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Project-Team Calvi

Scientific Computing and Visualization

Nancy - Grand Est

Theme : Computational models and simulation

Activity Report

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CALVI is a project associating Institut Elie Cartan (IECN, UMR 7502, CNRS, INRIA and Université Henri Poincaré, Nancy), Institut de Recherche Mathématique Avancée (IRMA, UMR 7501, CNRS and Université de Strasbourg) and Laboratoire des Sciences de l'Image, de l'Informatique et de la Télédétection (LSIIT, UMR 7005, CNRS and Université de Strasbourg) with close collaboration to Laboratoire de Physique des Milieux Ionisés et Applications (LPMIA, UMR 7040, CNRS and Université Henri Poincaré, Nancy).

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2. Overall Objectives

2.1. Introduction

CALVI was created in July 2003.
It is a project associating Institut Elie Cartan (IECN, UMR 7502, CNRS, INRIA and Université Henri Poincaré, Nancy), Institut de Recherche Mathématique Avancée (IRMA, UMR 7501, CNRS and Université de Strasbourg) and Laboratoire des Sciences de l'Image, de l'Informatique et de la Télédétection (LSIIT, UMR 7005, CNRS and Université de Strasbourg) with close collaboration to Laboratoire de Physique des Milieux Ionisés et Applications (LPMIA, UMR 7040, CNRS and Université Henri Poincaré, Nancy).

Our main working topic is modeling, numerical simulation and visualization of phenomena coming from plasma physics and beam physics. Our applications are characterized in particular by their large size, the existence of multiple time and space scales, and their complexity.

Different approaches are used to tackle these problems. On the one hand, we try and implement modern computing techniques like **parallel computing** and **grid computing** looking for appropriate methods and algorithms adapted to large scale problems. On the other hand we are looking for **reduced models** to decrease the size of the problems in some specific situations. Another major aspect of our research is to develop numerical methods enabling us to optimize the needed computing cost thanks to **adaptive mesh refinement** or **model choice**. Work in scientific visualization complement these topics including **visualization of multidimensional data** involving large data sets and **coupling visualization** and **numerical computing**.

2.2. Highlights of the year

The INRIA Large Scale Initiative Action on Modelling and Numerical Simulation for Magnetic Fusion and ITER has started at the beginning of 2009 with a strong involvment of the CALVI project-team.

Nicolas Besse has defended his 'Habilitation à diriger les recherches' in November, thanks to the one year and half on leave at INRIA Nancy-Grand-Est in the CALVI project-team.

We have gained a new understanding of conservative semi-Lagrangian solvers and implemented a conservative parabolic spline method (PSM) into the 5D GYSELA code on the way to simulating efficiently core plasma turbulence on a field aligned mesh of the torus.

3. Scientific Foundations

3.1. Kinetic models for plasma and beam physics

Plasmas and particle beams can be described by a hierarchy of models including N-body interaction, kinetic models and fluid models. Kinetic models in particular are posed in phase-space and involve specific difficulties. We perform a mathematical analysis of such models and try to find and justify approximate models using asymptotic analysis.

3.1.1. Models for plasma and beam physics

The **plasma state** can be considered as the **fourth state of matter**, obtained for example by bringing a gas to a very high temperature ($10^4\ K$ or more). The thermal energy of the molecules and atoms constituting the gas is then sufficient to start ionization when particles collide. A globally neutral gas of neutral and charged particles, called **plasma**, is then obtained. Intense charged particle beams, called nonneutral plasmas by some authors, obey similar physical laws.

The hierarchy of models describing the evolution of charged particles within a plasma or a particle beam includes N-body models where each particle interacts directly with all the others, kinetic models based on a statistical description of the particles and fluid models valid when the particles are at a thermodynamical equilibrium.

In a so-called *kinetic model*, each particle species s in a plasma or a particle beam is described by a distribution function $f_s(\mathbf{x},\mathbf{v},t)$ corresponding to the statistical average of the particle distribution in phase-space corresponding to many realisations of the physical system under investigation. The product $f_s\,d\mathbf{x}\,d\mathbf{v}$ is the average number of particles of the considered species, the position and velocity of which are located in a bin of volume $d\mathbf{x}\,d\mathbf{v}$ centered around $(\mathbf{x},\mathbf{v})$. The distribution function contains a lot more information than what can be obtained from a fluid description, as it also includes information about the velocity distribution of the particles.

A kinetic description is necessary in collective plasmas where the distribution function is very different from the Maxwell-Boltzmann (or Maxwellian) distribution which corresponds to the thermodynamical equilibrium, otherwise a fluid description is generally sufficient. In the limit when collective effects are dominant with respect to binary collisions, the corresponding kinetic equation is the *Vlasov equation*

$$\frac{\partial f_s}{\partial t} + \mathbf{v}\cdot\frac{\partial f_s}{\partial \mathbf{x}} + \frac{q}{m}(\mathbf{E}+\mathbf{v}\times\mathbf{B})\cdot\frac{\partial f_s}{\partial \mathbf{v}} = 0,$$

which expresses that the distribution function f is conserved along the particle trajectories which are determined by their motion in their mean electromagnetic field. The Vlasov equation which involves a self-consistent electromagnetic field needs to be coupled to the Maxwell equations in order to compute this field

$$\begin{aligned}
-\frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t} + \nabla\times\mathbf{B} &= \mu_0\,\mathbf{J},\\
\frac{\partial \mathbf{B}}{\partial t} + \nabla\times\mathbf{E} &= 0,\\
\nabla\cdot\mathbf{E} &= \frac{\rho}{\varepsilon_0},\\
\nabla\cdot\mathbf{B} &= 0,
\end{aligned}$$

which describes the evolution of the electromagnetic field generated by the charge density

$$\rho(\mathbf{x},t) = \sum_s q_s \int f_s(\mathbf{x},\mathbf{v},t)\,d\mathbf{v},$$

and current density

$$\mathbf{J}(\mathbf{x},t) = \sum_s q_s \int f_s(\mathbf{x},\mathbf{v},t)\mathbf{v}\,d\mathbf{v},$$

associated to the charged particles.

When binary particle-particle interactions are dominant with respect to the mean-field effects then the distribution function f obeys the Boltzmann equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} = Q(f, f),$$

where Q is the nonlinear Boltzmann collision operator. In some intermediate cases, a collision operator needs to be added to the Vlasov equation.

The numerical solution of the three-dimensional Vlasov-Maxwell system represents a considerable challenge due to the huge size of the problem. Indeed, the Vlasov-Maxwell system is nonlinear and posed in phase space. It thus depends on seven variables: three configuration space variables, three velocity space variables and time, for each species of particles. This feature makes it essential to use every possible option to find a reduced model wherever possible, in particular when there are geometrical symmetries or small terms which can be neglected.

3.1.2. Mathematical and asymptotic analysis of kinetic models

The mathematical analysis of the Vlasov equation is essential for a thorough understanding of the model as well for physical as for numerical purposes. It has attracted many researchers since the end of the 1970s. Among the most important results which have been obtained, we can cite the existence of strong and weak solutions of the Vlasov-Poisson system by Horst and Hunze [85], see also Bardos and Degond [65]. The existence of a weak solution for the Vlasov-Maxwell system has been proved by Di Perna and Lions [74]. An overview of the theory is presented in a book by Glassey [82].

Many questions concerning for example uniqueness or existence of strong solutions for the three-dimensional Vlasov-Maxwell system are still open. Moreover, their is a realm of approached models that need to be investigated. In particular, the Vlasov-Darwin model for which we could recently prove the existence of global solutions for small initial data [66].

On the other hand, the asymptotic study of the Vlasov equation in different physical situations is important in order to find or justify reduced models. One situation of major importance in tokamaks, used for magnetic fusion as well as in atmospheric plasmas, is the case of a large external magnetic field used for confining the particles. The magnetic field tends to incurve the particle trajectories which eventually, when the magnetic field is large, are confined along the magnetic field lines. Moreover, when an electric field is present, the particles drift in a direction perpendicular to the magnetic and to the electric field. The new time scale linked to the cyclotron frequency, which is the frequency of rotation around the magnetic field lines, comes in addition to the other time scales present in the system like the plasma frequencies of the different particle species. Thus, many different time scales as well as length scales linked in particular to the different Debye length are present in the system. Depending on the effects that need to be studied, asymptotic techniques allow to find reduced models. In this spirit, in the case of large magnetic fields, recent results have been obtained by Golse and Saint-Raymond [83], [87] as well as by Brenier [69]. Our group has also contributed to this problem using homogenization techniques to justify the guiding center model and the finite Larmor radius model which are used by physicist in this setting [80], [78], [79].

Another important asymptotic problem yielding reduced models for the Vlasov-Maxwell system is the fluid limit of collisionless plasmas. In some specific physical situations, the infinite system of velocity moments of the Vlasov equations can be closed after a few of those, thus yielding fluid models.

3.2. Development of simulation tools

The development of efficient numerical methods is essential for the simulation of plasmas and beams. Indeed, kinetic models are posed in phase space and thus the number of dimensions is doubled. Our main effort lies in developing methods using a phase-space grid as opposed to particle methods. In order to make such methods efficient, it is essential to consider means for optimizing the number of mesh points. This is done through different adaptive strategies. In order to understand the methods, it is also important to perform their mathematical analysis. Since a few years we are interested also with solvers that uses Particle In Cell method. This new issue allows us to enrich some parts of our research activities previously centered on the Semi-Lagrangian approach.

3.2.1. Introduction

The numerical integration of the Vlasov equation is one of the key challenges of computational plasma physics. Since the early days of this discipline, an intensive work on this subject has produced many different numerical schemes. One of those, namely the Particle-In-Cell (PIC) technique, has been by far the most widely used. Indeed it belongs to the class of Monte Carlo particle methods which are independent of dimension and thus become very efficient when dimension increases which is the case of the Vlasov equation posed in phase space. However these methods converge slowly when the number of particles increases, hence if the complexity of grid based methods can be decreased, they can be the better choice in some situations. This is the reason why one of the main challenges we address is the development and analysis of adaptive grid methods.

3.2.2. Convergence analysis of numerical schemes

Exploring grid based methods for the Vlasov equation, it becomes obvious that they have different stability and accuracy properties. In order to fully understand what are the important features of a given scheme and how to derive schemes with the desired properties, it is essential to perform a thorough mathematical analysis of this scheme, investigating in particular its stability and convergence towards the exact solution.

3.2.3. The semi-Lagrangian method

The semi-Lagrangian method consists in computing a numerical approximation of the solution of the Vlasov equation on a phase space grid by using the property of the equation that the distribution function f is conserved along characteristics. More precisely, for any times s and t, we have

$$f(\mathbf{x},\mathbf{v},t)=f(\mathbf{X}(s;\mathbf{x},\mathbf{v},t),\mathbf{V}(s;\mathbf{x},\mathbf{v},t),s),$$

where $(\mathbf{X}(s;\mathbf{x},\mathbf{v},t),\mathbf{V}(s;\mathbf{x},\mathbf{v},t))$ are the characteristics of the Vlasov equation which are solution of the system of ordinary differential equations

$$\begin{aligned}\frac{d\mathbf{X}}{ds}&=\mathbf{V},\\ \frac{d\mathbf{V}}{ds}&=\mathbf{E}(\mathbf{X}(s),s)+\mathbf{V}(s)\times\mathbf{B}(\mathbf{X}(s),s),\end{aligned}\tag{1}$$

with initial conditions $\mathbf{X}(t)=\mathbf{x}$, $\mathbf{V}(t)=\mathbf{v}$.

From this property, f^n being known one can induce a numerical method for computing the distribution function f^{n+1} at the grid points $(\mathbf{x}_i,\mathbf{v}_j)$ consisting in the following two steps:

1. For all i,j, compute the origin of the characteristic ending at $\mathbf{x}_i,\mathbf{v}_j$, i.e. an approximation of $\mathbf{X}(t_n;\mathbf{x}_i,\mathbf{v}_j,t_{n+1})$, $\mathbf{V}(t_n;\mathbf{x}_i,\mathbf{v}_j,t_{n+1})$.
2. As

$$f^{n+1}(\mathbf{x}_i,\mathbf{v}_j)=f^n(\mathbf{X}(t_n;\mathbf{x}_i,\mathbf{v}_j,t_{n+1}),\mathbf{V}(t_n;\mathbf{x}_i,\mathbf{v}_j,t_{n+1})),$$

   f^{n+1} can be computed by interpolating f^n which is known at the grid points at the points $\mathbf{X}(t_n;\mathbf{x}_i,\mathbf{v}_j,t_{n+1}),\mathbf{V}(t_n;\mathbf{x}_i,\mathbf{v}_j,t_{n+1})$.

This method can be simplified by performing a time-splitting separating the advection phases in physical space and velocity space, as in this case the characteristics can be solved explicitly.

3.2.4. Adaptive semi-Lagrangian methods

Uniform meshes are most of the time not efficient to solve a problem in plasma physics or beam physics as the distribution of particles is evolving a lot as well in space as in time during the simulation. In order to get optimal complexity, it is essential to use meshes that are fitted to the actual distribution of particles. If the global distribution is not uniform in space but remains locally mostly the same in time, one possible approach could be to use an unstructured mesh of phase space which allows to put the grid points as desired. Another idea, if the distribution evolves a lot in time is to use a different grid at each time step which is easily feasible with a semi-Lagrangian method. And finally, the most complex and powerful method is to use a fully adaptive mesh which evolves locally according to variations of the distribution function in time. The evolution can be based on a posteriori estimates or on multi-resolution techniques.

3.2.5. Particle-In-Cell codes

The Particle-In-Cell method [68] consists in solving the Vlasov equation using a particle method, i.e. advancing numerically the particle trajectories which are the characteristics of the Vlasov equation, using the equations of motion which are the ordinary differential equations defining the characteristics. The self-fields are computed using a standard method on a structured or unstructured grid of physical space. The coupling between the field solve and the particle advance is done on the one hand by depositing the particle data on the grid to get the charge and current densities for Maxwell's equations and, on the other hand, by interpolating the fields at the particle positions. This coupling is one of the difficult issues and needs to be handled carefully.

3.2.6. Maxwell's equations in singular geometry

The solutions to Maxwell's equations are *a priori* defined in a function space such that the curl and the divergence are square integrable and that satisfy the electric and magnetic boundary conditions. Those solutions are in fact smoother (all the derivatives are square integrable) when the boundary of the domain is smooth or convex. This is no longer true when the domain exhibits non-convex *geometrical singularities* (corners, vertices or edges).

Physically, the electromagnetic field tends to infinity in the neighbourhood of the re-entrant singularities, which is a challenge to the usual finite element methods. Nodal elements cannot converge towards the physical solution. Edge elements demand considerable mesh refinement in order to represent those infinities, which is not only time- and memory-consuming, but potentially catastrophic when solving time dependent equations: the CFL condition then imposes a very small time step. Moreover, the fields computed by edge elements are discontinuous, which can create considerable numerical noise when the Maxwell solver is embedded in a plasma (e.g. PIC) code.

In order to overcome this dilemma, a method consists in splitting the solution as the sum of a *regular* part, computed by nodal elements, and a *singular* part which we relate to singular solutions of the Laplace operator, thus allowing to calculate a local analytic representation. This makes it possible to compute the solution precisely without having to refine the mesh.

This *Singular Complement Method* (SCM) had been developed [64] and implemented [63] in plane geometry.

An especially interesting case is axisymmetric geometry. This is still a 2D geometry, but more realistic than the plane case; despite its practical interest, it had been subject to much fewer theoretical studies [67]. The non-density result for regular fields was proven [70], the singularities of the electromagnetic field were related to that of modified Laplacians [59], and expressions of the singular fields were calculated [60]. Thus the SCM was extended to this geometry. It was then implemented by F. Assous (now at Bar-Ilan University, Israel) and S. Labrunie in a PIC–finite element Vlasov–Maxwell code [61].

As a byproduct, space-time regularity results were obtained for the solution to time-dependent Maxwell's equation in presence of geometrical singularities in the plane and axisymmetric cases [81], [60].

3.3. Large size problems

3.3.1. Introduction

The applications we consider lead to very large size computational problems for which we need to apply modern computing techniques enabling to use efficiently many computers including traditional high performance parallel computers and computational grids.

The full Vlasov-Maxwell system yields a very large computational problem mostly because the Vlasov equation is posed in six-dimensional phase-space. In order to tackle the most realistic possible physical problems, it is important to use all the modern computing power and techniques, in particular parallelism and grid computing.

3.3.2. Parallelization of numerical methods

An important issue for the practical use of the methods we develop is their parallelization. We address the problem of tuning these methods to homogeneous or heterogeneous architectures with the aim of meeting increasing computing resources requirements.

Most of the considered numerical methods apply a series of operations identically to all elements of a geometric data structure: the mesh of phase space. Therefore these methods intrinsically can be viewed as a data-parallel algorithm. A major advantage of this data-parallel approach derives from its scalability. Because operations may be applied identically to many data items in parallel, the amount of parallelism is dictated by the problem size.

Parallelism, for such data-parallel PDE solvers, is achieved by partitioning the mesh and mapping the sub-meshes onto the processors of a parallel architecture. A good partition balances the workload while minimizing the communications overhead. Many interesting heuristics have been proposed to compute near-optimal partitions of a (regular or irregular) mesh. For instance, the heuristics based on space-filing curves [84] give very good results for a very low cost.

Adaptive methods include a mesh refinement step and can highly reduce memory usage and computation volume. As a result, they induce a load imbalance and require to dynamically distribute the adaptive mesh. A problem is then to combine distribution and resolution components of the adaptive methods with the aim of minimizing communications. Data locality expression is of major importance for solving such problems. We use our experience of data-parallelism and the underlying concepts for expressing data locality [89], optimizing the considered methods and specifying new data-parallel algorithms.

As a general rule, the complexity of adaptive methods requires to define software abstractions allowing to separate/integrate the various components of the considered numerical methods (see [86] as an example of such modular software infrastructure).

Another key point is the joint use of heterogeneous architectures and adaptive meshes. It requires to develop new algorithms which include new load balancing techniques. In that case, it may be interesting to combine several parallel programming paradigms, i.e. data-parallelism with other lower-level ones.

Moreover, exploiting heterogeneous architectures requires the use of a run time support associated with a programming interface that enables some low-level hardware characteristics to be unified. Such run time support is the basis for heterogeneous algorithmics. Candidates for such a run time support may be specific implementations of MPI such as MPICH-G2 (a grid-enabled MPI implementation on top of the GLOBUS tool kit for grid computing [77]).

Our general approach for designing efficient parallel algorithms is to define code transformations at any level. These transformations can be used to incrementally tune codes to a target architecture and they warrant code reusability.

4. Application Domains

4.1. Thermonuclear fusion

Controlled fusion is one of the major prospects for a long term source of energy. Two main research directions are studied: magnetic fusion where the plasma is confined in tokamaks using a large external magnetic field and inertial fusion where the plasma is confined thanks to intense laser or particle beams. The simulation tools we develop can be applied for both approaches.

Controlled fusion is one of the major challenges of the 21st century that can answer the need for a long term source of energy that does not accumulate wastes and is safe. The nuclear fusion reaction is based on the fusion of atoms like Deuterium and Tritium. These can be obtained from the water of the oceans that is widely available and the reaction does not produce long-term radioactive wastes, unlike today's nuclear power plants which are based on nuclear fission.

Two major research approaches are followed towards the objective of fusion based nuclear plants: magnetic fusion and inertial fusion. In order to achieve a sustained fusion reaction, it is necessary to confine sufficiently the plasma for a long enough time. If the confinement density is higher, the confinement time can be shorter but the product needs to be greater than some threshold value.

The idea behind magnetic fusion is to use large toroidal devices called tokamaks in which the plasma can be confined thanks to large applied magnetic field. The international project ITER[1] is based on this idea and aims to build a new tokamak which could demonstrate the feasibility of the concept.

The inertial fusion concept consists in using intense laser beams or particle beams to confine a small target containing the Deuterium and Tritium atoms. The Laser Mégajoule which is being built at CEA in Bordeaux will be used for experiments using this approach.

Nonlinear wave-wave interactions are primary mechanisms by which nonlinear fields evolve in time. Understanding the detailed interactions between nonlinear waves is an area of fundamental physics research in classical field theory, hydrodynamics and statistical physics. A large amplitude coherent wave will tend to couple to the natural modes of the medium it is in and transfer energy to the internal degrees of freedom of that system. This is particularly so in the case of high power lasers which are monochromatic, coherent sources of high intensity radiation. Just as in the other states of matter, a high laser beam in a plasma can give rise to stimulated Raman and Brillouin scattering (respectively SRS and SBS). These are three wave parametric instabilities where two small amplitude daughter waves grow exponentially at the expense of the pump wave, once phase matching conditions between the waves are satisfied and threshold power levels are exceeded. The illumination of the target must be uniform enough to allow symmetric implosion. In addition, parametric instabilities in the underdense coronal plasma must not reflect away or scatter a significant fraction of the incident light (via SRS or SBS), nor should they produce significant levels of hot electrons (via SRS), which can preheat the fuel and make its isentropic compression far less efficient. Understanding how these deleterious parametric processes function, what non uniformities and imperfections can degrade their strength, how they saturate and interdepend, all can benefit the design of new laser and target configuration which would minimize their undesirable features in inertial confinement fusion. Clearly, the physics of parametric instabilities must be well understood in order to rationally avoid their perils in the varied plasma and illumination conditions which will be employed in the National Ignition Facility or LMJ lasers. Despite the thirty-year history of the field, much remains to be investigated.

Our work in modelling and numerical simulation of plasmas and particle beams can be applied to problems like laser-matter interaction, the study of parametric instabilities (Raman, Brillouin), the fast ignitor concept in the laser fusion research as well as for the transport of particle beams in accelerators. Another application is devoted to the development of Vlasov gyrokinetic codes in the framework of the magnetic fusion programme in collaboration with the Department of Research on Controlled Fusion at CEA Cadarache. Finally, we work in collaboration with the American Heavy Ion Fusion Virtual National Laboratory, regrouping teams from laboratories in Berkeley, Livermore and Princeton on the development of simulation tools for the evolution of particle beams in accelerators.

4.2. Nanophysics

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[1] http://www.iter.org

Kinetic models like the Vlasov equation can also be applied for the study of large nano-particles as approximate models when ab initio approaches are too costly.

In order to model and interpret experimental results obtained with large nano-particles, ab initio methods cannot be employed as they involve prohibitive computational times. A possible alternative resorts to the use of kinetic methods originally developed both in nuclear and plasma physics, for which the valence electrons are assimilated to an inhomogeneous electron plasma. The LPMIA (Nancy) possesses a long experience on the theoretical and computational methods currently used for the solution of kinetic equation of the Vlasov and Wigner type, particularly in the field of plasma physics.

Using a Vlasov Eulerian code, we have investigated in detail the microscopic electron dynamics in the relevant phase space. Thanks to a numerical scheme recently developed by Filbet et al. [76], the fermionic character of the electron distribution can be preserved at all times. This is a crucial feature that allowed us to obtain numerical results over long times, so that the electron thermalization in confined nano-structures could be studied.

The nano-particle was excited by imparting a small velocity shift to the electron distribution. In the small perturbation regime, we recover the results of linear theory, namely oscillations at the Mie frequency and Landau damping. For larger perturbations nonlinear effects were observed to modify the shape of the electron distribution.

For longer time, electron thermalization is observed: as the oscillations are damped, the center of mass energy is entirely converted into thermal energy (kinetic energy around the Fermi surface). Note that this thermalization process takes place even in the absence of electron-electron collisions, as only the electric mean-field is present.

5. Software

5.1. Vlasy

Participants: Matthieu Haefelé [correspondant], Pierre Navaro.

The aim of the platform is to change the way numerical methods are implemented and tested. It has been initiated because most of the researchers of the CALVI project develop new numerical methods for almost the same equations. Until now, every researchers implemented their methods as stand-alone C or Fortran applications. So, each researcher, for each code, has to implement the validation process by himself without using previous implementation done by himself or another member of the project. The platform move the implementation from stand-alone application to a module oriented one. Thanks to standardized application programing interfaces (API), the different numerical methods can be swapped between them and can be validated within a common skeleton. This common skeleton plus the standard API is actually the platform. A better reuse of existing modules is expected as well as an increased efficiency in numerical methods implementation.

The whole implementation has been refactored this year according to remarks made by the team. So the python package called ’vlasy’, which stands for ’Vlasov’ + ’Python’, is born. Lot’s of things that were accessible to the user are now embedded in Python classes within the package. As a result, the user access objects at higher level of abstraction, thus making the usage easier. Some unit tests have been introduced in the skeleton part of the package and solver validation process is also implemented as unit tests. Two Vlasov solvers have been added as well as 4 test cases. The vlasy package is already used at CEA Cadarache in a physics team.

5.2. Vador

Participants: Francis Filbet [correspondant], Eric Sonnendrücker.

The development of the Vador code by Francis Filbet started during his PhD thesis. It solves the Vlasov equation on a uniform grid of phase-space. The two-dimensional version (four dimensions in phase-space) uses cartesian geometry and the Positive Flux Conservative (PFC) method [76], that is perfectly conservative and enables to preserve the positivity of the distribution function. The axisymmetric version is based on the use of the invariance of the canonical momentum and uses a semi-Lagrangian method following the characteristics exactly at the vicinity of $r = 0$. The method is described in [75]. It has been applied as well for plasma as for beam simulations.

The code is available at the following address:
http://math.univ-lyon1.fr/~filbet/open_vador.html

5.3. Obiwan

Participants: Nicolas Besse, Michaël Gutnic, Matthieu Haefelé, Guillaume Latu [correspondant], Eric Sonnendrücker.

Obiwan is an adaptive semi-Lagrangian code for the resolution of the Vlasov equation. It has up to now a cartesian 1Dx-1Dv version and a 2Dx-2Dv version. The 1D version is coupled either to Poisson's equation or to Maxwell's equations and solves both the relativistic and the non relativistic Vlasov equations. The grid adaptivity is based on a multiresolution method using Lagrange interpolation as a predictor to go from one coarse level to the immediately finer one. This idea amounts to using the so-called interpolating wavelets. A parallel version of the code exists and uses the OpenMP paradigm. Domain size of 512^4 has been considered and the method allows to save effectively memory and computation time compared to a non-adaptive code.

5.4. Yoda

Participants: Martin Campos Pinto, Olivier Hoenen [correspondant], Michel Mehrenberger, Eric Violard.

YODA is an acronym for Yet anOther aDaptive Algorithm. The sequential version of the code was developed by Michel Mehrenberger and Martin Campos-Pinto during CEMRACS 2003. The development of a parallel version was started by Eric Violard in collaboration with Michel Mehrenberger in 2003. It is currently continued with the contributions of Olivier Hoenen. It solves the Vlasov equation on a dyadic mesh of phase-space. The underlying method is based on hierarchical finite elements. Its originality is that the values required for interpolation at the next time step are determined in advance. In terms of efficiency, the method is less adaptive than some other adaptive methods (multi-resolution methods based on interpolating wavelets as examples), but data locality is improved.

5.5. Brennus

Participants: Pierre Navaro [correspondant], Eric Sonnendrücker.

The Brennus code is developed in the framework of a contract with the CEA Bruyères-Le-Châtel. It is based on a first version of the code that was developed at CEA. The new version is written in a modular form in Fortran 90. It solves the two and a half dimensional Vlasov-Maxwell equations in cartesian and axisymmetric geometry and also the 3D Vlasov-Maxwell equations. It can handle both structured and unstructured grids in 2D but only structured grids in 3D. Maxwell's equations are solved on an unstructured grid using either a generalized finite difference method on dual grids or a discontinuous Galerkin method in 2D. On the 2D and 3D structured meshes Yee's method is used. The Vlasov equations are solved using a particle method. The coupling is based on traditional PIC techniques.

5.6. LOSS

Participants: Nicolas Crouseilles [correspondant], Guillaume Latu, Eric Sonnendrücker, Stéphanie Salmon.

The LOSS code is devoted to the numerical solution of the Vlasov equation in four phase-space dimensions, coupled with the two-dimensional Poisson equation in cartesian geometry. It implements a parallel version of the semi-Lagrangian method based on a localized cubic splines interpolation we developed. It has the advantage compared to older versions of the cubic splines semi-Lagrangian method to be efficient even when the number of processors becomes important (several hundreds). It is written in Fortran 90 and MPI. The computation kernel of LOSS has been adapted and put in the GYSELA5D code owned by the CEA-Cadarache.

A slightly different version called LOSSx has been developed. The Lossx code is based on the previous one LOSS. It is also devoted to the numerical solution of the Vlasov equation in four phase-space dimensions, coupled with the two-dimensional Poisson equation in cartesian geometry. LOSSx, written in Fortran 90, is parallel in the configuration domain using MPI and uses a dynamic mesh evolving with the distribution function in the velocity domain.

5.7. SPIN

Participants: Sébastien Jund, Guillaume Latu [correspondant], Pierre Navaro, Eric Sonnendrücker.

The Scalable Particle-IN-cell (Spin) code is dedicated to the solving of Vlasov-Maxwell equations, using finite elements for the Maxwell solver. This code is designed to be able to scale well on parallel machine. We elaborated different strategies to balance both the computational loads of Vlasov part (Particle In Cell method) and the Maxwell part (Edge finite elements), in order to take into account the number of particles and elements per processor. The proposed load balancing schemes are for example: static, dynamic (several options), eulerian, lagrangian.

This code has run several 2D test cases, and the 3D version will be achieved soon. The 2D Maxwell solver is able to deal with hybrid grid (triangles and quadrangles) and has the capability of using high order elements. We built the numerical scheme in order to achieve a charge conserving property. An other characteristic of the solver concerns parallel work distribution. The computations on quadrangles are highly parallel: there are few communications and nearly no dependencies between computations. On the triangles, we use a sparse solver in order to solve Maxwell equation (all triangles are tightly coupled). The PASTIX solver (INRIA/Scalapplix team) or a classical Conjugate Gradient solver are used in order to perform the sparse computations.

5.8. calviExport library

Participants: Matthieu Haefelé, Guillaume Latu.

This library contains the different algorithms which can compress a 4D function which is known on a regular discretization. These algorithms have been designed to work on independent blocs of data if they share one point on their boundaries. So this library can be easily integrated into parallel codes. For example, it has been successfully integrated into LOSS, YODA and GYSELA5D (gyrokinetic code from CEA-Cadarache). The output is a set of binary files which contain the resulting compressed function and are structured thanks to a dedicated sparse data format. Typically, we have compressed a 32 GB particle beam distribution function (256^4 grid) into a 40 MB compressed function, which represent a compression factor of 819. This data export relies on the HDF5 library[2], so it is efficient and portable. Finally, these files are directly imported into the plasmaViz software for 4D visualization.

5.9. plasmaViz

Participant: Matthieu Haefelé.

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[2] http://www.hdfgroup.org/

This software is a multidimensional visualization tool. It enables the visualization of 4D functions thanks to an hyperslicing-based interactive visualization technique. So the user can explore at real-time frame rates large hyper-volumetric 4D scalar fields (*i.e.* datasets beyond 16GB) defined on regular structured grids. Thanks to the calviExport library, the parallel simulations export directly the compressed function and plasmaViz is able to load it into memory thanks to a sparse and efficient data structure. As the user selects different hyperslices, plasmaViz builds them from the compressed function on-the-fly. Thanks to hierarchical finite elements and efficient reconstruction algorithms, we can reach interactive frame rates. This software is currently used by physicists from Cadarache and CEA-Bruyère and its integration in the VTK[3] based visualization tool *VisIt*[4] is in progress.

6. New Results

6.1. Mathematical and numerical analysis

Participants: Nicolas Besse, Mihai Bostan, Nicolas Crouseilles, Sever Hirstoaga, Simon Labrunie, Sandrine Marchal, Thomas Respaud, Jean Roche, Eric Sonnendrücker.

We have established several existence and uniqueness results for collisionless kinetic models, the Vlasov-Poisson and Vlasov-Maxwell equations of plasma physics but also the Nordström-Vlasov equations used in astrophysics. We also investigated different asymptotic regimes for the Vlasov-Maxwell equations. Finally, this section includes recent results concerning the convergence of the numerical solution towards the solution of the model (Maxwell or Vlasov).

6.1.1. Asymptotic regimes and existence results for the Vlasov-Poisson and Vlasov-Maxwell equations

In [20] we study a special type of solution for the one dimensional Vlasov-Maxwell equations. We assume that initially the particle density is constant on its support in the phase space and we are looking for solutions with particle density having the same property at any time $t > 0$. More precisely, for each x the support of the density is assumed to be an interval $[p_-, p_+]$ with end-points varying in space and time. We analyze here the case of weak and strong solutions for the effective equations verified by the end-points and the electric field (water-bag model) in the relativistic setting.

We study the existence of weak solutions for the stationary Nordström-Vlasov equations in a bounded domain. The proof follows by fixed point method. The asymptotic behavior for large light speed is analyzed as well. We justify the convergence towards the stationary Vlasov-Poisson model for stellar dynamics [19], [48].

The subject matter of [18] concerns the existence of permanent regimes (*i.e.,* stationary or time periodic solutions) for the Vlasov-Maxwell system in a bounded domain. We are looking for equilibrium configurations by imposing specular boundary conditions. The main difficulty is the treatment of such boundary conditions. Our analysis relies on perturbative techniques, based on uniform a priori estimates.

We investigate the well posedness of stationary Vlasov-Boltzmann equations both in the simpler case of linear problems with a space varying force field, and, the non-linear Vlasov-Poisson-Boltzmann system. For the former we obtain existence-uniqueness results for arbitrarily large integrable boundary data and justify further a priori estimates. For the later the boundary data needs to satisfy an entropy condition guaranteeing classical statistical equilibrium at the boundary. This stationary problem relates to the existence of phase transitions associated with slab geometries [22].

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[3] http://www.vtk.org/

[4] http://www.llnl.gov/visit/

The subject matter of [50] concerns the asymptotic regimes for transport equations with advection fields having components of very disparate orders of magnitude. Such models arise in the magnetic confinement context, where charged particles move under the action of strong magnetic fields. According to the different possible orderings between the typical physical scales (Larmor radius, Debye length, cyclotronic frequency, plasma frequency) we distinguish several regimes: guiding-center approximation, finite Larmor radius regime, etc. The main purpose is to derive the limit models: we justify rigorously the convergence towards these limit models and we investigate the well-posedness of them.

One of the main applications in plasma physics is the energy production through thermo-nuclear fusion. Magnetic confinement controlled fusion requires the confinement of the plasma within a bounded domain using a strong magnetic field. Several models exist for describing the evolution of strongly magnetized plasmas. In [49] we provide a rigorous derivation of the guiding-center approximation in the general three dimensional setting under the action of large stationary inhomogeneous magnetic fields. The first order corrections are computed as well: electric cross field drift, magnetic gradient drift, magnetic curvature drift, etc. The mathematical analysis relies on averaging techniques and ergodicity.

On the other hand, in order to derive a drift-kinetic model, we consider in [54] a new scaling of the Vlasov equation under the hypothesis of large external nonstationary and inhomogeneous electromagnetic field and under the condition of low-Mach number, i.e. when the kinetic energy of the fluid motion is very small in comparison to the thermal energy. To this end, we first make the dimensionless cyclotron period appear in the scaled Vlasov equation. Then we decompose the particle velocity into the mean velocity and its random part and we deduce a system of two equations giving the evolution of the new distribution function and the mean velocity (of the fluid motion). Afterward, an asymptotic analysis is made for this model and a formal derivation of the drift-kinetic model (in a five dimensional phase space) is thus obtained.

We consider the equation $H(Du) = H(0), x \in R^N$. More precisely we investigate under which hypotheses the constant functions are the only bounded solutions. In arbitrary space dimension we prove that this happens when convexity and coercivity occur. In one space dimension we show that the above property holds true for Hamiltonians in a larger class. These results apply when studying the long time behaviour of solutions for time-dependent Hamilton-Jacobi equations [23].

We began [56] the analysis of the qualitative properties of the stationary solutions of the Vlasov-Poisson system in a model 2D singular domain (a polygon with a re-entrant corner). These functions satisfy the system:

$$\begin{aligned} f(x,v) &= \gamma\left(\frac{v^2}{2} + \phi(x) - \phi_e(x) - \beta\right), \\ -\Delta\phi(x) = \rho(x) &:= \int f(x,v)\,dv, \quad \int f(x,v)\,dx\,dv = M\,; \end{aligned} \tag{2}$$

where γ is a given function, ϕ is the potential created by the particles, ϕ_e is an external potential, M is the total mass of the particles, and $\beta \in \mathbb{R}$ is adjusted to satisfy the mass constraint. The qualitative properties of the solution have been established, with an emphasis on the behaviour of the potential ϕ and the density ρ in the neighbourhood of the re-entrant corner. Asymptotics (as a function of the total mass M) have been obtained in the case of a Maxwellian distribution, i.e. when $\gamma(s) = \exp(-s)$. This is the first step towards the analysis of singularities of the time-dependent Vlasov–Poisson and Vlasov–Maxwell systems, though considerable difficulties have to be overcome.

We studied in [57] the existence and uniqueness of solutions to the Vlasov–Poisson system with an initial data of bounded variation. Unlike the works of Cooper–Klimas, Glassey–Schaeffer–Strauss, Guo, ... we do not assume that the initial data (and hence the solution) are bounded, continuous or compactly supported. We were able to prove local existence and uniqueness in dimension 1+1, with an explicit lower bound of the existence time in function of the data. Generalization to higher dimensions is under progress.

6.1.2. Convergence studies of numerical methods

The subject matter of [21] concerns the numerical approximation of reduced Vlasov-Maxwell models by semi-Lagrangian schemes. Such reduced systems have been introduced recently in the literature for studying the laser-plasma interaction. We recall the main existence and uniqueness results on these topics, we present the semi-Lagrangian scheme and finally we establish the convergence of this scheme.

In the paper [58], we introduced a new class of forward Semi-Lagrangian schemes for the Vlasov-Poisson system based on a Cauchy Kovalevsky (CK) procedure for the numerical solution of the characteristic curves. Exact conservation properties of the first moments of the distribution function for the schemes were derived and a convergence study was performed that applies as well for the CK scheme as for a more classical Verlet scheme. The convergence in L1 norm of the schemes was proved and error estimates were obtained.

On a different topic, we analysed numerically the so-called Fourier–Singular Complement Method for the time-dependent Maxwell equations in an axisymmetric domain [52]. This work completes a series of articles on the numerical solution of the equations of electromagnetism in this type of domain : see [62] for Maxwell's equations in the case of axially symmetric data and [71] for Poisson's equation with arbitrary data. The method relies on a continuous approximation of the electromagnetic field, unlike, e.g., edge element methods. This has many advantages in the case of model coupling, e.g. if the Maxwell solver is embedded in a Vlasov–Maxwell code, either PIC or Eulerian. The symmetry of rotation is exploited by using finite elements in a meridian section of the domain only, and a spectral method in the azimuthal dimension. The analysis also incorporates the approach of [26], which allows one to handle both: - noisy or approximate data which fail to satisfy the charge conservation equation, as may happen in a Vlasov–Maxwell code - domains with geometrical singularities (non-convex edges and/or vertices) which cause the electromagnetic field to be less regular than in a smooth or convex domain.

6.1.3. Domain decomposition for the solution of nonlinear equations

This is a joint work with Noureddine Alaa, Professor at the Marrakech Cadi Ayyad University. Strongly degenerate parabolic problems have received considerable attentions, and various forms of this problems have been proposed in the literature, especially in the area of reaction-diffusion equations with cross-diffusion, such problems arise from biological, chemical and physical systems. Various methods have been proposed in the mathematical literature to study the existence, uniqueness and compute numerical approximation of solutions for quasi-linear partial differential equation problems.

In this work we give a result of existence of weak solutions for some quasi-linear parabolic and periodic problem and present a method to compute a numerical solution. The algorithm is based on the Schwarz overlapping domain decomposition method, combined with finite element method. In a first step a super-solution is computed. In a second step a weak solution of the nonlinear problem is computed using a Newton method, see [37]. New numerical analysis and simulation results are published in [13], [30].

6.1.4. Mathematical study of water-bag models

The multi-water-bag representation of the statistical distribution function of particles can be viewed as a special class of exact weak solution of the Vlasov equation, allowing to reduce this latter into a set of hydrodynamic equations while keeping its kinetic character. Therefore finding water-bag-like weak solutions of the gyrokinetic equations leads to the birth of the gyro-water-bag model.

The paper [17] addresses the derivation of the nonlinear gyro-water-bag model, its quasilinear approximation and their numerical approximations by Runge-Kutta semi-Lagrangian methods and Runge-Kutta discontinuous Galerkin schemes respectively.

In [32] the water-bag concept is used in a gyrokinetic context to study finite Larmor radius effects with the possibility of using the full Larmor radius distribution instead of an averaged Larmor radius. The resulting model is used to study the ion temperature gradient (ITG) instability.

In [16] we derive different multi-water-bag (MWB) models, namely the Poisson-MWB, the quasineutral-MWB and the electromagnetic-MWB models. Then we prove some existence and uniqueness results for classical solutions of these different models.

6.2. Development of Vlasov solvers

Participants: Nicolas Besse, Martin Campos Pinto, Nicolas Crouseilles, Alain Ghizzo, Michaël Gutnic, Matthieu Haefelé, Olivier Hoenen, Sébastien Jund, Guillaume Latu, Michel Mehrenberger, Thomas Respaud, Stéphanie Salmon, Eric Sonnendrücker.

6.2.1. Two-dimensional solvers

In [28], a Forward semi-Lagrangian method has been tested and validated. The main difference with the classical Backward semi-Lagrangian method are twofold. First, since the characteristics curves along with the unknown is constant are followed forward in time, this method then enables the use of classical high order time discretization (such as Runge-Kutta 4 algorithms). Second, the remapping (or the deposition) step which is based on cubic spline polynomials, enables to reconstruct the distribution function on a uniform mesh using the particles which have moved during one time step. Two main improvements have been performed during the present year. First, a Cauchy-Kovaleskaya procedure has been tested and validated. This procedure enables a completely explicit way to compute the end of the characteristics, as opposite to Runge-Kutta algorithms which needs intermediate and costly steps. Second, since the method has a lot of similarity with the PIC methods, a charge conservation preserving scheme has been implemented for both Runge Kutta and Cauchy-Kovaleskaya time algorithms.

Another strategy based on conservative semi-Lagrangian methods has been implemented and tested. Whereas semi-Lagrangian methods compute the distribution function on the grid points, conservative methods considers an average of the unknown on each cell. This approximation enables the solving of multi-dimensional problems by a successive solving of one-dimensional equations. This work started last year and has been achieved this year (see [27]). New formulations of conservative semi-Lagrangian methods have been introduced; this unified framework enables in particular to recover several numerical methods available in the literature (PFC, PPM, PSM). Moreover, new filters are proposed to ensure the unknown respects the extrema principles and limit the spurious oscillations created by high order interpolation operators.

A 2D version of LOSS that uses GPGPU computing units has been designed. On a personal computer, we obtain speedups up to 80 using the GPU versus the conventional processor. The domain decomposition strategy is the same as in our previous MPI version of LOSS. Porting codes on GPGPU is cost-effective, because high speedups could be achieved on a low-cost machine. But it is also time-consuming for the developer.

The conservative scheme PFC (developed in [76]) and a numerical scheme for a reformulation of the Poisson equation (similar to that in [72]) were tested in a slight different framework: the Vlasov-Poisson system with a collisional (BGK) term, for a two-species plasma with realistic electron-to-ion mass ratio and dimensionless Debye length (this problem is relevant for the numerical study of plasma-wall interactions).

6.2.2. CALVI platform

The aim of the platform is to change the way numerical methods are implemented and tested. It has been initiated because most of the researchers of the CALVI project develop new numerical methods for almost the same equations. Until now, every researchers implemented their methods as stand-alone C or Fortran applications. So, each researcher, for each code, has to implement the validation process by himself without using previous implementation done by himself or another member of the project. The platform move the implementation from stand-alone application to a module oriented one. Thanks to standardized application programing interfaces (API), the different numerical methods can be swapped between them and can be validated within a common skeleton. This common skeleton plus the standard API is actually the platform. A better reuse of existing modules is expected as well as an increased efficiency in numerical methods implementation.

The whole implementation has been refactored this year according to remarks made by the team. So the python package called 'vlasy', which stands for 'Vlasov' + 'Python', is born. Lot's of things that were accessible to the user are now embedded in Python classes within the package. As a result, the user access objects at higher level of abstraction, thus making the usage easier. Some unit tests have been introduced in the skeleton part of the package and solver validation process is also implemented as unit tests. Two Vlasov solvers have been added as well as 4 test cases. The vlasy package is already used at CEA Cadarache in a physics team.

6.2.3. Four-dimensional solvers

A four-dimensional cubic splines interpolation has been validated in the framework of the backward semi-Lagrangian method on the Vlasov-Poisson equations. This study was motivated to study the validity of the time splitting of the method when non-conservative advection terms are involved. The method is currently tested on more complex problems and appears to be competitive from a CPU time point of view. This approach benefits from the Local Splines strategy which enables a decomposition domain well suited for parallel implementation. This non split scheme has been recently added in the Gysela code. It provides a reference numerical scheme that avoids some approximations that come with splitting. Furthermore, it will allow in the future for alternative and more accurate ways to track the feet of the characteristics.

6.2.4. Adaptive solvers

In [40] a new adaptive semi-Lagrangian scheme based on wavelet approximations for solving transport equations with underlying smooth flow is presented. Inspired by a recent method of Besse, Filbet, Gutnic, Paun and Sonnendrücker, this new approach differs in the fact that it is mostly driven by the notion of good adaptation of a wavelet tree to a given function. Moreover it comes with guaranteed error estimates. In a previous joint work with Mehrenberger, we had designed a first adaptive semi-Lagrangian scheme based on multilevel, hierarchical meshes. The method consisted in predicting a new adaptive mesh for every time step by using a low-cost strategy, and next readapt it once according to the smoothness of the transported numerical solutions. By a rigorous analysis we could prove that our scheme had a prescribed accuracy, achieved by applying the prediction and correction algorithms only once per time step.

The present scheme implements similar ideas, but now in the framework of interpolatory wavelets. For this purpose we translate the property of being (strongly) well-adapted to a given function in the context of wavelet trees, and show that it is (weakly) preserved by a low-cost prediction algorithm which transports wavelet grids along any smooth flow. As a consequence, error estimates can be established for the resulting “predict and readapt” scheme under the essential assumption that the flow underlying the transport equation, as well as its numerical approximation, is a stable diffeomorphism. One complexity result is stated in addition.

6.2.5. Electromagnetic Particle In Cell (PIC) solvers

This project funded by ANR proposes to develop and compare Finite Element Time Domain (FETD) solvers based on the one hand on high order H(curl) conforming elements and on the other hand on high order Discontinuous Galerkin (DG) finite elements and investigate their coupling to the particles. These self consistent relativistic PIC solvers will be the first of this kind in this context and promise to have an impact for the simulation of realistic problems in accelerator and plasma physics.

During the last year we further developed a previous work on charge conserving Finite Element PIC schemes on general grids [51]. We proposed a general mathematical formulation for charge conserving finite elements Maxwell solvers coupled with particle schemes. In particular, we identified the finite-element continuity equations that must be satisfied by the discrete current sources for several classes of time domain Vlasov-Maxwell simulations to preserve the Gauss law at each time step, and proposed a generic algorithm for computing such consistent sources. Since our results cover a wide range of schemes (namely curl-conforming finite element methods of arbitrary degree, general meshes in 2 or 3 dimensions, several classes of time discretization schemes, particles with arbitrary shape factors and piecewise polynomial trajectories of arbitrary degree), we believe that they provide a useful roadmap in the design of high order charge conserving FEM-PIC numerical schemes.

A parallel code (Spin) has been developed to solve bigger test cases using the same numerical method. Spin solves Maxwell equations on hybrid meshes in 2D space (quadrangles and triangles) using edge finite elements. A Poisson solver, that uses also edge finite elements, is called once at the beginning of each run to find the initial self-consistent electric field. The work distribution on processors is well balanced on several dozens of cores in this 2D version. The 3D version of Spin is currently under development.

6.3. Multiple time scales solvers and Magneto HydroDynamics

Participants: Jean-Philippe Braeunig, Emmanuel Frénod, Michaël Gutnic, Philippe Helluy, Alexandre Mouton, Eric Sonnendrücker.

6.3.1. Multiple time scales solvers

One of the most important difficulties of numerical simulation of magnetized plasmas is the existence of multiple time and space scales, which can be very different. In order to produce good simulations of these multiscale phenomena, we have investigated the development of models and numerical methods which are adapted to these problems. The two-scale convergence theory introduced by G. Nguetseng and G. Allaire is one of the tools which can be used to rigorously derive multiscale limits and to obtain new limit models which can be discretized with a usual numerical method: we call this procedure a two-scale numerical method. Within the thesis of Alexandre Mouton we developed a two-scale semi-Lagrangian method and applied it on a gyrokinetic Vlasov-like model in order to simulate a plasma submitted to a large external magnetic field. In order to tackle this complex model, we first investigated this idea in simpler cases. First, we developed a two-scale finite volume method applied to the weakly compressible 1D isentropic Euler equations. Even if this mathematical context is far from a Vlasov-like model, it is a relatively simple framework in order to study the behaviour of a two-scale numerical method in front of a nonlinear model. In a second part, we developed a two-scale semi-Lagrangian method for the two-scale model developed by E. Frénod, F. Salvarani et E. Sonnendrücker in order to simulate axisymmetric charged particle beams. Even if the studied physical phenomena are quite different from magnetic fusion experiments, the mathematical context of the one-dimensional paraxial Vlasov-Poisson model is very simple for establishing the basis of a two-scale semi-Lagrangian method. Finally, we used the two-scale convergence theory in order to improve M. Bostan's weak-* convergence results about the finite Larmor radius model, and we developed a forward semi-Lagrangian method implementing the two-scale method.

6.3.2. Magneto HydroDynamics

The MagnetoHydroDynamics (MHD) equations are a simplified but rich model of conducting fluids. They can be used in some parts of ITER but also in stellar physics, geophysics and plasmas physics. The Discontinuous Galerkin (DG) method is already used for solving MHD problems. It has proved to be very efficient and accurate. However, several difficulties are still present:
-in some cases, the MHD first order equations admit several entropy solutions. The DG method can be designed in order to satisfy an entropy principle, but it is not clear how it behaves in case of multiple solutions;
-if in some parts of the mesh small cells are required, it is important, for efficiency reasons to be able to deal with several time step sizes;
-finally, the divergence free condition is treated by the hyperbolic divergence cleaning technique (see references in [14] and [45]).

As a conclusion, this project permitted to address relevant problems in the approximation of the MHD equations by DG schemes. The scheme has been implemented in CM2, a parallel and general purpose CFD code.

6.3.3. Numerical simulation of compressible multi-material fluid flows

Participant: Jean-Philippe Braeunig
This work is achieved in collaboration with J.-M. Ghidaglia (ENS Cachan), F. Dias (ENS cachan) and B. Desjardins (ENS Ulm) in the frame of the Laboratoire de Recherche Commun MESO (ENS cachan - CEA Bruyères-le-Châtel).

This collaboration has begun during Braeunig's PhD (2004-2007) which was a collaboration CEA-ENS Cachan. We have designed a novel pure eulerian Finite Volumes method for compressible multi-material fluid flows with sharp interface capturing called FVCF-NIP, (Finite Volumes with Characteristic Flux (VFFC) scheme of Ghidaglia et al, interface capturing Natural Interface Positioning (NIP)). A new concept is introduced, the condensate, which allows to handle mixed cells containing two or more materials and to calculate the evolution of the interface on the fixed eulerian grid. The main features of this method are: second order in time and space, local conservation of mass, momentum and total energy, no diffusion of any materials eulerian quantity on each others through the interface and free sliding of materials on each others at the interface. This work is described in Braeunig's PhD report 2007 and in a paper by Braeunig et al [24] published in 2009. A later INRIA report is published in 2009 by Braeunig [46], that describes some improvements of the NIP interface capturing method. The method is currently improved by the work of trainees and post-docs at LRC MESO. The PhD thesis of Daniel Chauveheid has begun in September 2009 on this topic at CEA Bruyères-le-Châtel with the collaboration of Braeunig.

This method is used for industrial applications. One of them is the simulation of Liquefied Natural Gas (LNG) sloshing in LNG carriers (LNG tanks in a boat). The issue was to study and design a procedure to extrapolate experimental results obtained in laboratory with a small scale model (scale 1/40) to the scale of the LNG carrier (scale 1) taking into account compressible effects. A scaling law has been proposed and validated numerically with a VFFC-NIP code. The code has been validated by comparing results with analytical solutions and with a reduced numerical model on academic benchmarks. This work has been presented by J.-M. Ghidaglia at ISOPE 2010 Conference and described in a paper in the ISOPE 2010 Conference Proceeding, see Braeunig et al [38].

6.4. Application of Vlasov codes to magnetic fusion

Participants: Pierre Bertrand, Nicolas Besse, Jean-Philippe Braeunig, Nicolas Crouseilles, Daniele Del Sarto, Sever Hirstoaga, Giovanni Manfredi, Michel Mehrenberger, Etienne Gravier, Guillaume Latu, Jean Roche, Amar Mokrani, Simon Labrunie, Hocine Sellama, Eric Sonnendrücker.

The computation of turbulent thermal diffusivities in fusion plasmas is of prime importance since the energy confinement is determined by these transport coefficients. Fusion plasmas are thus prompt to instabilities and required a self-consistent analysis of the plasmas and the electromagnetic fields. Since collisions between particles play a negligible role, the kinetic plasma behavior is described by the well-known Vlasov model. A key issue is the resonant interaction between particles and waves, which has to be accurately described. The self consistent coupling of the electromagnetic fields then exhibits resonant (Landau) interactions between charged particles and electromagnetic waves, a feature that cannot be addressed in the fluid limit.

6.4.1. Development of a 5D gyrokinetic code

The collaboration around the optimization of the GYSELA code used for gyrokinetic simulations of turbulence in tokamaks went on. The upgrade from four to five dimensions of the phase space is now efficient on several thousands of processors. Last year, several developments of the code enabled to achieve this task.

The aim of this work is to improve the accuracy and the physical relevance of the GYSELA 5D code. Mainly, we would like to perform simulations using a mesh based on curvilinear coordinates in such a way mesh lines are aligned with magnetic field lines. This will diminish numerical diffusion, reduce the size of the computations and improve results accuracy. Moreover, a conservative scheme for plasma turbulence simulations will be used. Using a conservative formalism is an asset for physical relevance of simulations and allows a directional splitting of the Vlasov equation, what is very convenient to deal with curvilinear meshes.
We started in this way by studying conservative numerical methods with curvilinear coordinates for the Guiding-Center (GC) model, which is a reduced 2D conservative model for plasma turbulence. We use the Parabolic Spline Method (PSM), which is a semi-lagrangian conservative scheme using a cubic spline reconstruction. It is a similar method to the Backward Semi-Lagrangian (BSL) scheme [88] (exactly the same scheme for linear constant advection), but based on the conservative form of the Vlasov equation, obviously for conservative models. Different curvilinear meshes are tested on linear advection benchmarks and on simulation

of the growth of unstable turbulent modes. This work has been presented at Conference "Numerical Models for Controlled Fusion" and described in the Conference Proceeding Braeunig et al [39] .
Afterward, the conservative semi-lagrangian PSM scheme has been integrated in the GYSELA code. We first have faced numerical difficulties about the velocity field characteristics. We noticed that cells geometric evolution through the scheme should conserve their volumes, what is equivalent to have a divergence free velocity field at the discrete level, and not only at the continuous level. It is important to obtain a robust scheme in the sense of getting nearby a maximum principle condition. In the same way of improving robustness, we propose an "entropic flux limiter" for the PSM scheme to cut off the spurious oscillations that may appear when dealing with small scales turbulent structures in the flow, below the mesh size. A different way of MPI parallel computing is used for this scheme (transposition), achieved by Guillaume Latu. Drift kinetic $4D$ benchmarks have been performed and compared with the former BSL scheme. This work is described in an INRIA report Braeunig et al [47]. Further validation will be done, especially for the full 5D gyrokinetic model in the GYSELA code which is already functional with the PSM scheme.

Physicists have improved the Gysela code in order to add heat flux driven ion turbulence. It involves large displacements during the advection phase of the Semi-Lagrangian method. In order to take care of this new feature, another parallel algorithm is needed to replace the *local spline method* that requires a too strong CFL-like condition. A 4D transposition parallel operator has been found that provides a solution. Even if the communication time is growing with this new algorithm, it remains less than the advection computing time, even for big runs. The overall parallel relative efficiency of Gysela decreased in this new configuration, nevertheless the asymptotic behaviour (for large number of processors) is still very scalable.

6.4.2. Numerical study of the gyroaverage operator

In this work, we are concerned with numerical approximation of the gyroaverage operators arising in plasma physics to take into account the effects of the finite Larmor radius corrections. Several methods are proposed in the space configuration and compared to the reference spectral method. In particular, a new method is proposed; the basic point is the expansion of the function on a basis (such as polynomial basis). Computing the gyroaverage of a function then reduces to compute the gyroaverage of its basis, which are known analytically. Hence, in the same way as finite element formulation, the method can be formulated into a matrix form. The approach presents other several advantages. On the one side, the number of quadrature points is automatically determined as the intersection between the mesh and the Larmor circle, which provides the necessary adaptivity to reach a good accuracy even for large Larmor circles. Contrary to previous works, the basis function are not evaluated at the quadrature points but integrated on a circle arc, which turns out to be more accurate. the gyroaverage operator also includes an integration with respect to the Larmor radius which belongs to $[0, +\infty]$. Hence a good accuracy when large Larmor radius are considered is required. But, it turns out that it is not sufficient since the numerical integration with respect to the Larmor radius is also important in order to reach a good accuracy for the gyroaverage operator. For example, traditional quadrature rules (such as trapezoidal or Laguerre ones) are not sufficiently efficient. In this context, we develop a new approach which appears to be very efficient for arbitrary wave numbers. The coupling with the guiding-center model leads to very good results compared to the analytical results in the linear regime and to the spectral method for the gyroaverage operator. We then investigate the influence of the different approximations considering the coupling with some guiding-center models available in the literature.

6.4.3. Plasma-wall interactions – application to ELM modes on JET

The vast majority of plasmas produced in the laboratory are in contact with a material surface. In fusion devices, the surface can be either the material vessel that contains the plasma, or some *ad-hoc* device (limiter or divertor) specifically designed to optimize the interaction with the charged particles. These surfaces are eroded by ion and neutral bombardment and may thus see their lifetime considerably reduced. This is one of the key issues for the ITER tokamak, and even more so, for future commercial power plants.

The heat load on the divertor plates can be considerably strained during violent events known as ELMs (edge-localized modes). Although the precise origin of ELMs is still under debate, in practice, these events result in the ejection of energetic charged particles beyond the magnetic separatrix. These particles travel along the magnetic field lines and end up hitting the divertor plates.

In order to model such a scenario, we have developed a 1D Vlasov-Poisson code with open boundaries, for both ions and electrons. The spatial co-ordinate represents the distance along the magnetic field line, whereas the absorbing boundaries are supposed to mimic the divertor plates. Appropriate diagnostics are set up to compute the particles and heat fluxes on the plates.

The main numerical bottleneck is represented by the very large ratio between the system size (~ 10m) and the Debye length ($\sim 10^{-4}$m). A possible approach is to use the recently developed "asymptotic preserving" schemes [72], which allows to work with very small Debye length without incurring numerical instabilities. We are currently implementing this type of scheme in the Vlasov-Poisson code. This project is developed in collaboration with W. Fundamenski and S. Devaux (JET).

6.4.4. Gyro-water-bag approach

In the Gyro-Water-Bag (GWB) approach, a discrete distribution function taking the form of a multi-step like function is used in place of the continuous distribution function along the velocity direction. According to Liouville's phase-space conservation property the distribution function remains constant in time between the bag contours. The time evolution of the system is completely described by the knowledge of the contours. We get a set of hydrodynamic equations, where the system behaves as N fluids coupled together by the electromagnetic fields (in our case the quasi-neutrality). As a matter of fact a small bag number (not more than 10) has been shown to be sufficient to correctly describe the Ion Temperature Gradient (ITG) instability observed in fusion plasmas. Thus the water-bag offers an exact description of the plasma dynamics even with a small bag number, allowing more analytical studies and bringing the link between the hydrodynamic description and the full Vlasov one. Encouraging results have been obtained using three nonlinear waterbag codes: a 3D nonlinear self-consistent gyro-water-bag code which is based on a semi-Lagrangian method (this code was subject to comparison with the GYSELA code dealing with curvilinear meshes); a 3D quasilinear self-consistent gyro-water-bag code and a 1D nonlinear self-consistent electromagnetic-water-bag code where the Discontinuous Galerkin methods are used.

6.4.5. Trapped-ion driven turbulence: gyrokinetic modeling

Drift wave instabilities and their subsequent turbulence are believed to be an important component of the experimentally observed anomalous transport of heat in tokamaks. It was known for several decades, that the transport is "anomalous" in the sense that it does not follow the standard magnitude scaling of collisional transport. Expressed in terms of diffusivities the transport of ions and electrons is comparable, in the range of one or fewer times $1m^2s^{-1}$ in the core region, which is indeed one order of magnitude larger than the collisional ion transport and three higher than collisional electron transport.

Most previous studies of ion-temperature-gradient-driven drift wave turbulence have utilized a simple one-field, nonlinear fluid model, known as the Hasegawa-Mima (HM) equation. This equation is an important paradigm for the description of drift-wave turbulence in magnetically confined plasmas and has a structure similar to that of the Charney equation, describing geostrophic motions in planetary atmospheres. This model is indeed connected to two-dimensional (2D) turbulence. However it is well known that, for 2D turbulence, the feature of turbulence are different from the standard 3D turbulence.

At this step, different remarks must be pointed out:

(i) At high temperature and taking into account the toroidal effects, collisionless kinetic effects allow an effective short time decoupling of particles and field lines ("defreezing effects") thereby introducing non fluid effects, as Landau resonances, strong finite Larmor radius effects and trapped particle resonances.

Trapped particles, in general have unfavorable magnetic drift, leading to the trapped particle instability, a localized low-frequency interchange. The most prominent type of long wavelength toroidal microinstability is Trapped Ion driven Mode (TIM) in the presence of a significant ion temperature gradient. The initial work by Kadomtsev and Pogutse 1971 indicates that the TIM mode has a real frequency below the diamagnetic drift frequency ω_* and below the bounce frequency ω_b. These instabilities are easier to excite in the core region of tokamak fusion plasmas where the plasma can be considered to be effectively collisionless. Thus these instabilities are characterized by frequencies of the order of the trapped particle precession frequency and radial scales of the order of several banana widths. These properties make TIM modes have a global nature *i.e.* large radial correlation lengths that can vary on the equilibrium scale length rather than on the ion gyro-radius scale length usually associated with kinetic micro-instabilities. It has been predicted that because of their large scales and in spite of their low frequencies, these instabilities could lead to a huge transport corresponding to a Bohm-like confinement observed in many experiments. Such Trapped-ion driven modes are thus a simple prototype of kinetic instability since they are driven through the resonant interaction between a wave and trapped ions via their precession motion and implies low toroidal numbers ($n < 100$), allowing fast numerical gyrokinetic simulations (see Depret el al 2000).

Although TIM have been studied during several decades, there exists a real interest today. Recently trapped particle modes seem to play a key role in nonambipolar transport in ITER-relevant regimes, where strong enhancement of transport is thus predicted by bounce-harmonic resonance.

(ii) Another feature concerns the fact that turbulent transport can be greatly reduced in the presence of a magnetic shear. It is well known that the stabilization effect of the precession drift reversal for trapped ion driven instabilities is efficient in nonlinear regime. Magnetic shear describes the dependence of field line direction on the coordinate across closed flux surfaces. In a toroidal field with circular flux surfaces with minor and major radii r and R, the shear is defined as $s = (r/q)\,\partial q/\partial r$. The quantity $q\,(r)$ is the winding number of magnetic field lines on any given flux surface, *i.e.* the ratio of the displacement in toroidal angle to displacement in poloidal angle between two points on a field line. Thus, in a toroidal plasma, the magnetic field is not uniform. Therefore, its magnitude varies both along and transverse to the field lines. The longitudinal variation traps particles (the projection of the guiding-center orbit onto a cross section at fixed toroidal angle traces out a "banana" shape). While the transverse variation, referred to as magnetic shear, has a strong stabilization effect on collective instabilities. This effect exists both in fluid and kinetic instabilities. For trapped particle drive instabilities (as TIM instabilities), it takes place through the reversal of the precession drift (see Kadomtsev and Pogutse 1971).

(iii) Although 5D gyrokinetic simulations are now possible with realistic geometry, such simulations require huge CPU time and memory resources. The most mature kinetic approach is the particle-in-cell (PIC) method. The method involves to integrate gyrokinetic Vlasov equation in time by advancing marker particles along a set of characteristics within the phase space. It basically involves a lagrangian formulation in which the dynamics of an ensemble of gyro-averaged "particles" are tracked.

Several previous points were addressed in a gyrokinetic model of ITG instabilities for TIM model: forward cascade processes, condensation process of turbulence toward low toroidal modes, turbulence stabilization for TIM modes due to reversed magnetic shear. Trapped-ion driven modes (TIMs) are studied by solving a Vlasov equation in action-angle variables using Hamiltonian formalism (see Depret et al 2000). This Vlasov equation is then averaged over the fast scales: cyclotron and bounce motion for trapped ions. The distribution is then calculated as a function of the poloidal flux ψ (normalized to 2π and which indeed plays the role of a radial coordinate) and the precession angle of trapped ions $\phi_3 = \varphi - q\theta$, parametrized by the particle energy E and the trapping parameter κ (depending of the adiabatic invariant μ).

The reduced gyrokinetic Vlasov equation is given by (see Garbet et al 1990, 1992, 1994 and 2001):

$$\frac{\partial f}{\partial t} + \omega_d\,(\kappa; s)\,\frac{E}{T_0}\frac{\partial f}{\partial \phi_3} + \frac{\partial \widehat{J}_0 \widetilde{U}}{\partial \psi}\frac{\partial f}{\partial \phi_3} - \frac{\partial \widehat{J}_0 \widetilde{U}}{\partial \phi_3}\frac{\partial f}{\partial \psi} = 0 \tag{3}$$

where the trapped ion distribution function is $f = f_{\kappa,E}\left(\phi_3, \psi, t\right)$. The self-consistency constraint is

$$C\left(U - \langle U\rangle_{\psi}\right) - C\alpha\nabla^2 U = \overline{n}_i - n_{pi} \tag{4}$$

where we have introduced $U = e_i\widetilde{U}/T_0$, n_{pi} the passing ion density and the gyro-averaged pseudo-density of trapped ions is given by:

$$\overline{n}_i\left(\phi_3, \psi, t\right) = \frac{2}{\sqrt{\pi}} \int_0^{\infty} d(E/T_0) \sqrt{\frac{E}{T_0}} \int_0^{\kappa_{max}} d\kappa\, \kappa K\left(\kappa\right) \widehat{J}_0 f_{\kappa,E}\left(\phi_3, \psi, t\right). \tag{5}$$

In the previous expression we have $C = \left(1 + T_i/T_e\right)/f_p$ where $f_p = 2\sqrt{2\varepsilon}/\pi$ is the fraction of trapped ions. Consequently we have reduced the six-dimensional Vlasov equation into a set of 2D Vlasov equations (indeed $N_\kappa \times N_E$ equations) acting on a two-dimensional phase space (ϕ_3, ψ) (precession angle $\phi_3 = \varphi - q_0\theta$, poloidal flux normalized to 2π), parametrized by the kinetic energy E and the trapping parameter κ ($\kappa \leqslant \kappa_{max}$ with a chosen value of $\kappa_{max} = 0.975$ for numerical simulations). $\widehat{J}_0$ is the gyroaverage operator - multiplication by $J_0\left(k_\perp \rho_c\right) J_0\left(k_\psi \widehat{\delta}_2\right)$ - in Fourier space, ρ_c being the gyro-radius and $\widehat{\delta}_2$ the banana width. The present implementation of this operator is based on a Padé approximation of the Bessel function J_0. Eqs (3), (4) and (5) constitute the basis of our Vlasov model for describing TIM instabilities.

Here the density refers to the density of banana centers which do not correspond to the real density of particles. For instance Hahm and Tang 1996 use a Taylor expansion to give an estimation of the potential value averaged along a field line in the form $\left\langle \widetilde{U} \right\rangle_{banana\ orbits} = U + \frac{1}{2}\delta_b^2\nabla^2\widetilde{U}$, which allows to take into account the difference between the real trapped ion particle density and the density of banana centers.

The trapped ion driven mode has been studied by solving a Vlasov equation averaged over the cyclotron and bounce motion of trapped particles in the presence of a magnetic shear. The magnetic shear parameter appears to play a major role in the stabilization process of the instability and allows us to study the occurring of turbulence inside the system. The major mechanism of turbulent transport is large-scale (electrostatic) convection of trapped particles. The dominant driving process is the temperature gradient over some critical value, and one of the stabilizing elements is reversed magnetic shear. Turbulent plasma is obtained when the magnetic shear reaches a limit value which is positive. The introduction of the magnetic shear parameter allows us to study the different regimes of turbulent transport from plasma state described by a small number of toroidal modes till the occurring of Kolmogorov-like cascade which implies the excitation of a large band of toroidal modes (fully developed turbulence). This is achieved by using a semi-Lagrangian Vlasov code which allows a very accurate description of the trapped particle distribution function in phase space.

6.4.6. *Full wave modeling of lower hybrid current drive in tokamaks*

This work is performed in collaboration with Yves Peysson (DRFC, CEA Cadarache). The goal of this work is to develop a full wave method to describe the dynamics of lower hybrid current drive problem in tokamaks. The propagation and the absorption of the lower hybrid electromagnetic wave is a powerful method to generate current drive by wave-particle resonance. However since the wavelength of the electromagnetic field at the LH frequency is very small, a conventional full wave analysis represents an extremely difficult numerical task, far beyond computer capabilities. The problem is addressed in our work, by full wave calculations based on a mathematical finite element technique, allowing for the first time to treat a large volume of plasma. This method is based on a mixed augmented variational (weak) formulation taking account of the divergence constraint and essential boundary conditions, which provides an original and efficient scheme to describe in a global manner both propagation and absorption of electromagnetic waves in plasmas, without the WKB approximation, as done in the conventional ray tracing techniques. This offers the possibility to investigate specific cases for which the usual description fails and may help therefore a general understanding of the LH physics. A first application to a realistic small tokamak configuration is considered in [42].

6.5. Application of Vlasov codes in nanophysics

Participants: Nicolas Crouseilles, Paul-Antoine Hervieux, Giovanni Manfredi, Omar Morandi.

For a few works, our team has been involved in several research projects involving the application of Vlasov-like equations to the physics of nano-sized objects, such as thin metal films, nanoparticles, quantum wells and quantum dots. It is a topic with tremendous potential for a broad spectrum of applications, ranging from materials science to biology and medicine. Our approach – based on a phase-space description of the dynamics – is not widely used in the nanophysics community, which constitutes one of the originalities of our project.

6.5.1. Quantum hydrodynamics with spin

In previous years, a quantum hydrodynamical (QHD) model was used to investigate the self-consistent electron dynamics in a thin metal film [73]. This QHD model can be viewed as a velocity-moment expansion of the quantum Vlasov (or Wigner) equation. More recently, we have extended the QHD model to include the effect of *spin*. In this model, the electron population is described by a two-component spinor that evolves according to a modified Pauli equation. The numerical code is currently being validated by comparison with some available exact solutions. It will also be necessary to develop a realistic physical model for the spin-spin interactions. The first relevant results are expected for 2010.

6.5.2. Breather mode in a confined quantum electron gas

This work was performed in collaboration with F. Haas and P. Shukla, from the Theoretical Physics Department of the Ruhr Universität, Bochum (Allemagne).

By using a version of the quantum hydrodynamic model, we have demonstrated the existence of a novel breather mode in the self-consistent dynamics of a confined electron gas. This mode corresponds to oscillations of *size* of the electron density, as measured by the variance $\sigma^2 = \int n_e(x,t)x^2 dx$. A variational method was used to determine the salient features of the electron breather mode. Numerical simulations of the time-dependent Wigner-Poisson equations were shown to be in excellent agreement with our analytical results. For asymmetric confinement, a signature of the breather mode is observed in the dipole response, which can be detected by standard optical means.

These results have potential applications to the electron dynamics of nanosized semiconductor devices, such as quantum dots and quantum wells.

6.5.3. Ultrafast magnetization dynamics in diluted magnetic semiconductors

We have developed a dynamical model that successfully explains the observed time evolution of the magnetization in diluted magnetic semiconductor quantum wells after weak laser excitation. Based on a many-particle expansion of the exact $p-d$ exchange interaction, our approach goes beyond the usual mean-field approximation. It includes both the sub-picosecond demagnetization dynamics and the slower relaxation processes which restore the initial ferromagnetic order on a nanosecond timescale. In agreement with experimental results, our numerical simulations show that, depending on the value of the initial lattice temperature, a subsequent enhancement of the total magnetization may be observed on a timescale of few hundreds of picoseconds.

More recently, our model was augmented in order to include the role played by the quantum confinement and the band structure. It was shown that the sample thickness and the background hole density strongly influence the phenomenon of demagnetization. Quantitative results were given for III-V ferromagnetic GaMnAs quantum wells of thickness 4 and 6 nm.

6.6. Inverse problem governed by Maxwell equations

Participant: Jean Roche.

This work is performed in collaboration with Jose Herskovits Norman (UFRJ, Rio de Janeiro, Bresil). Electromagnetic forces allow contactless heating, shaping and controlling of chemical aggressive, hot melts. Applications of this industrial technique are electromagnetic shaping of aluminium ingots using soft-contact confinement of the liquid metal, electromagnetic shaping of components of aeronautical engines made of superalloy materials (Ni,Ti,...), control of the structure solidification, etc ...

We study a two-dimensional magnetostatic inverse shaping problem: can one find a distribution of electric current in order that the horizontal cross-section of the molten metal have a prescribed shape? This is a very important problem that one needs to solve in order to define a process of electromagnetic liquid metal forming. In addition, from a practical point of view, the magnetic field has to be created by a simple configuration of inductors.

Under suitable assumptions, the equilibrated configurations are described by a set of equations expressing an equilibrium relation on the boundary between electromagnetic and surface tension forces (and gravity in three-dimensional models). This equilibrium relation involves the curvature of the boundary and the solution of an elliptic exterior boundary value problem. The equilibrated shape has been shown to be the stationary state of the total energy subject to the constraint that the surface area (the volume in three-dimensional problems) is prescribed.

The goal of this work is to give an algorithm to locate suitable inductors around the molten metal so that the equilibrated shape be as near as possible to a desired one. Two different approaches are proposed, the first one seeks for a set of inductors such that the distance between the equilibrated shape and the given target one is minimized. The second approach looks for a set of inductors such that a slack function related to the equilibrium relation on the boundary of the target shape is minimized.

In the two papers [25], [41] we consider the more realistic case where the inductors are composed by a set of bundled vertical electric wires made of insulated strands. We are interested to determine the position and shape of the package of strands in order to have an horizontal cross-section of the molten metal as close as possible to a prescribed shape.

7. Contracts and Grants with Industry

7.1. CEA Cadarache, gyrokinetic simulation and visualization

Participants: Jean-Philippe Braeunig, Nicolas Crouseilles, Guillaume Latu, Michel Mehrenberger, Ahmed Ratnani, Eric Sonnendrücker.

The object of this contract is the optimization of the semi-Lagrangian code GYSELA used for gyrokinetic simulations of a tokamak and the development of efficient visualization tools for the simulation results. One major development in the code this year was the upgrade from four to five phase space dimensions. This could not be done efficiently without a careful optimization which we helped to perform. Moreover, the 5D code needs to be run on a large number or processors. For this reason we integrated the new local spline interpolation technique we developed, which proved very efficient. On the other hand we parallelized the quasi-neutral Poisson solver used in the code.

7.2. LRC project with CEA Cadarache, Full wave modeling of lower hybrid current drive in tokamaks

Participants: Jean Roche, Simon Labrunie, Amar Mokrani.

The goal of this work is to develop a full wave method to describe the dynamics of lower hybrid current drive problem in tokamaks.

7.3. National initiatives

7.3.1. ANR Projects

Calvi members are involved in three ANR projects.

- Non thematic ANR: Study of wave-particle interaction for Vlasov plasmas (leader A. Ghizzo). In collaboration with F. Califano from the University of Pisa in Italy.

- ANR Calcul Intensif et Simulation: HOUPIC (ANR-06-CIS6-013-01, leader E. Sonnendrücker): Development of 3D electromagnetic PIC codes comparing conforming Finite Elements and Discontinuous Galerkin Solvers on unstructured grids. http://www-math.u-strasbg.fr/houpic/.

- Non thematic ANR: EGYPT project (leader Ph. Ghendrih). Study of gyrokinetic models and their numerical approximation. In collaboration with DRFC/CEA-Cadarache.

7.3.2. INRIA Large Scale Initiative "Fusion"

Eric Sonnendrücker is heading the Large Scale Initiative Fusion energy that started at the beginning of 2009 http://www-math.u-strasbg.fr/ae_fusion/.

7.4. European initiatives

7.4.1. DFG/CNRS project “Noise Generation in Turbulent Flows"

This projects involves several French and German teams both in the applied mathematics and in the fluid dynamics community. Its aim is the development of numerical methods for the computation of noise generated in turbulent flows and to understand the mechanisms of this noise generation.

The project is subdivided into seven teams each involving a French and a German partner. Our German partner is the group of C.-D. Munz at the University of Stuttgart. More details can be found on the web page http://www.iag.uni-stuttgart.de/dfg-cnrs/index_fr.htm

7.4.2. EUFORIA Project

This project is funded by European Union under the Seventh Framework Program (FP7) which will provide a comprehensive framework and infrastructure for core and edge transport and turbulence simulation, linking grid and High Performance Computing, to the fusion modeling community. It has started in January 2008 and ends in December 2010. CALVI is involved in this project to provide efficient and reliable visualization tools. Our proposal is based on the use of two tools: Python with numPy and Matplotlib packages and VisIt Software. Our contribution consists in three packages: getting data from fusion community into VisIt and Python, accessing VisIt and Python from Kepler which is the central software of the project, and providing 4D compression and visualization. This year we made the first point which was quite straight forward. More details can be found on the web page http://www.euforia-project.eu/EUFORIA/

7.5. International initiative

7.5.1. Project “Adaptive Multilevel Particle Schemes for Plasma Simulations”

Participant: Martin Campos Pinto.

Funded by a Fulbright grant this project is developed in collaboration with A. Friedman from the Lawrence Berkeley National Laboratory and J. Verboncoeur at the University of California, Berkeley.

8. Dissemination

8.1. Leadership within scientific community

8.1.1. Conferences, meetings and tutorial organization

- Giovanni Manfredi was co-organizer of the "Vlasovia 2009" conference, CIRM, Marseille, August 31st - September 4th, 2009.
- Nicolas Crouseilles and Eric Sonnendrücker organized the Summer school of the Large Scale Initiative "FUSION" : September 15-18, 2009, Strasbourg.
- Eric Sonnendrücker was co-organizer of the conference on "Numerical Methods for Controlled Fusion", 20-24 Avril 2009, Porquerolles, France
- Pierre Navaro and Eric Sonnendrücker organized the semestrial Euforia (European 7th FP project) meeting in Strasbourg, 25-27 November 2009.

8.1.2. Invitations at conferences and summer schools

- Nicolas Besse gave a lecture at the 7th International Conference of Numerical Analysis and Applied Mathematics, Rethymno, Crete (Greece) September 18-22, 2009. Title: Reduced models for gyrokinetic turbulence.
- Mihai Bostan gave the following lectures:
  - Equations cinétiques et applications
    Centre International de Rencontres Mathématiques Marseille, February 2009. Title: Asymptotic regimes for strongly magnetized plasmas. Gyro-kinetic models.
  - Numerical models for controlled fusion, Porquerolles, France 20-24 April 2009. Title: Gyro-kinetic models for strongly magnetized plasmas and ergodic theory.
  - Modeling and simulation for magnetic fusion, Strasbourg, France 15-18 september 2009. Title: Second order accurate models for strongly magnetized plasmas.
  - Physical and mathematical challenges in light of Iter, Marseille, France 26-30 October 2009. Title: Rigorous derivation of gyro-kinetic models for strongly magnetized plasmas.
  - International workshop on Hamiltonian approaches of Iter physics; Marseille, France 2nd-6th november 2009. Title: Asymptotic models for magnetic confinement.
  - Theory and Numerics of kinetic equations, University of Saarland, Saarbruecken Germany November 16-18 2009. Title: Asymptotic models for strongly magnetized plasmas.
- Martin Campos Pinto gave the following lectures:
  - “How to predict accurate grids in adaptive semi-Lagrangian schemes” at the Workshop Multiresolution and Adaptive Methods for Convection-Dominated Problems held at University Paris 6, January 22-23, 2009, Paris.
  - “Consistent coupling in FEM-PIC codes for Vlasov-Maxwell Simulation” at the 10th International Computational Accelerator Physics Conference, August 31st - September 4th, 2009, San Francisco.
- Nicolas Crouseilles taught a course ”New formulations of semi-Lagrangian methods” at the "Vlasovia 2009" conference, CIRM, Marseille, August 31st - September 4th, 2009.
- Alain Ghizzo gave the following lectures:
  - ”Eulerian-Vlasov models for plasma simulation”, at the 9th International School for Space Simulations, July 3-11, 2009, Paris

  - ”Gyrokinetic simulation of Trapped Ion Modes for ITG instabilities”, at the International Workshop on "Hamiltonian Approaches of ITER Physics" held in CIRM (Centre International de Rencontres Mathématiques), Marseille, November 2nd-6th, 2009.
- Giovanni Manfredi taught a course at the Summer school of the Large Scale Initiative "FUSION": September 15-18, 2009, Strasbourg. Title: Plasma-wall transition in magnetized plasmas.
- Jean-Rodolphe Roche gave the following invited lectures:
  - ”A domain decomposition method for second order non-linear PDE’s equations”, at Laboratoire National de Calcul Scientifique, Petropolis, Brasil.
  - ”Shape optimization for electromagnetic casting problem” at Instituto Balseiro, San Carlos de Bariloche, Argentina.
  - ”La méthode de décomposition de domaines” at Institut Jean Lamour, Nancy, France.
- Stéphanie Salmon gave the following invited lecture
  - "Exact Charge Conservation in a High-Order Conforming Maxwell Solver coupled with Particles" in the Minisymposium "High-order methods for the solution of wave propagation" organized by Stéphane Lanteri at Waves 2009, 15th-19th June 2009, Pau.
- Eric Sonnendrücker gave the following invited lectures:
  - "Adaptive methods for the Vlasov equation" at "Multiresolution and Adaptive Methods for Convection-Dominated Problems", January 22-23, 2009, Paris, France.
  - "Adaptive semi-Lagrangian methods for the Vlasov equation", at SMAI 2009 conference, mini-symposium on Multiresolution methods, 25-29 May 2009, La Colle sur Loup, France.
  - "Geometric formulation of the Vlasov-Maxwell" Equations at "Workshop on Hamiltonian methods for ITER physics", 2-6 November 2009, CIRM, Luminy.

8.1.3. Administrative duties

- Vladimir Latocha is assistant head of the Mathematics Department at the University Henri Poincaré Nancy 1. He is also in charge of the international relations.
- Vladimir Latocha gives lectures for "training of trainers" of the Education Office of Nancy-Metz on the theme of algorithmics at the secondary school.
- Jean Rodolphe Roche is the head of the Mathematics Science department of the “École Supérieure des Sciences et Technologies de l’Ingénieur de Nancy" .
- Jean Rodolphe Roche is the research coordinator of the L.R.C. projet ”Full wave modeling of lower hybrid current drive in tokamaks”
- Jean Rodolphe Roche is the research coordinator of a CAPES-COFECUB bilateral agreement with the Federal University of Rio de Janeiro and the National Laboratory of Scientific Computing of Brazil.
- Eric Sonnendrücker is a member of the National Committee of Universities (26th section: applied mathematics).
- Eric Sonnendrücker is a member of the Scientific Committee of CIRM.

8.2. Teaching

- Vladimir Latocha taught a course entitled "Basics of Scientific Programming" at the Master of Mathematics at the University Henri Poincaré Nancy 1.

- Giovanni Manfredi and Paul-Antoine Hervieux taught a 28-hour course at the Master "Condensed Matter and Nanophysics". Title of the course: Photon-matter interactions.
- Martin Campos Pinto taught a graduate course entitled "Mathematical Methods for Physics" at the Master of Computational Engineering at the "Institut de Mécanique des Fluides et des Solides" in Strasbourg.
- Jean Rodolphe Roche taught a course on Domain Decomposition in the M2 in mathematics of UHP.
- Eric Sonnendrücker taught a course on wavelets in the Master 2 in mathematics at University of Strasbourg.

8.3. Ph. D. Theses

8.3.1. Ph. D. defended in 2009

1. Alexandre Mouton, *Multiscale approximation of the Vlasov equation*. Advisors: Emmanuel Frénod and Eric Sonnendrücker. Defended September 16, 2009 (Jury: Grégoire Allaire, Christophe Besse, Laurent Desvillettes, Emmanuel Frénod, Philippe Helluy, Eric Sonnendrücker).

8.3.2. Ph. D. in progress

1. Aurore Back, *Hamiltonian derivation of gyrokinetic models*. Advisors: Emmanuel Frénod and Eric Sonnendrücker.
2. Anaïs Crestetto, since September 2009, *High order moments fluid model for plasmas and multiphase media.* Advisors: Philippe Helluy and Marc Massot.
3. Sandrine Marchal, *Domain decomposition methods to solve a system of hyperbolic equations*. Advisors: Simon Labrunie and Jean Rodolphe Roche.
4. Thomas Respaud, *Numerical coupling of Maxwell and Vlasov equations*. Advisor: Eric Sonnendrücker.
5. Ahmed Ratnani, *Study of the quasi-neutrality equation and its coupling with Vlasov equations*. Advisors: Nicolas Crouseilles and Eric Sonnendrücker.
6. Takashi Hattori, since september 2009, *Domain decomposition methods for full wave simulation in cold plasma*. Advisors: Simon Labrunie and Jean Rodolphe Roche.

8.3.3. Post Doc in progress

1. Omar Morandi, *Ultrafast magnetization dynamics in diluted magnetic semiconductors*. Advisor: Nicolas Crouseilles, Paul-Antoine Hervieux, Giovanni Manfredi.
2. Marc Sauget, *Algorithms and load-balancing strategies in Particle-In-Cell Codes*. Advisor: Guillaume Latu.
3. Hocine Sellama, *Numerical study of gyroaverage operators*. Advisor: Nicolas Crouseilles, Michel Mehrenberger, Eric Sonnendrücker.
4. Fahd Karami, *Singularities of the Vlasov-Poisson system*. Advisors : Xavier Antoine and Simon Labrunie.
5. Amar Mokrani, *Full-wave modeling of lower hybrid current drive in tokamaks*. Advisor: Jean Roche.

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