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Project-Team SIMPAF

Simulations and Modelling for PArticles and Fluids

IN COLLABORATION WITH: Laboratoire Paul Painlevé

RESEARCH CENTER
Lille - Nord Europe

THEME
Computational models and simulation

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Project-Team SIMPAF

Keywords: Scientific Computation, Fluid Dynamics, Particles

Creation of the Project-Team: July 01, 2007 , Updated into Team: January 01, 2013 .

1. Members

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Faculty Members

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Claire Chainais [Professor USTL, HdR]

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Stephan De Bièvre [Professor USTL, HdR]

Pauline Lafitte [Professor at ECP, HdR]

Frédéric Lagoutière [Prof. Univ. Paris 11 (until August 2012), HdR]

Ingrid Lacroix-Violet [Assistant Prof. USTL, on a temporary Inria position]

PhD Students

Émilie Soret [started in 2011, advised by S. De Bièvre]

Pierre-Louis Colin [started in 2012, advised by C. Chainais and I. Lacroix-Violet]

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Thomas Gallouët [since October 2012, advised by A. Gloria and C. Chainais]

Administrative Assistant

Karine Lewandowski [Secretary (SAR) Inria]

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. General framework

Partial Differential Equations, Kinetic Equations, Conservation Laws, Hyperbolic Systems, Fluid Mechanics, Parabolic Systems, Computational Fluid Dynamics, Plasma Physics, Asymptotic analysis

The scientific activity of the project is concerned with Partial Differential Equations (PDE) 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 motivated the introduction of the so-called kinetic schemes.

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 and it has evolved with the composition of the team. One may think of:

- charged particles: description of semi-conductor devices or plasmas;
- bacteria, individuals or genes as in models motivated by biology or population dynamics;
- 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...
- cross-links in polymer chains to describe rubber elasticity;
- oxide molecules to model corrosion phenomena at the microscopic scale and derive effective macroscopic equations;
- cold atoms...

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 and Simulations

Statistical Physics, Homogenization, Asymptotic Preserving Schemes

3.2.1. Homogenization methods

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

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

The team is interested in qualitative as well as quantitative results, and theoretical as well as numerical results. Challenging questions are mainly related to nonlinear problems (nonlinear elasticity for instance) and stochastic problems (especially regarding quantitative results).

3.2.2. *Statistical physics : molecular dynamics*

The team is concerned with the numerical simulation of stochastically perturbed Molecular Dynamics. The main goal is to handle in the same simulation the fastest time scales (e.g. the oscillations of molecular bindings), and the slowest time scales (e.g. the so-called reaction coordinates). Recently, M. Rousset co-authored a monograph [64] which summarizes standard and state-of-the-art free energy calculations, that are used to accelerate slow variables in MD simulations.

3.2.3. *Statistical physics: dynamical friction, fluctuations and approach to equilibrium*

In models of charge transport, say transport of electrons, a phenomenological friction force is generally introduced, which is proportional to the velocity v . The dissipation induced by such a term is essential for the description of phenomena such as Ohm's law and approach to equilibrium. Our idea is to go back to a microscopic framework, with a description of the energy exchanges between the electrons and the surrounding medium which is the ultimate source of the dissipation of energy by the medium and of an effective friction force. We have shown numerically and argued theoretically that the balance between the fluctuations and the dissipation by the medium drives the particle to thermal equilibrium. The goal is now to provide rigorous proof of this statement. As a first step in this program, results will be obtained in an appropriate weak coupling limit. This program requires efforts in modelling, probability and analysis, but the questions are also really challenging for numerics, due, notably, to the large number of degrees of freedom involved in the equation. The subject is at the heart of the PhD work of É. Soret, now in her second year as a PhD student.

3.2.4. *Cold Atoms*

In the framework of the Labex CEMPI, C. Besse, S. De Bièvre and G. Dujardin are working, in collaboration with J.-C. Garreau and the cold-atom team at PhLAM, on the mathematical analysis and the numerical simulation of kicked rotor systems. Such systems are experimentally realized at PhLAM. A triple goal is being pursued: understand the effect of non-linearities on dynamical localization, understand dynamical localization in systems other than kicked rotors, and exploring the limits of the analogy between kicked systems and the Anderson model.

3.3. Plasma

In the context of the Galileo satellite-positioning system, C. Besse and C. Yang, members of the ANR Iodissee project, developed a hierarchy of plasma models which describe ionospheric scintillations. This hierarchy involves many small parameters, and they introduced an asymptotic preserving scheme which allows one to take small parameters into account without solving the problem on a very fine grid [8]. The next step is to understand the fading and phase variations when waves propagate in this medium. This is a work in progress with P. Lafitte and S. Minjeaud (CNRS, Université de Nice).

3.4. Finite element and finite volume methods

Conservation Laws, Anti-Diffusive Schemes, Viscous Flows, Control, Turbulence, Finite element methods, Finite volume methods

3.4.1. Control in Fluid Mechanics

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

E. Creusé is involved in the development of open and closed active flow control, with applications to recirculation in engines or blood flows.

3.4.2. Numerical Methods for Viscous Flows

Numerical investigations are very useful to check the behavior of systems of equations modelling very complicate dynamics. In order to simulate the motion of mixtures of immiscible fluids having different densities, a recent contribution of the team was to develop an hybrid Finite Element / Finite Volume scheme for the resolution of the variable density 2D incompressible Navier-Stokes equations. The main points of this work were to ensure the consistency of the new method [56] as well as its stability for high density ratios [54]. In order to answer these questions, we have developed a MATLAB code and a C++ code. In the following of this work, C. Calgaro and E. Creusé now have in mind the following objectives, in collaboration with T. Goudon (team COFFEE, Inria Sophia-Antipolis) :

- Distribute the matlab version of the code (with an accurate documentation and a graphic interface) to promote new collaborations in the domain and compare alternative numerical solution methods (for instance to compare updating LU factorizations, see [55]);
- To generalize the stability results obtained in [54] for the scalar transport equation to the full 2D Euler system, in particular very low density values density (near vacuum);
- Complete the C++ code to treat more general hydrodynamic models (combustion theory, transport of pollutants). We plan to check the behavior of the equations (typically the Kazhikhov-Smagulov model of powder-snow avalanches) in the regime when the current existence theory does not apply, and extend our kinetic asymptotic-based schemes to such problems.

3.4.3. A posteriori error estimators for finite element methods

A posteriori estimates, finite element methods

The team works on a posteriori error estimators for finite element methods, applied to the resolution of several partial differential equations. The objective is to derive useful tools in order to control the global error between the exact solution and the approximated one (reliability of the estimator), and to control the local error leading to adaptive mesh refinement strategies (efficiency of the estimator).

More specifically, E. Creusé works on the derivation of some "reconstruction estimators" based on gradient averaging, for diffusion problems (with S. Nicaise, LAMAV, Valenciennes), the Reissner-Mindlin system (PhD of É. Verhille), and the Maxwell equations (PhD of Z. Tang).

3.5. Numerical analysis of Schrödinger equations

Dispersive equations, Schrödinger equations

3.5.1. Modelling of quantum dot-helium

In collaboration with G. Reinish (Nice Observatory) and V. Guðmundsson (University of Reykjavik), C. Besse and G. Dujardin are working on the numerical computation of the ground state and the first bound states of the non linear Schrödinger-Poisson system with confining quadratic potential in 2 space dimensions. This models quatum dot helium (*i.e.* the behavior of a pair of quantum electrons in a strong confining potential). The goal is to perform after that numerical time stepping methods to simulate the dynamics of the NLSP system and compute accurately some quantities of physical interest as functions of time, in order to be able to compare the competition between the Coulomb (repulsive) interaction and the binding (attractive) forces due to the confinement in this model as well as in other quantum mechanics models.

3.5.2. Dispersive Schrödinger-like equations

In collaboration with M. Taki (PhLAM laboratory, Lille), C. Besse and G. Dujardin are considering dispersive equations modelling the propagation of a laser beam in an optical fiber. They are trying to explain the possible ways of creating rogue waves in the propagation of laser beams. More generally, they are trying to explain which terms in the dispersive Schrödinger-like equations obtained by the physicists allow which physical behaviour of the solutions (e.g. the creation of rogue waves).

4. Application Domains

4.1. Fluid mechanics

4.1.1. Numerical methods for viscous flows

We are concerned with systems of PDEs describing the evolution of mixture flows. The fluid is described by its density, its velocity and its pressure. These quantities obey mass and momentum conservation. On the one hand, when we deal with the 2D variable density incompressible Navier-Stokes equations, we aim at studying some instabilities phenomena such as the Raileigh-Taylor instability.

Furthermore, diffuse interface models have gained renewed interest in the last few years in fluid mechanics applications. From a physical viewpoint, they allow to describe phase transition phenomena. In this case, a specific stress tensor, introduced originally by Korteweg, must be added to the momentum equation.

If we use in addition the Fick law to relate the divergence of the velocity to derivatives of the density, one obtains the so-called KS model. In this case, the density of the mixture is naturally highly heterogeneous, and may model powder-snow avalanches or specific pollutants. Similar models also appear in combustion theory.

4.1.2. Control

Flow control strategies using passive or active devices are crucial tools in order to save energy in transports (especially for cars, trucks or planes), or to avoid the fatigue of some materials arising in a vast amount of applications. Nowadays, shape optimization needs to be completed by other original means, such as porous media located on the profiles, as well as vortex generator jets in order to drive active control.

4.2. Rubber elasticity

At the continuum level, rubber is modelled by an energy E defined as the integral over a domain D of \mathbb{R}^d of some energy density W depending only locally on the gradient of the deformation u : $E(u) = \int_D W(\nabla u(x)) dx$. At the microscopic level (say 100nm), rubber is a network of cross-linked and entangled polymer chains (each chain is made of a sequence of monomers). At this scale the physics of polymer chains is well-understood in terms of statistical mechanics: monomers thermally fluctuate according to the Boltzmann distribution [61]. The associated Hamiltonian of a network is typically given by a contribution of the polymer chains (using self-avoiding random bridges) and a contribution due to steric effects (rubber is packed and monomers are surrounded by an excluded volume). The main challenge is to understand how this statistical physics picture yields rubber elasticity, and how this can be taken advantage of in order to devise physically-based constitutive laws for rubber. A rigorous derivation can be performed using tools of stochastic homogenization. The challenge is now to devise a numerical method to pass from polymer physics to an explicit continuum constitutive law, and to apply this approach to physically relevant models.

4.3. Maxwell equations

The a posteriori error estimators developed for the Maxwell equations are very useful tools. They are implemented in the software "Carmel-3D" (see the softwares section). This numerical code is used in order to study some original applications, like electrical machines or specific actuators. It is also devoted to nondestructive control by the use of Foucault currents, to the simulation of devices using magnetic fluids or of induced currents in human bodies.

4.4. Corrosion models

The application domains related to corrosion models are the following.

4.4.1. Corrosion modelling of iron based alloy in nuclear waste repository

The concept for long term storage of high-level radioactive waste in France is based on an underground repository. The waste shall be confined in a glass matrix and then placed into cylindrical steel canisters. These containers shall be placed into micro-tunnels in the highly impermeable Callovo-Oxfordian claystone layer at a depth of several hundred meters. At the request of the French nuclear waste management agency ANDRA, investigations are conducted to optimize and finalize this repository concept with the aim to ensure its long-term safety and its reversibility. The long-term safety assessment of the geological repository has to take into account the degradation of the carbon steel used for the waste overpacks and the cell disposal liners, which are in contact with the claystone formation. This degradation is mainly caused by generalized corrosion processes which form a passive layer on the metal surface consisting of a dense oxide inner layer and a porous hydroxide outer layer in contact with the groundwater in the pore space of the claystones. The processes take place under anaerobic conditions, since the groundwater is anoxic.

As a tool to investigate the corrosion processes at the surface of the carbon steel canisters, the Diffusion Poisson Coupled Model (DPCM) for corrosion has been developed by Bataillon *et al.* [47]. The numerical approximation of this corrosion model by accurate and efficient methods is challenging.

4.4.2. Corrosion modelling of Ni-base alloys in Pressurized Water Reactor primary water

The understanding of the oxidation behavior of Ni-base alloys in PWR primary water is of major importance due to the cations released due to corrosion of the steam generators which is a source of the radioactivity of the primary circuit. Moreover, the oxidation process is the reason of the initiation of intergranular stress corrosion cracking in some alloys. A numerical model, called EKINOX (Estimation KINetics OXYdation), has been developed at CEA [48] in order to simulate the oxide scale growth. This model should be able to calculate the evolutions of concentration profiles of the species and of their point defects in the oxide and in the substrate. Numerical experiments have shown the limits of this existing numerical model, especially the need of very small time steps for the computations ; a macroscopic model should be developed and numerical methods proposed for its simulation.

4.5. Plasmas

In the last decade, satellite-positioning devices have become one of the most powerful navigation assistance systems. Recently, Europe launched the first satellites of Galileo, a competitor to the constellation of satellites Navstar GPS American system. In order to guarantee the integrity service level, it is fundamental to take into account the various physical phenomena that can affect the mission and to identify all the potential sources of system unavailability. One of the main sources of data unavailability that has been identified is the phenomenon of ionospheric scintillations. Indeed scintillation causes radio frequency signal amplitude to fade and phase variations as satellite signals pass through the ionosphere. Such effects may induce loss of lock or cycle slips on ranging signals broadcast by Galileo satellites making them totally useless for accurate integrity information determination.

4.6. Optical fibers

When designing optical fibers, the question of the envelope dynamics of laser impulses is crucial because its answer decides how much information the fiber will actually be able to carry. Recent progresses in the optical fiber design now allow to choose specific physical parameters very precisely, and the main limitation for being able to design new and more efficient optical fibers is the understanding of the effect of specific conjunctions of parameter values. In other terms, a main issue is the understanding of the influence of several parameters on specific solutions of nonlinear dispersive equations of Schrödinger type.

5. Software

5.1. ns2ddv-M

Participants: Caterina Calgaro [correspondant (Univ. Lille 1)], Emmanuel Creusé [correspondant (Univ. Lille 1)].

Incompressible Navier-Stokes, Variable Density, Rayleigh-Taylor Instability The NS2DDV-M 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 [56]. The NS2DDV-M code will be available on the SIMPAF team web page before the end of 2011.

Here is the self-assessment of the team effort following the grid provided by Inria (see : <http://www.inria.fr/institut/organisation/instances/commission-d-evaluation>): A3, SO3-up4, SM2-up3, EM3, SDL4, DA1, CD4, MS4, TPM4.

Software web site : <http://math.univ-lille1.fr/~simpaf/SITE-NS2DDV/home.html>

5.2. ns2ddv-C++

Participants: Caterina Calgaro [correspondant (Univ. Lille 1)], Emmanuel Creusé [correspondant (Univ. Lille 1)], Thierry Goudon.

Incompressible Navier-Stokes, Variable Density, Kazhikhov-Smagulov model, Rayleigh-Taylor Instability, avalanches phenomena The NS2DVD-C++ code is based on a hybrid method coupling FV and FE approaches for solving the variable density Navier-Stokes equation in dimension 2. The code is developed around the GetFem++ and the Bamg softwares. It allows in particular mesh refinement strategies so that very relevant simulations can be reached (as the falling droplet with very high density ratios, see for example [54]). The current version of the code consider the additional terms in the Kazhikhov-Smagulov model.

Webpage : <http://math.univ-lille1.fr/~simpaf/SITE-NS2DDV>

Here is the self-assessment of the team effort following the grid provided by Inria (see : <http://www.inria.fr/institut/organisation/instances/commission-d-evaluation>): A1, SO3-up4, SM1, EM2, SDL1, DA1, CD4, MS4, TPM1.

5.3. RTcodes

Participants: Pauline Lafitte [correspondant (ECP)], Jean-François Coulombel [(CNRS & Univ. Nantes)], Christophe Besse [(Univ. Lille 1)], Thierry Goudon [(Inria)], Giovanni Samaey [(KU Leuven)].

Radiative Transfer, Radiative shocks, AP schemes

We have developed a set of numerical codes, written in Scilab, to compute the solutions of the system coupling the Euler equations to the radiation through energy exchanges, in the non equilibrium regime. This covers several situations in the hierarchy of asymptotic problems. The code treats the one-dimensional framework. In particular the code can be used to investigate radiative shocks profiles. The main advantage of our numerical codes is that they do not require any refinement near the singularities. The numerical tests show a very good agreement with the theoretical predictions. See reference [27].

Here is the self-assessment of the team effort following the grid provided by Inria (see : <http://www.inria.fr/institut/organisation/instances/commission-d-evaluation>): A2, SO3, SM2, EM1, SDL1.

5.4. FPcodes

Participants: Pauline Lafitte [correspondant (ECP)], Thierry Goudon [(Inria)], Benjamin Boutin [(Univ. Rennes)].

Fluid-Particles flows, Gravity driven flows, AP schemes

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 an asymptotic-based scheme, is described in details in [57].

Here is the self-assessment of the team effort following the grid provided by Inria (see : <http://www.inria.fr/institut/organisation/instances/commission-d-evaluation>): A2, SO3, SM2, EM1, SDL1.

5.5. CLAToolBox

Participant: Christophe Besse [correspondant].

Absorbant boundary conditions, Schrödinger equation

As a byproduct of the review paper [45], a user-friendly interface is offered¹ to trial and compare various numerical methods to solve the 1D Schrödinger equation with absorbant boundary conditions. We also mention [50] for a numerical investigation of blow-up phenomena in the nonlinear Schrödinger equation.

5.6. SPARCS

Participant: Christophe Besse.

Vlasov-Poisson system, Euler-Poisson system. Back-Trajectory method

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

5.7. Code-Carmel3D

Participant: Emmanuel Creusé [correspondant (Univ. Lille 1)].

This numerical code, developed in collaboration between EDF R&D and Lille 1 University, is devoted to the electromagnetic fields computation by the use of finite element methods. This code allows in particular to perform nondestructive control by the use of Foucault currents in steam generator pipes, and should be soon coupled with the thermal simulation of Code-Aster. Code-Carmel3D uses the Salomé platform (mesh-generator and post-processing) and Open Turns (uncertainties computation). It will consequently allow to solve multi-physics problems, both for the temporal and harmonic formulations.

6. New Results

6.1. Interactions of Macro- and Microscopic scales

6.1.1. Homogenization methods

We have obtained three types of results regarding the homogenization theory and its applications. The first series of results is related to nonlinear elasticity. In [44], A. Gloria has proved the convergence of a discrete model for rubber towards a nonlinear elasticity theory in collaboration with R. Alicandro and M. Cicalese. This analysis has motivated the study of a specific random point set to model the stochastic network of polymer

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

chains, namely the random parking measure, and results have been obtained by A. Gloria and M. Penrose (University of Bath) in [42]. The numerical simulation of the model with the random parking measure has been addressed by A. Gloria, P. La Tallec and M. Vidrascu (project team REO) in [21], and the comparisons with mechanical experiments are promising. A related inverse problem is currently under investigation by M. de Buhan, A. Gloria, P. Le Tallec, and M. Vidrascu.

A second type of results concerns a quantitative theory of stochastic homogenization of discrete linear elliptic equations. A breakthrough has been obtained by A. Gloria and F. Otto (MPI Leipzig) in [63] and [24], who gave the first optimal variance estimate of the energy density of the corrector field for stochastic discrete elliptic equations. The proof makes extensive use of a spectral gap estimate and of deep elliptic regularity theory, bringing in fact the probabilistic arguments to a minimum. This analysis has enabled A. Gloria to propose efficient numerical homogenization methods, both in the discrete and continuum settings [62], [20], see the review article [33]. In [23], A. Gloria and J.-C. Mourrat has pushed the approach forward and introduced new approximation formulas for the homogenized coefficient. In [22] they have considered a more probabilistic approach and given a complete error analysis of a Monte-Carlo approximation of the homogenized coefficients in the discrete case. Work in progress concerns the generalization of the results on discrete elliptic equations to the continuum case.

The third direction of research concerns the periodic homogenization of a coupled elliptic/parabolic system arising in the modelling of nuclear waste storage. This work is in collaboration with the French agency ANDRA. A. Gloria, T. Goudon, and S. Krell have made a complete theoretical analysis of the problem, derived effective equations, and devised an efficient method to solve the effective problem numerically, based on the reduced basis approach, see [41]. This subject has been pushed forward by Z. Habibi in collaboration with ANDRA.

6.1.2. *Statistical physics : molecular dynamics*

In [28], the analysis of constrained molecular dynamics is proposed, with associated numerical schemes.

In [29], the probabilistic derivation of the chemotaxis equation from the individual motion of bacteriae have been carried out. In [30], a numerical method with asymptotic variance reduction have been proposed.

6.2. Plasmas

We investigated a projective integration scheme for a kinetic equation in the limit of vanishing mean free path, in which the kinetic description approaches a diffusion phenomenon. The scheme first takes a few small steps with a simple, explicit method, such as a spatial centered flux/forward Euler time integration, and subsequently projects the results forward in time over a large time step on the diffusion time scale. We showed that, with an appropriate choice of the inner step size, the time-step restriction on the outer time step is similar to the stability condition for the diffusion equation, whereas the required number of inner steps does not depend on the mean free path. We also provided a consistency result. The presented method is asymptotic-preserving, in the sense that the method converges to a standard finite volume scheme for the diffusion equation in the limit of vanishing mean free path. This is a joint work with G. Samaey (K. U. Leuven) [27].

6.3. Finite element and finite volume methods

6.3.1. *Control in fluid mechanics*

Recently, open and closed active flow control were carried out in order to study the flow behavior over a backward-facing step in a transitional regime. It was done either by a global frequency destabilization at the entry of the domain, or by a local blowing or suction through the lower and upper parts of the step by the use of small jets ([58], E. Creusé, A. Giovannini (IMFT Toulouse) and I. Mortazavi (MC2 Inria EPI, Bordeaux)). The numerical computations were based on a vortex-in-cell method. Such controls were shown to be efficient in reducing the average recirculation length value, the global flow energy, as well as the global flow enstrophy. We have now in mind to apply such a strategy on cavity-stent flows, in order to study the effect of passive and/or active control on the average emptying time of the cavity, corresponding to a lot of possible industrial or health applications (combustion, blood circulation in arteries,...).

Passive as well as active control were also performed on the "Ahmed body geometry", which can be considered as a first approximation of a vehicle profile. This work was carried out in collaboration with the EPI Inria MC2 team in Bordeaux (C.H. Bruneau, I. Mortazavi and D. Depeyras), as well as with Renault car industry (P. Gillieron). We recently combined active and passive control strategies in order to reach efficient results, especially concerning the drag coefficient, for two and three dimensional simulations [51]. We recently worked on a 25° rear-window configuration of the Ahmed body, for which the 3D-effects are very important and have to be considered in the numerical simulations [9]. Moreover, the effect of the vortices dynamics on the drag coefficient of a square Ahmed body was addressed [53], as well as the impact of several Ahmed bodies on the same road [52].

In another field of applications, a work was performed with the TEMPO Laboratory of Valenciennes. The objective of this collaboration was to study the pressure wave generated by high-speed trains entering tunnels in order to improve the shape of the tunnel sections.

6.3.2. Numerical Methods for viscous flows

In the case of compressible models, as the Euler equations, a careful analysis of sharp and practical stability conditions to ensure the positivity of both density and pressure variables was performed [11]. We are also concerned with the numerical simulation of certain multi-fluids flows, which in particular arises in the modelling of powdersnow avalanches. The hybrid scheme works on unstructured meshes and can be advantageously coupled to mesh refinements strategies in order to follow fronts of high density variation [38]. In order to answer these questions, we have developed a MATLAB code (NS2DDV-M, see the softwares section), a Fortran code and a C++ code.

6.3.3. A posteriori error estimators for finite element methods

A recent work, in collaboration with S. Nicaise (LAMAV, Valenciennes), was devoted to the derivation of some so-called "reconstruction estimators" based on gradient averaging, in order to provide lower and upper bounds of the error arising from a discontinuous Galerkin approximation of a diffusion problem [59].

At the same time, some equilibrated-type estimators were developed for the Reissner-Mindlin system arising in solid mechanics applications, for conforming and locking-free approximations, in the context of the PhD. of É. Verhille.

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

Some residual-type a posteriori error estimators were developed in the context of magnetostatic and magnetodynamic Maxwell equations, given in their potential and harmonic formulations. Here, the task was to find a relevant decomposition of the error in order to obtain the reliability of the estimator, with the use of ad-hoc interpolations. This work was realized in collaboration with the L2EP Laboratory (Laboratoire d'Electrotechnique et d'Electronique de Puissance de Lille, Lille 1 University), and gave rise to several contributions [17], [18], [32], [31], [65], obtained in the context of the Ph-D thesis of Zuqi Tang [2]. Then, other results about reconstructed a posteriori error estimators were obtained for Discontinuous Galerkin methods, applied to convection-reaction-diffusion equations [16].

6.4. Numerical analysis of Schrödinger equations

6.4.1. Absorbing boundary conditions

C. Besse continues his collaboration with X. Antoine (EPI Corida) and P. Klein. They construct in [3] some classes of absorbing boundary conditions for the two-dimensional Schrödinger equation with a time and space varying exterior potential and for general convex smooth boundaries. The construction is based on asymptotics of the inhomogeneous pseudodifferential operators defining the related Dirichlet-to-Neumann

operator. Furthermore, a priori estimates are developed for the truncated problems with various increasing order boundary conditions. They propose in [34] some suitable discretization schemes of these ABCs and prove some semi-discrete stability results. Furthermore, the full numerical discretization of the corresponding initial boundary value problems is considered and simulations are provided to compare the accuracy of the different ABCs.

6.4.2. *Semi-classical limit of the nonlinear Schrödinger equation*

C. Besse works with R. Carles and F. Méhats (EPI Ipso). They consider in [36] the semiclassical limit for the nonlinear Schrödinger equation. They introduce a phase/amplitude representation given by a system similar to the hydrodynamical formulation, whose novelty consists in including some asymptotically vanishing viscosity. They prove that the system is always locally well-posed in a class of Sobolev spaces, and globally well-posed for a fixed positive Planck constant in the one-dimensional case. They propose a second order numerical scheme which is asymptotic preserving. Before singularities appear in the limiting Euler equation, they recover the quadratic physical observables as well as the wave function with mesh size and time step independent of the Planck constant. This approach is also well suited to the linear Schrödinger equation.

6.4.3. *Analysis and numerical simulation of the Schrödinger equation*

The linear or nonlinear Schrödinger equation with potential is one of the basic equations of quantum mechanics and it arises in many areas of physical and technological interest, e.g. in quantum semiconductors, in electromagnetic wave propagation, and in seismic migration. The Schrödinger equation is the lowest order one-way approximation (paraxial wave equation) to the Helmholtz equation and is called Fresnel equation in optics, or standard parabolic equation in underwater acoustics. The solution of the equation is defined on an unbounded domain. If one wants to solve such a whole space evolution problem numerically, one has to restrict the computational domain by introducing artificial boundary conditions. So, the objective is to approximate the exact solution of the whole-space problem, restricted to a finite computational domain. A review article [45] was written this year to describe and compare the different current approaches of constructing and discretizing the transparent boundary conditions in one and two dimensions. However, these approaches are limited to the linear case (or nonlinear with the classical cubic nonlinearity: an article written was dedicated to this case this year [49]) and constant potentials. Therefore, in collaboration with X. Antoine (IECN Nancy and Inria Lorraine), we proposed to P. Klein to study, in her PhD thesis, the case of the Schrödinger equation with variable potentials. The study of the non-stationary one-dimensional case has already led to one publication [46] and some preliminary results in the stationary case are really promising. These cases are relevant since for example the equations appear in the Bose Einstein condensate with a quadratic potential.

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

Dispersive equations, such as the Schrödinger equation are also considered as boundary-value problems. For example, in [60], G. Dujardin studies the long time asymptotics of the solutions of linear Schrödinger equations considered as initial-boundary value problems on the half-line and on bounded intervals when the boundary data are periodic functions of time. G. Dujardin obtains theoretical results using a transformation method introduced by T. Fokas and provides several numerical experiments to support them.

6.5. Other contributions

6.5.1. *Corrosion models*

The Diffusion Poisson Coupled Model [47] is a model of iron based alloy in a nuclear waste repository. It describes the growth of an oxide layer in this framework. The system is made of a Poisson equation on the electrostatic potential and convection-diffusion equations on the densities of charge carriers (electrons, ferric cations and oxygen vacancies), supplemented with coupled Robin boundary conditions. The DPCM model also takes into account the growth of the oxide host lattice and its dissolution, leading to moving boundary equations. In [12], C. Chainais-Hillairet and I. Lacroix-Violet consider a simplified version of this model,

where only two charge carriers are taken into account and where there is no evolution of the layer thickness. They prove the existence of a steady-state solution to this model. More recently, C. Chainais-Hillairet and I. Lacroix-Violet have also obtained an existence result for the time-dependent simplified model. This result will be soon submitted for publication.

In [4], C. Chainais-Hillairet and coworkers have studied some numerical methods for the approximation of the DPCM model. The choice of the numerical methods is justified by a stability analysis and by the study of their numerical performance. These methods have been implemented in the code CALIPSO developed at ANDRA. Numerical experiments with real-life data show the efficiency of the developed methods.

6.5.2. *Transparent boundary conditions for the Helmholtz equation*

C. Besse and I. Violet start a collaboration with S. Fliss (Poems), J. Coatleven and K. Ramdani (Corida) to build transparent boundary conditions for the Helmholtz equation. They propose in [6] a strategy to determine the Dirichlet-to-Neumann (DtN) operator for infinite, lossy and locally perturbed hexagonal periodic media. They obtain a factorization of this operator involving two non local operators. The first one is a DtN type operator and corresponds to a half-space problem. The second one is a Dirichlet-to-Dirichlet (DtD) type operator related to the symmetry properties of the problem. The half-space DtN operator is characterized via Floquet-Bloch transform, a family of elementary strip problems and a family of stationary Riccati equations. The DtD operator is the solution of an affine operator valued equation which can be reformulated as a non standard integral equation.

6.5.3. *Analysis of subcycling techniques*

Several physics situations involve phenomena which occur on very different time scales. A popular option to integrate the equations in time in this context is to use sub-cycling techniques, which allow to weaken the stability constraints. Several questions are still open for the asymptotic behavior of such methods, e.g. the preservation of equilibrium states. New results about the asymptotic orders if such methods have been derived on toy-model problems which allow a better understanding of these methods and their preservation of equilibrium states [40].

6.5.4. *Phase transitions*

We analyzed numerically a forward-backward diffusion equation with a cubic-like diffusion function, –emerging in the framework of phase transitions modelling– and its “entropy” formulation determined by considering it as the singular limit of a third-order pseudo-parabolic equation. Precisely, we proposed schemes for both the second and the third order equations, we discussed the analytical properties of their semi-discrete counter- parts and we compared the numerical results in the case of initial data of Riemann type, showing strengths and flaws of the two approaches, the main emphasis being put on the propagation of transition interfaces. This is a joint work with C. Mascia (Univ. La Sapienza) [25].

6.5.5. *Modelling of the biological populations*

We worked on two problems of biological populations: the understanding of the occurrence of collective behavior for large populations and the extinction probabilities in some population dynamics.

Several approaches are used in the modelling of collective behavior models for large populations of fish : we obtained results at the particle and kinetic levels for a model involving self-propulsion, friction and an attractive/repulsive potential. By introducing a new dimensionless setting, we identified five parameters that govern the possible asymptotic states for this system (clumps, spheres, dispersion, mills, rigid-body rotation, flocks) and performed a numerical analysis on the 3D particle-setting. Also, we described the kinetic system derived as the limit from the particle model as N tends to infinity; and we proposed, in 1D, a numerical scheme for the simulations, and performed a numerical analysis devoted to trying to recover asymptotically patterns similar to those emerging for the equivalent particle systems, when particles originally evolved on a circle. this is a joint work with J. Rosado (UCLA) and F. Vecil (Univ. Valencia) [43].

The extinction probabilities of a flower population may be modelled by an inhomogeneous random walk on the positive quadrant. On the one hand, introducing the generating function, that solves a PDE, we computed an explicit solution. On the other hand, we compared stochastic and deterministic resolutions of the random walk. This is a joint work with K. Raschel (Univ. Tours), V. C. Tran (Univ. Lille 1) [26].

7. Bilateral Contracts and Grants with Industry

7.1. Numerical homogenization for models of transfer of solutes in porous media

Participants: Antoine Gloria, Zakaria Habibi.

This is a contract (2011-2012) between Inria and ANDRA. The aim of this research is to determine the effective coefficients for models of transfer of solutes in porous media. This is a numerical homogenization problem for a coupled system of convection-diffusion equations. This enters the framework of the numerical simulation for radioactive waste disposal devices.

7.2. Study of the EKINOX model of corrosion

Participants: Claire Chainais, Antoine Gloria.

This is a CNRS Contract (2012-2013) with CEA, Univ Lille1, and Univ B. Pascal. In collaboration with C.Desgranges and F. Lequien (CEA), F. Bouchon (Univ. B. Pascal), A. Gloria and C. Chainais-Hillairet are considering the model EKINOX developed at CEA for the study of the corrosion of Ni-base alloys in PWR primary water. Starting from this numerical model (leading to an explicit in time scheme), they have established a macroscopic model (a system of coupled partial differential equations). Based on this model, the aim is to propose some new numerical methods taking into account correctly the relevant time scales or scales of parameters.

7.3. Numerical methods for the DPCM model

Participants: Claire Chainais, Thomas Gallouët, Antoine Gloria.

This is a contract (2012-2014) between Inria and ANDRA. Some numerical methods have already been developed for the approximation of the DPCM model (corrosion model of an iron based alloy in the nuclear waste repository), see [4]. These methods have been implemented in the code CALIPSO developed at ANDRA. They are devoted to the simulation of the time-dependent model and based on a implicit first order in time and second order in space scheme. For this problem, we want to develop second order in time schemes which remain unconditionally stable. We also want to design new schemes for the direct computation of a steady-state. This should be done during the post-doc of Thomas Gallouët. This is work in collaboration with C. Bataillon (CEA), F. Bouchon (Univ B. Pascal) and J. Fuhrmann (WIAS Berlin).

8. Partnerships and Cooperations

8.1. National Initiatives

8.1.1. Collaborations within Inria

MICMAC (M. Rousset)
REO (A. Gloria)
COFFEE (E. Creusé and C. Calgaro)
POEMS (C. Besse and I. Lacroix-Violet)
CORIDA (C. Besse)
IPSO (C. Besse)

8.1.2. ANR

8.1.2.1. ANR MICROWAVE (2009-2012)

Participants: Christophe Besse, Ingrid Lacroix-Violet.

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

8.1.2.2. ANR IODISSEE (2009-2012)

Participants: Christophe Besse, Pauline Lafitte.

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

8.1.2.3. ANR MEGAS (2009-2012)

Participant: Mathias Rousset.

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

8.1.2.4. ANR INTOCS (2009-2012)

Participant: Pauline Lafitte.

The main scientific subject of the project is the interaction of compressible waves, and more precisely the propagation of high frequency oscillations in hyperbolic boundary value problems. One of the physical motivations is the "Mach stems" formation in reacting gas flows. The head of the project is JF Coulombel (Univ. Nantes), former member of SIMPAF.

8.1.2.5. ANR AMAM (2011-2014)

Participant: Antoine Gloria.

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

8.1.2.6. ANR STAB (2013-2017)

Participant: Pauline Lafitte.

STAB (starting in 2013) : Most of the natural time-evolving systems that one encounters in Physics, Biology, Economics..., can be described by means of evolution equations, or systems of such equations. These equations may include randomness or not. During the last decade, a lot of progress has been made in the understanding of the stabilization of these dynamics, i.e. their convergence to equilibrium. In particular the picture of the qualitative description of the rate of convergence is now almost complete for symmetric models (reversible dynamics). However, the non-reversible setting is still insufficiently understood. One of the most fascinating features of this research area is the strong intricacy between the analysis of partial differential equations and stochastic methods, each approach enlightening the other one. The main goal of this project is to go further, developing tractable and efficient tools, in particular for numerical schemes and algorithms, based on the computation of explicit theoretical bounds. Hence, even if part of the project is devoted to the theoretical study of non-reversible or highly degenerate situations (we typically have to face kinetic or reaction-diffusion models for example), the heart of the project will include discretization schemes, approximating particle systems and concrete simulation situations (including boundary conditions). This concerns the stability of the discretization or numerical methods. The acronym STAB covers both aspects: stabilization and stability. Indeed, sensitivity to small perturbations (or to boundary conditions) is the first definition of large time stability for numerical schemes. The head of the project is I. Gentil (Univ. Lyon1).

8.1.3. Competitivity Clusters

8.1.3.1. LABEX Centre Européen pour les Mathématiques, la Physique et leurs Interactions – CEMPI (2012-2019)

The “Laboratoire d’Excellence” CEMPI was created by the French government within the framework of its “Projets d’Investissement d’Avenir” program, in February 2012. It is a joint venture of the Laboratoire Paul Painlevé (mathematics) and the Laboratoire Physique des Lasers, Atomes et Molécules (PhLAM). Several members of CEMPI participate actively in the CEMPI research and training project, notably through the focus area “The interaction of mathematics and physics”. The corresponding research is described in Sections 3.2.4 and 3.5.

8.2. European Initiatives

8.2.1. Collaborations with Major European Organizations

Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany (F. Otto)

Quantitative homogenization theory (see Section 3.2.1)

9. Dissemination

9.1. Scientific Animation

- A. Gloria is in charge with D. Bonheure of the "PDE and analysis" seminar at ULB since September 2012.
- M. Rousset was in charge of the PDE and numerical analysis seminar of the mathematics department Paul Painlevé until September 2012.
- S. de Bièvre was part of the organizing committee of the "CEMPI Inaugural Conference" in September 2012.

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

S. De Bièvre is in charge of the Doctoral formation in Applied Mathematics at the University of Lille.

E. Creusé is in charge of the first year of the master program "Ingénierie Mathématique" of the Lille 1 University.

C. Besse is in charge of the international Master degree at the University of Lille 1 devoted to Scientific Computing.

Members of the team are involved in MSc degrees at USTL (C. Calgaro, S. De Bièvre, G. Dujardin, M. Rousset).

P. Lafitte is involved in a MSc in Ile de France (M2S) and is in charge of the PDE teaching in first year at École Centrale Paris.

I. Lacroix-Violet teaches numerical analysis in L3 at Polytech Lille (98h).

A. Gloria teaches at ULB (licence 2, master 2, 120h).

9.2.2. Supervision

HdR : A. Gloria, "Qualitative and quantitative results in stochastic homogenization", Lille 1, February 24th 2012

PhD in progress : É. Soret, since September 2011, "Stochastic acceleration and equilibration, Supervision by S. De Bièvre and T. Simon (Painlevé)

PhD in progress : P.-L. Colin, "Étude théorique et numérique de modèles mathématiques de corrosion", 09/01/2012, C. Chainais-Hillairet et I. Lacroix-Violet

9.2.3. Juries

C. Chainais, G. Dujardin and P. Lafitte are members of the jury of the national hiring committee of the "Agrégation de mathématiques".

9.3. Popularization

C. Calgaro is in charge of the communication of "Laboratoire Paul Painlevé" and she is in charge of the relation between the University of Lille and high schools. Accordingly, she organizes various events like "Les Mathématiques itinérantes" and "Stage de seconde à contenu scientifique". With the help of the Communication Department of Inria, C. Calgaro, E. Creusé and T. Goudon produced a documentary fiction (in French) for a general audience on how research in applied mathematics is being done. The title is "Avis de recherche" (see <http://www.inria.fr/avisderecherche>).

On Wednesday, 19th of September 2012, C. Calgaro and C. Besse organized with the mathematics department P. Painlevé laboratory, the Société Mathématique de France, Inria, CNRS and Lille 1 University the conference "Un texte, un mathématicien" in Lille. The invited speaker was C. Villani, the 2010 Fields medalist. This conference had a great success with over 1200 participants.

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