



INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Project-Team Calvi

Scientific Computation and Visualization

Nancy - Grand Est

Theme : Computational models and simulation

Activity
R *eport*

2010

Table of contents

1. Team	1
2. Overall Objectives	2
2.1. Introduction	2
2.2. Highlights	2
3. Scientific Foundations	2
3.1. Kinetic models for plasma and beam physics	2
3.1.1. Models for plasma and beam physics	2
3.1.2. Mathematical and asymptotic analysis of kinetic models	4
3.1.3. Asymptotic analysis yielding fluid models	4
3.2. Development of simulation tools	4
3.2.1. Introduction	4
3.2.2. Convergence analysis of numerical schemes	5
3.2.3. The semi-Lagrangian method	5
3.2.4. Particle-In-Cell codes	6
3.2.5. Maxwell's equations in singular geometry	6
3.2.6. Symplectic and two-scale numerical methods	6
3.3. Large size problems	6
3.3.1. Introduction	6
3.3.2. Parallelization of numerical methods	7
4. Application Domains	7
4.1. Thermonuclear Fusion	7
4.2. Beams	8
4.3. Nanophysics	8
5. Software	9
5.1. Vlasv	9
5.2. Obiwan	9
5.3. Yoda	10
5.4. Brennus	10
5.5. LOSS	10
5.6. GYSELA	10
6. New Results	10
6.1. Mathematical and numerical analysis	10
6.1.1. Existence results for Vlasov-like equations	11
6.1.2. Gyrokinetic asymptotic analysis	11
6.1.3. Mathematical study of water-bag models	11
6.1.4. Mathematical properties of numerical methods	12
6.1.5. Domain decomposition for the solution of nonlinear equations	13
6.2. Vlasov solvers	13
6.3. Other numerical developments for magnetic fusion	13
6.3.1. Numerical study of approximated models	14
6.3.2. Plasma-wall interactions – application to ELM modes on JET	14
6.3.3. Gyro-water-bag approach	14
6.4. Application of Vlasov/Wigner codes in nanophysics	14
6.5. Maxwell and applications	15
6.5.1. Inverse problem governed by Maxwell equations	15
6.5.2. NURBS for solving Maxwell	16
6.5.3. Full wave modelling of lower hybrid current drive in tokamaks	16
6.6. Diffusion of knowledge and methods towards other fields	17
6.6.1. Numerical simulation of compressible multi-material fluid flows	17

6.6.2. Applications to environmental sciences	17
7. Contracts and Grants with Industry	17
7.1. CEA Cadarache, gyrokinetic simulation and visualization	17
7.2. LRC project with CEA Cadarache, Full wave modelling of lower hybrid current drive in tokamaks	18
7.3. National initiatives	18
7.3.1. ANR Projects	18
7.3.2. INRIA Large Scale Initiative "Fusion"	18
7.3.3. INRIA ADT SeLaLib	18
7.3.4. Cemracs 2010 projects	18
7.4. European initiatives	18
7.4.1. DFG/CNRS project "Noise Generation in Turbulent Flows"	18
7.4.2. EUFORIA Project	19
7.5. International initiative	19
8. Dissemination	19
8.1. Leadership within scientific community	19
8.1.1. Conferences, meetings and tutorial organization	19
8.1.2. Invitations at conferences and summer schools	19
8.1.3. Administrative duties	20
8.2. Teaching	21
8.3. Ph. D. Theses	21
8.3.1. Ph. D. defended in 2010	21
8.3.2. Ph. D. in progress	21
8.3.3. Post Doc in progress	21
9. Bibliography	22

1. Team

Research Scientists

Nicolas Besse [On leave from University Henri Poincaré from 1st September 2008 until August 2010, HdR]
Jean-Philippe Braeunig [INRIA, on leave from CEA since 1st September 2008]
Nicolas Crouseilles [INRIA Research Scientist, IRMA]
Emmanuel Frénod [Professor, on leave from Université de Bretagne-Sud since 1st September 2010, HdR]
Sever Hirstoaga [INRIA Research Scientist, IRMA]
Martin Campos Pinto [CNRS Research Scientist, IRMA, Visiting University of California–Lawrence Berkeley National Laboratory since March 2010]

Faculty Members

Michaël Gutnic [Assistant Professor at Université de Strasbourg]
Simon Labrunie [Vice-team Leader, Assistant Professor at University Henri Poincaré Nancy 1, HdR]
Vladimir Latocha [Assistant Professor at Université Henri Poincaré Nancy 1]
Guillaume Latu [Until August 2010, Assistant Professor Université de Strasbourg, Research Scientist at CEA-Cadarache from 1st september 2010]
Michel Mehrenberger [Assistant Professor at Université de Strasbourg]
Jean Roche [Professor at ESSTIN, HdR]
Stéphanie Salmon [Until August 2010, Assistant Professor at Université de Strasbourg, Professor at Université de Reims – Champagne-Ardenne since 1st September 2010, HdR]
Eric Sonnendrücker [Team Leader, Professor at Université de Strasbourg, HdR]

External Collaborators

Pierre Bertrand [Emeritus Professor, LPMIA, Nancy, HdR]
Mihai Bostan [Assistant Professor, Besançon, HdR]
Alain Ghizzo [Professor, LPMIA, Nancy, HdR]
Etienne Gravier [Assistant Professor, LPMIA, Nancy, HdR]
Philippe Helluy [Professor, IRMA, Strasbourg, HdR]
Paul-Antoine Hervieux [Professor, IPCMS, Strasbourg, HdR]
Giovanni Manfredi [CNRS Research Scientist, IPCMS, Strasbourg, HdR]
Thierry Réveillé [Assistant Professor, LPMIA, Nancy]

Technical Staff

Edwin Chacon Golcher [Since 1st December 2010, INRIA Senior Engineer, ADT SeLaLib Engineer Team Leader]
Pierre Navaro [CNRS Research Engineer, Université de Strasbourg]

PhD Students

Aurore Back [Université de Strasbourg, Advisors: Emmanuel Frénod and Eric Sonnendrücker]
Céline Caldini [Since October 2010, INRIA - AEN Fusion, Advisor: Mihai Bostan]
Anaïs Crestetto [INRIA, Advisors: Philippe Helluy and Marc Massot]
Pierre Glanc [Since October 2010, INRIA, Advisors: Nicolas Crouseilles, Emmanuel Frénod, Philippe Helluy and Michel Mehrenberger]
Takashi Hattori [Université Henri Poincaré Nancy, Advisors: Simon Labrunie and Jean Roche]
Sandrine Marchal [Université Henri Poincaré Nancy, Advisors: Simon Labrunie and Jean Roche]
Mathieu Lutz [Since September 2010, Université de Strasbourg, Advisors: Emmanuel Frénod and Eric Sonnendrücker]
Ahmed Ratnani [INRIA, Advisors: Nicolas Crouseilles and Eric Sonnendrücker]
Thomas Respaud [Université de Strasbourg, Advisor: Eric Sonnendrücker, PhD defended in november 2010]

Post-Doctoral Fellows

Morgane Bergot [Since December 2010, INRIA, Advisor: Eric Sonnendrücker]
Sébastien Jund [Until August 2010, ANR HOUPIC, IRMA, Advisor: Eric Sonnendrücker]
Olivier Hoenen [Université de Strasbourg - Euforia Project financing, Advisor: Eric Sonnendrücker]

Administrative Assistants

Sophie Drouot [TR, part-time in project]

Christel Wiemert [TR, part-time in project]

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

- Launch of ADT SeLaLib

3. Scientific Foundations

3.1. Kinetic models for plasma and beam physics

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,
- fluid models valid when the particles are at a thermodynamical equilibrium.

Calvi team mainly focuses on kinetic models, but not exclusively. In particular, every kind of models are mathematically analyzed, approximate models are built and studied and model hierarchies are set out.

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

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

which describes the evolution of the electromagnetic field generated by the charge and current densities

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

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.

Beside this, **enriching and making more rigorous the model hierarchy** is also an important challenge which requires a deep knowledge of different models in use in plasma physics (e.g. Magneto-Hydro-Dynamics, Laser-Matter Interaction, Waves In Plasma, etc.) and their connections with Vlasov-like models.

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 [77], see also Bardos and Degond [56]. The existence of a weak solution for the Vlasov-Maxwell system has been proved by Di Perna and Lions [66]. An overview of the theory is presented in a book by Glassey [74].

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 [57].

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 [75], [79] as well as by Brenier [62]. 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 [70], [68], [69].

3.1.3. *Asymptotic analysis yielding fluid models*

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 equation can be closed after a few of those, thus yielding fluid models.

3.2. **Development of simulation tools**

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. For a few years, we also have been interesting in solvers that use Particle In Cell method. This new issue allows us to enrich some parts of our research activities previously centered on the Semi-Lagrangian approach. We also have been initiating to insert asymptotic analysis products and geometry products within numerical methods in order to enforce their robustness and their ability to perform long term simulations.

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.

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 this case a variants, called adaptive semi-Lagrangian methods, of semi-Lagrangian methods was set out better to better fit the distribution of particles.

3.2.4. Particle-In-Cell codes

The Particle-In-Cell method [59] 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.

3.2.5. 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 [55] and implemented [54] 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 [58]. The non-density result for regular fields was proven [63], the singularities of the electromagnetic field were related to that of modified Laplacians [50], and expressions of the singular fields were calculated [51]. 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 [52].

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 [73], [51].

3.2.6. Symplectic and two-scale numerical methods

In order to set out numerical methods that can be valid even for long term simulations, two strategies may be followed. The first one is to incorporate in them asymptotic analysis concepts allowing to take into account, precisely, only the resulting mean effect of oscillations. This yields Two-Scale-Numerical-Methods which were introduced in [71] and [72] and which constitutes an active research activity.

The second, which also gives rise to an active research activity, consists in incorporating Hamiltonian mechanics and symplectic geometry concepts while building numerical schemes.

3.3. Large size problems

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 [76] 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 [80], 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 [78] 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.

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

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. Deuterium can be obtained from the water of the oceans that is widely available and Tritium can be produced from Lithium directly in a tokamak. Moreover, 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.

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

Our work in modelling and numerical simulation of plasmas and 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. 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.

4.2. Beams

Vlasov equation, Vlasov-Poisson and Vlasov-Maxwell systems are also used to model transport of particle beams in accelerators. As a consequence our work also applies to this field. In particular, 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.

4.3. 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.

¹<http://www.iter.org>

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. [67], 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. Vlasy

Participant: Pierre Navaro [correspondant].

The aim of the platform is to change the way numerical methods are implemented and tested. It has been initiated because most of the researchers of the CALVI project develop new numerical methods for almost the same equations. Until now, all researchers implemented their methods as stand-alone C or Fortran applications. So, each researcher, for each code, has to implement the validation process by himself without using previous implementation done by himself or another member of the project. The platform moves the implementation from a stand-alone application to a module oriented one. Thanks to standardized application programming interfaces (API), the different numerical methods can be swapped between them and can be validated within a common skeleton. This common skeleton plus the standard API is actually the platform. A better reuse of existing modules is expected as well as an increased efficiency in numerical methods implementation.

The whole implementation has been refactored this year according to remarks made by the team. So the python package called 'vlasy', which stands for 'Vlasov' + 'Python', is born. Lots of things that were accessible to the user are now embedded in Python classes within the package. As a result, the user accesses objects at a higher level of abstraction, thus making the usage easier. Some unit tests have been introduced in the skeleton part of the package and the solver validation process is also implemented as unit tests. Two Vlasov solvers have been added as well as 4 test cases. The vlasy package is already used at CEA Cadarache in a physics team.

5.2. Obiwan

Participants: Nicolas Besse, Michaël Gutnic, Guillaume Latu [correspondant], Eric Sonnendrücker.

Obiwan is an adaptive semi-Lagrangian code for the resolution of the Vlasov equation. It has up to now a cartesian 1Dx-1Dv version and a 2Dx-2Dv version. The 1D version is coupled either to Poisson's equation or to Maxwell's equations and solves both the relativistic and the non relativistic Vlasov equations. The grid adaptivity is based on a multiresolution method using Lagrange interpolation as a predictor to go from one coarse level to the immediately finer one. This idea amounts to using the so-called interpolating wavelets. A parallel version of the code exists and uses the OpenMP paradigm. Domain size of 512^4 has been considered and the method allows to save effectively memory and computation time compared to a non-adaptive code.

5.3. Yoda

Participants: Martin Campos Pinto, Olivier Hoenen [correspondant], Michel Mehrenberger.

YODA is an acronym for Yet another Adaptive Algorithm. The sequential version of the code was developed by Michel Mehrenberger and Martin Campos-Pinto during CEMRACS 2003. The development of a parallel version was started by Eric Violard in collaboration with Michel Mehrenberger in 2003. It is currently continued with the contributions of Olivier Hoenen. It solves the Vlasov equation on a dyadic mesh of phase-space. The underlying method is based on hierarchical finite elements. Its originality is that the values required for interpolation at the next time step are determined in advance. In terms of efficiency, the method is less adaptive than some other adaptive methods (multi-resolution methods based on interpolating wavelets as examples), but data locality is improved.

5.4. Brennus

Participants: Pierre Navaro [correspondant], Eric Sonnendrücker.

The Brennus code is developed in the framework of a contract with the CEA Bruyères-Le-Châtel. It is based on a first version of the code that was developed at CEA. The new version is written in a modular form in Fortran 90. It solves the two and a half dimensional Vlasov-Maxwell equations in cartesian and axisymmetric geometry and also the 3D Vlasov-Maxwell equations. It can handle both structured and unstructured grids in 2D but only structured grids in 3D. Maxwell's equations are solved on an unstructured grid using either a generalized finite difference method on dual grids or a discontinuous Galerkin method in 2D. On the 2D and 3D structured meshes Yee's method is used. The Vlasov equations are solved using a particle method. The coupling is based on traditional PIC techniques.

5.5. LOSS

Participants: Nicolas Crouseilles, Guillaume Latu [correspondant].

The LOSS code is devoted to the numerical solution of the Vlasov equation in four phase-space dimensions, coupled with the two-dimensional Poisson equation in cartesian geometry. It implements a parallel version of the semi-Lagrangian method based on a localized cubic splines interpolation we developed. It has the advantage compared to older versions of the cubic splines semi-Lagrangian method to be efficient and scalable even when the number of processors becomes important (several hundreds). It is written in Fortran 90 and MPI. The computation kernel of LOSS has been adapted and put in the GYSELA5D code owned by the CEA-Cadarache.

5.6. GYSELA

Participants: Eric Sonnendrücker [correspondant], Virginie Grandgirard.

The GYSELA code is a 5D global gyrokinetic code that simulates a ring of confined plasma in a torus with circular cross-section. The evolution of the ion distribution function and of the electric potential are computed self-consistently, assuming quasi-neutrality and that the electrons are in Maxwell-Boltzmann equilibrium with this potential.

6. New Results

6.1. Mathematical and numerical analysis

Participants: Nicolas Besse, Mihai Bostan, Nicolas Crouseilles, Emmanuel Frénod, Sever Hirstoaga, Simon Labrunie, Sandrine Marchal, Michel Mehrenberger, Alexandre Mouton, Thomas Respaud, Jean Roche, Eric Sonnendrücker.

6.1.1. Existence results for Vlasov-like equations

In [45] **existence and uniqueness of solutions to the Vlasov–Poisson system with an initial data with bounded variation** is gotten. Unlike in works of Cooper–Klimas, Glassey–Schaeffer–Strauss, Guo, ... bound, continuity and compact support on initial data (and hence the solution) are not assumed. Local existence and uniqueness are proved in dimension 1+1, with an explicit lower bound of the existence time in terms of the data. Generalization to higher dimensions is under progress.

In [16], in the continuity of [61], **existence of weak solutions for the stationary Nordström-Vlasov equations in a bounded domain** is set out. The proof follows by a fixed point method. The asymptotic behavior for large light speed is analyzed as well. Convergence towards the stationary Vlasov-Poisson model for stellar dynamics is also studied.

[18] investigates the **well-posedness of stationary Vlasov-Boltzmann equations** both in the simpler case of linear problems with a space varying force field, and, the non-linear Vlasov-Poisson-Boltzmann system. For the former we obtain existence-uniqueness results for arbitrarily large integrable boundary data and justify further a priori estimates. For the later the boundary data needs to satisfy an entropy condition guaranteeing classical statistical equilibrium at the boundary. This stationary problem relates to the existence of phase transitions associated with slab geometries.

6.1.2. Gyrokinetic asymptotic analysis

The subject matter of [17] concerns asymptotic regimes for **transport equations with advection fields having components of very disparate orders of magnitude**. Such models arise in the magnetic confinement context, where charged particles move under the action of strong magnetic fields. According to the different possible orderings between the typical physical scales (Larmor radius, Debye length, cyclotron frequency, plasma frequency) we distinguish several regimes: guiding-center approximation, finite Larmor radius regime, etc. The main purpose is to derive the limit models: we justify rigorously the convergence towards these limit models and we investigate the well-posedness of them.

In [36] we provide a rigorous **derivation of the guiding-center approximation in the general three dimensional** setting under the action of large stationary inhomogeneous magnetic fields. The first order corrections are computed as well: electric cross field drift, magnetic gradient drift, magnetic curvature drift, etc. The mathematical analysis relies on averaging techniques and ergodicity.

In order to derive a **drift-kinetic model**, we consider in [43] a new scaling of the Vlasov equation under the hypothesis of **large external nonstationary and inhomogeneous electromagnetic field and under the condition of low-Mach number**, i.e. when the kinetic energy of the fluid motion is very small in comparison to the thermal energy. To this end, we first make the dimensionless cyclotron period appear in the scaled Vlasov equation. Then we decompose the particle velocity into the mean velocity and its random part and we deduce a system of two equations giving the evolution of the new distribution function and the mean velocity (of the fluid motion). Afterward, an asymptotic analysis is made for this model and a formal derivation of the drift-kinetic model (in a five dimensional phase space) is thus obtained.

In [23] the **Two-dimensional Finite Larmor Radius asymptotic regime** (previously reached in [69] and [60]) is addressed using a two scale convergence methods after rewriting the Vlasov-Poisson system in a coordinate system so called **canonical gyrokinetic coordinate** system.

6.1.3. Mathematical study of water-bag models

In [13] we prove the **existence and uniqueness of classical solution for a system of PDEs recently developed to model the nonlinear gyrokinetic turbulence in magnetized plasma**. From the analytical and numerical point of view this model is very promising because it allows to recover kinetic features (wave-particle interaction, Landau resonance) of the dynamic flow with the complexity of a multi-fluid model. This model, called the gyro-water-bag model, is derived from two phase space variable reductions of the Vlasov equation through the existence of two underlying invariants. The first one, the magnetic moment, is adiabatic and the second, a geometric invariant named "water-bag", is exact and is just the direct consequence of the Liouville Theorem.

The aim [14] is to study the **existence of classical solution for the waterbag model with a continuum of waterbag**, which can be viewed as an infinite dimensional system of first-order conservation laws. The waterbag model, which constitutes a special class of exact weak solution of the Vlasov equation, is well known in plasma physics and its applications in gyrokinetic theory and laser-plasma interaction are very promising. The proof of the existence of a continuum of regular waterbag relies on a generalized definition of hyperbolicity for integrodifferential hyperbolic system of equations, some results in singular integral operators theory and harmonic analysis, Riemann-Hilbert boundary value problem and energy estimates.

In [35] we consider the **relativistic waterbag continuum** which is a useful PDE for collisionless kinetic plasma modelling recently developed. 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 nonlinear resonant wave-particle interaction). These models are very promising because they reveal to be very useful for analytical theory and numerical simulations of laser-plasma and gyrokinetic physics. The relativistic waterbag continuum is derived from two phase-space variable reductions of the relativistic Vlasov-Maxwell equations through the existence of two underlying exact invariants, one coming from physic properties of the dynamics is the canonical transverse momentum, and the second, named the "water-bag" and coming from geometric property of the phase-space is just the direct consequence of the Liouville Theorem. In this paper we prove existence and uniqueness of global weak entropy solutions of the relativistic waterbag continuum. Existence is based on vanishing viscosity method and bounded variations (BV) estimates to get compactness while proof of uniqueness relies on kinetic formulation of the relativistic waterbag continuum and the associated kinetic entropy defect measure.

6.1.4. *Mathematical properties of numerical methods*

[39] analyses numerically the so-called **Fourier–Singular Complement Method for the time-dependent Maxwell equations in an axisymmetric domain**. This work completes a series of articles on the numerical solution of the equations of electromagnetism in this type of domain (see [53] for Maxwell's equations in the case of axially symmetric data and [64] for Poisson's equation with arbitrary data). The method relies on a continuous approximation of the electromagnetic field, unlike, e.g., edge element methods. This has many advantages in the case of model coupling, e.g. if the Maxwell solver is embedded in a Vlasov–Maxwell code, either PIC or Eulerian. The symmetry of rotation is exploited by using finite elements in a meridian section of the domain only, and a spectral method in the azimuthal dimension. The analysis incorporates an approach which allows one to handle both noisy or approximate data which fail to satisfy the charge conservation equation, as may happen in a Vlasov–Maxwell code and domains with geometrical singularities (non-convex edges and/or vertices) which cause the electromagnetic field to be less regular than in a smooth or convex domain.

[12] consider the **spherically symmetric Vlasov-Einstein system in the case of asymptotically flat spacetimes**. From the physical point of view this system of equations can model the formation of a spherical black hole by gravitational collapse or describe the evolution of galaxies and globular clusters. We present **high-order numerical schemes based on semi-Lagrangian** techniques. The convergence of the solution of the discretized problem to the exact solution is proven and high-order error estimates are supplied. More precisely the metric coefficients converge in L^∞ and the statistical distribution function of the matter and its moments converge in L^2 with a rate of $\mathcal{O}(\Delta t^2 + h^m/\Delta t)$, when the exact solution belongs to H^m .

In [21], **conservative semi-Lagrangian schemes** are presented for the Vlasov equation. In particular, a Hermite reconstruction enables to unify several numerical schemes of the literature (PSM, PPM, PFC). Moreover, slope limiters have been compared and proposed to ensure positivity or monotonicity of the numerical solution.

In [41] and [29] a new method for the solving of the charge conservation problem is proposed and applied to the Vlasov-Poisson equation. It is based on the **Forward semi-Lagrangian method** (see [65]) which bears similarities with Particle In Cell (PIC) method. Using strategies employed in PIC methods, a charge conserving numerical method is then obtained for a semi-Lagrangian method.

In [40], an **asymptotic preserving scheme** is designed for the collisional Vlasov-Poisson equation using the so-called micro-macro decomposition. This approach enables to get a numerical scheme which is stable for every mean free path in the diffusion or high-field limit, and the limit of which is consistent with the continuous limit model.

6.1.5. Domain decomposition for the solution of nonlinear equations

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

Strongly problems of parabolic equations have received considerable attentions, and various forms of this problems have been proposed in the literature, especially in the area of reaction-diffusion equations with cross-diffusion, such problems arise from biological, chemical and physical systems. Various methods have been proposed in the mathematical literature to study the existence, uniqueness and compute numerical approximation of solutions for quasi-linear partial differential equation problems. This year our work was about the periodic case. We develop a numerical method to solve periodic non linear parabolic equations based on domain decomposition and optimization interior points method.

6.2. Vlasov solvers

Participants: Nicolas Besse, Martin Campos Pinto, Nicolas Crouseilles, Alain Ghizzo, Michaël Gutnic, Olivier Hoenen, Sébastien Jund, Guillaume Latu, Michel Mehrenberger, Thomas Respaud, Stéphanie Salmon, Eric Sonnendrücker.

In [42], we present a **discontinuous Galerkin scheme for the numerical approximation of the one-dimensional periodic Vlasov-Poisson equation**. The scheme is based on a Galerkin-characteristics method in which the distribution function is projected onto a space of discontinuous functions. Comparisons with a classical semi-Lagrangian method are shown to emphasize the good behavior of the present scheme when applied to Vlasov-Poisson test cases.

The purpose of [34] is simulation of magnetized plasmas in the ITER project framework. In this context, Vlasov-Poisson like models are used to simulate core turbulence in the tokamak in a toroidal geometry. Accurate schemes, parallel algorithms need to be designed to bear these simulations.

This report describes a Hermite formulation of the conservative **PSM scheme** which is very generic and allows to implement different semi-Lagrangian schemes. We also test and propose **numerical limiters** which should improve the robustness of the simulations by diminishing spurious oscillations. This work involved a trainee (J. Guterl, advised by J.-P. Braeunig) and their results were incorporated in GYSELA.

Concerning plasma simulation, the purpose of this report ([34]) is **core turbulence in tokamak plasma** in toroidal geometry. The natural 6-dimensional problem (3D in space and 3D in velocity) is reduced to a 5D gyrokinetic model, taking advantage of the particular motion of particles due to the presence of a strong magnetic field. Using previously built **Semi-Lagrangian Methods with Flux Limiters** applied to the **Vlasov-Poisson system, Plasma Turbulence simulations** are performed and reported.

In [30] **turbulent transport governed by the toroidal ion temperature gradient driven instability is analyzed** with the full-f global gyrokinetic code GYSELA when the system is driven by a prescribed heat source.

In [37], a general mathematical formulation for charge conserving **Finite Elements Maxwell solvers coupled with Particle-In-Cell schemes** is proposed. A particular care is taken to finite-element continuity equations that must be satisfied by the discrete current sources for several classes of time domain Vlasov-Maxwell simulations. The results cover a wide range of schemes (namely curl-conforming finite element methods of arbitrary degree, general meshes in 2 or 3 dimensions, several classes of time discretization schemes, particles with arbitrary shape factors and piecewise polynomial trajectories of arbitrary degree).

6.3. Other numerical developments for magnetic fusion

Participants: Pierre Bertrand, Nicolas Besse, Jean-Philippe Braeunig, Nicolas Crouseilles, Daniele Del Sarto, Sever Hirstoaga, Giovanni Manfredi, Michel Mehrenberger, Etienne Gravier, Guillaume Latu, Jean Roche, Amar Mokrani, Simon Labrunie, Hocine Sellama, Eric Sonnendrücker.

6.3.1. Numerical study of approximated models

The **validity of quasilinear theory (QL) describing the weak warm beam–plasma instability** has been a controversial topic for several decades. In [15] it is tackled anew, both analytically and by numerical simulations which benefit from the power of modern computers and from the development in the last decade of Vlasov codes endowed with both accuracy and weak numerical diffusion. Self-consistent numerical simulations within the Vlasov–wave description show that QL theory remains valid in the strong chaotic diffusion regime. However there is a non-QL regime before saturation, which confirms previous analytical work and numerical simulation, but contradicts another analytical work. We show analytically the absence of mode coupling in the saturation regime of the instability where a plateau is present in the tail of the particle distribution function. This invalidates several analytical works trying to prove or to contradict the validity of QL theory in the strongly nonlinear regime of the weak warm beam–plasma instability.

In [20], a general framework is proposed for the **numerical approximation of the gyroaverage operator with finite gyroradius guiding-center** which enables to unify several methods existing in the literature. A new approach is also presented and some comparisons are performed through a guiding-center model.

6.3.2. Plasma-wall interactions – application to ELM modes on JET

The aim of [25] is to model the effect of energetic charged particles (generated during violent events known as edge-localized modes) on the divertor plates of a tokamak. We thus have developed a 1D Vlasov-Poisson code with open boundaries for both ions and electrons. The spatial co-ordinate represents the distance along the magnetic field line, whereas the absorbing boundaries are supposed to mimic the divertor plates. Appropriate diagnostics are set up to compute the particles and heat fluxes on the plates. The relevant physical regime is determined by two dimensionless parameters: the ion-to-electron mass ratio and the ratio of the Debye length to the parallel connection length. The latter is particularly important as its small values correspond to the quasineutral limit. In order to lift numerical constraints on the time and space steps, inherent to this limit, we use an asymptotic preserving scheme. This is done first, by reformulating the Poisson equation into a strictly equivalent equation which is not singular in the quasineutral limit and second, by implicit time-discretization of the reformulated Poisson equation.

The results of numerical simulations performed with our model were compared systematically to analytical solutions obtained with a simplified free-streaming model [W. Fundamenski et al., Plasma Phys. Control. Fus. **48**, 109 (2006)]. Several comparisons with numerical results obtained with a PIC code (developed at the University of Innsbruck) were also performed. Despite the differences in the numerical methods and in the model, a fairly good agreement was observed. Comparisons with a fluid code (developed at Culham, UK) and with experimental results from JET are under way.

6.3.3. Gyro-water-bag approach

[48] addresses the gyrokinetic water-bag model in toroidal geometry. Our previous works were focused on the water-bag concept in magnetized cylindrical plasmas. Here we report on the possibility to improve the water-bag model by taking into account the curvature and gradient drifts. After a presentation of the model, a linear analysis with some approximations is performed. Interchange and Ion Temperature Gradient instabilities are examined with this new gyro-water-bag model in order to show its ability in describing kinetic instabilities in toroidal geometry.

We report in a paper to be published a new modelling method to study multiple species dynamics in magnetized plasmas. Such a method is based on the gyro water bag modelling, which consists in using a multi step-like distribution function along the velocity direction parallel to the magnetic field. Such a model has been very recently ported to the context of strongly magnetized plasmas. We present its generalization to the case of multi species magnetized plasmas: each ion species being modelled via a multi water bag distribution function. We discuss in details the modelling procedure. As an illustration, we present results obtained in the linear framework.

6.4. Application of Vlasov/Wigner codes in nanophysics

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

For a few years, our team has been involved in several research projects involving the application of Vlasov-like equations to the physics of nano-sized objects, such as thin metal films, nanoparticles, quantum wells and quantum dots. It is a topic with tremendous potential for a broad spectrum of applications, ranging from materials science to biology and medicine. Our approach – based on a phase-space description of the dynamics – is not widely used in the nanophysics community, which constitutes one of the originalities of our project.

6.4.1. Ultrafast magnetization dynamics in diluted magnetic

We have developed (see [33] [24] and [26]) a dynamical model that successfully explains the observed time evolution of the magnetization in diluted magnetic semiconductor quantum wells after weak laser excitation. Based on a many-particle expansion of the exact $p - d$ exchange interaction, our approach goes beyond the usual mean-field approximation. It includes both the sub-picosecond demagnetization dynamics and the slower relaxation processes which restore the initial ferromagnetic order on a nanosecond timescale. In agreement with experimental results, our numerical simulations show that, depending on the value of the initial lattice temperature, a subsequent enhancement of the total magnetization may be observed on a timescale of few hundreds of picoseconds.

More recently, our model was augmented in order to include the role played by the quantum confinement and the band structure. It was shown that the sample thickness and the background hole density strongly influence the phenomenon of demagnetization. Quantitative results were given for III-V ferromagnetic GaMnAs quantum wells of thickness 4 and 6 nm.

Finally, in [28], **third-order effects in the many-particle expansion** of the exact $p - d$ exchange interaction were taken into account. Dynamical RKKY-like interactions and double-exchange mechanism based on the Kondo interaction emerge naturally from our approach. Our analysis reveals that the many-particle expansion is not generally well defined and an infrared Kondo-like divergence can occur. In particular, the bare polarization propagator fails to converge in the presence of a highly confined hole gas and an enhancement of the ion-hole spin correlation is found for low-dimensional systems. Finally, numerical simulations have been performed on GaMnAs and show that dynamical many-particle correlations play a significant role in the time evolution of the total magnetization.

6.5. Maxwell and applications

Participants: Paul-Antoine Hervieux, Giovanni Manfredi, Omar Morandi, Ahmed Ratnani, Jean Roche, Eric Sonnendrücker.

6.5.1. Inverse problem governed by Maxwell equations

This work is performed in collaboration with Jose 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 [32]. 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, see [38].

6.5.2. *NURBS for solving Maxwell*

In [49], high order methods for solving the time domain **Maxwell equations using spline finite elements on domains defined by NURBS** is studied. Convenient basis functions for the discrete exact sequence of spaces are exhibited which provided the same discrete structure as for classical Whitney Finite Elements. An analysis of stability of the time scheme is also developed.

6.5.3. *Full wave modelling of lower hybrid current drive in tokamaks*

This work is performed in collaboration with Yves Peysson (DRFC, CEA Cadarache).

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 provide 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 fill 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 modelling* 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 and boundary conditions. The variational formulation is then discretized using modified Taylor-Hood (nodal) elements.

One of the objectives in 2010 was the evolution of the MatLab finite element code " FullWaveFEM" developed to handle more real cases, in particular we introduce a new boundary condition in order to take account of the antenna and essential condition are considered.

6.6. Diffusion of knowledge and methods towards other fields

Methods, results and more generally knowledge produced within Calvi team are used in other fields.

6.6.1. Numerical simulation of compressible multi-material fluid flows

[47] and [19] resume a research programme on simulation of compressible multi-material fluid flows with sharp interface capturing called FVCF-NIP (Finite Volumes with Characteristic Flux).

This work is achieved in collaboration with J.-M. Ghidaglia (ENS Cachan), F. Dias (ENS Cachan) and B. Desjardins (ENS Ulm) in the frame of the Laboratoire de Recherche Commun MESO (ENS cachan - CEA Bruyères-le-Châtel).

[19] sets out a **method to control pressure in compressible multi-material fluid flows**. The multi-material character is characterized by the fact that several fluids, separated by interfaces, coexist within the system. Conservation and gliding property preserving numerical reconstruction of interfaces are proposed to fit well every fluid.

[47] improves NIP interface numerical reconstruction which was initially proposed by J.-P. Braeunig in his PhD thesis.

6.6.2. Applications to environmental sciences

In [11] and [22] asymptotic methods initially designed for tokamak plasmas were applied to coastal ocean waters linked phenomena.

Methods for mass transfer modelling was applied in the haulage context in [44].

In [46] parallel simulation methods was applied on a biological question.

7. Contracts and Grants with Industry

7.1. CEA Cadarache, gyrokinetic simulation and visualization

Participants: Jean-Philippe Braeunig, Nicolas Crouseilles, Guillaume Latu, Michel Mehrenberger, Ahmed Ratnani, Eric Sonnendrücker.

We have been involved for the last few years in the development and optimization of the full-f semi-Lagrangian gyrokinetic code GYSELA 5D originally written by V. Grangirard at CEA-Cadarache. The code is based on a 5D gyrokinetic approximation of the Vlasov equation (for the description of the ions) coupled to a quasi-neutrality equation for the computation of the self-consistent electrostatic potential. The code, which is written in toroidal geometry, has been optimized to run efficiently on up to 4096 processors to study the effects of zonal flows on the development of turbulence in a Tokamak plasma.

The major achievements of the year have been the following:

- Introduction of magnetic coordinates to separate the fast motion of particles along the magnetic field lines from the slow perpendicular motion.
- Introduction of a conservative semi-Lagrangian scheme (PSM) in the GYSELA code that allows a 1D directional splitting procedure to solve the 4D Vlasov equations in the gyrokinetic model.
- Modification of the parallelization strategy to take benefits of the 1D directional splitting procedure.
- Development of a new very accurate quasi-neutral solver based on NURBS that can handle arbitrary geometries.
- The numerical techniques to deal with the gyroaverage operator have been adapted to the GYSELA code framework and especially to deal with boundary conditions. Moreover, a new formulation of the quasi-neutral equation has been proposed in the frame of a collaboration IRMA-LATP Marseille that has to be further studied and validated.
- Development of a new Forward Semi-Lagrangian scheme for the Vlasov equation.

7.2. LRC project with CEA Cadarache, Full wave modelling of lower hybrid current drive in tokamaks

Participants: Jean Roche, Simon Labrunie, Amar Mokrani.

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

7.3. National initiatives

7.3.1. ANR Projects

Calvi members are involved in ANR projects.

- Non thematic ANR: Study of wave-particle interaction for Vlasov plasmas (leader A. Ghizzo). In collaboration with F. Califano from the University of Pisa in Italy.
- ANR Calcul Intensif et Simulation: HOUPIC (ANR-06-CIS6-013-01, leader E. Sonnendrücker): Development of 3D electromagnetic PIC codes comparing conforming Finite Elements and Discontinuous Galerkin Solvers on unstructured grids. <http://www-math.u-strasbg.fr/houpic/>.
- Non thematic ANR: EGYPT project (leader Ph. Ghendrih). Study of gyrokinetic models and their numerical approximation. In collaboration with DRFC/CEA-Cadarache.

7.3.2. INRIA Large Scale Initiative "Fusion"

- Eric Sonnendrücker is heading the Large Scale Initiative Fusion energy that started at the beginning of 2009 http://www-math.u-strasbg.fr/ae_fusion/.
- Every member of Calvi is involved within this Large Scale Initiative.

7.3.3. INRIA ADT SeLaLib

- ADT SeLaLib was launch in fall 2010.
- Edwin Chacon-Golcher joined Calvi team in december as Senior Engineer as leader of the future Engineer team.
- An API for SeLaLib is being defined (in collaboration with the CEA Gysela team).

7.3.4. Cemracs 2010 projects

(Details on Cemracs projects may be found on the web page: http://smai.emath.fr/cemracs/cemracs10/fr_projects.html)

- Guillaume Latu, Ahmed Ratnani and Eric Sonnendrücker were involved in Cemracs Project "Gyronurbs" whose target was to solve the Vlasov equation in complex geometry using Nurbs.
- Aurore Back, Anaïs Crestetto, Ahmed Ratnani and Eric Sonnendrücker were involved in Cemracs Project "IsoPic" whose target was to develop an axisymmetric PIC code based on isogeometric analysis.
- Nicolas Crouseilles and Michel Mehrenberger were involved in Cemracs Project "VlasovDG" whose target was to develop a Discontinuous Galerkin Vlasov code.

7.4. European initiatives

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

This project involves several French and German teams both in the applied mathematics and in the fluid dynamics community. Its aim is the development of numerical methods for the computation of noise generated in turbulent flows and to understand the mechanisms of this noise generation.

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

7.4.2. EUFORIA Project

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

7.5. International initiative

7.5.1. Project "Adaptive Multilevel Particle Schemes for Plasma Simulations"

Participant: Martin Campos Pinto.

Funded by a Fulbright grant this project is developed in collaboration with A. Friedman from the Lawrence Berkeley National Laboratory and J. Verboncoeur at the University of California, Berkeley.

8. Dissemination

8.1. Leadership within scientific community

8.1.1. Conferences, meetings and tutorial organization

- Nicolas Crouseilles and Eric Sonnendrücker organized Cemracs 2010 in Marseille (120 participants over 6 weeks) (<http://smai.emath.fr/cemracs/cemracs10/>)
 - During the first week : Summer school on numerical methods for fusion.
 - During the five other weeks : Projects supported by INRIA, CEA, Universities, CNRS.
- Giovanni Manfredi jointly edited the proceedings of the international workshop "Vlasovia 2009" (Luminy, Marseille, 2009), which are to be published in the journal "Transport theory and statistical physics".
- Jean Rodolphe Roche is the research coordinator of the L.R.C. projet - Full wave modelling of lower hybrid current drive in tokamaks.

8.1.2. Invitations at conferences and summer schools

- Jean-Philippe Braeunig
 - was invited to give a talk at the meeting of ANR Project Espoir in June.
 - was invited by Prof. Dias to give the following talk: "Some improvements and applications of the Finite Volumes FVCF-NIP method for the simulation of compressible multi-material fluid flows" at the "Seminary of the School of Mathematical Sciences", University College Dublin, Ireland in January.
 - gave the following conferences:
 - * "Some numerical aspects of conservative schemes in a 4D Vlasov drift-kinetic code"

* "The Enhanced NIP method for multi-material fluid flows"

at the "Workshop on the Physical and Numerical Modeling of Turbulent and Multi-Phase Flows" in Cargèse, Corsica in September.

- Nicolas Crouseilles gave talks in
 - Canum 2010 in Carcans-Maubuisson; June 2 (<http://smai.emath.fr/canum2010/>).
 - Program "Partial Differential Equations in Kinetic Theories" in Cambridge - satellite workshop in Edinburgh; 8-12 november : "PDEs in kinetic theories: kinetic description of biological models" (<http://www.icms.org.uk/workshops/kintheories>).
- Emmanuel Frénod was invited by "Doctorials" of "École Doctorale de Mathématiques et d'Informatique de Dakar" to give a conference on "Usefulness of Modelling and Asymptotic Analysis", February 8 and 9.
- Paul-Antoine Hervieux gave the following talk : "Electron dynamics and ultrafast ionization of clusters and fullerenes", at the European Conference on Atoms, Molecules and Photons in Salamanca (Spain); July.
- Simon Labrunie was invited to make conferences:
 - Sixth Singular Days on Asymptotic Methods for PDEs in Berlin; April 29 - May 1.
 - ECCM 10 ("Fourth European Conference on Computational Mechanics") in Paris; May 16 - 21.
- Giovanni Manfredi gave the following talks:
 - "Electron dynamics and ultrafast ionization of clusters and fullerenes", at the European Conference on Atoms, Molecules and Photons, Salamanca (Spain), July.
 - "Electron Thermalization and Decoherence in Thin Metal Films", at the annual meeting of the European COST action CUSPFEL (Chemistry With Ultrashort Pulses and Free-Electron Lasers) in Heraklion (Greece); October 23-25.
 - "Quantum fidelity for many-particle systems", at QCHAOS 2010: 4th Workshop on Quantum Chaos, Theory and Applications, Castro Urdiales (Spain), September 13-17.
- Eric Sonnendrücker was invited for talks at:
 - Plasma day at university Paris 6, mars 15.
 - Mini-symposium at the SIAM meeting on Dynamical Systems and Partial Differential Equations, Barcelona, May 31-June 4.
 - Symposium on new trends in numerical methods for plasma physics, Garching, Germany, July 8.
 - Workshop Frontiers in Computational Astrophysics, ENS Lyon, October 11-15.
 - Day on mathematics for energy organized by GdR Momas and CHANT, Paris, November 5.
 - Workshop Classical and Quantum Mechanical Models of Many-Particle Systems, Oberwolfach, Germany, December 6-10.

8.1.3. Administrative duties

- Nicolas Crouseilles was member of board of examiners for the position "MdC chaire INRIA" at Pau.
- Jean Rodolphe Roche is the research coordinator of a CAPES-COFECUB bilateral agreement with the Federal University of Rio de Janeiro and the National Laboratory of Scientific Computing of Brazil.

- Eric Sonnendrücker is a member of CNU 26, applied mathematics and applications of mathematics.
- Eric Sonnendrücker was a member of the board of examiners for professor positions at the university of Mulhouse and the ENS Cachan.
- Eric Sonnendrücker is a member of panel 6 (mathematics and computer science) of GENCI for the attribution of computing hours on the french supercomputing systems

8.2. Teaching

- Emmanuel Frénod was invited by "Département de Mathématiques et Informatique" to give a 10-hour course for Master and Ph. D. students in Mathematics and Computer Sciences on "Two-Scale Convergence and Application to Seabed Morpho-dynamics in Tide-Influenced Coastal Ocean Waters".
- Vladimir Latocha gave lectures on Scientific Computation in the Master in mathematics of UHP.
- Giovanni Manfredi and Paul-Antoine Hervieux taught a 28-hour course at the Master "Condensed Matter and Nanophysics". Title of the course: Photon-matter interactions.
- Jean Rodolphe Roche gave lectures on Domain Decomposition in the M2 in mathematics of UHP.
- Eric Sonnendrücker taught a course on numerical methods for the Vlasov-Maxwell equations in the Master 2 of mathematics at the University of Strasbourg.

8.3. Ph. D. Theses

8.3.1. Ph. D. defended in 2010

1. Thomas Respaud, *Numerical coupling of Maxwell and Vlasov equations*. Advisor: Eric Sonnendrücker, defended: 2nd November.

8.3.2. Ph. D. in progress

1. Aurore Back, *Hamiltonian derivation of gyrokinetic models*. Advisors: Emmanuel Frénod and Eric Sonnendrücker.
2. Anaïs Crestetto, *High order moments fluid model for plasmas and multiphase media*. Advisors: Philippe Helluy and Marc Massot.
3. Céline Caldini, since October 2010, *Mathematical and numerical analysis of gyro-kinetic models - Application to magnetic confinement*. Advisor: Mihai Bostan
4. Pierre Glanc, since October 2010, *Numerical approximation of Vlasov's equations with conservative remapping methods*. Advisors: Nicolas Crouseilles, Emmanuel Frénod, Philippe Helluy and Michel Mehrenberger
5. Takashi Hattori, *Domain decomposition methods for full wave simulation in cold plasma*. Advisors: Simon Labrunie and Jean Rodolphe Roche.
6. Sandrine Marchal, *Domain decomposition methods to solve a system of hyperbolic equations*. Advisors: Simon Labrunie and Jean Rodolphe Roche.
7. Mathieu Lutz, since September 2010, *Mathematical and numerical study of a gyrokinetic model including electromagnetic effects for Tokamak plasma simulation*. Advisors: Emmanuel Frénod and Eric Sonnendrücker.
8. Ahmed Ratnani, *Study of the quasi-neutrality equation and its coupling with Vlasov equations*. Advisors: Nicolas Crouseilles and Eric Sonnendrücker.

8.3.3. Post Doc in progress

1. Morgane Bergot, since December 2010, *High order time schemes for conservative semi-Lagrangian Vlasov solvers*. Advisors: Eric Sonnendrücker.
2. Olivier Hoenen, *Visualisation tools for fusion*. Advisors: Eric Sonnendrücker

9. 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).
- [2] N. BESSE, M. MEHRENBERGER. *Convergence of classes of high-order semi-Lagrangian schemes for the Vlasov Poisson system*, in "Math. Comp.", 2005, vol. 77, p. 93–123, <http://www.ams.org/journals/mcom/2008-77-261/S0025-5718-07-01912-6/home.html>.
- [3] M. CAMPOS PINTO, M. MEHRENBERGER. *Convergence of an adaptive semi-Lagrangian scheme for the Vlasov-Poisson system*, in "Numer. Math.", 2008, vol. 108, n^o 3, p. 407-444, <http://hal.archives-ouvertes.fr/inria-00070487/en/>.
- [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>.
- [5] N. CROUSEILLES, M. MEHRENBERGER, E. SONNENDRÜCKER. *Conservative semi-Lagrangian schemes for the Vlasov equation*, in "J. Comput. Phys.", 2010, vol. 229, p. 1927-1953, <http://dx.doi.org/10.1006/jcph.2001.6818>.
- [6] F. FILBET, E. SONNENDRÜCKER, P. BERTRAND. *Conservative numerical schemes for the Vlasov equation*, in "J. Comput. Phys.", 2001, vol. 172, n^o 1, p. 166–187, <http://dx.doi.org/10.1006/jcph.2001.6818>.
- [7] F. FILBET, E. SONNENDRÜCKER. *Modeling and numerical simulation of space charge dominated beams in the paraxial approximation*, in "Math. Models Methods Appl. Sci.", 2006, vol. 16, n^o 5, p. 763–791, <http://hal.archives-ouvertes.fr/inria-00070460/en/>.
- [8] E. FRÉNOT, E. SONNENDRÜCKER. *The finite Larmor radius approximation*, in "SIAM J. Math. Anal.", 2001, vol. 32, n^o 6, p. 1227–1247, <http://hal.archives-ouvertes.fr/inria-00072809/en/>.
- [9] V. GRANDGIRARD, Y. SARAZIN, P. ANGELINO, A. BOTTINO, N. CROUSEILLES, G. DARMET, G. DIF-PRADALIER, X. GARBET, P. GHENDRIH, S. JOLLIET, G. LATU, E. SONNENDRÜCKER, L. VILLARD. *Global full-f gyrokinetic simulations of plasma turbulence*, in "Plasma Physics and Controlled Fusion", 2007, vol. 49, n^o 12B, p. B173-B182, <http://stacks.iop.org/0741-3335/49/B173>.
- [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

Articles in International Peer-Reviewed Journal

- [11] P. AILLIOT, E. FRÉNOT, V. MONBET. *Modeling the Coastal Ocean over a Time Period of Several Weeks*, in "Journal of Differential Equations", Feb 2010, vol. 246, n^o 4, p. 639 - 659, <http://hal.inria.fr/hal-00202638/en>.
- [12] P. BECHOUCHE, N. BESSE. *Analysis of a semi-Lagrangian method for the spherically symmetric Vlasov-Einstein system*, in "ESAIM-M2AN: Math. Mod. Numer. Anal.", 2010, vol. 44, p. 573-595, <http://dx.doi.org/10.1051/m2an/2010012>.
- [13] N. BESSE. *On the Cauchy problem for the gyro-water-bag model*, in "Math. Mod. Meth. Appl. Sci.", 2011, Accepted.
- [14] N. BESSE. *On the water-bag continuum*, in "Arch. Rational Mech. Ana.", 2011, Accepted.
- [15] N. BESSE, Y. ELSKENS, D. ESCANDE, P. BERTRAND. *Validity of the quasilinear theory: refutations and new numerical confirmation*, in "Plasma Phys. Control. Fusion", 2011, Accepted.
- [16] M. BOSTAN. *Boundary value problem for the stationary Nordström-Vlasov system*, in "J. Korean Math. Soc.", 2010, vol. 47, n^o 4, p. 743-766.
- [17] M. BOSTAN. *Transport equations with disparate advection fields. Application to the gyrokinetic models in plasma physics*, in "J. Differential Equations", 2010, vol. 249, p. 1620-1663, <http://dx.doi.org/10.1016/j.jde.2010.07.010>.
- [18] M. BOSTAN, I. GAMBA, T. GOUDON, A. VASSEUR. *Boundary value problems for the stationary Vlasov-Boltzmann-Poisson equation*, in "Indiana University Mathematical Journal", 2010, to appear, <http://rene.ma.utexas.edu/users/gamba/papers/slab-BTE-poisson-08.pdf>.
- [19] J.-P. BRAEUNIG. *An algorithm to control the pressure evolution for the FVCF-NIP method for compressible multi-material fluid flows*, in "International Journal on Finite Volumes", Nov 2010, vol. 1, n^o 7, p. pp 101-132, <http://hal.inria.fr/hal-00531586/en>.
- [20] N. CROUSEILLES, M. MEHRENBERGER, H. SELLAMA. *Numerical solution of the gyroaverage operator for the finite gyroradius guiding-center model.*, in "Communications in Computational Physics", Sep 2010, vol. 8, n^o 3, p. 484-510, <http://hal.inria.fr/inria-00507301/en>.
- [21] N. CROUSEILLES, M. MEHRENBERGER, E. SONNENDRÜCKER. *Conservative semi-Lagrangian schemes for the Vlasov equation*, in "J. Comput. Phys.", 2010, vol. 229, p. 1927-1953, <http://www.sciencedirect.com/science/article/B6WHY-4XSTDBW-1/2/ed303f797cb08e5769bc541b055ce745>.
- [22] I. FAYE, E. FRÉNOT, D. SECK. *Singularly perturbed degenerated parabolic equations and application to seabed morphodynamics in tided environment*, in "Discrete and Continuous Dynamical Systems: Series A", 2011, vol. 29, n^o 3, p. 1001-1030, <http://hal.archives-ouvertes.fr/hal-00433133/en/>.
- [23] E. FRÉNOT, A. MOUTON. *Two-dimensional Finite Larmor Radius approximation in canonical gyrokinetic coordinates*, in "Journal of Pure and Applied Mathematics: Advances and Applications", 2010, vol. 4, n^o 2, p. 135-166, <http://hal.inria.fr/hal-00531361/en>.

- [24] R. JASIAK, G. MANFREDI, P.-A. HERVIEUX. *Electron thermalization and quantum decoherence in metal nanostructures*, in "Phys. Rev. B", Jun 2010, vol. 81, n^o 24, 241401, <http://link.aps.org/doi/10.1103/PhysRevB.81.241401>.
- [25] G. MANFREDI, S. HIRSTOAGA, S. DEVAUX. *Vlasov modelling of parallel transport in a tokamak scrape-off layer*, in "Plasma Physics and Controlled Fusion", 2011, vol. 53, n^o 1, 015012, <http://stacks.iop.org/0741-3335/53/i=1/a=015012>.
- [26] O. MORANDI, P.-A. HERVIEUX, G. MANFREDI. *Pseudo-fermion formalism applied to nonequilibrium Kondo-type problems*, in "Nuovo Cim.", Jan 2010, vol. 33C, n^o 1, p. 173-180, <http://paperseek.sif.it/index.php?doi=10.1393/ncc/i2010-10577-1>.
- [27] O. MORANDI, P.-A. HERVIEUX, G. MANFREDI. *Time-dependent model for diluted magnetic semiconductors including band structure and confinement effects*, in "Phys. Rev. B", Apr 2010, vol. 81, n^o 15, 155309, <http://link.aps.org/doi/10.1103/PhysRevB.81.155309>.
- [28] O. MORANDI, P.-A. HERVIEUX. *Third-order many-body perturbation theory applied to Kondo-type dynamics in diluted magnetic semiconductors*, in "Phys. Rev. B", May 2010, vol. 81, n^o 19, 195215, <http://link.aps.org/doi/10.1103/PhysRevB.81.195215>.
- [29] T. RESPAUD, E. SONNENDRÜCKER. *Analysis of a new class of Forward Semi-Lagrangian schemes for the 1D Vlasov-Poisson Equations*, in "Numerische Mathematik / Numerical Mathematics", 2011, MSC: 65M12, 78A35 [DOI : 10.1007/s00211-010-0351-2], <http://hal.archives-ouvertes.fr/hal-00442957/en/>.
- [30] Y. SARAZIN, V. GRANDGIRARD, J. ABITEBOUL, S. ALLFREY, X. GARBET, P. GHENDRIH, G. LATU, A. STRUGAREK, G. DIF-PRADALIER. *Large scale dynamics in flux driven gyrokinetic turbulence*, in "Nuclear Fusion", 2010, vol. 50, n^o 5, 054004, <http://stacks.iop.org/0029-5515/50/i=5/a=054004>.

International Peer-Reviewed Conference/Proceedings

- [31] A. CANELAS, J. HERSKOVITS, J.-R. ROCHE. *Shape Optimization for Inverse Electromagnetic Casting Problems*, in "Inverse Problems, Design and Optimization Symposium - IPDO2010", Brésil João Pessoa, Nov 2010, <http://hal.inria.fr/inria-00532882/en>.

Workshops without Proceedings

- [32] A. CANELAS, J.-R. ROCHE, J. HERSKOVITS. *Shape Optimization for Direct and Inverse Electromagnetic Casting Problem*, in "IV European Conference on Computational Mechanics – ECCM 2010", France Paris, ECCOMAS, Nov 2010, <http://hal.inria.fr/inria-00532909/en>.

Scientific Books (or Scientific Book chapters)

- [33] G. MANFREDI, P.-A. HERVIEUX, Y. YIN, N. CROUSEILLES. *Collective Electron Dynamics in Metallic and Semiconductor Nanostructures*, in "Advances in the Atomic-Scale Modeling of Nanosystems and Nanostructured Materials", C. MASSOBRIO, H. BULOUE, C. GOYHENEX (editors), Lecture Notes in Physics, Springer Berlin / Heidelberg, 2010, vol. 795, p. 1-44, 10.1007/978-3-642-04650-6_1, http://dx.doi.org/10.1007/978-3-642-04650-6_1.

Research Reports

- [34] J. GUTERL, J.-P. BRAEUNIG, N. CROUSEILLES, V. GRANDGIRARD, G. LATU, M. MEHREBERGER, E. SONNENDRÜCKER. *Test of some numerical limiters for the conservative PSM scheme for 4D Drift-Kinetic simulations.*, INRIA, 2010, <http://hal.archives-ouvertes.fr/inria-00540948/en/>.

Other Publications

- [35] N. BESSE. *Global weak solution for the relativistic waterbag continuum*, submitted.
- [36] M. BOSTAN. *Gyrokinetic Vlasov equation in three dimensional setting. Second order approximation*, 2010, to appear, http://hal.archives-ouvertes.fr/docs/00/43/12/89/PDF/main_CentreGuide3D.pdf.
- [37] M. CAMPOS PINTO, S. JUND, S. SALMON, E. SONNENDRÜCKER. *Charge conserving FEM-PIC schemes on general grids*, submitted, <http://hal.archives-ouvertes.fr/hal-00311429/fr/>.
- [38] A. CANELAS, J.-R. ROCHE, J. HERSKOVITS. *Shape optimization for inverse electromagnetic casting problems*, 2010, <http://hal.inria.fr/inria-00533699/en>.
- [39] P. CIARLET, S. LABRUNIE. *Numerical solution of Maxwell's equations in axisymmetric domains with the Fourier Singular Complement Method*, 2010, 37 pages, <http://hal.inria.fr/hal-00365391/en>.
- [40] N. CROUSEILLES, M. LEMOU. *An asymptotic preserving scheme based on a micro-macro decomposition for collisional Vlasov equations: diffusion and high-field scaling limits.*, 2010, <http://hal.inria.fr/hal-00533327/en>.
- [41] N. CROUSEILLES, T. RESPAUD. *A charge preserving scheme for the numerical resolution of the Vlasov-Ampère equations*, 2010, <http://hal.inria.fr/hal-00533390/en>.
- [42] N. CROUSEILLES, M. MEHREBERGER, F. VECIL. *Discontinuous Galerkin semi-Lagrangian method for Vlasov-Poisson*, Submitted, <http://hal.archives-ouvertes.fr/hal-00544677/en/>.
- [43] P. DEGOND, S. HIRSTOAGA, M.-H. VIGNAL. *The Vlasov model under large magnetic fields in the low-Mach number regime*, 2010, in revision, <http://hal.archives-ouvertes.fr/hal-00384345/fr/>.
- [44] W. DESPAGNE, E. FRÉNOT. *Transport hub flow modelling*, <http://hal.inria.fr/hal-00522938/en>.
- [45] S. LABRUNIE, S. MARCHAL, J.-R. ROCHE. *Local existence and uniqueness of the mild solution to the 1D Vlasov-Poisson system with an initial condition of bounded variation*, 2010, <http://hal.inria.fr/hal-00397497/en>.
- [46] M. LANGLAIS, G. LATU, J. ROMAN, P. SILAN. *Highly scalable parallel simulator of a host-parasite system*, 2010, <http://hal.inria.fr/hal-00453501/en>.
- [47] R. LOUBÈRE, J.-P. BRAEUNIG, J.-M. GHIDAGLIA. *A totally Eulerian Finite Volume solver for multi-material fluid flows: Enhanced Natural Interface Positioning (ENIP)*, 2010, 28 pages, <http://hal.inria.fr/hal-00527765/en>.
- [48] P. MOREL, E. GRAVIER, N. BESSE, R. KLEIN, A. GHIZZO, X. GARBET, P. BERTRAND. *Water-bag modeling of a multispecies plasma*, submitted.

- [49] A. RATNANI, E. SONNENDRÜCKER. *Arbitrary High-Order Spline Finite Element Solver for the Time Domain Maxwell equations*, 2010, <http://hal.inria.fr/hal-00507758/en>.

References in notes

- [50] F. ASSOUS, P. CIARLET, S. LABRUNIE. *Theoretical tools to solve the axisymmetric Maxwell equations*, in "Math. Meth. Appl. Sci.", 2002, vol. 25, p. 49–78.
- [51] F. ASSOUS, P. CIARLET, S. LABRUNIE. *Solution of axisymmetric Maxwell equations*, in "Math. Meth. Appl. Sci.", 2003, vol. 26, p. 861–896.
- [52] 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. Comp. Phys.", 2003, vol. 191, p. 147–176.
- [53] 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, p. 147–176.
- [54] F. ASSOUS, P. CIARLET, J. SEGRÉ. *Numerical solution to the time dependent Maxwell equations in two dimensional singular domains: the Singular Complement Method*, in "J. Comput. Phys.", 2000, vol. 161, p. 218–249.
- [55] F. ASSOUS, P. CIARLET, E. SONNENDRÜCKER. *Resolution of the Maxwell equations in a domain with reentrant corners*, in "M 2 AN", 1998, vol. 32, p. 359–389.
- [56] C. BARDOS, P. DEGOND. *Global existence for the Vlasov-Poisson equation in 3 space variables with small initial data*, in "Ann. Inst. H. Poincaré Anal. Non Linéaire", 1985, vol. 2, n^o 2, p. 101–118.
- [57] S. BENACHOUR, F. FILBET, P. LAURENÇOT, E. SONNENDRÜCKER. *Global existence for the Vlasov-Darwin system in \mathbb{R}^3 for small initial data*, in "Math. Methods Appl. Sci.", 2003, vol. 26, n^o 4, p. 297–319.
- [58] C. BERNARDI, M. DAUGE, Y. MADAY. *Spectral methods for axisymmetric domains*, Series in Applied Mathematics, Gauthier-Villars, Paris and North Holland, Amsterdam, 1999.
- [59] C. BIRDSALL, A. LANGDON. *Plasma Physics via Computer Simulation*, McGraw-Hill, New York, 1985.
- [60] M. BOSTAN. *The Vlasov-Poisson system with strong external magnetic field. Finite Larmor radius regime*, in "Asymptot. Anal.", 2007, vol. 62, n^o 2, p. 91-123, <http://hal.archives-ouvertes.fr/docs/00/25/80/24/PDF/Bostan2.pdf>.
- [61] M. BOSTAN. *Stationary solutions for the one dimensional Nordström-Vlasov system*, in "Asymptot. Anal.", 2009, vol. 64, n^o 3-4, p. 155-183.
- [62] Y. BRENIER. *Convergence of the Vlasov-Poisson system to the incompressible Euler equations*, in "Comm. Partial Differential Equations", 2000, vol. 25, n^o 3-4, p. 737–754.

- [63] P. CIARLET, N. FILONOV, S. LABRUNIE. *Un résultat de fermeture pour les équations de Maxwell en géométrie axisymétrique*, in "C. R. Acad. Sci. Paris série I", 2000, vol. 331, p. 293–298.
- [64] P. CIARLET, B. JUNG, S. KADDOURI, S. LABRUNIE, J. ZOU. *The Fourier–Singular Complement method for the Poisson problem. Part II: axisymmetric domains*, in "Numer. Math.", 2006, vol. 102, p. 583–610.
- [65] N. CROUSEILLES, T. RESPAUD, E. SONNENDRÜCKER. *A forward semi-Lagrangian method for the numerical solution of the Vlasov equation*, in "Comput. Phys. Comm.", 2009, vol. 180, p. 1730 - 1745.
- [66] R. DIPERNA, P.-L. LIONS. *Global weak solutions of the Vlasov-Maxwell systems*, in "Comm. Pure. Appl. Math.", 1989, vol. XLII, p. 729–757.
- [67] F. FILBET, E. SONNENDRÜCKER, P. BERTRAND. *Conservative numerical schemes for the Vlasov equation*, in "J. Comput. Phys.", 2001, vol. 172, n^o 1, p. 166–187.
- [68] E. FRÉNOT, E. SONNENDRÜCKER. *Long time behavior of the Vlasov equation with a strong external magnetic field*, in "Math. Models Methods Appl. Sci.", 2000, vol. 10, n^o 4, p. 539–553.
- [69] E. FRÉNOT, E. SONNENDRÜCKER. *The finite Larmor radius approximation*, in "SIAM J. Math. Anal.", 2001, vol. 32, n^o 6, p. 1227–1247.
- [70] E. FRÉNOT, E. SONNENDRÜCKER. *Homogenization of the Vlasov equation and of the Vlasov-Poisson system with a strong external magnetic field*, in "Asymptot. Anal.", 1998, vol. 18, n^o 3-4, p. 193–213.
- [71] E. FRÉNOT, A. MOUTON, E. SONNENDRÜCKER. *Two-scale numerical simulation of the weakly compressible 1D isentropic Euler equations*, in "Numerische Mathematik / Numerical Mathematics", 2007, vol. 108, n^o 2, p. 263-293, <http://hal.archives-ouvertes.fr/hal-00173412/en/>.
- [72] E. FRÉNOT, F. SALVARANI, E. SONNENDRÜCKER. *Long time simulation of a beam in a periodic focusing channel via a two-scale PIC-method*, in "Mathematical Models and Methods in Applied Sciences", 2009, vol. 19, n^o 2, p. 175-197, ACM 82D10 35B27 76X05, <http://hal.archives-ouvertes.fr/hal-00180700/en/>.
- [73] E. GARCIA, S. LABRUNIE. *Régularité spatio-temporelle de la solution des équations de Maxwell dans des domaines non-convexes*, in "C. R. Acad. Sci. Paris, série I", 2002, vol. 334, p. 293–298.
- [74] R. T. GLASSEY. *The Cauchy problem in kinetic theory*, Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 1996.
- [75] F. GOLSE, L. SAINT-RAYMOND. *The Vlasov-Poisson system with strong magnetic field in quasineutral regime*, in "Math. Models Methods Appl. Sci.", 2003, vol. 13, n^o 5, p. 661–714.
- [76] M. GRIEBEL, G. ZUMBUSCH. *Hash based adaptive parallel multilevel methods with space-filling curves*, 2000.
- [77] E. HORST, R. HUNZE. *Weak solutions of the initial value problem for the unmodified nonlinear Vlasov equation*, in "Math. Methods Appl. Sci.", 1984, vol. 6, n^o 2, p. 262–279.

- [78] M. PARASHAR, J. C. BROWNE, C. EDWARDS, K. KLIMKOWSKI. *A common data management infrastructure for adaptive algorithms for PDE solutions*, 1997.
- [79] L. SAINT-RAYMOND. *The gyrokinetic approximation for the Vlasov-Poisson system*, in "Math. Models Methods Appl. Sci.", 2000, vol. 10, n^o 9, p. 1305–1332.
- [80] E. VIOLARD. *A Semantic Framework To Adress Data Locality in Data Parallel Programs*, in "Parallel Computing", 2004, vol. 30, n^o 1, p. 139–161.