INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Project-Team Calvi

Scientific Computing and Visualization

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Activity Report

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1. Team

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 Louis Pasteur, Strasbourg) and Laboratoire des Sciences de l'Image, de l'Informatique et de la Télédétection (LSIIT, UMR 7005, CNRS and Université Louis Pasteur, 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. Overall Objectives

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 Louis Pasteur, Strasbourg) and Laboratoire des Sciences de l'Image, de l'Informatique et de la Télédétection (LSIIT, UMR 7005, CNRS and Université Louis Pasteur, 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**.

3. Scientific Foundations

3.1. Kinetic models for plasma and beam physics

Keywords: *Vlasov equation*, *asymptotic analysis*, *beam physics*, *existence*, *kinetic models*, *mathematical analysis*, *modeling*, *plasma physics*, *reduced models*, *uniqueness*.

3.1.1. Abstract

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.

3.1.2. 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

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

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 resolution 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.

3.1.3. 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 [68], see also Bardos and Degond [50]. The existence of a weak solution for the Vlasov-Maxwell system has been proved by Di Perna and Lions [56]. An overview of the theory is presented in a book by Glassey [64].

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 [51].

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 [66], [70] as well as by Brenier [54]. 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 [62], [60], [61].

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

Keywords: *Numerical methods*, *Vlasov equation*, *adaptivity*, *convergence*, *numerical analysis*, *semi-Lagrangian method*, *unstructured grids*.

3.2.1. Abstract

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.

3.2.2. 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.

3.2.3. 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.

3.2.4. 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.

3.2.5. 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.

3.2.6. Particle-In-Cell codes

The Particle-In-Cell method [53] 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 diffential 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.

3.2.7. 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 reentrant 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 instationary 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 [48] and implemented [49] 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 [52]. The non-density result for regular fields was proven [55], the singularities of the electromagnetic field were related to that of modified Laplacians [45], and expressions of the singular fields were calculated [46]. 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 [47].

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 [63], [46].

3.3. Large size problems

Keywords: *GRID*, *Parallelism*, *code transformation*, *domain decomposition*.

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 ressources 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 partitionning the mesh and mapping the submeshes 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 [67] 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 [71], 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 [69] 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 runtime support associated with a programming interface that enables some low-level hardware characteristics to be unified. Such runtime support is the basis for heterogeneous algorithmics. Candidates for such a runtime 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 [59]).

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.

3.4. Scientific visualization of plasmas and beams

Visualization of multi-dimensional data and more generally of scientific data has been the object of numerous research projects in computer graphics. The approaches include visualization of three-dimensional scalar fields looking at iso-curves and iso-surfaces. Methods for volume visualization, and methods based on points and flux visualization techniques and vectorial fields (using textures) have also been considered. This project is devoted to specific techniques for fluids and plasmas and needs to introduce novel techniques for the visualization of the phase-space which has more than three dimensions.

Even though visualization of the results of plasma simulations is an essential tool for the physical intuition, today's visualization techniques are not always well adapted tools, in comparison with the complexity of the physical phenomena to understand. Indeed the volume visualization of these phenomena deals with multidimensional data sets and sizes nearer to terabytes than megabytes. Our scientific objective is to appreciably improve the reliability of the numerical simulations thanks to the implementation of suitable visualization techniques. More precisely, to study these problems, our objective is to develop new physical, mathematical and data-processing methods in scientific visualization: visualization of larger volume datasets, taking into account the temporal evolution. A global access of data through 3D visualization is one of the key issues in numerical simulations of thermonuclear fusion phenomena. A better representation of the numerical results will lead to a better understanding of the physical problems. In addition, immersive visualization helps to extract the complex structures that appear in the plasma. This work is related to a real integration between numerical simulation and scientific visualization. Thanks to new methods of visualization, it will be possible to detect the zones of numerical interest, and to increase the precision of calculations in these zones. The integration of this dynamical side in the pipeline “simulation then visualization" will not only allow scientific progress in these two fields, but also will support the installation of a unique process “simulation-visualization".

4. Application Domains

4.1. Thermonuclear fusion

Keywords: *ITER*, *Inertial fusion*, *laser-matter interaction*, *magnetic fusion*, *particle accelerators*.

Controled 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

[1] http://www.iter.gouv.fr/index.php

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

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. [58], 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. Vador

Keywords: *2D and axisymmetric geometry*, *PFC method*, *Vlasov*, *beam simulation*, *conservative*, *plasma simulation*, *positivity preserving*.

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 [58], 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 [57]. It has been applied as well for plasma as for beam simulations.

The code is available at the following address:
http://www.univ-orleans.fr/mapmo/membres/filbet/index_vad.html

5.2. Obiwan

Keywords: *Vlasov*, *adaptive*, *interpolet*, *multiresolution*, *semi-Lagrangian*.

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.

5.3. Yoda

Keywords: *Vlasov*, *adaptive*, *hierarchical finite elements*, *multiresolution*, *semi-Lagrangian*.

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. The implementation is generic n dimensional ($2n$-dimensions in phase-space).

5.4. Brennus

Keywords: *Maxwell*, *Particle-In-Cell (PIC)*, *Vlasov*, *axisymmetric*, *beam simulation*, *finite volume*, *plasma simulation*, *unstructured grids*.

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. 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 and Nedelec finite elements in 3D. 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.

5.5. LOSS

Keywords: *MPI*, *Vlasov*, *local cubic splines*, *scalability*, *semi-Lagrangian*.

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

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 goemetry. 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.

6. New Results

6.1. Existence results and qualitative behaviour for the Vlasov-Poisson and Vlasov-Maxwell equations

Keywords: *Vlasov-Maxwell equations*, *Vlasov-Poisson equations*, *harmonic solutions*, *laser-plasma interaction*, *permanent regimes*, *weak/mild formulation*.

Participants: Mihai Bostan, Simon Labrunie.

We proved existence and/or uniqueness results of different weak and mild solutions for the Vlasov-Poisson equations in different situations and asymptotic behaviour of the solutions.

In [3], we study the existence of time periodic weak solution for the N dimensional Vlasov-Poisson system with boundary conditions. We start by constructing time periodic solutions with compact support in momentum and bounded electric field for a regularized system. Then, the a priori estimates follow by computations involving the conservation laws of mass, momentum and energy. One of the key points is to impose a geometric hypothesis on the domain: we suppose that its boundary is strictly star-shaped with respect to some point of the domain. These results apply for both classical and relativistic case and for systems with several species of particles.

In [5], we consider a stationary $1D$ Vlasov-Maxwell system which describes the laser-plasma interaction. Three cases are analyzed: the classical case, the quasi-relativistic case and the relativistic case. We prove the existence of a stationary solution and we establish estimates for the charge and current densities

in [6], we construct weak solutions for the three dimensional Vlasov-Poisson initial-boundary value problem with bounded electric field. The main ingredient consists of estimating the change in momentum along characteristics of regular electric fields inside bounded spatial domains. As direct consequences we obtain the propagation of the momentum moments and the existence of a weak solution satisfying the balance of total energy

In [4], we study a reduced $1D$ Vlasov-Maxwell system which describes the laser-plasma interaction. The unknowns of this system are the distribution function of charged particles, satisfying a Vlasov equation, the electrostatic field, verifying a Poisson equation and a vector potential term solving a nonlinear wave equation. The nonlinearity in the wave equation is due to the coupling with the Vlasov equation through the charge density. We prove here the existence and uniqueness of the mild solution (*i.e.*, solution by characteristics) in the relativistic case by using the iteration method.

In [7], we study the permanent regimes of the reduced Vlasov–Maxwell system for laser-plasma interaction. A non-relativistic and two different relativistic models are investigated. We prove the existence of solutions where the distribution function is Boltzmannian and the electromagnetic variables are time-harmonic and circularly polarized.

In [2], we study the behavior of time periodic weak solutions for the relativistic Vlasov-Maxwell boundary value problem in a three dimensional bounded domain with strictly star-shaped boundary when the light speed becomes infinite. We prove the convergence toward a time periodic weak solution for the classical Vlasov-Poisson equations.

6.2. Periodic solutions for nonlinear elliptic equations. Applications to charged particles beam focusing systems

Keywords: *Nonlinear elliptic equations*, *electron beam focusing system*, *existence and uniqueness*, *periodic solutions*.

Participants: Mihai Bostan, Eric Sonnendrücker.

We study the existence of spatial periodic solutions for nonlinear elliptic equations $-\Delta u + g(x, u(x)) = 0,\ x \in R^N$ where g is a continuous function, nondecreasing w.r.t. u. We give necessary and sufficient conditions for the existence of periodic solutions. Some cases with nonincreasing functions g are investigated as well. As an application we analyze the mathematical model of electron beam focusing system and we prove the existence of positive periodic solutions for the envelope equation. We present also numerical simulations [8].

6.3. Development of semi-Lagrangian Vlasov solvers

Keywords: *MPI*, *Vlasov*, *cubic splines*, *semi-Lagrangian*.

Participants: Nicolas Besse, Nicolas Crouseilles, Alain Ghizzo, Michael Gutnic, Olivier Hoenen, Guillaume Latu, Stéphanie Salmon, Eric Sonnendrücker, Eric Violard.

During the last year we continued the development of our semi-Lagrangian Vlasov solvers based on different interpolation techniques on adaptive and uniform grids.

A major improvement of the classical semi-Lagrangian method based on a cubic spline intepolation was obtained in order to get a good scalability on several hundreds of processors which are needed in realistic applications. The main drawback of cubic spline interpolation which works very well in practice, is that this interpolation is non-local since all the values of the distribution function on a line of the grid are needed. Therefore previous parallel implementations used a global transpose of the distribution function at each split step which does not scale well over around a hundred processors even with a careful implementation and overlapping of computations and communications. To overcome this problem, we developed a method using patches decomposing the phase-space domain, each patch being devoted to one processor. Each patch computes its own local cubic spline coefficients which are necessary to interpolate the distribution function on the subdomain. Such an approach would involve a large amount of data exchange, but a condition on the time step allows us to control the shifts generated by the solve of the equations of motion, so that the communications are only done between adjacent processors. Hence, this communication scheme enables us to obtain competitive results from a scalability point of view. Moreover, thanks to an adapted treatment of the boundary conditions, the numerical results obtained with this new method are in very good agreement with those obtained with the sequential version of the code. In particular, several numerical tests applied to plasma physics or beam physics showed the good behavior of the method [34], [12]. In addition to the newly developed code LOSS, this method was also integrated into the code GYSELA in the framework of a contract with CEA Cadarache.

On the other hand, in many physical situations Vlasov simulations on a uniform grid are inefficient because at any given time nothing is happening in some regions of phase space. Moving grid techniques can then be used to save a lot of computation time. In this context, we developed a relativistic Vlasov-Maxwell solver for laser-plasma interaction based on a moving grid. We work on a semi-Lagrangian code, initially developed by Alain Ghizzo to study the interaction of ultrashort electromagnetic pulse with plasma. During the major part of the simulation, many of the grid points are useless as the distribution function is zero on these points. We thus introduce a dynamic mesh (or moving grid) following the development of instabilities which allows us to considerably decrease the number of points in the computational grid where the distribution function is zero. All the details and results of this work are described in [41].

Concerning our adaptive wavelet based semi-Lagrangian Vlasov solvers, two main improvements where obtained during the past year. First we developed a new solver for the 1D relativistic Vlasov-Maxwell equations and second we completed and optimized our 4D phase space code.

Two major extensions were made in our parallel adaptive 1D code. First we developed a 1D Maxwell solver and then we replaced the non relativistic Vlasov equation by its relativistic counterpart, thus introducing new difficulties. In this case the splitting method does not yield constant coefficient advections in each direction and is therefore not used. Instead a second order predictor corrector type non split method was introduced. On the other hand, in the computation of the current density from the wavelet decomposition of the distribution we had to take into account the Lorentz factor γ which is a non polynomial function of the momentum. This code was used to study parametric instabilities in laser-plasma interaction. A characteristic feature of the numerical experiments performed with this code was the use of a finer mesh in x-direction than in v-direction. This has been documented in [39].

On the other hand we completed the developement of the adaptive parallel 2D Vlasov solver (4D in phase space) and applied it to several problems in beam physics and plasma physics [21], [11]. In this new simulator, we consider a large phase space domain. The use of an adaptive scheme leads to a severe reduction of memory usage. A new data structure based on two levels of arrays, one for the coarse grid and one for the finer levels has been introduced for efficiency. This application was parallelized on a shared memory architecture to shorten the simulation run-time.

The development of the adaptive code based on hierarchical finite elements was also continued. One main advantage of this method, is that the underlying dyadic partition of cells allows an efficient parallelization. We studied in particular new interpolation schemes based on Hermite polynomials, as the old scheme based on $\mathbb{Q}_2$ interpolation seems to dissipative and the use of higher order methods is not straightforward in that context. Numerical results on uniform and adaptive grids were obtained and compared with biquadratic Lagrange interpolation introduced in in the case of a rotating Gaussian [25].

6.4. Two-scale simulation of Maxwell and acoustics equations

Participants: Sébastien Jund, Stéphanie Salmon, Eric Sonnendrücker.

We have developped a numerical method for solving second order formulation of Maxwell's and the linear acoustics equations on a grid involving zones with cells of very different sizes, in order for example to compute sources, coming from particles in the case of Maxwell's equations or from a direct numerical simulation of the flow in the case of the acoustics equations, which need to be resolved locally on a very fine grid.

In order to devise a two-scale algorithm that can be used on a coarse grid with fine patches, we chose to extend the method developed by Glowinski and al. [65] for the steady-stage Poisson equation using scalar Lagrange Finite Elements to the time dependent two-dimensional Maxwell and linear acoustics equations solved using Nédélec edge Finite Elements in the first case and Raviart-Thomas face Finite Elements in the second case. The idea is based on domain decomposition and multigrid techniques. We first developped our method in the steady-state case and then extended it naturally to the time-dependent case using an implicit time discretization.

This work began in CEMRACS 2005 and the results are presented in the proceedings of CEMRACS 2005 for Maxwell's equations [1] and the proceedings of the ECCOMAS CFD 2006 conference for the linear acoustics [31].

6.5. Solution of Maxwell's equations in singular geometry

Participant: Simon Labrunie.

We completed a series of papers aimed at some efficient numerical methods for solving the Poisson problem in three-dimensional prismatic and axisymmetric domains. In the first and second parts the Fourier singular complement method (FSCM) was introduced and analysed for prismatic and axisymmetric domains with reentrant edges, as well as for the axisymmetric domains with sharp conical vertices. In this last part we conduct numerical experiments to check and compare the accuracies and efficiencies of FSCM and some other related numerical methods for solving the Poisson problem in the aforementioned domains. In the case of prismatic domains with a reentrant edge, we shall compare the convergence rates of three numerical methods: 3D finite element method using prismatic elements, FSCM, and the 3D finite element method combined with the FSCM. For axisymmetric domains with a non-convex edge or a sharp conical vertex we investigate the convergence rates of the Fourier finite element method (FFEM) and the FSCM, where the FFEM will be implemented on both quasi-uniform meshes and locally graded meshes. The complexities of the considered algorithms are also analysed [40].

We also developed an improved version of the Singular Complement Method (SCM) for Maxwell's equations, which relies on an asymptotic expansion of the solution near non-regular points. This method allows to recover an optimal error estimate when used with $\mathbb{P}_1$ Lagrange finite elements; extension to higher-degree elements is possible. It can be applied to static, harmonic, or time-dependent problems [42].

6.6. Domain decomposition for the resolution of nonlinear equations

Participant: Jean Roche.

This a joint work with Noureddine Alaa, Professor at the Marrakech Cadi Ayyad University.

The principal objective of this work was to study existence, uniqueness and present a numerical analysis of weak solutions for a quasi-linear elliptic problem that arises in biological, chemical and physical systems. Various methods have been proposed for studying the existence, uniqueness, qualitative properties and numerical simulation of solutions. We were particularly interested in situations involving irregular and arbitrarily growing data.

Another approach studied here was the numerical approximation of the solution of the problem. The most important difficulties are in this approach the uniqueness and the blowup of the solution.

The general algorithm for numerical solution of this equations is one application of the Newton method to the discretized version of the problem. However, in our case the matrix which appears in the Newton algorithm is singular. To overcome this difficulty we introduced a domain decomposition to compute an approximation of the iterates by the resolution of a sequence of problems of the same type as the original problem in subsets of the given computational domain. This domain decomposition method coupled with a Yosida approximation of the nonlinearity allows us to compute a numerical solution. In the 2-d case we consider the case where the data belong to $L^1(\Omega)$ and the gradient dependent non-linearity is quadratic. We show the existence and present a numerical analysis of a weak solution.

These results were published in [38], [43], [28].

6.7. Visualization of transparent structures

Participants: Jean-Michel Dischler, Olivier Genevaux.

Accurate refraction, thanks to raytracing, has always been a popular effect in computer graphics. However, devising a technique that produces realistic refractions at interactive rates remains an open problem.

We proposed a method to achieve realistic and interactive refractive effects through complex static geometry. It relies on an offline step where many light paths through the object are pre-evaluated. During rendering, these precomputed paths are used to provide approximations of actual refracted paths through the geometry, enabling further sampling of an environment map. The relevant information of the light paths, namely the final output direction when leaving the refractive object, is compressed using frequency domain based spherical harmonics. The matching decompression procedure, entirely offloaded onto graphics hardware, is handled at interactive speed.

6.8. Dynamic load balancing for volume data visualization

Participant: Jean-Michel Dischler.

Parallel volume rendering is one of the most efficient techniques to achieve real time visualization of large datasets by distributing the data and the rendering process over a cluster of machines. However, when using level of detail techniques or when zooming on parts of the datasets, load unbalance becomes a challenging issue that has not been widely studied in the context of hardware-based rendering. We addressed this issue and showed how to achieve good load balancing for parallel level of detail volume rendering. We do so by dynamically distributing the data among the rendering nodes according to the load of the previous frame. We illustrate the efficiency of our technique on large datasets.

6.9. GPU Based Interactive 4D+t visualization of plasma simulation data

Participants: Jean-Michel Dischler, Yuetong Luo.

Based on DVR (direct volume rendering) technology and GPU programming technology, we developed a new interactive visualization technique for exploring plasma behaviors resulting from 4D+t (x, y, t, v_x, v_y) numerical simulations on regular grids. For given (v_x, v_y) pair, the corresponding 3D subspace (x, y, t) is shown, and the user can browse the whole data by changing (v_x, v_y) interactively. To utilize general-purpose computing ability of modern GPU for achieving interactive frame rate, we used a novel data structure (nested tile-board), so that we can implement multi-resolution decompression and rendering on GPU directly. A technical report is being currently written.

6.10. Full wave modeling of lower hybrid current drive in tokamaks

Participants: Pierre Bertrand, Jean-Hugues Chatenet, Christoph Kirsch, Jean Roche.

This work is performed in collaboration with Yves Peysson (DRFC, CEA Cadarrache). 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 wave dynamics may be accurately described in the cold plasma approximation, which supports two independent modes of propagation, the slow wave which correspond to a cold electrostatic plasma wave, and the fast wave, namely the whistler mode. Because of the simultaneous presence of the slow and fast propagation branches a vectorial wave equation must be solved. The wave equation is obtained from the Maxwell equations with a time harmonic approximation. We consider a toroidal formulation of the Maxwell equations. Simulations will be carried out using domain decomposition techniques.

6.11. Numerical experiments of stimulated Raman scattering using semi-lagrangian Vlasov-Maxwell codes

Participants: Alain Ghizzo, Pierre Bertrand, Daniele DelSarto, Thierry Réveillé.

We have investigated Vlasov-Maxwell numerical experiments for realistic plasmas in collaboration of the group of Dr B. Afeyan of Polymath research Inc. (in an international collaboration program of the Department of Energy of USA) and T. W. Johnston of I.N.R.S. Energie et MatÂriaux (QuéÂbec Canada). Our studies so far indicate that a promising way to deter these undesirable processes is by instigating the externally controlled creation of large amplitude plasma fluctuations making the plasma an inhospitable host for the growth of coherent wave-wave interactions. The area where we plan to focus most of our attention is in Vlasov-Maxwell (semi-lagrangian) simulations in 1D. In several works, see for example [44], the nonlinear evolution of the electron plasma waves which have been generated by optical mixing (pump plus probe beams) is investigated to understand the kinetic effects that saturate the growth of these modes. Both the electron plasma wave and ion acoustic wave generation and SRS interaction problems are treated in great detail. Fluid and kinetic degrees of freedom to saturate SRS and to limit the growth of the optical mixing generated waves will be elucidated by Vlasov simulations.

In particular we have considered laser plasma instabilities in kinetic regimes assigning an essential role to trapped particles. These regimes of SRS are relevant to plasma conditions expected in ignition designs to be felted at the National Ignition Facility (NIF), as will the Laser MegaJoule project (LMJ) in France, currently under construction.

It is widely admitted that in this strong Landau regime referred as a new "kinetic" regime of the instability, the nonlinear behavior of the plasma is dominantly kinetic and not fluid, through an initial phase fluid phase and a possible transition from this phase to a kinetic one. It becomes clear that in that new kinetic regime (see [16]) , trapping effects and the associated nonlinear shift in frequency are expected to dominate since the Langmuir Decay Instability is too heavily Landau damped to compete.

On the other hand, recent Vlasov simulations [17] have shown the importance of Kinetic Electron Electrostatic Nonlinear waves (KEEN waves) characterized by phase space (trapping) vortices which may survive in strong Landau regime. This aspect is likely to be of considerable interest for a wide variety of applications, such as those related to the Fast Ignitor in laser fusion of high-energy ion acceleration in laser interactions with ultra-thin foils.

This work was performed in the context of a project of ANR (Agence Nationale de la Recherche) concerning *the study of wave-particle interaction for Vlasov plasmas*. In this project our main working topic is modeling and numerical simulation in hot plasma physics and we focus on the physical behavior of complex systems. The project involves cross-interactions between plasma physicists of LPMIA of Nancy and of the University of Pisa in Italy (F. Califano), applied mathematicians of the Calvi Group and computer scientists.

6.12. Plasma-wall interaction

Participants: Stéphane Devaux, Giovanni Manfredi.

A Vlasov code was used to model the transition region between an equilibrium plasma and an absorbing wall in the presence of a tilted magnetic field, for the case of a weakly collisional plasma ($\lambda_{\rm mfp} \gg \rho_i$, where $\lambda_{\rm mfp}$ is the ion-neutral mean free path and ρ_i is the ion Larmor radius). The phase space structure of the plasma-wall transition was analyzed in detail and theoretical estimates of the magnetic presheath width were tested numerically. It was shown that the distribution near the wall is far from Maxwellian, so that temperature measurements should be interpreted with care. Particular attention was devoted to the angular distribution of ions impinging on the wall, which is an important parameter to determine the level of wall erosion and sputtering.

6.13. Loschmidt echo in a system of interacting electrons

Participants: Paul-Antoine Hervieux, Giovanni Manfredi.

In a famous controversy with Ludwig Boltzmann at the dawn of modern statistical mechanics, Joseph Loschmidt pointed out that, if one reverses the velocities of all particles in a physical system, the latter would evolve back to its initial state, thus violating the second law of thermodynamics. The main objection to this line of reasoning is that velocity reversal is an extremely unstable operation and that tiny errors would quickly restore "normal" entropy increase. Nevertheless, time reversal is indeed possible, as was shown in spin echo experiments performed since the 1950s.

Loschmidt's idea has recently experienced a resurgence of interest in the context of quantum information theory. Indeed, any attempt at coding information using quantum bits is prone to failure if a small coupling to the environment destroys the unitary evolution of the wave function (decoherence). In order to estimate the robustness of a physical system, the following procedure has been suggested: a single quantum particle evolves under the action of a chaotic Hamiltonian H_0 until a time T; then, it is evolved backwards in time until 2T with the original Hamiltonian plus a small perturbation (the "environment"). The square of the scalar product of the initial and final states defines the Loschmidt echo or fidelity of the system. Theoretical and numerical studies showed that the Loschmidt echo decays exponentially with the time delay T.

What happens when one deals, not with a single particle, but with a large system of interacting particles, such as the electrons in a metallic or semiconductor nanostructure? In order to answer this question, we devised a quantum hydrodynamic model that includes electron-electron interactions via the self-consistent Coulomb field. The results of our numerical experiments were intriguing: the fidelity does not decay exponentially, but rather stays close to unity until a critical time, after which it drops abruptly. This unusual behaviour is related to the fact that the unperturbed Hamiltonian H_0 depends on the electron density n_e. When the perturbation induces a small change in n_e, H_0 is itself modified, which in turns affects n_e, and so on. Thanks to this "snowball effect", the perturbed and unperturbed solutions can diverge very fast. This effect could be a generic feature of interacting many-particle systems. If so, it would have an impact on the decoherence properties of solid-state quantum computation devices, which may then behave differently in the single-electron and many-electron regimes.

7. Contracts and Grants with Industry

7.1. CEA Bruyères-Le-Châtel, PIC code

Participants: Pierre Navaro, Eric Sonnendrücker.

The object of the contract is the development of an efficient parallel Particle-In-Cell (PIC) solver for the numerical resolution of the two configuration space - three momentum space dimensions Vlasov-Maxwell equations in cartesian and axisymmetric geometries. In this year's work we added a Discontinuous Galerkin Maxwell solver. This code is written in a modular way using the fortran 90 language.

7.2. CEA Bruyères-Le-Châtel, simulation of particle beams

Participants: Nicolas Crouseilles, Guillaume Latu, Eric Sonnendrücker, Xinting Zhang.

The object of this contract is the development of efficient Vlasov-Poisson solvers based on a phase space grid for the study of intense particle beams. We investigated different ideas to decrease the loss of particles close to the axis in axisymmetric geometry. We also coupled the new codes developed this year LOSS and OBIWAN to the envelope solver used to compute beams matched to a given focusing lattice in order to be able to use them for particle beam simulations.

7.3. CEA Cadarache, gyrokinetic simulation and visualization

Participants: Nicolas Crouseilles, Guillaume Latu, Eric Sonnendrücker, Eric Violard.

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.

7.4. National initiatives

7.4.1. INRIA ARC Project

Calvi members are involved in the ARC project "Modelling of magnetized plasmas". This project is headed by Eric Sonnendrücker and also involves the INRIA projects MC2, SCALAPPLIX, SIMPAF all in INRIA Futurs, as well as the MIP laboratory in Toulouse. It is devoted to the mathematical justifications of models used for Tokamak simulation as well as their efficient implementation http://www-irma.u-strasbg.fr/annexes/arc_plasma/.

7.4.2. ANR Projects

Calvi members are involved in two ANR projects.

- ANR Masse de données : MASSIM project (leader J.-M. Dischler).
  Simulation and visualization of problems involving large data sets in collaboration with O. Coulaud (project Scalapplix). https://dpt-info.u-strasbg.fr/~dischler/massim/massim.html
- 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.

7.4.3. Participation to GdR Research groups from CNRS

The members of Calvi participate actively in the following GdR:

- GdR Groupement de recherche en Interaction de particules (GRIP, CNRS 2250):
  This research group is devoted to the modelling and simulation of charged particles. It involves research teams form the fields of Partial Differential Equations and Probability. http://smai4.emath.fr/grip/
- GdR équations Cinétiques et Hyperboliques : Aspects Numériques, Théoriques, et de modélisation (CHANT, CNRS 2900):
  This research group is devoted to the modelling and numerical simulation of hyperbolic and kinetic equations. http://chant.univ-rennes1.fr/

7.5. European initiatives

7.5.1. 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

8. Dissemination

8.1. Leadership within scientific community

8.1.1. Conferences, meetings and tutorial organization

- Eric Sonnendrücker was chair of the scientific program committee of the 16th Symposium on Heavy Ion Fusion, Saint-Malo, France 9-14 July 2006 http://hif06.lpgp.u-psud.fr.
- G. Manfredi was co-organizer of the Second international workshop on the theory and applications of the Vlasov equation ("Vlasovia 2006"), which took place in Florence, Italy, 18-21 September 2006.
- Eric Sonnendrücker was in the scientific committee of the Workshop Plasmas Magnétisés, Nice, France, 23-24 November 2006 http://www-math.unice.fr/~bertheli/Page_Web/Plasmas.

8.1.2. Invitations at conferences and summer schools

- Eric Sonnendrücker gave an invited talk at HIF 06, Saint-Malo, 9-14 July 2006.
- Eric Sonnendrücker gave an invited talk at HYP 06, Lyon, 17-21 July 2006.

- Eric Sonnendrücker gave a lecture on numerical methods for kinetic equations at the Ecole d'Aquitaine, Maubuisson, 11-14 September 2006.

8.1.3. Administrative duties

- Jean-Michel Dischler is the vice-head of the LSIIT laboratory of CNRS and University Louis Pasteur in Strasbourg.
- Jean-Michel Dischler is vice-president of the Eurographics french chapter association and member of the professional board of Eurographics.
- 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 participate to organization of the European Master (Master Erasmus Mundus) in Computational Physics.
- Jean Rodolphe Roche participate to organization of the French Master "Fusion".
- Jean Rodolphe Roche is the research coordinator of the "École Supérieure des Sciences et Technologies de l'Ingénieur de Nancy" .
- Eric Sonnendrücker is the head of the Center of studies in parallel computing and visualization of the University Louis Pasteur in Strasbourg, which makes parallel computing ressources and a workbench for immersed visualization available to the researchers of the University.
- Eric Sonnendrücker is a member of the National Commitee of Universities (26th section: applied mathematics).

8.2. Teaching

- *Jean Rodolphe Roche* taught an optional graduate course entitled "Parallel Architecture and Domain Decomposition Method" in the Master of Mathematics of the University Henri Poincaré (Nancy I).
- *Simon Labrunie and Jean Rodolphe Roche* taught an optional graduate course entitled "Numerical Analysis of Hyperbolic Problems" in the Master of Mathematics at the University Henri Poincaré (Nancy I).
- *Eric Sonnendrücker* taught an optional graduate course entitled "Modelling and numerical simulation of charged particles" in the Master of Mathematics at the University Louis Pasteur of Strasbourg.

8.3. Ph. D. Theses

8.3.1. Ph. D. defended in 2006

1. Olivier Géneveaux, *Realistic visualization of fluid - solid body interactions* Université Louis Pasteur, Strasbourg, 27 November 2006. Advisor: Jean-Michel Dischler.

8.3.2. Ph. D. in progress

1. Alexandre Mouton, *Multiscale approximation of the Vlasov equation*. Advisors: Emmanuel Frénod and Eric Sonnendrücker.
2. Matthieu Haefele, *High performation visualization of particle beams*. Advisors: Jean-Michel Dischler and Eric Sonnendrücker.
3. Sébastien Jund, *High order Finite Element methods for Maxwell's equations and acoustics*. Advisors: Stéphanie Salmon and Eric Sonnendrücker.
4. Sandrine Marchal, *Domain decomposition methods to solve a system of hyperbolic equations*. Advisors: Simon Labrunie and Jean Rodolphe Roche.
5. Olivier Hoenen, *Parallelization of adaptive methods for the Vlasov equation*. Advisor: Eric Violard.

8.3.3. Post Doc in progress

- Christoph Kirsch, *Numerical analysis of the full wave model*, Advisor: Jean Rodolphe Roche.
- Mohammed Iguernane, *Domain decomposition method applied to reaction diffusion equations*. Advisor: Jean Rodolphe Roche.

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