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Computer and Computational Sciences at Exascale

Postdoctoral project proposal

High order hybridized implicit DGTD method for the numerical modeling of electromagnetic wave interaction with plasma media in 3d

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Controlled fusion is one of the major challenges of the 21st century that can answer the need for a long term source of energy that does not accumulate wastes and is safe. The nuclear fusion reaction is based on the fusion of atoms like atoms of deuterium and tritium. This reaction does not produce long-term radioactive wastes, unlike todays nuclear power plants which are based on nuclear fission. In order either to achieve a sustained fusion reaction or simply to obtain a positive energy balance, it is necessary to confine sufficiently the plasma for a long enough time. One major research approach is based on magnetic fusion : the plasma is confined thanks to large applied magnetic fields produced by a large toroidal device called *tokamak*. The international project ITER (International Thermonuclear Experimental Reactor) is based on this idea and aims to build a new tokamak which could demonstrate the feasibility of the concept. This approach leads to study hot plasmas, which constitute an important field in physics and applied mathematics, spanning many different length and time scales. Accurately simulating hot plasmas requires solving the physics of hydrodynamics, electron transport, and wave-plasma interactions, to name a few processes. This postdoctoral project is more particularly concerned with the numerical modeling of wave-plasma interaction. Under certain conditions of excitation, electromagnetic wave propagation in a plasma is characterized by different spatial scales generating different time scales. Moreover, for applications that are specific to the ITER problem, geometrical features of the problems also play an important role. Numerical methods must take into account these modeling features, and must be adapted to the characteristics of modern parallel computing platforms taking into account their architecture in order to answer to the computational resources requirements of the uderlying large-scale simulations. Appropriate parallelization strategies need to be designed that combine distributed memory (MIMD) and shared memory (SIMD) paradigms. Most algorithms are not yet ready to exploit these available architecture capabilities and developing large-scale scientific computing tools that efficiently exploit this processing power, of the order of petaflops with current generation systems, is a very complicated task and will be an even more challenging one with future exascale systems.

From the point of view of mathematical modeling, plasma-wave interaction can be studied by considering the system of time-domain Maxwell equations coupled to an appropriate model of the plasma behavior. In general (such as in the cold plasma approximation), the plasma response is taken into account through the equation of electron motion (given an applied, background magnetic field) which allows determining the plasma current. The latter is itself taken into account in the right-hansd side of the Maxwell-Ampere equations. In practice the time evolution of the plasma current is given by an auxiliary differential equations (i.e. an ordinary differential equation). Very often, this coupled system of space-time differential equations is solved using a variant of the well known and widely adopted Finite Difference Time Domain (FDTD) method [Yee66] such as in [Smi07] among others. The great success of FDTD methods for realistic time-domain computational electromagnetics, is largely due to the simplicity and rather straightforward implementation of the algorithm, combined to ever increasing processing capabilities of computing systems. In a FDTD method, the whole computational domain is discretized using a structured (cartesian) grid. This greatly simplifies the discretization process but also represents the main limitation of the method when complicated geometrical objects come into play. Unfortunately, the discretization of objects with complex shapes or small geometrical details using cartesian meshes hardly yields an efficient numerical methodology. Indeed, the so-called stair-casing approximation may lead to local zeroth-order and at most first-order accuracy; it may also produce locally non-convergent results. In the present application context, the complexity of the geometry of the tokamak is particularly challenging for a discretization based on cartesian meshes. Numerical methods able to deal with non-uniform unstructured meshes would be more appropriate in this setting. Furthermore, the variety of wave phenomena supported even by cold plasmas include waves that are much slower than the vacuum wave speed. Since explicit time-domain approaches have a limited maximum time step determined by the vacuum wave speed, simulating the solwer waves requires extremely dense sampling in time to get waves which are decently resolved in space. Implicit (or locally implicit) time stepping could be a viable alternative to tackle the restriction on the time step and improve the overall computational efficiency.

The present postdoctoral project is a first step towards the development of a new unstructured mesh based, time-domain solver, adapted to massively parallel computers, for the numerical modeling of plasma-wave interaction in 3d. The system of time-domain Maxwell equations augmented by a differential model of cold plasmas will be solved by a high order discontinuous Galerkin method for the discretization in space coupled to a second order Crank-Nicholson implicit time stepping scheme.

During the last 10 years, discontinuous Galerkin (DG) methods have been extensively considered for obtaining approximate solution of Maxwell's equations modeling electromagnetic wave propagation. Thanks to the discontinuity of the approximation, this kind of methods has many advantages, such as adaptivity to complex geometries through the use of unstructured possibly non-conforming meshes, easily obtained high order accuracy, *hp*-adaptivity and natural parallelism. However, despite these advantages, DG methods have one main drawback particularly sensitive for stationary problems: the number of globally coupled degrees of freedom (DOFs) is much greater than the number of DOFs required by conforming finite element methods for the same accuracy. Consequently, DG methods are expensive in terms of both CPU time and memory consumption, especially for steady-like problems, or in the context of implicit time-stepping schemes which require solving a large sparse linear system at each time step. Hybridization of DG methods [CGL09] is devoted to address this issue while keeping all the advantages of DG methods. Such a hybridizable discontinuous Galerkin (HDG) method for the discretization of the system of 3d time-harmonic Maxwell's equations will be at the heart of the present project. HDG methods introduce an additional *hybrid* variable on the faces of the elements, on which the definition of the local (element-wise) solutions is based. A so-called *conservativity condition* is imposed on the numerical trace, whose definition involved the hybrid variable, at the interface between neighboring elements. As a result, HDG methods produce a linear system in terms of the DOFs of the additional hybrid variable only. In this way, the number of globally coupled DOFs is reduced. The local values of the electromagnetic fields can be obtained by solving local problems element-by-element. Recently, researchers of teh NACHOS project-team at Inria Sophia Antipolis - Méditerranée have studied such a HDG formulation for the system of 2d time-domain Maxwell equations [LP11]. A first objective of this postdoctoral project will be to extend the formulation presented in [LP11] to the 3d case, and to implement the resulting implicit HDGTD (Hybridized Discontinuous Galerkin Time Domain) formulation in a computer code adapted to parallel computing platforms.

Though the HDG method results in a smaller linear system than the one associated with a classical upwind flux-based DG method, the size of this system is often too large to be solved by a direct solver as soon as one considers realistic 3d problems. In addition, for very large-scale propagation problems, exploiting a multi-processor system is a mandatory path to reduce the solution time and have access to the required memory capacity. Therefore, a second objective of the present work will be the study of parallel algebraic solution strategies for the HDGTD linear system. The focus will be on hybrid iterative/direct approaches based on domain decomposition principles, amenable to a mixed MIDM/SIMD parallelization, by adapting ideas behind similar solvers studied by reserachers of the HiePACS project-team at Inria Bordeaux - Sud-Ouest [AGGR11].

For this postdoctoral project, applications are invited from recently graduated Ph.D students in applied mathematics or scientific computing with emphasis on the numerical treatment of PDE systems. A first research experience in computational electromagnetics will be an asset. A good knowledge of high performance computing principles and a first experience in parallel programming is required, as is the ability to manipulate complex computer codes in a Linux/Unix environment. This project will be conducted in the Nachos project-team at Inria Sophia Antipolis - Méditerranée (Stéphane Lanteri) for waht concern the HDG method for time-domain electromagnetics, in close collaboration with researchers from the Hipeacs project-team at Inria Bordeaux - Sud-Ouest for what concern aspected related to parallel algebraic sparse linear solvers.

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