

Project-Team calvi

Calcul Scientifique et Visualisation

Lorraine

THEME NUM

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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 Louis Pasteur, Strasbourg) and Laboratoire des Sciences de l'Image, de l'Informatique et de la Télédétection (LSIIT, UMR 7005, CNRS and Université Louis Pasteur, Strasbourg) with close collaboration to Laboratoire de Physique des Milieux Ionisés et Applications (LPMIA, UMR 7040, CNRS and Université Henri Poincaré, Nancy).

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

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

- Simon Labrunie has been seconded as a CR INRIA from october 1, 2003 to september 30, 2005.
- Guillaume Latu who is a Maître de Conférences in computer science, specialized in parallel computing, at the Université Louis Pasteur joined the project in May 2004.
- Saïd Benachour left the project.

3. Scientific Foundations

3.1. Kinetic models for plasma and beam physics

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

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

3.1.1. Models for plasma and beam physics

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

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

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

what can be obtained from a fluid description, as it also includes information about the velocity distribution of the particles.

A kinetic description is necessary in collective plasmas where the distribution function is very different from the Maxwell-Boltzmann (or Maxwellian) distribution which corresponds to the thermodynamical equilibrium, 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*

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

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

$$\begin{aligned} -\frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} + \nabla \times \mathbf{B} &= \mu_0 \mathbf{J}, \\ \frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} &= 0, \\ \nabla \cdot \mathbf{E} &= \frac{\rho}{\epsilon_0}, \\ \nabla \cdot \mathbf{B} &= 0, \end{aligned}$$

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

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

and current density

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

associated to the charged particles.

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

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

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

The numerical resolution of the three-dimensional Vlasov-Maxwell system represents a considerable challenge due to the huge size of the problem. Indeed, the Vlasov-Maxwell system is 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 essential the 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 [50], see also Bardos and Degond [32]. The existence of weak solution for the Vlasov-Maxwell system has been proved by Di Perna and Lions [39]. The state of the theory is presented in a recent book by Glassey [47].

Many questions concerning for example uniqueness or existence of strong solutions for the three-dimensional 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 [33].

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 [48][54] 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 [45][43][44].

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

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

The development of efficient numerical methods is essential for the simulation of plasmas and beams. Indeed, kinetic models are posed in phase space and thus the number of dimensions is doubled. Our main effort lies in developing methods using a phase-space grid as opposed to particle methods. In order to make such methods efficient, it is essential to consider means for optimizing the number of mesh points. This is done through different adaptive strategies. In order to understand the methods, it is also important to perform their mathematical analysis.

3.2.1. Introduction

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

3.2.2. Convergence analysis of numerical schemes

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

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

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

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

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

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

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

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

3.2.4. Adaptive semi-Lagrangian methods

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

3.2.5. Particle-In-Cell codes

The Particle-In-Cell method [36] 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 in a function space such that the curl and the divergence are square integrable and that satisfy the electric and magnetic boundary conditions. Those solutions are in fact smoother (all the derivatives are square integrable) when the boundary of the domain is smooth or convex. This is no longer true when the domain exhibits non-convex *geometrical singularities* (corners, vertices or edges).

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

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

This *Singular Complement Method* (SCM) had been developed [30] and implemented [31] 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 [34]. The non-density result for regular fields was proven [38], the singularities of the electromagnetic field were related to that of modified Laplacians [27], and expressions of the singular fields were calculated [28]. 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 [29].

3.2.6.2. Other results, extensions.

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 [46][28].

3.3. Large size problems

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

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. Parallelization of numerical methods

An important issue for the practical use of the method 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 [49] 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 [56], 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 [42]).

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

3.4. Scientific visualization of plasmas and beams

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

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

4. Application Domains

4.1. Thermonuclear fusion

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

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 ITER¹ 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.

Our work in modelling 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 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. [41], 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

¹<http://www.iter.gov.fr>

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, positive.*

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 [41], 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 [40]. It has been applied as well for plasma as for beam simulations.

The code is available at the following address:

http://www.univ-orleans.fr/SCIENCES/MAPMO/membres/filbet/index_vad.html

5.2. Obiwan

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

Participants: Michaël Gutnic [correspondant], Matthieu Haefelé, Guillaume Latu, 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 an axisymmetric 1Dr-1Dv version using one fixed value of the canonical angular momentum. The grid adaptivity is based on a multiresolution method using Lagrange interpolation as a predictor to go from one coarse level to the immediately finer one. This idea amounts to using the so-called interpolating wavelets.

5.3. Yoda

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

Participants: Olivier Hoenen [correspondant], Michel Mehrenberger, Isabelle Metzmeier, 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 and Isabelle Metzmeier. It solves the Vlasov equation on a dyadic mesh of phase-space. The underlying method is based on hierarchical finite elements. Its originality is that the values required for interpolation at the next time step are determined in advance. In terms of efficiency, the method is less adaptive than some other adaptive methods (multi-resolution methods based on interpolating wavelets as examples), but data locality is improved. The implementation is generic n dimensional ($2n$ -dimensions in phase-space).

5.4. M2V

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

Participants: Pierre Navaro [correspondant], Eric Sonnendrücker.

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. Reduced modelling of plasmas

Participants: Simon Labrunie, Pierre Bertrand.

In collaboration with J.A. Carrillo (Universitat Autònoma de Barcelona) we have studied mathematically a reduced kinetic model for laser-plasma interaction. Global existence and uniqueness of solutions and the stability of certain equilibria were obtained [22].

Despite its one-dimensional character, this system is strongly non-linear and already embeds some features of higher-dimensional, relativistic Vlasov-Maxwell systems. Thus it had been subject to many physical [35] and computational investigations by fluid [52] and kinetic semi-Lagrangian [51] methods. The study of its qualitative properties by numerical simulation is currently under way (see §6.4) and might open the way for the definition of more complex, but still tractable models.

6.2. Convergence of semi-Lagrangian methods

Participants: Nicolas Besse, Michel Mehrenberger.

The convergence of several semi-Lagrangian numerical schemes for the one-dimensional Vlasov-Poisson equations has been proved and error estimates given in the case of several interpolation schemes: linear interpolating polynomials on an unstructured mesh of phase-space, [4]; high order schemes using symmetric Lagrange interpolation, B-Spline interpolation or wavelet interpolation, [21]; Hermite interpolation with the propagation of gradients of f on a uniform grid of phase-space [19].

6.3. Convergence of discontinuous Galerkin methods for the MHD system

Participant: Nicolas Besse.

We developed and proved, in collaboration with D. Kröner (Freiburg, Germany), the convergence of a locally divergence free discontinuous Galerkin finite element method for the induction equations of the MHD system [20]

6.4. WENO simulations of plasmas

Participants: Simon Labrunie, Vladimir Latocha.

We are presently working on the definition and parallelization of a WENO code for the simulation of laser-plasma interactions. It is based on the 1D code already used in [8] and uses the model of §6.1. Of course, the study of more realistic situations: complex, multi-dimensional geometries... is still the objective in the long run.

6.5. Moment conservation in the adaptive method based on interpolating wavelets

Participants: Michaël Gutnic, Matthieu Haefelé, Eric Sonnendrücker.

The first version of our adaptive method did not exactly conserve mass, when grid points were removed. Even though we can always get sufficient conservation by lowering the threshold for removing grid points, this is not efficient for some problems. Therefore, we developed a procedure enabling to conserve any desired

number of moments. The idea is based on the lifting procedure introduced by Sweldens [55] which consists in modifying the wavelet using a linear combination of the old wavelet and the translates of the scaling function at the coarser level. The coefficients involved in this linear combination are easy to compute and this procedure has been implemented in Obiwan. Mass conservation (order 0 moment) gives already satisfactory results since the lack of numerical stability in some numerical simulations is now avoided.

6.6. Moment conservation in the adaptive method based on hierarchical finite elements

Participants: Olivier Hoenen, Michel Mehrenberger, Isabelle Metzmeier, Eric Violard.

We currently investigate techniques for mass conservation in the hierarchical finite element method. The basic idea here is associating an average mass with each cell of the dyadic mesh. During time evolution, mass conservation is achieved by redistributing the mass amongst cells. The mass of each cell of the predicted mesh is determined from the mass contribution of the backward advected cells of the initial mesh.

6.7. Optimization of Obiwan

Participants: Michaël Gutnic, Matthieu Haefelé, Guillaume Latu.

A first sequential simulator was developed using a numerical scheme based on wavelets. From one time step to the other, two advections in variables x and v are performed on a given space containing N points. Only a percentage p of all the points (x, v) are effectively advected in the considered space, as the adaptive wavelet method allows us to reconstruct the remaining points if necessary. For small values of p , one can expect to reduce the total computing cost because the advection concerns only pN points instead of N . Nevertheless, the use of this method has an overhead since we have to deal with the wavelet coefficients after each advection. In order to obtain an efficient application, we considered the complexity of the advection algorithm, and of the overhead. We performed a reduction of the overhead in several ways. We first reduced the complexity in memory consumption and improved the use of cache memory. We replaced the data structure used to keep the wavelet coefficient (a hashtable) with a sparse data structure that has better properties in term of access time (for reading and writing). Furthermore, we evaluated a possible parallelization of the application. The dependencies between data and computation are currently under evaluation. Because of access of coefficients at different levels, necessary with the wavelet method, data locality is not very good. Therefore, we will probably consider a parallel version of the application that will use a shared memory machine. Thus, the wavelet coefficients will be easily accessible from each processor.

6.8. Parallelization of Yoda

Participants: Olivier Hoenen, Michel Mehrenberger, Eric Violard.

We investigated the parallel implementation of an adaptive method based on hierarchical finite elements. The underlying numerical method uses a dyadic mesh which is particularly well suited to manage data locality. We have developed an adapted data distribution pattern based on a division of the computational domain into *regions* and integrated a load balancing mechanism which periodically redefines regions to follow the evolution of the physics. In order to reduce communications, the regions which are built should be connex. We use the Hilbert's space filling curve to achieve this goal. Experimental results show the good efficiency of our code and confirm the adequacy of our implementation choices.

We are also looking at simplifications of the "forward-backward" scheme: We investigate a new numerical method with a simpler time evolution scheme: in this new scheme, the compressed mesh at next time step is predicted directly. Only backward advections are performed. Forward advections and compression phase are eliminated from the old scheme. The notion of regions may advantageously be reused for defining a suitable load balancing mechanism. Another issue addresses targeting of heterogeneous parallel architectures.

We are also extending the Yoda code to 4D phase-space. In order to validate the simulations we shall compare them with simulations performed with Vador which uses a uniform dense mesh and is based on

a conservative method. We want to characterize the advantages of a given method relatively to the others. Our experiments show that this could depend on the test case and the required level of accuracy. Better implementations could be obtained by integrating several methods together.

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

Participants: Alain Ghizzo, Pierre Bertrand, Thierry Réveillé.

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

For these reasons, we have investigated Vlasov-Maxwell numerical experiments for realistic plasmas in collaboration of the group of Dr B. Afeyan of Polymath research Inc. (in an international collaboration program of the Department of Energy of USA). Our studies so far indicate that a promising way to deter these undesirable processes is by instigating the externally controlled creation of large amplitude plasma fluctuations making the plasma an inhospitable host for the growth of coherent wave-wave interactions. The area where we plan to focus most of our attention is in Vlasov-Maxwell (semi-lagrangian) simulations in 1D. In several works, see for example [15], the nonlinear evolution of the electron plasma waves which have been generated by optical mixing (pump plus probe beams) is investigated to understand the kinetic effects that saturate the growth of these modes. Both the electron plasma wave and ion acoustic wave generation and SRS interaction problems are treated in great detail. Fluid and kinetic degrees of freedom to saturate SRS and to limit the growth of the optical mixing generated waves will be elucidated by Vlasov simulations.

6.10. Resolution of the Vlasov equation on a moving grid of phase-space

Participants: Stéphanie Salmon, Eric Sonnendrücker.

This work is performed in collaboration with Edouard Oudet (University of Chambéry).

We extended the idea of solving the Vlasov equation on moving grids of phase space. In our first work [12], we developed a moving grid technique that follows the envelope motion of a beam. This method is a semi-Lagrangian method using a uniform logical grid which is mapped at each time step to a physical grid adapted to the evolution of the particles. The mapping is for example a rotation and a dilatation to follow the envelope motion. Different kinds of mappings can be used in different situations. As in general, the particle motion in a beam is a small non linear perturbation of a linear motion. A mapping associated to the linear motion can be

used. This has the advantage that the particles always stay close to the grid points, which reduces diffusion in the semi-Lagrangian method.

6.11. Coupling particles with a Maxwell solver in PIC codes

Participants: Régine Barthelmé, Eric Sonnendrücker.

When using the classical charge and current deposition algorithms in PIC codes, the continuity equation $\partial_t \rho + \nabla \cdot J = 0$ is not satisfied at the discrete level. Therefore when using only Ampere and Faraday's laws to compute the electromagnetic field, Gauss's law $\nabla \cdot E = \rho$ is violated over long time computations yielding unphysical results. Specific current deposition techniques need to be introduced. The most widely used is that of Villasenor and Buneman which works for linear deposition algorithms. We extended this method to higher order deposition schemes and to non uniform meshes.

6.12. High order finite element method for the wave equation

Participants: Sébastien Jund, Stéphanie Salmon, Eric Sonnendrücker.

In the frame of the DFG/CNRS project "Noise Generation in Turbulent Flows", we need to develop very precise solvers for the acoustics wave equation on unstructured grids. This solver will then be coupled to an Euler solver to compute the noise generation. In collaboration with our partners from the University of Stuttgart in Germany we want to compare the efficiency of high order solvers based on continuous finite elements to high order solvers based on the discontinuous Galerkin method. In order for the finite element solvers to be efficient, we developed a new strategy to lump the mass matrix which can be applied at any order. It has already been implemented for \mathbb{P}_k elements with $k \leq 6$.

6.13. Maxwell's equation in singular geometry

Participant: Simon Labrunie.

We have been carrying on the joint work with P. Ciarlet's team at ENSTA and J. Zou (Chinese University of Hong-Kong). Our *Singular Complement Method* (SCM) has been applied to simple, but genuinely three-dimensional situations, namely prismatic and axisymmetric domains with arbitrary data. Complete convergence proofs and error estimates have been obtained, and numerical tests have been performed in the electrostatic case [23][24]. Feasibility in the general case has been investigated [26]. Later on, approximate symmetries (i.e. domains that are nearly axisymmetric if one neglects small peripheral parts) could be treated by using perturbative expansion techniques in addition to this method.

6.14. 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. (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.

From a numerical point of view several algorithms have been conceived and implemented. Moreover their features (convergence, accuracy) have been analyzed [2]. The resulting code has been the object of a contract with EADS.

We are now developing a two dimensional version using domain decomposition methods. We are also interested in the coupled problem between radiation and Navier Stokes equation.

6.15. Domain decomposition for the resolution of non linear equations

Participant: Jean Roche.

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

The principal objective of this work is to study existence, uniqueness and present a numerical analysis of weak solutions for a quasi-linear elliptic problem that arises in biological, chemical and physical systems. Various methods have been proposed for study the existence, uniqueness, qualitative properties and numerical simulation of solutions. We were particularly interested in situations involving irregular and arbitrarily growing data ([14]).

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

The general algorithm for numerical solution of this equations is one application of the Newton method to the discretized version of the problem. However, in our case the matrix which appears in the Newton algorithm is singular. To overcome this difficulty we introduced a domain decomposition to compute an approximation of the iterates by the resolution of a sequence of problems of the same type as the original problem in subsets of the given computational domain. This domain decomposition method coupled with a Yosida approximation of the non linearity allows us to compute a numerical solution, see ([14] and [18]).

6.16. Interactive 4D+t visualization of a plasma

Participants: Christophe Mion, Florence Zara, Jean-Michel Dischler.

We developed a new interactive visualization technique for exploring plasma behaviors resulting from 4D+t numerical simulations on regular grids. It implements a new out-of-core 4D+t visualization technique, based on a "focus and context" approach using a hybrid data compression method. The originality of this work consists in coupling the 3D visualization with the progressive load and decompression of data in such a way that it still guaranties real-time frame rates even on low-end PCs while maintaining a high degree of numerical precision.

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: Matthieu Haefele, 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. This contract focused on the development of new confinement fields and new particle distributions for the VADOR solver. We also continued our development of new visualization techniques.

7.3. European initiatives

7.3.1. 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>.

7.3.2. 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 is the development of numerical methods for the computation of noise generated in turbulent flows and to understand the mechanisms of this noise generation.

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

8. Dissemination

8.1. Leadership within scientific community

8.1.1. Conferences, meetings and tutorial organization

- Michaël Gutnic, Stéphanie Salmon and Eric Sonnendrücker organized CANUM 2004, the major french conference on numerical analysis. It took place in Obernai, near Strasbourg, from May 31 to June 4, 2004.
- Simon Labrunie and Vladimir Latocha organized with Jan Sokolowski the "Quatrièmes Journées singulières", 7 – 9 June 2004, Pont-à-Mousson, Lorraine, France <http://www.iecn.u-nancy.fr/~js4/>

8.1.2. Administrative duties

- Jean-Michel Dischler is the head of the Computer Science department of the University Louis Pasteur in Strasbourg.
- Jean-Michel Dischler is vice-president of the Eurographics french chapter association and member of the professional board of Eurographics.
- 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 is a member of the National Committee of Universities (26th section: applied mathematics).

8.2. Teaching

- *Jean-Michel Dischler* taught a graduate course (DEA) entitled "Rendering and visualization" in DEA of Computer Science at the University Louis Pasteur of Strasbourg.
- *Jean Rodolphe Roche* taught a DESS course entitled "Parallel Architecture and Domain Decomposition Method" in DESS IMOI of the University Henri Poincare-Nancy I.
- *Eric Sonnendrücker* taught 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* taught 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.

8.3. Ph. D. Theses

8.3.1. Ph. D. earned in 2004

1. Michel Mehrenberger, *Observability inequalities and adaptive resolution of the Vlasov equation using hierarchical finite elements*. Université Louis Pasteur, Strasbourg, 15 December 2004. Jury: A. Cohen (referee), A. Haraux (referee), Bopeng Rao (internal referee), P. Loretto, V. Komornik (advisor), Eric Sonnendrücker (advisor).

8.3.2. Ph. D. in progress

1. Régine Barthelmé, *Analysis of charge conservation problems in Particle-In-Cell codes and development of new methods*. Advisor: Eric Sonnendrücker.
2. Olivier Géneveaux, *Realistic visualization of fluid - solid body interactions*. Advisor: Jean-Michel Dischler.
3. Matthieu Haefele, *High performance visualization of particle beams*. Advisors: Jean-Michel Dischler and Eric Sonnendrücker.
4. Sébastien Jund, *Mathematical and numerical analysis of weakly compressible flows*. Advisors: Stéphanie Salmon and Eric Sonnendrücker.
5. Isabelle Metzmeier, *Conservative adaptive methods for the Vlasov equation*. Advisor: Eric Sonnendrücker.
6. Olivier Hoenen, *Parallelization of adaptive methods for the Vlasov equation*. Advisor: Eric Violard.

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