. Chehab, K. Jbilou and H. Sadok, to be held March 17-20, 2008, Lille.

- Workshop "Finite Element and Finite Volume Methods in CFD", organized by P. Deuring, Th. Goudon and S. Nicaise, to be held March 27-28, 2008.

- Congrès National d'Analyse Numérique, a conference of the Society of Applied and Industrial Mathematics (SMAI), organized also with Univ. Paris 13, to be held May 26-30, 2008.

8.2. Teaching Activities

Th. Goudon and P. Lafitte are members of the jury of the national hiring committee of the “Agrégation de mathématiques”.

S. De Bièvre is member of the jury of the national hirring committee of the “CAPES de mathématiques”.

Th. Goudon is responsible of the Doctoral formation in Applied Mathematics at the University of Lille.

S. De Bièvre published a book chapter [19] containing the notes of courses he taught at several summer schools, one in Norway in august 2003 (quantum field theory), another in Montreal in july 2005 and at the Academy of Sciences in Beijing, also in july 2005 (quantum chaos). Within the framework of his regular teaching duties at the Université de Lille, he furthermore wrote a book [2] destined to help students in the preparation for the national exams for high school teachers (CAPES).

9. Bibliography

Year Publications

Books and Monographs

[1] C. CALGARO, J.-F. COULOMBEL, T. GOUDON. *Analysis and Simulation of Fluid Dynamics*, Advances in Mathematical Fluid Mechanics, Birkhauser, 2007.

[2] S. DE BIÈVRE. *L'oral du CAPES de mathématiques–Face au jury*, Ellipses, 2007.

Doctoral dissertations and Habilitation theses

[3] E. CREUSÉ. *Simulation et contrôle actif d'écoulements, estimations dÕerreurs a posteriori pour les méthodes d'éléments finis*, Habilitation à diriger les recherches, Univ. Valenciennes, 2007.

[4] A. DEVYS. *Etude d'un modèle de croissance de cellules cancéreuses*, Mémoire Mastère 2, ENS Cachan, Antenne de Bretagne Ker Lann, 2007.

[5] P. KLEIN. *Etude du choix d'une condition aux limites artificielle pour l'équation de Schrödinger avec potentiel en dimension un*, Mémoire Mastère 2, Univ. des Sciences et Technologies Lille, 2007.

[6] M. LARGEN. *Etude de la capacitance d'un équipement électromagnétique*, Mémoire Mastère 2, Univ. Bordeaux 1, 2007.

[7] C. LIN. *Modèles mathématiques de la théorie du transfert radiatif*, Ph. D. Thesis, Univ. des Sciences et Technologies Lille, 2007.

Articles in refereed journals and book chapters

[8] M. ABOUNOUH, H. AL MOATASSIME, J.-P. CHEHAB, S. DUMONT, O. GOUBET. *Discrete Schrödinger Equations and dissipative dynamical systems*, in "Comm. in Pure and Applied Analysis", to appear, 2007.

[9] C. BESSE, R. CARLES, N. J. MAUSER, H.-P. STIMMING. *Monotonicity properties of the Blow-Up time for nonlinear Shrödinger equations: numerical evidence*, in "DCDS-B", to appear, 2007.

[10] C. BESSE, P. DEGOND, H. J. HWANG, R. PONCET. *Nonlinear Instability of the Two-Dimensional Striation Model About Smooth Steady States*, in "Communication in Partial Diff. Eqs.", vol. 32, 2007, p. 1017–1041.

[11] M. BOSTAN, T. GOUDON. *Low field regime for the relativistic Vlasov-Maxwell-Fokker-Planck system; the one and one half dimensional case*, in "Kinetic and Related Models", to appear, 2007.

[12] C. CALGARO, E. CREUSÉ, T. GOUDON. *An hybrid finite volume-finite element method for variable density incompressible flows*, in "J. Comput. Phys.", to appear, 2007.

[13] J. A. CARRILLO, T. GOUDON, P. LAFITTE, F. VECIL. *Numerical schemes of diffusion asymptotics and moment closures for kinetic equations*, in "J. Scientific Computing", to appear, 2007.

[14] F. CASTELLA, P. DEGOND, T. GOUDON. *Asymptotic problems for wave-particle interactions; quantum and classical models*, in "Nonlinearity", vol. 20, 2007, p. 1677–1720.

[15] F. CASTELLA, P. DEGOND, T. GOUDON. *Large time dynamics of a classical system subject to a fast varying force*, in "Comm. Math. Phys.", vol. 276, 2007, p. 23–49.

[16] J.-F. COULOMBEL, T. GOUDON. *The strong relaxation limit of the multidimensional isothermal Euler equations*, in "Transactions of the American Mathematical Society", vol. 359, n^{o} 2, 2007, p. 637–648.

[17] E. CREUSÉ, M. FARHLOUL, L. PAQUET. *A posteriori error estimation for the dual mixed finite element method for the p-Laplacian in a polygonal domain*, in "Comput. Methods Appl. Mech. Engrg.", vol. 196, n^{o} 25-28, 2007, p. 2570–2582.

[18] E. CREUSÉ, S. NICAISE. *A posteriori error estimations of a coupled mixed and standard Galerkin method for second order operators*, in "Journal of Computational and Applied Mathematics", 2007.

[19] S. DE BIÈVRE. *An introduction to quantum equidistribution*, in "Equidistribution in Number Theory", Nato Science Series II: Mathematics, Physics, Chemistry, vol. 237, Springer, 2007, p. 305–330.

[20] L. DESVILLETTES, C. LIN. *NON-LTE Line Radiative Transfer Quasi-stationary Approximation*, in "WSPC - Proceedings", to appear, 2007.

[21] T. GOUDON, V. MILJANOVIC, C. SCHMEISER. *On the Shockey-Read-Hall model: generation and recombination in semiconductors*, in "SIAM J. Appl. Math.", vol. 67, 2007, p. 1183–1201.

[22] T. GOUDON, F. POUPAUD. *Homogenization of transport equations: A simple PDE approach to the Kubo formula*, in "Bulletin Sciences Mathématiques", vol. 131, 2007, p. 72–88.

[23] S. JAOUEN, F. LAGOUTIÈRE. *Numerical transport in multlifluids with arbitrary number of components*, in "Comput. Methods Appl. Mech. Engrg.", vol. 196, 2007, p. 3127–3140.

[24] A. JÜNGEL, I. VIOLET. *First-order entropies for the Derrida-Lebowitz-Speer-Spohn equation*, in "Discrete and Continuous Dynamical Systems, Series B (DCDS-B)", vol. 8, n^{o} 4, 2007, p. 861–877.

[25] A. JÜNGEL, I. VIOLET. *The quasi-neutral limit in the quantum drift-diffusion equations*, in "Asymptotic Anal.", vol. 53, n^{o} 3, 2007, p. 139–157.

[26] T. LELIÈVRE, M. ROUSSET, G. STOLTZ. *Computation of free energy differences through nonequilibrium stochastic dynamics: the reaction coordinate case*, in "Journal of Computational Physics", vol. 222, n^{o} 2, 2007, p. 624-643.

[27] T. LELIÈVRE, M. ROUSSET, G. STOLTZ. *Computation of free energy profiles with adaptive parallel dynamics*, in "J. Stat. Phys.", vol. 126, n^{o} 13, 2007, 134111.

[28] C. LIN, J.-F. COULOMBEL, T. GOUDON. *Asymptotic stability of shock profiles in radiative hydrodynamics*, in "C. R. Acad. Sci. Paris Sér. I Math.", to appear, 2007.

[29] I. VIOLET. *High order expansions in quasi-neutral limit of the Euler-Poisson system for a potential flow*, in "Proceedings of the Royal Society of Edinburgh : section A", vol. 137, 2007, p. 1101-1118.

Internal Reports

[30] X. ANTOINE, A. ARNOLD, C. BESSE, M. EHRHARDT, A. SCHÄDLE. *A Review of Transparent and Artificial Boundary Conditions Techniques for Linear and Nonlinear Schrödinger Equations*, Technical report, 2007.

[31] M. BOSTAN, T. GOUDON. *High-electric-field limit for the Vlasov-Maxwell-Fokker-Planck system*, Technical report, INRIA, 2007.

[32] C. CALGARO, J.-P. CHEHAB, J. LAMINIE, E. ZAHROUNI. *Schémas multiniveaux pour les équations d'ondes en dimension 1*, Technical report, 2007.

[33] J. A. CARRILLO, T. GOUDON, P. LAFITTE. *Simulation of Fluid & Particles Flows: Asymptotic Preserving Schemes for Bubbling and Flowing Regimes*, Technical report, 2007.

[34] C. CHAINAIS, Y.-J. PENG, I. VIOLET. *Numerical solutions of the Euler-Poisson systems for the potential flows*, Technical report, 2007.

[35] C. CHALONS, J.-F. COULOMBEL. *Relaxation approximation of the Euler equations*, Technical report, 2007.

[36] J.-P. CHEHAB, M. REYDAN. *Preconditioned residual methods for solving steady fluid flows*, Technical report, INRIA, 2007, http://hal.inria.fr/inria-00145783.

[37] J.-F. COULOMBEL. *Stability of finite volume schemes for hyperbolic systems in two space dimensions*, Technical report, 2007.

[38] J.-F. COULOMBEL, P. LAFITTE. *Computation of shock profiles in radiative hydrodynamics*, Technical report, 2007.

[39] J.-F. COULOMBEL, P. SECCHI. *Nonlinear compressible vortex sheets in two space dimensions*, Technical report, 2007.

[40] E. CREUSÉ, A. GIOVANNINI, I. MORTAZAVI. *Vortex simulation of active control strategies for transitional backward-facing step flows*, Technical report, 2007.

[41] S. DE BIÈVRE, P. LAFITTE, P. PARRIS. *Normal transport at positive temperatures in classical Hamiltonian systems*, to appear, Technical report, 2007.

[42] S. DE BIÈVRE, P. LAFITTE, P. PARRIS. *Ohmic Response of a Classical Particle Coupled to a non-Ohmic Bath*, Technical report, 2007.

[43] O. GOUBET, E. ZAHROUNI. *On a time discretization of a weakly damped forced nonlinear Schrödinger equation*, Technical report, 2007.

[44] T. GOUDON, A. VASSEUR. *Regularity analysis for systems of reaction-diffusion equations*, Technical report, INRIA, 2007.

[45] T. LELIÈVRE, M. ROUSSET, G. STOLTZ. *Long-time convergence of an Adaptive Biasing Force method*, arXiv:0706.1695v1, Technical report, 2007.