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1. Team

Caiman is a joint team with the "École Nationale des Ponts et Chaussées" (French national civil engineering school) through the CERMICS *("Centre d'Enseignement et de Recherche en Mathématiques et Calcul Scientifique", Teaching and Research Center on Mathematics and Scientific Computing), the CNRS (French National Center of Scientific Research) and the Nice-Sophia Antipolis University (NSAU), through the Dieudonné Laboratory (UMR 6621).*

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2. Overall Objectives

2.1. Overall Objectives

The project-team aims at proposing innovative numerical methods for the computer simulation of wave propagation problems in heterogeneous media. Scientific activities are concerned with the formulation and mathematical analysis of numerical methods for the underlying systems of partial differential equations (PDEs), as well as their implementation on modern high performance computing platforms, and their application to realistic configurations.

In the time domain, we construct numerical methods based on finite volumes or discontinuous finite elements on unstructured or locally refined meshes. We investigate several topics dealing with the accuracy, efficiency and flexibility of the proposed methods and in particular, high order interpolation methods on simplicial meshes in connection with discontinuous finite element formulations, discretization methods on non-conforming meshes, locally implicit time integration schemes and domain decompositition algorithms. To a lesser extent, we investigate several aspects related to the numerical solution of frequency domain problems. Current application domains of the proposed numerical methodologies pertain to computational electromagnetics and computational geophysics.

3. Scientific Foundations

3.1. First-order linear systems of PDEs and discontinuous finite element methods

Finite volume methods numerical methods based on a partition of the computational domain into control volumes, where an approximate for the average value of the solution is computed. These methods are very well suited for conservation laws, especially when the problem solution has very low regularity. These methods find natural extensions in discontinuous finite elements approaches.

Discontinuous finite element methods numerical methods based on a partition of the computational domain into finite elements, where the basis functions used are local to finite elements (absolutely no continuity between elements is required through element interfaces). These methods are also well suited for conservation laws. In general, they are more expensive than classical finite elements, but lead to very simple algorithms for the coupling of different element types or for the use of locally refined, possibly non-conforming grids.

The systems of PDEs that are at the heart of the team activities can be rewritten as hyperbolic systems of conservation laws or balance equations. The Euler equations of gaz dynamics form a non-linear strictly hyperbolic system of conservation laws. The non-linearity leads to irregular (weak) solutions, even if the initial flow is smooth. Then the use of very low order finite elements was proposed and finite volumes were introduced to match the conservative nature of the initial physical system: the computational domain is partitioned in control volumes and the numerical unknowns are defined as the mean values of the fields inside the control volumes (this is different from finite difference methods, where unknowns are approximates to point-wise values, and from finite element methods where unknowns are coordinates relatively to a functional basis of solutions). The hyperbolic systems of PDEs that are currently considered in the team are the Maxwell equations modeling the propagation of electromagnetic waves and the elastodynamic equations modeling the propagation of acoustic waves in elastic materials.

Finite volume methods can easily deal with complex geometries and irregular solutions [40]. They can simply lead to conservative methods (where for example no fluid mass is lost). They are based on numerical flux functions, yielding an accurate approximation of the variable flux through control volume interfaces (these interfaces separate two distinct average fields on the two control volumes). The construction of these numerical flux functions is itself based on approximate Riemann solvers [41] and interpolation and slope limitation can yield higher accuracy (outside discontinuity zones) [44].

These methods can be used in many application fields: complex fluid dynamics (with several species or phases), wave propagation in the time domain in heterogeneous media (acoustics, electromagnetics, etc.). For wave propagation problems, finite volume methods based on local Riemann solvers induce a numerical diffusion which pollutes the simulation results (the artificial dissipation is necessary for flow problems, in order to build a viscous approximation of the problem, i.e. in order to obtain some monotonicity properties, ensuring that variables like density and pressure always remain positive).

We have recently proposed a simple and very efficient finite volume method [7] for the numerical simulation of wave propagation in heterogeneous media, which can be used on arbitrary unstructured meshes and compares well with commonly used finite difference methods such as the finite difference method due to Yee [51], in terms of numerical properties and computational efficiency. This method has been extended to higher orders of accuracy in the framework of non-dissipative discontinuous Galerkin time domain (DGTD) formulations [4].

3.2. Domain decomposition methods

Keywords: *Schur complement*, *Schwarz method*, *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 [46], 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 [46]- [45]- [48]. Related activities of the team are concerned with the design of Schwarz type domain decomposition methods in conjunction with discontinuous Galerkin discretization formulations on unstructured meshes for the resolution of time domain and time harmonic Maxwell equations. A first contribution for the latter equations is described in [24] and in more details in the PhD thesis of Hugo Fol [8].

3.3. High performance parallel and distributed computing

Keywords: *distributed computing*, *domain partitioning*, *grid computing*, *message passing*, *parallel computing*.

The design of algorithms together with the development of software adapted to modern high performance computing platforms is recognized as a mandatory path for the numerical simulation of realistic three-dimensional physical problems in all fields of computational science. The team has a long experience in the development of parallel finite element solvers using a classical SPMD (Single Program Multiple Data) strategy that combines a partitioning of the computational domain and a message passing programming model based on MPI (Message Passing Interface) [5]-[3] in the context of fluid dynamics applications. A similar strategy has recently been applied to unstructured tetrahedral mesh finite volume and discontinuous Galerkin solvers for the time domain Maxwell equations [9]. These solvers assume that the underlying platform consists of a tightly coupled and homogeneous set of processing nodes. However, two major evolutions concerning computing platforms have taken place in the recent years:

- at the scale of a LAN (Local Area Network), the computing platform is a cluster of multiprocessors systems which can be viewed as an hybrid distributed-shared memory system. Moreover, multiple core systems are progressively adopted thus introducing an additional level in the local memory hierarchy.
- at the scale of a WAN (Wide Area Network), the Grid concept has recently appeared and is currently the subject of numerous studies worldwide both at the system and application levels. A Grid is by definition a geographically distributed computing platform gathering an heterogeneous set of resources (supercomputer systems, clusters of PCs, storage systems, visualization systems, etc.).

It is clear that the standard SPMD strategy that has been adopted so far does not yield a software that efficiently exploit the modern computing platforms outlined above. Such a platform can be viewed as a three level architecture:

- (a) the highest level consists of a small number (< 10) of clusters with between a few hundreds to one thousand nodes. These clusters are interconnected by a wide area network (WAN).
- (b) the intermediate level is materialized by the LAN connecting the nodes of a given cluster. This level is characterized by the fact the LAN may differ from one cluster to the other (Gigabit Ethernet, Myrinet, Infiniband, etc.).
- (c) the lower level is used to characterize the architecture of a node: single versus multiprocessor systems, single versus multiple-core systems and memory structure.

Beside the design of numerical algorithms that take into account this hierarchical structure, the team is collaborating with computer scientists in order to take benefit from the recent advances in distributed computing methodologies [1].

4. Application Domains

4.1. Computational electromagnetics for engineering design

Keywords: *electromagnetic compatibility*, *electromagnetic waves*, *furtivity*, *telecommunications*, *transportation systems*, *vulnerability of weapon systems*.

We develop numerical methods and algorithms for the computer solution of time and frequency domain electromagnetic wave propagation equation. These methods can be applied to many different physical settings and several very rich application domains, like telecommunications, transportation engineering and weapon systems engineering (optimum design of antennas, electromagnetic compatibility, furtivity, modelling of new absorbing media).

In the time domain, we aim at proposing accurate and efficient methods for complex geometries and heterogeneous materials (possibly with small elements like point sources, lines, etc.). We first adapted existing finite volume methods, initially designed for the solution of compressible fluid dynamics problems on unstructured grids. Their upwind nature [6] lead to numerical dissipation of the electromagnetic energy. We then proceeded with dissipation-free finite volume methods based on centered fluxes [7]. For the Maxwell system, they compared well with commonly used finite difference methods in terms of accuracy and efficiency on regular meshes, but with spurious propagation modes on highly distorted meshes for example. Moreover, these methods can be coupled with Yee's finite difference method [51], in order to use different numerical methods in the context where they are the most efficient. Finally, we are now developing methods based on the discontinuous Galerkin setting, which can be seen as high order extensions of finite volume methods [33]. These methods can easily and accurately deal with highly heterogeneous materials [4], highly distorted meshes and non-conforming meshes as well. These methods are the robust and necessary bricks towards one of the goals we are aiming at: the construction of a complete chain of numerical methods, allowing the use of unstructured meshes and heterogeneous materials, based on space schemes designed on a conforming or non-conforming discretization of the computational domain combined to hybrid explicit/implicit time integration schemes.

We are also considering adapting discontinuous Galerkin methods for the treatment of frequency domain problems. Here, our goal is to design accurate and efficient finite element methods for heterogeneous materials that could be further coupled to a boundary element method.

4.2. Bioelectromagnetics

Keywords: *bioheat*, *electromagnetic waves*, *geometrical modeling*, *health*, *mobile phone radiation*, *numerical dosimetry*.

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. Typical applications are concerned with the evaluation of biological effects of electromagnetic waves and their use for medical applications. Beside questions related to mathematical and numerical modelling, 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 [36] 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 modelling 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).

4.3. 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.

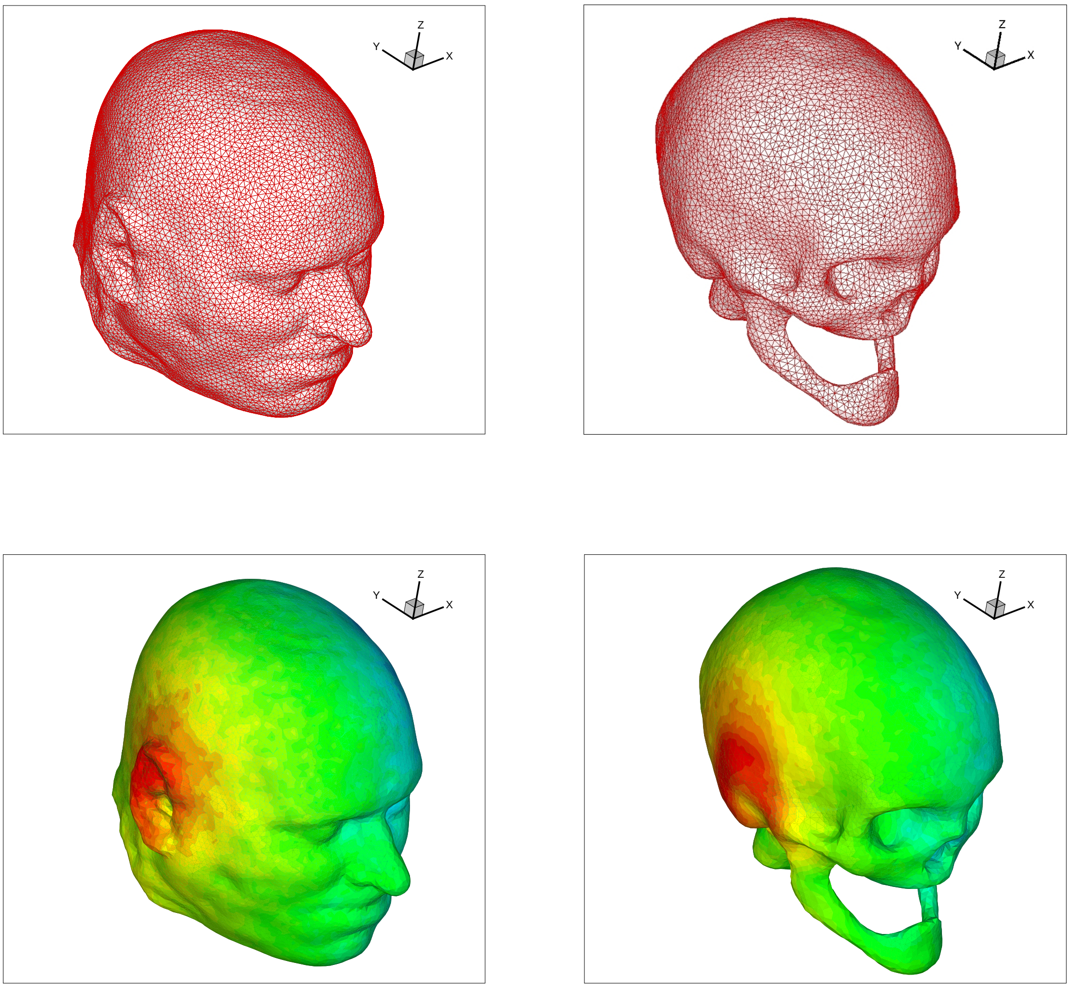

Figure 1.

Triangulated surfaces for meshes of the skin and the skull (top figures)
Local SAR over maximum local SAR in log scale (bottom figures)

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 [49] and based on the first order velocity-stress hyperbolic system of elastic waves equations, which is an extension of the scheme derived by Yee [51] 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 [17]-[27] 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.

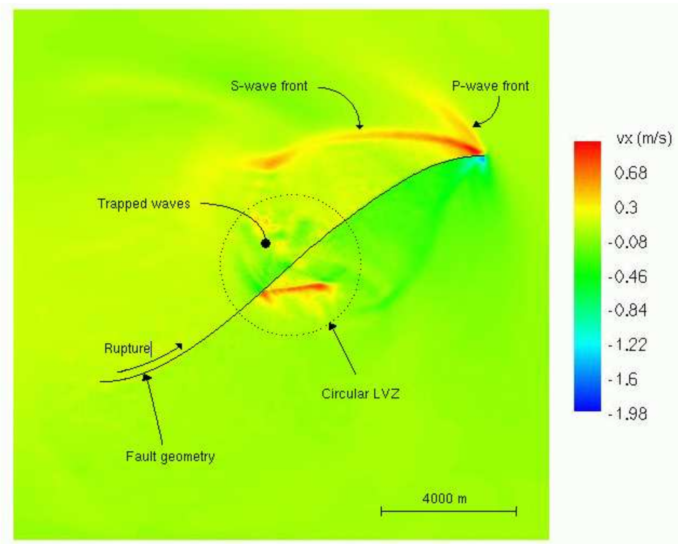

Figure 2.

Propagation of a non-planar fault in an heterogeneous medium
Rupture is 14.3 Km long with a 1 Km long nucleation zone
Contour lines of v_x (4 sec after rupture initiation)

5. Software

5.1. MAXDGk

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

Participants: Loula Fezoui, Stéphane Lanteri [correspondant].

The team develops the MAXDGk [37] 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 (DG-Pk) [4]. This software and the underlying algorithms are adapted to distributed memory parallel computing platforms [9].

5.2. MAXDGHk

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

Participants: Victorita Dolean, Hugo Fol, 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 [30]. 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 [24].

5.3. ELASTODGk

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

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

The team has initiated in 2006 the development of the ELASTODGk [37] 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 (DG-Pk).

6. New Results

6.1. Electromagnetic wave propagation

6.1.1. *High order DGTD methods on simplicial meshes*

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

Participants: Loula Fezoui, Stéphane Lanteri, Serge Piperno.

Electromagnetic wave propagation problems often involve irregularly shaped objects. Therefore, the use of locally refined simplicial meshes (triangles in the 2D case and tetrahedra in the 3D case) is mandatory for many applications. We have proposed in [4] a high order non-dissipative discontinuous Galerkin method for the numerical solution of the time domain Maxwell equations over 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 [4]. We are now considering possible implementations of discontinuous Galerkin methods on tetrahedra for arbitrary interpolation orders. We are currently investigating the use of nodal polynomial basis functions prior to consider in a near future hierarchical interpolation bases.

6.1.2. DGTD methods on locally refined structured meshes

Keywords: *Maxwell system*, *discontinuous Galerkin*, *finite volume*, *locally refined mesh*, *non-conforming mesh*, *non-dissipative*, *structured mesh*, *time domain*.

Participants: Antoine Bouquet, Serge Piperno, 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 methods for the numerical simulation of the three-dimensional Maxwell equations on locally refined, possibly non-conforming structured meshes. The DGTD method developed on block-cartesian grids [2] (divergence-free basis functions with varying accuracy, second-order leap-frog scheme, centered fluxes) has been re-implemented in a cartesian grid setting in the context of PhD thesis subject of Antoine Bouquet (fully funded by France Télécom R&D). We consider returning to full P1 elements rather than only the P1_{div} elements and we are also investigating the possibility to couple DGTD methods with the fictitious domain approach.

6.1.3. DGTD methods on non-conforming simplicial meshes

Keywords: *Maxwell system*, *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 Yee [51]. However, in the recent years, there has been an increasing interest in discontinuous Galerkin time domain methods designed on unstructured meshes [42]-[4] 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 design of non-conforming discontinuous Galerkin methods is still in its infancy. The non-conformity can result from a local refinement of the mesh, of the interpolation order or of both of them. We have initiated in 2006 a study concerning the design of 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 [4], the DGTD-Pk methods that we consider in this study are 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 methods is studied using an energetic approach similarly to what has been done in [4]. However, the novelty here stems from the fact that we extend this analysis to the case of non-conforming meshes. Then, we prove that the non-conforming DGTD-Pk methods conserve a certain form of discrete energy under a CFL-like condition. Furthermore, we obtain explicit expressions of the maximum allowable time step that include geometrical parameters related to the non-conformity of the underlying mesh [31].

6.1.4. Implicit DGTD methods for the Maxwell equations

Keywords: *Maxwell system*, *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 investigating 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 [4]. We currently consider the 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. A preliminary implementation of this method has been realized in 2D on triangular meshes. Our ultimate goal is to design hybrid time integration strategies, coupling an implicit scheme applied locally in regions where the mesh is highly refined, with an explicit scheme elsewhere.

6.1.5. DGTD methods for acoustics using symplectic local time-stepping

Keywords: *discontinuous Galerkin*, *linear waves propagation problems*, *local time-stepping*, *stability*, *symplectic scheme*, *time domain*, *unstructured mesh*.

Participant: Serge Piperno.

The discontinuous Galerkin time domain (DGTD) methods are now popular for the solution of wave propagation problems. Able to deal with unstructured, possibly locally-refined meshes, they handle easily complex geometries and remain fully explicit with easy parallelization and extension to high orders of accuracy. Non-dissipative versions exist, where some discrete electromagnetic energy is exactly conserved. However, the stability limit of the methods, related to the smallest elements in the mesh, calls for the construction of local time-stepping algorithms. These schemes have already been developed for example for N-body mechanical problems and are known as symplectic schemes. Totally explicit algorithms have been applied here to DGTD methods on two-dimensional acoustic problems, as well as locally implicit time-schemes [15]. Although the proposed algorithm perform very well on real-life two-dimensional unstructured meshes (like those produced by an automatic mesh generator around objects with small details), some instabilities may (rarely) appear. More, numerical tests show disappointing instabilities on one-dimensional settings where the mesh size has discontinuities. A theoretical study is under way, which aims at giving a sufficient stability condition on the time step involving the mesh size distribution. The question is the following: will the stability limit on the time-step get more severe as the symplectic scheme uses more different time steps (and then the CPU time gain would be destroyed)? There are hopes to lose efficiency only by a global factor of $\sqrt{2}$.

6.1.6. DGTD methods for dispersive materials

Keywords: *Debye model*, *Maxwell system*, *auxiliary differential equation*, *discontinuous Galerkin*, *finite volume*, *non-dissipative*, *time domain*, *triangular mesh*.

Participants: Papa Ibou Diouf, Loula Fezoui, Stéphane Lanteri.

A medium is called dispersive if the speed of the wave that propagates in this medium depends on the frequency. There exists different physical models of dispersion whose characteristics mainly depend on the considered medium. Two main strategies can be considered for the numerical treatment of a model characterizing a dispersive material: the recursive convolution method and the auxiliary differential equation method [47]. In this study, a numerical methodology combining a high order discontinuous Galerkin method on triangular meshes with an auxiliary differential equation modeling the time evolution of the electric polarization for a dispersive medium of Debye type, has been developed for the resolution of the two-dimensional time domain Maxwell equations. Preliminary results have been obtained that are in agreement with the expected physical behaviour of such a material. The next steps are to realize a detailed validation of the proposed methodology and to conduct a theoretical analysis of its stability.

6.1.7. 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, Hugo Fol, Stéphane Lanteri, Ronan Perrussel, Serge Piperno.

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. 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 [4], 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 [43]. Moreover, such formulations are necessary to prevent the apparition of spurious modes when solving the Maxwell eigenvalue problem [50]. In this study we aim at comparing DG methods relying on centered and upwind fluxes in terms of accuracy, well posedness of the resulting discrete problems and efficiency. Moreover, discontinuous Galerkin frequency domain (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. From the algorithmic point of view, if linear systems are solved using an iterative solution method, then it is necessary to devise appropriate preconditioners that take care of the matrix properties. This is an important component of our study that lead us to investigate two strategies: domain decomposition methods (additive, non-overlapping, Schwarz algorithms) and algebraic preconditioning methods.

6.2. Seismic wave propagation

6.2.1. Dynamic fault modeling in the context of a finite volume method

Keywords: *P-SV wave propagation*, *centered scheme*, *dynamic fault modelling*, *finite volume*, *linear elasto-dynamics equations*, *time domain*, *velocity-stress system*.

Participants: Mondher Benjemaa, Nathalie Glinsky-Olivier, Serge Piperno, Jean Virieux [NSAU and Géo-sciences Azur].

We are interested in the numerical simulation of seismic activity, including wave propagation and dynamic fault modelling. As a first step, we have modelled the two-dimensional P-SV wave propagation in a vertical, linear, isotropic, and heterogeneous medium (parameters for the medium are the density ρ and the Lamé coefficients λ and μ) by solving the first order hyperbolic linear system of elastodynamics, using an adaptation of the centered finite volume scheme initially proposed for the time domain Maxwell equations [7] whose particularity is the absence of dissipation and the conservation of a discrete energy. The finite volumes are the elements of the triangular mesh: this allows for an easy inclusion of the physical heterogeneities and meshing around faults (or the free surface).

The validation of this method has been done by studying the P-SV wave propagation in an homogeneous medium with a horizontal free surface. Solutions have been compared to analytical seismograms for horizontal and vertical velocities. This method also provides satisfying solutions for a heterogeneous medium with a free surface (weathered-layer test case). Several boundary conditions have been compared for the artificial boundaries: a new absorbing flux condition, coming from the methods dedicated to the Maxwell equations, a classical absorbing boundary conditions of PML type (with quadrangular elements surrounding the triangular mesh) and a PML type condition on the initial triangular mesh.

We are also interested in the simulation of a fault, whose location is prescribed, but with a prescribed or dynamic transient behaviour. This problem has already been solved especially by finite difference methods, for which the fault is represented by a spread set of local sources following the fault's geometry. This approach is not easy to extend in three space dimensions and in configurations where the set of faults becomes complex. Using Finite Volume methods (where the finite volumes coincide with the simplices), two techniques can be proposed. In two space dimensions, the first one considers the fault as the set of triangles neighbouring a line (meshed as triangle edges) and the solutions obtained have been validated by confrontation with results of the finite difference method. A second method, new and more original, consists of a representation of the fault by the set of edges themselves (infinitely thin segments instead of elements). A study of the conservation of the total energy of the system provides a condition on the numerical fluxes computed through the fault in order to obtain stability (and accuracy). This condition has been applied to study the dynamic rupture of a complex geometrical fault. Arbitrary non-planar faults (following element edges) can be explicitly included in the mesh. Different shapes of faults are analyzed, as well as the influence of the mesh refinement on the fault solutions. Several models for the propagation of the rupture have been proposed, especially a more physical one based on a slip-weakening friction law [19].

These results are very promising and encourage us to go further into three space dimensions. The algorithms developed in two space dimensions (formulations, centered fluxes, fluxes through fault edges, dynamic rupture) should be readily extendable to three space dimensions. We are also considering the application of discontinuous Galerkin methods to the solution of these equations (in particular to get more accuracy near the dynamically rupturing fault).

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 system*.

Participants: Nathalie Glinsky-Olivier, Loula Fezoui.

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 time domain elastodynamic equations. Indeed, these methods share some ingredients of the DG-Pk methods developed for the time domain Maxwell equations among which, the nodal polynomial basis functions, a leap-frog time intregration scheme and a centered scheme for the evaluation of the numerical flux at the interface between neighboring elements.

6.3. Domain decomposition methods for the Maxwell equations

Keywords: *Maxwell equations*, *Schwarz algorithm*, *domain decomposition*, *frequency domain*, *natural interface conditions*, *optimized interface conditions*.

Participants: Victorita Dolean, Hugo Fol, Stéphane Lanteri, Ronan Perrussel.

The linear systems resulting from the discretization of the three-dimensional frequency domain Maxwell equations using discontinuous Galerkin methods on unstructured tetrahedral meshes are characterized by large sparse, complex coefficients and irregularly structured matrices. Therefore, if one wants to reach a prescribed accuracy at a manageable computational cost, parallel computing is a mandatory path and it is required to look for (almost) scalable resolution strategies. A standard approach for solving these systems calls for sparse direct solvers. However, such an approach is not feasible for reasonably large systems due to the memory requirements of direct solvers. Moreover, parallel computing is a mandatory route for the design of solution algorithms capable of solving problems of realistic importance. Several parallel sparse direct solvers have been developed in the recent years such as MUMPS [38]. 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. In this context, domain decomposition algorithms are popular strategies that can be used to design parallel preconditioning techniques for Krylov type iterative methods or as coordination methods for sparse direct solvers applied at the subdomain level.

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 first order condition is imposed at the interfaces between neighboring subdomains that corresponds to a Dirichlet condition for characteristic variables associated to incoming waves. From the discretization viewpoint, 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) [8]-[24].

On the other hand, we also study optimized Schwarz methods that make use of more effective transmission conditions than the classical Dirichlet conditions at the interfaces between subdomains. New transmission conditions were originally proposed for three different reasons: first, to obtain Schwarz algorithms that are convergent without overlap; second, 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. In this context, we investigate the benefits of using discontinuous Galerkin formulations for obtaining compact discretizations of the interface conditions of non-overlapping optimized Schwarz algorithms designed for the first order time harmonic Maxwell equations. This work is in progress.

6.4. High performance parallel and distributed computing

6.4.1. Parallel and distributed programming models for unstructured mesh solvers

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

Participants: Guillaume Alléon [EADS-CCR, Toulouse], Françoise Baude [Oasis team, INRIA Sophia Antipolis], Denis Caromel [Oasis team, INRIA Sophia Antipolis], Serge Chaumette [LABRi, Bordeaux], Thierry Gautier [ID-IMAG, Moais, Grenoble], Hervé Guillard [Smash team, INRIA Sophia Antipolis], Fabrice Huet [Oasis team, INRIA Sophia Antipolis], Youssef Mesri [Smash team, INRIA Sophia Antipolis], Stéphane Lanteri, Christian Perez [Paris team, IRISA Rennes], Thierry Priol [Paris team, IRISA Rennes].

In close collaboration we computer scientists actively involved in the Grid computing field, we investigate the combination of standard parallel programming models (message passing programming with MPI and shared memory programing with OpenMP) with modern distributed programming methodologies for the development of high performance grid-enabled unstructured mesh solvers for the three-dimensional Maxwell equations. This activity if for a great part undertaken in the context of the ANR DiscoGrid project that aims at studying and promoting a new paradigm for programming non-embarrassingly parallel scientific computing applications on a distributed, heterogeneous, computing platform. The proposed programming model assumes a hierachical partitioning of the underlying unstructured (tetrahedral) mesh in order to take into account the heterogeneity of the computational nodes and interconnection networks, as well as the multi-processing and memory characteristics of a computational node. In particular, the proposed parallelization strategy relies on the application of distinct treatments to the data migration operations taking place on the various levels of a hierarchical partition.

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, 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. In particular, the experimental software developed by N. Canouet during his PhD thesis [39] has been reprogrammed and parallelized in a cartesian grid framework.

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

Participants: Loula Fezoui, Stéphane Lanteri, Serge Piperno, Muriel Sesques [CEA/CESTA, Bordeaux].

CEA/DAM (Division of Military Applications) takes part with EADS (for the DGA) in the development of a software for the numerical simulation of the interaction of transient electromagnetic fields with particles. In this context, CEA/CESTA is evaluating the finite volume and discontinuous Galerkin methods developed by the team, as a basis for the development of a Vlasov/Maxwell software.

7.3. DG methods for the frequency domain Maxwell equations

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

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 discontinuous Galerkin methods on unstructured tetrahedral meshes for the solution of the frequency domain Maxwell equations.

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, Jean Virieux [NSAU and Géosciences Azur].

This new 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 (Caimanteam), 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) will be 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-CCR, Toulouse], Françoise Baude [Oasis team, INRIA Sophia Antipolis], Denis Caromel [Oasis team, INRIA Sophia Antipolis], Serge Chaumette [LABRi, Bordeaux], Thierry Gautier [ID-IMAG, Moais, Grenoble], Hervé Guillard [Smash team, INRIA Sophia Antipolis], Fabrice Huet [Oasis team, INRIA Sophia Antipolis], Youssef Mesri [Smash team, INRIA Sophia Antipolis], Stéphane Lanteri, Christian Perez [Paris team, IRISA Rennes], Thierry Priol [Paris team, IRISA Rennes].

The team is coordinating the DiscoGrid [34] (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 [35]. 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.

During this first year, the team has actively participated in the definition of an approppriate SPMD programming model for the unstructured mesh finite element and finite volume solvers considered in the DiscoGrid project. This programming model assumes that the underlying mesh is decomposed using a hierarchical partitioning algorithm which takes into account the heterogeneity of the computational nodes and interconnection networks. The next step will consist in the specification of an application programming interface in conjunction with the various parallel and distributed programming environments and methodologies that will be used in the project.

9. Dissemination

9.1. Editing, scientific committees

Stéphane Lanteri is a member of the scientific committee of the ANR program "Calcul Intensif et Simulation".
Stéphane Lanteri is the scientific coordinator of the Grid5000@Sophia project [35].
Stéphane Lanteri co-organized with Raymond Namyst (LABRi, Bordeaux) and Olivier Richard (ID-IMAG, Montbonnot Saint Martin) the "Experimental Grid testbeds for the assessment of large-scale distributed applications and tools" workshop that was held in conjunction with the 15th International Symposium on High Performance Distributed Computing (HPDC-15) June 19-23 2006, Paris
Stéphane Lanteri co-organized with Jean Roman (Scalaplix team at INRIA Futurs) and Thierry Priol (Paris team at IRISA) the CEA-EDF-INRIA school "High performance scientific computing: algorithms, software tools and applications", that tokk place on November 6-9, 2006 at INRIA Rocquencourt.
Serge Piperno participated to INRIA's CR2 local admissibility jury at Rocquencourt.
Serge Piperno is a member of the editing committee of "Progress in computational fluid dynamics" (Inderscience).
Serge Piperno is an external member of the steering committee of the Federative Research Program MAHPSO (high accuracy models for wave propagation systems of equations) of ONERA (the French national aerospace research establishment).
Serge Piperno co-organized (with Raphael Gillard and Lionel Pichon) a meeting on "Time domain methods for waves" of the GDR Ondes (GT1) at Institute Henri Poincaré.

9.2. 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).
"Calcul Scientifique", Serge Piperno, cours de première année, Ecole Nationale des Ponts et Chaussées (30h).
"Interactions fluide-structure", Serge Piperno, Mastère de Mécanique Numérique, Ecole Nationale Supérieure des Mines de Paris (6h).
Organization by Serge Piperno of an "opening week" at INRIA Sophia Antipolis for "Maths-Info" students, Ecole Nationale des Ponts et Chaussées.
"Introduction à l'électromagnétisme computationnel", Francesca Rapetti, Master de Mathématiques, seconde année, Université de Nice/Sophia Antipolis.

9.3. Prize

Serge Piperno received the 2006 Blaise Pascal GAMNI-SMAI prize.

9.4. Ongoing PhD theses

Mondher Benjemaa, "Simulation numérique de la rupture dynamique des séismes par des méthodes volumes finis en maillages non structurés", Nice-Sophia Antipolis University.
Antoine Bouquet, "Adaptation de méthodes des domaines fictifs aux schémas de type Galerkin discontinu avec sous-maillage", 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.
Hugo Fol, "Méthodes de type Galerkin discontinu pour la résolution numérique des équations de Maxwell en régime harmonique", Nice-Sophia Antipolis University.

9.5. PhD thesis supervision activity

Victorita Dolean is co-advisor of the thesis of Adrien Catella.
Stéphane Lanteri is supervising the thesis of Adrien Catella, Hassan Fahs and Hugo Fol.
Nathalie Glinsky-Olivier is co-advisor of the thesis of Mondher Benjemaa.
Serge Piperno is supervising the thesis of Antoine Bouquet and co-advisor of the thesis of Mondher Benjemaa (with Jean Virieux).
Francesca Rapetti is co-advisor of the thesis of Hassan Fahs.

9.6. Reviewing activity and participation to jurys

Serge Piperno took part to the jury of the HDR defense of Elisabeth Longatte (UST Lille) and to the jury (as reviewer) of the PhD thesis defense of Yoann Ventribout (Supaero Toulouse).

9.7. Invitations, seminars, communications

Plenary lecture of Stéphane Lanteri at the Numelec 2006 (5ème Conférence Europénne sur les Méthodes Numériques en Electromagnétisme) Conference, Lille, November 29-30 and December 1, 2006.
Seminar of Stéphane Lanteri during the short course "Méthodes performantes en algèbre linéaire pour la résolution de systèmes et le calcul de valeurs propres", Coll'ege de Polytechnique, March 28-30, 2006.
Seminars of Serge Piperno at Laboratoire Jacques-Louis Lions and at ONERA Chatillon.
Communications of Serge Piperno at ECCOMAS CFD 2006 Conference, Egmond aan Zee, The Netherlands, September 5-8, 2006.

9.8. International collaborations

We have initiated this year a collaboration with the Department of Geological Sciences at San Diego State University (with VÃctor Manuel Cruz-Atienza, Steven .M. Day and Kim B. Olsen) which is concerned with the development of finite volume methods for the numerical modeling of earthquake dynamics and wave propagation in the three-dimensional case.

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