Activity Report 2017

Team TONUS

TOkamaks and NUmerical Simulations

Inria teams are typically groups of researchers working on the definition of a common project, and objectives, with the goal to arrive at the creation of a project-team. Such project-teams may include other partners (universities or research institutions).

RESEARCH CENTER
Nancy - Grand Est

THEME
Earth, Environmental and Energy Sciences

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Team TONUS

Creation of the Team: 2012 January 01

Keywords:

Computer Science and Digital Science:

A6. - Modeling, simulation and control
A6.1. - Mathematical Modeling
A6.1.1. - Continuous Modeling (PDE, ODE)
A6.1.4. - Multiscale modeling
A6.1.5. - Multiphysics modeling
A6.2. - Scientific Computing, Numerical Analysis & Optimization
A6.2.1. - Numerical analysis of PDE and ODE
A6.2.7. - High performance computing
A6.3.4. - Model reduction
A7.1. - Algorithms
A8.9. - Performance evaluation

Other Research Topics and Application Domains:

B1.1.10. - Mathematical biology
B4.2.2. - Fusion
B5.2.3. - Aviation
B6.1.1. - Software engineering

1. Personnel

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2. Overall Objectives

2.1. Overall Objectives

TONUS started in January 2014. It is a team of the Inria Nancy-Grand Est center. It is located in the mathematics institute (IRMA) of the University of Strasbourg.

The International Thermonuclear Experimental Reactor (ITER) is a large-scale scientific experiment that aims to demonstrate that it is possible to produce energy from fusion, by confining a very hot hydrogen plasma inside a toroidal chamber, called tokamak. In addition to physics and technology research, tokamak design also requires mathematical modelling and numerical simulations on supercomputers.

The objective of the TONUS project is to deal with such mathematical and computing issues. We are mainly interested in kinetic, gyrokinetic and fluid simulations of tokamak plasmas. In the TONUS project-team we are working on the development of new numerical methods devoted to such simulations. We investigate several classical plasma models, study new reduced models and new numerical schemes adapted to these models. We implement our methods in two software projects: Selalib [1] and SCHNAPS [2] adapted to new computer architectures.

We have strong relations with the CEA-IRFM team and participate in the development of their gyrokinetic simulation software GYSELA. We are involved in two Inria Project Labs, respectively devoted to tokamak mathematical modelling and high performance computing. The numerical tools developed from plasma physics can also be applied in other contexts. For instance, we collaborate with a small company in Strasbourg specialized in numerical software for applied electromagnetism. We also study kinetic acoustic models with the CEREMA and multiphase flows with EDF.

Finally, our topics of interest are at the interaction between mathematics, computer science, High Performance Computing, physics and practical applications.

3. Research Program

3.1. Kinetic models for plasmas

The fundamental model for plasma physics is the coupled Vlasov-Maxwell kinetic model: the Vlasov equation describes the distribution function of particles (ions and electrons), while the Maxwell equations describe the electromagnetic field. In some applications, it may be necessary to take relativistic particles into account, which leads to consider the relativistic Vlasov equation, even if in general, tokamak plasmas are supposed to be non-relativistic. The distribution function of particles depends on seven variables (three for space, three for the velocity and one for time), which yields a huge amount of computations.

To these equations we must add several types of source terms and boundary conditions for representing the walls of the tokamak, the applied electromagnetic field that confines the plasma, fuel injection, collision effects, etc.

Tokamak plasmas possess particular features, which require developing specialized theoretical and numerical tools.

[1] http://selalib.gforge.inria.fr/
[2] http://schnaps.gforge.inria.fr

Because the magnetic field is strong, the particle trajectories have a very fast rotation around the magnetic field lines. A full resolution would require a prohibitive amount of calculations. It is then necessary to develop reduced models for large magnetic fields in order to obtain tractable calculations. The resulting model is called a gyrokinetic model. It allows us to reduce the dimensionality of the problem. Such models are implemented in GYSELA and Selalib.

On the boundary of the plasma, the collisions can no more be neglected. Fluid models, such as the MagnetoHydroDynamics (MHD) become again relevant. For the good operation of the tokamak, it is necessary to control MHD instabilities that arise at the plasma boundary. Computing these instabilities requires special implicit numerical discretizations with excellent long time behavior.

In addition to theoretical modelling tools, it is necessary to develop numerical schemes adapted to kinetic, gyrokinetic and fluid models. Three kinds of methods are studied in TONUS: Particle-In-Cell (PIC) methods, semi-Lagrangian and fully Eulerian approaches.

3.1.1. Gyrokinetic models: theory and approximation

In most phenomena where oscillations are present, we can establish a three-model hierarchy: (i) the model parameterized by the oscillation period, (ii) the limit model and (iii) the two-scale model, possibly with its corrector. In a context where one wishes to simulate such a phenomenon where the oscillation period is small and the oscillation amplitude is not small, it is important to have numerical methods based on an approximation of the Two-Scale model. If the oscillation period varies significantly over the domain of simulation, it is important to have numerical methods that approximate properly and effectively the model parameterized by the oscillation period and the Two-Scale model. Implementing Two-Scale Numerical Methods (for instance by Frénod et al. [23]) is based on the numerical approximation of the Two-Scale model. These are called of order 0. A Two-Scale Numerical Method is called of order 1 if it incorporates information from the corrector and from the equation of which this corrector is a solution. If the oscillation period varies between very small values and values of order 1, it is necessary to have new types of numerical schemes (Two-Scale Asymptotic Preserving Schemes of order 1 or TSAPS) that preserve the asymptotics between the model parameterized by the oscillation period and the Two-Scale model with its corrector. A first work in this direction has been initiated by Crouseilles et al. [22].

3.1.2. Semi-Lagrangian schemes

The Strasbourg team has a long and recognized experience in numerical methods of Vlasov-type equations. We are specialized in both particle and phase space solvers for the Vlasov equation: Particle-in-Cell (PIC) methods and semi-Lagrangian methods. We also have a long-standing collaboration with the CEA of Cadarache for the development of the GYSELA software for gyrokinetic tokamak plasmas.

The Vlasov and the gyrokinetic models are partial differential equations that express the transport of the distribution function in the phase space. In the original Vlasov case, the phase space is the six-dimension position-velocity space. For the gyrokinetic model, the phase space is five-dimensional because we consider only the parallel velocity in the direction of the magnetic field and the gyrokinetic angular velocity instead of three velocity components.

A few years ago, Eric Sonnendrücker and his collaborators introduced a new family of methods for solving transport equations in the phase space. This family of methods are the semi-Lagrangian methods. The principle of these methods is to solve the equation on a grid of the phase space. The grid points are transported with the flow of the transport equation for a time step and interpolated back periodically onto the initial grid. The method is then a mix of particle Lagrangian methods and Eulerian methods. The characteristics can be solved forward or backward in time leading to the Forward Semi-Lagrangian (FSL) or Backward Semi-Lagrangian (BSL) schemes. Conservative schemes based on this idea can be developed and are called Conservative Semi-Lagrangian (CSL).

GYSELA is a 5D full gyrokinetic code based on a classical backward semi-Lagrangian scheme (BSL) [27] for the simulation of core turbulence that has been developed at CEA Cadarache in collaboration with our team [24].

More recently, we have started to apply the Semi-Lagrangian methods to more general kinetic equations. Indeed, most of the conservation laws of physics can be represented by a kinetic model with a small set of velocities and relaxation source terms [7]. Compressible fluids or MHD equations have such representations. Semi-Lagrangian methods then become a very appealing and efficient approach for solving these equations.

3.1.3. PIC methods

Historically PIC methods have been very popular for solving the Vlasov equations. They allow solving the equations in the phase space at a relatively low cost. The main disadvantage of this approach is that, due to its random aspect, it produces an important numerical noise that has to be controlled in some way, for instance by regularizations of the particles, or by divergence correction techniques in the Maxwell solver. We have a long-standing experience in PIC methods and we started implementing them in Selalib. An important aspect is to adapt the method to new multicore computers. See the work by Crestetto and Helluy [21].

3.2. Fluid and Reduced kinetic models for plasmas

As already said, 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.

Assuming that the distribution function has a Maxwellian shape, for instance, we obtain the MagnetoHydroDynamic (MHD) model. It is physically valid only in some parts of the tokamak (at the edges for instance). The fluid model is generally obtained from the hypothesis that the collisions between particles are strong.

But the reduction is not necessarily a consequence of collisional effects. Indeed, even without collisions, the plasma may still relax to an equilibrium state over sufficiently long time scales (Landau damping effect).

In the fluid or reduced-kinetic regions, the approximation of the distribution function could require fewer data while still achieving a good representation, even in the collisionless regime.

Therefore, a fluid or a reduced model is a model where the explicit dependency on the velocity variable is removed. 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 the solution of a first order hyperbolic system.

Another way to reduce the model is to try to find an abstract kinetic representation with an as small as possible set of kinetic velocities. The kinetic approach has then only a mathematical meaning. It allows solving very efficiently many equations of physics [13].

3.2.1. Numerical schemes

As previously indicated, an efficient method for solving the reduced models is the Discontinuous Galerkin (DG) approach. It is possible to make it of arbitrary order. It requires limiters when it is applied to nonlinear PDEs occurring for instance in fluid mechanics. But the reduced models that we intent to write are essentially linear. The nonlinearity is concentrated in a few coupling source terms.

In addition, this method, when written in a special set of variables, called the entropy variables, has nice properties concerning the entropy dissipation of the model. It opens the door to constructing numerical schemes with good conservation properties and no entropy dissipation, as already used for other systems of PDEs [28], [20], [26], [25].

3.2.2. Matrix-free Implicit schemes

In tokamaks, the reduced model generally involves many time scales. Among these time scales, many of then, associated to the fastest waves, are not relevant. In order to filter them out, it is necessary to adopt implicit solvers in time. When the reduced model is based on a kinetic interpretation, it is possible to construct implicit schemes that do not impose solving costly linear systems. In addition the resulting solver is stable even at very high CFL number [13].

3.3. Electromagnetic solvers

Precise resolution of the electromagnetic fields is essential for proper plasma simulation. Thus it is important to use efficient solvers for the Maxwell systems and its asymptotics: Poisson equation and magnetostatics.

The proper coupling of the electromagnetic solver with the Vlasov solver is also crucial for ensuring conservation properties and stability of the simulation.

Finally, plasma physics implies very different time scales. It is thus very important to develop implicit Maxwell solvers and Asymptotic Preserving (AP) schemes in order to obtain good behavior on long time scales.

3.3.1. Coupling

The coupling of the Maxwell equations to the Vlasov solver requires some precautions. The most important one is to control the charge conservation errors, which are related to the divergence conditions on the electric and magnetic fields. We will generally use divergence correction tools for hyperbolic systems presented for instance in [18] (and the references therein).

3.3.2. Implicit solvers

As already pointed out, in a tokamak, the plasma presents several different space and time scales. It is not possible in practice to solve the initial Vlasov-Maxwell model. It is first necessary to establish asymptotic models by letting some parameters (such as the Larmor frequency or the speed of light) tend to infinity. This is the case for the electromagnetic solver and this requires implementing implicit time solvers in order to efficiently capture the stationary state, the solution of the magnetic induction equation or the Poisson equation.

4. Application Domains

4.1. Controlled fusion and ITER

The search for alternative energy sources is a major issue for the future. Among others, controlled thermonuclear fusion in a hot hydrogen plasma is a promising possibility. The principle is to confine the plasma in a toroidal chamber, called a tokamak, and to attain the necessary temperatures to sustain nuclear fusion reactions. The International Thermonuclear Experimental Reactor (ITER) is a tokamak being constructed in Cadarache, France. This was the result of a joint decision by an international consortium made of the European Union, Canada, USA, Japan, Russia, South Korea, India and China. ITER is a huge project. As of today, the budget is estimated at 20 billion euros. The first plasma shot is planned for 2020 and the first deuterium-tritium operation for 2027. Many technical and conceptual difficulties have to be overcome before the actual exploitation of fusion energy. Consequently, much research has been carried out around magnetically confined fusion. Among these studies, it is important to carry out computer simulations of the burning plasma. Thus, mathematicians and computer scientists are also needed in the design of ITER. The reliability and the precision of numerical simulations allow a better understanding of the physical phenomena and thus would lead to better designs. TONUS's main involvement is in such research. The required temperatures to attain fusion are very high, of the order of a hundred million degrees. Thus it is imperative to prevent the plasma from touching the tokamak inner walls. This confinement is obtained thanks to intense magnetic fields. The magnetic field is created by poloidal coils, which generate the toroidal component of the field. The toroidal plasma current also induces a poloidal component of the magnetic field that twists the magnetic field lines. The twisting is very important

for the stability of the plasma. The idea goes back to research by Tamm and Sakharov, two Russian physicists, in the 50's. Other devices are essential for the proper operation of the tokamak: divertor for collecting the escaping particles, microwave heating for reaching higher temperatures, fuel injector for sustaining the fusion reactions, toroidal coils for controlling instabilities, etc.

4.2. Other applications

The software and numerical methods that we develop can also be applied to other fields of physics or of engineering.

- For instance, we have a collaboration with the company AxesSim in Strasbourg for the development of efficient Discontinuous Galerkin (DG) solvers on hybrid computers. The applications is electromagnetic simulations for the conception of antennas, electronic devices or aircraft electromagnetic compatibility.
- The acoustic conception of large rooms requires huge numerical simulations. It is not always possible to solve the full wave equation and many reduced acoustic models have been developed. A popular model consists in considering "acoustic" particles moving at the speed of sound. The resulting Partial Differential Equation (PDE) is very similar to the Vlasov equation. The same modelling is used in radiation theory. We have started to work on the reduction of the acoustic particles model and realized that our reduction approach perfectly applies to this situation. A new PhD with CEREMA (Centre d'études et d'expertise sur les risques, l'environnement, la mobilité et l'aménagement) has started in October 2015 (PhD of Pierre Gerhard). The objective is to investigate the model reduction and to implement the resulting acoustic model in our DG solver.
- In september 2017, we started a collaboration with EDF Chatou (PhD of Lucie Quibel) on the modelling of multiphase fluids with complex equations of state. The goal is to simulate the high temperature liquid-vapor flow occurring in a nuclear plant. Among others, we will apply our recent kinetic method for designing efficient implicit schemes for this kind of flows.

5. Highlights of the Year

5.1. Highlights of the Year

We have developed [7] a new numerical method for solving any hyperbolic system of conservation laws (and among them the reduced plasma models). The method is based on a vectorial kinetic representation of the equations, an efficient transport solver (suc as DG or Semi-Lagrangian) and palindromic time integration. The resulting scheme is unconditionally stable, matrix-free and high order. We applied it successfully to the simulation of Rayleigh-Taylor instabilities and we are extending it to the simulation of MHD instabilities.

6. New Software and Platforms

6.1. CLAC

Conservation Laws Approximation on many Cores
SCIENTIFIC DESCRIPTION: It is clear now that future computers 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 kind of 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 coarse grain parallelism, while the OpenCL library will efficiently operate the fine grain parallelism.

We have invested for several years until 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.

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.
FUNCTIONAL DESCRIPTION: CLAC is a generic Discontinuous Galerkin solver, written in C/C++, based on the OpenCL and MPI frameworks.

- Partner: AxesSim
- Contact: Philippe Helluy
- URL: http://clac.gforge.inria.fr/

6.2. Selalib

SEmi-LAgrangian LIBrary
KEYWORDS: Plasma physics - Semilagrangian method - Parallel computing - Plasma turbulence
SCIENTIFIC DESCRIPTION: The objective of the Selalib project (SEmi-LAgrangian LIBrary) is to develop a well-designed, organized and documented library implementing several numerical methods for kinetic models of plasma physics. Its ultimate goal is to produce gyrokinetic simulations.

Another objective of the library is to provide to physicists easy-to-use gyrokinetic solvers, based on the semi-lagrangian techniques developed by Eric Sonnendrücker and his collaborators in the past CALVI project. The new models and schemes from TONUS are also intended to be incorporated into Selalib.
FUNCTIONAL DESCRIPTION: Selalib is a collection of modules conceived to aid in the development of plasma physics simulations, particularly in the study of turbulence in fusion plasmas. Selalib offers basic capabilities from general and mathematical utilities and modules to aid in parallelization, up to pre-packaged simulations.

- Partners: Max Planck Insitute - Garching - Université de Strasbourg
- Contact: Philippe Helluy
- URL: http://selalib.gforge.inria.fr/

6.3. SCHNAPS

Solver for Conservative Hyperbolic Nonlinear Applications for PlasmaS
KEYWORDS: Discontinuous Galerkin - StarPU - Kinetic scheme
FUNCTIONAL DESCRIPTION: Generic systems of conservation laws. Specific models: fluids, Maxwell, Vlasov, acoustics (with kinetic representation). Multitasking with StarPU. Explicit solvers (RK2, RK3, RK4): accelerated with OpenCL Implicit solvers: through kinetic representations and palindromic time integration.

- Contact: Philippe Helluy
- URL: http://schnaps.gforge.inria.fr/

7. New Results

7.1. Palindromic methods

7.1.1. Palindromic discontinuous Galerkin method in 2D and 3D

Participants: David Coulette, Florence Drui, Emmanuel Franck, Philippe Helluy, Laurent Navoret.

In the previous year (see [7]) we have proposed a method to solve hyperbolic systems like the Euler equations with an unconditionally stable high-order method. This method is based on a kinetic representation of the hyperbolic system. The kinetic equations are solved with an upwind DG method. It requires no matrix storage. High order is obtained through palindromic composition methods. The concept has been test in 1D. During this year we extend the method to 2D and 3D and applied it to fluid mechanics. Currently we are working on improving this method on realistic cases for MHD instabilities. The objective is to compare the results with the European code JOREK.

We are also working on methods for applying boundary conditions in a stable way with the palindromic method (postdoc of Florence Drui).

7.1.2. Kinetic model for palindromic methods

Participants: David Coulette, Emmanuel Franck, Laurent Navoret.

One of the most important drawbacks of the Palindromic method is the numerical dispersion associated to the high-order time scheme. To limit this problem we propose to replace the DG method by a semi-Lagrangian method and design new kinetic representations which are more accurate. We also studied the stability of these news models. The first results were good and currently we are working on the 2D extension and the coupling with limiter technics.

7.1.3. Finite element relaxation methods for fluid models

Participants: David Coulette, Emmanuel Franck.

In parallel to our work on the Palindromic method based on a kinetic relaxation model, we studied in [17] a variant based on the Xin-Jin relaxation model. Coupled with a finite element method we obtain an implicit solver for Euler equations where we invert only Laplacians and mass matrices. The first results show that the method is more efficient in CPU costs and memory. The finite elements used are the same as in JOREK.

7.2. MHD problems

Participant: Emmanuel Franck.

7.2.1. Compatible Implicit finite element for linear MHD

In this work we consider a linear MHD problem. The aim is to design an implicit method able to preserve the energy equation and the divergence free constraints in realistic Tokamak geometry. The first idea is to use a splitting scheme between the wave and convection parts coupled with an implicit scheme for each subsystem. In order to discretize each sub-system we use compatible B-Splines FE method wich allows us to preserve the invariants and to use a reduction of the implicit problem to be inverted. The idea was improved on simple geometries. We are currently extending the method on realistic geometries.

7.2.2. Splitting and relaxation for JOREK code

The Jorek code is the main European code for the simulation of Tokamak instabilities. The inversion of the full matrix is based on Block Jacobi preconditioning which is not efficient in some cases and very greedy in memory. We are investigating a new splitting scheme similar to the one used in works on compatible Finite Elements. We have also just begun to investigate the relaxation method used in the Palindromic scheme to solve the reduced MHD model of JOREK.

7.3. Finite Volume approximations of the Euler system with variable congestion

Participants: Pierre Degond, Piotr Minakowski, Laurent Navoret, Ewelina Zatorska.

We are interested in the numerical simulations of the Euler system with variable congestion encoded by a singular pressure. This model describes for instance the macroscopic motion of a crowd with individual congestion preferences. In [3] we propose an asymptotic preserving (AP) scheme based on a conservative formulation of the system in terms of density, momentum and density fraction. A second order accuracy version of the scheme is also presented. We validate the scheme on one-dimensional test cases and compare it with a scheme developed in a previous work and extended here to higher order accuracy. We finally carry out two-dimensional numerical simulations and show that the model exhibits typical crowd dynamics.

7.4. Numerical scheme for sheath equilibria

Participants: Mehdi Badsi, Michel Mehrenberger, Laurent Navoret.

We are interested in developing a numerical method for capturing stationary sheaths that a plasma forms in contact with a metallic wall. This work is based on a bi-species (ion/electron) Vlasov-Ampère model proposed in [19]. The main question addressed in this work is to know if classical numerical schemes can preserve stationary solutions with boundary conditions, since these solutions are not a priori conserved at the discrete level. In the context of high-order semi-Lagrangian method, due to their large stencil, interpolation near the boundary of the domain also requires a specific treatment. Moreover, for preventing instabilities from developing in large time, the proposed method guaranties that the discrete Gauss equation is satisfied in time.

7.5. Recurrence phenomenon for finite element grid based Vlasov solver

Participants: Michel Mehrenberger, Laurent Navoret, Thi Nhung Pham.

When using a grid based solver (finite element/DG scheme, discontinuous Galerkin semi-Lagrangian scheme) and spatial periodic boundary conditions, the simulations of the Vlasov-Poisson system exhibit numerical reappearance of initial perturbations at some time called recurrence time. This time depends on the numerical parameters (degree and mesh size of the finite element mesh). With a given number of degrees of freedom, considering a large degree approximation makes the phenomenon appear earlier in the simulation and thus makes this choice less attractive. In our work [9], we highlight that the time and the intensity of the recurrence are related to the quadrature rules used for computing the charge density. In particular, quadratures that are exact on trigonometric polynomials weaken the recurrence effect.

7.6. PICSL

Participants: Yann Barsamian, Joackim Bernier, Sever Hirstoaga, Michel Mehrenberger.

7.6.1. Particle in Cell and Semi-Lagrangian schemes for two species plasma simulations

Thanks to a classical first order dispersion analysis, we are able to check the validity of 1D$\times$1D two species Vlasov-Poisson simulations; the extension to second order is performed and shown to be relevant for explaining further details. In order to validate multidimensional effects, we propose in [14] a 2D $\times$ 2D single species test problem that has true 2D effects coming from the sole second order dispersion analysis. Finally, we perform, in the same code, full 2D×2D nonlinear two species simulations with mass ratio and consider the mixing of semi-Lagrangian and Particle-in-Cell methods. This work has been initiated at CEMRACS 2016.

7.7. TARGET

Participants: Nicolas Bouzat, Guillaume Latu, Camilla Bressan, Michel Mehrenberger, Virginie Grandgirard.

7.7.1. TArgeting Realistic GEometry in Tokamak code gysela

The framework of the work in [16] is the Semi-Lagrangian setting for solving the gyrokinetic Vlasov equation and the Gysela code. A new variant for the interpolation method is proposed that can handle the mesh singularity in the poloidal plane at $r = 0$ (a polar system is used for the moment in Gysela). A non-uniform meshing of the poloidal plane is proposed, instead of a uniform one, in order to save memory and computations. The interpolation method, the gyroaverage operator, and the Poisson solver are revised in order to cope with non-uniform meshes. A mapping that establishes a bijection from polar coordinates to more realistic plasma shapes is used to improve the realism. Convergence studies are provided to establish the validity and robustness of our new approach. This work has been initiated at CEMRACS 2016.

7.8. Field-aligned interpolation for gyrokinetics

Participants: Yaman Güclü, Philippe Helluy, Guillaume Latu, Michel Mehrenberger, Laura Mendoza, Eric Sonnendrücker, Maurizio Ottaviani.

This work is devoted to the study of field-aligned interpolation in semi-Lagrangian codes. This work has been initiated in 2013; this year the article has been accepted [5]. In the context of numerical simulations of magnetic fusion devices, this approach is motivated by the observation that gradients of the solution along the magnetic field lines are typically much smaller than along a perpendicular direction. In toroidal geometry, field-aligned interpolation consists of a 1D interpolation along the field line, combined with 2D interpolations on the poloidal planes (at the intersections with the field line). A theoretical justification of the method is provided in the simplified context of constant advection on a 2D periodic domain: unconditional stability is proven, and error estimates are given which highlight the advantages of field-aligned interpolation. The same methodology is successfully applied to the solution of the gyrokinetic Vlasov equation, for which we present the ion temperature gradient (ITG) instability as a classical test case: first we solve this in cylindrical geometry (screw-pinch), and next in toroidal geometry (circular Tokamak). In the first case, the algorithm is implemented in Selalib (semi-Lagrangian library), and the numerical simulations provide linear growth rates that are in accordance with the linear dispersion analysis. In the second case, the algorithm is implemented in the Gysela code, and the numerical simulations are benchmarked with those employing the standard (not aligned) scheme. Numerical experiments show that field-aligned interpolation leads to considerable memory savings for the same level of accuracy; substantial savings are also expected in reactor-scale simulations.

We are also currently implementing into SCHNAPS a general transport solver for addressing non-conforming patches in complex geometries. The objective is to be able to design meshes that are able to deal with magnetic aligned geometries. The resulting scheme will be used for solving kinetic equations, of course. But it can also be the building block of a palindromic method applied on curved and non-conforming meshes.

7.9. InKS

Participants: Olivier Aumage, Julien Bigot, Ksander Ejjaaouani, Michel Mehrenberger.

7.9.1. A programming model to decouple performance from semantics in simulation codes

Existing programming models lead to a tight interleaving of semantics and computer optimization concerns in high-performance simulation codes. With the increasing complexity and heterogeneity of supercomputers this requires scientists to become experts in both the simulated domain and the optimization process and makes the code difficult to maintain and port to new architectures. The report in [12] proposes InKS, a programming model that aims to improve the situation by decoupling semantics and optimizations in code so as to ease the collaboration between domain scientists and experts in high-performance optimizations. We define the InKS language that enables developers to describe the semantics of a simulation code with no concern for performance. We describe the implementation of a compiler able to automatically execute this code without making any explicit execution choice. We also describe a method to manually specify these choices to reach high-performance. Our preliminary evaluation on a 3D heat equation solver demonstrates the feasibility of the automatic approach as well as the ability to specify complex optimizations while not altering the semantic part. It shows promising performance where two distinct specifications of optimization choices in InKS offer similar performance as existing hand-tailored versions of the solver.

7.10. Performance of Particle-in-Cell methods

Participants: Yann Barsamian, Sever Hirstoaga, Eric Violard.

In a two-dimensional framework, in [6] we optimized a Particle-in-Cell (PIC) code by analyzing different data structures for the particles and for the grid fields with the aim of improving the cache reuse and by using the vectorization from the compiler. We also parallelized the code with OpenMP/MPI and satisfactory strong and weak scaling up to 8192 cores were obtained on the supercomputer CURIE.
Currently [15] we are extending and improving this work to a three-dimensional electrostatic PIC code.

7.11. Comparison of multiscale PIC methods

Participants: Nicolas Crouseilles, Sever Hirstoaga, Xiaofei Zhao.

In [2] we study different types of multiscale methods to numerically study the long-time Vlasov–Poisson equation with a strong magnetic field. The multiscale methods are an asymptotic preserving Runge–Kutta scheme, an exponential time differencing scheme, the stroboscopic averaging method and a uniformly accurate two-scale formulation. Extensive numerical experiments are conducted to investigate and compare the accuracy, efficiency, and long-time behavior of all the methods. The methods with the best performance under different parameter regimes are identified.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Grants with Industry

We are involved in the PhD direction of Lucie Quibel in collaboration with EDF Chatou (CIFRE support). The objective is to design new Equations Of States (EOS) for the simulation of multiphase flows. The EOS cannot be chosen arbitrarily if one wants to ensure the stability of the fluid model. We are also interested to apply our palindromic method for computing low-Mach liquid-vapor flows.

9. Partnerships and Cooperations

9.1. Regional Initiatives

The thesis of Pierre Gerhard devoted to numerical simulation of room acoustics is supported by the Alsace region. It is a joint project with CEREMA (Centre d'études et d'expertise sur les risques, l'environnement, la mobilité et l'aménagement) in Strasbourg.

9.2. National Initiatives

9.2.1. Contracts with Industry

We are involved in a common project with the company AxesSim in Strasbourg. The objective is to help to the development of a commercial software for the numerical simulation of electromagnetic phenomena. The applications are directed towards antenna design and electromagnetic compatibility. This project was partly supported by DGA through "RAPID" (régime d'appui à l'innovation duale) funds. A CIFRE PhD has started in AxesSim on the same kinds of subjects in March 2015 (Bruno Weber). The new project is devoted to the use of runtime system in order to optimize DG solvers applied to electromagnetism [10]. The resulting software will be applied to the numerical simulation of connected devices for clothes or medicine. The project is supported by the "Banque Publique d'Investissement" (BPI) and coordinated by the Thales company.

9.2.2. ANR

ANR project PEPPSI (models for edge plasma physic in Tokamak) in *Programme Blanc* SIMI 9, started in 2013, ended this year.
Participants: David Coulette, Giovanni Manfredi [coordinator], Sever Hirstoaga.

9.2.3. IPL FRATRES

The TONUS project belongs to the IPL FRATRES (models and numerical methods for Tokamak).
Funded by the IPL, Xiaofei Zhao was a post-doctoral fellow until September 2017, under the joint supervision of Nicolas Crouseilles (team IPSO, Inria Rennes) and Sever Hirstoaga.

9.2.4. IPL C2S@exa

The TONUS and HIEPACS projects have obtained the financial support for the PhD thesis of Nicolas Bouzat thanks to the IPL C2S@exa (computational sciences at exascale). Nicolas Bouzat works at CEA Cadarache and is supervised locally by Guillaume Latu; the PhD advisors are Michel Mehrenberger and Jean Roman.

9.2.5. HPC resources

- GENCI project *Simulation numérique des plasmas par des méthodes semi-lagrangiennes et PIC adaptées*: 450 000 scalar computing hours on CURIE_standard (January 2016-January 2017). Coordinator: Michel Mehrenberger
  Participants: Sever Hirstoaga, Guillaume Latu, Michel Mehrenberger, Thi Nhung Pham, Christophe Steiner, Yann Barsamian.
- GENCI project *Simulations 3D de plasmas deux espèces avec des méthodes particulaires et semi-lagrangiennes*: 400 000 scalar computing hours accepted in October 2017 on supercomputer OCCIGEN. Coordinator: Sever Hirstoaga
  Participants: Yann Barsamian, Sever Hirstoaga, Michel Mehrenberger.
- PRACE project *SME HPC Adoption Programme in Europe: full simulation of an electromagnetic wave inside and ouside a fully modeled human body*: 40 000 GPU computing hours accepted in October 2017 on supercomputer Piz Daint. Coordinator: Bruno Weber
  Participants: Philippe Helluy, Bruno Weber.

9.3. European Initiatives

9.3.1. FP7 & H2020 Projects

9.3.1.1. EUROfusion 2015-2017

- Eurofusion Enabling Research Project ER15-IPP01 (1/2015-12/2017) "Verification and development of new algorithms for gyrokinetic codes" (Principal Investigator: Eric Sonnendrücker, Max-Planck Institute for Plasma Physics, Garching).
  Participants: Philippe Helluy, Sever Hirstoaga, Michel Mehrenberger.
- Eurofusion Enabling Research Project ER15-IPP05 (1/2015-12/2017) "Global non-linear MHD modelling in toroidal geometry of disruptions, edge localized modes, and techniques for their mitigation and suppression" (Principal Investigator: Matthias Hoelzl, Max-Planck Institute for Plasma Physics, Garching).
  Participant: Emmanuel Franck.

9.4. International Initiatives

9.4.1. Participation in Other International Programs

Participants: David Coulette, Conrad Hillairet, Emmanuel Franck, Philippe Helluy [local coordinator].

ANR/SPPEXA "EXAMAG" is a joint French-German-Japanese project. Its goal is to develop efficient parallel MHD solvers for future exascale architectures. With our partners, we plan to apply highly parallelized and hybrid solvers for plasma physics. One of our objectives is to develop Lattice-Boltzmann MHD solvers based on high-order implicit Discontinous Galerkin methods, using SCHNAPS and runtime systems such as StarPU.

9.5. International Research Visitors

9.5.1. Visits of International Scientists

Christian Klingenberg from Würzburg university was invited several times in 2017, by Philippe Helluy.

Roberto Ferretti was invited one month in 2017 at IRMA, by Michel Mehrenberger, for working on the stability of semi-Lagrangian schemes.

9.5.2. Visits to International Teams

9.5.2.1. Research Stays Abroad

Philippe Helluy, Emmanuel Franck and David Coulette visited Christian Klingenberg at Würzburg university.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. Member of the Organizing Committees

Philippe Helluy is member of the French candidature committee for the organization of the International Congress of Mathematics in 2022 in Paris and Strasbourg https://www.icm2022-paris.com/.

10.1.2. Journal

10.1.2.1. Member of the Editorial Boards

Philippe Helluy is in the editorial board of

International Journal of Finite Volume

Computational and Applied Mathematics

10.1.2.2. Reviewer - Reviewing Activities

Emmanuel Franck was a reviewer for

Communication in computation physics

Computer Methods in Applied Mechanics and Engineering

Journal of Computational Physics

Philippe Helluy has done reviews for

Numerical Methods for Partial Differential Equations

Journal of Computational Physics

Computers and Fluids

M2AN

Esaim Proceedings and reviews

Sever Hirstoaga was a reviewer for

Journal of Computational and Applied Mathematics (2 papers)

Journal of Approximation Theory

SIAM Journal on Optimization

Multiscale Modeling and Simulation: A SIAM Interdisciplinary Journal

MathSciNet/Mathematical Reviews

Michel Mehrenberger participates in reviewing for

SIAM Journal on Scientific Computing

Mathematical Methods in the Applied Sciences

Evolution Equations and Control Theory

Journal of Computational Physics

International Conference on Physics, Mathematics and Statistics 2018

Applied Mathematics and Computation

Computer Physics Communications

Laurent Navoret was a reviewer for

Kinetic and Related Models

10.1.3. Invited Talks

Emmanuel Franck was invited at

Enumath conference, Bergen, September 2017.

the Workshop JOREK, Prague, March 2017.

the IPL Fratres Meeting, Rennes, November 2017.

Philippe Helluy was invited at

NUMKIN 2017, Garching November 2017

Fast high order DG methods for future architectures Heidelberg July 2017

Workshop - "Modeling and Numerical Methods for Hot Plasmas III": 12-13 octobre 2017 Bordeaux

Sever Hirstoaga was invited at

the “Séminaire d’analyse numérique”, at IRMAR, Rennes, February 2nd, 2017.

Michel Mehrenberger

gave a talk entitled «About recurrence time for a semi-Lagrangian discontinuous Galerkin Vlasov solver» at Collisionless Boltzmann (Vlasov) Equation and Modeling of Self-Gravitating Systems and Plasmas, CIRM (Marseille), 30 october-3 november 2017.

was invited at the seminar «Analyse Numérique et Calcul Scientifique» of Besançon “Méthodes numériques pour la physique des plasmas”, February 16, 2017.

Larent Navoret was invited at

the Seminar of the Interdisciplinary Center for Scientific Computing, Heidelberg, Germany

10.1.4. Scientific Expertise

Philippe Helluy is in the evaluation committee of the “réseau calcul” of CNRS.

10.1.5. Research Administration

Philippe Helluy

has been elected as the Director of the IRMA mathematics institute (official start in september 2018).

Sever Hirstoaga

was member of the hiring committee for an associate professor position at the ENS Mécanique et des Microtechniques, Besançon.

Michel Mehrenberger

is in the IREM ("Institut de recherche sur l'enseignement des mathématiques") team "Modélisation" for the year 2017-2018, Université de Strasbourg.

is in the committee of the Ecole Doctorale ED269, EDMSII, Université de Strasbourg.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

M1: Philippe Helluy, algorithmes pour les graphes 30 HETD

M2: Philippe Helluy, Contrôle optimal 30 HETD

M2: Philippe Helluy, EDP hyperboliques 30 HETD

L2: Philippe Helluy, Calcul scientifique 64 HETD

Ecole d'ingénieurs: Philippe Helluy, recherche opérationnelle 40 HETD, analyse numérique 40 HETD

Licence: Michel Mehrenberger, Calcul scientifique, 65 h eq. TD, L3, Université de Strasbourg, France.

Licence: Michel Mehrenberger, Optimisation Non-Linéaire, 54h eq. TD, Cours et TD, L3 Maths-Eco, Université de Strasbourg, France

Master: Michel Mehrenberger, Calcul scientifique, 32.5h eq. TD, Cours et TP, M1 CSMI, Université de Strasbourg, France.

Master: Michel Mehrenberger, PIP: certification python, 13h eq. TD, TP, M1 Mathématiques, Université de Strasbourg, France.

Master: Michel Mehrenberger, Calcul scientifique, 22 h eq. TD, TP, M2 Agrégation, Université de Strasbourg, France.

Licence : Laurent Navoret, Nonlinear optimization (18h eq. TD), L3 Maths-Eco, Université de Strasbourg, France.

Master 1: Laurent Navoret, Python (32,5h eq. TD), Université de Strasbourg, France.

Master 2 (Agrégation) : Laurent Navoret, scientific computing (60h eq. TD), Université de Strasbourg, France.

Master 2 (Cell physics) : Laurent Navoret, Basics in maths (24h eq. TD), Université de Strasbourg, France.

Master 2 (Agrégation) : Laurent Navoret, Head of the master, Université de Strasbourg, France.

10.2.2. Supervision

Philippe Helluy has been Habilitation "garant" of Olivier Hurisse (EDF) and Marcela Szopos (IRMA), at université de Strasbourg.

PhD in progress: Lucie Quibel (CIFRE support): in collaboration with EDF Chatou, from October 2017, Advisor: Philippe Helluy.

PhD in progress: Marie Houillon: "Modeling of thin wires in electromagnetic software", Advisors: Philippe Helluy and Laurent Navoret, from October 2017, Labex Irmia support.

PhD in progress: Bruno Weber(CIFRE support): "Optimization of DG software on GPU in the AxesSim company". Advisor: Philippe Helluy.

PhD in progress: Maxime Schmitt: “Optimization of scientific software with arbirary mesh refinement”, Advisors: Philippe Helluy and Cédric Bastoul (CAMUS team). Labex Irmia support.

PhD in progress: Ksander Ejjaaouani, "Conception of a programmation model, application to gyrokinetic simulations", from October 2016, Advisors: Michel Mehrenberger, Julien Bigot, Olivier Aumage.

PhD in progress: Nicolas Bouzat, "Conception of a programmation model, application to gyrokinetic simulations", from October 2015, Advisors: Michel Mehrenberger, Jean Roman, Guillaume Latu.

PhD in progress: Pierre Gerhard, "Résolution des modèles cinétiques. Application à l'acoustique du bâtiment", from October 2015, Advisors: Philippe Helluy, Laurent Navoret.

Conrad Hillairet: interrupted thesis at the request of the student.

10.2.3. Juries

Philippe Helluy was member of the following juries

jury of the PhD committee of Tohir Akramov, in astrophysics, université de Strasbourg, 28 September 2017.

jury of the PhD committee of Thomas Altazin, in scientific computing, université de Toulon, 7 September 2017.

jury of the PhD committee of Laura Mendoza, in plasma physics, Max Planck Institut for Plasma Physics, Garching.

jury of the PhD committee of Florence Drui, in multiphase models, Ecole Centrale Paris, 7 July 2017.

Michel Mehrenberger was member of the jury of the PhD committee of Mohammad Akil (Université de Limoges), 6 October 2017.

11. Bibliography

Publications of the year

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International Conferences with Proceedings

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Conferences without Proceedings

[9] L. NAVORET, M. MEHRENBERGER. *About recurrence time for a semi-Lagrangian discontinuous Galerkin Vlasov solver*, in "Collisionless Boltzmann (Vlasov) Equation and Modeling of Self-Gravitating Systems and Plasmas", Marseille, France, October 2017, https://hal.archives-ouvertes.fr/hal-01653023

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