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Project-Team Calvi

Scientific Computing and Visualization

Nancy - Grand Est

THEME NUM

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CALVI is a project associating Institut Elie Cartan (IECN, UMR 7502, CNRS, INRIA and Université Henri Poincaré, Nancy), Institut de Recherche Mathématique Avancée (IRMA, UMR 7501, CNRS and Université 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. Introduction

CALVI was created in July 2003.
It is a project associating Institut Elie Cartan (IECN, UMR 7502, CNRS, INRIA and Université Henri Poincaré, Nancy), Institut de Recherche Mathématique Avancée (IRMA, UMR 7501, CNRS and Université 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 topic of interest is modeling, numerical simulation and visualization of phenomena coming from plasma physics and beam physics. Our applications are characterized in particular by their large size, the existence of multiple time and space scales, and their complexity.

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

2.2. Highlights of the year

A first version of the CALVI platform integrating most of the 1D codes for the simulation of plasmas has been completed.

Stéphanie Salmon has obtained her Habilitation à Diriger les Recherches.

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 non neutral 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 realizations 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_s 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 [74], see also Bardos and Degond [57]. The existence of a weak solution for the Vlasov-Maxwell system has been proved by Di Perna and Lions [63]. An overview of the theory is presented in a book by Glassey [71].

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 [58].

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 [72], [77] as well as by Brenier [61]. 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 [69], [67], [68].

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*, *PIC method*, *Vlasov equation*, *adaptivity*, *convergence*, *numerical analysis*, *semi-Lagrangian method*, *unstructured grids*.

3.2.1. Introduction

The numerical integration of the Vlasov equation is one of the key challenges of computational plasma physics. Indeed, kinetic models are posed in phase space and thus the number of dimensions is doubled. Since the early days of this discipline, an intensive work on this subject has produced many different numerical schemes. We have been interested in two of the most promising. The first and by far the most widely used is the Particle In Cell (PIC) method which approximates the distribution function, solution of the Vlasov equation, by Dirac measures which act like macro-particles. It is independent of dimension and thus becomes very efficient when dimension increases which is interesting for the Vlasov equation posed in phase space. However its convergence rate is slow. The second uses a phase-space grid for the solution of the Vlasov equation. In both cases, the Vlasov solver is coupled with a physical grid based field solver. At the beginning of the project we were mainly involved in the latter approach. 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. However it is still out of reach to address full three-dimensional problems with a phase-space grid method. For these kind of large problems we have also started recently to work on efficient PIC methods for three-dimensional problems with complex geometries.

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 origin of the characteristics $\mathbf{X}(t_n;\mathbf{x}_i,\mathbf{v}_j,t_{n+1})$, $\mathbf{V}(t_n;\mathbf{x}_i,\mathbf{v}_j,t_{n+1})$.

This method can be simplified using a time-splitting procedure 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 [60] consists in solving the Vlasov equation using a particle method, i.e. advancing numerically the particle trajectories which are the characteristics of the Vlasov equation, using the equations of motion which are the ordinary differential equations defining the characteristics. The self-fields are computed using a standard method on a structured or unstructured grid of physical space. The coupling between the field solve and the particle advance is done on the one hand by depositing the particle data on the grid to get the charge and current densities for Maxwell's equations and, on the other hand, by interpolating the fields at the particle positions. This coupling is one of the difficult issues and needs to be handled carefully.

3.2.6. Maxwell's equations in singular geometry

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

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

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

This *Singular Complement Method* (SCM) had been developed [56] and implemented [55] 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 [59]. The non-density result for regular fields was proven [62], the singularities of the electromagnetic field were related to that of modified Laplacians [52], and expressions of the singular fields were calculated [53]. 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 [54].

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 [70], [53].

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 resources requirements.

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

Parallelism, for such data-parallel PDE solvers, is achieved by partitioning the mesh and mapping the 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 [73] 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 [78], 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 [75] as an example of such modular software infrastructure).

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

Moreover, exploiting heterogeneous architectures requires the use of a run-time support associated with a programming interface that enables some low-level hardware characteristics to be unified. Such run-time support is the basis for heterogeneous algorithmic. Candidates for such a run-time support may be specific implementations of MPI such as MPICH-G2 (a grid-enabled MPI implementation on top of the GLOBUS tool kit for grid computing [66]).

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 re-usability.

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*.

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.

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. Two major research approaches are followed towards the objective of fusion based nuclear plants: magnetic fusion and inertial fusion. We develop simulation tools for both approaches.

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

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

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 under-dense 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 inter-depend, 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 modeling 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 program 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. [65], 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 [65], 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 [64]. 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. A parallel version of the code exists and uses the OpenMP paradigm. Domain size of 512^4 has been considered and the method allows to save effectively memory and computation time compared to a non-adaptive code.

5.3. 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.

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 was fisrt 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, Stéphanie Salmon, 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 geometry. It implements a parallel version of the semi-Lagrangian method based on a localized cubic splines interpolation we developed. It has the advantage compared to older versions of the cubic splines semi-Lagrangian method to be efficient even when the number of processors becomes important (several hundreds). It is written in Fortran 90 and MPI. The computation kernel of LOSS has been adapted and put in the GYSELA5D code owned by the CEA-Cadarache.

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

5.6. SPIN

Keywords: *Particle In Cell*, *Unstructured Grid*, *Vlasov*, *finite elements*, *parallelization*.

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

The Scalable Particle-IN-cell (Spin) code is dedicated to the solving of Vlasov-Maxwell equations, using finite elements for the Maxwell solver. This code is designed to be able to scale well on parallel machines. We have elaborated different strategies to balance both the computational loads of the Vlasov part (Particle In Cell method) and the Maxwell part (Edge finite elements). In order to do that we take into account the number of particles and elements per processor. This code has run several 2D test cases, and we are working now on a 3D version.
The Maxwell solver can handle hybrid grids (triangles and quadrangles) and has the capability of using high order elements. We built the numerical scheme in order to achieve a charge conserving property. Another characteristic of the solver concerns parallel work distribution. The computations on quadrangles are highly parallel: there are few communications and nearly no dependencies between computations. On the triangles, we use a sparse solver in order to solve Maxwell equation (all triangles are tightly coupled). The PASTIX solver (INRIA/Scalapplix team) or a classical Conjugate Gradient solver are used in order to perform the sparse computations.

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

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

5.8. 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-Bruyères-Le-Châtel and its integration in the VTK[3] based visualization tool *VisIt*[4] is in progress.

6. New Results

6.1. Existence and other theoretical results

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

Participants: Mihai Bostan, Nicolas Crouseilles, Sever Hirstoaga, Simon Labrunie, Jean Roche, Eric Sonnendrücker.

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

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

The papers [20], [19] are devoted to the asymptotic analysis of a system of PDEs describing the evolution of charged particles. The unknown are the distribution function of a particle population and the electro-magnetic field. The particles are subject to collisional mechanisms and to the action of electro-magnetic forces. The latter are defined in a self-consistent way by the Maxwell equations. We are interested in hydrodynamic limits where the relaxation effects induced by the collisional processes are strong enough and force the distribution function to tend towards an equilibrium state. Hence, in such a regime the behavior of the particles can be described by means of a finite set of macroscopic quantities, that is certain averages with respect to momentum of the distribution function. We distinguish two asymptotic regimes:

- the high-field regime corresponds to a situation where the force field has the same order as the collision term [19],

- the low-field regime corresponds to a situation where the convection and the force field are also singular terms within the equations, but at lower order than the leading contribution of the collisions [20].
Roughly speaking, the latter regime leads to convection-diffusion limit equations, while the former yields a purely hyperbolic model. The question has been pointed out by Poupaud [76] motivated by the modeling of semi-conductors devices.

In [17] we investigate the homogenization of the one dimensional Vlasov-Maxwell system. We indicate the convergence rate for the electric fields and establish weak convergence for the particle densities. In the non relativistic case we compute explicitly the limit solution. The theoretical results are illustrated by some numerical simulations.

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

An important problem we have been interesting in for some time in the context of models for magnetic fusion is the gyrokinetic limit of the Vlasov equation in a large non uniform magnetic field. More precisely, we consider the Vlasov equation which describes the dynamics of charged particles in an external electromagnetic field, in terms of a distribution function. When the magnetic field is assumed to be large, the rotation period of the particles around the magnetic field lines becomes small. Since this time scale is very detrimental for the stability of numerical schemes, our aim is to find a model where this time scale is removed. There is already a large literature on the subject in physics and also some preliminary mathematical results in simplified cases. We got some new results in this direction during the past year.

In [18] we study the finite Larmor radius regime for the Vlasov-Poisson equations with strong external magnetic field. The derivation of the limit model follows by formal expansion in power series with respect to a small parameter. If we replace the particle distribution by the guiding center distribution of the Larmor circles the limit of these densities satisfies a transport equation, whose velocity is given by the gyro-average of the electric field. We justify rigorously the convergence towards the above model and we investigate the well-posedness of it.

On the other hand in [48] we consider a new scaling of the Vlasov equation in order to derive a drift-kinetic model. To this end, we first make dimensionless cyclotron period appear in the scaled Vlasov equation. Then we decompose the particle velocity into the mean velocity and its random part and we deduce a system of two equations giving the evolution of the new distribution function and the mean velocity. Afterward, an asymptotic analysis is made for this model and a formal derivation of the gyrokinetic model (in a five dimension phase space) is thus obtained.

6.1.2. Convergence studies of numerical methods

In [16] we present a particle method for solving numerically the one dimensional Vlasov-Maxwell equations. This method is based on the formulation by characteristics. We perform the error analysis and we investigate the properties of this new scheme. The main point here is that the computation of the electric field do not require neither the calculation of the charge and current densities nor the explicit resolution of the Maxwell equations. In fact such schemes rely only on the approximation of the characteristics and the electric field, which are generally more regular than the particle distribution (think that f can be a L^1 function or even a measure). We do not need to ask for the smoothness of the particle distribution of the exact solution since no interpolation is performed.

In [43], a numerical analysis of the semi-Lagrangian scheme applied to the reduced Vlasov-Maxwell model is performed. This model has been recently introduced in the literature for studying laser-plasma interaction and some theoretical results has been established so far. This work is devoted to the proof of convergence of a semi-Lagrangian numerical solution towards the unique solution of the problem. The main interest of this work consists in the fact that a two dimensional advection is studied whereas split problems were studied so far in this framework. Numerical experiments proved the good behavior of the scheme even if the use of higher order interpolation operators is strongly advised.

We (in collaboration with P. Ciarlet) performed in [22] a numerical analysis of the time-dependent Maxwell equations with elliptic correction and with divergence constraint. These slightly generalized formulations are used to avoid a numerical drift of the numerical solution to Maxwell's equations when the continuity equation $\partial_t \varrho + \mathrm{div} J = 0$ (or a discrete version of it) is not exactly satisfied. This issue may arise when simulating plasmas, or more generally systems of charged particles, by PIC or Eulerian (Vlasovian) codes. This is (to our knowledge) the first comprehensive numerical analysis of the various nodal finite element methods for Maxwell's equations, including the treatment of both the divergence condition $\mathrm{div}\, E = \varrho/\varepsilon_0$ and the geometrical singularities. We concentrated on continuous (nodal) finite elements because they do not create spurious discontinuities of the force experienced by the particles. We obtained error estimates for the elliptic correction and for the mixed (saddle-point) formulation of the constraint; the two approaches are not equivalent at discrete level when nodal elements are used, unlike what happens with edge elements. The estimates are valid for the three main versions of nodal element method for Maxwell's equations: the basic one (which

can be used when the domain is regular or convex), the weighted regularization and the singular complement method (which are used to take geometrical singularities into account).

6.1.3. Domain decomposition for the resolution of nonlinear equations

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

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

where A is a second order derivatives 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 study the existence, uniqueness, qualitative properties and numerical simulation of solutions.

Another approach studied 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 equation 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 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 non-linearity 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. We apply this method to better understand the nickel-iron electrodeposition process, we have developed one-dimensional numerical model. This model addresses dissociation, diffusion, electromigration, convection and deposition of multiple ion species. To take account of the anisotropic behavior of the solution we introduce a domain decomposition numerical method. Simulations with experimental data show that our model can predict characteristic features of the nickel-iron system. New numerical analysis and simulation are published in [13], [14].

6.2. Development of Vlasov solvers

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

Participants: Nicolas Besse, Jean-Philippe Braeunig, Nicolas Crouseilles, Alain Ghizzo, Michael Gutnic, Matthieu Haefele, Olivier Hoenen, Guillaume Latu, Michel Mehrenberger, Thomas Respaud, Stéphanie Salmon, Eric Sonnendrücker, Eric Violard.

6.2.1. Two-dimensional solvers

In [45] a new Forward semi-Lagrangian method has been developed and validated. The main differences with the classical Backward semi-Lagrangian method are twofold. First, since the characteristics curves along with the unknown is constant are followed forward in time, this method enables the use of classical high order time discretization (such as Runge-Kutta 4 algorithms). Second, the remapping (or the deposition) step which is based on cubic spline polynomials, enables to reconstruct the distribution function on a uniform mesh using the particles which have moved during one time step. The analogous step for the backward method involves an interpolation to update the unknown. Several steps of the algorithm are identical or very close to those using in PIC methods. Hence, some strategies used in PIC methods for example in order to enforce the exact conservation of charge at the discrete level should be straightforward to adapt.

Another strategy based on conservative semi-Lagrangian methods has been implemented and tested. Whereas semi-Lagrangian methods compute the distribution function on the grid points, conservative methods considers an average of the unknown on each cell. This approximation enables to solve multi-dimensional problems by a successive solution of one-dimensional equations with a time splitting method. This is not the case for non-conservative methods when the advection field is not constant. In such a case, the conservative methods exhibit a very good behavior on long time simulations compared to traditional semi-Lagrangian methods. The possibility to deal with one-dimensional problems has a huge advantage from a memory point of view or for parallel algorithms. Finally, we have proved that in the particular case of a constant advective field, the two methods are algebraically equivalent.

6.2.2. CALVI platform

The aim of the platform is to change the way numerical methods are implemented and tested. It has been initiated because most of the researchers of the CALVI project develop new numerical methods for almost the same equations. Until now, every researchers implemented their methods as stand-alone C or Fortran applications. So, each researcher, for each code, has to implement the validation process by himself without using previous implementation done by himself or another member of the project. The platform moves the implementation from stand-alone application to a module oriented one. Thanks to standardized application programing interfaces (API), the different numerical methods can be swapped between them and can be validated within a common skeleton. This common skeleton plus the standard API is actually the platform. A better reuse of existing modules is expected as well as an increased efficiency in numerical methods implementation. The basis of the CALVI platform has been built this year and the main work consisted in architecture and API design. A first release has been provided. It contains skeleton modules: initial functions (8 test-cases with 3 validating ones), silo exports (Python bindings to the silo library), time diagnostics, and 5 drivers for validation purpose. It contains also solvers which are codes that have been modified in order to respect the API: 3 Vlasov solvers, 2 Rho solvers, and 4 Poisson solvers.

6.2.3. Four-dimensional solvers

A four-dimensional cubic splines interpolation has been validated in the framework of the backward semi-Lagrangian method on the Vlasov-Poisson equations. This study was motivated to study the validity of the time splitting of the method when non-conservative advection terms are involved. The method is currently tested on more complex problems and appears to be competitive from a CPU time point of view. This approach benefits from the Local Splines strategy which enables a decomposition domain well suited for parallel implementation.

Otherwise, a basic uniform semi-Lagrangian Vlasov-Poisson solver in $2D \times 2D$, named split4D which takes the benefit of total directional splitting has been written in C. In order to keep data locality, we have considered some local splines and quasi-interpolants. The code has been tested for the Landau damping. The benefit of using quasi-interpolants should be further developed. A straightforward parallelization of this uniform code has been implemented with calls to MPI and OpenMP directives. Some investigations are currently done about how to best use the memory hierarchy within this code.

6.2.4. Adaptive solvers

We contributed to the development of the 2D adaptive MPI parallel code (referred to as Yoda4D). This code targets distributed memory architectures and clusters. We added a fast geometric mesh partitioner and data redistribution is now overlapped with computations in order to reduce overheads during the dynamic load balancing phase. This balancing scheme and the efficiency of the code up to 32 processors has been validated in [36].

A lecture has been given by Martin Campos-Pinto [39]. A new class of adaptive semi-Lagrangian schemes-based on performing a semi-Lagrangian method on adaptive interpolation grids – in the context of solving Vlasov equations with underlying smooth flow, such as the one-dimensional Vlasov-Poisson system. After recalling the main features of the semi-Lagrangian method and its error analysis in a uniform setting, we describe two frameworks for implementing adaptive interpolations, namely multilevel finite elements and

interpolating wavelets. For both discretizations we introduce a notion of good adaptivity to a given function, and show that it is preserved by a low-cost prediction algorithm which transport multilevel grids along any smooth flow. As a consequence, error estimates are established for the resulting "predict and re-adapt" schemes under the essential assumption that the flow underlying the transport equation, as well as its approximation, is a diffeomorphism. Some complexity results are stated in addition, together with a conjectured convergence rate for the overall adaptive scheme. As for the wavelet case, these results are new and also apply to high order interpolation.

6.2.5. Electromagnetic Particle In Cell (PIC) solvers

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

We have developed a general mathematical framework for electromagnetic Particle-In-Cell (PIC) codes that can be used on structured as well as unstructured or hybrid grids. It can accommodate high order Maxwell finite element solvers conforming in $H(\mathrm{curl})$ that prevent to create spurious electromagnetic modes which could be amplified by the numerical noise of the PIC method (see [49] for high order Maxwell finite solvers and their properties). A 2D code, named HYBRID_FEM_PIC_2D, coupling a $H(\mathrm{curl})$ conforming finite element solver of any order 1, 2 or 3 on hybrid grid for the Maxwell equations and a PIC solver for the Vlasov equation was developed including an exact discrete continuity equation. We have also developed a 3D code on a regular grid (STRUCTURED_FEM_PIC_3D) including the same features and finally we are working on an unstructured one (UNSTRUCTURED_FEM_PIC_3D). One of the key points in the coupling between Maxwell and PIC solvers is the continuity equation. Indeed, the computation of the current density created by the particles and entering as the source for the electromagnetic solver must enforce the discrete charge conservation to ensure that the numerical solution is physical. This equation reads $\frac{\partial \rho}{\partial t} + \mathrm{div} J = 0$, where ρ is the charge density and J the current density. We have shown that if the charge density is given by $\rho_h^n(\mathbf{x}) := \sum_{k=1}^{N_p} w_k S(\mathbf{x} - \mathbf{x}_k^n)\Delta t$, where S is a local smooth shape function such as a B-spline, and $w_k,\ \mathbf{x}_k,\ \mathbf{v}_k$ are respectively the weight, the position and velocity of the k-th particle, then the discrete continuity equation is guaranteed by the following formula for the current density:

$$\overline{\mathbf{J}}_h^{n+\frac{1}{2}}(\mathbf{x}) := \sum_{k=1}^{N_p} w_k \mathbf{v}_k^{n+\frac{1}{2}} \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} S(\mathbf{x} - \mathbf{x}_k(t)) dt. \tag{3}$$

We have given a practical algorithm for implementing this new method, which requires the same computational tools as the classical PIC scheme. We also have shown in [47] that the lowest order version of our formulation (order 1 for the finite element) corresponds, on a rectangular grid, to the traditional Cloud-In-Cell (CIC) version of the PIC method coupled to a Yee Maxwell solver and the Villasenor-Buneman charge deposition scheme.

A parallel code (Spin) has been developed to solve bigger test cases using the same numerical method. Spin solves Maxwell equations on hybrid meshes (quadrangles and triangles) using edge finite elements. The work distribution on processors is expected to be balanced because the Maxwell solver on quadrangles is highly parallel.

6.3. Multiple time scales solvers and Magneto HydroDynamics

Participants: Emmanuel Frénod, Michael Gutnic, Philippe Helluy, Hélène Mathis, Alexandre Mouton, Eric Sonnendrücker.

6.3.1. Multiple time scales solvers

Problems in which two very different time scales co-exist put a strong constraint on the time step which needs to be adapted to the smallest time scale in order to avoid instabilities. We have developed a new technique based on two-scale convergence tools for handling such problems. The idea is to find the two-scale limit of the original equation and to solve numerically this two-scale limit, in which the fast scale is handled via an integral term and where the small time step constraint is removed. We have used this technique in order to develop a two-scale PIC method for a problem in accelerator physics [25] and also for the gyrokinetic limit in the thesis of Alexandre Mouton.

6.3.2. Magneto HydroDynamics

The CALVI project is mainly devoted to the construction of numerical schemes for kinetic plasma physics simulations. We have started a new research effort directed towards fluid models such as the ideal magneto-hydro-dynamics (MHD) model. A summer research session has been organized in Luminy in July and august 2008 during the CEMRACS'08 http://smai.emath.fr/cemracs/cemracs08/fr_projects.html

The project, entitled "GADMHD: approximation GAlerkin Discontinu pour la MagnétoHydroDynamique" allowed to achieve several objectives: to develop a new high order discontinuous galerkin code for solving the MHD equations, to investigate several practical aspects of this kind of problems (validation, analytical solution, Riemann problem, multiplicity of the entropy solutions, *etc.*), and finally to test and analyze a new general multi-time step algorithm based on the Adams-Bashforth time integration. This last algorithm permits to reduce significantly the computational cost when large and big cells are mixed in the mesh. The results obtained during the research session are available in the final report [41].

6.4. Visualization

Keywords: *Multi-GPU*, *Pre-integrated*, *Sort Last Volume*.

Participants: Jean-Michel Dischler, Stéphane Marchesin.

6.4.1. Higher order Pre-integrated Volume Rendering

In the field of Volume Rendering, pre-integration techniques for arbitrary transfer functions has certainly led to the most significant and convincing results on standard PC consumer graphics with regard to both quality and performance. By showing that the ideal scalar signal along the cast rays is better approximated by a succession of polynomial curves as opposed to linear segments, we have proposed a new method for pre-integrated volume rendering. This method is based on a second and third order polynomial interpolation of the scalar values, allowing it to converge more rapidly towards the integration of a volume reconstructed by a trilinear filter. Our approach manages to capture the smoothness of the volume's details without the need of further ray re-sampling, and consequently succeeds in reducing the visual artifacts in comparison to previous techniques. Our experiments showed that second order polynomials improve framerates and visual quality while third order does not provide significant further improvements, which is related to the fact that sample positions are equispaced for real-time rendering purposes. We published second order pre-integration in [35].

6.4.2. Multi-Sort Last Volume Visualization

We conducted an experimental study of an inexpensive off-the-shelf sort-last volume visualization architecture based upon multiple GPUs and a single CPU. This study showed how to efficiently make use of this architecture to achieve high performance sort-last volume visualization of large datasets. We analyzed the bottlenecks of this architecture and compared it to a classical sort-last visualization system using a cluster of commodity machines interconnected by a gigabit Ethernet network. As a result of this experimental study we showed that this solution competes very well with a mid-sized PC cluster, while it significantly improves performance compared to a single standard PC. The results of our study have been published in [38].

6.5. Application of Vlasov codes to magnetic fusion

Participants: Pierre Bertrand, Nicolas Besse, Jean-Philippe Braeunig, Nicolas Crouseilles, Daniele DelSarto, Nicolas Dubuit, M Elmounden, Etienne Gravier, Rudy Klein, Guillaume Latu, Jean Roche, Eric Sonnendrücker.

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

6.5.1. Development of a 5D gyrokinetic code

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

In the frame of gyrokinetic models in Magnetic Confinement Fusion, we are interested in simulation of plasma motion with a strong anisotropy in the velocity field. This situation occurs in tokamaks and ITER in particular, where the magnetic field is so strong that the particles are mostly following magnetic field lines. Parallel (to the magnetic field lines) velocity and perpendicular velocities are then of different magnitudes and should be treated specifically. Therefore, considering that the magnetic field is constant, a gyrokinetic model written in curvilinear coordinates is currently investigated, which should allow to make simulations using a mesh aligned to the magnetic field lines. Such a mesh should reduce significantly numerical diffusion in magnetic lines direction. Early tests using a simple model show that numerical diffusion is reduced even for not strictly aligned meshes. However, this technique introduces some difficulties on boundary conditions. In fact, the physical location of domain boundaries could be complex curves and for periodic boundary conditions, one has to find values on one side of the domain to imposes equal values on the other side. If a curvilinear cartesian mesh is not aligned with the periodic direction, one has to find values at boundaries taking into account the lag between mesh lines and periodic direction. Curvilinear coordinates impose also to work on data post-treatment, adapting visualization tools to this kind of meshes.

We investigate a modification of the scheme in order to have field aligned coordinates. This feature, used by many other gyrokinetic codes, will improve the numerical quality of the simulations. Nevertheless the numerical method and the parallelization should be deeply revised.

6.5.2. Gyro-water-bag approach

In the Gyro-Water-Bag (GWB) approach, a discrete distribution function taking the form of a multi-step like function is used in place of the continuous distribution function along the velocity direction. According to Liouville's phase-space conservation property the distribution function remains constant in time between the bag contours. The time evolution of the system is completely described by the knowledge of the contours. We get a set of hydrodynamic equations, where the system behaves as N fluids coupled together by the electromagnetic fields (in our case the quasi-neutrality). As a matter of fact a small bag number (not more than 10) has been shown to be sufficient to correctly describe the Ion Temperature Gradient (ITG) instability observed in fusion plasmas (see [32]). Thus the water-bag offers an exact description of the plasma dynamics even with a small bag number, allowing more analytical studies and bringing the link between the hydrodynamic description and the full Vlasov one. First very encouraging results have been obtained with a 3-D code in cylindrical geometry and for electrons following the adiabatic law (see [15]) based on discontinuous-Galerkin type methods.

6.5.3. Trapped-ion driven turbulence (4D model)

The work focuses on trapped-ion driven modes (TIM), which belong to the family of ion gradient driven modes. Theses instabilities are characterized by frequencies of the order of the trapped precession frequency and radial scales of the order of several banana orbits. Trapped-ion driven 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. Averaging the kinetic equation over both cyclotron and bounce motions allows the number of independent variables in phase space to be reduced. The new Vlasov equation function depends on only two variables (precession angle and poloidal flux), the final problem is 2D, parametrized by the particle energy and trapping parameter, allowing for an efficient parallelization of the code. The goal is here to take into account the effects of the magnetic shear on the stabilization of the instability for an ensemble of values of the trapping parameter. The development (and optimization) of a 4D Vlasov code on a parallel computer is thus in progress. The step is necessary to check the validity and the accuracy of this method of reduction based on action-angle formalism. First numerical results of the code implemented on a parallel IBM-Power4 supercomputer show a very good stability of the numerical scheme taking into account a marginally stable initial condition. This very good stability of the Vlasov method (which is noiseless in comparison with the standard Particles-In-Cell codes) allows us to control the start up of the ITG instability (which grows from the round-off errors of the computer).

A key element in the understanding of the role played by trapped ions in the turbulence may be obtained by making numerical simulations using the full-gyrokinetic GYSELA code (which describes of course trapped and passing particles) and the reduced action-angle code which indeed takes into account only TIM. A major goal in the future is to implement the closed-loop strategy combining the implementation of reduced models (which are faster and cheaper than the full gyrokinetic treatment) with a series of numerical comparisons using the GYSELA 5D code. The existing cooperation with teams of CEA makes this a realistic objective on a long time (more than one year) with potentially large overall impact.

6.5.4. 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 corresponds 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 et al. 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. We develop a new version introducing domain decomposition techniques and source terms.

6.6. Application of Vlasov codes nanophysics

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

6.6.1. 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 In order to include quantum effects, a quantum hydrodynamic model 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 traveling through the film. These results published in [23] confirm that the hydrodynamic model is well suited to describe the electron dynamics in finite-size nano-objects.

6.6.2. Quantum electron dynamics in thin metal films

In the past few years, we carried out a series of studies on the ultra-fast electron dynamics in thin metal films. Self-consistent simulations of the electron dynamics and transport were performed using a semi-classical Vlasov-Poisson model. In particular, we showed that, after the excitation energy has been absorbed by the film, slow nonlinear oscillations appear, with a period proportional to the film thickness. These oscillations were attributed to non-equilibrium electrons bouncing back and forth on the film surfaces. Recently, we have extended this semi-classical study to the quantum regime, by employing the Wigner-Poisson equations. It was found that the Vlasov and Wigner results coincide for large excitations. In contrast, for small excitations, the period of the oscillations diverges from the semi-classical “ballistic" value obtained previously. Closer inspection of the Wigner functions reveals that, in the fully quantum regime, the phase-space structures that are responsible for the ballistic transport cannot form. Simple analytical arguments are provided in support of the above numerical findings.

6.6.3. Ultra-fast magnetization dynamics in diluted magnetic semiconductors

In [31], we have developed a dynamical model that successfully explains the observed time evolution of the magnetization in diluted magnetic semiconductor quantum wells after weak laser excitation. Based on a many-particle expansion of the exact $p-d$ exchange interaction, our approach goes beyond the usual mean-field approximation. It includes both the sub-picosecond demagnetization dynamics and the slower relaxation processes which restore the initial ferromagnetic order on a nanosecond timescale. In agreement with experimental results, our numerical simulations show that, depending on the value of the initial lattice temperature, a subsequent enhancement of the total magnetization may be observed on a timescale of few hundreds of picoseconds.

6.6.4. Quasilinear approximation of the Wigner-Poisson equations

The Wigner equation is the quantum analog of the classical Vlasov equation. Although many important results have been obtained in the field of classical phase-space (or Langmuir) turbulence, comparatively few works have investigated the important question of quantum plasma turbulence. A reasonable strategy to attack these problems would consist in extending well-known techniques issued from the theory of classical plasmas in order to include quantum effects. In this context, the simplest approach is given by the weak turbulence kinetic equations first derived by Vedenov and Drummond in the 1960s – the so-called quasilinear theory. In a recent work [27], we re-examined the quasilinear theory of the Wigner-Poisson system in one spatial dimension. It was found that quantum effects manifest themselves in transient periodic oscillations of the averaged Wigner function in velocity space. The quantum quasilinear theory was checked against numerical simulations of the bump-on-tail and two-stream instabilities. The predicted wavelength of the oscillations in velocity space agrees well with the numerical results.

6.7. Inverse problem governed by Maxwell equations

Participant: Jean Roche.

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

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

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

The goal of this work is to give an algorithm to locate suitable inductors around the molten metal so that the equilibrated shape be as near as possible to a desired one. Two different approaches are proposed, the first one seeks for a set of inductors such that the distance between the equilibrated shape and the given target one is minimized. The second approach looks for a set of inductors such that a slack function related to the equilibrium relation on the boundary of the target shape is minimized. New results are obtained in [21], [33]. In a new paper to appear [44] we consider the more realistic case where the inductors are composed by a set of bundled vertical electric wires made of insulated strands. We are interested to determine the position and shape of the package of strands in order to have an horizontal cross-section of the molten metal as close as possible to a prescribed shape.

7. Contracts and Grants with Industry

7.1. CEA Cadarache, gyrokinetic simulation and visualization

Participants: Jean-Philippe Braeunig, Nicolas Crouseilles, Guillaume Latu, Michel Mehrenberger, Ahmed Ratnani, Eric Sonnendrücker, 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. LRC project with CEA Cadarache, Full wave modeling of lower hybrid current drive in tokamaks

Participants: Jean Roche, Simon Labrunie, E. Natarajan.

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

7.3. National initiatives

7.3.1. ANR Projects

Calvi members are involved in three ANR projects.

- 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): Development of 3D electromagnetic PIC codes comparing conforming Finite Elements and Discontinuous Galerkin Solvers on unstructured grids. http://www-math.u-strasbg.fr/houpic/.

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

7.3.2. Participation to GdR Research groups from CNRS

The members of Calvi participate actively in the following GdR:

- GdR équations Cinétiques et Hyperboliques : Aspects Numériques, Théoriques, et de modélisation (CHANT, CNRS 2900): this research group is devoted to the modeling 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

7.4.2. EUFORIA Project

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

8. Dissemination

8.1. Leadership within scientific community

8.1.1. Invitations at conferences and summer schools

- E. Sonnendrücker gave an invited lecture at the Workshop "Méthodes multi-échelles pour la turbulence plasma et fluide: Applications à la fusion dans les plasmas avec confinement magnétique" at CIRM Luminy (April 21-25, 2008).
- E. Sonnendrücker gave an invited lecture at the ITER workshop at University Paris 6 (May 22-23, 2008).
- E. Sonnendrücker gave an invited lecture at the France-Canada Conference in Montréal (June 1-5, 2008).
- E. Sonnendrücker gave an invited lecture at the EDF-CEA-INRIA summer school at Nice on the topic "Numerical models for controlled fusion" (September 8-12, 2008).
- E. Sonnendrücker gave an invited lecture at the Workshop on Gyrokinetic models in Vienna, Austria (September 15-18, 2008).

8.1.2. 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 Committee of the university.
- Jean-Michel Dischler is a member of the professional board of Eurographics.
- Jean Rodolphe Roche is the head of the Mathematics Department of the École Supérieure des Sciences et Technologies de l'Ingénieur de Nancy.
- Jean Rodolphe Roche is the research coordinator of the "École Supérieure des Sciences et Technologies de l'Ingénieur de Nancy" .
- Jean Rodolphe Roche is the research coordinator of a CAPES-COFECUB bilateral agreement with the Federal University of Rio de Janeiro and the National Laboratory of Scientific Computing of Brazil.
- Eric Sonnendrücker is 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 taught an optional graduate course entitled "Scientific computing" in the Master of Mathematics at the University Henri Poincaré (Nancy I).
- Eric Sonnendrücker taught an optional graduate course entitled "Kinetic models for fusion" 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 2008

1. Olivier Hoenen, *Parallelization of Adaptive Methods for the Vlasov Equation*. Advisor: Eric Violard. Defended June 18, 2008 (Jury: Jacques Bahi, Olivier Coulaud, Catherine Mongenet, Eric Sonnendrücker, Stéphane Vialle, Eric Violard).

8.3.2. Ph. D. in progress

1. Aurore Back, *Hamiltonian derivation of gyrokinetic models*. Advisors: Emmanuel Frénod, Eric Sonnendrücker.
2. Sandrine Marchal, *Domain decomposition methods to solve a system of hyperbolic equations*. Advisors: Simon Labrunie, Jean Rodolphe Roche.
3. Alexandre Mouton, *Multiscale approximation of the Vlasov equation*. Advisors: Emmanuel Frénod, Eric Sonnendrücker.

4. Thomas Respaud, *Numerical coupling of Maxwell and Vlasov equations*. Advisors: Eric Sonnendrücker.
5. Ahmed Ratnani, *Study of the quasi-neutrality equation and its coupling with Vlasov equations*. Advisors: Nicolas Crouseilles, Eric Sonnendrücker.

8.3.3. Post Doc in progress

1. Fahd Karami, *Analytical and numerical study of singularities of the Vlasov-Poisson and Vlasov-Maxwell systems*. Advisor: Simon Labrunie, Xavier Antoine.
2. Omar Morandi, *Ultrafast magnetization dynamics in diluted magnetic semiconductors*. Advisor: Nicolas Crouseilles, Paul-Antoine Hervieux, Giovanni Manfredi.
3. Hocine Sellama, *Numerical study of gyroaverage operators*. Advisor: Nicolas Crouseilles, Michel Mehrenberger, Eric Sonnendrücker.

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