INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Project-Team nachos

Numerical modeling and high performance computing for evolution problems in complex domains and heterogeneous media

Sophia Antipolis - Méditerranée

THEME NUM

Activity Report

2008

Table of contents

The NACHOS project-team has been launched on July 2007. It is a follow-up to the CAIMAN project-team which was stopped at the end of June 2007. NACHOS is a joint team with CNRS and the University of Nice-Sophia Antipolis (UNSA), through the J.A. Dieudonné Mathematics Laboratory (UMR CNRS 6621).

1. Team

Research Scientist

Loula Fezoui [Research Director, INRIA]
Stéphane Lanteri [Research Director, Team leader, INRIA, HdR]
Nathalie Glinsky-Olivier [Research Scientist, Cermics[1], ENPC]

Faculty Member

Victorita Dolean [Faculty Member, UNSA[2], J.A. Dieudonné Laboratory (UMR CNRS 6621)]
Francesca Rapetti [Faculty Member, UNSA, J.A. Dieudonné Laboratory (UMR CNRS 6621)]

External Collaborator

Martin Gander [External Collaborator, Mathematics Section, University of Geneva, Switzerland]
Luc Giraud [External Collaborator, Parallel Algorithms and Optimization Group, ENSEEIHT-IRIT, Toulouse]
Stéphane Operto [External Collaborator, UNSA and Géosciences Azur Laboratory (UMR CNRS 6526)]
Ronan Perrussel [External Collaborator, Ampère Laboratory, Ecole Centrale de Lyon (UMR CNRS 5005)]
Muriel Sesques [External Collaborator, CEA/CESTA, Bordeaux]
Jean Virieux [External Collaborator, Joseph Fourier University and Géophysique Interne et Tectonophysique (LGIT) Laboratory]
Joe Wiart [External Collaborator, France Télécom R&D, Issy-les-Moulineaux]

PhD Student

Adrien Catella [PhD Student, INRIA]
Joseph Charles [PhD Student, INRIA]
Hassan Fahs [PhD Student, MENSR-INRIA]
Mohamed El Bouajaji [PhD Student, INRIA]

Post-Doctoral Fellow

Sarah Delcourte [Post-Doctoral Fellow, until 09/2008]
Siham Layouni [Post-Doctoral Fellow, from 10/2008]

Visiting Scientist

Serge Moto Pong [Visiting Scientist, University of Yaoundé 1, Cameroon, from 11/2007 until 08/2008]

Administrative Assistant

Montserrat Argente [Administrative Assistant, INRIA]

Other

Clément Durochat [Master intern, Paul Sabatier University, Toulouse, from 05/2007 until 08/2007]
Antoine Jarrier [Master intern, UNSA, from 06/2007 until 09/2007]
Antoine Bouquet [Research engineer, from 01/2008 until 04/2008]
Christian Konrad [Master intern, from 01/2008 until 07/2008 - Research engineer, from 09/2008 until 12/2008]

---

[1] Mathematics and scientific computing joint École Nationale des Ponts et Chaussées - INRIA research center
[2] University of Nice-Sophia Antipolis

2. Overall Objectives

2.1. Overall objectives

The research activities of the NACHOS project-team are concerned with the formulation, analysis and evaluation of numerical methods and high performance resolution algorithms for the computer simulation of evolution problems in complex domains and heterogeneous media. The team concentrates its activities on mathematical models that rely on first order linear systems of partial differential equations (PDEs) with variable coefficients and more particularly, PDE systems pertaining to electrodynamics and elastodynamics with applications to computational electromagnetics and computational geoseismics. These applications involve the interaction of the underlying physical fields with media exhibiting space and time heterogeneities such as when studying the propagation of electromagnetic waves in biological tissues or the propagation of seismic waves in complex geological media. Moreover, in most of the situations of practical relevance, the computational domain is irregularly shaped or/and it includes geometrical singularities. Both the heterogeneity and the complex geometrical features of the underlying media motivate the use of numerical methods working on non-uniform discretizations of the computational domain. In this context, ongoing research efforts of the team aim at the development of unstructured (or hybrid unstructured/structured) mesh based methods with activities ranging from the mathematical analysis of numerical methods for the solution of the systems of PDEs of electrodynamics and elastodynamics, to the development of prototype 3D simulation software that efficiently exploit the capabilities of modern high performance computing platforms.

In the case of electrodynamics, the mathematical model of interest is the full system of unsteady Maxwell equations [35] which is a first-order hyperbolic linear system of PDEs (if the underlying propagation media is assumed to be linear). This system can be numerically solved using so-called time domain methods among which the Finite Difference Time Domain (FDTD) method introduced by K.S. Yee [43] in 1996 is the most popular et which often serves as a reference method for the works of the team. In the vast majority of existing time domain methods, time advancing relies on an explicit time scheme. For certain types of problems, a time harmonic evolution can be assumed leading to the formulation of the frequency domain Maxwell equations whose numerical resolution requires the solution of a linear system of equations (i.e in that case, the numerical method is naturally implicit). Heterogeneity of the propagation media is taken into account in the Maxwell equations through the electrical permittivity, the magnetic permeability and the electric conductivity coefficients. In the general case, the electrical permittivity and the magnetic permeability are tensors whose entries depend on space (i.e heterogeneity in space) and frequency (i.e physical dispersion and dissipation). In the latter case, the time domain numerical modeling of such materials requires specific techniques in order to switch from the frequency evolution of the electromagnetic coefficients to a time dependency. Moreover, there exists several mathematical models for the frequency evolution of these coefficients (Debye model, Lorentz model, etc.).

In the case of elastodynamics, the mathematical model of interest is the system of elastodynamic equations [30] for which several formulations can be considered such as the velocity-stress system. For this system, as with Yee's scheme for time domain electromagnetics, one of the most popular numerical method is the finite difference method proposed by J. Virieux [41] in 1986. Heterogeneity of the propagation media is taken into account in the elastodynamic equations through the Lamé and mass density coefficients. A frequency dependence of the Lamé coefficients allows to take into acount physical attenuation of the wave fields and characterizes a viscoelastic material. Again, several mathematical models exist for expressing the frequency evolution of the Lamé coefficients.

The research activities of the team are currently organized along four main directions: (a) arbitrary high order finite element type methods on simplicial meshes for the discretization of the considered systems of PDEs, (b) efficient time integration methods for dealing with grid induced stiffness when using non-uniform (locally refined) meshes, (c) domain decomposition algorithms for solving the algebraic systems resulting from the discretization of the considered systems of PDEs when a time harmonic regime is assumed or when time integration relies on an implicit scheme and (d) adaptation of numerical algorithms to modern high performance computing platforms. From the point of view of applications, the objective of the team is to demonstrate the capabilities of the proposed numerical methodologies for the simulation of realistic wave propagation problems in complex domains and heterogeneous media.

2.2. Highlights of the year

Arbitrary high order in space and time Discontinuous Galerkin Time Domain (DGTD) methods on simplicial meshes have been developed for the solution of the systems of time domain Maxwell and elastodynamic equations in 2D and 3D. These methods extend our previous achievements by using a family of high order leap-frog schemes for time integration.

For time domain electromagnetic simulations involving locally refined simplicial meshes, a hybrid explicit/implicit discontinuous Galerkin method has been designed which allows for a substantial gain in computing time as compared to a fully explicit solution strategy, at the expense of a moderate memory overhead.

3. Scientific Foundations

3.1. Arbitrary high order discontinuous Galerkin methods on simplicial meshes

Keywords: *conforming mesh*, *discontinuous Galerkin*, *finite element*, *finite volume*, *hp-adaptivity*, *non-confoming mesh*, *polynomial interpolation*, *simplicial mesh*.

The applications in computational electromagnetics and computational geoseismics that are considered by the team lead to the numerical simulation of wave propagation in heterogeneous media or/and involve irregularly shaped objects or domains. The underlying wave propagation phenomena can be purely unsteady or they can be periodic (because the imposed source term follows a time harmonic evolution). In this context, the overall objective of the research activities undertaken by the team is to develop numerical methods that fulfill the following features:

- Accuracy. The foreseen numerical methods should ideally rely on discretization techniques that best fit to the geometrical characteristics of the problems at hand. For this reason, the team focusses on methods working on unstructured, locally refined, even non-conforming, simplicial meshes. These methods should also be capable to accurately describe the underlying physical phenomena that may involve highly variable space and time scales. With reference to this characteristic, two main strategies are possible: adaptive local refinement/coarsening of the mesh (i.e h-adaptivity) and adaptive local variation of the interpolation order (i.e p-adaptivity). Ideally, these two strategies are combined leading to the so-called hp-adaptive methods.

- Numerical efficiency. The simulation of unsteady problems most often rely on explicit time integration schemes. Such schemes are constrained by a stability criteria linking the space and time discretization parameters that can be very restrictive when the underlying mesh is highly non-uniform (especially for locally refined meshes). For realistic 3D problems, this can represent a severe limitation with regards to the overall computing time. In order to improve this situation, one possible approach which is considered by the team consists in resorting to an implicit time scheme in regions of the computational domain where the underlying mesh is refined while an explicit time scheme is applied to the remaining part of the domain. The resulting hybrid explicit/implicit time integration strategy raises several challenging questions both at the mathematical analysis level (stability and accuracy, especially for what concern numerical dispersion), and from the computer implementation viewpoint (data structures, parallel computing aspects). On the other hand, for implicit time integration schemes on one hand, and for the numerical treatment of time harmonic problems on the other hand, numerical efficiency also refers to a foreseen property of linear system solvers.

- Computational efficiency. Despite the ever increasing performances of microprocessors, the numerical simulation of realistic 3D problems is hardly performed on a high-end workstation and parallel computing is a mandatory path. Realistic 3D wave propagation problems lead to the processing of very large volumes of data. The latter results from two combined parameters: the size of the mesh i.e the number of mesh elements, and the number of degrees of freedom per mesh element which is itself linked to the degree of interpolation and to the number of physical variables (for systems of partial differential equations). Hence, numerical methods must be adapted to the characteristics of modern parallel computing platforms taking into account their hierarchical nature (e.g multiple processors and multiple core systems with complex cache and memory hierarchies). Appropriate parallelization strategies need to be designed that combine distributed memory and shared memory programming paradigms. Moreover, maximizing the effective floating point performances will require the design of numerical algorithms that can benefit from the optimized BLAS linear algebra kernels.

The discontinuous Galerkin method (DG) was introduced in 1973 by Reed and Hill to solve the neutron transport equation. From this time to the 90's a review on the DG methods would likely fit into one page. In the meantime, the finite volume approach has been widely adopted by computational fluid dynamics scientists and has now nearly supplanted classical finite difference and finite element methods in solving problems of non-linear convection. The success of the finite volume method is due to its ability to capture discontinuous solutions which may occur when solving non-linear equations or more simply, when convecting discontinuous initial data in the linear case. Let us first remark that DG methods share with finite volumes this property since a first order finite volume scheme can be viewed as a 0th order DG scheme. However a DG method may be also considered as a finite element one where the continuity constraint at an element interface is released. While it keeps almost all the advantages of the finite element method (large spectrum of applications, complex geometries, etc.), the DG method has other nice properties which explain the renewed interest it gains in various domains in scientific computing as witnessed by books or special issues of journals dedicated to this method [24]- [25]- [26]- [33]:

- it is naturally adapted to a high order approximation of the unknown field. Moreover, one may increase the degree of the approximation in the whole mesh as easily as for spectral methods but, with a DG method, this can also be done very locally. In most cases, the approximation relies on a polynomial interpolation method but the DG method also offers the flexibility of applying local approximation strategies that best fit to the intrinsic features of the modeled physical phenomena.

- When the discretization in space is coupled to an explicit time integration method, the DG method leads to a block diagonal mass matrix independently of the form of the local approximation (e.g the type of polynomial interpolation). This is striking difference with classical, continuous finite element formulations. Moreover, the mass matrix is diagonal if an orthogonal basis is chosen.

- It easy handles complex meshes. The grid may be a classical conforming finite element mesh, a non-conforming one or even a hybrid mesh made of various elements (tetrahedra, prisms, hexahedra, etc.). The DG method has been proved to work well with highly locally refined meshes. This property makes the DG method more suitable to the design of a hp-adaptive solution strategy (i.e where the characteristic mesh size h and the interpolation degree p changes locally wherever it is needed).

- It is flexible with regards to the choice of the time stepping scheme. One may combine the DG spatial discretization with any global or local explicit time integration scheme, or even implicit, provided that the resulting scheme is stable,

- it is naturally adapted to parallel computing. As long as an explicit time integration scheme is used, the DG method is easily parallelized. Moreover, the compact nature of DG discretization schemes is in favor of high computation to communication ratio especially when the interpolation order is increased.

As with standard finite element methods, a DG method relies on a variational formulation of the continuous problem at hand. However, due to the discontinuity of the global approximation, this variational formulation has to be defined at the element level. Then, a degree of freedom in the design of a DG method stems from the approximation of the boundary integral term resulting from the application of an integration by parts to the elementwise variational form. In the spirit of finite volume methods, the approximation of this boundary integral term calls for a numerical flux function which can be based on either a centered scheme or an upwind scheme, or a blending between these two schemes.

For the numerical solution of the time domain Maxwell equations, we have first proposed a non-dissipative high order DG method working on unstructured conforming simplicial meshes [5]-[2]. This DG method combines a central numerical flux function for the approximation of the integral term at an interface between two neighboring elements with a second order leap-frog time integration scheme. Moreover, the local approximation of the electromagnetic field relies on a nodal (Lagrange type) polynomial interpolation method. Recent achivements in the framework of the team deal with the extension of these methods towards non-conforming meshes and hp-adaptivity [17]-[16], their coupling with hybrid explicit/implicit time integration schemes in order to improve their efficiency in the context of locally refined meshes [18], and their extension to the numerical resolution of the elastodynamic equations modeling the propagation of seismic waves [12].

3.2. Domain decomposition methods

Keywords: *Schur complement method*, *Schwarz algorithm*, *artificial interface*, *non-overlapping algorithm*, *overlapping algorithm*, *substructuring*, *transmission condition*.

Domain Decomposition (DD) methods are flexible and powerful techniques for the parallel numerical solution of systems of PDEs. As clearly described in [39], they can be used as a process of distributing a computational domain among a set of interconnected processors or, for the coupling of different physical models applied in different regions of a computational domain (together with the numerical methods best adapted to each model) and, finally as a process of subdividing the solution of a large linear system resulting from the discretization of a system of PDEs into smaller problems whose solutions can be used to devise a parallel preconditioner or a parallel solver. In all cases, DD methods (1) rely on a partitioning of the computational domain into subdomains, (2) solve in parallel the local problems using a direct or iterative solver and, (3) calls for an iterative procedure to combine the local solutions to obtain the solution of the global (original) problem. Subdomain solutions are connected by means of suitable transmission conditions at the artificial interfaces between the subdomains. The choice of these transmission conditions greatly influences the convergence rate of the DD method. One generally distinguish three kinds of DD methods:

- overlapping methods use a decomposition of the computational domain in overlapping pieces. The so-called Schwarz method belongs to this class. Schwarz initially introduced this method for proving the existence of a solution to a Poisson problem. In the Schwarz method applied to the numerical resolution of elliptic PDEs, the transmission conditions at artificial subdomain boundaries are simple Dirichlet conditions. Depending on the way the solution procedure is performed, the iterative process is called a Schwarz multiplicative method (the subdomains are treated in sequence) or an additive method (the subdomains are treated in parallel).
- non-overlapping methods are variants of the original Schwarz DD methods with no overlap between neighboring subdomains. In order to ensure convergence of the iterative process in this case, the transmission conditions are not trivial and are generally obtained through a detailed inspection of the mathematical properties of the underlying PDE or system of PDEs.
- substructuring methods rely on a non-overlapping partition of the computational domain. They assume a separation of the problem unknowns in purely internal unknowns and interface ones. Then, the internal unknowns are eliminated thanks to a Schur complement technique yielding to the formulation of a problem of smaller size whose iterative resolution is generally easier. Nevertheless, each iteration of the interface solver requires the realization of a matrix/vector product with the Schur complement operator which in turn amounts to the concurrent solution of local subproblems.

Schwarz algorithms have enjoyed a second youth over the last decades, as parallel computers became more and more powerful and available. Fundamental convergence results for the classical Schwarz methods were derived for many partial differential equations, and can now be found in several books [39]- [38]- [40].

The research activities of the team on this topic aim at the formulation, analysis and evaluation of Schwarz type domain decomposition methods in conjunction with discontinuous Galerkin approximation methods on unstructured simplicial meshes for the solution of time domain and time harmonic wave propagation problems. Ongoing works in this direction are concerned with the design of non-overlapping Schwarz algorithms for the solution of the time harmonic Maxwell equations. A first achievement has been a Schwarz algorithm for the time harmonic Maxwell equations, where a first order absorbing condition is imposed at the interfaces between neighboring subdomains [4]. This interface condition is equivalent to a Dirichlet condition for characteristic variables associated to incoming waves. For this reason, it is often referred as a natural interface condition [19]. Beside Schwarz algorithms based on natural interface conditions, the team also investigates algorithms that make use of more effective transmission conditions [15]-[14]. From the theoretical point of view, this represents a much more challenging goal since most of the existing results on optimized Schwarz algorithms have been obtained for scalar partial differential equations. For the considered systems of PDEs, the team plan to extend the techniques for obtaining optimized Schwarz methods previously developed for the scalar partial differential equations to systems of partial differential equations by using appropriate relationships between systems and equivalent scalar problems [32].

3.3. High performance numerical computing

Keywords: *SPMD model*, *distributed memory*, *hierarchical architecture*, *multicore*, *multiprocessor*, *parallel computing*, *shared memory*.

Beside basic research activities related to the design of numerical methods and resolution algorithms for the wave propagation models at hand, the team is also committed to demonstrate the benefits of the proposed numerical methodologies in the simulation of challenging three-dimensional problems pertaining to computational electromagnetics and computation geoseismics. For such applications, parallel computing is a mandatory path. Nowadays, modern parallel computing platforms most often take the form of clusters of multiprocessor systems which can be viewed as hybrid distributed-shared memory systems. Moreover, multiple core systems are increasingly adopted thus introducing an additional level in local memory hierarchies. Developing numerical algorithms that efficiently exploit such platforms raise several challenges, especially in the context of a massive parallelism. In this context, the efforts of the team are towards the exploitation of multiple levels of parallelism and the study hierachical SPMD (Single Program Multiple Data) strategies for the parallelization of unstructured mesh based solvers.

4. Application Domains

4.1. Computational electromagnetics and bioelectromagnetics

Keywords: *biological effects*, *electromagnetic compatibility*, *electromagnetic vulnerability*, *electromagnetic waves*, *furtivity*, *living tissues*, *numerical dosimetry*, *telecommunications*, *transportation systems*.

Electromagnetic devices are ubiquitous in present day technology. Indeed, electromagnetism has found and continues to find applications in a wide array of areas, encompassing both industrial and societal purposes. Applications of current interest include (among others) those related to communications (e.g transmission through optical fiber lines), to biomedical devices and health (e.g tomography, power-line safety, etc.), to circuit or magnetic storage design (electromagnetic compatibility, hard disc operation), to geophysical prospecting, and to non-destructive evaluation (e.g crack detection), to name but just a few. Equally notable and motivating are applications in defense which include the design of military hardware with decreased signatures, automatic target recognition (e.g bunkers, mines and buried ordnance, etc.) propagation effects on communication and radar systems, etc. Although the principles of electromagnetics are well understood, their application to practical configurations of current interest, such as those that arise in connection with the examples above, is significantly complicated and far beyond manual calculation in all but the simplest cases. These complications typically arise from the geometrical characteristics of the propagation medium (irregular shapes, geometrical singularities), the physical characteristics of the propagation medium (heterogeneity, physical dispersion and dissipation) and the characteristics of the sources (wires, etc.).

The significant advances in computer modeling of electromagnetic interactions that have taken place over the last two decades have been such that nowadays the design of electromagnetic devices heavily relies on computer simulation. Computational electromagnetics has thus taken on great technological importance and, largely due to this, it has become a central discipline in present-day computational science. The team currently considers two applications dealing with electromagnetic wave propagation that are particularly challenging for the proposed numerical methodologies.

Interaction of electromagnetic waves with biological tissues. Electromagnetic waves are increasingly present in our daily environment, finding their sources in domestic appliances and technological devices as well. With the multiplication of these sources, the question of potential adverse effects of the interaction of electromagnetic waves with humans has been raised in a number of concrete situations quite recently. It is clear that this question will be a major concern for our citizens in a near future, especially in view of the ever-rising adoption of wireless communication systems. Beside, electromagnetic waves also find applications in the medical domain for therapeutic and diagnostic purposes. Two main reasons motivate our commitment to consider this type of problem for the application of the numerical methodologies developed in the NACHOS project-team:

- first, from the numerical modeling point of view, the interaction between electromagnetic waves and biological tissues exhibit the three sources of complexity listed above and are thus particularly challenging for pushing one step forward the state-of-the art of numerical methods for computational electromagnetics. The propagation media is strongly heterogeneous and the electromagnetic characteristics of the tissues are frequency dependent. Interfaces between tissues have rather complicated shapes that cannot be accurately discretized using cartesian meshes. Finally, the source of the signal often takes the form of a complicated device (e.g a mobile phone or an antenna array).
- second, the study of the interaction between electromagnetic waves and living tissues finds applications of societal relevance such as the assessment of potential adverse effects of electromagnetic fields or the utilization of electromagnetic waves for therapeutic or diagnostic purposes. It is widely recognized nowadays that numerical modeling and computer simulation of electromagnetic wave propagation in biological tissues is a mandatory path for improving the scientific knowledge of the complex physical mechanisms that characterize these applications.

Despite the high complexity both in terms of heterogeneity and geometrical features of tissues, the great majority of numerical studies have been conducted using the widely known FDTD method. In this method, the whole computational domain is discretized using a structured (cartesian) grid. Due to the possible straightforward implementation of the algorithm and the availability of computational power, FDTD is currently the leading method for numerical assessment of human exposure to electromagnetic waves. However, limitations are still seen, due to the rather dificult departure from the commonly used rectilinear grid and cell size limitations regarding very detailed structures of human tissues. In this context, the general objective of the works of the NACHOS project-team is to demonstrate the benefits of high order unstructured mesh based Maxwell solvers fr a realistic numerical modeling of the interaction of electromagnetic waves and living tissues.

Interaction of electromagnetic waves with charged particle beams. Physical phenomena involving charged particles take place in various physical and technological situations such as in plasmas, semiconductor devices, hyper-frequency devices, charged particle beams and more generally, in electromagnetic wave propagation problems including the interaction with charged particles by taking into account self consistent fields. The numerical simulation of the evolution of charged particles under their self-consistent or applied electromagnetic fields can be modeled by the three dimensional Vlasov-Maxwell equations. The Vlasov equation describes the transport in phase space of charged particles submitted to external as well as self-consistent electromagnetic fields. It is coupled non-linearly to the Maxwell equations which describe the evolution of the self-consistent electromagnetic fields. The numerical method which is mostly used for the solution of these equations is the Particle-In-Cell (PIC) method. Its basic idea is to discretize the distribution function f of the particles which is the solution of the Vlasov equation, by a particle method, which consists in representing f by a finite number of macro-particles and advancing those using the Lorentz equations of motion. On the other hand, Maxwell equations are solved on a computational mesh of the physical space. The coupling is done by gathering the charge and current densities from the particles on the mesh to get the sources for the Maxwell equations, and by interpolating the field data on the particles when advancing them. In summary the Particle-In-Cell algorithm, after the initialization phase, is based on a time loop which consists of the following steps: 1) particle advance, 2) charge and current density deposition on the mesh, 3) field solve, 4) field interpolation at particle positions. More physics, like particle injection or collisions can be added to these basic steps.

PIC codes have become a major research tool in different areas of physics involving self-consistent interaction of charged particles, in particular in plasma and beam physics. Two-dimensional simulations have now become very reliable and can be used as well for qualitative as for quantitative results that can be compared to experiments with good accuracy. As the power of supercomputers was increasing three dimensional codes have been developed in the recent years. However, even in order to just make qualitative 3D simulations, an enormous computing power is required. Today's and future massively parallel supercomputers allow to envision the simulation of realistic problems involving complex geometries and multiple scales. In order to achieve this efficiently, new numerical methods need to be designed. This includes the investigation of high order Maxwell solvers, the use of hybrid grids with several homogeneous zones having their own structured or unstructured mesh type and size, and a fine analysis of load balancing issues. These issues are studied in details in the team in the context of discontinuous Galerkin discretization methods on simplicial meshes. Indeed, the team is one of the few groups worldwide [36] considering the development of parallel unstructured mesh PIC solvers for the three-dimensional Vlasov-Maxwell equations.

4.2. Computational geoseismics

Keywords: *elastodynamic waves*, *environment*, *seismic hazard*, *seismic waves*.

Computational challenges in geoseismics span a wide range of disciplines and have significant scientific and societal implications. Two important topics are mitigation of seismic hazards and discovery of economically recoverable petroleum resources. In the realm of seismic hazard mitigation alone, it is worthwhile to recall that despite continuous progress in building numerical modeling methodologies, one critical remaining step is the ability to forecast the earthquake ground motion to which a structure will be exposed during its lifetime. Until such forecasting can be done reliably, complete success in the design process will not be fulfilled. Our involvement in this scientific thematic is rather recent and mainly result from the setup of an active collaboration with geophysicians from the Géosciences Azur laboratory in Sophia Antipolis. In the framework of this collaboration, our objective is to develop high order unstructured mesh based methods for the numerical solution of the time domain elastodynamic equations modeling the propagation of seismic waves in heterogeneous media on one hand, and the design of associated numerical methodologies for modeling the dynamic formation of a fault resulting from an earthquake.

To understand the basic science of earthquakes and to help engineers better prepare for such an event, scientists want to identify which regions are likely to experience the most intense shaking, particularly in populated sediment-filled basins. This understanding can be used to improve building codes in high risk areas and to help engineers design safer structures, potentially saving lives and property. In the absence of deterministic earthquake prediction, forecasting of earthquake ground motion based on simulation of scenarios is one the most promising tools to mitigate earthquake related hazard. This requires intense modeling that meets the spatial and temporal resolution scales of the continuously increasing density and resolution of the seismic instrumentation, which record dynamic shaking at the surface, as well as of the basin models. Another important issue is to improve our physical understanding of the earthquake rupture processes and seismicity.

Large scale simulations of earthquake rupture dynamics, and of fault interactions, are currently the only means to investigate these multi-scale physics together with data assimilation and inversion. High resolution models are also required to develop and assess fast operational analysis tools for real time seismology and early warning systems. Modeling and forecasting earthquake ground motion in large basins is a challenging and complex task. The complexity arises from several sources. First, multiple scales characterize the earthquake source and basin response: the shortest wavelengths are measured in tens of meters, whereas the longest measure in kilometers; basin dimensions are on the order of tens of kilometers, and earthquake sources up to hundreds of kilometers. Second, temporal scales vary from the hundredths of a second necessary to resolve the highest frequencies of the earthquake source up to as much as several minutes of shaking within the basin. Third, many basins have a highly irregular geometry. Fourth, the soils' material properties are highly heterogeneous. And fifth, geology and source parameters are observable only indirectly and thus introduce uncertainty in the modeling process. Because of its modeling and computational complexity and its importance to hazard mitigation, earthquake simulation is currently recognized as a grand challenge problem.

Numerical methods for the propagation of seismic waves have been studied for many years. Most of existing numerical software rely on finite element or finite difference methods. Among the most popular schemes, one can cite the staggered grid finite difference scheme proposed by Virieux [41] and based on the first order velocity-stress hyperbolic system of elastic waves equations, which is an extension of the scheme derived by K.S. Yee [43] for the solution of the Maxwell equations. The use of cartesian meshes is a limitation for such codes especially when it is necessary to incorporate surface topography or curved interface. In this context, our objective is to solve these equations by finite volume or discontinuous Galerkin methods on unstructured triangular (2D case) or tetrahedral (3D case) meshes. This is a recent activity of the team (launched in mid-2004), which is conducted in close collaboration with the *Déformation active, rupture et ondes* team of the Géosciences Azur laboratory in Sophia Antipolis. Our first achievement in this domain has been a centered finite volume software on unstructured triangular meshes [1] which has been validated and evaluated on various problems, ranging from academic test cases to realistic situations.

5. Software

5.1. MAXDGk

Keywords: *Maxwell equations*, *discontinuous Galerkin*, *electromagnetic waves*, *parallel computing*, *time domain*.

Participants: Loula Fezoui, Stéphane Lanteri [correspondant].

The team develops the MAXDGk [27] software suite for the solution of the 2D and 3D Maxwell equations in the time domain. This software implements a high order discontinuous Galerkin method on unstructured triangular (2D case) or tetrahedral (3D case) meshes [5]. The local approximation of the electromagnetic field currently relies on a nodal (Lagrange type) polynomial interpolation method. The underlying algorithms are adapted to distributed memory parallel computing platforms [2].

5.2. MAXDGHk

Keywords: *Maxwell equations*, *discontinuous Galerkin*, *electromagnetic waves*, *frequency domain*, *parallel computing*.

Participants: Victorita Dolean, Stéphane Lanteri [correspondant].

The team develops the MAXDGHk software suite for the numerical solution of the 2D and 3D Maxwell equations in the frequency domain. This software currently implements a high order discontinuous Galerkin method on unstructured triangular (2D case) or tetrahedral (3D case) meshes [13]. The local approximation of the electromagnetic field currently relies on a nodal (Lagrange type) polynomial interpolation method. The underlying algorithms are adapted to distributed memory parallel computing platforms. In particular, the resolution of the sparse, complex coefficients, linear systems resulting from the discontinuous Galerkin formulation is performed by a hybrid iterative/direct solver whose design is based on domain decomposition principles [4].

5.3. ELASTODGk

Keywords: *discontinuous Galerkin*, *elastodynamic waves*, *finite volume*, *parallel computing*, *time domain*, *velocity-stress system*.

Participants: Loula Fezoui [correspondant], Nathalie Glinsky-Olivier, Stéphane Lanteri.

The team develops the ELASTODGk [27] software for the numerical resolution of the 2D and 3D velocity-stress equations in the time domain. This software implements a high order discontinuous Galerkin method on unstructured triangular (2D case) or tetrahedral (3D case) meshes [12]. The local approximation of the electromagnetic field currently relies on a nodal (Lagrange type) polynomial interpolation method. The underlying algorithms are adapted to distributed memory parallel computing platforms.

6. New Results

6.1. Electromagnetic wave propagation

6.1.1. Arbitrary high order DGTD method on simplicial meshes

Keywords: *Maxwell equations*, *discontinuous Galerkin*, *finite volume*, *leap-frog scheme*, *tetrahedral mesh*, *time domain*, *triangular mesh*, *unstructured mesh*.

Participants: Hassan Fahs, Loula Fezoui, Stéphane Lanteri.

The DGTD-$\mathbb{P}_p$ method previsouly developed in the team for the numerical solution of the time domain Maxwell equations on unstructured simplicial meshes [5] has been extended to arbitrary high order in space and time. The resulting method relies on the following ingredients: a central numerical flux function for the approximation of the integral term at an interface between two neighboring elements, a high order nodal (Lagrange type) polynomial interpolation method for the approximation of the electromagnetic field components within a simplex element and a high order leap-frog scheme for time integration. The improvement of the accuracy properties of the DGTD-$\mathbb{P}_p$ method thanks to the use of high order leap-frog scheme is illustrated on Fig. 1 in the context of the numerical solution of the 2D Maxwell equations, and by considering the problem of the propagation of an eigenmode in a unitary square cavity with perfectly conducting walls. The figures show the observed numerical h-convergence of the DGTD-$\mathbb{P}_p$ methods based on the second order (left) and fourth order (right) leap-frog scheme and confirm the theoretical *a priori* estimates [9].

6.1.2. Arbitrary high order DGTD method on non-conforming simplicial meshes

Keywords: *Maxwell equations*, *discontinuous Galerkin*, *finite volume*, *leap-frog scheme*, *locally refined mesh*, *non-conforming mesh*, *tetrahedral mesh*, *time domain*, *triangular mesh*, *unstructured mesh*.

Participants: Hassan Fahs, Loula Fezoui, Stéphane Lanteri, Francesca Rapetti.

Two important features of discontinuous Galerkin methods are their flexibility with regards to the local approximation of the field quantities and their natural ability to deal with non-conforming meshes. The non-conformity can result from a local refinement of the mesh (h-adaptivity), or of the approximation order (p-adaptivity) or of both of them (hp-adaptivity). In the context of the PhD thesis of Hassan Fahs [9], we have studied non-dissipative discontinuous Galerkin methods for solving the 2D time domain Maxwell equations on non-conforming, locally refined, triangular meshes. Similarly to the method described in [5], the DGTD method considered in this study is based on two basic ingredients: a centered approximation for the calculation of numerical fluxes at inter-element boundaries and an explicit leap-frog time integration scheme [17]. In this context, a hp-like DGTD method which allows for both a local non-conforming refinement of the mesh and a locally defined approximation order has been designed, anlayzed and evaluated in the context of the numerical solution of the 2D time domain Maxwell equations on triangular meshes [16]. The use of a locally refined triangular mesh is illustrated on Fig. 2 for the simulation of the propagation of an eigenmode in a wedge-shaped cavity with perfectly conducting walls, using the DGTD-$\mathbb{P}_1$ method.

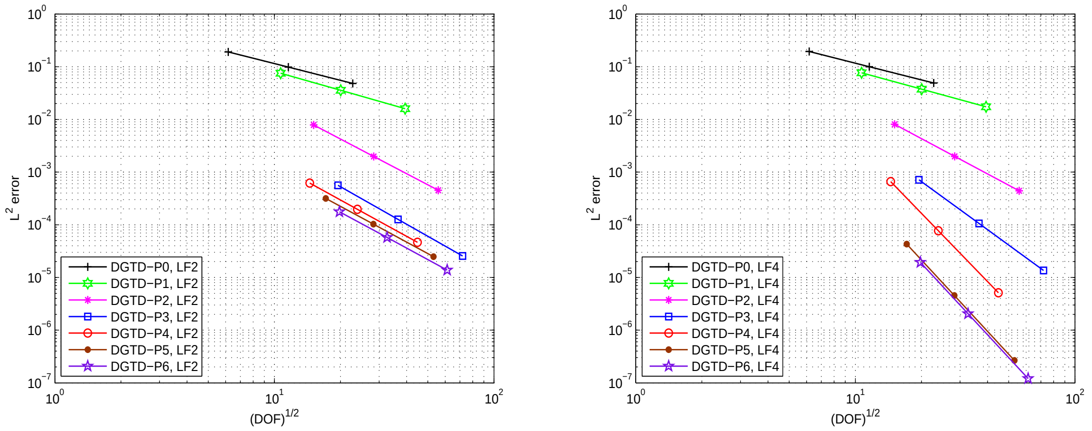

Figure 1. Square-shaped PEC resonator: h-convergence of the DGTD-$\mathbb{P}_p$ methods based on the second order (left) and fourth order (right) leap-frog schemes.

6.1.3. High order polynomial interpolation in DGTD methods

Keywords: *Maxwell equations*, *discontinuous Galerkin*, *hierachical basis*, *modale basis*, *nodal basis*, *polynomial interpolation*, *time domain*.

Participants: Loula Fezoui, Antoine Jarrier, Joseph Charles, Stéphane Lanteri.

In the high order DGTD-$\mathbb{P}_p$ methods developed by the team so far, the local approximation of the electromagnetic field relies on a nodal (Lagrange type) polynomial interpolation method however it is clear that other polynomial interpolation methods could be adopted as well. The choice of a set ot basis functions should ideally take into account several criteria among which, the modal or nodal nature of the functions, the orthogonality of the functions, the hierachical structure of the functions, the conditioning of the elemental matrices to be inverted (e.g the mass matrix in explicit DGTD methods) and the programming simplicity. We have started this year a study aiming at the choice of an appropriate polynomial interpolation method in view of the development of a p-adaptive DGTD-$\mathbb{P}_p$ method on simplicial meshes. As a preliminary step, several candidate polynomial interpolation methods are numerically assessed in details in the context of the solution of the 1D and 2D Maxwell equations.

6.1.4. Hybrid FVDT/DGTD method on multi-element meshes

Keywords: *Maxwell equations*, *discontinuous Galerkin*, *finite volume*, *hybrid trangular/quadrangular mesh*, *quadrangular mesh*, *time domain*, *triangular mesh*.

Participants: Clément Durochat, Stéphane Lanteri.

For some propagation problems, the use of a single geometrical element type (a simplex in the DGTD methods developed by the team so far) in the discretization process may not be optimal. Instead, one would ideally allow the combined use of different types of element e.g. quandrangles and triangles in the 2D case, or hexahedra and tetrahedra in the 3D case. We have initiated this year a study in this direction by considering the coupling of a non-dissipative FVTD method designed on quadrangular meshes with the non-dissipative high order DGTD method on triangular meshes introduced in [5]. In this preliminary study, the underlying hybrid quadrangular/triangular mesh has been assumed to be a conforming mesh i.e hanging nodes are not allowed and we focussed on the stability analysis of the resulting hybrid FVDT/DGTD method on multi-element meshes, while accuracy and efficiency issues will be considered in a sequel study.

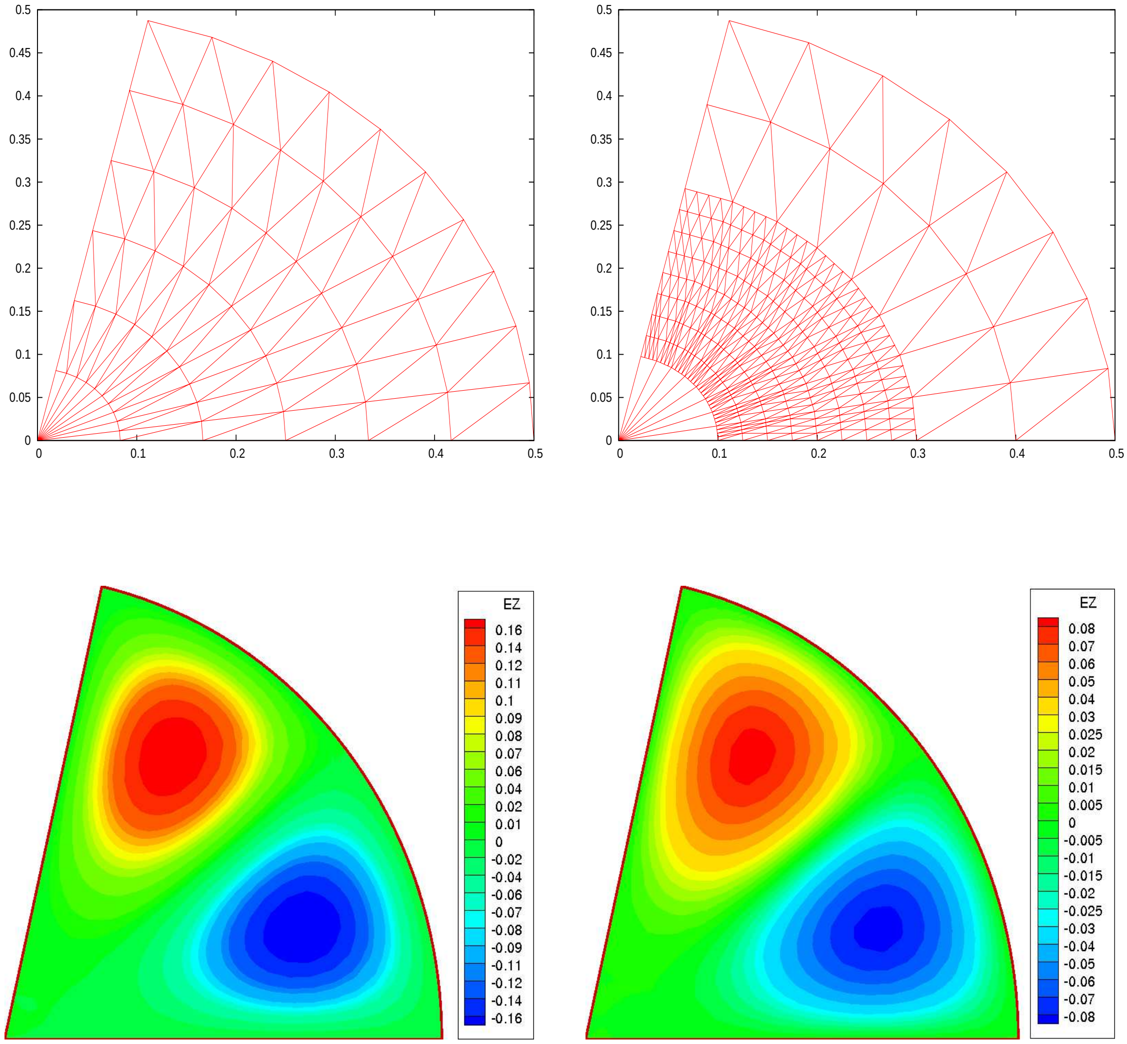

Figure 2. Wedge-shaped PEC resonator: conforming and non-conforming triangular meshes (top) and contour lines of E_z at different times.

6.1.5. Hybrid explicit/implicit DGTD method

Keywords: *Maxwell equations*, *discontinuous Galerkin*, *finite volume*, *hybrid explicit-implicit time integration*, *implicit time integration*, *locally refined mesh*, *tetrahedral mesh*, *time domain*, *triangular mesh*, *unstructured mesh*.

Participants: Adrien Catella, Victorita Dolean, Stéphane Lanteri.

Existing numerical methods for the solution of the time domain Maxwell equations often rely on explicit time integration schemes and are therefore constrained by a stability condition that can be very restrictive on highly refined meshes. An implicit time integration scheme is a natural way to obtain a time domain method which is unconditionally stable. In the context of the PhD thesis of Adrien Catella [8], we have studied the applicability of implicit time integration schemes in conjunction with discontinuous Galerkin methods for the solution of the 2D time domain Maxwell equations [10]. The starting-point of this study is the explicit, non-dissipative, DGTD-$\mathbb{P}_p$ method introduced in [5] and we have proposed to use of Crank-Nicholson scheme in place of the explicit leap-frog scheme adopted in this method. As a result, we obtain an unconditionally stable, non-dissipative, implicit DGTD-$\mathbb{P}_p$ method, but at the expense of the inversion of a global linear system at each time step, thus obliterating one of the attractive features of discontinuous Galerkin formulations. A more viable approach for 3D simulations consists in applying an implicit time integration scheme locally i.e in the refined regions of the mesh, while preserving an explicit time scheme in the complementary part, resulting in an hybrid explicit-implicit (or locally implicit) time integration strategy. We have studied such a hybrid explicit-implicit DGTD method for solving the time domain Maxwell equations on unstructured simplicial meshes. The hybrid explicit-implicit DGTD method considered in this study was initially introduced by Piperno in [37]. However, to our knowledge, this hybrid explicit-implicit DGTD method had not been investigated numerically. An illustration of the application of the resulting hybrid explicit-implicit DGTD-$\mathbb{P}_1$ method is shown on Fig. 3 below. The underlying tetrahedral mesh consists of 360,495 vertices and 2,024,924 elements. When 6381 elements are treated implicitly (i.e $\approx$ 0.2% of the tetrahedra of the mesh), the simulation time is reduced from $\approx$ 25 h to $\approx$ 4 h. This hybrid explicit-implicit DGTD-$\mathbb{P}_p$ opens the route for large-scale time domain electromagnetic wave simulations using highly refined meshes. Our short-term objectives in this direction will be, to study the stability and convergence of the method, to adapt the method to distributed memory parallel computing platforms. Beside, we also plan to investigate the extension of the proposed hybrid explici-implicit strategy to higher order time schemes.

6.1.6. High order DGTD Particle-in-Cell method on simplicial meshes

Keywords: *Maxwell equations*, *Particle-in-Cell*, *discontinuous Galerkin*, *tetrahedral mesh*, *time domain*.

Participants: Loula Fezoui, Christian Konrad, Siham Layouni, Stéphane Lanteri.

In the context of the ANR HOUPIC project (starting date: january 2007 - duration: 3 years), we are considering the development of a parallel DGTD/PIC solver for the solution of the system of Vlasov-Maxwell equations. This work entails several aspects ranging from numerical analysis questions (charge conservation property, methods of assignment of current and charge densities to physical space) to algorithimc concerns (parallel particle localization algorithm in a tetrahedral mesh, parallelization and load balancing strategies). In particular, we have studied the applicability of Space filling Curves (SFCs) as a basis for designing a fast and scalable strategy for solving the two-constraint partitioning problem raised by the parallelization of a tetrahedral mesh coupled DG/PIC solver. A new SFC based method which is well adapted to multi-constraint partitioning problems has been proposed [23]. This method has been compared to graph based partitioning methods from the widely used MeTiS tool. Experimental results show that the proposed SFC based method is at least 100 times faster than MeTiS to the disadvantage of edge-cuts that are between 2 to 4 times worse than those achieved by the MeTiS methods.

6.1.7. Numerical modeling of human tissues exposure to electromagnetic fields

Keywords: *Maxwell equations*, *Visible Human*, *discontinuous Galerkin*, *tetrahedral mesh*, *time domain*.

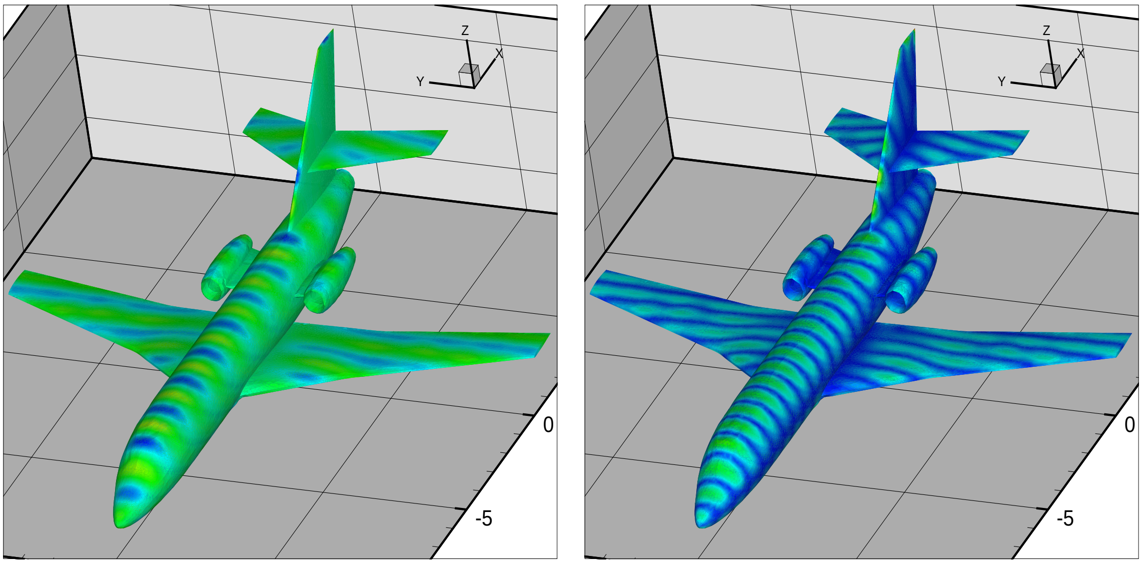

Figure 3. Scattering of a plane wave by a Falcon jet geometry: contour lines of E_z and $|\mathbf{E}|$ on the aircraft surface

Participants: Stéphane Lanteri, Laurent Rineau [Geometry Factory, Sophia Antipolis], Mariette Yvinec [GEOMETRICA project-team], Joe Wiart [France Télécom R&D, Issy-les-Moulineaux].

The Visible Human project [29] aimed at the construction of complete, anatomically detailed, three-dimensional representations of male and female human bodies. Among other achievements, high resolution images of representative male and female cadavers have been completed. These image data sets are used for various research purposes among which numerical dosimetry studies of human tissues exposure to electromagnetic fields. As a matter of fact, the Visible Human model is now used by several groups worldwide involved in such studies and, in almost all the cases, the FDTD method is directly applied to the voxel grid defining the images. In this study, we have constructed realistic geometrical models of the Visible Human, based on tetrahedral meshes, using the tetrahedral mesh generator co-developed by the GEOMETRICA project-team and the Geometry Factory company. Then, the high order DGTD methods developed in the team are used to simulate the propagation of an electromagnetic wave in homogeneous and heterogeneous tissue models. The objective is to obtain highly accurate distributions of the SAR (Specific Absorption Rate) which is a basic quantity of interest in microwave numerical dosimetry studies, and to assess whether localized effects (so called hot spots) appear that are not correctly modeled by the FDTD method due to the use of cartesian meshes. In particular, the staircasing which is typical of cartesian meshes does not allow for a correct representation of tissue (i.e media) interfaces. Thus, one of the challenges of the present study is to construct geometrical models which include an accurate discretization of tissue interfaces (at least for a few tissues of the body such as the skin, the fat, the skull and the muscle) through the use of appropriate geometrical modeling tools. A preliminary result is shown on Fig. 4 for the propagation of a plane wave (F=2.14 GHz) in a homogeneous model of the visible human using the DGTD-$\mathbb{P}_2$ method. The underlying tetraedral mesh consists of 899,872 vertices and 5,335,521 elements. The total number of unknowns of this problem is 320,131,260 (there are 60 degrees of freedom per element for the $\mathbb{P}_2$ interpolation method). Worthwhile to note, this large scale simulation has been conducted on 512 cores of the Bull supercomputer operated by the CCRT (Centre de Calcul Recherche et Technologie) with a simulation time of 1 h 45 mn.

6.1.8. DG methods for the frequency domain Maxwell equations

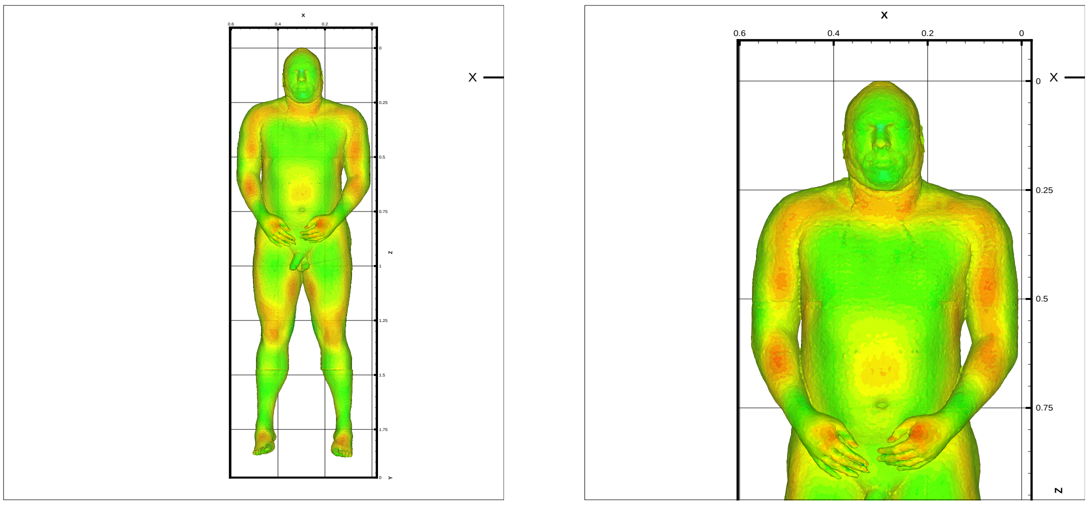

Figure 4. Propagation of a plane wave in a homogeneous model of a human body.

Keywords: *Maxwell equations*, *centered schemes*, *discontinuous Galerkin*, *finite volume*, *frequency domain*, *simplicial mesh*, *time harmonic*, *unstructured mesh*, *upwind schemes*.

Participants: Victorita Dolean, Mohamed El Bouajaji, Stéphane Lanteri, Ronan Perrussel [Ampère Laboratory, Ecole Centrale de Lyon].

A large number of electromagnetic wave propagation problems can be modeled by assuming a time harmonic behavior and thus considering the numerical solution of the time harmonic (or frequency domain) Maxwell equations. In this study, we investigate the applicability of discontinuous Galerkin methods on simplicial meshes for the calculation of time harmonic electromagnetic wave propagation in heterogeneous media. Although there are clear advantages of using DG methods based on a centered scheme for the evaluation of surface integrals when solving time domain problems [5], such a choice is questionable in the context of time harmonic problems. Penalized DG formulations or DG formulations based on an upwind numerical flux have been shown to yield optimally convergent high order DG methods [34]. Moreover, such formulations are necessary to prevent the apparition of spurious modes when solving the Maxwell eigenvalue problem [42]. We have developed this year a arbitrary high order discontinuous Galerkin frequency domain DGFD-$\mathbb{P}_p$ method on triangular meshes, relying on either a centered or an upwind flux, for solving the 2D time harmonic Maxwell equations. Moreover, as a first step towards the development of a p-adaptive DGFD-$\mathbb{P}_p$ method, the approximation order is allowed to be defined at the element level based on a local geometrical criterion.

6.2. Seismic wave propagation

6.2.1. Arbitrary high order DGTD method on simplicial meshes

Keywords: *P-SV wave propagation*, *discontinuous Galerkin*, *finite volume*, *leap-frog scheme*, *tetrahedral mesh*, *triangular mesh*, *unstructured mesh*, *velocity-stress equations*.

Participants: Sarah Delcourte, Nathalie Glinsky-Olivier, Loula Fezoui, Serge Moto Pong [University of Yaoundé 1, Cameroon].

We continue developing high order non-dissipative discontinuous Galerkin methods on simplicial meshes (triangles in the 2D case and tetrahedra in the 3D case) for the numerical solution of the first order hyperbolic linear system of elastodynamic equations. These methods share some ingredients of the DGTD-$\mathbb{P}_p$ methods developed by the team for the time domain Maxwell equations among which, the use of nodal polynomial (Lagrange type) basis functions, a second order leap-frog time integration scheme and a centered scheme for the evaluation of the numerical flux at the interface between neighboring elements. The resulting DGTD-$\mathbb{P}_p$ methods have been validated and evaluated in detail in the context of propagation problems in both homogeneous and heterogeneous media including problems for which analytical solutions can be computed. Particular attention was given to the study of the mathematical properties of these schemes such as stability, convergence and dispersion.

In the 2D case, the source modeling has been studied via the Garvin test case i.e the propagation of an explosive source in a half-space with a free surface. A class of high order leap-frog schemes has also been studied. These schemes improve the accuracy of the highest orders spatial schemes (fpr $p \geq 3$) while being efficient since they allow the use of larger time steps as compared to the DGTD-$\mathbb{P}_p$ method based on the second order leap-frog scheme.

In the 3Dcase, in the framework of the ANR QSHA project, canonical problems are studied such as semi-spherical or ellipsoidal canyon/basin in order to compare results of several numerical methods. More realistic test cases are examined via our participation to the Euroseistest Numerical Benchmark initiative. The objective of this benchmark, organized in the framework of the Cashima project (CEA Cadarache, the LGIT in Grenoble and Aristotle University of Thessaloniki), is to perform simulations of real events on the Volvi area (a well documented region near Thessaloniki) including complex characteristics of the medium.

6.3. Domain decomposition methods

6.3.1. Optimized Schwarz algorithms for the time harmonic Maxwell equations discretized by DG methods

Keywords: *Maxwell equations*, *Schwarz algorithm*, *discontinuous Galerkin*, *domain decomposition*, *natural interface conditions*, *optimized interface conditions*, *time harmonic*.

Participants: Victorita Dolean, Mohamed El Bouajaji, Martin Gander [Mathematics Section, University of Geneva], Stéphane Lanteri, Ronan Perrussel [Ampère Laboratory, Ecole Centrale de Lyon].

The linear systems resulting from the discretization of the 3D time harmonic Maxwell equations using discontinuous Galerkin methods on simplicial meshes are characterized by large sparse, complex coefficients and irregularly structured matrices. Classical preconditioned iterative methods (such as the GMRES Krylov method preconditioned by an incomplete LU factorization) generally behave poorly on these linear systems. A standard alternative solution strategy calls for sparse direct solvers. However, this approach is not feasible for reasonably large systems due to the memory requirements of direct solvers. On the other hand, parallel computing is recognized as a mandatory path for the design of algorithms capable of solving problems of realistic importance. Several parallel sparse direct solvers have been developed in the recent years such as MUMPS [31]. Even if these solvers efficiently exploit distributed memory parallel computing platforms and allow to treat very large problems, there is still room for improvements of the situation. Iterative methods can be used to overcome this memory problem. The main difficulty encountered by these methods is their lack of robustness and, generally, the unpredictability and unconsistency of their performance when they are used over a wide range of different problems. Because an iterative solver will usually require fewer iterations and less time if more fill-in is allowed in the preconditioner, some approaches combine the direct solvers techniques with other iterative preconditioning techniques in order to build robust preconditioners. For example, a popular approach in the domain decomposition framework is to use a direct solver inside each subdomain and to use an iterative solver on the interfaces between subdomains.

Even if they have been introduced for the first time two centuries ago, over the last two decades, classical Schwarz methods have regained a lot of popularity with the developpement of parallel computers. First developped for the elliptic problems, they have been recently extended to systems of hyperbolic partial differential equations, and it was observed that the classical Schwarz method can be convergent even without overlap in certain cases. This is in strong contrast to the behavior of classical Schwarz methods applied to elliptic problems, for which overlap is essential for convergence. Over the last decade, optimized versions of Schwarz methods have been developed for elliptic partial differential equations. These methods use more effective transmission conditions between subdomains, and are also convergent without overlap for elliptic problems. The extension of such methods to systems of equations and more precisely to Maxwell's system (time harmonic and time discretized equations) has been done recently in [19]- [32].

These new transmission conditions were originally proposed for three different reasons: first, to obtain Schwarz algorithms that are convergent without overlap; secondly, to obtain a convergent Schwarz method for the Helmholtz equation, where the classical Schwarz algorithm is not convergent, even with overlap; and third, to accelerate the convergence of classical Schwarz algorithms. Several studies towards the development of optimized Schwarz methods for the time harmonic Maxwell equations have been conducted this last decade, most often in combination with conforming edge element approximations. Optimized Schwarz algorithms can involve transmission conditions that are based on high order derivatives of the interface variables. However, the efectiveness of the new optimized interface conditions has been proved so far only for simple geometries and applications.

In order to extend them to more realistic applications and geometries, and high order approximation methods, our first strategy for the design of parallel solvers in conjunction with discontinuous Galerkin methods on simplicial meshes relies on a Schwarz algorithm where a classical condition is imposed at the interfaces between neighboring subdomains which corresponds to a Dirichlet condition for characteristic variables associated to incoming waves. From the discretization point of view, this interface condition gives rise to a boundary integral term which is treated using a flux splitting scheme similar to the one applied at absorbing boundaries. The Schwarz algorithm can be used as a global solver or it can be reformulated as a Richardson iterative method acting on an interface system. In the latter case, the resolution of the interface system can be performed in a more efficient way using a Krylov method. This approach has been implemented in the context of low order discontinuous Galerkin methods (finite volume method and discontinuous Galerkin method based on linear interpolation) [4]. Preliminary investigations of optimized Schwarz algorithms combined to high order discontinuous Galerkin time harmonic methods on triangular meshes for the discretization of the 2D Maxwell equations are reported in [15].

7. Contracts and Grants with Industry

7.1. High order DGTD-PIC solver for the Vlasov/Maxwell equations

Participants: Adrien Catella, Joseph Charles, Loula Fezoui, Stéphane Lanteri, Muriel Sesques [CEA/CESTA, Bordeaux].

The subject of this research grant with CEA/CESTA in Bordeaux is the development of a coupled Vlasov/Maxwell solver combining the high order DGTD-$\mathbb{P}_p$ method on tetrahedral meshes developed in the team [5] and a Particle-In-Cell method. The resulting DGTD-PIC solver will be used for electrical vulnerability studies of the experimental chamber of the *Laser Mégajoule* system. The PhD thesis of Adrien Catella is fully funded by this grant.

7.2. DGTD methods on non-conforming simplicial meshes

Participants: Hassan Fahs, Stéphane Lanteri, Joe Wiart [France Télécom R&D, Issy-les-Moulineaux].

A collaboration with the IOP team of France Télécom R&D (center of Issy-les-Moulineaux) was initiated in 2003 in the framework of the HeadExp Concerted Research Action. This collaboration currently goes on in the context of a research grant which aims at the development of high order DGTD-$\mathbb{P}_p$ methods on non-conforming simplicial meshes for the numerical modeling of the interaction of electromagnetic waves with biological tissues. The PhD thesis of Hassan Fahs is partially funded by this grant.

8. Other Grants and Activities

8.1. Quantitative Seismic Hazard Assessment (QSHA)

Keywords: *discontinuous Galerkin*, *finite volume*, *seismic hazard*, *seismic wave propagation*.

Participants: Nathalie Glinsky-Olivier, Serge Piperno [Cermics, ENPC], Jean Virieux [Joseph Fourier University and LGIT laboratory].

This project if funded by the ANR in the framework of the program *Catastrophes Telluriques et Tsunami*, at the end of 2005. The participants are: CNRS/Géosciences Azur, BRGM (Bureau de Recherches Géologiques et Minières, Service Aménagement et Risques Naturels, Orléans), CNRS/LGIT (Laboratoire de Géophysique Interne et Technophysique, Observatoire de Grenoble), CEA/DAM (Bruyères le Chatel), LCPC, INRIA Sophia Antipolis (NACHOS team), ENPC (Cermics), CEREGE (Centre europeen de Recherche et d'Enseignement des Géosciences de l'Environnement, Aix en Provence), IRSN (Institut de Radioprotection et de Surete Nucléaire), CETE Méditerranée (Nice), LAM (Laboratoire de Mécanique, Université de Marne la Vallée), LMS (Laboratoire de Mécanique des Solides, Ecole Polytechnique). The activities planned in the QSHA project aim at (1) obtaining a more accurate description of crustal structures for extracting rheological parameters for wave propagation simulations, (2) improving the identification of earthquake sources and the quantification of their possible size, (3) improving the numerical simulation techniques for the modeling of waves emitted by earthquakes, (4) improving empirical and semi-empirical techniques based on observed data and, (5) deriving a quantitative estimation of ground motion. From the numerical modeling viewpoint, essentially all of the existing families of methods (boundary element method, finite difference method, finite volume method, spectral element method and discrete element method) are extended for the purpose of the QSHA objectives.

8.2. Distributed objects and components for high performance scientific computing (DiscoGrid)

Keywords: *Grid computing*, *component models*, *distributed objects*, *hierarchical mesh partitioning*, *high performance computing*, *message passing programming*, *unstructured mesh solvers*.

Participants: Antoine Bouquet, Matthieu Cargnelli [EADS Innovation Works, Toulouse], Françoise Baude [OASIS project-team, INRIA Sophia Antipolis], Denis Caromel [OASIS project-team, INRIA Sophia Antipolis], Vincent Cave [OASIS project-team, INRIA Sophia Antipolis], Serge Chaumette [LABRi, Bordeaux], Thierry Gautier [ID-IMAG, MOAIS team, Grenoble], Hervé Guillard [SMASH project-team, INRIA Sophia Antipolis], Stéphane Lanteri, Raul Lopez [PARIS project-team, IRISA Rennes], Alexandre Moyer [SMASH project-team, INRIA Sophia Antipolis], Christian Perez [PARIS project-team, IRISA Rennes], Frédéric Wagner [ID-IMAG, MOAIS team, Grenoble].

The project-team is coordinating the DiscoGrid (Distributed objects and components for high performance scientific computing on the Grid'5000 test-bed) project which is funded by ANR in the framework of *Calcul Intensif et Grilles de Calcul* program (this project has started in January 2006 for a duration of 3,5 years). The DiscoGrid project aims at studying and promoting a new paradigm for programming non-embarrassingly parallel scientific computing applications on a distributed, heterogeneous, computing platform. The target applications require the numerical resolution of systems of partial differential equations (PDEs) modeling electromagnetic wave propagation and fluid flow problems. More importantly, the underlying numerical methods share the use of unstructured meshes and are based on well known finite element and finite volume formulations.

8.3. High order finite element particle-in-cell solvers on unstructured grids (HOUPIC)

Keywords: *Maxwell equations*, *Particle-In-Cell*, *discontinuous Galerkin*, *high performance computing*, *time domain*.

Participants: Loula Fezoui, Christian Konrad, Stéphane Lanteri, Muriel Sesques [CEA/CESTA, Bordeaux], Eric Sonnendrücker [IRMA, Strasbourg].

The project-team is a partner of the HOUPIC project which is funded by ANR in the framework of *Calcul Intensif et Simulations* program (this project has started in January 2007 for a duration of 3 years). This project is coordinated by Eric Sonnendrücker for the IRMA (Institut de Recherche Mathématique Avancée) Laboratory in Strasbourg, and the other partners are the LSIIT (Laboratoire des Sciences de l'Image, de l'Informatique et de la Télédétection) in Strasbourg, the CEA/CESTA in Bordeaux, the PSI (Paul Scherrer Institut) in Villigen (Switzerland) and the IAG (Institut für Aerodynamik und Gasdynamik) in Stuttgart (Germany). The main objective of this project is to develop and compare Finite Element Time Domain (FETD) solvers based on high order Hcurl conforming elements and high order Discontinuous Galerkin (DG) finite elements and investigate their coupling to a PIC method.

8.4. Ultra-wideband microwave imaging and inversion (MAXWELL)

Keywords: *Maxwell equations*, *discontinuous Galerkin*, *frequency domain*, *high performance computing*.

Participants: Victorita Dolean, Mohamed El Bouajaji, Stéphane Lanteri, Christian Pichot [LEAT].

The project-team is a partner of the MAXWELL project (Novel, ultra-wideband, bistatic, multipolarization, wide offset, microwave data acquisition, microwave imaging, and inversion for permittivity) which is funded by ANR under the non-thematic program (this project has started in January 2008 for a duration of 4 years). This project is coordinated by Christian Pichot from the LEAT (Laboratoire d'Electronique Antennes et Télécommunications) in Sophia Antipolis and the other partners are the Géosciences Azur Laboratory in Sophia Antipolis and the MIGP (Laboratoire de Modélisation et Imagerie en Géosciences de Pau) Laboratory. This project aims at the development of a complete microwave imaging system, with a frequency bandwidth of 1.87 GHz, ranging from 130 MHz to 2 GHz, using unstructured mesh solvers of the time harmonic Maxwell equations which drive a generalized least-squares inversion engine, whose output is a subsurface map of the relative permittivity. Subsidiary goals of the project are: (a) the construction and calibration of two ultra-wideband antennas, (b) the construction of two types of carriages for performing data acquisition, (c) the acquisition of dense microwave data with very wide offset for the entire bandwidth from 130 MHz to 2 GHz and for 2 orthogonal co-polarizations and one cross-polarization, (d) the reprocessing of data, including gain and kinematic inversion using conventional seismic processing formulations and (e) the development of discontinuous Galerkin solvers on simplicial meshes for the numerical solution of the time harmonic Maxwell equations and their integration into an inversion system.

9. Dissemination

9.1. Teaching

"Éléments finis", Victorita Dolean, Master de Mathématiques, première année, Université de Nice/Sophia Antipolis (48h).

"Analyse numérique", Victorita Dolean, Master de Mathématiques, première année, Université de Nice/Sophia Antipolis (36h).

"Méthodes numériques", Victorita Dolean, Master de Mathématiques, seconde année, Université de Nice/Sophia Antipolis (30h).

"Analyse numérique", Victorita Dolean, première année ingénieur, EPU de Nice/Sophia Antipolis (78h).

"Méthodes numériques pour les EDP", Victorita Dolean, seconde année ingénieur, filière Mathématiques Appliquées et Modélisation, EPU de Nice/Sophia Antipolis (39h).

"Calcul Numérique Parallèle", Stéphane Lanteri, Mastère de Mécanique Numérique, Ecole Nationale Supérieure des Mines de Paris (9h).

9.2. Ongoing PhD theses

Mondher Benjemaa, "Etude et simulation numérique de la rupture dynamique des séismes par des méthodes d'éléments finis discontinus", Nice-Sophia Antipolis University.

Antoine Bouquet, "Caractérisation de structures rayonnantes par une méthode Galerkin discontinue associée à une technique de domaines fictifs", Nice-Sophia Antipolis University.

Adrien Catella, "Méthode de type Galerkin discontinu d'ordre élevé en maillages tétraédriques non-structurés pour la résolution numérique des équations de Maxwell en domaine temporel", Nice-Sophia Antipolis University.

Hassan Fahs, "Méthodes de type Galerkin discontinu en maillages non-conformes pour la résolution numérique des équations de Maxwell en domaine temporel", Nice-Sophia Antipolis University.

9.3. International collaborations

Since January 2008, the NACHOS project-team is a partner of the PhyLeaS [28] INRIA associate team (Design and high performance implementation of parallel hybrid sparse linear solvers) which is coordinated by Jean Roman (ScAlApplix project-team, INRIA Bordeaux â Sud-Ouest Research Center) and associates the following partners: Yousef Saad (Department of Computer Science and Engineering, University of Minnesota, USA), Matthias Bollhoefer (Institute of Computational Mathematics Department of Mathematics and Computer Science, TU Brunswick, Germany), Luc Giraud (Parallel Algorithms and Optimization Group, LIMA-IRIT UMR CNRS 5505, ENSEEIHT, Toulouse). The research activities undertaken in the framework of the PhyLeaS associate team aim at the design and efficient implementation of parallel hybrid linear system solvers which combine the robustness of direct methods with the implementation flexibility of iterative schemes. These approaches are candidate to get scalable solvers on massively parallel computers.

The team is collaborating with Martin Gander (Mathematics Section of the University of Geneva) on the design of optimized Schwarz type domain decomposition algorithms for the time domain and time harmonic Maxwell equations. Martin Gander spent two weeks in the team this year.

10. Bibliography

Major publications by the team in recent years

[1] M. BENJEMAA, N. GLINSKY-OLIVIER, V. CRUZ-ATIENZA, J. VIRIEUX, S. PIPERNO. *Dynamic non-planar crack rupture by a finite volume method*, in "Geophys. J. Int.", vol. 171, 2007, p. 271-285.

[2] M. BERNACKI, L. FEZOUI, S. LANTERI, S. PIPERNO. *Parallel unstructured mesh solvers for heterogeneous wave propagation problems*, in "Appl. Math. Model.", vol. 30, n^{o} 8, 2006, p. 744–763.

[3] M. BERNACKI, S. LANTERI, S. PIPERNO. *Time-domain parallel simulation of heterogeneous wave propagation on unstructured grids using explicit non-diffusive, discontinuous Galerkin methods*, in "J. Comp. Acoustics", vol. 14, n^{o} 1, 2006, p. 57–81.

[4] V. DOLEAN, S. LANTERI, R. PERRUSSEL. *A domain decomposition method for solving the three-dimensional time-harmonic Maxwell equations discretized by discontinuous Galerkin methods*, in "J. Comput. Phys.", vol. 227, n^{o} 3, 2007, p. 2044–2072.

[5] L. FEZOUI, S. LANTERI, S. LOHRENGEL, S. PIPERNO. *Convergence and stability of a discontinuous Galerkin time-domain method for the 3D heterogeneous Maxwell equations on unstructured meshes*, in "ESAIM: Math. Model. Num. Anal.", vol. 39, n^{o} 6, 2005, p. 1149–1176.

[6] S. PIPERNO, M. REMAKI, L. FEZOUI. *A nondiffusive finite volume scheme for the three-dimensional Maxwell's equations on unstructured meshes*, in "SIAM J. Num. Anal.", vol. 39, n^{o} 6, 2002, p. 2089–2108.

[7] G. SCARELLA, O. CLATZ, S. LANTERI, G. BEAUME, S. OUDOT, J.-P. PONS, S. PIPERNO, P. JOLY, J. WIART. *Realistic numerical modelling of human head tissue exposure to electromagnetic waves from cellular phones*, in "Comptes Rendus Physique", vol. 7, n^{o} 5, 2006, p. 501–508.

Year Publications

Doctoral Dissertations and Habilitation Theses

[8] A. CATELLA. *Schémas d'intégration en temps efficaces pour la résolution numérique des équations de Maxwell instationnaires par des méthodes Galerkin discontinues d'ordre élevé en maillages non-structurés*, Thèse de Mathématiques, Université de Nice-Sophia Antipolis, Décembre 2008.

[9] H. FAHS. *Méthodes de type Galerkin discontinu d'ordre élevé pour la résolution numérique des équations de Maxwell instationnaires sur des maillages simplexes non-conformes*, Thèse de Mathématiques, Université de Nice-Sophia Antipolis, Décembre 2008.

Articles in International Peer-Reviewed Journal

[10] A. CATELLA, V. DOLEAN, S. LANTERI. *An implicit discontinuous Galerkin time-domain method for two-dimensional electromagnetic wave propagation*, in "COMPEL", to appear, 2008.

[11] A. CATELLA, V. DOLEAN, S. LANTERI. *An unconditionally stable discontinuous Galerkin method for solving the 2D time-domain Maxwell equations on unstructured triangular meshes*, in "IEEE. Trans. Magn.", vol. 44, n^{o} 6, 2008, p. 1250–1253.

[12] S. DELCOURTE, L. FEZOUI, N. GLINSKY-OLIVIER. *A high-order discontinuous Galerkin method for the seismic wave propagation*, in "ESAIM: proceedings", to appear, 2008.

[13] V. DOLEAN, H. FOL, S. LANTERI, R. PERRUSSEL. *Solution of the time-harmonic Maxwell equations using discontinuous Galerkin methods*, in "J. Comp. Appl. Math.", vol. 218, n^{o} 2, 2008, p. 435-445.

[14] V. DOLEAN, M. GANDER, L. GERARDO-GIORDA. *Optimized Schwarz methods for Maxwell equations*, in "SIAM J. Scient. Comp.", to appear, 2008, https://hal.archives-ouvertes.fr/ccsd-00107263.

[15] V. DOLEAN, S. LANTERI, R. PERRUSSEL. *Optimized Schwarz algorithms for solving time-harmonic Maxwell's equations discretized by a discontinuous Galerkin method*, in "IEEE. Trans. Magn.", vol. 44, n^{o} 6, 2008, p. 954–957.

[16] H. FAHS. *Development of a hp-like discontinuous Galerkin time-domain method on non-conforming simplicial meshes for electromagnetic wave propagation*, in "Int. J. Numer. Anal. Mod.", to appear, 2008.

[17] H. FAHS, L. FEZOUI, S. LANTERI, F. RAPETTI. *Preliminary investigation of a non-conforming discontinuous Galerkin method for solving the time-domain Maxwell equations*, in "IEEE. Trans. Magn.", vol. 44, n^{o} 6, 2008, p. 1254–1257.

International Peer-Reviewed Conference/Proceedings

[18] A. CATELLA, V. DOLEAN, L. FEZOUI, S. LANTERI. *Efficient time integration strategies for high-order discontinuous Galerkin time-domain methods*, in "24th International Review of Progress in Applied Computational Electromagnetics (ACES 2008), Niagara Falls, Canada", april 2008.

[19] V. DOLEAN, M. GANDER. *Why classical Schwarz methods applied to hyperbolic systems can converge even without overlap*, in "17th International Conference on Domain Decomposition Methods in Science

and Engineering, St. Wolfgang-Strobl, Austria", Lecture Notes in Computational Science and Engineering (LNCSE), vol. 60, Springer Verlag, 2008, p. 467–475.

[20] H. FAHS, S. LANTERI. *A high-order non-conforming discontinuous Galerkin method for time-domain electromagnetics*, in "13th International Congress on Computational and Applied Mathematics (ICCAM 08), Ghent, Belgium", july 2008.

[21] H. FAHS, S. LANTERI, F. RAPETTI. *Development of a non-conforming discontinuous Gakerkin method on simplex meshes for electromagnetic wave propagation*, in "4th International Conference on Advanced COmputational Methods in ENgineering (ACOMEN'08), Liège, Belgium", may 2008.

Research Reports

[22] H. FAHS, S. LANTERI. *Convergence and stability of a high-order leap-frog based discontinuous Galerkin method for the Maxwell equations on non-conforming meshes*, Technical report, n^{o} RR-6699, INRIA, 2008, http://hal.inria.fr/inria-00332277.

[23] C. KONRAD. *On domain decomposition with space filling curves for the parallel solution of the coupled Maxwell/Vlasov equations*, Technical report, n^{o} RR-6693, INRIA, 2008, http://hal.inria.fr/inria-00331382.

References in notes

[24] B. COCKBURN, G. KARNIADAKIS, C. SHU (editors). *Discontinuous Galerkin methods. Theory, computation and applications*, Lecture Notes in Computational Science and Engineering, vol. 11, Springer-Verlag, 2000.

[25] B. COCKBURN, C. SHU (editors). *Special issue on discontinuous Galerkin methods*, J. Sci. Comput., vol. 22-23, Springer, 2005.

[26] C. DAWSON (editor). *Special issue on discontinuous Galerkin methods*, Comput. Meth. App. Mech. Engng., vol. 195, Elsevier, 2006.

[27] *MAXDGk software*, http://www-sop.inria.fr/caiman/personnel/Stephane.Lanteri/maxdgk/maxdgk.html.

[28] *PhyLeaS associate team*, http://www-sop.inria.fr/nachos/phyleas.

[29] *Visible Human Project*, http://www.nlm.nih.gov/research/visible/visible_human.html.

[30] K. AKI, P. RICHARDS. *Quantitative seismology*, University Science Books, Sausalito, CA, USA, 2002.

[31] P. AMESTOY, I. DUFF, J.-Y. L'EXCELLENT. *Multifrontal parallel distributed symmetric and unsymmetric solvers*, in "Comput. Meth. App. Mech. Engng.", vol. 184, 2000, p. 501–520.

[32] V. DOLEAN, M. GANDER. *The relation between optimized Schwarz methods for scalar and systems of partial differential equations*, in "6th International Congress on Industrial and Applied Mathematics (ICIAM 07), ETH Zurich, Switzerland", 2007.

[33] J. HESTHAVEN, T. WARBURTON. *Nodal discontinuous Galerkin methods: algorithms, analysis and applications*, Springer Texts in Applied Mathematics, Springer Verlag, 2007.

[34] P. HOUSTON, I. PERUGIA, A. SCHNEEBELI, D. SCHOTZAU. *Interior penalty method for the indefinite time-harmonic Maxwell equations*, in "Numer. Math.", vol. 100, 2005, p. 485–518.

[35] J. JACKSON. *Classical Electrodynamics*, Third edition, John Wiley and Sons, INC, 1998.

[36] G. JACOBS, J. HESTHAVEN. *High-order nodal discontinuous Galerkin Particle-in-Cell methods on unstructured grids*, in "J. Comput. Phys.", vol. 121, 2005, p. 96–121.

[37] S. PIPERNO. *Symplectic local time stepping in non-dissipative DGTD methods applied to wave propagation problem*, in "ESAIM: Math. Model. Num. Anal.", vol. 40, n^{o} 5, 2006, p. 815–841.

[38] A. QUARTERONI, A. VALLI. *Domain decomposition methods for partial differential equations*, Numerical Mathematics and Scientific Computation, Oxford University Press, 1999.

[39] B. SMITH, P. BJORSTAD, W. GROPP. *Domain decomposition and parallel multilevel methods for elliptic partial differential equations*, Cambridge University Press, 1996.

[40] A. TOSELLI, O. WIDLUND. *Domain Decomposition Methods. Algorithms and theory*, Springer Series in Computational Mathematics, vol. 34, Springer Verlag, 2004.

[41] J. VIRIEUX. *P-SV wave propagation in heterogeneous media: velocity-stress finite difference method*, in "Geophysics", vol. 51, 1986, p. 889–901.

[42] T. WARBURTON, M. EMBREE. *On the role of the penalty in the local Discontinuous Galerkin method for Maxwell's eigenvalue problem*, in "Comput. Meth. App. Mech. Engng.", vol. 195, 2006, p. 3205–3223.

[43] K. YEE. *Numerical solution of initial boundary value problems involving Maxwell's equations in isotropic media*, in "IEEE Trans. Antennas and Propagation", vol. 14, n^{o} 3, 1966, p. 302–307.