Project-Team calvi

Calcul Scientifique et Visualisation

Lorraine
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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

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
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.

- Simon Labrunie has been seconded as a CR INRIA from october 1, 2003 to september 30, 2004.
- Vladimir Latocha has been hired on september 1, 2003 as a Maître de Conférences in applied mathematics at the Université Henri Poincaré and joins the project.

3. Scientific Foundations

3.1. Kinetic models for plasma and beam physics

**Key words:** plasma physics, beam physics, kinetic models, reduced models, Vlasov equation, modeling, mathematical analysis, asymptotic analysis, existence, 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 $f_s(x, v, t)$ corresponding to the statistical average of the particle distribution in phase-space corresponding to many realisations of the physical system under investigation. The product $f_s dx dv$ is the average number of particles of the considered species, the position and velocity of which are located in a bin of volume $dx dv$ centered around $(x, v)$. 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.
else 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

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

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

\[
-\frac{1}{c^2} \frac{\partial E}{\partial t} + \nabla \times B = \mu_0 J,
\]

\[
\nabla \cdot E = \frac{\rho}{\varepsilon_0},
\]

\[
\nabla \cdot B = 0,
\]

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

\[
\rho(x, t) = \sum_s q_s \int f_s(x, v, t) \, dv,
\]

and current density

\[
J(x, t) = \sum_s q_s \int f_s(x, v, t)v \, dv,
\]

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

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

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

The numerical resolution of the three-dimensional Vlasov-Maxwell system represents a considerable challenge due to the huge size of the problem. Indeed, the Vlasov-Maxwell system is non-linear 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 mathematic 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 [52], see also Bardos and Degond [33]. The existence of weak solution for the Vlasov-Maxwell system has been proved by Di Perna and Lions [40]. The state of the theory is presented in a recent book by Glassey [48].

Many questions concerning uniqueness in particular and strong solutions for the Vlasov-Maxwell system are still open. Moreover, there 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 [4].

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 who 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 [49][55] as well as by Brenier [37]. 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 [46][44][45].

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 close after a few of them, thus yielding fluid models.

3.2. Development of simulation tools

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

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. Numerical simulation of plasmas started in the 1960s and developed according to the available computing resources: at the beginning in the 1960s and 1970s, only 1D simulations were possible and many different approaches where introduced. Each of them had advantages and drawbacks. Then in the 1980s qualitatively accurate 2D simulations became accessible using the Particle-In-Cell (PIC) technique. Resulting codes have proven to be useful in studying plasma dynamics even for 2D and 3D problems and complex geometries. It thus became by far the method of choice in most simulations. However, only a few particles per cell have been used particularly in 3D PIC codes leading to a high level of numerical noise, especially in regions of phase space where the density is low. Thus, in the 1990s, when computers became powerful enough, it was interesting again to use solvers based on a phase-space grid which are more precise and better in some situations. However complexity, on uniform grids, becomes too important when dimension increases. For this reason it is important to optimize the number of grid points that are used according to the evolution of the solution and use adaptive grid methods.

Our aim is to develop and analyze new and efficient solvers for the Vlasov-Maxwell equations and related models, in particular adaptive 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 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

$$f(x, v, t) = f(X(s; x, v, t), V(s; x, v, t), s),$$

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

$$\frac{dX}{dt} = V,$$
$$\frac{dV}{dt} = E(X(s), s) + V(s) \times B(X(s), s), \quad (1)$$

with initial conditions $X(t) = x, V(t) = v$.

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 $(x_i, v_j)$ consisting in the following two steps:

1. For all $i, j$, compute the origin of the characteristic ending at $x_i, v_j$, i.e. an approximation of $X(t_n; x_i, v_j, t_{n+1}), V(t_n; x_i, v_j, t_{n+1})$.
2. As

$$f^{n+1}(x_i, v_j) = f^n(X(t_n; x_i, v_j, t_{n+1}), V(t_n; x_i, v_j, t_{n+1})).$$

$f^{n+1}$ can be computed by interpolating $f^n$ which is known at the grid points at the points $X(t_n; x_i, v_j, t_{n+1}), V(t_n; x_i, v_j, t_{n+1})$.

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 [35] 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

3.2.6.1. The Singular Complement Method

The solutions to Maxwell’s equations are a priori defined within the variational spaces $X = H_0(\text{rot}, \Omega) \cap H(\text{div}, \Omega)$ and $Y = H(\text{rot}, \Omega) \cap H_0(\text{div}, \Omega)$, i.e. the space of vector fields in $L^2(\Omega)$ with $L^2$ divergence and curl, satisfying the electric and magnetic boundary conditions. Those solutions are in fact smoother (i.e. $H^1(\Omega)$) when the boundary of the domain $\Omega$ is smooth or convex. This is no longer true when $\Omega$ exhibits non-convex geometrical singularities (corners, vertices or edges). In this case, the spaces $X$ and $Y$ do not admit any dense subspace contained within $H^1(\Omega)$.

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 (i.e. $H^1(\Omega)$) 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 [30] and implemented [32] in plane geometry. Theoretical studies had been performed in polyhedral geometry [29][36][31].

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 [34]. The non-density result for regular fields was proven [38], the singularities of the electromagnetic field were related to that of modified Laplacians [26], and expressions of the singular fields were calculated [27]. 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 [28].

3.2.6.2. Other results, extensions.

As a byproduct, space-time regularity results of the type $C^{0,\alpha}([0, T]; H^s(\Omega))$ were obtained for the solution to time-dependent Maxwell’s equation in presence of geometrical singularities in the plane and axisymmetric cases [47][27]. The exponents $\alpha$ and $s$ depend on the nature and geometry of the singularities.

3.3. Large size problems

Key words: Parallelism, domain decomposition, GRID, code transformation.

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.

3.3.1. Introduction

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. Parallelisation of numerical methods

We are concerned with the parallel implementation of the numerical methods that we use to solve the Vlasov equation. We address the problem of tuning them 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 [50] give very good results for a very low cost.

Adaptive methods include a mesh refinement step and can highly reduce memory usage and computations volume. In return, they induce a load imbalance and require to dynamically distribute the (so-called 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 [15], 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 [53] 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 [43]).

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.

In the area of thermonuclear fusion, the numerical simulations showed their great utility. These simulations consist in solving the Vlasov equation which describes the behavior of the particles in the plasma. Numerical simulations often make it possible to improve the theory in order to get a better agreement with laboratory experiments. The visualization of the results of these simulations is currently used but the visualization techniques are not always well adapted tools, in comparison with the complexity of the physical phenomena to understand. Indeed the volume visualization of these phenomena deals with multidimensional data sets and sizes nearer to terabytes than megabytes. Our scientific objective is to appreciably improve the reliability of
the numerical simulations thanks to the implementation of suitable visualization techniques. More precisely, to study these problems, our objective is to develop new physical, mathematical and data-processing methods in scientific visualization: visualization of larger volume datasets, taking into account the temporal evolution. A global access of data through 3D visualization is one of the key issues in numerical simulations of thermonuclear fusion phenomena. A better representation of the numerical results will lead to a better understanding of the physical problems. In addition, immersive visualization helps to extract the complex structures that appear in the plasma. This work is related to a real integration between numerical simulation and scientific visualization. Thanks to new methods of visualization, it will be possible to detect the zones of numerical interest, and to increase the precision of calculations in these zones. The integration of this dynamical side in the pipeline "simulation then visualisation" will not only allow scientific progress in these two fields, but also will support the installation of a unique process "simulation-visualisation".

4. Application Domains

4.1. Thermonuclear fusion

Key words: Inertial fusion, magnetic fusion, ITER, particle accelerators, laser-matter interaction.

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

Our work in modeling and numerical simulation of plasmas and particle beams can be applied to problems like laser-matter interaction in particular for particle accelerators, the study of parametric instabilities (Raman, Brillouin), the fast ignitor concept in the laser fusion research. Another application is devoted to the development of Vlasov gyrokinetic codes in the framework of the magnetic fusion programme. 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 nanoparticles as approximate models when ab initio approaches are too costly.

\(^1\)http://www.iter-gouv.fr
In order to model and interpret experimental results obtained with large nanoparticles, 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. [42], 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 nanostructures could be studied.

The nanoparticle 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

Participants: Francis Filbet [correspondant], Eric Sonnendrücker.

Key words: Vlasov, 2D, axisymmetric, beam simulation, plasma simulation, PFC method, conservative, positive.

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 [42] 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 [41]. It has been applied as well for plasma as for beam simulations.

The code is available at the following address:

5.2. Obiwan

Participants: Michaël Gutnic [correspondant], Matthieu Haefelé, Eric Sonnendrücker.

Key words: Vlasov, semi-Lagrangian, adaptive, multiresolution, interpollet.

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 an axisymmetric 1Dr-1Dv version using one fixed value of the canonical angular momentum. The grid adaptivity is base 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. M2V

Participants: Pierre Navaro [correspondant], Eric Sonnendrücker.
**Key words:** Vlasov, Maxwell, Particle-In-Cell (PIC), axisymmetric, beam simulation, plasma simulation, unstructured grids, finite volume.

The M2V code is developed in the framework of a contract with the CEA. 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. Maxwell’s equations are solved on an unstructured grid using a finite volume type method. The Vlasov equations are solved using a particle method. The coupling is based on traditional PIC techniques.

## 6. New Results

### 6.1. Existence of weak solutions for the Vlasov-Darwin model

**Participants:** Said Bénachour, Francis Filbet, Eric Sonnendrücker.

This work has been performed in collaboration with Philippe Laurençot (Toulouse).

The Darwin model is an approximation of Maxwell’s equations where the transverse part of the displacement current is neglected in Ampère’s law. Doing this, the hyperbolic Maxwell’s system is transformed into the Darwin model which can also be written as a set of three elliptic problems, hence changing completely the nature of the problem. The Darwin model has been studied in connection with the Maxwell system, and it has been proved in [54] that it is intermediate between Maxwell and Poisson’s equations. However, there exist no results concerning the coupled Vlasov-Darwin equations. We prove the existence of global weak solutions for this problem for small initial data. The major difficulty in this problem comes from the lack of energy type estimate for the transverse part of the electric field. We overcome this problem using a duality argument which yields an estimate for small initial data. This work is presented in [4].

### 6.2. Fluid limits of the Vlasov-Maxwell system

**Participants:** Simon Labrunie, Pierre Bertrand.

We have been investigating some simple situations, such as waves in 1D plasmas, which exemplify the fluid limits without accumulating technical difficulties. Indeed, these approximations are of thermodynamic nature and do not depend on the dimensionality or geometry.

#### 6.2.1. Numerical method.

Several “toy” codes for plasma simulation have been written in joint work with J.A. Carrillo (now at the University of Barcelona) using the WENO (Weighted Essentially Non-Oscillatory) method. The latter is one of the most precise methods available for conservation laws [56]. These codes allow to perform an extensive experimental study of some of the simplified models mentioned in the previous paragraph. More specifically, we were able to:

- Make meaningful comparisons between “exact” and simplified models: kinetic and fluid, two- and one-species.
- Check the underlying hypotheses of the fluid derivation (i.e. the equations of state for the various species) using kinetic simulations.
- Assess the accuracy of the quasi-neutrality criteria: equality of the concentrations of positive and negative species, or their proportionality to the Boltzmann factor.

This work helped to set the limits of validity of these approximations [21]. Some findings are rather novel:

- Fluid modelling appears justified even in the absence of collisions, provided certain relationships hold between the characteristic speed of the phenomenon under consideration and the thermal velocities of the various species.
• The Boltzmann criterion for quasi-neutrality, though seemingly more “sensible” than the simple equality of concentrations, appears to fail when one tends to neutrality.

We are presently working on another WENO code, incorporating some magnetic field effects in order to model laser-plasma interactions. Of course, the study of more realistic situations: complex, multi-dimensional geometries... is still the objective in the long run.

6.3. Convergence of semi-Lagrangian methods

**Participant:** Nicolas Besse.

The convergence of several semi-Lagrangian numerical schemes for the one-dimensional Vlasov-Poisson equations has been proved:

• Proof of convergence of a semi-Lagrangian scheme for the Vlasov-Poisson equations based on linear interpolating polynomials on an unstructured mesh of phase-space. The error estimate in $L^\infty$ norm is in $O(h^{4/3})$.

• Proof of convergence of high order semi-Lagrangian schemes for the Vlasov-Poisson equations using different kinds of interpolation: symmetric Lagrange interpolation, B-Spline interpolation, wavelet interpolation. The error estimate in $L^2$ norm is in $O(\Delta t^2 + h^{m+1} \Delta t^\alpha)$.

• Proof of convergence of a semi-Lagrangian scheme for the Vlasov-Poisson equations based on Hermite interpolation and the propagation of gradients of $f$ on a uniform grid of phase-space.

6.4. Semi-Lagrangian methods for the resolution of the Vlasov equation

**Participants:** Nicolas Besse, Pierre Bertrand, Alain Ghizzo, Eric Sonnendrücker.

6.4.1. Semi-Lagrangian method for unstructured grids

A thorough study of the semi-Lagrangian method for the Vlasov-Poisson system on unstructured grids of triangles has been performed in the thesis work of Nicolas Besse. The time discretization is based on a splitting scheme. Different kinds of interpolation steps based on finite element interpolants have been tested. A first negative result was that Lagrange interpolants of order at least three yield an unstable scheme. Note that high order Lagrange interpolation can be used on uniform grids as long as the interpolating polynomial covers several cells and is only used in its stability zone, which is identified. Good interpolants in the case of unstructured triangular meshes are based on high order Hermite interpolation and the propagation of $\nabla f$ as well as $f$ to update the degrees of freedom. Conservation of mass and positivity can be recovered using a posteriori methods. This work is described in Nicolas Besse’s thesis and in [5].

6.4.2. Semi-Lagrangian method in the relativistic case

The semi-Lagrangian method can make use of a time splitting scheme and thus in some case reduce the resolution to two successive constant coefficient advection problems. However, in the strongly relativistic regime of the laser-plasma interaction, an unadapted use of the splitting scheme may lead to a bad density conservation and triggers numerical instability in the case of a one-dimensional system. A direct integration using a two-dimensional full advection based on B-Spline interpolation was initially proposed in [57].

This method was extended to the relativistic case in paper [14] for achieving accurate solution of the Vlasov-Maxwell system.

In the paper [11] we present results of 2D open Semi-Lagrangian Vlasov (SLV) simulations of the ultra-intense electromagnetic pulse with an slightly overdense (or underdense) plasma and describe the new features of the 2D SLV code that made it possible for the first time to simulate, using a 2D causal Vlasov code, the penetration of a strong electromagnetic pulse in an overdense plasma by relativistic self-induced transparency, and the relativistic filamentation instability (RFI) in an underdense plasma. In this code, the integration of the Vlasov equation is made along their exact characteristics. The code exists in 1D1/2 and 2D geometries and...
6.5. Adaptive semi-Lagrangian methods

Participants: Michaël Gutnic, Matthieu Haefelé, Michel Mehrenberger, Eric Sonnendrücker.

6.5.1. An adaptive method based on interpolating wavelets

If we want to use the semi-Lagrangian method for realistic problems involving high-dimensional phase-space, it is essential to optimize the number of mesh points used according to the variations of the distribution function. We are thus investigating adaptive grid methods. As an essential building block of the semi-Lagrangian method is interpolation, a first idea is to perform this interpolation on nested grids, whence the idea of multi-resolution analysis and interpolating wavelets.

The method is based on the use of a hierarchy of nested grids. In order to bind one level to the next, restriction and prediction operators are used. The restriction operator consists in keeping only the values at the even grid points. The prediction operator consists in keeping the same value at the even grid points and reconstructing the value at the odd grid points with the underlying interpolation operator (e.g. cubic Lagrange interpolation). Instead of storing the value at the odd grid points, one can store a so-called detail which is the difference between this value, and the value predicted from the coarser mesh. Then, when the detail is small, the value can be reconstructed with good accuracy from the coarser mesh and does not need to be computed. This enables to eliminate the corresponding grid point from the mesh.

This strategy enables to construct an initial adaptive grid by compressing the initial value of the distribution function. The time evolution is then performed in two steps: first we predict a new adaptive grid using a forward advection, then we compute the values of the distribution function on the adaptive grid and compress again for the next time step. A first description of this method can be found in [17].

6.5.2. An adaptive method based on hierarchical finite elements

The idea in this method is to use an algorithm based on hierarchical finite element decomposition. At each time step, the distribution function is given by the local finite element bases associated to the (dyadic) cells of an adaptive mesh whose underlying cell tree is consistent in the sense that no cell is partially refined.

Like in the interpolation wavelet method, a “forward-backward” scheme is used. From an initial adaptive mesh, we predict a new mesh by forward advection along the characteristics, we next compute the new data on the new grid by backward advection, compress it and go further. We notice that the computation of the function at the origin of the characteristic only involves the nodes associated to the leaf cell where this origin lie. The compression of the cell tree is based on the idea that where the nodal reconstruction on a ‘mother’ cell is close to the reconstruction on its ‘daughters’ leaves, then the mesh can be locally coarsened. So we loop over the levels in decreasing order and ask whether we can discard the daughters or not.

In addition to tree structure storage, we have another data structure (we use a hash map) in order to loop faster over one level. The implementation is generic \(N\) dimensional (tensor products of intervals).

This work was started during CEMRACS 2003 in collaboration with Martin Campos-Pinto and Albert Cohen.

6.6. Collision models

Participant: Francis Filbet.

6.6.1. Approximation of Landau equation for plasma physics

We investigate the approximation of the solution to the Vlasov equation coupled with the Fokker-Planck-Landau collision operator using a phase space grid. On the one hand, the algorithm is based on the conservation of the flux of particles and the conservation of the total energy. Then, the distribution function is reconstructed allowing to control spurious oscillations or preserving the positivity. On the other hand, the methods preserve the main properties of the collision operators in order to reach the correct stationary state. Several numerical
results are presented in one dimension in space and three dimensions in velocity. This work is in collaboration with N. Crouseilles (MIP, Toulouse and CEA-CESTA Bordeaux).

6.6.2. Accurate numerical methods for the Boltzmann equation

We are interested in the construction of an accurate method for the space non homogeneous Boltzmann equation. The discretization of the transport step has to be done carefully because it induces physical oscillations in the velocity space. Then, we construct a fractional step deterministic scheme for the time dependent Boltzmann equation, which is based on five main ingredients

Fractional step in time allows to treat separately the transport and the collision.

Fourier-Spectral method for the evolution of the collision step allows a very accurate discretization in velocity domain, at a reasonable computational cost.

Positive and Flux Conservative (PFC) finite volume method for the free transport provides a third order (in space) accurate scheme for the evolution of distribution function during the transport step. The scheme is conservative, and preserves positivity. It is much less dissipative than Essentially Non Oscillatory (ENO) and Weighted Essentially Non Oscillatory (WENO) schemes usually used for hyperbolic systems of conservation laws.

Positive time discretization A suitable time discretization of the collisional equation is used, which allows a large stability time step, even for problems with considerably small Knudsen number. The time discretization method for the collision step is based on a modified Time Relaxed scheme.

Multiple resolution A different resolution will be used in velocity space in the transport and in the collision step. Considering that the collision step is more expensive, and more accurate (spectral accuracy) than the transport step, it is convenient to use more points in velocity space during the transport step.

6.7. Maxwell’s equation in singular geometry

Participant: Simon Labrunie.

We have been working with P. Ciarlet Jr. (ENSTA) and J. Zou (Chinese University of Hong-Kong) on the extension of the Singular Complement Method (SCM) to axisymmetric domains and non-axisymmetric data. This method is based on the coupling of finite elements, complemented with singularities, in a meridian half-plane, and a spectral method in the azimuthal direction (the principle in given in [51]). Numerical experimentations are being conducted by B. Jung at ENSTA. This is the first implementation of the SCM in a genuinely three-dimensional case. Later on, approximate symmetries (i.e. domains that are nearly axisymmetric if one neglects small peripheral parts) could be treated by using domain decomposition techniques in addition to this method.

6.8. Transport equations

Participants: Jean Roche, Didier Schmitt.

This work consists in the theoretical and numerical analysis of transport equations in collaboration with G. Jeandel and F. Asllanaj (LEMTA).

Our main application is the propagation of heat by radiation and conduction in so-called semi-transparent media like those used for the isolation of houses or satellites. This project that started during the thesis of F. Asllanaj has yielded many theoretical results: existence and uniqueness of the solution of the considered model as well as a priori estimates of the behavior of the solution (the luminance). This results can be considered new even from a physics point of view [2].

From a numerical point of view several algorithms have been conceived and implemented. Moreover their features (convergence, accuracy) have been analyzed [1]. The resulting code has been the object of a contract with EADS.
6.9. Domain decomposition for the resolution of non linear equations

Participant: Jean Roche.

In collaboration with Nour Eddine Alaa, professor in Marrakech, we work on the numerical and theoretical analysis of the following nonlinear equation:

\[
\begin{aligned}
- u''(t) + G(t, u'(t)) &= F(t, u(t)) + f 	ext{ in } (0, 1) \\
 u(0) &= u(1) = 0
\end{aligned}
\]

with \( G, F : [0, 1] \times \mathbb{R} \rightarrow [0, +\infty] \) measurable and continuous with respect to \( u' \) and \( u, f \) being a nonnegative measure. Such problems come from reaction-diffusion problems in physics, biology and chemistry.

We have considered the cases when \( f \) is nonsmooth and the behavior of \( G \) with respect to \( u' \) and of \( F \) with respect to \( u \) are arbitrary.

We have established the existence of a solution in \( W^{1, \infty}_{loc}(0, 1) \) and developed a numerical domain decomposition method coupled with Newton’s method for the computation of an approximate solution [23].

6.10. Parallelization of numerical methods

Participants: Francis Filbet, Eric Violard.

We first focussed on the study of a code named VADOR and its adaptation to an heterogeneous architecture like the computational grid.

VADOR is a C++/MPI parallel code which implements a Positive Flux Conservative (PFC) scheme to solve the Vlasov equation. PFC is representative for methods using a regular mesh of the phase space.

The parallelization of this code is based on a well-known parallelization technique called regular domain decomposition. However, the numerical method induces drastic constraints on the data distribution scheme. We have to overcome this problem in order to adapt the code to an heterogeneous architecture.

We defined a code transformation based on the emulated process notion. This transformation respects distribution constraints and enables load balancing at runtime [39]. We investigated its use to take into account the heterogeneity of processor speeds.

We applied this transformation to the VADOR code and obtained a new version which is better tuned for the grid. Performances of this new code were measured on a test grid made of an aggregate of various processors. Experiments validated and confirmed the advantages of our transformation [58].

We are now interested in the parallelization of the OBIRAN code which implements an adaptive numerical method. Our first goal is to tune it to an homogeneous parallel machine. Then we plan to target an heterogeneous architecture.

We currently develop a mechanism which balance workload during execution: some code transformations will then incrementally be applied to adapt this mechanism to its utilization in the numerical method.

6.11. Visualization of tokamaks

Participants: Gilles Dépret, Bruno Lévy.

This work is based on a volume visualization software “Fusion”. It is a research platform for 3D modeling and texturing which is developed by the ISA research project at the INRIA Lorraine. It contains tools for interactive constrained texturing of polygonal models, multi-resolution analysis and decimation of triangulated surfaces, volume rendering and iso-surfaces extraction for polyhedral grids. Fusion is written in portable C++, and available on many different platforms (linux, unix, windows) with a user-friendly and intuitive interface.

The volume rendering functionalities of Fusion allow a suitable representation for the results of numerical simulation of turbulent plasma phenomena as shown in Figure 1 (distribution function for all energy levels at one time step in phase space) and in Figure 2 (volume rendering of electrostastical potential with a slice in phase space).
Figure 1. Distribution function for all energy levels at one time step in phase space.

Figure 2. Volume rendering of electrostatic potential with a slice in phase space.
6.12. Scalable volume Visualization

**Participants:** Stéphane Marchesin, Jean-Michel Dischler.

The 2D real time optimally adapting meshes (ROAM) algorithm has proved to be very useful for real-time visualization of large scale terrains, because of its good error-controlling properties. In this work, we have proposed a generalization of this algorithm in 3D suitable for scalable volume visualization. Our algorithm, builds a volumetric mesh from a voxel object, replacing the triangle of 2D ROAM with its 3D equivalent, the tetrahedron. We then compute a bounded error inside the tetrahedron to build a hierarchical tetrahedral mesh and refine this mesh in real time to adapt it to the viewing conditions. With this algorithm, we further achieve cell sorting in linear time, thus obtaining real-time view-dependent display of the volumetric object.

Because of continuous improvements in simulation techniques, the amount of 3D data that visualization systems have to handle is increasing rapidly. These large datasets often cannot be visualized without previous compression by classical visualization methods using only video card hardware, because they are often many times larger than what a video card’s memory can hold. Visualizing such datasets “as-is” is not possible either, again because of their size. There is therefore a need for highly accurate volume visualization methods that are able to handle very large data sets. The method that we propose provides a new real time volume visualization technique using a level-of-detail-based approach. This method is scalable, and allows large dataset visualization. We applied the method to the visualization of 4D plasma data by projecting it into a 3D space.

6.13. Hardware accelerated volume visualization using precomputed visibility

**Participant:** Jean-Michel Dischler.

Visibility computations generally represent a very time consuming part of illumination algorithms. The cost is amplified by the fact that quite often identical or similar information is recomputed multiple times. We describe a general method of precomputing, storing and reusing visibility information for light transport in a number of different types of scenes. In particular we consider participating media useful for high quality volume visualization.

In collaboration with the graphics group of the Max Planck Institut of Saarbruecken, we have proposed a method for accelerating the rendering of volumetric scalar fields (clouds for instance) by reordering the light transport in such a way that the visibility information is accessed in structured memory access patterns. This yields a method that is well suited for SIMD-style parallelization of the light transport. We obtained a near interactive volume lighting including shadows and inter-reflections published in [6].

6.14. 5D volume fields visualization

**Participants:** Olivier Géneveaux, Jean-Michel Dischler.

Interactively visualizing the surface of liquids simulated by the Navier-Stokes equations as developed in [19] requires a hybrid surface and volume visualization technique to take into account both the surface aspect and the semi-transparent nature of the fluid. We propose a hybrid rendering technique for visualization this light-dependent (e.g. five-dimensional) information. Compression of the high-dimensional data is performed using a Fourier transformation, keeping only the lowest frequencies. Decompression is performed directly by the graphics card thus yielding interactive rates. We intend to apply this decompression technique to the 2D plasma visualization in phase space (e.g. 4D data fields).

7. Contracts and Grants with Industry

7.1. CEA Bruyères-Le-Châtel, PIC code

**Participants:** Pierre Navaro, Eric Sonnendrücker.
The object of the contract is the development of an efficient parallel Particle-In-Cell (PIC) solver for the numerical resolution of the two configuration space - three momentum space dimensions Vlasov-Maxwell equations in cartesian and axisymmetric geometries. This code is written in a modular way using the fortran 90 language, so that it will be easy to add more physics.

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

Participants: Francis Filbet, Eric Sonnendrücker.

The object of this contract is the development of efficient Vlasov-Poisson solvers based on a phase space grid for the study of intense particle beams. Due to the important motion of the beam in phase-space during the evolution in the focusing lattice, it is very inefficient to use uniform grids. Hence the effort is put on adaptive techniques.

8. Other Grants and Activities

8.1. National projects

- French Ministry of Research grant for young researchers (ACI "Jeunes Chercheurs") obtained by Eric Sonnendrücker to develop a research team on the topic "numerical simulation of charged particles" (2000-2003). The objectives of the proposal were to develop and analyze simulation tools for the numerical simulation of charge particles.

8.2. European initiatives

8.2.1. RTN HYKE: HYperbolic and Kinetic Equations

The HYKE network is a Research Training Network (RTN) financed by the European Union in the 5th Framework Programme "Improving the Human Potential" (IHP). It puts together the major European teams involved in the mathematics of conservation laws and kinetic theory. See the HYKE web page for more details http://www.hyke.org.

8.2.2. DFG/CNRS project "Noise Generation in Turbulent Flows"

This project involves several French and German teams as well in the applied mathematics as in the fluid dynamics community. Its aim 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. More details can be found on the web page http://www.iag.uni-stuttgart.de/DFG-CNRS/index_fr.htm

9. Dissemination

9.1. Leadership within scientific community

9.1.1. Conferences, meetings and tutorial organization

- Michaël Gutnic and Eric Sonnendrücker organized CEMRACS 2003 with Stéphane Cordier (Orléans) and Thierry Goudon (Lille).

CEMRACS is a six week summer research center that takes place every summer at CIRM in Luminy. CEMRACS 2003 was devoted to "Numerical methods for hyperbolic and kinetic problems". The mornings of the first week lectures were given by Albert Cohen (Paris 6), Frédéric Coquel (Paris 6) and Pierre Degond (Toulouse). The rest of the time was spent working on modeling and simulation projects submitted by industrial and academic partners.

- Michaël Gutnic, Stéphanie Salmon and Eric Sonnendrücker are the organizers of CANUM 2004, the major French conference on numerical analysis that will take place in Obernai, near Strasbourg, from May 31 to June 4, 2004.

9.1.2. Administrative duties

- Jean-Michel Dischler is the head of the Computer Science department of the University Louis Pasteur in Strasbourg.
- J.M. Dischler is vice-president of the Eurographics french chapter association and member of the professional board of Eurographics.
- 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 resources and a workbench for immersed visualization available to the researchers of the university.
- Eric Sonnendrücker has been nominated member of the National Committee of Universities (26th section: applied mathematics).

9.2. Teaching

- Jean-Michel Dischler is teaching a graduate course (DEA) entitled “Rendering and visualization” in DEA of Computer Science at the University Louis Pasteur of Strasbourg.
- Jean Rodolphe Roche is teaching a DESS course entitled "Parallel Architecture and Domain Decomposition Method" in DESS IMOI of the University Henri Poincare-Nancy I.
- Eric Sonnendrücker is teaching an optional graduate course (DEA) entitled “Adaptive numerical methods for scalar conservation laws” in DEA of Mathematics at the University Louis Pasteur of Strasbourg.
- Eric Violard is teaching an optional graduate course of DEA entitled “Transformations and adaptations of parallel programs” in DEA of Computer Science at the University Louis Pasteur of Strasbourg.

9.3. Ph. D. Theses

9.3.1. Ph. D. earned in 2003


9.3.2. Ph. D. in progress

9.3.3. Talks and posters given at conferences and seminars

10. Bibliography

Articles in referred journals and book chapters


Publications in Conferences and Workshops


Internal Reports


Miscellaneous


Bibliography in notes


