TONUS – TOkamaks and NUmerical Simulations – Inria project-team in Strasbourg.

IRMA (CNRS UMR 7501), Inria Nancy-Grand Est, Université de Strasbourg.

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1 TONUS in a few words

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. It consists in confining a very hot hydrogen plasma inside a toroidal chamber, called a tokamak. In addition to physics and technology research, tokamak design also requires mathematical modeling 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 and gyrokinetic simulations of collisionless plasmas. Together with other Inria teams, we will also address related subjects: fluid plasma models; collisions; reduced, multiscale and asymptotic models; electromagnetism, etc. TONUS is a team of the Inria Nancy-Grand Est center. It is located in the mathematics institute¹ of the university of $Strasbourg^2$.

TONUS is an evolution of the CALVI³ project, created in 2003 by Éric Sonnendrücker. Éric Sonnendrücker has been hired by the Max Planck Institute in Munich. TONUS will be directed by Philippe Helluy, professor in applied mathematics at the university of Strasbourg.

In the TONUS project-team we will develop research on new numerical methods devoted to plasma physics simulation. We will investigate several classical plasma models, create new reduced models and new powerful numerical schemes adapted to these models.

We will implement our methods in our two software projects: Selalib⁴ and CLAC⁵, adapted to new computer architectures. We will run challenging simulations on high performance computers with thousands of nodes.

In order to achieve these aims, we will collaborate with several Inria and international teams working on related subjects. We will also keep strong relations with the CEA-IRFM team⁶ and participate to the development of their gyrokinetic simulation software GYSELA. We will be involved into two Inria Project Labs: FUSION and C2S@exa, respectively devoted to tokamak mathematical modeling and high performance computing on future exascale supercomputers.

Finally, we want the TONUS project-team to be at the interaction between mathematics, computer science, High Performance Computing, physics and practical applications.

2 TONUS members

2.1 Current composition

- Head: Philippe Helluy (PR⁷, Université de Strasbourg (UdS)).
- Permanent members: Michaël Gutnic (MCF, UdS), Sever Hirstoaga (CR, Inria), Michel Mehrenberger (MCF HDR, UdS), Laurent Navoret (MCF, UdS).
- Temporary research engineers: Edwin Chacon-Golcher (Inria)
- Permanent research engineer: Pierre Navaro (CNRS, UdS).
- PhD students: Pierre Glanc, Mathieu Lutz (ATER 2013-2014), Michel Massaro, Nhung Pham, Christophe Steiner, Thomas Strub.

¹"Institut de Recherche Mathématique Avancée" (IRMA)

²"Université de Strasbourg" (UdS)

³CALcul scientifique et VIsualisation

⁴Semi-Lagrangian Library http://selalib.gforge.inria.fr/

⁵Conservation Laws Approximation on many Cores

⁶CEA: "Commissariat à l'Energie Atomique", french atomic energy agency. IRFM: "Institut de Recherche sur la Fusion Magnétique", research team working on magnetic confinement fusion in CEA.

⁷PR: full professor, MCF: assistant professor, CR: researcher.

- Postdoc: Adnane Hamiaz (Inria, UdS).
- Associate members: Nicolas Besse (MCF HDR, Université Henri Poincaré), Emmanuel Frénod (PR, Université de Bretagne-Sud).

2.2 Participants' résumés

Head: Philippe Helluy

45 years old, full professor since 2006, Université de Strasbourg (UdS). Applied mathematics, scientific computing for multiphase flows and plasma physics.

PhD thesis in 1994, ONERA Toulouse on numerical methods for electromagnetism. 1994-2006: assistant professor in the University of Toulon. Habilitation thesis in 2005 on multiphase flows.

1) Barberon, Thomas; Helluy, Philippe; Rouy, Sandra Practical computation of axisymmetrical multifluid flows. Int. J. Finite Vol. 1 (2004), no. 1, 34 pp.

2) Helluy, P.; Mathis, H. Pressure laws and fast Legendre transform. Math. Models Methods Appl. Sci. 21 (2011), no. 4, pp. 745-775.

3) Crestetto, A.; Helluy, P. Resolution of the Vlasov-Maxwell system by PIC discontinuous Galerkin method on GPU with OpenCL. ESAIM Proc. 38 (2012) pp. 257-274

Current doctoral supervision: J. Jung, M. Massaro, N. Pham, T. Strub.

Award: fourth prize of the AMD international OpenCL innovation challenge 2012.

A more complete CV can be found at http://www-irma.u-strasbg.fr/helluy/ADMIN/ cv-helluy.pdf

Nicolas Besse

36 years old, assistant professor since 2005 at Université de Nancy.

PhD thesis in 2003, Université Louis Pasteur, Strasbourg. HDR thesis in 2009, Université Henri Poincaré, Nancy.

1) N. Besse, E. Sonnendrücker, Semi-Lagrangian schemes for the Vlasov equation on an unstructured mesh of phase space, J. Comput. Phys., 191 (2003), 341-376,

2) N. Besse, Convergence of a high-order semi-Lagrangian scheme with propagation of gradients for the Vlasov-Poisson system, SIAM, J. Numer. Anal., 46 (2008), 639-670

3) N. Besse, Y. Elskens, D. Escande, P. Bertrand, Validity of quasilinear theory: refutations and new numerical confirmation, Plasma Phys. Control. Fusion, 53 (2011), 025012

Current doctoral supervision: David Coulette, PhD student in Plasma Physics, CNRS/Région Lorraine Fellowship 2010-2013

Edwin Chacon-Golcher

40 years old, Specialist Engineer at Inria.

PhD thesis in 2002, University of California at Berkeley 2002-2004 Postdoc, Los Alamos National Laboratory, 2004-2010 Staff Member Los Alamos National Laboratory, 2010-present: Specialist Engineer Inria

1) E. Chacon-Golcher and Kevin J. Bowers. Particle-in-Cell with Monte Carlo Collisions Gun Code Simulations of a Surface-Conversion H- Ion Source. Commun. Comput. Phys., 4 (2008), pp. 647-658. International Conference on Numerical Simulation of Plasmas, 2007.

2) E. Chacon-Golcher and F. Neri. A Symplectic Integrator with Arbitrary Vector and Scalar Potentials. Physics Letters A. http://dx.doi.org/10.1016/j.physleta.2008.04.058

3) A. Anders and E. Chacon-Golcher. Time Resolved Emittance of a Bismuth Ion Beam from a Pulsed Metal Vacuum Arc Ion Source. J. Appl. Phys. Vol 93 No. 5. Mar. 2003.

Emmanuel Frénod

44 years old, Professor since 2006 Université de Bretagne-Sud, France.

PhD in 1994, Université Paris-Nord, habilitation thesis in 1999, Université de Bretagne-Sud

1) N. Crouseilles, E. Frénod, S. Hirstoaga & A. Mouton (2013) Two-Scale Macro-Micro decomposition of the Vlasov equation with a strong magnetic Field. Mathematical Models and Methods in Applied Sciences, vol. 23, No. 8, pp 1527–1559

2) E. Frénod & A
 . Rousseau (2013) Paralic Confinement - Models and Simulations. Acta
 Applicanda Mathematicae, vol $123,\,{\rm No}$ 1, pp
 $1\!-\!19$

3) I. Faye, E. Frénod & D. Seck (2011) Singularly perturbed degenerated parabolic equations and application to seabed morphodynamics in tided environment. Discrete and Continuous Dynamical Systems, Series A (DCDS-A), Vol. 29, No 3, pp 1001–1030

Current doctoral supervision:

Tarik Chakour - Développement, analyse et implémentation d'un modèle financier continu - Financement sur contrat de recherche (avec MGDIS) - Ecole Doctorale SICMA (Soutenance prévue fin 2015).

Mathieu Lutz - Etude mathématique et numérique d'un modèle gyrocinétique incluant des effets électromagnétiques pour la simulation d'un plasma de Tokamak - Codirection avec Eric Sonnendrücker - Bourse MESR - École Doctorale de Strabourg (Soutenance prévue en 2013)

Michaël Gutnic

44 years old, assistant professor since 1999, Université de Strasbourg.

PIC methods for plasma physics. Finite Volume for porous medium flows.

1) Frénod, Emmanuel; Gutnic, Michaël; Hirstoaga, Sever A. First order Two-Scale Particlein- Cell numerical method for Vlasov equation, submitted to Proceedings of CEMRACS 2011, in ESAIM Proc.

2) Gutnic, Michaël; Latu, Guillaume; Sonnendrücker, Eric, Adaptive two-dimensional Vlasov simulation of heavy ion beams, Nucl. Instr. and Meth. A, doi :10.1016/j.nima.2007.02.043 (2007).

3) Eymard, R.; Gallouët, T.; Herbin, R.; Gutnic, M.; Hilhorst, D. Approximation by the finite volume method of an elliptic-parabolic equation arising in environmental studies. Math. Models Methods Appl. Sci. 11 (2001), no. 9, 1505–1528.

Sever Hirstoaga

35 years old, Inria junior researcher since 2008

2007-2008: Inria post-doctoral position, Institut Mathématique de Toulouse, Toulouse 2006-2007: ATER, Université Paris-Dauphine, Paris. PhD thesis in 2006, Université Pierre et Marie Curie, Paris

1) Vlasov modelling of parallel transport in a tokamak scrape-off layer, Plasma Physics and Controlled Fusion, 53(1), 015012, 2011; with G. Manfredi, S. Devaux

2) Two-Scale Macro-Micro decomposition of the Vlasov equation with a strong magnetic field, M3AS, 23 (8), 2013, 1527–1559; with N. Crouseilles, E. Frénod, A. Mouton

3) First order Two-Scale Particle-In-Cell numerical method for the Vlasov equation ESAIM Proceedings, 38, 2012, 348-360; with E. Frénod, M. Gutnic.

Michel Mehrenberger

36 years old, Assistant professor since 2006, Université de Strasbourg

PhD thesis in 2004, Université Louis Pasteur, Strasbourg HDR thesis in 2012, Université de Strasbourg 2005-2006, post-doctoral position INRIA GAMMA project, Rocquencourt

1) Convergence of classes of high order semi-Lagrangian schemes for the Vlasov equation, Math. of Comp. 77 (2008), 93–123, with Nicolas Besse

2) Conservative semi-Lagrangian schemes for Vlasov equations, Journal of Computational Physics 229 (2010), 1927–1953, with Nicolas Crouseilles and E. Sonnendrücker.

3) Enhanced convergence estimates for semi-Lagrangian schemes. Application to the Vlasov-Poisson equation, SIAM J. Numer. Anal 51 (2013), no. 2, 840–863, with F. Charles and B. Després.

Current doctoral supervision:

P. Glanc (2010-2013) "Numerical approximation of the Vlasov equation with conservative remapping methods", with N. Crouseilles.

C. Steiner (2011-2014), '"Study of the numerical resolution of the gyroaverage operator and of some advection schemes", with N. Crouseilles.

Pierre Navaro.

41 years old, Research Engineer in Scientific Computing since 2004 CNRS.

PhD thesis in 2002, Université du Havre

Senior developer in project Selalib http://selalib.gforge.inria.fr

Laurent Navoret

30 years old, Assistant Professor since 2011 Université de Strasbourg.

PhD thesis in 2010, Université Paul Sabatier, Toulouse Postdoctoral position in 2010-2011, Université Paris Descartes, Paris

1) P. Degond, F. Deluzet, L. Navoret, A.-B. Sun, M.-H. Vignal, Asymptotic-Preserving Particle-In-Cell method for the Vlasov-Poisson system near quasi-neutrality, J. Comp. Phys., vol. 229, n°16, pp. 5630-5652 (2010)

2) P. Degond, L. Navoret, R. Bon, D. Sanchez, Congestion in a macroscopic model of self-driven particles modeling gregariousness, J. Stat. Phys., vol. 138, pp. 85-125 (2010)

3) P. Degond, J. Hua, L. Navoret, Numerical simulations of the Euler system with congestion constraint, J. Comput. Phys., vol. 230, n 22, pp. 8057–8088 (2011)

Doctoral supervision : Mme Thi Trang Nhung PHAM (co-supervision with Philippe Helluy).

2.3 Other members

Several PhD students and postdocs are currently working in TONUS. We give here briefly their research subjects.

Pierre Glanc (directed by M. Mehrenberger): conservative semi-Lagrangian schemes.

Adnane Hamiaz (postdoc): Vlasov solvers on curvilinear meshes.

Mathieu Lutz (directed by E. Frénod): theoretical geometrical aspects of the gyrokinetic theory.

Michel Massaro (directed by P. Helluy and the CAMUS team): MHD solvers, algorithms for multicore solvers.

Nhung Pham (directed by P. Helluy and L. Navoret): reduced and velocity-Fourier-transformed Vlasov solvers.

Christophe Steiner (directed by M. Mehrenberger): theoretical and numerical studies of semi-Lagrangian schemes and of gyroaverage operators.

Thomas Strub (directed by P. Helluy and the AxesSim company staff): Maxwell solvers in the CLAC software.



Figure 1: Poloidal coils and magnetic field lines geometry inside a tokamak.

3 Tokamak plasma modeling

3.1 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 a result of a joint decision by an international consortium made of the European Union, Canada, the 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. It is thus 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 (see Figure 1). 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*.

3.2 A challenge for scientific computing

The main unknown of the problem is the distribution function f(x, v, t) that counts the number of ions at point x and time t having velocity v. The problem is time-dependent in



Figure 2: Gyrokinetic trajectories

a six-dimensional phase space. The distribution function satisfies the Vlasov equation with weak collisions

$$\partial_t f + v \cdot \nabla_x f + (E + v \times B) \cdot \nabla_v f = C(f) \simeq 0.$$

The equation is coupled with Maxwell's equations for the electric field E and the magnetic field B. Generally one can assume that the particle velocities are small compared to the speed of light. In a first approximation, the magnetic field is also supposed to be known. It is then sufficient to solve the Poisson equation for the electric potential Φ in order to compute the electric field

$$\nabla \cdot E = \rho - \rho_0, \quad E = -\nabla \Phi,$$

while the charge ρ is given by

$$\rho(x,t) = \int_{v} f(x,v,t) dv.$$

The model has to be supplemented by boundary conditions. Of course, the model can be refined with many others physical phenomena: electron effects, magnetic fluctuations, *etc*.

As of today, solving the full Vlasov-Poisson model in a tokamak is way too expensive, even in modern supercomputers. It is thus necessary to derive more tractable models, taking into account several asymptotics.

Charged particles follow helicoidal trajectories around magnetic field lines, this is called cyclotron motion. See Figure 2. Inside a tokamak, because of the high intensity of the magnetic fields, the rotation occurs at high cyclotron frequency.

Moreover, the central plasma density is very low and the collisions are rare. It is thus possible to neglect them on long time scale. The consequence is that classical fluid models, such as MagnetoHydroDynamics (MHD), are not able to precisely represent the plasma in the core region. More expensive models that capture kinetic effects are required. The gyrokinetic models [Gar11] are obtained by supposing that the cyclotron frequency tends to infinity.

The gyrokinetic models are widely adopted in tokamak simulation software written by physicists. Depending on the effects considered, these models may become very complicated. Despite the asymptotic hypotheses, they remain very expensive to solve numerically. In the TONUS project we participate to the tokamak numerical simulation challenge. We have three main objectives, which are to

- justify rigorously the models obtained by the physicists and propose new models;
- construct adaptive and efficient numerical methods;
- implement the numerical methods in useful software adapted to supercomputer architectures.

3.3 State of the art

Several teams worldwide are developing models and simulation software for gyrokinetic tokamak plasmas. We give here a list of representative developments in this field.

We can distinguish two kinds of work:

- numerical analysis for plasma physics is developed by mathematicians, physicists or computer scientists. In this work, small teams, specialized in scientific computing, design new numerical methods, models and algorithms. The methods are rigorously analyzed and tested in simplified configurations. Depending on their efficiency, and if they are designed for production simulation codes, they can be incorporated into larger software. The numerical analysis is not limited to the development of direct simulation tools. New tools are emerging: reduced model and adaptive model analysis, uncertainty quantification, asymptotic-preserving approximations.
- tokamak gyrokinetic simulation codes are mainly developed by teams of physicists and often supported by national energy agencies (Department Of Energy in the US, EURATOM in Europe, CEA in France, Max Planck Institute in Germany, Atomic Energy Agency in Japan). These codes require complex physical models and algorithms that scale on supercomputers. They are developed by teams of several physicists, computer scientists and, sometimes, mathematicians. Thus, they require rigorous software engineering and once an architecture is chosen they are not necessarily adapted to new methods and algorithms. In addition, the focus is often set on physical modeling and intensive parallel computations. Physical models and software engineering are thus carefully designed, but the numerical methods are not necessarily the most recent.

In TONUS, we are interested in the two kinds of works: design of new methods, implementation in applied simulation tools, like the CEA code GYSELA.

3.3.1 Research on general methods

We now mention some applied mathematicians working on numerical methods for plasma physics. Such researchers are developing general numerical methods that can be applied to many fields of science. They can also be interested in numerical fluid mechanics or electromagnetic simulations, for instance. Therefore it is not possible to give a complete list of applied mathematicians who have worked on numerical methods for plasma physics. We only review a few well-established researchers. **United States** Phillip Colella is a well known researcher from the Lawrence Berkeley National Laboratory working on numerical methods for hyperbolic systems. With collaborators, he has written recently several papers on adaptive numerical approximation of the Vlasov equation [BMC12].

Irene Gamba is professor at the university of Texas. She is specialized in the numerical resolution of Vlasov and other kinetic equations. She is interested in the applications of the Discontinuous Galerkin approach to plasma models [CGFLM13].

Andrew Chriestlieb is associate professor at the university of Michigan. He is working on meshless Vlasov solvers and parallel time integrators [QC10]

Leslie Greengard is professor at the Courant Institute in New York. He is specialized on fast numerical solvers for electromagnetism [GG13].

Cory Hauck is a researcher at Oak Ridge National Laboratory. He is interested in computational aspects of kinetic theory and hyperbolic balance laws, including entropy dissipative moment methods, asymptotic analysis, and numerical schemes for multi-scale problems [HL08].

Jan Hesthaven is professor at Brown University. He is well known for his works on discontinuous Galerkin methods, Particle-In-Cell solvers and GPU computing [KWBH09]. He as also worked on uncertainty quantification, Padé interpolants of discontinuous functions and general strategies for constructing reduced models.

Chi-Wang Shu is professor at Brown University. He is a specialist of numerical solutions of conservation laws: non oscillatory finite difference, DG approximations and spectral methods [ZGS01].

Europe José Carrillo is professor at Imperial College in London. He is a specialist of the numerical analysis of PDEs. He has written several papers on the numerical approximation of the Vlasov equation. For a recent work on Discontinuous Galerkin method applied to Vlasov Poisson system, see [DCS12].

Pierre Degond, previously in Toulouse, has also recently been hired by Imperial College in London. He has worked many years on theoretical and numerical methods for kinetic or fluid plasma physics. Recently he has studied many schemes derived from the Asymptotic Preserving approach. See [DDNSV10] for instance.

Bengt Elliasson is a theoretical physicist from University of Bochum, Germany. He has recently published a series of paper on the Fourier transformed Vlasov equation [Eli10]. We will extend his approach for constructing reduced plasma models.

Dietmar Kröner is professor at the Freiburg University, in Germany. He has developed several methods for plasma physics and already collaborated with us. For instance, he has constructed a divergence cleaning technique for the finite volume MHD solvers, which is widely used and cited [DKKMSW02].

Claus-Dieter Munz is professor at the University of Stuttgart. He has developed with Dietmar Kröner the divergence cleaning for MHD. He has also a long experience on Discontinuous Galerkin solver with ADER time integration and Particle-In-Cell methods for beam physics [Mu12]. **Japan** Yasuhiro Idomura is a researcher at the Japan Atomic Energy Agency. He is specialized in HPC and eulerian conservative schemes for tokamak simulations [IIKAT08]. He is also developer of the code GT5D.

Takashi Yabe is a Professor at the Department of Mechanical Sciences and Engineering, Tokyo Institute of Technology. He is specialist both of numerical methods for fluid mechanics and for plasma physics [TYN02].

3.3.2 Simulation tools

The typical tokamak simulation software relies on the gyrokinetic approximation. It is generally based on one of the three main approaches: the Lagrangian approach (Particle-In-Cell methods), Eulerian approaches (finite volumes or finite elements) or semi-Lagrangian approaches. A review of the physicists' favorite methods and software is given in the review [Gar11]. We list here some of them.

PIC solvers In the Particle-In-Cell (PIC) approach, the distribution function is approximated by particles, which are accelerated by the electromagnetic field. The electric potential is solved on a grid with a Poisson solver. The source term of the Poisson solver is obtained from a particle deposition algorithm on the grid.

- ELMFIRE ⁸ is a gyrokinetic code for studies of both turbulence and neoclassical effects in tokamaks. It is developed by J. Heikkinen and his team in Finland [HJKO08]. It is based on a so called full-f approach. The δf approach consist in splitting the distribution function f into a main Maxwellian part f_0 and a perturbation δf , which is represented by particles. The full-f approach is more general but also more computationally intensive.
- GTS⁹ is PIC solver developed by W. Wang at the Princeton Plasma Physics Laboratory (PPPL). The code uses a δf approach, it can handle adiabatic or kinetic electrons. It can be coupled to experimental or coupled magnetic configurations. XGC is another gyrokinetic Particle-in-Cell code developed at PPPL¹⁰ by S. Ku and C. S. Chang. XGC is devoted to the simulation of kinetic turbulence in edge plasmas. It is adapted to diverted magnetic geometries with wall boundary conditions.
- ORB5¹¹ is a global gyrokinetic δf PIC solver: the distribution function is represented by numerical particles. The code solves the Fokker-Planck-Poisson system, in the electrostatic limit, for gyrokinetic ions and drift-kinetic or adiabatic electrons. It is developed in EPFL in Switzerland by the team of L. Villard
- VORPAL ¹² is a PIC solver initially developed at the university of Colorado. It is now commercially distributed by the company Tech-X.

⁸http://physics.aalto.fi/groups/fusion/research/elmfire/

 $^{^{9} \}rm http://theorycodes.pppl.wikispaces.net/GTS$

 $^{^{10} \}rm http://theorycodes.pppl.wikispaces.net/XGC1$

¹¹http://crpp.epfl.ch/ORB5

¹²http://www.txcorp.com/

Eulerian and semi-Lagrangian solvers In the Eulerian approach, the distribution function is solved on a five-dimensional grid by finite difference (or similar) methods. In the semi-Lagrangian approach, the particles are initially located at grid nodes. They are projected back on grid nodes after each time step.

- GKWGKW (Gyro-Kinetics at Warwick)¹³ is a dedicated software tool for the study of turbulence in a tokamak plasma in the local limit. It includes the full toroidal geometry of the tokamak, with real MHD equilibria, kinetic electrons and an arbitrary number of ion species, electro-magnetic effects, collision effects.
- GENE¹⁴, FEFI : GENE is a plasma gyrokinetic code developed by the team of F. Jenko at the Garching Institut for Plasma Physics (IPP) in Germany. FEFI is another similar software developed by B. Scott at IPP. GENE can be coupled to various MHD equilibrium codes for both tokamak and stellarator geometries. GENE can be used for two-scale simulations involving ions and electrons. It can solve a single flux tube or a full tokamak [GJ11]. GENE uses a numerical discretization that follows the magnetic field lines.
- GT5D¹⁵ is a full-*f* gyrokinetic software developed at Japan Atomic Energy Agency. It is based on high order conservative finite difference approximation and semi-implicit time integration. It solves ions and supposes that the electrons are adiabatic. The equations are solved in aligned curvilinear coordinates. The code has been highly optimized on recent supercomputers architectures with 10,000-100,000 cores [IJ11].
- GYRO and NEO¹⁶ are computational plasma physics code developed and maintained at General Atomics, an american private company working in the nuclear domain. GYRO solves the five-dimensional coupled gyrokinetic and Maxwell equations using a combination of finite difference, finite element and spectral methods. It has the capability to treat a flux-tube or global radial domain, in a full or partial torus. It also handles adiabatic, drift-kinetic or gyrokinetic electrons.
- GYSELA¹⁷ is a semi-Lagrangian solver developed by the team of V. Grandgirard at CEA Cadarache in France. GYSELA computes a full-*f* model with ions. The semi-Lagrangian approach allows using arbitrary time-step, which is an important advantage over other methods. Recently, GYSELA ran on a supercomputer with 500,000 processors. GYSELA is the only important gyrokinetic semi-Lagrangian solver worldwide [G07].
- TEMPEST¹⁸ is an edge simulation software developed at the Lawrence Livermore National Laboratory. It allows gyro-kinetic continuum simulations to study the boundary plasma over a region extending from inside the H-mode pedestal across the separatrix to the divertor plates [X10].

 $^{^{13}}$ http://code.google.com/p/gkw/

 $^{^{14} \}rm http://www.ipp.mpg.de/{\sim}fsj/gene/$

 $^{^{15} \}rm http://www-jt60.naka.jaea.go.jp/english/theory/staff/idomura.html$

 $^{^{16} \}rm https://fusion.gat.com/theory/Gyro$

 $^{^{17}} http://www-drfc.cea.fr/cea/ts/resultats/gyrocinetique/$

 $^{^{18} \}rm http://www.mfescience.org/Tempest/index.html$

3.3.3 American CERF project

The Co-design for Exascale Research in Fusion (CERF) Center is a recent American project, headed by Alice Koniges from Berkeley¹⁹. It puts together a team with physicists, mathematicians, computer scientists and hardware engineers. Physicists guide the integrated development through real user codes. Solver technology, advanced numerics, and programming models are also included. The multidisciplinary nature of the project is very interesting.

Inria supports two IPL²⁰ projects where tokamak fusion simulation is involved. The FUSION IPL, which should be launched in 2014, is devoted to mathematical and numerical analysis of plasma models. The C2S@EXA IPL, which started in May 2013, is devoted to research on future exascale computers and algorithms. One of the large scale challenges addressed by C2S@EXA is the simulation of a tokamak core plasma on supercomputer architectures. The American CERF project could be compared, in its spirit, to the combination of those two IPL projects.

4 Project

We will describe now the main lines of our research project. On the methodology side, we have decided to concentrate on the following points:

- kinetic simulations,
- reduced simulations,
- electromagnetic solvers for plasma physics.

We will also continue two software projects:

- Selalib, devoted to kinetic simulations,
- CLAC, devoted to reduced and electromagnetic models.

For each point, we recall the context and give our objectives for the next year.

In Section 6 we present our main collaborations and conclude on our positioning in the international context.

4.1 Kinetic models for plasmas

Participants: N. Besse, E. Chacon-Golcher, E. Frénod, M. Gutnic, P. Helluy, S. Hirstoaga, M. Mehrenberger, P. Navaro, L. Navoret.

¹⁹http://cerf.nersc.gov/

²⁰Inria Project Labs

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 into account relativistic particles, which lead to consider the relativistic Vlasov equation, but generally, tokamak plasmas are supposed to be non relativistic. The particles' distribution function depends on seven variables (three for space, three for velocity and one for time), which leads to very heavy 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.

Because the magnetic field is strong, the particle trajectories have a very fast rotation around the magnetic field lines. A full resolution would require excessive calculations. It is thus necessary to develop models where the cyclotron frequency tends to infinity 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. Those models require averaging of the acting fields during a rotation period along the trajectories of the particles. This averaging is called the gyroaverage and requires specific discretizations.

The tokamak and its magnetics fields present a very particular geometry. Some authors have proposed to return to the intrinsic geometrical versions of the Vlasov-Maxwell system in order to build better gyrokinetic models and adapted numerical schemes. This implies the use of sophisticated tools of differential geometry: differential forms, symplectic manifolds, and hamiltonian geometry.

In addition to theoretical modeling tools, it is necessary to develop numerical schemes adapted to kinetic and gyrokinetic models. Three kinds of methods will be developed: Particle-In-Cell (PIC) methods, semi-Lagrangian and fully Eulerian approaches.

4.1.1 Gyrokinetic models: theory and approximation

Context In most phenomena where oscillations are present, we can establish a three-model hierarchy:

- the model parameterized by the oscillation period,
- the limit model,
- 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 where 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. Implemented Two-Scale Numerical Methods (for instance by Allaire, et al. and Frénod et al. [AB05, FSS09]) are 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 to 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) with the property being able to 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. [CFHM].

Objectives On the mathematical side, following the works of Mathieu Lutz' PhD thesis [FL11], we will generalize the geometric Gyro-Kinetic theory by writing it when the phase space is the cotangent bundle of a regular manifold and Maxwell equations are written using differential forms. This will be connected with the works to adapt the Two-Scale convergence to objects like differential forms developed in the PhD thesis of Aurore Back [Bac11].

Beyond the mathematical motivation of this task, these geometric concepts will then be used to validate Two-Scale Numerical Methods (meaning that we ask for the numerical scheme to preserve the Hamiltonian, invariants, geometrical structure *etc.*) and thus make them more robust with respect to their behavior over time spans of a few tens of milliseconds.

In the end, the objective is to implement Two-Scale Numerical Methods within software products dedicated to Tokamak simulation. The chosen software product for this is Selalib, described in Section 5.1. Following previous works of the CALVI team on two-scale numerical methods, we will progressively incorporate two-scale gyrokinetic solvers into Selalib. We will consider two families of solvers: the Particle-In-Cell (PIC) approach and the Semi-Lagrangian approach (see below).

4.1.2 Semi-lagrangian schemes

Context 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 longstanding 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 introduce a new family of methods for solving transport equations in the phase space. This family of methods are the semiLagrangian 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 thus 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) [SRBG99] for the simulation of core turbulence that has been developed at CEA Cadarache in collaboration with our team [GBBa06]. Although GYSELA was carefully developed to be conservative at lowest order, it is not exactly conservative, which might be an issue when the simulation is under-resolved, which always happens in turbulence simulations due to the formation of vortices which roll up.

Objectives In the last years, we have developed two alternatives: a conservative semi-Lagrangian method (CSL) that is based on the conservative form of the Vlasov equation [CMS10b] and a forward semi-Lagrangian (FSL) method that involves a PIC like conservative deposition in the whole phase-space [CMS09]. Our aim is to continue the validation of FSL and CSL in Selalib and GYSELA.

The tokamak plasma is strongly anisotropic due to the large magnetic field. It is essential for an accurate an robust numerical solver to decouple the fast and slow advections in the gyrokinetic equations. For this, two options are envisaged. The first one consists in working with curvilinear coordinates, which are aligned with the motion of the particles in the equilibrium state. Some first developments are being done for reduced Vlasov-Poisson models and will be continued.

Another option is to work in the original system of coordinates but split the fast and slow advections using an operator splitting technique. The fast advection would contain only terms known at the beginning of the simulation, the self-consistent part being in the slow advection. For the fast advection, a FSL scheme can be considered or some cascade interpolation variants, which should permit to replace the costly four-dimensional interpolation/deposition step by a succession of one-dimensional steps. The fast advection can then be coupled with a CSL/Finite Volume method; this has already been investigated [BCMS09] for the slow motion.

Associated to this problem is the study of the gyroaverage operator; several techniques have been developed in the framework of a cartesian mesh [CMS10a]. We plan to develop a robust gyroaverage solver in the circular geometry and even on more general geometries. More generally, development of Vlasov and Poisson solvers in curvilinear geometries will be continued. Reduced models in two dimensions for specific circular geometries will be envisaged in the framework of the library Selalib.

4.1.3 PIC methods

Context 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 the method 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 longstanding experience in PIC methods. Our objective will be to continue to study them and implement them in Selalib. An important aspect is to adapt the method to new multicore computers. See the preliminary work by Crestetto and Helluy [CH12].

Objectives As we have already explained, several different time scales make the numerical resolution of the particle trajectories difficult. We will implement in Selalib new Asymptotic Preserving (AP) PIC algorithms. These algorithms will be obtained from the theoretical studies detailed in 4.1.1. We will also implement recent PIC methods for the quasineutral limit [Na11].

Recently Martin Campos Pinto, from Laboratoire Jacques Louis Lions (LJLL) in Paris introduced a new class of particle methods for solving abstract transport equations. In this method, the "particles" are represented by functions, such as splines localized around centers that follow the characteristic trajectories of the problem. Their shapes are modified during the evolution according to local approximations of the characteristic flow. A novelty of the method is that the particles are not regularized. In the new approach, the projection step is not necessary for proving the convergence of the method.

We will implement in Selalib, in collaboration with Martin Campos Pinto, the new PIC solver and will provide extensive validations on classical problems and in the asymptotic gyrokinetic limit.

4.2 Reduced kinetic models for plasmas

Participants: N. Besse, P. Helluy, S. Hirstoaga, L. Navoret

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. Fine collision models will be mainly investigated in the KALIFFE team. In our approach we will not assume that the collisions are strong, but rather try to adapt the representation of the distribution function according to its shape, keeping the kinetic effects. 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). Recently, a team at



Figure 3: Space a velocity fluctuations spectra (from [HNT12])

the Plasma Physics Institut (IPP) in Garching has carried out a statistical analysis of the 5D distribution functions obtained from gyrokinetic tokamak simulations [HNT12]. They discovered that the fluctuations are much higher in the space directions than in the velocity directions. See Figure 3.

This indicates that the approximation of the distribution function could require fewer data while still achieving a good representation, even in the collisionless regime.

Our approach is different from the fluid approximation. 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 and will be studied theoretically and numerically: waterbag approximations, velocity space transforms, *etc.*

4.2.1 Velocity space transformations

Context An experiment made in the 60's [MW64] 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 Villani [Vil10], 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 damping [MV11, Vil12].

More practically, this experiment and its theoretical framework show that it is interesting to represent the distribution function by an 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 Eliasson in [Eli01] with the Fourier expansion.

In long time scales, filamentation phenomena result in high frequency oscillations in velocity space that numerical schemes cannot resolve. For stability purposes, most numerical schemes contain dissipation mechanisms that may affect the precision of the finest oscillations that could be resolved.

Objective One way to reduce the dissipation is to consider the absorbing boundary conditions developed by Eliasson for the Fourier-transformed (in the velocity variables) Vlasov-Maxwell system: it consists in removing the high velocity modes in a lowest dissipative way. We aim to develop such strategies in the context of Finite Element Methods, which enable us to develop high order numerical schemes.

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 will be 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 will compare the DG approach with semi-Lagrangian or PIC methods on classical test cases: Landau damping, two-stream instability, echoes. This work has already started during a research session at CEMRACS 2012. It will also be the subject of the Ph. D. of Nhung Pham, started in October 2012.

For studying charged particles beams, the approach has to be extended to the relativistic case. Paradoxically the relativistic case seems to be simpler, because the velocity space is bounded by the speed of light.

The method will then be extended to two-dimensional cases. Anaïs Crestetto, during her thesis, implemented a DG/PIC coupling for solving particle beams, which is very efficient and runs on GPU computers. Nhung Pham will implement in this software the full DG Vlasov-Maxwell model, which will allow precision and performance comparisons.

On the other hand, we develop a three-dimensional DG generic DG solver called CLAC (for "Conservation Laws Approximation on many Cores") for approximating systems of hyperbolic equations. It is based on the MPI and OpenCL libraries, in order that it can be run on a cluster of GPUs. This work will be fully exploited because the velocity expansion approach perfectly enters this framework. The PhD of Michel Massaro, started in november 2012, will be devoted partly to this objective, in collaboration with the CAMUS team, specialized in the programming of multicore processors. Another objective of Michel Massaro will be to study numerically the magnetic reconnection problem that occurs in astrophysical plasmas. This work is in collaboration with the Strasbourg astrophysics team.

In the long term, we want to apply the method to the simulation of an axisymmetric tokamak. The simulation of a full three-dimensional tokamak plasma is also envisaged. This will require of course to access supercomputers such as the CEA TGCC Curie [TGCC].

For this purpose, we have to extend the velocity expansion approach to gyrokinetic equations. Gyrokinetic models, as the original Vlasov equation, are transport equations, but in a modified phase space [Gar11]. Consequently, the velocity expansion technique will also lead to hyperbolic systems and the previous method, and the numerical codes, can also apply to gyrokinetic models.

Generally, the collisions can be neglected in the central part of the tokamak plasma. On long time scales, however, this hypothesis is no longer valid. In addition, if we want to also solve the edge plasma, it is necessary to take into account the collision effects. In the hyperbolic systems framework, some authors have constructed entropy-conservative schemes [Ta86, Ba06]. For non-linear systems of fluid mechanics, these schemes are rather theoretical tools for constructing entropy dissipative schemes. We will use this kind of approaches, based on the Legendre transform [Hel09] for solving Vlasov and constructing minimal dissipation schemes together with simplified collision models, consistent with the second principle of thermodynamics. A more precise description of these ideas is given in the report of a CEM-RACS 2012 project, also corresponding to beginning of the Ph. D. thesis of Nhung Pham [HP12].

The velocity expansion is a promising numerical method. However, in some cases, other representations of the distribution function are better adapted. A popular approach is the waterbag representation, which assumes that the distribution is piecewise constant. Each piece is called a "waterbag". It allows computing only the boundaries of the waterbags, which leads to simpler resolutions [BBBB09, Cres12]. This is interesting, for instance, for some gyrokinetic models studied by Nicolas Besse [BB09]. Another representation often used by physicists is the moment representation. We also have worked on such topics [Cres12]. All these approaches lead to hyperbolic systems in space and time. Thus, the most efficient methods will also be incorporated into CLAC.

4.2.2 Adaptive modeling

Context Another trend in scientific computing is to optimize the computation time through adaptive modeling. This approach consists in applying the more efficient model locally, in the computational domain, according to an error indicator. In tokamak simulations, this kind of approach could be very efficient, if we are able to choose locally the best intermediate kinetic-fluid model as the computation runs. This field of research is very promising. It requires developing a clever hierarchy of models, rigorous error indicators, versatile software architecture, and algorithms adapted to new multicore computers.

Objectives An important application of adaptive modeling is the study of the so-called Edge Localized Modes (ELM) in a tokamak. ELM are instabilities that develop in the region between the central plasma and the boundary of the tokamak. In reality, some particles may escape from the confinement zone; these are collected by surfaces called divertor plates and

sent there by the specially-shaped magnetic field near the so-called "X" point. In the edge region, it is no longer possible to neglect collisions, and the fluid models become relevant again.

ELMs are studied in the team CASTOR with the JOREK software. The main approach is based on MHD models and Braginskii closures [BGNK11]. Here, we want to also model kinetic effects. Such problem is typically a question where all Inria teams working on fusion must collaborate.

In TONUS, we are concerned with kinetic simulation of ELMs and the plasma-wall transition. Hence, the principal mathematical tools will be the coupled Vlasov and Poisson equations. The Vlasov equation will further be augmented by including suitable collision and ionization terms. Thus, three directions of research will be pursued: (a) the development of efficient reduced Vlasov solvers well-adapted to the study of plasma-wall transition problems; (b) the development of Asymptotic Preserving schemes, which allow us to deal in an optimal manner with singular regimes characterized by very small or vanishing dimensionless parameters; (c) the investigation of alternative approaches such as the 'water-bag' method. Concerning the first direction, we have developed two Eulerian Vlasov-Poisson codes: a 1D1V time-dependent code for the ELMs dynamics [GM11] and a 1D3V code for the study of the magnetized plasma-wall transition in the stationary regime [SD08].

4.2.3 Numerical schemes

Context 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 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 [Ta86, Ba06, Lev97, HL08].

Objectives We will incorporate those models into CLAC, the DG parallel code that we currently develop in TONUS. CLAC runs on clusters of GPUs. Many improvements of the current version of CLAC will be explored, for instance: variable order, local time-stepping strategies, *etc*.

For validating our DG solver, we will rely on our collaborations inside the IPL FUSION. We could for instance define with Francis Filbet's KALIFFE team test cases of varying sizes to compare the semi-Lagrangian methods and the new reduced model algorithms. We will also use the tools developed in the CASTOR team, which has created inside the PlaTo project a database of practical tools such as: tokamak meshes (ITER or JET configurations), collections of initial conditions, tools for computing the initial magnetic confinement field from the Grad–Shafranov equation, numerical results for the ELM problem, *etc.* We will also define test cases in collaboration with astrophysicists from the Strasbourg Observatory.

Finally, we are also collaborating inside the IPL C2S@exa. We will define a big challenge inside this project to be solved within a few years. This challenge will consist in simulating central tokamak plasma on a realistic geometry. This case will be solved on a supercomputer made of thousands of multicore processors.

4.3 Electromagnetic solvers

Participants: M. Gutnic, P. Helluy, P. Navaro

Context A precise resolution of the electromagnetic fields is essential for proper plasma simulation. It thus 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.

4.3.1 Maxwell solvers

Objectives A possible approach for solving the Maxwell equations is again to apply the Discontinuous Galerkin (DG) approach. This is what we are currently developing in CLAC with the AxesSim company. However, our generic solver, which can be used with other hyperbolic models, will not necessarily be the most efficient. We will thus collaborate with other Inria teams, specialists of electromagnetic simulations, such as the NACHOS team of Stéphane Lanteri, in order to have access to the most efficient solvers and numerical methods. One possible joint project could be, within the context of the C2S@exa project, to address the microwave plasma heating modeling, which requires intensive computations.

4.3.2 Coupling

Context The coupling of the Maxwell equations to the Vlasov solver requires some precautions. The most important 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 [ABGHMS09] (and included references).

Objectives For the coupling design, we will collaborate with Martin Campos Pinto from the University Paris 6, who has recently constructed a new PIC solver based on generalized representations of particles. See Section 4.1.3.

For the applications, we will continue the work of Anaïs Crestetto on charged particles beams solved on GPUs. In a first simpler step, we will consider beam physics simulations in which the charged particles are relativistic. In this case the resolution of the time-dependent Maxwell equations is relevant.

Like pseudo-compressible methods in fluid mechanics, it is possible to use a time-dependent solver as a numerical tool for computing the stationary state. A simple approach is to set an artificial speed of light in the model in order to accelerate the convergence to the stationary state. In some cases and for some computer architectures, such algorithms can be competitive compared to implicit solvers.

4.3.3 Implicit solvers

Context 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.

Objectives We have thus to solve large linear systems on parallel computers. It is clear that efficient linear algebra algorithms implemented on parallel computers are essential for our project. We will rely on these topics on collaborations inside the IPL C2S@exa. We will probably couple the PastiX library, developed in Bordeaux in the HiePACS project, with Selalib and CLAC. The work has already started for Selalib. We will also participate in discussions about the design of an adequate interface.

At the same time, we will pursue our works in Selalib on FFT-based Poisson solvers.

We will also collaborate with the CASTOR team, which has a long experience of implicit solvers for high-order finite volume schemes applied to fluid mechanics and MHD flows. We will organize workshop sessions in order to compare and validate our numerical results.

5 Software development

Several software projects are already running in our team and will be continued, mainly the Selalib project, which aims at developing semi-Lagrangian solvers for gyrokinetic plasmas, and the CLAC solver devoted to simulations of reduced plasma models on GPU clusters.

5.1 Selalib

The objective of the ADT Selalib (SEmi-LAgrangian LIBray) 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 provide to physicists easy-to-use gyrokinetic solvers, based on the semi-lagrangian techniques developed by Eric Sonnendrücker and his collaborators in the CALVI project. The new models and schemes from TONUS are also intended to be incorporated into Selalib.

In addition, the CEA of Cadarache and the team of Virginie Grandgirard are interested by the development of this library, which picks up and extends many methods implemented in GYSELA. Éric Sonnendrücker in Munich will continue to work on Selalib. A joint development of Selalib between Strasbourg and Munich will allow the two sides to benefit of each other's work.

Selalib is a library of FORTRAN modules. The CEA Cadarache has advised this language, because it is widespread in the engineering and physics communities. In this way, we hope that it will diffuse among researchers interested in plasma simulations.

Selalib is under GPL license and available on the Inria forge²¹.

5.2 CLAC

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. 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.

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

²¹http://selalib.gforge.inria.fr/

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^{22} deposit of the first version of CLAC in October 2012.

For the time of the TONUS evaluation, the source code can be browsed on our svn repository $_{\rm 23}$

5.3 Software engineering

Our objective will be to unify these developments in order to construct a practical tool for the numerical simulation of ITER plasmas, with good visibility. A good software design is essential if we want to go towards adaptive modeling and to have an application field as large as possible. It is also very important for possible future technology transfers.

The unification work is very important. We will rely on the engineers enrolled in the Selalib project. In addition to programming the new numerical schemes, it is important to respect strict implementation rules, for a team efficient work. This implies documenting the software inside the sources as long as it is developed. The conception has to be explicit (thanks to UML diagrams, for instance). The licensing has to be thought in advance, in such a way that the libraries can be used by several collaborators, including industrial partners.

In a more prospective way we will explore several other tracks.

Generally, scientific software is not easy to use by people who are not experts in computer science. People would like to express their problem in the natural language of their domain. This is the objective of Domain Specific Embedded Language (DSEL). In the applied mathematical community, Freefem++ is a well-known research and teaching software, that uses these ideas. It allows expressing in a natural mathematical way the geometry and the variational formulation of a boundary value problem, without having to cope with low-level details (meshing, assembling, linear solver, visualizations, etc.). Christophe Prud'homme is a new colleague at the mathematical institute in Strasbourg. He has developed the library Feel++ [Pr12], which is based on the DSEL idea. For a better diffusion of our software, we could envisage to couple our codes with a DSEL. No doubt that we will discuss this possibility with Christophe Prud'homme.

Another trend is to observe that the architecture of supercomputers becomes more and more complex. Such supercomputers are made of connected computers. And each computer itself is made of several multicore processors. The computation power is important (we should reach the exaflopic power in 2019), but programming becomes more complicated. We have to access computation and memory resources with several hierarchical levels and very different speeds. It thus important to manage in a clever way the delay caused by communications and the memory bandwidth bottlenecks. In the future it is probable that the complexity of an algorithm will be in some cases less important than the data transfers that it implies in the computer memory. Thus scientific computing has to care not only about the

²²http://www.app.asso.fr/en/

²³http://www-irma.u-strasbg.fr/subversion/CM2/sources/GPU/CLAC/, login: guest, no password.

computations but also about the organization of data in memory. On a single core computer this problem is often hidden by the processor cache prefetch mechanism. The members of the Inria project-team CAMUS, directed by Philippe Clauss, are specialized in compiler automatic parallelism. We have decided to supervise together the PhD of Michel Massaro. The objective is to improve our existing codes in order to reach optimal performance. This collaboration could also be a good occasion to explore new more abstract programming models for scientific computing. Several studies could be followed around loop optimizations with the polyhedric approach, or graph tools for organizing and optimally distribute the computations on massively parallel computers.

6 TONUS collaborations

As of May 2013, TONUS is a team of the Inria Nancy-Grand Est center. We describe our main current collaborations and involvement in other projects that will be continued in the future Inria project-team.

6.1 Inria teams working on Fusion

Inria has invested for several years in the research on numerical simulations for plasma physics. We describe here the current context within Inria on this subject.

We can very schematically identify three main problems that are relevant to the numerical simulation of a tokamak plasma. These three main subjects are at the heart of three Inria teams working on plasma modeling in collaboration with TONUS:

- In the core plasma, it is necessary to use a full kinetic or gyrokinetic modeling. The plasma is almost collisionless. The numerical simulation of such plasmas is mainly the task of the TONUS team in Strasbourg. TONUS is the continuation of the CALVI project (CALcul and VIsualization) created in 2003 by Éric Sonnendrücker. It is devoted to the mathematical and numerical studies for plasma and particle beam physics.
- In the edge plasma, it is important to take into account the collisions for a proper modeling. It is also interesting to construct intermediate models between kinetic and fluid models in order to improve the coupling strategy between these. This task would mainly be developed by the KALIFFE team in Lyon. Francis Filbet is currently launching the KALIFFE team in Lyon (Kinetic models AppLIed for Future of Fusion Energy). His main research topics are the kinetic-fluid plasma theory, the collision kernels and associated numerical schemes.
- Other models are useful in other parts of the tokamak. For instance, the MHD model is relevant to the edge plasma, with some approximations. It is also important to compute and adapt the magnetic configuration in accordance with the plasma current. Those problems are mainly studied by the CASTOR team in Nice under the direction of Jacques Blum.

Of course, the three teams have also common research subjects. They can compare different approaches on analogous problems.

6.2 Inria Project Lab (IPL) "fusion"

Inria plans to continue an Inria Project Lab $(IPL)^{24}$ devoted to fusion. The FUSION IPL is specialized in the mathematical modeling and simulations for magnetic fusion and in particular for the ITER project. The first project was directed by Éric Sonnendrücker, former leader of the CALVI project. The new project would now be led by Jacques Blum, leader of the CASTOR Inria team. In addition to the three teams at the heart of the Inria fusion strategy, the IPL will encourage the collaboration with other teams:

- COFFEE in Nice, working on general mathematical models for complex flows. Thierry Goudon is head of the COFFEE project (COmplex Flows For Energy and Environment). His team is studying PDEs of hydrodynamic type or hybrid fluid-kinetic systems. It is also interested in numerical methods for coupling multiscale models.
- IPSO in Rennes. In this team, Nicolas Crouseilles, a former member of the CALVI team, is a specialist of asymptotic modeling for plasmas.
- CEA-IRFM (magnetic fusion research institute of the French atomic agency) in Cadarache. The IPL collaborates on two important software developments of the CEA devoted to tokamak simulations: GYSELA, a five-dimensional gyrokinetic core plasma solver and JOREK, a MHD edge plasma solver.
- Bruno Després and Martin Campos-Pinto in Paris VI university: they are specialists of general plasma modeling, electromagnetic modeling and Particle-In-Cell methods.
- Claudia Negulescu's team in Toulouse: is specialized in Asymptotic Preserving numerical methods for kinetic, fluid and multiscale models.

In the context of the first FUSION action, Inria has funded two software projects ("Action de Développement Technologique" ADT):

- PlaTo (Platform for Tokamak simulation) is a suite of data and softwares dedicated to the geometry and physics of Tokamaks. It contains tools for computing initial magnetic configurations and adapted meshes. It also contains MHD solvers and drift approximation solvers. The modules developed in PlaTo could be reused in the CEA software JOREK.
- The Selalib (Semi-Lagrangian Library) is a Fortran library devoted to the numerical simulation of kinetic equations arising in plasma physics. It contains semi-Lagrangian solvers and Poisson solvers necessary for full Vlasov simulations of gyrokinetic simulations. The modules developed in Selalib can be integrated later on into the CEA software GYSELA.

²⁴formerly called "Action d'Envergure" (AE) or "Large Scale Initiative" (LSI)

6.3 Inria Project Lab C2S@exa

The C2S@Exa²⁵ is another Inria IPL concerned with the development of numerical modeling methodologies that fully exploit the processing capabilities of modern massively parallel architectures. C2S@Exa is a multidisciplinary project gathering applied mathematicians and computer scientists from Inria project-teams.

The IPL has been recently launched by Stéphane Lanteri leader of the NACHOS²⁶ Inria project-team. C2S@Exa has identified several simulation challenges that will be addressed within the four next years. TONUS is involved in this project, with the CEA, through one of the IPL challenge, which is to simulate gyrokinetic plasmas on exascale computer architectures.

6.4 Other collaborations

During the years, several collaborations have been established with industrial and scientific partners. The Strasbourg team is also involved in several research projects. We now focus on some collaborations and programs that we want to continue or enforce.

6.4.1 CEA-IRFM

CEA-IRFM in Cadarache: the team of Virginie Grandgirard is involved in the development of CEA software, GYSELA for five-dimensional gyrokinetic plasma simulations, and JOREK for three-dimensional fluid plasma simulations. We have a long-range collaboration that we want to pursue on GYSELA, and thus on the development of Selalib. We also want to have more collaboration on MHD or reduced models simulations. The collaboration will be on algorithms design, GPU developments, *etc.*

6.4.2 Max Planck Institute in Munich

Éric Sonnendrücker, former head of the CALVI project-team, is now member of the Max Planck Institute. We will keep strong interactions with his new team in Munich in order to bring together in an efficient way various research and software developments, such as Selalib. Éric Sonnendrücker has a long established international reputation in the community of plasma physics mathematical modeling. Together with our colleagues from CEA-IRFM (Virginie Grandgirard) he will be our entry point in order to reach the international teams working on tokamak fusion.

 $^{^{25}\}mathrm{Computer}$ and Computational Sciences at Exascale

 $^{^{26}\}mathrm{Numerical}$ modeling and high perform Ance computing for evolution problems in Complex domains and Heterogene OuS media

6.4.3 IRMIA

IRMIA "Labex": the Mathematics Institute in Strasbourg has proposed with several partners, including the Inria team CAMUS, a new project. This project, called IRMIA, received french "Labex" label. An important part of the project is devoted to HPC research in industry and physics. This project gives thus new funding (PhD and post-doc grants) and opportunities to develop better collaborations between mathematicians and computer scientists for developing algorithms adapted to multicore architectures. The university of Strasbourg applied last year to the French program "EquipEx" and successfully obtained support for computing facilities through the "Equip@meso" project. Our project will also rely on these computing facilities.

6.4.4 Strasbourg physicists

For obtaining relevant numerical methods, it is very important to collaborate with physicists. We will continue our current collaborations with physicists of Strasbourg, working on astrophysics, plasma physics and particle physics. Our collaboration are with Jerome Petri, Hubert Baty at the Observatoire de Strasbourg and Giovanni Manfredi, Paul-Antoine Hervieux at the Institut de Physique et de Chimie des Matériaux de Strasbourg (IPCMS).

6.4.5 AxesSim

For plasma simulations, we are developing a generic Discontinuous Galerkin solver, CLAC (see Section 5.2). CLAC is developed in collaboration 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 electromagnetism.

6.5 International positioning

From the state of the art presented in Section 3.3, we have observed some tendencies in the plasma numerical simulation community.

On the one hand, it is necessary to include relevant physical models and perform huge computations on supercomputers made of thousands of cores. These constraints imply stable software engineering.

On the other hand, an objective of a tokamak simulation is to predict and control plasma instabilities. It is therefore very important to ensure that the computed plasma stability is indeed physical and not a numerical artifact. This requires rigorous mathematical and numerical analysis in the model derivations and in the design of the simulation tools. For addressing larger and larger simulations, it is also necessary to improve the precision and efficiency of the numerical methods. Several tracks must thus be explored: higher order methods, reduced modeling, adaptive modeling and error indicators, *etc.*

In our opinion we are well inserted in the tokamak numerical simulation competition and we propose an innovative project that combines several aspects: rigorous mathematical analysis, HPC, new numerical methods and models.

On some points, we inherited the experience developed in the CALVI project. Some of our works are internationally recognized: semi-Lagrangian numerical methods, mathematical analysis of the gyrokinetic models, for instance. We participate in the GYSELA project through Selalib. GYSELA is well positioned among the existing gyrokinetic codes because of the relevance of its physical models, the parallelization capabilities and its high order innovative semi-Lagrangian numerical methods. We will maintain this activity, which is the base of good tokamak simulations.

Our objective is to develop new numerical methods and reduced models for tokamak plasma simulations. In order to convince the physicists that our new methods are good alternatives compared to older tools, it is necessary to test these methods in realistic plasma configurations. Therefore, our plan for the end of the next four years is to be able to simulate a simplified tokamak core plasma on a parallel computer in Selalib and CLAC with the new approaches. The best methods could then be implemented in GYSELA. On a longer range we plan to incorporate finer physical descriptions in our software, such as electron effects and self-consistent magnetic fields.

For achieving our goal, we have to improve some aspects that are already addressed by other international teams. In our opinion, the hottest required features are:

- The capability to deal with curved meshes and magnetic-aligned coordinates.
- The integration of finer physical modeling into Selalib: fine collision models (collaboration with the KALIFFE team), electrons effects, better gyroaverage operators (collaboration with CEA IRFM), AP approaches.
- The possibility to couple the core simulation with other models: magnetic configuration and edge plasma fluid models (collaboration with the CASTOR team).
- The kinetic representation in the velocity directions has to be improved. That's why we plan to incorporate velocity-Fourier-transformed and other reduced models in CLAC or Selalib.
- Finally, we have to ensure that our algorithms will scale on future exascale computers. This implies that we will have probably to mix fully-Eulerian solvers, which are well adapted to parallel algorithms and small timescale models, with semi-Lagrangian solvers, which allow arbitrary time steps, but at the cost of larger parallel communications. These topics will be addressed within C2S@EXA project collaborations.

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