INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Project-Team Simpaf

SImulation and Modelling for PArticles and Fluids

Futurs

THEME NUM

Activity Report

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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).

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2. Overall Objectives

2.1. Overall Objectives

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). 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 problems.

3. Scientific Foundations

3.1. Scientific Foundations: PDEs for Particles and Fluids

Keywords: *Conservation Laws*, *Fluid Mechanics*, *Hyperbolic Systems*, *Kinetic Equations*, *PDEs*, *Parabolic Systems*.

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, as 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 physicsrequires 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*, *Hydrodynamic Limit*, *Statistical Physics*.

3.2.1. 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. Moreover, purely macroscopic models of radiative transfer exhibit some shock profiles that are only piecewise smooth. A first study of these phenomena appears in the PhD thesis of Ch. Lin where we describe small amplitude radiative shocks. 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 plan to 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 now able to treat numerically the full coupling of radiation with hydrodynamics (Euler equations) in the non equilibrium diffusion regime.

3.2.2. 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 will be 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 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. It is quite promising to 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.

3.2.3. 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 our asymptotic preserving splitting methods and anti-diffusive schemes for transport equations. Therefore, we can compare various limited flux models and discuss on numerics their properties and advantages.

3.3. Charged Particles

Keywords: *Ohm's law*, *Plasmas Physics*.

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, 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 computatinal 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 techniques.
Ch. Besse worked recently on the modelling of ionospheric plasma. 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-type models, in which the self-consistent force field satisfies a complex equation, linked to the gyrokinetic effects.
On such questions of modelling, asymptotic analysis, and simulations for magnetized plasmas natural interactions must be considered with E. Sonnendrucker of the CALVI project. To this end, we have initiated a specific INRIA action, the ARC “Magnetized plasmas”, involving CALVI, SIMPAF, MC2, SCALLAPLIX, and the CNRS laboratory MIP in Toulouse, together with the researchers of the Atomic Energy Agency in Cadarache.

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 is the object of a strong collaboration with the Department Research and Technology of the company Alcatel Alenia Space and the PhD of S. Borghol will be 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.

We simulate 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. We submit the whole system to an external constant force field and check the validity of the linear response theory and of the Einstein relation, which relates the diffusion constant to the mobility. To that end, we first compute the diffusion constant 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, we obtain the mobility 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. The results show 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.

3.4. Simulations of Complex Fluid Flows

Keywords: *Anti-Diffusive Schemes*, *Conservation Laws*, *Control*, *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. A challenging question is the large time behavior of the scheme. 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. New schemes for conservation laws are currently under study that satisfy error estimates independent of the final time. We are also interested in the new approach referred to as the "pressure relaxation method" through collaborations with Ch. Chalons (Paris 7).

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. Motion of Solid Bodies in Fluids

Considering the motion of solid bodies in a fluid leads to several mathematical difficulties and numerical challenges. A first difficulty is related to the motion of the body itself and the position it occupies with respect to the discrete mesh on which the solution of the evolution equations is evaluated. Examples of applications as well as numerical methods can be found in works by Maury and Lagoutière. Approaches are very different depending on the compressibility of the fluid. A second difficulty arises when the fluid evolves in an unbounded domain. It is then necessary to truncate the computation domain, which yields a new boundary condition. Of course, it is expected that the artificial boundary does not perturb too much the solution in the domain we are interested in. Another approach consists in restricting to laminar flows around a body having a given velocity. The resolution of the stationary Navier-Stokes equation leads, at each non linear iteration step, to a convection-diffusion problem of Oseen type. Numerical methods, which use domain decomposition arguments, are proposed to treat the problem, with the aim of solving a fully three-dimensional situation. We wish to combine the different aspects of the problem and to further compare the efficiency of the different approaches.

We are also concerned with direct simulation of fluid-particle flows. As particles are treated as individuals, with their actual geometry, this approach has long been considered as too expensive to be expected to handle many-particle problems. Yet, with the increase of the speed of up-to-date processors and memory capacities, together with the developpement of new techniques to compute such flows, those approaches can now be seen as a powerful tool to provide essential information on the fine scale phenomena which have an influence on the overall behaviour of complex mixtures. From our point of view, this approach raises two main issues:

1) In order to provide information concerning many-particle problems, periodic boundary conditions have to be considered, which is not a standard problem as soon as moving boundary problems are concerned.

2) Even if the number of computed particles is reduced by the use of periodic conditions, the study of complex phenomena requires the actual computation of relatively large numbers of particles (say, from 1000 to 10000), which is still a challenge, especially in the three-dimensional case.

Point 1 has been completed for two dimensional problems, in the framework of Arbitrary Lagrangian Eulerian methods (based on a moving, unstructured mesh) but is still unaddressed in 3D. In our minds, Points 1 and 2 call for the development of methods which rely on a fixed, cartesian mesh. They allow to handle the periodicity (in all directions) in a natural way, and make it possible to use fast solvers. This kind of approach (with the use of Lagrange multipliers to take into account the rigid bodies) has been followed by Glowinski's team, in Houston, to which some participants of this project are connected, but we also began to develop our own approach (based on a domain decomposition with overlapping, which decouples global and local problems). As for today, this method makes it possible to handle a thousand particles (with a prescribed motion) in a Navier-Stokes fluid, and we plan to extend it to more general situations.

3.4.3. 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 depending on the flow itself. 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 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 gas vary.

The objective of the SIMPAF project, in collaboration with members of the project MC2 in Bordeaux (C.-H. Bruneau, I. Mortavazi), will be to extend this approach to transient states. The plan splits into the development of rigorously justified control strategy, based on optimal control theory, and less academic approaches which are able to treat complex geometries, and lead to efficient and practically reasonable control.

3.4.4. 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 fluctuant 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 limitated 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 a certain low Mach number model arising in combustion theory. The interesting thing is that the 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 will be 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 connection of the SIMULA+ code to the SIMPAF project relies on the fact that FEMOL++ allows to develop several a posteriori error estimators related to fluid-mechanics problems. Moreover, the mesh generation procedures of FEMOL+ will naturally be used in the codes developed by the project. In particular, computations for complex fluid flows will need more involved mesh generation methods and will interact with Simula+.
- 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 developped by the LPMM.

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 nonoverlapping 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: this strategy 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.

5. New Results

5.1. Dynamical Multi-level and Domain Decomposition Schemes

Dynamical multilevel algorithms issued from the theory of approximate inertial manifolds and from the nonlinear Galerkin method have been used mainly for the discretization of the viscous Burgers equations. For highly non stationary regimes of the incompressible Navier-Stokes equations in 2D geometries and primitive variables (velocity and pressure), some mixed finite element methods, with hierarchical basis, are used to discretize the equations. Following a nonoverlapping domain decomposition approach, we write the original problem as an interface problem which involves a Lagrange multiplier corresponding to the velocity (the FETI approach). A dynamical multilevel method is now developed locally on each subdomain: after a splitting of the velocity and pressure unknowns in their large structures and fluctuating corrections, and following theoretical and numerical criteria, during some intervals of time, only the equation which governs the large scales is solved in some subdomains, when the whole solution is computed in the rest of the domain. During these intervals of time, the correction scales are locally frozen and the interacting terms depending on the small scales, which vary slowly, are introduced in the large scale equation. This approach shows to be efficient in order to compute non stationary flows. First results are obtained for the 2D-lid driven cavity benchmark Other physical benchmarks (channel flows, flows behind a backward-facing step, flows past a cylinder,...) must be developed. The numerical analysis of these schemes and a rigorous justification of the modelling is in progress.

5.2. The Steady Navier-Stokes Problem in Exterior Domain

We are interested in numerical simulations of the laminar flow for the incompressible Navier-Stokes equations in a three-dimensional exterior domain. The exterior domain is cut by a sphere of radius R and some suitable approximate boundary conditions are imposed to the truncation boundary of the computational domain: the minimal requirement of these conditions is to ensure the solvability of the truncated system and the decay of the truncation error if R grows. We associate to the truncated problem a mesh made of homothetic layers, called exponential mesh, such that the number of degrees of freedom only grows logarithmically with R and such that the optimal error estimate holds. In order to reduce the storage, only discretizations by equal-order velocity-pressure finite elements with additional stabilization terms are considered. Therefore, the linearization inside a quasi-Newton or fixed-point method leads to a generalized saddle-point problem, that may be solved by a Krylov method applied to the preconditioned complete system matrix. We introduce a bloc-triangular preconditioner such that the decay rate of the Krylov method is independent of the mesh size h. For the exterior domain problem, theoretical and numerical estimates of the decay rate of the Krylov method are given in function of the truncation radius and of the Reynolds number.

5.3. 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 ad P. Parris are now extending this work to stationary non-equilibrium situations, 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.

Comparisons of their results to experimental data for charge transport in appropriate physical systems such as organic molecular crystals are envisaged.

5.4. Estimators and Control

1. 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.
2. 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. The originality of the analysis consists in combining two different finite element methods in both the subdomains into which the computational domain splits.
3. 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.

5.5. Radiative Transfer

Th. Goudon and P. Lafitte are interested in 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 investigate a simplified exchange model and we justify both the equilibrium and non equilibrium asymptotics, taking into account Doppler corrections. They also introduce a numerical method, based on a splitting strategy, which is specifically designed to treat efficiently the asymptotic regime. Their most recent work in this field takes into account the coupling of the kinetic equation and the full Euler system.

On the other hand, C. Lin, J.-F. Coulombel and Th. Goudon have studied shock profiles for radiative hydrodynamics in non equilibrium regimes. For small amplitude shocks, the existence of smooth profiles is justified, the smaller the shocks, the smoother the profile.

5.6. 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. 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 fonction 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. 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.

5.7. 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). A classical approach relies on suitable closures of moment systems obtained by integrating the kinetic equation with respect to the velocity variable. Such a closure is required to fulfill a flux limited property, crucial for applications. J.F. Coulombel, Th. Goudon with F. Golse deal with the closure obtained by a Entropy Minimization Principle, in the spirit of D. Levermore's contributions. They justify the global existence of smooth solutions for small initial data. The difficulty consists in showing that this approach can be used uniformly with respect to the Knudsen number ϵ and that the smallness condition does not depend on this parameter. Then, they prove that the moment system is consistent with the diffusion asymptotics as ϵ tends to 0.

This is completed by a numerical study performed by J. A. Carrillo, Th. Goudon, P. Lafitte and F. Vecil, working on new relaxation numerical strategies to deal with these equations in order to investigate on numerical grounds the relevance, depending on the value of ϵ, of the different approximate models.

5.8. Conservation Laws, Fluid Mechanics

F. Lagoutière develops anti-diffusive numerical strategies. A crucial requirement for the applications is that the method should work on non structured meshes. In particular he is interested in multiphase flows.

Ch. Chalons and J.-F. Coulombel are able to justify the convergence of the so called "pressure relaxation" model to the Euler equations. 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.

6. Contracts and Grants with Industry

6.1. ALCATEL

Participants: Christophe Besse, Thierry Goudon, Jean-Michel Sellier, Saja Borghol.

We started a new collaboration with Alcatel concerning the modelling and simulation of spacecraft/plasma interaction.

7. Other Grants and Activities

7.1. Actions nationales

7.1.1. ARC "Plasmas Magnétisés"

Participants: Thierry Goudon, Christophe Besse, 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. Sonnendrucker, 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.

7.2. Actions internationales

7.2.1. Projet 3+3 Méditerrannée MASOH

In 2006 the SIMPAF team has initiated a collaborating program "3+3 Méditerranée" funded by INRIA. This program is devoted to Modelling, Analysis and Simulation of Hydodynamic 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 (described at the URL:http://math.univ-lille1.fr/ chehab/MASOH/masoh.html) merges together various collaborations the node of which is SIMPAF; the involved teams are

- France: SIMPAF, Amiens, Paris-Sud,

- Marrocco : Marrakech,

- Tunisia: Monastir,

- Spain: Granada.

As a consequence, two PhD theses were started in 2006 co-advised by SIMPAF's members.

7.3. Visites, et invitations de chercheurs

Th. Goudon has been invited for lectures in the University of Vienna (Homogenization theory), the Autonomous University of Barcelona (Hydrodynamic limits), the University of Grenada (Collisionless kinetic equations), Saint Louis du Sénégal (Fluid mechanics); He has also been invited at the University of Maryland (Nov. 2005), CRM Barcelona (Jan.-Feb. 2006), ICES Austin Texas (April 2006, Jan. 2007), and Texas A & M, College Station (Nov. 2006).

P. Lafitte spent two weeks at the CRM Barcelona in February 2006.

J.-F. Coulombel has been invited by the University of Brescia (Italy), pursuing a collaboration with P. Secchi.

In the context of the MASOH program, C. Besse and O. Goubet have visited the University of Monastir, while J.-P. Chehab and O. Goubet went to Marrakech.

8. Dissemination

8.1. Animation de la Communauté scientifique

Th. Goudon is the head of the CNRS network "Interacting Particles" (GDR 2255) and he is member of the scientific comittee of the CNRS European network GREFI-MEFI.

C. Calgaro is responsible of Communication in the Department of Mathematics of the University of Lille.

She organized a first colloquium in December 2005 and a second one in December 2006 addressed to the undergraduate students, on "Les métiers des Mathématiques".

She organized (with D. Poirette) the exposition "Au delà du compas, la géométrie des courbes", which took place in Lille, in the period March-April 2006.

C. Calgaro and P. Lafitte organized the workshop "Rencontres Numériques en mécanique des fluides", which took place in Lille, March 9-10 2006.

C. Calgaro, J.-F. Coulombel and Th. Goudon are editors of the book "Analysis and Simulation of Fluid Dynamics" to appear in the series Advances in Mathematical Fluid Mechanics, Birkhauser.

P. Lafitte and Th. Goudon have organized, with N. Ben Abdallah and K. Domelevo, a summer school devoted to Multiscale aspects of transport phenomena, June 2006.

P. Lafitte and Th. Goudon organize a SMF session devoted to mathematical models and numerical methods in radiative transfer, August 2007.

8.2. Enseignement

Ch. Besse has been invited for a lecture at the CEA-EDF-INRIA School at Maubuisson.

Th. Goudon has been invited for a lecture at the CIRM for a summer school devoted to Radiative Transfer, Sept. 2005.

S. De Bièvre published two book chapters (see [37], [38]) 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 destined to help students in the preparation for the national exams for high school teachers (CAPES) [1]. He has also given a public interest lecture on “Chaos in physics and mathematics”, in the framework of a series of such lectures organized by the mathematics department of the Université Lille 1, and co-organized by C. Calgaro.

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