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

2007

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1. Team

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 6621).

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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. We consider in the first place mathematical models that rely on first order linear systems of partial differential equations with variable coefficients and more particularly those pertaining to electrodynamics and elastodynamics with applications to computational electromagnetics and computational geoseismics.

We focus on applications in these domains which 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, our research efforts 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 discretization of systems of partial differential equations (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 [41] 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 [47] in 1996 is the most popular. 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 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 permittivityand 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 swicth 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 [32] 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 [45] 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.

From the point of view of applications, our objective is to demonstrate the capabilities of the proposed numerical methodologies for the study of realistic wave propagation problems in complex domains and heterogeneous media. Three physical situations currently attract our attention which respectively involve the interaction of:

- electromagnetic waves with dispersive media focussing on biological tissues,
- electromagnetic waves with charged particles considering particle-in-cell methods,
- seismic waves with viscoelastic geological media.

3. Scientific Foundations

3.1. High order discontinuous Galerkin methods on simplicial meshes

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

The applications in computational electromagnetics and computational geoseismics that are considered in the NACHOS project-team lead to the numerical simulation of wave propagation in heterogeneous media and often involve complex shape objects or domains including geometrical details or singularities. The underlying wave propagation phenomena can be purely unsteady or they can be periodic (because the imposed source term follows a time harmonic evolution). Although time domain formulations of wave propagation problems correspond to the most general situation, time harmonic problems are interesting for at least two reasons: they lead to more challenging mathematical problems (define on complex valued quantities) and thus motivate the research of powerful numerical methods (especially in the case of highly heterogeneous media) and, their solutions can be used to validate that of equivalent time domain problems. When a time harmonic behavior applies, numerical methods can take into account this fact as soon as the initial phase of their design. The overall objective of NACHOS is to develop unstructured (or hybrid structured/unstructured) mesh based numerical methods for solving time domain and time harmonic electromagnetic and geoseismic PDE models with a particular attention to several distinguishing features that are discussed below.

Accuracy. We consider numerical methods relying on discretization techniques that best fit to the geometrical characteristics of the problems at hand. For this reason, we favor 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. Also, both strategies are all local in nature.

Numerical efficiency. The numerical simulation of unsteady problems most often rely on explicit time integration schemes. Such schemes are subjected to 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 three-dimensional problems, this simply translates into unfeasible computing times. In order to improve this situation, one possible approach consists in applying an implicit time scheme in regions of the computational domain where the underlying mesh is highly refined. The resulting hybrid explicit/implicit time integration strategy raises several challenges both from the mathematical analysis viewpoint (stability and accuracy, especially for what concern numerical dispersion) and from the computer implementation viewpoint (data structures, parallel computing aspects). 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 three-dimensional problems is hardly performed on a high-end workstation and parallel computing is a mandatory path. This is all the more true that we aim at demonstrating the benefits of the numerical methods that we will propose through the simulation of large-scale wave propagation problems leading to the processing of very large volumes of data. The latter results from two combined parameters: the size of the mesh (measured by the total number of 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 [25]- [26]- [27]- [39]. Let us point out here some of these properties:

- easy extension to higher order interpolation. One may increase the degree of the polynomials in the whole mesh as easily as for spectral methods and moreover this can be done very locally,
- no global mass matrix to invert. In fact this is true if advancing in time is done using an explicit scheme. Let us note that the mass matrix is diagonal if an orthogonal basis is chosen,
- easy handling of 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 deal with the hp strategy (i.e the characteristic mesh size h and the interpolation degree p changes locally wherever it is needed),
- large choice of time stepping schemes. One may combine the DG spatial discretization with any global or local explicit time integration scheme or even implicit provided that the resulting scheme will be stable,
- nice parallelization properties. 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 for high order interpolation methods.

For the numerical resolution of the time domain Maxwell equations, we have recently proposed a family of non-dissipative high order DG methods working on unstructured simplicial meshes [5]-[1]. These DG methods combine a central scheme for the numerical flux at the interfaces between neighboring elements with a second order leap-frog time integration scheme. Moreover, the local approximation of the electromagnetic field relies on nodal (Lagrange type) polynomials. Ongoing works in NACHOS are concerned with the extension of these methods towards non-conforming hp-adaptivity, their coupling with hybrid explicit/implicit time integration schemes in order to improve their efficiency in the context of locally refined meshes, and their extension to the numerical resolution of the elastodynamic equations modeling the propagation of seismic waves.

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 resolution of systems of PDEs. As clearly described in [43], 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 [43]- [42]- [44].

Our research activities on this topic aim at the formulation, analysis and concrete evaluation of Schwarz type domain decomposition methods in conjunction with discontinuous Galerkin approximation methods on unstructured simplicial meshes for the calculation of time domain and time harmonic wave propagation problems in heterogeneous media. Ongoing works in this direction are concerned with the design of overlapping and non-overlapping Schwarz algorithms for the solution of the time harmonic Maxwell equations. In these algorithms, a first order absorbing condition is imposed at the interfaces between neighboring subdomains. 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 [20]. Whatsoever is the overlapping strategy, 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 iterative resolution of the interface system can be performed in a more efficient way using a Krylov method. Beside Schwarz algorithms based on natural interface conditions, we also study algorithms that make use of more effective transmission conditions. 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. We 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 [19].

3.3. Hybrid explicit/implicit time integration schemes

Keywords: *grid induce stiffness*, *hybrid explicit/implicit time scheme*, *stability*.

Explicit time integration schemes are subjected to stability conditions that become very restrictive when the underlying mesh is locally refined since the global time step is deduced from the volume of the smallest mesh element. Two main strategies can be considered to improve this situation: local time stepping and implicit time integration. Although the adoption of an implicit time integration scheme will allow to overcome the restrictive constraint on the time step for locally refined meshes, it is still not clear whether the resulting numerical methodology will demonstrate a superiority in terms of accuracy and overall computing cost over the original methodology based on an explicit time integration scheme. On one hand, the dispersion error should be minimized while taking care to the increase in complexity of the time integration technique. On the other hand, the computing cost is also directly impacted by the fact that at each time step, an implicit time integration scheme yields the inversion of a large sparse linear system. For certain linear systems of partial differential equations, the matrix of this system is constant as far as the time step is fixed during the simulation. The linear system solver can certainly exploit this fact but this will probably not translate into a drastic reduction of the cost of a single time step. Taking into account all these issues, a locally implicit time integration scheme could be the best compromise when solving an unsteady wave propagation problem on a locally refined mesh. Such a hybrid explicit/implicit time integration strategy raises several challenges both from the mathematical analysis viewpoint (stability and accuracy, especially for what concern numerical dispersion) and from the computer implementation viewpoint (data structures, parallel computing aspects). Our activities in this domain aim at the design of hybrid explicit/implicit integration schemes in conjunction with high order discontinuous Galerkin methods on locally refined triangular or tetrahedral meshes.

3.4. High performance numerical computing

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

Beside basic research activities related to the topics discussed above, we are also committed to assessing the numerical methods and resolution algorithms that we propose through the numerical simulation of large-scale three-dimensional problems pertaining to computational electromagnetics and computation geoseismics. In practice, accuracy constraints bring the challenge of processing very large data sets corresponding to high resolution discretized geometrical models. In addition, the physical phenomena of interest are in essence unsteady and stability issues impose rather small time steps meaning that numerical simulations require a lot of time iterations. In this context, 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 an hybrid distributed-shared memory systems. Moreover, multiple core systems are increasingly adopted thus introducing an additional level in the local memory hierarchy. Developing numerical algorithms that efficiently exploit such platforms raise several challenges, especially in the context of a massive parallelism. In this context, our activites are concerned with (a) the exploitation of multiple levels of parallelism in domain decomposition algorithms for solving the large algebraic systems resulting from the DG discretization of the systems of PDEs that we consider and, (b) 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. Part of the research efforts of the NACHOS team in this domain actually aim at demonstrating the benefits of our unstructured mesh based electromagnetic solvers in some relevant industrial contexts (see section). However, we also consider in details situations that deal with the propagation of electromagnetic waves in biological tissues. Two main reasons motivate our commitment to study this type of problems:

- first, from the numerical modeling point of view, the interaction between electromagnetic waves and living 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.

The numerical methods that we develop for the solution of the time domain Maxwell equations in heterogeneous media call for their application to the study of the interaction of electromagnetic waves with living tissues. Beside questions related to mathematical and numerical modeling, these applications most often require to deal with very complex structures like the tissues of the head of a cellular phone user. For a realistic computer simulation of such problems, it is most often necessary to build discretized geometrical models starting from medical images. In the context of the HeadExp [30] cooperative research action (from January 2003 to December 2004), we have set up a collaboration with computer scientists that are experts in medical image processing and geometrical modeling in order to build unstructured, locally refined, tetrahedral meshes of the head tissues. Using these meshes, we consider the adaptation of our finite volume and discontinuous Galerkin methods for their application to the numerical dosimetry, that is the evaluation of the specific absorption rate (SAR), of an electromagnetic wave emitted by a mobile phone (see Fig. 1).

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.

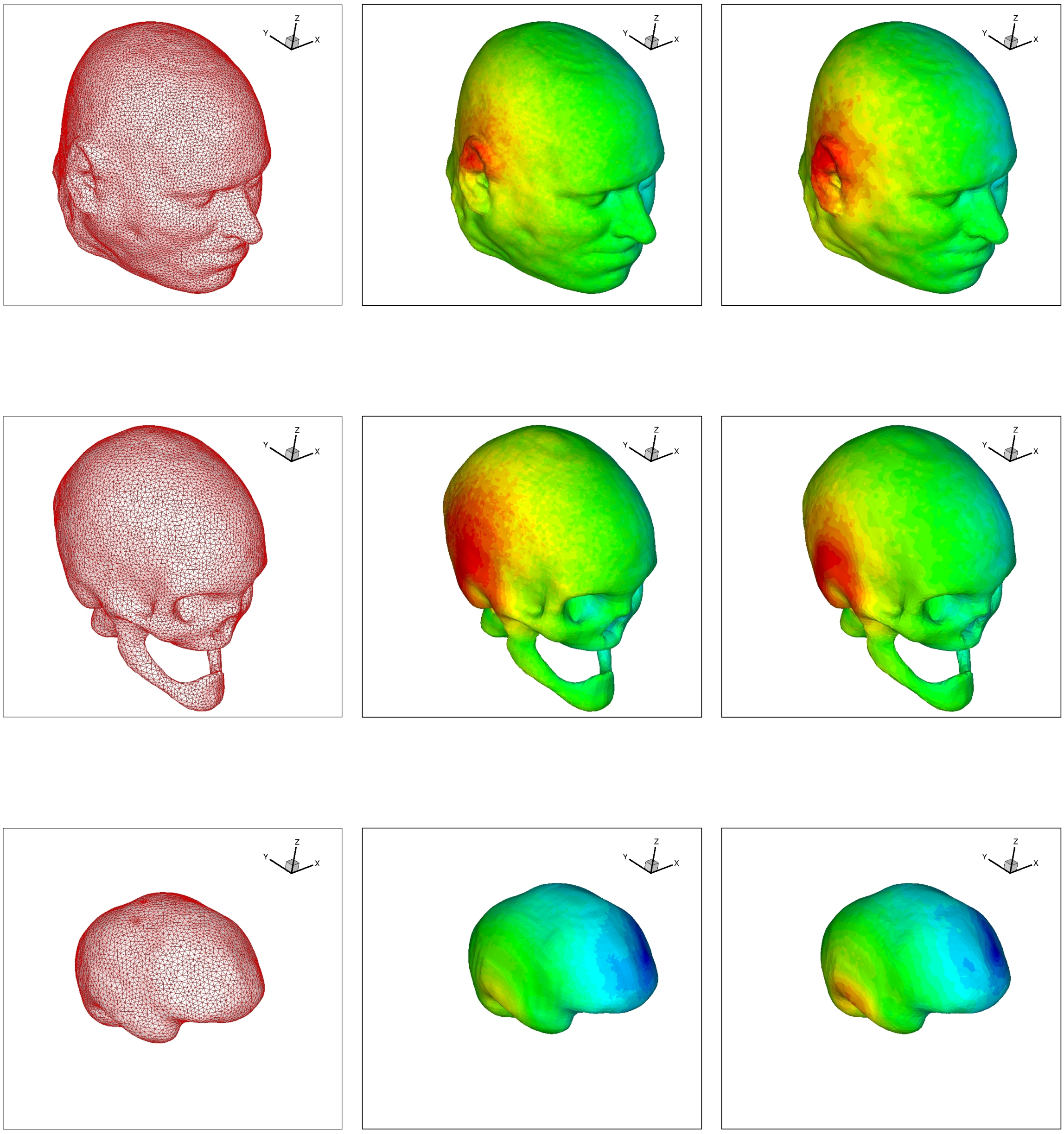

Figure 1. Exposition of head tissues to mobile phone radiation

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 [45] 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 [47] 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 is a centered finite volume software on unstructured triangular meshes [10] which has been validated and evaluated on various problems, ranging from academic test cases to realistic situations such as the one illustrated on Fig 2, showing the propagation of a non-planar fault in an heterogeneous medium.

5. Software

5.1. MAXDGk

Keywords: *Maxwell equations*, *discontinuous Galerkin*, *electromagnetic waves*, *finite volume*, *heterogeneous medium*, *parallel computing*, *time domain*.

Participants: Loula Fezoui, Stéphane Lanteri [correspondant].

The team develops the MAXDGk [31] software for the numerical resolution of the three-dimensional Maxwell equations in the time domain, for heterogeneous media. The software implements a high order discontinuous Galerkin method on unstructured tetrahedral meshes based on nodal polynomial interpolation (DGTD-Pk) [5]. This software and the underlying algorithms are adapted to distributed memory parallel computing platforms [1].

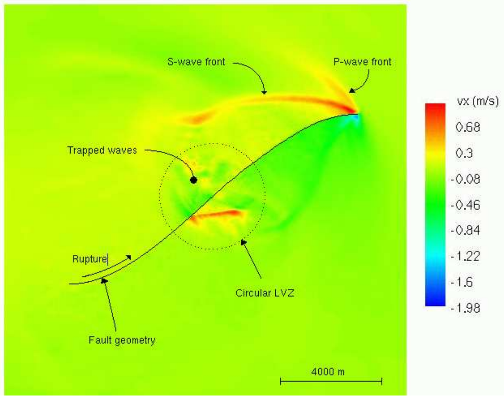

Figure 2. Propagation of a non-planar fault in an heterogeneous medium

5.2. MAXDGHk

Keywords: *Maxwell equations*, *discontinuous Galerkin*, *electromagnetic waves*, *finite volume*, *frequency domain*, *heterogeneous medium*, *parallel computing*.

Participants: Victorita Dolean, Stéphane Lanteri [correspondant].

The team develops the MAXDGHk software for the numerical resolution of the three-dimensional Maxwell equations in the frequency domain, for heterogeneous media. The software currently implements low order discontinuous Galerkin methods (finite volume method and discontinuous Galerkin method based on linear interpolation) on unstructured tetrahedral meshes. This software and 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 formulations is obtained with an overlapping Schwarz domain decomposition method [13].

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 [31] software for the numerical resolution of the three-dimensional velocity-stress equations in the time domain. The software implements a high order discontinuous Galerkin method on unstructured tetrahedral meshes based on nodal polynomial interpolation (DGTD-Pk).

6. New Results

6.1. Electromagnetic wave propagation

6.1.1. High order DGTD methods on simplicial meshes

Keywords: *Maxwell equations*, *discontinuous Galerkin*, *finite volume*, *non-dissipative*, *tetrahedral mesh*, *time domain*, *triangular mesh*, *unstructured mesh*.

Participants: Loula Fezoui, Medhi Fhima, Stéphane Lanteri.

We have recently proposed in [5] a high order non-dissipative discontinuous Galerkin method for the numerical solution of the time domain Maxwell equations on unstructured meshes (DGTD-Pk method). The method relies on the choice of a local basis of polynomial functions, a centered approximation for the surface integrals (i.e numerical fluxes at the interface between neighboring elements) and a second order leap-frog scheme for advancing in time. The method is proved to be stable for a large class of basis functions and a discrete analog of the electromagnetic energy is also conserved. A proof for the convergence has been established for arbitrary orders of accuracy on tetrahedral meshes, as well as a weak divergence preservation property [5]. This year, we have developed and experimented discontinuous Galerkin methods of arbitrary interpolation orders based on nodal polynomial basis functions. Nevertheless, for a polynomial degree $k \geq 2$, the accuracy of the resulting DGTD method is limited by the second order accuracy of the adopted leap-frog scheme. Thus a short term objective is to devise ways of increasing the accuracy of the time integration scheme while still preserving the non-dissipative nature of the overall DGTD method.

6.1.2. DGTD methods on locally refined structured meshes

Keywords: *Maxwell equations*, *UPML model*, *discontinuous Galerkin*, *fictitious domain*, *finite volume*, *locally refined mesh*, *non-conforming mesh*, *structured mesh*, *time domain*.

Participants: Antoine Bouquet, Serge Piperno [Cermics, ENPC], Claude Dedeban [France Télécom R&D, La Turbie].

Electromagnetic wave propagation problems often involve objects of very different scales. In collaboration with France Télécom R&D, we have studied discontinuous Galerkin time domain (DGTD) methods for the numerical simulation of the three-dimensional Maxwell equations on block-structured, non-conforming, locally refined grids. Starting from the work of Nicolas Canouet in his PhD thesis [3], we have compared in this context the uses of full P1 elements and P1_{div} elements. In his PhD thesis (defence planned for end 2007), Antoine Bouquet has also developed a DGTD version of the quite classical UPML approach (which is closer to the original Maxwell equations than standard PML models, and allows simulation with infinite conductors with extensions inside the PML regions). Finally, a DGTD method has been coupled with a fictitious domain approach initially developed for the FDTD of K.S. Yee [47]. Results are satisfactory (comparable to FDTD) and allow the use of complex geometric details inside small loaclly refined zones. However, the method seems to reach a limit in accuracy, probably linked to the incomplete treatment of the boundary condition inside elements meeting the metallic boundary (it is not a problem in FDTD, equivalent to a *conformal* FETD method, which DGTD is not).

6.1.3. DGTD methods on non-conforming simplicial meshes

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

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

The numerical resolution of the time domain Maxwell equations most often relies on finite difference methods on structured meshes which find their roots in the original work of K.S. Yee [47]. However, in the recent years, there has been an increasing interest in discontinuous Galerkin time domain methods designed on unstructured meshes [38]-[5] since the latter are particularly well suited to the discretization of geometrical details that characterize applications of practical relevance. 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. Whereas high order discontinous Galerkin time domain methods have been developed rather readily, the development of non-conforming discontinuous Galerkin methods has been less impressive. The non-conformity can result from a local refinement of the mesh, of the interpolation order or of both of them. In the context of the PhD thesis of Hassan Fahs, we study non-dissipative discontinuous Galerkin methods for solving the two-dimensional time domain Maxwell equations on non-conforming, locally refined, triangular meshes. Similarly to the method described in [5], the DGTD-Pk method that we consider 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. The stability of the resulting method is studied using an energetic approach [4]. This year concentrated our efforts on a detailed evaluation of the numerical convergence properties of a hp-like (i.e non-conforming in h and p) DGTD-Pk method [24]-[23].

6.1.4. Implicit DGTD methods for the Maxwell equations

Keywords: *Maxwell equations*, *discontinuous Galerkin*, *finite volume*, *implicit time integration*, *locally refined mesh*, *non-dissipative*, *tetrahedral mesh*, *time domain*, *triangular mesh*, *unconditional stability*, *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 or unstructured simplicial meshes. An implicit time integration scheme is a natural way to obtain a time domain method which is unconditionally stable. We are studying the applicability of implicit time integration schemes in conjunction with discontinuous Galerkin methods for the solution of the time domain Maxwell equations. The starting-point of this study is the explicit, non-dissipative, DGTD-Pk method introduced in [5]. We 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 uncnonditionally stable, non-dissipative, implicit DGTD-Pk method. So far, the method has been implemented and evaluated in 2D on triangular meshes [11]-[22]. The implementation in 3D is a work in progress. Our ultimate goal is to design an hybrid time integration strategy, coupling an implicit scheme applied locally in regions where the mesh is highly refined, with an explicit scheme elsewhere. In this context, we also investigate the use of higher order time integration schemes.

6.1.5. High order DGTD particle-in-cell method on simplicial meshes

Keywords: *Maxwell equations*, *discontinuous Galerkin*, *particle-in-cell*, *tetrahedral mesh*, *time domain*.

Participants: Loula Fezoui, Christian Konrad, Stéphane Lanteri.

We have started this year a study aiming at the development of a coupled high order discontinuous Galerkin/Particle-In-Cell (PIC) parallel solver. This work, which is taking place in the framework of the ANR HOUPIC project (starting date: january 2007 - duration: 3 years), entails several aspects ranging from numerical analysis questions (charge conservation property, methods of assignment of current and charge densities to physical space, methods of interpolation of electric and magnetic fields to phase space) to algorithimc concerns (parallel particle localization algorithm in a tetrahedral mesh, parallelization and load balancing strategies).

6.1.6. DG methods for the frequency domain Maxwell equations

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

Participants: Victorita Dolean, 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 resolution 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 [40]. Moreover, such formulations are necessary to prevent the apparition of spurious modes when solving the Maxwell eigenvalue problem [46]. We consider discontinuous Galerkin frequency domain (DGFD) methods relying on centered or upwind fluxes for solving the first order form of the time harmonic Maxwell equations [12]. Moreover, DGFD methods lead to the inversion of a sparse (complex) linear system whose matrix operator may exhibit scale discrepancies in the coefficients due on one hand, to the non uniformity of the mesh and, on the other hand, to the heterogeneity of the underlying medium. Appropriate solution strategies have to be designed for such linear systems and this lead lead us to investigate hybrid/iterative strategies based on domain decomposition principles [18].

6.2. Seismic wave propagation

6.2.1. Wave propagation and dynamic fault modeling in the context of a finite volume method

Keywords: *P-SV wave propagation*, *centered scheme*, *dynamic fault modeling*, *finite volume*, *linear elastodynamic equations*, *time domain*, *velocity-stress equations*.

Participants: Mondher Benjemaa, Victor Manuel Cruz-Atienza [Department of Geological Sciences, San Diego State University], Nathalie Glinsky-Olivier, Stéphane Lanteri, Serge Piperno [Cermics, ENPC], Jean Virieux [Joseph Fourier University and LGIT laboratory].

We are interested in the numerical simulation of seismic activity, including wave propagation and dynamic fault modeling. We concentrated our efforts this year on the extension of the previously proposed non-dissipative finite volume method for the numerical resolution of the first order hyperbolic linear system of elastodynamic equations in two space dimensions [10], to the three dimensional case based on tetrahedral meshes. Moreover, the resulting numerical methodology has been adapted to distributed memory parallel computing platforms using a classical SPMD strategy combining a partitioning of the computational problem with a message passing programming model. Preliminary numerical experiments have been conducted for planar and non-planar faults including comparisons with a state of the art finite difference method.

We are interested in the numerical simulation of seismic activity, including wave propagation and dynamic fault modeling. We concentrated our efforts this year on the extension of the previously proposed non-dissipative finite volume method for the numerical resolution of the first order hyperbolic linear system of elastodynamic equations in two space dimensions[10], to the three dimensional case based on tetrahedral meshes. Moreover, the resulting numerical methodology has been adapted to distributed memory parallel computing platforms using a classical SPMD strategy combining a partitioning of the computational problem with a message passing programming model. In the framework of the ANR project QSHA, several three-dimensional test-cases are studied to compare the results of the wave propagation due to various seismic point sources by different numerical methods (boundary element method, finite difference method, spectral element method, discrete element method and finite volume method). Concerning the dynamic rupture, numerical experiments have been conducted for planar and non planar faults. The first test case is the dynamic rupture of a planar fault proposed by the SCEC[1] Community for the second SCEC spontaneous rupture code validation workshop in 2004 [37]. Solutions have been compared to those provided by a finite-difference technique [36]. Another benchmark problem is concerned with a non-planar parabolic-shaped rupture problem [35]. Solutions for this difficult exercise are compared with those computed with a boundary integral equation (BIE) method [34]. These results are the first ever obtained for the study of the dynamic fault rupture by a finite-volume method.

6.2.2. High order DGTD methods on simplicial meshes

Keywords: *P-SV wave propagation*, *centered scheme*, *discontinuous Galerkin*, *finite volume*, *locally refined mesh*, *non-dissipative*, *tetrahedral mesh*, *time domain*, *triangular mesh*, *unstructured mesh*, *velocity-stress equations*.

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

We have initiated this year the development of high order non-dissipative discontinuous Galerkin methods on simplicial meshes (triangles in the 2D case and tetrahedra in the 3D case) for the numerical resolution of the first order hyperbolic linear system of elastodynamic equations. These methods share some ingredients of the DG TD-Pk methods previously developed 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-Pk 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. In 2D, 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. More realistic 2D and 3D test cases are now tackled.

[1] South California Earthquake Center

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, 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 three-dimensional 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 [33]. 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 the 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 [20]-[19].

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) [13]. Preliminary investigations of optimized Schwarz algorithms combined to high order discontinuous Galerkin time harmonic methods on triangular meshes for the discretization of the two-dimensional Maxwell equations are reported in [14]. The extension to the three-dimensional case is a work in progress.

6.3.2. Algebraic preconditioning of interface formulations of Schwarz algorithms

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

Participants: Luc Giraud [Parallel Algorithms and Optimization Group, ENSEEIHT-IRIT, Toulouse], Azzam Haidar [Parallel Algorithms, CERFACS, Toulouse], Stéphane Lanteri.

We have initiated this year a collaboration with Luc Giraud from ENSEEIHT-IRIT and one of his PhD students, Azzam Haidar from CERFACS. This works addresses the study of algebraic preconditioning techniques for the interface systems characterizing the Schwarz algorithms. These approaches are based on natural interface conditions for the numerical solution of the three-dimensional. The focus is on the first order system of time harmonic Maxwell equations discretized by discontinuous Galerkin methods on simplicial meshes. Once the internal variables are eliminited using a sparse direct solver (MUMPS in our case), the resulting linear system on the interface $T\lambda = d$ is sparse by blocks with identity blocks on the diagonal. The matrix T naturally writes $T = L + I + U$ where L (U) denotes the strictly lower (respectively strictly upper) triangular part. Consequently $(L + I)^{-1} = I - L$ and $(U + I)^{-1} = I - U$, so that a natural parallel preconditioner, which is easy and cheap to construct, is $(L + I)^{-1} + (U + I)^{-1}$. This preconditioner can be interpreted as an additive variant of a symmetric relaxation preconditioner. It is easy and cheap to construct because it relies on sub-matrices computed to perform the matrix-vector product and its application as a preconditioner in a Krylov suspace method comes at a cost identical to the cost of a matrix-vector product. Some variants based on this kernel can also be derived and will be studied as well. We also plan to study some approaches that attempt to reduce the cost of the preconditioner in the iterative loop.

7. Contracts and Grants with Industry

7.1. Expertise in the parallelization of structured mesh solvers

Participants: Antoine Bouquet, Claude Dedeban [France Télécom R&D, La Turbie], Serge Piperno [Cermics, ENPC], Stéphane Lanteri.

In the framework of this collaboration, we advise France Télécom R&D (center of La Turbie) in the parallelization of structured mesh time domain solvers on distributed memory computing platforms.

7.2. High order DGTD methods for a coupled Vlasov/Maxwell software

Participants: Adrien Catella, 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 based on the high order DGTD-Pk methods on tetrahedral meshes developed in the team. The resulting coupled Vlasov/Maxwell 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.

7.3. DG methods for the time harmonic Maxwell equations

Participants: Claude Dedeban [France Télécom R&D, La Turbie], Stéphane Lanteri, Serge Piperno [Cermics, ENPC].

France Télécom R&D (center of La Turbie) is developing its own software (SR3D) for the solution of the time harmonic Maxwell equations using a Boundary Element Method (BEM). FT R&D is interested in coupling SR3D with a finite element software able to deal with multi-material media. This grant is a first step in this direction as we study the development of finite volume and linear discontinuous Galerkin methods on unstructured tetrahedral meshes for the solution of the frequency domain Maxwell equations.

7.4. 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-Pk 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: Mondher Benjemaa, Nathalie Glinsky-Olivier, Stéphane Lanteri, Serge Piperno [Cermics, ENPC], Jean Virieux [Joseph Fourier University and LGIT laboratory].

This project has been selected 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: Guillaume Alléon [EADS France Campus Engineering, 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], Fabrice Huet [OASIS 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], Thierry Priol [PARIS project-team, IRISA Rennes], Frédéric Wagner [ID-IMAG, MOAIS team, Grenoble].

The project-team is coordinating the DiscoGrid [28] (Distributed objects and components for high performance scientific computing on the Grid'5000 test-bed) project which has been selected by ANR following the 2005 call for projects of the new program *Calcul Intensif et Grilles de Calcul* (this project has started in January 2006 for a duration of 3 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. The ultimate goal of the DiscoGrid project are to design parallel numerical algorithms and develop simulation software that efficiently exploit a computational grid and more particularly, the Grid'5000 test-bed [29]. In particular, the DiscoGrid project will study the applicability of modern distributed programming principles and methodologies for the development of high performance parallel simulation software.

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].

Particle-In-Cell (PIC) codes have become an essential tool for the numerical simulation of many physical phenomena involving charged particles, in particular beam physics, space and laboratory plasmas including fusion plasmas. Genuinely kinetic phenomena can be modeled by the Vlasov-Maxwell equations which are discretized by a PIC method coupled to a Maxwell field solver. Today's and future massively parallel supercomputers allow to envision the simulation of realistic problems involving complex geometries and multiple scales. However, in order to achieve this efficiently new numerical methods need to be investigated. This includes the investigation of high order very accurate 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. To this aim this project proposes to develop and compare Finite Element Time Domain (FETD) solvers based on the one hand on high order Hcurl conforming elements and on the other hand on high order Discontinuous Galerkin (DG) finite elements and investigate their coupling to the particles.

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

Collaboration with Victor Manuel Cruz-Atienza (Department of Geological Sciences at San Diego State University) on the development of finite volume methods for the numerical modeling of earthquake dynamics and wave propagation in the three-dimensional case.

Collaboration with Martin Gander (Mathematics Section, 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.

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Major publications by the team in recent years

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Year Publications

Doctoral dissertations and Habilitation theses

[8] M. BENJEMAA. *Etude et simulation numérique de la rupture dynamique des séismes par des méthodes d'éléments finis discontinus*, Thèse de Mathématiques, Université de Nice-Sophia Antipolis, Décembre 2007.

[9] A. BOUQUET. *Caractérisation de structures rayonnantes par une méthode Galerkin discontinue associée à une technique de domaines fictifs*, Thèse de Mathématiques, Université de Nice-Sophia Antipolis, Décembre 2007.

Articles in refereed journals and book chapters

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