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Project-Team CALVI

Scientific computation and visualization

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

RESEARCH CENTER
Nancy - Grand Est

THEME
Computational models and simulation

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Project-Team CALVI

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2. Overall Objectives

2.1. Introduction

CALVI was created in June 2003.

It is a project that initially associates Institut Elie Cartan de Lorraine (IECL, UMR 7502, CNRS, Inria and Université de Lorraine), 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 de Lorraine).

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**. The visualization topics were discontinued after the departure of one of our collaborator.

The CALVI project ended on December 2013. The main research subjects developed in CALVI will be continued through the new project TONUS, which started in January 2014.

2.2. Highlights of the Year

The Selalib project has made important progress in its development as it prepares for a release in 2014 with new additions in terms of capabilities and contributors.

3. Research Program

3.1. Kinetic models for plasma and beam physics

plasma physics, beam physics, kinetic models, reduced models, Vlasov equation, modeling, mathematical analysis, asymptotic analysis, existence, uniqueness

Plasmas and particle beams can be described by a hierarchy of models including N -body interaction, kinetic models and fluid models. Kinetic models in particular are posed in phase-space and involve specific difficulties. We perform a mathematical analysis of such models and try to find and justify approximate models by using asymptotic analysis or other approximations. The resulting reduced models can be of several natures: gyrokinetic, fluid-like, *etc.*

3.1.1. Models for plasma and beam physics

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

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

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

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

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

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

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

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

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

and current density

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

associated to the charged particles.

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

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

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

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

3.1.2. *Mathematical and asymptotic analysis of kinetic models*

The mathematical analysis of the Vlasov equation is essential for a thorough understanding of the model as well for physical as for numerical purposes. It has attracted many researchers since the end of the 1970s. Among the most important results which have been obtained, we can cite the existence of strong and weak solutions of the Vlasov-Poisson system by Horst and Hunze [73], see also Bardos and Degond [55]. The existence of a weak solution for the Vlasov-Maxwell system has been proved by Di Perna and Lions [63]. An overview of the theory is presented in a book by Glassey [70].

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 [56].

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 [71], [76] as well as by Brenier [59]. 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 [68], [66], [67].

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

3.2. Development of simulation tools

Numerical methods, Vlasov equation, unstructured grids, adaptivity, numerical analysis, convergence, Semi-Lagrangian method The development of efficient numerical methods is essential for the simulation of plasmas and beams. Indeed, kinetic models are posed in phase space and thus the number of dimensions is doubled. Our main effort lies in developing methods using a phase-space grid as opposed to particle methods. In order to make such methods efficient, it is essential to consider means for optimizing the number of mesh points. This is done through different adaptive strategies. In order to understand the methods, it is also important to perform their mathematical analysis. Since a few years we are interested also with solvers that uses Particle In Cell method. This new issue allows us to enrich some parts of our research activities previously centered on the Semi-Lagrangian approach.

3.2.1. *Introduction*

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

3.2.2. Convergence analysis of numerical schemes

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

3.2.3. The semi-Lagrangian method

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

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

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

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

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

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

1. For all i, j , compute the origin of the characteristic ending at $\mathbf{x}_i, \mathbf{v}_j$, i.e. an approximation of $\mathbf{X}(t_n; \mathbf{x}_i, \mathbf{v}_j, t_{n+1}), \mathbf{V}(t_n; \mathbf{x}_i, \mathbf{v}_j, t_{n+1})$.
2. As $f^{n+1}(\mathbf{x}_i, \mathbf{v}_j) = f^n(\mathbf{X}(t_n; \mathbf{x}_i, \mathbf{v}_j, t_{n+1}), \mathbf{V}(t_n; \mathbf{x}_i, \mathbf{v}_j, t_{n+1}))$, f^{n+1} can be computed by interpolating f^n which is known at the grid points at the points $\mathbf{X}(t_n; \mathbf{x}_i, \mathbf{v}_j, t_{n+1}), \mathbf{V}(t_n; \mathbf{x}_i, \mathbf{v}_j, t_{n+1})$.

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

3.2.4. Adaptive semi-Lagrangian methods

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

3.2.5. Particle-In-Cell codes

The Particle-In-Cell method [58] consists in solving the Vlasov equation using a particle method, i.e. advancing numerically the particle trajectories which are the characteristics of the Vlasov equation, using the equations of motion which are the ordinary differential equations defining the characteristics. The self-fields are computed using a standard method on a structured or unstructured grid of physical space. The coupling between the field solve and the particle advance is done on the one hand by depositing the particle data on the grid to get the charge and current densities for Maxwell's equations and, on the other hand, by interpolating the fields at the particle positions. This coupling is one of the difficult issues and needs to be handled carefully.

3.2.6. Fully Eulerian solvers

Recently, we have started to work on fully Eulerian solvers for approximating the Vlasov equation. Such solvers can be more expensive than semi-Lagrangian solvers. However they are more adapted to full parallelism and the resolution of the small time scales required for taking into account light particles effects.

3.2.7. Electromagnetic solvers

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 [54] and implemented [53] 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 [57]. The non-density result for regular fields was proven [62], 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 [69], [51].

3.3. Large size problems

Parallelism, domain decomposition, code transformation

3.3.1. Introduction

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

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

3.3.2. Parallelization of numerical methods

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

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

Parallelism, for such data-parallel PDE solvers, is achieved by partitioning the mesh and mapping the sub-meshes onto the processors of a parallel architecture. A good partition balances the workload while minimizing the communications overhead. Many interesting heuristics have been proposed to compute near-optimal partitions of a (regular or irregular) mesh. For instance, the heuristics based on space-filling curves [72] 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 [77], 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 [74] as an example of such modular software infrastructure).

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

Moreover, exploiting heterogeneous architectures requires the use of a run time support associated with a programming interface that enables some low-level hardware characteristics to be unified. Such run time support is the basis for heterogeneous algorithmics. Candidates for such a run time support may be specific implementations of MPI such as MPICH-G2 (a grid-enabled MPI implementation on top of the GLOBUS tool kit for grid computing [65]).

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

4. Application Domains

4.1. Thermonuclear fusion

Inertial fusion, magnetic fusion, ITER, particle accelerators, laser-matter interaction

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

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

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

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

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

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

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

4.2. Nanophysics

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

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

Using a Vlasov Eulerian code, we have investigated in detail the microscopic electron dynamics in the relevant phase space. Thanks to a numerical scheme recently developed by Filbet et al. [64], 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.

¹ <http://www.iter.org>

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 and Platforms

5.1. SeLaLib

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

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

This year many developments have incorporated into Selalib: semi-Lagrangian solvers on curvilinear grids, new models, new fully-Eulerian solvers, new linear solvers for the Poisson or quasineutrality equation. More details are given in the corresponding sections, because we always try to test our new algorithms within Selalib.

Selalib is available on the Inria Forge <http://selalib.gforge.inria.fr/>

5.2. CLAC

Participants: Philippe Helluy, Michel Massaro, Thomas Strub.

CLAC is a generic Discontinuous Galerkin solver, written in C/C++, based on the OpenCL and MPI frameworks. CLAC means "Conservation Laws Approximation on many Cores".

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

We have invested for several years now into scientific computing on GPUs, using the open standard OpenCL (Open Computing Language). We were recently awarded a prize in the international AMD OpenCL innovation challenge thanks to an OpenCL two-dimensional Vlasov-Maxwell solver that fully runs on a GPU. OpenCL is a very interesting tool because it is an open standard now available on almost all brands of multicore processors and GPUs. The same parallel program can run on a GPU or a multicore processor without modification.

CLAC is also a joint project with a Strasbourg small company, AxesSim, which develops software for electromagnetic simulations.

Because of the envisaged applications of CLAC, which may be either academic or commercial, it is necessary to conceive a modular framework. The heart of the library is made of generic parallel algorithms for solving conservation laws. The parallelism can be both fine-grained (oriented towards GPUs and multicore processors) and coarse-grained (oriented towards GPU clusters). The separate modules allow managing the meshes and some specific applications. In this way, it is possible to isolate parts that should be protected for trade secret reasons. The open source part of CLAC will be made freely available on the web later on. We have made an APP deposit of the first version of CLAC in October 2012. The versioning of CLAC project is also registered in the Inria Forge <http://clac.gforge.inria.fr>.

6. New Results

6.1. Software development

6.1.1. New methods in Selalib

The Selalib library has seen important developments during the year 2013 as we move towards a release in 2014. Several existing modules were improved in terms of their interfaces or implementations, while many other modules were added. Notably, we have improved our interaction with external software (Pigasus, developed by Dr. Ahmed Ratnani) capable of producing NURBS-based coordinate transformations and introduced a general elliptic PDE solver based on finite elements and arbitrary degree splines that can be used as a field solver in domains deformed by an arbitrary coordinate transformation. Preliminary results of these developments have been published ². In addition, we have included new abstractions to facilitate the development of parallel codes using domain decomposition methods. Modules like these have been already used in some of the multiple pre-packaged simulations also included during this period. For instance, it allows us to implement a new Vlasov-Poisson solver by the Eulerian reduced approach, with applications to four-dimensional Landau-Damping. The latest simulations also use newly developed interfaces related with the semi-lagrangian methodology, such as generic interfaces for advections and calculation of characteristics. At the end of 2013 virtually all conceivable abstractions related with the semi-lagrangian methodology have a natural place to live within the library.

Many new and classical methods and models have been cleanly incorporated into our software Selalib:

- Vlasov-Poisson solver by the Eulerian reduced approach. Application to 4D Landau-Damping.
- cartesian semi-Lagrangian 2D guiding center sequential simulation tested on periodic Kelvin Helmholtz instability
- polar semi-Lagrangian 2D guiding center sequential simulation tested on diocotron instability
- general curvilinear semi-Lagrangian 2D guiding center sequential simulation; first results, still in progress
- cartesian semi-Lagrangian 2D Vlasov-Poisson parallel simulation with high order splitting tested on Landau damping, bump on tail, two stream instability and beam
- cartesian semi-Lagrangian 2D Vlasov-Poisson sequential simulation without splitting tested on beam
- cartesian semi-Lagrangian 4D Vlasov-Poisson parallel simulation on cartesian grid with high order splitting tested on Landau-Damping
- polar semi-Lagrangian 4D drift kinetic parallel simulation tested on a simple ITG instability
- general curvilinear semi-Lagrangian 4D drift kinetic parallel simulation (in development)

²A. Back, E. Chacon-Golcher, V. Grandgirard, A. Ratnani, E. Sonnendrücker, A 4D semi-Lagrangian Vlasov solver based on an arbitrary curvilinear grid in physical space, poster at Vlasovia, 25-28 November 2013, Nancy

6.1.2. New developments in CLAC

CLAC is a generic DG solver for hyperbolic conservation laws. It is optimized for running efficiently on GPU clusters. We have reorganized the software conception in order to accelerate the computations. A first point is to group the finite-elements into uniform zones in order to get optimized kernels for SIMD architectures. A second point is to manage efficiently the data transfers between the zone. An important last point is to consider a non blocking parallel task management. This is achieved through a coupling between the event mechanisms of OpenCL and MPI. Some ideas and results are presented in [44]. In addition to these developments, we have started to test some parallel programming approaches in order to achieve good efficiency on multicore processors. These ideas have been tested on fluid models [27] and the MHD model [47]. They are very efficient and will be incorporated into CLAC later on.

6.2. Mathematical analysis of kinetic models

Participants: N. Besse, M. Bostan.

Contribution [13] concerns a one-dimensional version of the Vlasov equation dubbed the Vlasov-Dirac-Benney equation (in short V-D-B) where the self interacting potential is replaced by a Dirac mass. Emphasis is put on the relations between the linearized version, the full nonlinear problem and equations of fluids. In particular the connection with the so-called Benney equation leads to new stability results. Eventually the V-D-B appears to be at the cross road of several problems of mathematical physics which have as far as stability is concerned very similar properties.

The subject matter of paper ³ concerns anisotropic diffusion equations: we consider heat equations whose diffusion matrices have disparate eigenvalues. We determine first and second order approximations, we study their well-posedness and then, we establish convergence results. The analysis relies on averaging techniques, which have been used previously for studying transport equations whose advection fields have disparate components.

In ⁴ we perform an asymptotic analysis of general particle systems arising in collective behavior in the limit of large self-propulsion and friction forces. These asymptotics impose a fixed speed in the limit, and thus a reduction of the dynamics to a sphere in the velocity variables. The limit models are obtained by averaging with respect to the fast dynamics. We can include all typical effects in the applications: short-range repulsion, long-range attraction, and alignment. For instance, we can rigorously show that the Cucker-Smale model is reduced to the Vicsek model without noise in this asymptotic limit. Finally, a formal expansion based on the reduced dynamics allows us to treat the case of diffusion. This technique follows closely the gyroaverage method used when studying the magnetic confinement of charged particles. The main new mathematical difficulty is to deal with measure solutions in this expansion procedure.

6.2.1. Gyrokinetic approximation

Participants: E. Frénod, M. Lutz.

Considering a Hamiltonian Dynamical System describing the motion of charged particle in a Tokamak or a Stellarator, we build in [42] a change of coordinates to reduce its dimension. This change of coordinates is in fact an intricate succession of mappings that are built using Hyperbolic Partial Differential Equations, Differential Geometry, Hamiltonian Dynamical System Theory and Symplectic Geometry, Lie Transforms and a new tool which is here introduced : Partial Lie Sums.

6.3. Development of semi-Lagrangian methods

Participants: N. Crouseilles, P. Glanc, A. Hamiaz, S. Hirstoaga, M. Mehrenberger, J. Petri, E. Sonnendrücker, C. Steiner.

³M. Bostan, Strongly anisotropic diffusion problems; asymptotic analysis, in *J. Differential Equations*, vol. 256 pp. 1043-1092 (2013)

⁴M. Bostan, J.-A. Carrillo, Asymptotic fixed speed reduced dynamics for kinetic equations in swarming, *Math. Models Methods Appl. Sci.*, Vol.23, No. 13 pp. 2353-2393 (2013)

The development of numerical methods - here semi-Lagrangian schemes for plasma physic applications- is continued and strengthened in the context of the on-going library Selalib. We intend to improve the robustness of the numerical tools in order to be prepared for future more realistic test problems.

6.3.1. Vlasov-Poisson simulations on cartesian grids

We have developed a 1D x 1D Vlasov-Poisson solver on GPU using optimized FFT of CUDA and applied it on KEEN waves test case, which needs a fine resolution in velocity [46]. An efficiency of 100 Gflops on 4096x4096 grid is obtained while using single precision, and about 30 GFlops on a 2048x3048 grid using double precision. The approach is valid: implementation effort is reduced, because we rely on external optimizations and the speed-up is quite impressive (only 1 or 2 GFlops were obtained using CPU). We emphasize that FFT is used for the implementation but not (necessarily) for the numerical method. Classical methods like splines or arbitrary high order odd Lagrange interpolation are used, as they can be fitted in this framework. In order to reduce mass conservation issues while using single precision, a delta-f method is validated. The limitation is here the grid size; we were not able to run the code for bigger sizes. We then developed other strategies based on non uniform grids in velocity with cubic splines and two grid strategies⁵ and with the semi-Lagrangian discontinuous Galerkin (SLDG) scheme⁶. Integration of the code in Selalib with upgraded interface to deal with non uniform grids has been thought but remains to be done. Thanks to the MPI Parallelization of the Selalib code, we should be able to run the code for more interesting physical parameters, in particular, when the drive amplitude goes to zero, which leads to even more localized delta-f function in velocity.

Considering the SLDG scheme, we were able to prove a super convergence property in the case of constant linear advection [48].

6.3.2. Guiding-center based simulations on polar grids

We continue our work on polar grids, which are intermediate, between cartesian and general curvilinear grids. We have revisited a diocotron simulation previously done with the PIC method [75] by using a (classical) semi-Lagrangian approach. A detailed study of boundary conditions, energy and mass conservation as well as linear growth rates is performed and validated with the code [33]. We then have extended the code to a first drift kinetic simulation⁷ using at first the classical cubic splines method and then a new 2D conservative method, called CSL2D (conservative semi-Lagrangian 2D), based on mesh intersections and displacement of volumes [11]. For the latter method to work, we had to take care of the Jacobian and we used a delta-f method, in order to treat more easily non zero boundary conditions. We have benefitted from previous experience on the FSL2D (forward semi-Lagrangian) method. Again, the integration in Selalib is under development. Linear growth rate is here validated, by solving numerically the dispersion relation using recent results of [21].

6.3.3. Guiding-center simulations on general curvilinear grids

In order to deal with more complex geometries or to consider field aligned coordinates, we work on generalizing existing methods for curvilinear grids. Guiding center simulations have been successfully performed with the classical cubic splines method and a finite element solver for the Poisson equation developed by A. Back [32]. Further works concern integration in Selalib, in a more modular way. This should help the comparison with other methods as for example the recent CSL2D method [11] but also the previous CSL1D method [5].

6.4. Development of reduced Eulerian methods

Participants: E. Chacon Golcher, P. Helluy, L. Navoret, N. Pham.

⁵M. Mehrenberger, N. Crouseilles, E. Sonnendrücker, B. Afeyan High-Order Numerical Methods for KEEN Wave Vlasov-Poisson Simulations, Poster at PPPS, 16-21 June 2013, San Francisco

⁶C. Steiner, M. Mehrenberger, A semi-Lagrangian discontinuous Galerkin scheme for Vlasov-Poisson equation, poster at Vlasovia, 25-28 November 2013, Nancy

⁷N. Crouseilles, P. Glanc, S. Hirstoaga, E. Madaule, M. Mehrenberger, J. Pétri, Semi-Lagrangian simulations on polar grids: from diocotron instability to ITG turbulence, poster at Vlasovia, 25-28 November 2013, Nancy

6.4.1. Eulerian methods in the physical phase-space

Kinetic plasmas computer simulations are very intensive, because of the gyrokinetic turbulence. In some situations, it is possible to make assumptions on the shape of the distribution function that simplify the model. We obtain in this way a family of fluid or reduced models. If the distribution function has a Maxwellian shape (strong collisions), we obtain the MagnetoHydroDynamic (MHD) model. Even without collisions, the plasma may still relax to an equilibrium state over sufficiently long time scales (Landau damping effect). This indicates that the approximation of the distribution function could require fewer data while still achieving a good representation, even in the collisionless regime. In what follows we call this the “reduced model” approach. A reduced model is a model where the explicit dependence on the velocity variable is suppressed. In a more mathematical way, we consider that in some regions of the plasma, it is possible to exhibit a (preferably small) set of parameters α that allows us to describe the main properties of the plasma with a generalized “Maxwellian” M . Then $f(x, v, t) = M(\alpha(x, t), v)$. In this case it is sufficient to solve for $\alpha(x, t)$. Generally, the vector α is solution of a first order hyperbolic system.

Several approaches are possible that we have started to study theoretically and numerically: waterbag approximations, velocity space transforms, etc.

It is also possible to construct in this way intermediate models between the kinetic and the fluid models by truncating the velocity expansion. The unknowns α of the problem become the coefficients of the expansion, which depend only on space and time. They obey a first order hyperbolic PDE system. And then it is possible to capitalize on the large theoretical and numerical machinery developed for such PDEs.

A first step is to develop the one-dimensional models in order to test several numerical methods. The chosen approach is the high order Discontinuous Galerkin (DG) family of methods for solving the hyperbolic system. We compare the reduced Eulerian model with semi-Lagrangian or PIC methods on classical test cases: Landau damping, two-stream instability [28].

6.4.2. Eulerian method in the Fourier transformed phase-space

An experiment made in the 60's⁸ exhibits in a spectacular way the reversible nature of the Vlasov equations. When two perturbations are applied to a plasma at different times, at first the plasma seems to damp and reach an equilibrium. But the information of the perturbations is still here and “hidden” in the high frequency microscopic oscillations of the distribution function. At a later time a resonance occurs and the plasma produces an echo. The time at which the echo occurs can be computed (see Villani⁹, page 74). The fine mathematical study of this phenomenon allowed C. Villani and C. Mouhot to prove their famous result on the rigorous nonlinear Landau damping¹⁰.

More practically, this experiment and its theoretical framework show that it is interesting to represent the distribution function by an truncated expansion on an orthonormal basis of oscillating functions in the velocity variables. This representation allows a better control of the energy transfer between the low frequencies and the high frequencies in the velocity direction, and thus provides more relevant numerical methods. This kind of approach is studied for instance by Eliasson¹¹.

We have started to study such kind of approaches in [43]. An interesting point is that the truncated reduced model is also an hyperbolic system in the space direction only. This allows the classical methods for hyperbolic systems to be reused.

6.5. Two-Scale numerical methods

Participant: E. Frénod.

⁸Malmberg, J. and Wharton, C. Collisionless damping of electrostatic plasma waves. Phys. Rev. Lett. 13, 6 (1964), 184–186.

⁹Villani, C. Landau damping. CEMRACS 2010 lectures.

¹⁰Mouhot, C. ; Villani, C. On Landau damping, Acta Mathematica 207 (September 2011), 29-201.

¹¹Eliasson, B. Outflow boundary conditions for the Fourier transformed one-dimensional Vlasov-Poisson system. J. Sci. Comput. 16 (2001), no. 1, 1–28.

In note [39] a classification of Homogenization-Based Numerical Methods and (in particular) of Numerical Methods that are based on the Two-Scale Convergence is done. In this classification stand: Direct Homogenization-Based Numerical Methods, H-Measure-Based Numerical Methods, Two-Scale Numerical Methods and TSAPS (Two-Scale Asymptotic Preserving Schemes).

In [34] we develop and we explain the two-scale convergence in the covariant formalism, i.e. using differential forms on a Riemannian manifold. For that purpose, we consider two manifolds M and Y , the first one contains the positions and the second one the oscillations. We establish some convergence results working on geodesics on a manifold. Then, we apply this framework on examples.

6.6. Spline Discrete Differential Forms and applications

Participant: E. Sonnendrücker.

In [36] we construct a new set of discrete differential forms based on B-splines of arbitrary degree as well as an associated Hodge operator. The theory is first developed in 1D and then extended to multi-dimension using tensor products. We link our discrete differential forms with the theory of chains and cochains. The spline discrete differential forms are then applied to the numerical solution of Maxwell's equations.

The notion of B-spline based discrete differential forms is recalled and along with a Finite Element Hodge operator, it is used in [35] to design new numerical methods for solving the Vlasov-Poisson equations.

6.7. Simulations of highly oscillatory Vlasov-Poisson system

Participants: E. Frénod, S. Hirstoaga, M. Lutz, E. Sonnendrücker.

In paper [45] a Lie Transform method is applied for a charged beam under the action of a radial external electric field. The aim of the Lie transform method that is used here is to construct a change of variable which transforms the 2D kinetic problem into a 1D problem. This reduces the dimensionality of the problem and make it easier to solve numerically.

In paper [41], in the framework of a Particle-In-Cell scheme for some 1D Vlasov-Poisson system depending on a small parameter, we propose a time-stepping method which is numerically uniformly accurate when the parameter goes to zero. Based on an exponential time differencing approach, the scheme is able to use large time steps with respect to the typical size of the fast oscillations of the solution.

6.8. Waterbag models: analysis and simulations

Participant: N. Besse.

Ion temperature gradient instabilities play a major role in the understanding of anomalous transport in core fusion plasmas. In the considered cylindrical geometry, ion dynamics is described in [20] using a drift-kinetic multi-water-bag model for the parallel velocity dependency of the ion distribution function. In a first stage, global linear stability analysis is performed. From the obtained normal modes, parametric dependencies of the main spectral characteristics of the instability are then examined. Comparison of the multi-water-bag results with a reference continuous Maxwellian case allows us to evaluate the effects of discrete parallel velocity sampling induced by the Multi-Water-Bag model. Differences between the global model and local models considered in previous works are discussed. Using results from linear, quasilinear, and nonlinear numerical simulations, an analysis of the first stage saturation dynamics of the instability is proposed, where the divergence between the three models is examined.

In paper [21] we present two new codes devoted to the study of ion temperature gradient (ITG) driven plasma turbulence in cylindrical geometry using a drift-kinetic multi-water-bag model for ion dynamics. Both codes were developed to complement the Runge-Kutta semi-lagrangian multi-water-bag code GMWB3D-SLC described in [1]. The CYLGYR code is an eigenvalue solver performing linear stability analysis from given mean radial profiles. It features three resolution schemes and three parallel velocity response models (fluid, multi-water-bag, continuous Maxwellian). The QUALIMUWABA quasilinear code is an initial value code allowing the study of zonal flow influence on drift-waves dynamics. Cross-validation test performed between the three codes show good agreement on both temporal and spatial characteristics of unstable modes in the linear growth phase.

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

Participants: Takashi Hattori, Simon Labrunie, Jean R. Roche.

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

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

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

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

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

The domain considered is as near as possible of the cavity 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 modeling* in the literature: the original Maxwell's equations are used to obtain a second order equation for the time-harmonic electric field. These are written in a weak form using an augmented variational formulation (AVF), which takes into account the divergence. The variational formulation is then discretized using modified Taylor-Hood (nodal) elements.

The analyze of the model considered, existence and unicity of solution, equivalence of the formulation for the domain decomposition formulation was completed in the frame of Takashi Hattori Phd thesis.

During 2013 we continue to develop the domain decomposition method introduced in 2012 and a new preconditioned system was considered in the code "FullWaveFEM", [31].

6.10. Eulerian simulations of parallel transport in the SOL

Participants: S. Hirstoaga, G. Manfredi.

During the year 2013, we have progressed in the implementation of an asymptotic preserving (AP) Eulerian Vlasov code (VESPA: Vlasov Eulerian Simulator of PARallel transport) for the study of parallel transport in the scrape-off layer of tokamaks. An AP Vlasov-Poisson code had already been partially developed for the quasi-neutral regime. In this case the small parameter is the Debye length λ (normalized to the parallel connection length). The Poisson equation becomes singular when $\lambda \rightarrow 0$: the AP solution consists in reformulating Poisson's equation in a way that is no longer singular in this limit. In theory, any value of λ can be used, including $\lambda = 0$, without numerical instability and without any constraint on the grid spacing and time-step. In practice, we have observed a CFL stability condition (although not very restrictive) and a limit on the smallness of λ . During the past year, we have performed systematic tests on the code, which is now capable of attaining very small values of λ , down to 10^{-4} or even lower. Meaningful results can be obtained with just 1-2 hours of computation on a standard desktop computer (see for example [29]).

The next upgrade of the VESPA code concerns the modelling of collisions, which have been implemented through a relaxation (BGK) term that also retains the possibility to include ionization and recombination in the model. The BGK term has been tested and validated against analytical results. In particular, the AP scheme had to be modified in order to correctly treat the BGK term. These upgrades are now fully integrated into the VESPA code.

Using the VESPA code, we have studied the dynamical response of a stationary sheath-presheath system to an external perturbation, which takes the form of a small density disturbance in the central region of the plasma, far from the sheaths. The numerical results suggest that, for most regimes of physical interest, the perturbation is damped away before it reaches the wall and does not have a significant impact on the structure of the sheath. This scenario has been studied for different temperatures and density profiles of the disturbance.

We have started to look at the impact of secondary electrons (SE) on the structure and the formation of the sheath. SEs were neglected in previous versions of the code but can play a significant role on the wall potential. In the VESPA code, they are now modelled as a Maxwellian electron source located near the wall. First results indicate that a large yield rate of SEs reduces the potential drop between the plasma bulk and the wall.

6.11. Other application domains

6.11.1. Applications of Two-Scale numerical methods

Participant: E. Frénod.

In paper [37] we consider a model for short term dynamics of dunes in tidal area. We construct a Two-Scale Numerical Method based on the fact that the solution of the equation which has oscillations Two-Scale converges to the solution of a well-posed problem. This numerical method uses on Fourier series.

In [18] we present Chapman–Enskog and Hilbert expansions applied to the $O(v/c)$ Boltzmann equation for the radiative transfer of neutrinos in core-collapse supernovae. Based on the Legendre expansion of the scattering kernel for the collision integral truncated after the second term, we derive the diffusion limit for the Boltzmann equation by truncation of Chapman–Enskog or Hilbert expansions with reaction and collision scaling. We also give asymptotically sharp results obtained by the use of an additional time scaling. The diffusion limit determines the diffusion source in the *Isotropic Diffusion Source Approximation (IDSA)* of Boltzmann’s equation for which the free streaming limit and the reaction limit serve as limiters. Here, we derive the reaction limit as well as the free streaming limit by truncation of Chapman–Enskog or Hilbert expansions using reaction and collision scaling as well as time scaling, respectively. Finally, we motivate why limiters are a good choice for the definition of the source term in the IDSA.

6.11.2. Inverse problem governed by Maxwell equations

Participant: Jean R. Roche.

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

The industrial technique of electromagnetic casting allows for contactless heating, shaping and controlling of chemical aggressive, hot melts. The main advantage over the conventional crucible shape forming is that the liquid metal does not come into contact with the crucible wall, so there is no danger of contamination. This is very important in the preparation of very pure specimens in metallurgical experiments, as even small traces of impurities, such as carbon and sulphur, can affect the physical properties of the sample. Industrial applications are, for example, electromagnetic shaping of aluminum ingots using soft-contact confinement of the liquid metal, electromagnetic shaping of components of aeronautical engines made of superalloy materials (Ni,Ti, etc.), 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 [61]. In order to look for configurations of inductors considering different topologies we introduce a new formulation for the inverse problem using a shape functional based on the Kohn-Vogelius criterion. A topology optimization procedure is defined by means of topological derivatives, a new method that simplifies computation issues was considered, see [60] and [49].

During 2013 we rewrite the inverse electromagnetic casting model in order to have a quadratic programming problem, this simplified the numerical solution and simulation [19].

7. Bilateral Contracts and Grants with Industry

7.1. Bilateral Contracts with Industry

CLAC is a joint project with a Strasbourg small company, AxesSim, which develops software for electromagnetic simulations. Thomas Strub, who is employed in AxesSim with a CIFRE position, is doing his PhD on the design and development of CLAC applied to electromagnetic problems.

8. Partnerships and Cooperations

8.1. National Initiatives

8.1.1. ANR

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

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

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

8.1.2. Euratom-CEA projects

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

8.2. International Research Visitors

8.2.1. Visits to International Teams

Michel Mehrenberger, since September 2013, Institut für Plasma Physics (IPP) Munich, Germany.

9. Dissemination

9.1. Scientific Animation

9.1.1. Invitations at conferences and schools

- S. Labrunie gave the invited talk «Singular Solutions and Large Solutions to some Nonlinear Elliptic Equations in Polygonal Domains», Journées Singulières Augmentées en l'honneur de Martin Costabel, Rennes, 2013. <http://jsa2013.sciencesconf.org/>
- G. Manfredi gave the invited talk «Non-relativistic limits of Maxwell's equations» at the Workshop Asymptotic and Multiscale methods, Ile de Porquerolles, 9-15 June 2013, <http://www.math.univ-toulouse.fr/~cnegules/WAMs2013.html>
- E. Frénod gave
 - the invited talk « Sand transport in coastal ocean waters submitted to tide » at the Workshop Asymptotic and Multiscale methods, Ile de Porquerolles, 9-15 June 2013.
 - the invited course «Two-Scale Convergence and Two-Scale Numerical Methods », at "École de mécanique des fluides numérique", Ile de Porquerolles, 3-8 June 2013, <http://ecolemf.n.limsi.fr/doku.php?id=programme>.
 - the invited talk « The Geometrical Gyro-Kinetic Approximation » at the Institute of Natural Sciences, Shanghai Jiao Tong University, China, 8-27 May 2013.
 - the invited course « Two-Scale Convergence and Two-Scale Numerical Methods » at the Institute of Natural Sciences, Shanghai Jiao Tong University, China, 8-27 May 2013.
- M. Bostan, N. Crouseilles, P. Helluy, S. Hirstoaga and M. Mehrenberger gave invited talks at NumKin 2013, 2-6 September 2013, Garching, Germany, <http://www.ipp.mpg.de/ippcms/eng/for/veranstaltungen/konferenzen/2013/numkin2013/>.

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

Licence :

A. Hamiaz, Analyse numérique, 28h, L3, Université de Strasbourg, France.
 P. Helluy, Analyse numérique, 50h, L3, Université de Strasbourg, France.
 S. Hirstoaga, Analyse numérique, 42h, L3, Université de Strasbourg, France.
 S. Labrunie, Mathématiques générales en DUT génie civil, 100h, L1, Université de Lorraine, France
 S. Labrunie, Mathématiques générales en DUT génie civil, 20h, L2, Université de Lorraine, France
 M. Mehrenberger, Optimisation non linéaire, 39h, L3, Université de Strasbourg, France.
 M. Mehrenberger, Analyse numérique, 36h30, L2, Université de Strasbourg, France.
 M. Mehrenberger, Méthodes d'Analyse Numérique, 39h, L3, ENSIIE (ecole d'ingénieur, antenne de Strasbourg), France.
 Jean R. Roche, Mathématiques, 162h, L2, ESSTIN, Univ. de Lorraine, France.

Master :

A. Hamiaz, Mathématiques, 20h, Agrégation, Université de Strasbourg, France.
 M. Mehrenberger, Modélisation : Option Calcul Scientifique, 20h, M2, Université de Strasbourg, France.
 Jean R. Roche, Optimization, 30h, M1, ESSTIN, Univ. de Lorraine, France.
 Jean R. Roche, Décomposition de domaines , Cours 15h, Univ. de Hamman Sousse, Tunisie.

9.2.2. Supervision

PhD in Progress : Pierre Glanc, Méthodes numériques pour Vlasov par remapping conservatif, Université de Strasbourg, Advisors: Philippe Helluy, Michel Mehrenberger.

PhD in Progress : Nhung Pham, Méthodes numériques pour Vlasov, Université de Strasbourg, Advisors: Philippe Helluy, Laurent Navoret.

PhD in Progress : Michel Massaro, Résolution numérique de lois de conservation sur architectures multicores, Université de Strasbourg, Advisors: Philippe Helluy, Vincent Loechner (EPI CAMUS).

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

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

PhD in progress : Christophe Steiner, Résolution numérique de l'opérateur de gyromoyenne, schémas d'advection et couplage. Applications à l'équation de Vlasov. Université de Strasbourg Advisors: Michel Mehrenberger.

PhD in progress : Thomas Strub, Résolution des équations de maxwell tridimensionnelles instationnaires sur calculateur massivement multicoeur. Université de Strasbourg Advisors: Philippe Helluy.

9.2.3. Juries

N. Besse (advisor) and S. Labrunie participated in the PhD defense committee of David Coulette, Université de Lorraine, 6 December 2013.

E. Frénod participated in the following PhD defense committees :

Céline Caldini-Queiros, PhD at Université de Besançon, 15 November 2013. E. Frénod was referee.

Mathieu Lutz, PhD at Université de Strasbourg, 24 October 2013. E. Frénod was advisor.

G. Manfredi participated in the following PhD and HdR defense committees :

Philippe Coche, PhD at Université de Toulouse, 23 May 2013.

Stephen Jowan GALLAGHER, PhD at Warwick University (Royaume Uni), 2 October 2013.

Nicolas Lemoine, HdR at Université de Lorraine, 10 December 2013.

P. Helluy participated in the following PhD and HdR defense committees :

Clément Durochat, PhD at Inria Sophia Antipolis, 30 January 2013.

Jean-Baptiste Laurent, PhD at ONERA Toulouse, July 2013.

Yu Jie, PhD at EDF Chatou, 11 September 2013.

Sophie Gerald, PhD at ONERA Chatillon. November 2013.

Mathieu Lutz, PhD at Université de Strasbourg, October 2013.

9.3. Popularization

C. Caldini-Queiros wrote the popularization paper "Les schémas numériques : les mathématiques au service de la physique", published in "Presses universitaires de Franche-Comté", rewarded with Prix A' Doc de la jeune recherche en Franche-Comté 2013.

E. Frénod wrote the following popularization papers

- Mon littoral, c'est de la dynamique. Brève pour : 2013 - Mathématiques pour la planète Terre - <http://mpt2013.fr/mon-littoral-cest-de-la-dynamique/>.
- Aquaculture en milieux confinés : le cas de l'étang de Thau. Brève pour : 2013 Mathématiques pour la planète Terre. - <http://mpt2013.fr/aquaculture-en-milieux-confinés-le-cas-de-letang-de-thau/>.
- Un exemple d'application des mathématiques à l'environnement littoral : La dynamique à long terme des dunes marines dans les zones soumises à la marée. Modélisation, Analyse, Homogénéisation et Simulation. Matapli (Smai), No 100, pp 129–140.

10. Bibliography

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Doctoral Dissertations and Habilitation Theses

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- [12] M. LUTZ. , *Etude mathématique et numérique d'un modèle gyrocinétique incluant des effets électromagnétiques pour la simulation d'un plasma de Tokamak*, Université de Strasbourg, October 2013, <http://hal.inria.fr/tel-00875703>

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