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Project-Team Calvi

Scientific Computing and Visualization

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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*.

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 [68], see also Bardos and Degond [48]. The existence of a weak solution for the Vlasov-Maxwell system has been proved by Di Perna and Lions [55]. 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 [49].

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 [65], [72] as well as by Brenier [52]. 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 [61], [59], [60].

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*.

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.

3.2.1. 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 [51] 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.

3.2.6. 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 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 [46] and implemented [47] 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 [50]. The non-density result for regular fields was proven [53], the singularities of the electromagnetic field were related to that of modified Laplacians [43], and expressions of the singular fields were calculated [44]. 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 [45].

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 [62], [44].

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 [73], 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 [71] 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 [58]).

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 data-sets, 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.

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

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

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. [57], 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 [57], 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 [56]. 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

5.2. 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 sequential version of the code is available at the following address:
http://www-rocq.inria.fr/who/Michel.Mehrenberger/#logi The parallel code designed for distributed memory architectures is managed by version control system Subversion (SVN) and can be downloaded at :
http://icps.u-strasbg.fr/~hoenen/yoda/yoda4D.tgz

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 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.

5.5. 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.

5.6. calviExport library

Keywords: *compression*, *hierarchical finite elements*, *multidimensional visualization*.

Participants: Matthieu Haefele, 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 boudaries. So this library can be easily integrated into parallel codes. For example, it has been sucessfully integrated into LOSS, YODA and GYSELA5D (gyro-kynetic 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.

5.7. plasmaViz

Keywords: *compression*, *hierarchical finite elements*, *multidimensional visualization*.

Participant: Matthieu Haefele.

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-Bruyere and its integration in the VTK[3] based visualization tool *visit*[4] is in progress.

[2] http://www.hdfgroup.org/
[3] http://www.vtk.org/
[4] http://www.llnl.gov/visit/

6. New Results

6.1. Existence and other theoretical results

Keywords: *Guiding center approximation*, *Nordström-Vlasov equations*, *Propagation speed*, *Vlasov-Maxwell equations*, *Vlasov-Poisson equations*.

Participants: Mihai Bostan, Nicolas Crouseilles, Jean Roche.

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

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. In particular we have studied the Vlasov-Maxwell equations with strong self-consistent magnetic field, which plays a crucial role for the magnetic confinement fusion (MCF).

In [16], we have analyzed the Nordström-Vlasov system which describes the evolution of a population of self-gravitating collisionless particles. We studied the existence and uniqueness of mild solutions for the Cauchy problem in one dimension. This approach does not require any derivative for the initial particle density. For any initial particle density uniformly bounded with respect to the space variable by some function with finite kinetic energy and any initial smooth data for the field equation we could construct a global solution, preserving the total energy. Moreover the solution propagates with finite speed. The propagation speed coincides with the light speed.

In [15], we investigated the continuous dependence with respect to the initial data of the solutions of the 1D and 1.5D relativistic Vlasov-Maxwell system. More precisely we prove that these solutions propagate with finite velocity: the propagation velocity does not exceed the velocity of light. We formulate our results in the framework of mild solutions, *i.e.*, the particle densities are solutions by characteristics and the electromagnetic fields are Lipschitz continuous functions. Obviously this feature inherits from the hyperbolic structure of the Maxwell equations combined with the relativistic character of the particle dynamics. This leads to a better understanding of the transport of relativistic charged particles: we justify the existence of a dependence domain in space. From the numerical point of view this property has important consequences: it shows that the numerical approximation of these equations can be localized with respect to the space variable.

The motivations of [17] are to understand the models used in magnetic fusion devices where the particles are evolving in a large external magnetic field. The dynamics of charged particles is described in terms of a number density by the Vlasov equation, coupled to the Maxwell equations for the electromagnetic field. Generally the numerical solution of this model requires important computational efforts, since we are working in a phase space with three spatial dimensions and three momentum dimensions. Moreover new difficulties appear when studying strong magnetic field regimes: large magnetic fields introduce a new time scale, related to the period of rotation of the particles around the magnetic field lines. Since the cyclotron period is proportional to the inverse of the magnitude of the magnetic field, the above time scale is very restrictive from the numerical point of view. Hence it is worth looking for simpler approximate models, like the gyro-kinetic model or the guiding center model. In [17], we study the asymptotic behavior of the Vlasov-Maxwell equations with strong magnetic field. More precisely we investigate the Cauchy problems associated to strong initial magnetic fields. We justify the convergence towards the so-called "guiding center approximation" when the dynamics is observed on a slower time scale than the plasma frequency. Our proofs rely on the modulated energy method.

6.1.2. Domain decomposition for the resolution of nonlinear equations

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

The principal aim of this work was to give an existence result and present a numerical analysis of weak solutions for the following quasi-linear elliptic problem in one and two dimensions:

$$\begin{cases} -Au(x) + G(x, Du(x)) = F(x, u(x)) + f(x) & \text{in } \Omega\,, \\ u(x) = 0 \quad \text{on } \partial\Omega \end{cases} \tag{2}$$

where A is a second order differential operator in one dimension and the Laplace operator in two dimensions, G, F are Caratheodory non negative functions. The function f is given, finite and non negative. The domain $\Omega \subset \mathbb{R}^N,\ N = 1, 2$ is open and bounded.

Such problems arise from biological, chemical and physical systems and various methods have been proposed for studying the existence, uniqueness and qualitative properties of solutions as well as for the numerical simulation of such models.

In addition to existence and uniqueness we investigated 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 the numerical solution of this equations is an application of the Newton method to the discretized version of the problem. However, in our case the matrix which appears in the Newton algorithm can be 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 2D setting we consider the case where the data belong to $L^1(\Omega)$ and the gradient dependent non-linearity is quadratic. These results have been published in [40].

6.2. Development of Vlasov solvers

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

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

6.2.1. Development of semi-Lagrangian Vlasov solvers

We have developed in the last years a new interpolation method for semi-Lagrangian solvers on regular grids. This method is based on local splines on patches which are designed to be a very good approximation to global splines but have the huge advantage of scaling very well on several hundreds of processors. This method has been implemented in the code LOSS and has been successfully tested for several applications [19], [54]. Moreover, comparisons with the wavelet based adaptive code OBIWAN have been performed [34], [35], [32], [33] for beam physics applications. In this context however, the total charge is not equal to zero, and the Poisson solver based on FFT had to be modified. This has been done together with the integration of finite differences solvers. Moreover, a so-called envelope solver is required to initialize the semi-Lagrangian codes and to compute applied focusing electromagnetic fields. Some improvements have also been done at this level, in particular a quasi-Newton type method has been implemented in place of the shooting method. Numerical simulations involving the theoretical KV beam and more realistic beams show that these modifications lead to more accurate results.

6.2.2. Moving grid techniques

In many physical situations, Vlasov simulations on a uniform grid are inefficient because during the time evolution the distribution function vanishes in different regions of phase space, moving grid techniques can be used to save a lot of computation time by being able to follow closely the support of the distribution function. In this context, we introduced a dynamic mesh (or moving grid) following the evolution of the distribution function which allows us to considerably decrease the number of points in the computational grid. This technique already used with success in the last years for 1D problems was introduced in the newly developed 2D code LOSS (LOcal Spline Simulator). This solver is based on local cubic spline interpolations. The phase-space domain is decomposed in patches, each patch being devoted to one processor. Then each patch computes its own local cubic spline coefficients which are necessary to interpolate the distribution function on the subdomain. As such an approach involves a large amount of data exchange, a strict condition on the time step was necessary to control the shifts generated by the solve of the equations of motion, so that the communications were only done between adjacent processors. To improve the results obtained by this solver LOSS which was parallel in the velocity domain, we have developed a new code named LOSSx which is parallel in the configuration domain and uses a dynamic mesh in the velocity domain. This new code allowed us to save a large number of points in the velocity grid in particular for beam focusing problems where the evolution can be predicted by the envelope equation. Moreover, it overcomes one of the problem of LOSS as the time step is less constrained. This work has been described in [39].

6.2.3. Adaptive solvers based on hierarchical interpolation

We have investigated the use of different higher order interpolation operators in a hierarchical finite element context. It came out that the better option is to use centered Lagrange interpolation, in order to avoid unstable behaviours (cf [14]). The current implementation, even though it is adaptive, is however costly when going to higher degrees of interpolation. So, we have also developed a new uniform semi-Lagrangian code that solves the Vlasov equation in $1D \times 1D$ phase space as a testbed for new interpolation operators. It uses time-splitting, and several interpolation schemes have been implemented (for e.g. Lagrange interpolation from degree 1 to 9). Classical simulations have been successfully tested: Landau damping, two stream instability, semi-Gaussian beam with uniform and periodic focusing. In comparison with the adaptive code, this new code is generally faster even if the grid contains more points and can even use less memory, since the distribution function is only stored once. We plan to develop parallelization and adaptive strategies in the future, having in mind that we have to go faster (for some beam simulations) than this code which may be viewed as a reference; the implementation in $2D \times 2D$ has naturally also to be considered.

Following the semi-Lagrangian and finite hierarchical element approach, we also designed a new adaptive scheme to solve the 4D Vlasov equation. Improving data locality was kept in mind for designing this scheme and reaching an efficient parallel implementation. This scheme uses a block-based adaptation of a dyadic mesh and a $(1D \times 1D) \times 2D$ splitting of the equation which yields three successive advections at each time step. As it only involves predictable dependencies between blocks, this scheme is particularly well-suited to parallelization on distributed memory architectures [36]. We developed some parallelization techniques to reduce communications overhead and workload imbalance. Remaining communications are overlapped with computations and a new partitioning algorithm is used to build a dynamic load balancing mechanism. These mechanisms are included into the code which shows good scalability and efficiency on a PC cluster.

6.2.4. 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.

To begin with, we focus on 2D problems and develop a new Vlasov-Maxwell solver (named PADME) that couples a PIC solver written during her PhD thesis by R. Barthelmé and a structured H(curl) conforming finite elements solver for Maxwell's equations written by S. Jund during his PhD thesis. The key point in using H(curl) conforming finite elements is to not create spurious electromagnetic modes which could be amplified by the numerical noise of the PIC method. The other important point in the coupling is the computation of the current density created by the particles and entering as the source for the electromagnetic solver. This computation must enforce the charge conservation at the discrete level in order to ensure that the numerical solution is the physical one.

6.2.5. Asymptotic preserving numerical schemes

In the framework of the ARC fusion, we initiated a joint work with Pierre Degond from Toulouse on stable quasi-neutral Vlasov simulations. In such regimes, kinetic numerical simulations are complex since explicit schemes suffer from the severe constraint related to the small Debye length. To overcome this drastic constraint, we follow the strategy used in a previous work by Pierre Degond's group for the Euler-Poisson system: the Poisson equation is re-written in an equivalent form we called Reformulated Poisson Equation (RPE). They also coupled this new equation to the Vlasov model which was solved using a Particle In Cell method. However the results were noisy and the energy was not well conserved. So we tried using a semi-Lagrangian solver to approximate the Vlasov model in order to improve the noisy results obtained with the PIC approach. To do this, a new time integration of the characteristics together with the coupling with the RPE have been done. Stable simulations were then obtained, even for very small Debye lengths. Moreover, the solver enables to get a good conservation of the total energy.

A stability analysis has also been performed proving that the numerical scheme is stable for small values of the Debye length even if the time step does not resolve it. To that purpose, the dispersion relation of the linearized Vlasov equation coupled with the RPE is derived. The roots of the so-obtained dispersion relation provide an indication of the stability of the numerical scheme. Contrary to the Vlasov-Poisson system, the new scheme is proved to be stable even when the time step does not resolve the Debye length.

6.3. Multiple time scales solvers

Participants: Emmanuel Frénod, Alexandre Mouton, Eric Sonnendrucker.

We have developed specific numerical methods for problems involving a fast and a slow time scale. It consists in first deriving a homogenized equation which is averaged over the fast time scale and then developing a numerical method for the solution of this homogenized model. This technique has been applied to the 1D weakly compressible Euler equations [22] and to the paraxial Vlasov equation used in accelerator physics [42]. In both cases the new solvers approximate very well the original model for very different time scales at a fraction of the cost.

6.4. Visualization

Keywords: *compression*, *hierarchical finite elements*, *multidimensional visualization*.

Participants: Matthieu Haefele, Guillaume Latu, Florence Zara, Jean-Michel Dischler, Stéphane Marchesin.

6.4.1. A dedicated compression scheme for the visualization of large multidimensional functions

The interactive exploration of multidimensional data sets remains highly challenging as soon as the data size exceeds a certain threshold. We have designed a hyper-slicing based interactive visualization technique designed to explore at real-time frame rates large hyper-volumetric 4D scalar fields (*i.e.* data sets beyond 16GB) defined on regular structured grids. The key issue consists in coupling the visualization with a new efficient data representation scheme, in such a way that it can handle the different steps of scientific visualization, namely simulation post-processing, visualization pre-processing and finally interactive display. By introducing a hierarchical finite element representation, our technique allows users to explore the full data set at real-time frame-rates on low-end PCs. Its effectiveness has been evaluated on the interactive exploration of 4D phase space particle beams, resulting from the different numerical semi-Lagrangian simulations of the project.

The main contribution of this work is the design of a dedicated compression scheme that both reduces significantly the size of the data and can be easily integrated into parallel simulation codes. The sparse data structure gives an efficient memory representation to store the compressed function and provides random accesses efficient enough to make the reconstruction process interactive. This work has been published in [25] and two pieces of software calviExport 5.6 and plasmaViz 5.7 have been developed.

6.4.2. Improving feature visibility in data sets using locally adaptive volume rendering

Classical direct volume rendering techniques accumulate color and opacity contributions using the standard volume rendering equation approximated by alpha blending. However, such standard rendering techniques, often also aiming at visual realism, are not always adequate for efficient data exploration, especially when large opaque areas are present in a data set, since such areas can occlude important features and make them invisible. On the other hand, the use of highly transparent transfer functions allows viewing all the features at once, but often makes these features barely visible. In this paper we introduce a new, straightforward rendering technique called locally adaptive volume rendering, that consists in slightly modifying the traditional volume rendering equation in order to improve the visibility of the features, independently of any transfer function. Our approach is fully automatic and based only on an initial binary classification of empty areas. This classification is used to dynamically adjust the opacity of the contributions per-pixel depending on the number of non-empty contributions to that pixel. As will be shown by our comparative study with standard volume rendering, this makes our rendering method much more suitable for interactive data exploration at a low extra cost. Thereby, our method avoids feature visibility restrictions without relying on a transfer function and yet maintains a visual similarity with standard volume rendering.

6.4.3. Optimizing a commodity cluster for high performance volume visualization

Thanks to the advent of low-cost graphics hardware, commodity-based clusters have become an increasingly interesting solution to the large scale high-performance visualization problem. In the context of the ANR MASSIM project, we have developed a system for parallel large-scale volume visualization based on a 16 node commodity cluster. Our system includes both a hardware setup and a software setup. On the hardware side, we have explored how to make use of an inexpensive dual-card gigabit Ethernet network. On the software side, we have developed various stages of a volume rendering pipeline. In order to make efficient use of our hardware setup, we have to customize all the stages of the pipeline, specifically load balancing, compression, and communication optimization. As we are interested in high quality volume visualization, we only focus on lossless compression techniques. We have compared a number of compression methods including a GPU-based implementation, both theoretically and experimentally with different network speeds. Our extensive study highlights the most relevant compression methods in each case. A large number of performance results have been obtained that show the influence of each stage of the pipeline, in terms of frame rates. The performance we get on large scale data sets demonstrates that a commodity cluster can be efficiently used in this context as long as it is properly customized, both on the hardware and on the software side.

6.5. Application of Vlasov codes to inertial confinement fusion

Participants: Alain Ghizzo, Pierre Bertrand, Nicolas Besse, Thierry Réveillé.

This work was performed in the context of the ANR project VLASOV concerning the study of Wave-Particle interaction for Vlasov plasmas.

We have considered the Stimulated Raman Scattering in the Backward direction, sometimes called SRS-B and laser-plasma instabilities involving Electron Plasma waves in large plasmas in kinetic regimes, for which an essential role is played by well-trapped electrons. Parabolic profiles were considered as well as homogeneous plasmas.

The regimes studied are relevant to the plasmas conditions expected in ignition designs to be fielded at the National Ignition Facility (NIF), as well as the Laser MégaJoule (LMJ) project, currently under construction at the CEA of Bordeaux. The nonlinear behavior of the plasma is dominated by kinetic effects ant not by fluid effects, through an initial fluid phase and its transition to the kinetic one. Vlasov simulations have shown that the plasma wave undergoes a frequency decrease, according to the basic idea of Morales and O'Neil regarding the effect of trapped particles on the frequency of the Langmuir wave, while the the wave vector increases slightly so as to maintain the SRS resonance. In [12] the simulations show that the main process that limits the continuation of the BSRS instability by Langmuir wave frequency-wavevector chirping and retuning is provided by a process which begins with pairwise vortex merging of phase space vortices or "electron holes”. This vortex-merging process then evolves towards a resonant spectrum resembling that of a weak electrostatic inverse cascade induced by weak turbulence effects (see also [23]). This process may be thus responsible of SRS saturation in that regime of instability.

We have also investigated the high laser intensity regime of laser-plasma interaction using a full relativistic Semi-Lagrangian scheme presented in [20]. Relativistic effects allow the wave propagation in homogeneous over dense plasmas under conditions that allow for self-induced transparency. Vlasov-Maxwell simulations, based on a semi-Lagrangian scheme, revealed a rich variety of new phenomena associated with the trapped particles dynamics, which cannot be described in fluid models. Most notably is the observation, during the penetration phase of the pump electromagnetic wave, of a beat-wave heating scenario induced by a Doppler shift on the reflected wave at the (moving) wave front. This first phase of the instability was studied in detail in [24]. Our investigation reveals that it is the beating of the pump with the reflected wave that determines the resonance condition and the characteristics of the low-frequency driven electron wave. For a large range of physical parameters we have demonstrated the possibility of strong growth of this new beat wave process.

Once the plasma layer crossing by the front wave is achieved, this process ceases. A second instability, involving now a new "radiating pseudo cavity" electromagnetic mode is observed. This allows the initial narrow-band excitation of the kinetic electrostatic electron nonlinear (KEEN) waves at a frequency lower than the plasma frequency. Details of this process may be found in [63]. An adaptive semi-Lagrangian Vlasov-Maxwell model was also developed to study these highly relativistic regimes of the laser-plasma interaction in [13] The adaptative code was found to describe the nonlinear particle dynamics details in good agreement with a classical Vlasov model. This new version allows us to consider now the acceleration of ions usually characterized by fine filaments in the ion phase space.

6.6. Application of Vlasov codes to magnetic fusion

Participants: Pierre Bertrand, Nicolas Besse, Nicolas Crouseilles, Etienne Gravier, Christoph Kirsch, Guillaume Latu, Jean Roche, Eric Sonnendrücker.

Our team has been involved during the last few years in the Vlasov gyro-kinetic modelling of tokamak plasmas. The aim here is to develop the most physical appropriate ground for the gyrokinetic framework and to define the most apt approach on mathematical grounds for numerical simulations. To do that different approaches were investigated. First the Department of Research on the Controlled Fusion of the CEA of Cadarache has developed the code GYSELA 5D (see [66]) in which we have been closely collaborating and on the other hand we have investigate a different cheaper approach: the multi-water-bag model.

6.6.1. 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. Several developments of the code enabled to achieve this task. The major development during the past year consisted in the efficient parallelization of the quasi-neutral Poisson solver. This part of the code includes an important inter-processors communication step which penalized the global speedup of the code. A new method to solve the quasi-neutrality equation has been tested independently on academic tests and then integrated in the GYSELA code. Then, a new communication scheme has been implemented, leading to a scalable algorithm. For example, the global speedup is about 80% of efficiency using 2048 processors [37].

6.6.2. Multi-water-bag models

In order to make numerical comparisons with the full gyrokinetic approach, we have developed new techniques based on the dimension reduction of the phase space performed in the Hamiltonian framework, such as the multifluid approach (usually called the Gyro-Water-Bag model in [30], [31]) or using action-angle Hamiltonian formalism. The water-bag model was thus extended to the more complex situation relevant to magnetized plasmas for tokamaks. We have also developed a 4D Vlasov code for describing the trapped ion driven modes (TIM), which belong to the family of ion gradient driven modes (ITG instabilities). These instabilities were characterized by frequencies of the order of the trapped precession frequency and radial scales of the order of several "banana" orbits. Trapped-ion modes are a prototype of kinetic instability since they are driven through the resonant interaction between a wave and trapped ions via their precession motion. The code was implemented on the parallel computer of the IDRIS center. This model depends on only two variables (precession angle and poloidal flux), parametrized by the particle energy and trapping parameter (adiabatic invariant). The code uses again a Vlasov solver based on a semi-Lagrangian scheme.

6.6.3. Plasma-wall interaction

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. The ions' energy and angle of impact are of particular importance, as they determine the level of wall erosion and sputtering. Their dependence on the plasma parameters (magnitude and angle of incidence of the magnetic field, ion and electron temperatures, ...) is investigated in detail. The numerical results indicated that a magnetic field with grazing incidence and a low electron-to-ion temperature ratio have a beneficial effect, as far as wall erosion and sputtering are concerned.

6.6.4. 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 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.

We have developed a P_1 finite element method (FEM) in the spirit of F. Assous and all. method, which is based on a mixed augmented variational formulation (MAVF) of the problem. We have written a Matlab code for the method, which gives correct results in academic examples. Is currently being tested with real physical data.

6.7. Application of Vlasov codes nanophysics

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

6.7.1. Quantum hydrodynamics.

The dynamical properties of a finite system of electrons (thin metal film) have been recently investigated using a semi classical Vlasov-Poisson model [70]. In order to include quantum effects, a quantum hydrodynamic model [69] has been implemented in this context. First, the ground state was determined numerically using a relaxation technique. A systematic comparison with a stationary Schrödinger-type model enabled us to validate the accuracy of the hydrodynamic approach. Second, the electron dynamics was excited by perturbing the computed ground state. The quantum hydrodynamic model was shown to reproduce the most salient features of the Vlasov simulations: the thermal energy initially increases (heating) and, after saturation, low-frequency oscillations appear, corresponding to ballistic electrons travelling through the film. These results confirm that the hydrodynamic model is well suited to describe the electron dynamics in finite-size nano-objects. A journal article on this topic is currently in preparation.

6.7.2. Fidelity decay in a trapped Bose-Einstein condensate

The quantum coherence of a Bose-Einstein condensate is studied using the concept of quantum fidelity (Loschmidt echo). The condensate is confined in an elongated anharmonic trap and subjected to a small random potential such as that created by a laser speckle. Numerical experiments show that the quantum fidelity stays constant until a critical time, after which it drops abruptly over a single trap oscillation period. The critical time depends logarithmically on the number of condensed atoms and on the perturbation amplitude. This behavior may be observable by measuring the interference fringes of two condensates evolving in slightly different potentials. This work was published in [28].

6.7.3. Auto-resonant control of the electron dynamics in semiconductor quantum wells

Small semiconductor devices, such as quantum dots and quantum wells, have attracted considerable attention in recent years, particularly for possible applications in the emerging field of quantum computing. For quantum devices working with many electrons, it is therefore crucial to understand the properties of the self-consistent electron dynamics and its response to external electric fields. The optical response of nonparabolic quantum wells is generally dominated by a strong peak at the plasmon frequency. However, when the electrons reach the anharmonic regions of the confining potential, the laser frequency will no longer match the oscillation frequency of the potential, so that the resonance condition is lost and absorption of the laser light becomes inefficient. This limitation can be overcome by using a chirped laser pulse. By direct simulations using the Wigner phase-space approach, we prove that, with a sequence of just a few pulses, electrons can be efficiently detrapped from a nonparabolic well. For an array of multiple quantum wells, we can create and control an electronic current by suitably applying an auto-resonant laser pulse and a slowly varying dc electric field. This work was published in [27].

6.8. Inverse problem governed by Maxwell equations

Participant: Jean Roche.

This work was 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, ...

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 equilibrium 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 equilibrium 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 paper is to give an algorithm to locate suitable inductors around the molten metal so that the equilibrium 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 equilibrium 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. New result are presented in [41].

7. Contracts and Grants with Industry

7.1. 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.

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

Participants: Pierre Bertrand ,, Jean Roche.

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. 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-math.u-strasbg.fr/arc/.

7.3.2. ANR Projects

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

7.3.3. 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/

7.4. 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

8. Dissemination

8.1. Leadership within scientific community

8.1.1. Conferences, meetings and tutorial organization

- S. Salmon and E. Sonnendrücker edited with C.-D. Munz and M. Dumbser the proceedings of CEMRACS 2005 Computational Aeroacoustics and Computational Fluid Dynamics in Turbulent Flows, Volume 16 of ESAIM Proceedings, 2007.
- P. Helluy and E. Sonnendrücker co-organized with H. Guillard the conference *Numerical Flow Models for Controlled Fusion* in Porquerolles, 16-20 April 2007.
- E. Sonnendrücker co-organized with F. Filbet and P. Degond a workshop on numerical methods and kinetic equations in Toulouse, 2-4 July 2007.

8.1.2. Invitations at conferences and summer schools

- E. Sonnendrücker gave an invited talk at the Workshop on Computational Electromagnetism and Acoustics at Oberwolfach (February 5-9, 2007).

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 a member of the Scientific Council of the university.
- Jean-Michel Dischler is a 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 participated 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).
- Eric Sonnendrücker is a member of the Scientific Commitee of CIRM.

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 “Wavelets. Theory and application to adaptive numerical methods for PDEs” in the Master of Mathematics at the University Louis Pasteur of Strasbourg.
- *Eric Violard* taught an optional graduate course entitled ?Transformations and Adaptation of Parallel and Distributed Programs" in the Master of Computer Science at the University Louis Pasteur of Strasbourg.
- *Stéphanie Salmon* taught a graduate course entitled “Numerical methods for Maxwell’s equations” in the Master of “Calcul Scientifique et Visualisation” at the University Louis Pasteur of Strasbourg.

8.3. Ph. D. Theses

8.3.1. Ph. D. defended in 2007

1. Matthieu Haefelé, *Simulation and visualization of charged particle beams*. Advisors: J.-M. Dischler and Eric Sonnendrücker. Defended April 5, 2007 (Jury : Olivier Coulaud, Wilfried Lefer, Catherine Mongenet, Guillaume Latu, Florence Zara, J.-M. Dischler, Eric Sonnendrücker).
2. Sébastien Jund, *High order Finite Element methods for Maxwell’s equations and acoustics*. Advisors: Stéphanie Salmon and Eric Sonnendrücker. Defended November 28, 2007 (Jury : P. Ciarlet, Jr, G. Cohen, S. Piperno, P. Helluy, J. Segré, S. Salmon, E. Sonnendrücker.)

8.3.2. Ph. D. in progress

1. Alexandre Mouton, *Multiscale approximation of the Vlasov equation*. Advisors: Emmanuel Frénod and Eric Sonnendrücker.
2. Thomas Respaud, *Numerical coupling of Maxwell and Vlasov equations*. Advisors: Eric Sonnendrücker.
3. Sandrine Marchal, *Domain decomposition methods to solve a system of hyperbolic equations*. Advisors: Simon Labrunie and Jean Rodolphe Roche.
4. 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.
- Radoin Belaour, *Asymptotic preserving semi-Lagrangian quasi-neutral Poisson solvers*. Advisor: Nicolas Crouseilles.
- Matthieu Haefele, *Compression methods and Visualization tools*. Advisor: Eric Sonnendrücker

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Major publications by the team in recent years

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