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Project-Team CALVI

Scientific computation and visualization

IN COLLABORATION WITH: Institut Elie Cartan Nancy (IECN), Institut de recherche mathématique avancée (IRMA)

RESEARCH CENTER
Nancy - Grand Est

THEME
Computational models and simulation

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Project-Team CALVI

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Eric Sonnendrücker, head of the CALVI project has obtained a position at the Max Planck Institute in Garching near Munich. He is temporarily replaced by Philippe Helluy, professor at IRMA. The team will propose a new project-team in 2013, called TONUS, for “TOKamak NUmerical Simulations”

Creation of the Project-Team: June 01, 2003 .

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2. Overall Objectives

2.1. Introduction

CALVI was created in July 2003.

It is a project associating Institut Elie Cartan (IECN, UMR 7502, CNRS, Inria and Université Henri Poincaré, Nancy), Institut de Recherche Mathématique Avancée (IRMA, UMR 7501, CNRS and Université de Strasbourg) and Laboratoire des Sciences de l'Image, de l'Informatique et de la Télédétection (LSIIT, UMR 7005, CNRS and Université de 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 modelling, numerical simulation and visualization of phenomena coming from plasma physics and beam physics. Our applications are characterized in particular by their large size, the existence of multiple time and space scales, and their complexity.

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

2.2. Highlights of the Year

January 2012 : Anaïs Crestetto and Philippe Helluy have been awarded the fourth prize of the international "OpenCL Innovation Challenge" organized by the AMD company. They have simulated the electron beam inside an X ray generator on GPU. See <http://developer.amd.com/community/events/amd-opencl-coding-competition-2/>

September 2012 : Eric Sonnendrücker has obtained a position at the Max Planck Institute in Garching.

October 2012 : Michel Mehrenberger has defended his 'Habilitation à diriger des recherches'.

3. Scientific Foundations

3.1. Kinetic models for plasma and beam physics

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 $f_s(\mathbf{x}, \mathbf{v}, t)$ corresponding to the statistical average of the particle distribution in phase-space corresponding to many realisations of the physical system under investigation. The product $f_s d\mathbf{x} d\mathbf{v}$ is the average number of particles of the considered species, the position and velocity of which are located in a bin of volume $d\mathbf{x} d\mathbf{v}$ centered around (\mathbf{x}, \mathbf{v}) . The distribution function contains a lot more information than what can be obtained from a fluid description, as it also includes information about the velocity distribution of the particles.

A kinetic description is necessary in collective plasmas where the distribution function is very different from the Maxwell-Boltzmann (or Maxwellian) distribution which corresponds to the thermodynamical equilibrium, otherwise a fluid description is generally sufficient. In the limit when collective effects are dominant with respect to binary collisions, the corresponding kinetic equation is the *Vlasov equation*

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

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

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

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

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

and current density

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

associated to the charged particles.

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

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

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

The numerical solution of the three-dimensional Vlasov-Maxwell system represents a considerable challenge due to the huge size of the problem. Indeed, the Vlasov-Maxwell system is nonlinear and posed in phase space. It thus depends on seven variables: three configuration space variables, three velocity space variables and time, for each species of particles. This feature makes it essential to use every possible option to find a reduced model wherever possible, in particular when there are geometrical symmetries or small terms which can be neglected.

3.1.2. *Mathematical and asymptotic analysis of kinetic models*

The mathematical analysis of the Vlasov equation is essential for a thorough understanding of the model as well for physical as for numerical purposes. It has attracted many researchers since the end of the 1970s. Among the most important results which have been obtained, we can cite the existence of strong and weak solutions of the Vlasov-Poisson system by Horst and Hunze [74], see also Bardos and Degond [51]. The existence of a weak solution for the Vlasov-Maxwell system has been proved by Di Perna and Lions [59]. An overview of the theory is presented in a book by Glassey [71].

Many questions concerning for example uniqueness or existence of strong solutions for the three-dimensional Vlasov-Maxwell system are still open. Moreover, 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 [52].

On the other hand, the asymptotic study of the Vlasov equation in different physical situations is important in order to find or justify reduced models. One situation of major importance in tokamaks, used for magnetic fusion as well as in atmospheric plasmas, is the case of a large external magnetic field used for confining the particles. The magnetic field tends to incurve the particle trajectories which eventually, when the magnetic field is large, are confined along the magnetic field lines. Moreover, when an electric field is present, the particles drift in a direction perpendicular to the magnetic and to the electric field. The new time scale linked to the cyclotron frequency, which is the frequency of rotation around the magnetic field lines, comes in addition to the other time scales present in the system like the plasma frequencies of the different particle species. Thus, many different time scales as well as length scales linked in particular to the different Debye length are present in the system. Depending on the effects that need to be studied, asymptotic techniques allow to find reduced models. In this spirit, in the case of large magnetic fields, recent results have been obtained by Golse and Saint-Raymond [72], [80] as well as by Brenier [57]. 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 [67], [65], [66].

Another important asymptotic problem yielding reduced models for the Vlasov-Maxwell system is the fluid limit of collisionless plasmas. In some specific physical situations, the infinite system of velocity moments of the Vlasov equations can be closed after a few of those, thus yielding fluid models.

3.2. Development of simulation tools

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. Since a few years we are interested also with solvers that uses Particle In Cell method. This new issue allows us to enrich some parts of our research activities previously centered on the Semi-Lagrangian approach.

3.2.1. Introduction

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

3.2.2. Convergence analysis of numerical schemes

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

3.2.3. The semi-Lagrangian method

The semi-Lagrangian method consists in computing a numerical approximation of the solution of the Vlasov equation on a phase space grid by using the property of the equation that the distribution function f is conserved along characteristics. More precisely, for any times s and t , we have

$$f(\mathbf{x}, \mathbf{v}, t) = f(\mathbf{X}(s; \mathbf{x}, \mathbf{v}, t), \mathbf{V}(s; \mathbf{x}, \mathbf{v}, t), s),$$

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

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

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

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

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

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

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

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

3.2.4. Adaptive semi-Lagrangian methods

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

3.2.5. Particle-In-Cell codes

The Particle-In-Cell method [56] consists in solving the Vlasov equation using a particle method, i.e. advancing numerically the particle trajectories which are the characteristics of the Vlasov equation, using the equations of motion which are the ordinary differential equations defining the characteristics. The self-fields are computed using a standard method on a structured or unstructured grid of physical space. The coupling between the field solve and the particle advance is done on the one hand by depositing the particle data on the grid to get the charge and current densities for Maxwell's equations and, on the other hand, by interpolating the fields at the particle positions. This coupling is one of the difficult issues and needs to be handled carefully.

3.2.6. Maxwell's equations in singular geometry

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

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

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

This *Singular Complement Method* (SCM) had been developed [49] and implemented [48] 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 [54]. The non-density result for regular fields was proven [58], the singularities of the electromagnetic field were related to that of modified Laplacians [45], and expressions of the singular fields were calculated [46]. Thus the SCM was extended to this geometry. It was then implemented by F. Assous (now at Bar-Ilan University, Israel) and S. Labrunie in a PIC–finite element Vlasov–Maxwell code [47].

As a byproduct, space-time regularity results were obtained for the solution to time-dependent Maxwell’s equation in presence of geometrical singularities in the plane and axisymmetric cases [70], [46].

3.3. Large size problems

Parallelism, domain decomposition, code transformation

3.3.1. Introduction

The applications we consider lead to very large size computational problems for which we need to apply modern computing techniques enabling to use efficiently many computers including traditional high performance parallel computers and computational grids.

The full Vlasov-Maxwell system yields a very large computational problem mostly because the Vlasov equation is posed in six-dimensional phase-space. In order to tackle the most realistic possible physical problems, it is important to use all the modern computing power and techniques, in particular parallelism and grid computing.

3.3.2. Parallelization of numerical methods

An important issue for the practical use of the methods we develop is their parallelization. We address the problem of tuning these methods to homogeneous or heterogeneous architectures with the aim of meeting increasing computing resources requirements.

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

Parallelism, for such data-parallel PDE solvers, is achieved by partitioning the mesh and mapping the sub-meshes 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-filling curves [73] give very good results for a very low cost.

Adaptive methods include a mesh refinement step and can highly reduce memory usage and computation volume. As a result, they induce a load imbalance and require to dynamically distribute the adaptive mesh. A problem is then to combine distribution and resolution components of the adaptive methods with the aim of minimizing communications. Data locality expression is of major importance for solving such problems. We use our experience of data-parallelism and the underlying concepts for expressing data locality [81], 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 [79] as an example of such modular software infrastructure).

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

Moreover, exploiting heterogeneous architectures requires the use of a run time support associated with a programming interface that enables some low-level hardware characteristics to be unified. Such run time support is the basis for heterogeneous algorithmics. Candidates for such a run time support may be specific implementations of MPI such as MPICH-G2 (a grid-enabled MPI implementation on top of the GLOBUS tool kit for grid computing [64]).

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.

4. Application Domains

4.1. Thermonuclear fusion

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 a large external magnetic field and inertial fusion where the plasma is confined thanks to intense laser or particle beams. The simulation tools we develop can be applied for both approaches.

Controlled fusion is one of the major challenges of the 21st century that can answer the need for a long term source of energy that does not accumulate wastes and is safe. The nuclear fusion reaction is based on the fusion of atoms like Deuterium and Tritium. These can be obtained from the water of the oceans that is widely available and the reaction does not produce long-term radioactive wastes, unlike today's nuclear power plants which are based on nuclear fission.

Two major research approaches are followed towards the objective of fusion based nuclear plants: magnetic fusion and inertial fusion. In order to achieve a sustained fusion reaction, it is necessary to confine sufficiently the plasma for a long enough time. If the confinement density is higher, the confinement time can be shorter but the product needs to be greater than some threshold value.

The idea behind magnetic fusion is to use large toroidal devices called tokamaks in which the plasma can be confined thanks to large applied magnetic field. The international project ITER ¹ is based on this idea and aims to build a new tokamak which could demonstrate the feasibility of the concept.

The inertial fusion concept consists in using intense laser beams or particle beams to confine a small target containing the Deuterium and Tritium atoms. The Laser Mégajoule which is being built at CEA in Bordeaux will be used for experiments using this approach.

Nonlinear wave-wave interactions are primary mechanisms by which nonlinear fields evolve in time. Understanding the detailed interactions between nonlinear waves is an area of fundamental physics research in classical field theory, hydrodynamics and statistical physics. A large amplitude coherent wave will tend to couple to the natural modes of the medium it is in and transfer energy to the internal degrees of freedom of that system. This is particularly so in the case of high power lasers which are monochromatic, coherent sources of high intensity radiation. Just as in the other states of matter, a high laser beam in a plasma can give rise to stimulated Raman and Brillouin scattering (respectively SRS and SBS). These are three wave parametric instabilities where two small amplitude daughter waves grow exponentially at the expense of the pump wave, once phase matching conditions between the waves are satisfied and threshold power levels are exceeded. The illumination of the target must be uniform enough to allow symmetric implosion. In addition, parametric instabilities in the underdense coronal plasma must not reflect away or scatter a significant fraction of the incident light (via SRS or SBS), nor should they produce significant levels of hot electrons (via SRS), which can 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

¹<http://www.iter.org>

saturate and interdepend, all can benefit the design of new laser and target configuration which would minimize their undesirable features in inertial confinement fusion. Clearly, the physics of parametric instabilities must be well understood in order to rationally avoid their perils in the varied plasma and illumination conditions which will be employed in the National Ignition Facility or LMJ lasers. Despite the thirty-year history of the field, much remains to be investigated.

Our work in modelling and numerical simulation of plasmas and particle beams can be applied to problems like laser-matter interaction, the study of parametric instabilities (Raman, Brillouin), the fast ignitor concept in the laser fusion research as well as for the transport of particle beams in accelerators. Another application is devoted to the development of Vlasov gyrokinetic codes in the framework of the magnetic fusion programme in collaboration with the Department of Research on Controlled Fusion at CEA Cadarache. Finally, we work in collaboration with the American Heavy Ion Fusion Virtual National Laboratory, regrouping teams from laboratories in Berkeley, Livermore and Princeton on the development of simulation tools for the evolution of particle beams in accelerators.

4.2. Nanophysics

Kinetic models like the Vlasov equation can also be applied for the study of large nano-particles as approximate models when ab initio approaches are too costly.

In order to model and interpret experimental results obtained with large nano-particles, ab initio methods cannot be employed as they involve prohibitive computational times. A possible alternative resorts to the use of kinetic methods originally developed both in nuclear and plasma physics, for which the valence electrons are assimilated to an inhomogeneous electron plasma. The LPMIA (Nancy) possesses a long experience on the theoretical and computational methods currently used for the solution of kinetic equation of the Vlasov and Wigner type, particularly in the field of plasma physics.

Using a Vlasov Eulerian code, we have investigated in detail the microscopic electron dynamics in the relevant phase space. Thanks to a numerical scheme recently developed by Filbet et al. [63], the fermionic character of the electron distribution can be preserved at all times. This is a crucial feature that allowed us to obtain numerical results over long times, so that the electron thermalization in confined nano-structures could be studied.

The nano-particle was excited by imparting a small velocity shift to the electron distribution. In the small perturbation regime, we recover the results of linear theory, namely oscillations at the Mie frequency and Landau damping. For larger perturbations nonlinear effects were observed to modify the shape of the electron distribution.

For longer time, electron thermalization is observed: as the oscillations are damped, the center of mass energy is entirely converted into thermal energy (kinetic energy around the Fermi surface). Note that this thermalization process takes place even in the absence of electron-electron collisions, as only the electric mean-field is present.

5. Software

5.1. SeLaLib

Participants: Raphaël Blanchard, Edwin Chacon Golcher, Samuel De Santis, Aliou Diouf, Pierre Navaro, Morgane Bergot, Emmanuel Frénod, Philippe Helluy, Sever Hirstoaga, Michel Mehrenberger, Laurent Navoret, Eric Sonnendrücker.

Under the 'Fusion' large scale initiative, we have continued our work in the development of the ADT Selalib (the Semi-Lagrangian Library), now finishing its second year. This library provides building blocks for the development of numerical simulations for the solution of the fundamental equation of plasma physics: the Vlasov equation. In this context we have continued to add new modules improved interfaces and implemented 'continuous integration' software development techniques to improve code robustness and portability. Furthermore, we continue to involve other researchers within France and abroad to aid in the further development of this software product.

One of the aims of the ADT is to provide numerical building blocks for the GYSELA code developed at CEA Cadarache in collaboration with the Calvi project-team. GYSELA is used by physicists for simulating the development of turbulence in magnetic fusion plasmas in particular in view of the ITER project.

5.2. CLAC

Participants: Anaïs Crestetto, Philippe Helluy.

The objective of the three-dimensional parallel software CM2 (Code Multiéchelle Multiphysique) software is to implement a general solver for hyperbolic conservation laws. It is for instance able to solve the MHD model. CLAC is a C++ OpenCL/MPI based library derived from algorithms and ideas developed in CM2. CLAC means "Compute Language Approximation of Conservation laws".

It is clear now that a future supercomputer will be made of a collection of thousands of interconnected multicore processors. Globally it appears as a classical distributed memory MIMD machine. But at a lower level, each of the multicore processors is itself made of a shared memory MIMD unit (a few classical CPU cores) and a SIMD unit (a GPU). When designing new algorithms, it is important to adapt them for this architecture. Our philosophy will be to program our algorithms in such a way that they can be run efficiently on this kind of computers. Practically, we will use the MPI library for managing the high level parallelism, while the OpenCL library will efficiently operate the low level parallelism.

We have invested for several years now into scientific computing on GPU, using the open standard OpenCL (Open Computing Language). With Anaïs Crestetto, who is preparing a PhD in the CALVI project, we were recently awarded a prize in the international AMD OpenCL innovation challenge thanks. We have developed an OpenCL 2D Vlasov-Maxwell solver, coupling a PIC and a DG algorithms, which fully runs on a GPU. OpenCL is a very interesting tool because it is an open standard now available on almost all brands of multicore processors and GPU. The same parallel program can run on a GPU or a multicore processor without modification.

CLAC is written in C++, which is almost mandatory, because we use the OpenCL library. It also uses the MPI paradigm and is thus able to run on a cluster of GPU. CLAC is also inside a collaboration with a Strasbourg SME, AxesSim, which develops software for electromagnetic simulations. Thomas Strub, who is employed in AxesSim with a CIFRE position, is doing his Ph. D. on the conception and the development of CLAC applied to electromagnetic problems.

Because of the envisaged applications of CLAC, which may be either academical or commercial, it is necessary to conceive a modular framework. The heart of the library is made of generic parallel algorithms for solving conservation laws. The parallelism can be both fine grain (oriented towards GPU and multicore processors) and large grain (oriented towards GPU clusters). The separated modules allow managing the meshes and some specific applications. In this way, it is possible to isolate parts that can be protected by trade secret.

6. New Results

6.1. Mathematical analysis of kinetic models

6.1.1. Gyrokinetic and Finite Larmor radius approximations

Participants: Mihai Bostan, Céline Caldini, Emmanuel Frénod, Mathieu Lutz.

In a work in progress by E. Frénod and M. Lutz, the deduction of the Geometrical Gyro-Kinetic Approximation, which was originally obtained by Littlejohn in [75], [76], [77] using a physical approach which was mathematically formal, is done. The rigorous mathematical theory is built and explained in a form for providing it, especially, for analysts, applied mathematicians and computer scientists.

In the Note [16], we present the derivation of the finite Larmor radius approximation, when collisions are taken into account. We concentrate on the Boltzmann relaxation operator whose study reduces to the gyroaverage computation of velocity convolutions, which are detailed here. We emphasize that the resulting gyroaverage collision kernel is not local in space anymore and that the standard physical properties (i.e., mass balance, entropy inequality) hold true only globally in space and velocity. This work is a first step in this direction and it will allow us to handle more realistic collisional mechanisms, like the Fokker-Planck or Fokker-Planck-Landau kernels.

The subject matter of the paper [34] concerns the derivation of the finite Larmor radius approximation, when collisions are taken into account. Several studies are performed, corresponding to different collision kernels. The main motivation consists in computing the gyroaverage of the Fokker-Planck-Landau operator, which plays a major role in plasma physics. We show that the new collision operator enjoys the usual physical properties ; the averaged kernel balances the mass, momentum, kinetic energy and dissipates the entropy.

6.1.2. Singularities of the stationary Vlasov–Poisson system in a polygon

Participant: Simon Labrunie.

In collaboration with Fahd Karami (Université Cadi Ayyad, Morocco) and Bruno Pinçon (Université de Lorraine and project-team CORIDA), we conducted in [43] a theoretical and numerical study of the so-called “point effect” in plasma physics. The model (stationary Vlasov–Poisson system with external potential) corresponds a fully ionised plasma considered on a time scale much smaller than that of ions, but much larger than that of electrons. It appears as the relevant non-linear generalisation of the electrostatic Poisson equation. This may be a first step toward a quasi-equilibrium model valid on a larger time scale, where the equilibrium description of the electrons would be coupled to a kinetic or fluid model for the ions. This approximation is classical in plasma physics. We proved a general existence result for our model in a bounded domain $\Omega \subset \mathbb{R}^N$, which is not assumed to be smooth. When Ω is a polygonal domain of \mathbb{R}^2 , we described the singular behavior of the solution near a reentrant corner. In the important case of the Maxwell–Boltzmann distribution, we established a link between various asymptotics of the problem and the (suitably extended) theory of large solutions to nonlinear elliptic problems (for a review of this theory, see e.g. [50]). This allowed us to determine the dependence of the singularity coefficients on the parameters of the problem, such as the total mass of the distribution, or the boundary conditions of the potential. Numerical tests confirmed the theory.

6.2. Two-Scale Asymptotic-Preserving schemes

Participants: Nicolas Crouseilles, Emmanuel Frénod, Michaël Gutnic, Sever Hirstoaga.

In paper [20], we build a Two-Scale Macro-Micro decomposition of the Vlasov equation with a strong magnetic field. This consists in writing the solution of this equation as a sum of two oscillating functions with circumscribed oscillations. The first of these functions has a shape which is close to the shape of the Two-Scale limit of the solution and the second one is a correction built to offset this imposed shape. The aim of such a decomposition is to be the starting point for the construction of Two-Scale Asymptotic-Preserving schemes.

During CEMRACS 2011, we have started the project to test on a simplified model the Two-Scale Asymptotic-Preserving Schemes. The model, a two dimensional in phase space Vlasov-Poisson equation with small parameter, is used for a long time simulation of a beam in a focusing channel. This work was already done in [68] in the case where the solution is approximated by the two scale limit. The first goal is to improve this approximation, by going further, to the first order one; this was done in [41]. The second goal is to replace this approximation by an exact decomposition, using the macro-micro framework. This last approach will permit to treat the case of a not necessary small parameter. In order to accomplish the first task we have written a Particle-In-Cell code in SeLaLib.

6.3. Development of numerical methods

Participants: Morgane Bergot, Anaïs Crestetto, Nicolas Crouseilles, Pierre Glanc, Michel Mehrenberger, Hocine Sellama, Eric Sonnendrücker, Christophe Steiner.

The work [19] is devoted to the numerical simulation of the Vlasov equation in the fluid limit using particles. To that purpose, we first perform a micro-macro decomposition as in [53] where asymptotic preserving schemes have been derived in the fluid limit. In [53], a uniform grid was used to approximate both the micro and the macro part of the full distribution function. Here, we modify this approach by using a particle approximation for the kinetic (micro) part, the fluid (macro) part being always discretized by standard finite volume schemes. There are many advantages in doing so: (i) the so-obtained scheme presents a much less level of noise compared to the standard particle method; (ii) the computational cost of the micro-macro model is reduced in the fluid regime since a small number of particles is needed for the micro part; (iii) the scheme is asymptotic preserving in the sense that it is consistent with the kinetic equation in the rarefied regime and it degenerates into a uniformly (with respect to the Knudsen number) consistent (and deterministic) approximation of the limiting equation in the fluid regime.

In [39] we present finite volumes schemes for the numerical approximation of the one-dimensional Vlasov-Poisson equation (FOV CEMRACS 2011 project). Stability analysis is performed for the linear advection and links with semi-Lagrangian schemes are made. Finally, numerical results enable to compare the different methods using classical plasma test cases.

In [40], we test an innovative numerical scheme for the simulation of the guiding-center model, of interest in the domain of plasma physics, namely for fusion devices. We propose a 1D Discontinuous Galerkin (DG) discretization, whose basis are the Lagrange polynomials interpolating the Gauss points inside each cell, coupled to a conservative semi-Lagrangian (SL) strategy. Then, we pass to the 2D setting by means of a second-order Strang splitting strategy. In order to solve the 2D Poisson equation on the DG discretization, we adapt the spectral strategy used for equally-spaced meshes to our Gauss-point-based basis. The 1D solver is validated on a standard benchmark for the nonlinear advection; then, the 2D solver is tested against the swirling deformation ow test case; finally, we pass to the simulation of the guiding-center model, and compare our numerical results to those given by the Backward Semi-Lagrangian method.

In [44] we have developed the guiding-center model in polar coordinates; numerical issues/difficulties can be tackled in such a test case which thus may be viewed as a first intermediate step between a classical center guide simulation in a 2D cartesian mesh and a 4D drift kinetic simulation.

In [25] and [28], we are interested in the numerical solution of the collisionless kinetic or gyrokinetic equations of Vlasov type needed for example for many problems in plasma physics. Different numerical methods are classically used, the most used is the Particle In Cell method, but Eulerian and Semi-Lagrangian (SL) methods that use a grid of phase space are also very interesting for some applications. Rather than using a uniform mesh of phase space which is mostly done, the structure of the solution, as a large variation of the gradients on different parts of phase space or a strong anisotropy of the solution, can sometimes be such that it is more interesting to use a more complex mesh. This is the case in particular for gyrokinetic simulations for magnetic fusion applications. We develop here a generalization of the Semi-Lagrangian method on mapped meshes. Classical Backward Semi-Lagrangian methods (BSL), Conservative Semi-Lagrangian methods based on one-dimensional splitting or Forward Semi-Lagrangian methods (FSL) have to be revisited in this case of mapped meshes. We consider here the problematic of conserving exactly some equilibrium of the distribution function, by using an adapted mapped mesh, which fits on the isolines of the Hamiltonian. This could be useful in particular for Tokamak simulations where instabilities around some equilibrium are investigated. We also consider the problem of mass conservation. In the cartesian framework, the FSL method automatically conserves the mass, as the advective and conservative form are shown to be equivalent. This does not remain true in the general curvilinear case. Numerical results are given on some gyrokinetic simulations performed with the GYSELA code and show the benefit of using a mass conservative scheme like the conservative version of the FSL scheme. Inaccurate description of the equilibrium can yield to spurious effects in gyrokinetic turbulence simulations. Also, the Vlasov solver and time integration schemes impact the conservation of

physical quantities, especially in long-term simulations. Equilibrium and Vlasov solver have to be tuned in order to preserve constant states (equilibrium) and to provide good conservation property along time (mass to begin with). Several illustrative simple test cases are given to show typical spurious effects that one can observe for poor settings. We explain why Forward Semi-Lagrangian scheme bring us some benefits. Some toroidal and cylindrical GYSELA runs are shown that use FSL.

In [12] we present the Semi-Lagrangian method which is composed by essentially two ingredients : the computation of the characteristics along which the distribution function is constant and the interpolation step. We analyse high order schemes in time based on directional splitting, which are a succession of linear transport steps. We then study the Semi-Lagrangian methods in this particular case and we make the link between different formulations. We also obtain a convergence theorem for the Vlasov-Poisson system in this framework, which remains valid in the case of small displacements. We then develop this type of methods in a more general framework, by using one dimensionnal conservative splitting. We also consider a discontinuous Galerkin variant of such schemes. In a last part, we study the gyroaverage operator which appears in plasma physics by taking care of finite Larmor radius corrections. Finally, we discuss the problematic of zero discrete divergence which gives a compatibility between field computations and the numerical method of transport.

6.4. Finite Element Methods

6.4.1. Gyrokinetic quasi-neutrality equation

Participants: Nicolas Crouseilles, Eric Sonnendrücker.

In [21], a new discretization scheme of the gyrokinetic quasi-neutrality equation is proposed. We discretised the gyrokinetic Poisson equation using arbitrary order spline finite elements which enables to accommodate more complex domains. Moreover in standard polar coordinates we developed a fast solver which is comparable in computational time to the original FFT-second order finite differences, but can become more efficient for higher order as fewer grid points are needed for the same accuracy.

6.4.2. Dissipative boundary conditions for finite element codes

Participants: Philippe Helluy, Laurent Navoret, Eric Sonnendrücker.

We are developing finite-element codes for the Vlasov-Poisson system that would be able to capture the filamentation phenomenon. The filamentation is a mechanism that transfers the space fluctuations of the distribution function to high frequency oscillations in the velocity direction. For stability purpose, most numerical schemes contain dissipation that may affect the precision of the finest oscillations that could be resolved. In [60], [61], [62] Eliasson constructs a non reflecting and dissipative condition for the Fourier-transformed Vlasov-Poisson system. The condition enables the high velocity-frequency oscillations to leave the computational domain in a clean way.

We are currently developing a finite-element code based on this dissipative boundary condition. The code is part of the Selalib library. We also propose an approximation of the Eliasson method, based on the Béranger's PML formalism. Contrary to the original boudary conditions that requires a space Fourier transformation, this method is local and thus could be extended to higher dimensionnal problems and more complex geometries.

6.4.3. High order finite element methods for Maxwell

Participants: Stéphanie Salmon, Eric Sonnendrücker.

In paper [23], we study high order discretization methods for solving the Maxwell equations on hybrid triangle-quad meshes. We have developed high order finite edge element methods coupled with different high order time schemes and we compare results and efficiency for several schemes. We introduce in particular a class of simple high order low dissipation time schemes based on a modified Taylor expansion.

6.5. Waterbag models: analysis and simulations

Participant: Nicolas Besse.

In paper [33], we revisit the linear theory of kinetic flute-like modes such as ionic instabilities by using the exact geometric reduction of Vlasov equation yielded by waterbag invariants which are reminiscent to the geometric Liouville invariants. The waterbag representation of the statistical distribution function of particles can be viewed as a special class of exact weak solution of the Vlasov equation, allowing to reduce this latter into a set of hydrodynamic equations (with the complexity of a multi-fluid model) while keeping its kinetic features (Landau damping and resonant wave-particle interaction). For high toroidal-number-mode, from ballooning transformation and multi-scale WKB-type analysis, we demonstrate that one can construct eigenmode solutions of the two-dimensional integro-differential gyrowaterbag operator by solving a nested one-dimensional Fredholm-type integral equation. Qualitatively, the solution of the nested one-dimensional Fredholm-type equation is equivalent to first solving for the mode structure along the field lines locally in radius, and then constructing the two-dimensional global mode structure through a radially weighted superposition of local solutions. The radial weighted function is solution of a Schrödinger equation or a Riccati equation in the dual space. Solving the linear turning points problem and using connection formulas, the global dispersion relation arises from the WKB-type phase integral quantization condition which involves the local eigenfrequency. Finally we perform the spectral analysis of the nested one-dimensional Fredholm-type operator which constitutes a meromorphic family of compact operators and extend all the results proved for unstable eigenmodes to stable and damped ones by analytic continuation.

In paper [36], we present two new codes devoted to the study of ion temperature gradient (ITG) driven plasma turbulence in cylindrical geometry using a drift-kinetic multi-water-bag model for ion dynamics. Both codes were developed to complement the Runge-Kutta semi-lagrangian multi-water-bag code GMWB3D-SLC described in [55]. The CYLGYR code is an eigenvalue solver performing linear stability analysis from given mean radial profiles. It features three resolution schemes and three parallel velocity response models (fluid, multi-water-bag, continuous Maxwellian). The QUALIMUWABA quasi-linear code is an initial value code allowing the study of zonal flow influence on drift-waves dynamics. Cross-validation test performed between the three codes show good agreement on both temporal and spatial characteristics of unstable modes in the linear growth phase.

In paper [32], we first present the derivation of the anisotropic Lagrangian averaged gyrowaterbag continuum (LAGWBC) equations. The gyrowaterbag continuum can be viewed as a special class of exact weak solution of the Vlasov-gyrokinetic equation, allowing to reduce this latter into an infinite dimensional set of hydrodynamic equations (i.e. an infinite dimensional hyperbolic system of first-order conservation laws in several space dimensions with non-local fluxes) while keeping its kinetic features (Landau damping and nonlinear resonant wave-particle interaction). These models are very promising because they reveal to be very useful for analytical theory (such as the resolution of the eigenvalue problem for analytical description of various instabilities) and numerical simulations (when the continuum is converted into a small finite set of “fluid” or waterbag, the problem has the complexity of a multifluid model instead of a kinetic one) of laser-plasma and gyrokinetic physics (electrostatic turbulence problem). The gyrowaterbag waterbag continuum is derived from two phase-space variable reductions of the Vlasov equation through the existence of two underlying invariants. The first one, coming from physic properties of the dynamics (the fast gyromotion of particles around magnetic field lines) is adiabatic and called the magnetic moment. The second one, named “waterbag” and coming from geometric invariance property of the phase-space, is just the direct consequence of the Liouville Theorem and is reminiscent to the geometric Liouville invariant. In order to obtain the LAGWBC equations from the gyrowaterbag continuum we use an Eulerian variational principle and Lagrangian averaging techniques. Regarding to the original gyrowaterbag continuum, the LAGWBC equations show some additional properties and several advantages from the mathematical and physical viewpoints, which make this model a good candidate for describing accurately gyrokinetic turbulence in magnetically confined plasma. In the second part of this paper we prove local in time well-posedness of an approximated version of the anisotropic LAGWBC equations, that we call the “isotropic” LAGWBC equations, by using quasilinear PDE type methods and elliptic regularity estimates for several operators.

6.6. Simulations for Vlasov-Maxwell model

Participants: Anaïs Crestetto, Philippe Helluy.

In [37] (see also [11]), we present an implementation of a Vlasov-Maxwell solver for multicore processors. The Vlasov equation describes the evolution of charged particles in an electromagnetic field, solution of the Maxwell equations. We propose to solve the Vlasov equation by a Particle-In-Cell method (PIC), while the Maxwell system is computed by a Discontinuous Galerkin method. These methods are detailed, as well as the emission law for the particles and the implementation of the boundary conditions. We use the OpenCL framework, which allows our code to run on multicore processors or recent Graphic Processing Units (GPU). The key points of the implementation on this architecture are presented. We then study several numerical applications to two-dimensional test cases in cartesian geometry. The acceleration between the computation on a CPU and on a graphic card is very high, especially for the Maxwell part.

We have started a new software project called CLAC (for “Conservation Laws Approximation on many Cores”). This is a 3D Discontinuous Galerkin solver, which runs on a cluster of GPU’s, thanks to the OpenCL environment and the MPI library. CLAC is open source and developed in collaboration with the AxesSim company, a SME near Strasbourg. For the moment, it is applied to the Maxwell equations. But we plan to apply it to the MHD equations or mixed kinetic/fluid plasma models.

6.7. Free-streaming ELM formulae vs. Vlasov simulations

Participants: Sever Hirstoaga, Giovanni Manfredi.

One of the main challenges for future tokamak operation, such as ITER, is constituted by the large heat load on the divertor plates. The divertor surfaces are constantly bombarded with high-energy particles and may see their lifetime considerably reduced. The intensity of the particles and energy fluxes is particularly high during transient events known as edge-localised modes (ELMs). Our purpose here is to propose and investigate a kinetic model for ELMs.

The free-streaming model [69] is a simple analytical model for ELM transport in the scrape-off layer (SOL) of a tokamak. It is a force-free Vlasov equation with a source term for the ions distribution function (the Coulomb forces are ignored). Even though this model reproduces with good accuracy some of the main features of an ELM signal, it has two main drawbacks: (i) the self-consistent electric potential is not accounted for and (ii) only solutions for the ion distribution are considered.

In this contribution [24] we propose a set of modified free-streaming equations in order to overcome the above drawbacks. More precisely, some hypotheses on the Maxwellian initial condition lead to a model that includes the self-consistent electric potential. Assuming quasineutrality and using energy conservation we could derive analytical formulae for the electron quantities. This augmented free-streaming model was benchmarked to the Vlasov-Poisson simulations reported in [78]. The match is encouragingly good, thus justifying the applicability of the free-streaming approach.

Finally, from a computational point of view, transport in the SOL was studied by means of three different approaches – fluid, Vlasov and particle-in-cell (PIC). In spite of kinetic effects due to fast electrons which are not captured in the fluid code, the overall agreement between the codes was found to be quite satisfactory [22].

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

Participants: Pierre Bertrand, Takashi Hattori, Simon Labrunie, Jean Rodolphe Roche.

This work is performed in collaboration with Yves Peysson (DRFC, CEA Cadarache). Since September 2012 this work is included in the ANR CHROME.

The aim of this project is to develop a finite element numerical method for the full-wave simulation of electromagnetic wave propagation in plasma. Full-wave calculations of the LH wave propagation is a challenging issue because of the short wave length with respect to the machine size. In the continuation of the works led in cylindrical geometry, a full toroidal description for an arbitrary poloidal cross-section of the plasma has been developed.

Since its wavelength λ at the LH frequency is very small as compared to the machine size R , a conventional full wave description represents a considerable numerical effort. Therefore, the problem is addressed by an appropriate mathematical finite element technique, which incorporates naturally parallel processing capabilities. It is based on a mixed augmented variational (weak) formulation taking account of the divergence constraint and essential boundary conditions, which provides an original and efficient scheme to describe in a global manner both propagation and absorption of electromagnetic waves in plasmas.

With such a description, usual limitations of the conventional ray tracing related to the approximation $\lambda \ll \phi_B \ll R$, where ϕ_B is the size of the beam transverse to the rf power flow direction, may be overcome. Since conditions are corresponding to $\lambda \ll \phi_B \sim R$, the code under development may be considered as a WKB full wave, dielectric properties being local.

This formulation provides a natural implementation for parallel processing, a particularly important aspect when simulations for plasmas of large size must be considered.

The domain considered is as near as possible of the cavity filled by a tokamak plasma. Toroidal coordinates are introduced. In our approach we consider Fourier decomposition in the angular coordinate to obtain stationary Maxwell equations in a cross-section of the tokamak cavity.

A finite element method is proposed for the simulation of time-harmonic electromagnetic waves in a plasma, which is an anisotropic medium. The approach chosen here is sometimes referred to as *full-wave modeling* in the literature: the original Maxwell's equations are used to obtain a second order equation for the time-harmonic electric field. These are written in a weak form using an augmented variational formulation (AVF), which takes into account the divergence. The variational formulation is then discretized using modified Taylor-Hood (nodal) elements.

During 2012 we have developed a domain decomposition method and a new behavior of the plasma density was considered in the code "FullWaveFEM". A analyze of the model considered, existence and unicity of solution, equivalence of the formulation for the domain decomposition formulation was completed in the frame of Takashi Hattori Phd thesis.

6.9. Nearby fields to plasma physics

6.9.1. Neutrino transport in supernova

Participant: Emmanuel Frénod.

In [31] we give an introduction to the Boltzmann equation for neutrino transport used in core collapse supernova models as well as a detailed mathematical description of the Isotropic Diffusion Source Approximation (IDSA). Furthermore, we present a numerical treatment of a reduced Boltzmann model problem based on time splitting and finite volumes and revise the discretization of the IDSA for this problem. Discretization error studies carried out on the reduced Boltzmann model problem and on the IDSA show that the errors are of order one in both cases. By a numerical example, a detailed comparison of the reduced model and the IDSA is carried out and interpreted. For this example the IDSA modeling error with respect to the reduced Boltzmann model is numerically determined and localized.

In [30] we present Chapman–Enskog and Hilbert expansions applied to the $O(v/c)$ Boltzmann equation for the radiative transfer of neutrinos in core collapse supernovae. Based on the Legendre expansion of the scattering kernel for the collision integral truncated after the second term, we derive the diffusion limit for the Boltzmann equation by truncation of Chapman–Enskog or Hilbert expansions with reaction and collision scaling. We also give asymptotically sharp results obtained by the use of an additional time scaling. The diffusion limit determines the diffusion source in the Isotropic Diffusion Source Approximation (IDSA) of Boltzmann's equation for which the free streaming limit and the reaction limit serve as limiters. Here, we derive the reaction limit as well as the free streaming limit by truncation of Chapman–Enskog or Hilbert expansions using reaction and collision scaling as well as time scaling, respectively. Finally, we motivate why limiters are a good choice for the definition of the source term in the IDSA.

6.9.2. Inverse problem governed by Maxwell equations

Participant: Jean Rodolphe Roche.

This work is performed in collaboration with José Herskovits Norman of UFRJ, Rio de Janeiro, Antonio André Novotny from the LNCC, Petropolis, both from Brazil and Alfredo Canelas from the University of the Republic, Montevideo, Uruguay.

The industrial technique of electromagnetic casting allows for contactless heating, shaping and controlling of chemical aggressive, hot melts. The main advantage over the conventional crucible shape forming is that the liquid metal does not come into contact with the crucible wall, so there is no danger of contamination. This is very important in the preparation of very pure specimens in metallurgical experiments, as even small traces of impurities, such as carbon and sulphur, can affect the physical properties of the sample. Industrial applications are, for example, electromagnetic shaping of aluminum ingots using soft-contact confinement of the liquid metal, electromagnetic shaping of components of aeronautical engines made of superalloy materials (Ni,Ti, ...), control of the structure solidification.

The electromagnetic casting is based on the repulsive forces that an electromagnetic field produces on the surface of a mass of liquid metal. In the presence of an induced electromagnetic field, the liquid metal changes its shape until an equilibrium relation between the electromagnetic pressure and the surface tension is satisfied. The direct problem in electromagnetic casting consists in determining the equilibrium shape of the liquid metal. In general, this problem can be solved either directly studying the equilibrium equation defined on the surface of the liquid metal, or minimizing an appropriate energy functional. The main advantage of this last method is that the resulting shapes are mechanically stable.

The inverse problem consists in determining the electric currents and the induced exterior field for which the liquid metal takes on a given desired shape. This is a very important problem that one needs to solve in order to define a process of electromagnetic liquid metal forming.

In a previous work we studied the inverse electromagnetic casting problem considering the case where the inductors are made of single solid-core wires with a negligible area of the cross-section. In a second paper we considered the more realistic case where each inductor is a set of bundled insulated strands. In both cases the number of inductors was fixed in advance, see [18]. In this year we aim to overcome this constraint, and look for configurations of inductors considering different topologies with the purpose of obtaining better results. In order to manage this new situation we introduce a new formulation for the inverse problem using a shape functional based on the Kohn-Vogelius criterion. A topology optimization procedure is defined by means of topological derivatives, a new method that simplifies computation issues was considered, see [35] and [29].

7. Bilateral Contracts and Grants with Industry

7.1. Bilateral Grants with Industry

We have started a collaboration with the SME (Small and Medium Enterprise) AxesSim on the development of Maxwell solvers. AxesSim is specialized on scientific software for airplane electromagnetic compatibility. For the moment, one CIFRE thesis is supported by DGA. Gary Cohen from Inria Rocquencourt is also involved in the project.

8. Partnerships and Cooperations

8.1. National Initiatives

8.1.1. ANR

- Takashi Hattori, Simon Labrunie and Jean-Rodolphe Roche participate in the ANR project “CHROME” (Heating, Reflectometry and Waves for Magnetized Plasma), grouping researchers from Université Paris 6 (B. Després, M. Campos Pinto and others), the Inria project-team POEMS (E. Bécache, C. Hazard and P. Joly) and Université de Lorraine (S. Heuraux). Simon Labrunie is the head of the Lorraine team.

The CHROME project seeks to develop advanced mathematical and numerical tools for the simulation of electromagnetic waves in strongly magnetized plasmas (e.g., tokamak plasmas) in the context of reflectometry (a technique for probing the plasma by analysing the propagation of electromagnetic waves) and heating.

- GYPSI project (2010–2014), <https://sites.google.com/site/anrgypsi/>: coordinator Philippe Ghendrih (CEA Cadarache), other participants, University of Marseille, Universities of Strasbourg and Nancy (CALVI project-team). The aim is to understand the physics of turbulence in magnetically confined plasma using numerical simulation
- accepted ANR project “PEPPSI” in Programme Blanc SIMI 9 – Sciences de l’ingénierie (Edition 2012). Participants : Giovanni Manfredi (coordinator), Sever Hirstoaga.
- Stéphanie Salmon is a major member of ANR Project “VIVABRAIN” (Modèles Numériques, 2012) from 2013 to 2016.

8.1.2. Euratom-CEA projects

- Michel Mehrenberger is the coordinator of the project FR FCM (CNRS Federation on Magnetic Confinement Fusion), within Euratom-CEA association, Title: “Numerical Methods for GYSELA”, the goal is to help improving the numerical algorithms used by the GYSELA code developed at CEA Cadarache for the simulation of turbulence in magnetic fusion plasmas.
- Jean Roche is the coordinator of the FR FCM project with Euratom-CEA association, Title: “Full wave modeling of lower hybrid current drive in tokamaks”. The goal of this project is to develop a full wave method to describe the dynamics of lower hybrid current drive problem in tokamaks.

8.2. European Initiatives

8.2.1. Collaborations with Major European Organizations

E. Sonnendrücker: Max Planck Institut, Munich (Germany)

We will continue to collaborate with Eric Sonnendrücker on numerical and mathematical studies for plasma physics. We also collaborate on the SeLaLib project.

9. Dissemination

9.1. Scientific Animation

9.1.1. Invitations at conferences and summer schools

- Michel Mehrenberger gave invited talks at
 - ICOPS 2012, Edinburgh (Scotland, UK), 8-12 July 2012, “Conservative semi-lagrangian schemes on mapped meshes”, <http://icops2012.lboro.ac.uk/>
 - 4th Summer school on numerical modelling for fusion, 8-12 October 2012, IPP, Garching near Munich “High Order Semi-Lagrangian Schemes for the Vlasov equation”, http://www.ipp.mpg.de/ippcms/eng/for/veranstaltungen/konferenzen/su_school/
- Sever Hirstoaga gave an invited talk at The 9th AIMS Conference, in the Special Session 79 : “Numerical Methods based on Homogenization and on Two-Scale Convergence”, 1-5 July 2012, Orlando.

- Eric Sonnendrücker gave an invited talk on “Numerical Algorithms for Gyrokinetic simulations” at the Workshop on Computational Challenges in Magnetized Plasma, IPAM, UCLA, April 16-20, 2012.
- Jean Roche gave invited talks at
 - Engopt 2012, Rio de Janeiro, Brazil, July 2012, on “Interior Point Methods for Shape Optimization in Electromagnetic Casting”
 - 10th WCCM, Sao Paulo, Brazil, 8-13 July 2012, on “Adaptivity in Shape Optimization with an exterior state equation”

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

Philippe Helluy is responsible for the second year of Master CSSI (*Calcul Scientifique et Sécurité Informatique*) of the UFR Mathématique et Informatique, Université de Strasbourg.

Laurent Navoret is responsible for *Master Enseignement - parcours Agrégation* of the UFR Mathématique et Informatique, Université de Strasbourg, since September 2012.

- Nicolas Besse
 - Licence : Analyse, 90H, L2, Université de Lorraine Faculté des Sciences et Techniques, France
 - Licence : Analyse complexe, 16H, L3, Université de Lorraine Faculté des Sciences et Techniques, France
 - Licence : Analyse, 38H, L1, Université de Lorraine Faculté des Sciences et Techniques, France
 - Master : Modélisation mathématique et méthodes numériques pour les plasmas de fusion, 45H, M2-Fusion, Université de Lorraine, France
- Philippe Helluy
 - Master: EDP hyperboliques, 30 HETD, M2, Université de Strasbourg, France
 - Master: Contrôle Optimal, 30 HETD, M2, Université de Strasbourg, France
 - Master: Calcul Scientifique, 30 HETD, M1, Université de Strasbourg, France
 - Master: Elemental numerical methods, 30 HETD, M1 physique, Université de Strasbourg, France
 - Master: Recherche Opérationnelle, 30 HETD, école d’ingénieurs ENSIIE, Strasbourg, France.
 - Doctorat : Modèles mathématiques et numériques de la transition de phase, 30 HETD, M2, Université de Strasbourg, France
- Simon Labrunie
 - Licence : Mathématiques générales en DUT génie civil, 55h, L1, Université de Lorraine, France
 - Licence : Mathématiques générales en DUT génie civil, 55h, L2, Université de Lorraine, France
- Michel Mehrenberger
 - Licence : Optimisation non lineaire, 54h, L3, Université de Strasbourg, France
 - Licence : Méthodes d’Analyse Numérique, 39h, L3, ENSIIE (ecole d’ingenieur, antenne de Strasbourg), France
 - Licence : Analyse Numérique, 72h, L2, Université de Strasbourg, France

Licence : Calcul Formel et Simulation Numérique, 18h, L2, Université de Strasbourg, France

Master : Mathematical methods for physics, 30h, M1, Université de Strasbourg, France

Master : Spectral Analysis, 30h, M1, Université de Strasbourg, France

Master: Méthodes numériques pour les EDP, TP, 20h, M1, Université de Strasbourg, France

- Laurent Navoret

Licence : TD Technique d'Analyse Numérique, 36h eq. TD, L3, Université de Strasbourg, France

Licence : Introduction numérique aux E.D.P., 43.75h eq. TD, L3, Université de Strasbourg, France

Master : Modélisation : Option Calcul Scientifique, 72 eq. TD, M2, Université de Strasbourg, France

- Jean R. Roche

Licence: Mathématiques, 162 h eq. TD, L2, ESSTIN, Université de Lorraine, France.

Master : Optimisation, 30 h eq. TD, M1, ESSTIN, Université de Lorraine, France.

9.2.2. Supervision

HdR : Michel Mehrenberger, *Inégalités d'Ingham et schémas semi-lagrangiens pour l'équation de Vlasov*, 5 October 2012, Coordinator: Eric Sonnendrücker

PhD in progress : Céline Caldini , *Collisions dans les modèles gyrocinétiques*, Advisor: Mihai Bostan

PhD in progress : Pierre Glanc, *Approximation numérique des équations de Vlasov par des méthodes de "remapping" conservatifs*, Advisors: Nicolas Crouseilles, Emmanuel Frénod, Philippe Helluy and Michel Mehrenberger

PhD in progress : Nhung Pham, *Méthodes fluides généralisées pour les plasmas*, Advisor: Philippe Helluy

PhD in Progress : Michel Massaro, *Résolution numérique de lois de conservation sur architectures multicores*, Advisors: Philippe Helluy, Catherine Mongenet.

PhD in progress : Christophe Steiner, *Etudes de l'opérateur de gyromyenne et de son couplage avec les équations de Vlasov gyrocinétiques*, Advisors: Nicolas Crouseilles and Michel Mehrenberger

PhD in progress : Mathieu Lutz, *Etude théorique et numérique de l'approximation gyrocinétique*, Advisors: Emmanuel Frénod and Eric Sonnendrücker

PhD in progress : Mohamed Ghattassi, *Analyse et Contrôle d'un Four*, Université de Lorraine, Advisor: Jean Roche.

PhD in progress : Takashi Hattori, *Full wave modeling of lower hybrid current drive in tokamaks*, Université de Lorraine, Advisors: Simon Labrunie and Jean Roche.

9.2.3. Juries

Simon Labrunie participated to the following Ph.D. defense committees :

- Jean-Yves Moller, Ph.D. at Université de Lorraine, Title: *Eléments fins courbes et accélération pour le transport de neutrons*, January 2012. Simon Labrunie was co-director together with Richard Sanchez from CEA Saclay.
- Sébastien Cambon, Ph.D. at INSA Toulouse. Title: *Méthodes d'éléments fins d'ordre élevé et d'équations intégrales pour la résolution de problèmes de furtivité radar d'objets à symétrie de révolution*, July 2012.

9.3. Popularization

- October 2012 : Laurent Navoret gave a popularization talk, entitled "La valse relaxante des particules" and about the Landau damping, for the "Fête des sciences 2012" in Strasbourg.
- December 2012 : Philippe Helluy gave a talk entitled: "How to solve PDE on GPU" to high school students at IUFM d'Alsace.

10. Bibliography

Major publications by the team in recent years

- [1] F. ASSOUS, P. CIARLET, S. LABRUNIE, J. SEGRÉ. *Numerical solution to the time-dependent Maxwell equations in axisymmetric singular domains: the singular complement method*, in "J. Comput. Phys.", 2003, vol. 191, n^o 1, p. 147–176, [http://dx.doi.org/10.1016/S0021-9991\(03\)00309-7](http://dx.doi.org/10.1016/S0021-9991(03)00309-7).
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- [4] J. A. CARRILLO, S. LABRUNIE. *Global Solutions for the One-Dimensional Vlasov-Maxwell System for Laser-Plasma Interaction*, in "Math. Models Methodes Appl. Sci.", 2006, vol. 16, p. 19–57, <http://dx.doi.org/10.1142/S0218202506001042>.
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- [10] E. SONNENDRÜCKER, J. R. ROCHE, P. BERTRAND, A. GHIZZO. *The semi-Lagrangian method for the numerical resolution of the Vlasov equation*, in "J. Comput. Phys.", 1999, vol. 149, n^o 2, p. 201–220, <http://hal.archives-ouvertes.fr/inria-00073296/en/>.

Publications of the year

Doctoral Dissertations and Habilitation Theses

- [11] A. CRESTETTO. *Optimisation de méthodes numériques pour la physique des plasmas. Application aux faisceaux de particules chargées.*, Université de Strasbourg, October 2012, <http://hal.inria.fr/tel-00735569>.
- [12] M. MEHREMBERGER. *Inegalites d'Ingham et schemas semi-lagrangiens pour l'equation de Vlasov*, Université de Strasbourg, October 2012, Habilitation à Diriger des Recherches, <http://hal.inria.fr/tel-00735678>.

Articles in International Peer-Reviewed Journals

- [13] R. ABDELKHALEK, H. CALANDRA, O. COULAUD, G. LATU, J. ROMAN. *Fast seismic modeling and reverse time migration on a graphics processing unit cluster*, in "Concurrency and Computation: Practice and Experience", 2012, vol. 24, n^o 7, p. 739-750 [DOI : 10.1002/CPE.1875], <http://hal.inria.fr/hal-00653499>.
- [14] M. BERGOT, M. DURUFLE. *Approximation of $H(\text{div})$ with High-Order Optimal Finite Elements for Pyramids, Prisms and Hexahedra*, in "Communications in Computational Physics", 2012, submitted, submitted, <http://hal.inria.fr/hal-00723472>.
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- [22] E. HAVLICKOVA, W. FUNDAMENSKI, D. TSKHAKAYA, G. MANFREDI, D. MOULTON. *Comparison of fluid and kinetic models of target energy fluxes during edge localized modes*, in "Plasma Phys. Control. Fusion", 2012, vol. 54, 045002.

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Invited Conferences

- [25] M. MEHRENBERGER, M. BERGOT, V. GRANDGIRARD, G. LATU, H. SELLAMA, E. SONNENDRÜCKER. *Conservative Semi-Lagrangian solvers on mapped meshes*, in "ICOPS International Conference on Plasma Science", Edinburgh, United Kingdom, December 2012, <http://hal.inria.fr/hal-00759823>.

International Conferences with Proceedings

- [26] J.-P. BRAEUNIG, N. CROUSEILLES, M. MEHRENBERGER, E. SONNENDRÜCKER. *Guiding-center simulations on curvilinear meshes using semi-Lagrangian conservative methods*, in "Numerical Models for Controlled Fusion", Porquerolles, France, April 2012, vol. 5, p. 271-282, <http://hal.inria.fr/hal-00605870>.

Research Reports

- [27] G. LATU, M. BECOULET, G. DIF-PRADALIER, V. GRANDGIRARD, M. HOELZL, G. HUYSMANS, X. LACOSTE, E. NARDON, F. ORAIN, C. PASSERON, P. RAMET, A. RATNANI. *Non regression testing for the JOREK code*, Inria, November 2012, n^o RR-8134, 17, <http://hal.inria.fr/hal-00752270>.
- [28] G. LATU, V. GRANDGIRARD, J. ABITEBOUL, M. BERGOT, N. CROUSEILLES, X. GARBET, P. GHENDRIH, M. MEHRENBERGER, Y. SARAZIN, H. SELLAMA, E. SONNENDRÜCKER, D. ZARZOSO. *Accuracy of unperturbed motion of particles in a gyrokinetic semi-Lagrangian code*, Inria, September 2012, n^o RR-8054, 17, <http://hal.inria.fr/hal-00727118>.

Other Publications

- [29] M. AROZTEGUI, J. HERSKOVITS, J. R. ROCHE. *A feasible direction interior point algorithm for nonlinear semidefinite programming*, 2012, <http://hal.inria.fr/hal-00758803>.
- [30] H. BERNINGER, E. FRÉNOT, M. GANDER, M. LIEBENDÖRFER, J. MICHAUD. *Derivation of the Isotropic Diffusion Source Approximation (IDSA) for Supernova Neutrino Transport by Asymptotic Expansions*, 2012, <http://hal.inria.fr/hal-00762621>.
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- [36] D. COULETTE, N. BESSE. *Numerical comparisons of gyro-kinetic multi-water-bag models*, 2012, preprint, submitted, <http://hal.archives-ouvertes.fr/hal-00764904>.
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