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Project-Team caiman

Calcul scientifique, modélisation et analyse numérique

Sophia Antipolis

THEME NUM

Activity Report

2005

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1. Team

Caiman is a joint project-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, as well as their parallel implementation. A particular emphasis is put on the validation of the proposed methods on realistic (industrial or pre-industrial) 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, local time-stepping strategies (building on algorithms we first proposed for fluid-structure interactions), high order interpolation methods on triangular and tetrahedral meshes in connection with discontinuous finite element formulations, discretization methods on non-conform meshes and domain decompositition solution algorithms. Current applications relate to heterogeneous electromagnetics, acoustics, propagation of acoustic waves in a non-uniform steady compressible flow (aeroacoustics) and geophysics.

We also investigate several aspects related to the numerical simulation of acoustic and electromagnetic wave propagation problems in the frequency domain (time harmonic finite volumes and discontinuous finite elements, coupling with integral equations, solution algorithms).

3. Scientific Foundations

3.1. Conservation laws and discontinuous finite element methods

Keywords: *Riemann problem, computational fluid dynamics, discontinuous Galerkin, electromagnetics, finite volume, monotonicity, unstructured mesh*.

Participants: Serge Piperno, Stéphane Lanteri, Loula Fezoui, Nathalie Glinsky-Olivier, Alexandre Ern, Marc Bernacki, Mondher Benjemaa, Hugo Fol, Maud Poret.

Conservation law a conservation law is a partial differential balance equation of a scalar field (system of conservation laws for a vector field), where all terms are first-order space- or time-derivatives of functions of the unknown (for example, $\partial_t u + \partial_x f(u) = 0$).

Riemann solver a Riemann solver yields an exact or approximate solution of a local Riemann problem (initial value problem with two constant states). It is used in finite volume methods, for example in Godunov-type numerical fluxes.

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 choices of element types or for the use of locally refined, possibly non-conform grids.

Several systems of PDEs are at the heart of the project-team activities. However, they are all mainly similar to fluid dynamics equations, because they can be rewritten as hyperbolic systems of conservation laws or balance equations (Euler, Navier-Stokes, Maxwell equations). Fluid Dynamics equations are a non linear strictly hyperbolic system of conservation laws. Computational Fluid Dynamics started decades ago (see [40] for early references). 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 approximates to the mean values of the fields inside the control volumes (it 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).

Finite volume methods can easily deal with complex geometries and irregular solutions [4]. 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 [34] and interpolation and slope limitation can yield higher accuracy (outside discontinuity zones) [36].

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 [8] (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 proposed a simple and very efficient finite volume method 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 TDTD method due to Yee [42] in terms of numerical properties and computational efficiency [7]. This method has been extended to higher orders of accuracy with discontinuous Galerkin approaches[14].

Finally, we should recall here that finite volume methods can very simply deal with moving meshes (classically, for fluid-structure interaction simulations, Fluid Dynamics equations are rewritten in an Arbitrary Lagrangian-Eulerian (ALE) form, allowing the use of deforming meshes past a deforming structure). We have recently made some efforts to propose finite volume extensions on variable meshes [10] (both the coordinates and the topology of the unstructured mesh vary), excluding classical remeshing of mesh adaptation [32].

3.2. Coupling of models and methods

Keywords: *computational fluid dynamics*, *coupling*, *electromagnetics*, *finite element*, *finite volume*, *fluid-structure interaction*, *numerical analysis*, *unstructured mesh*.

Participants: Stéphane Lanteri, Loula Fezoui, Serge Piperno, Hugo Fol.

Coupling: interaction between several subsystems with simultaneous evolutions each depending on one-another. For example, a physical coupling can take place between different sub-systems. Similarly, different numerical methods solving different PDEs can be coupled to solve a coupled physical problem.

Coupling algorithm: a particular algorithm, built for the numerical simulation of a coupled problem, allowing the modular use of existing numerical procedures. If no particular attention is paid to the construction of the algorithm, it does not inherit the numerical properties of the coupled procedures (in particular stability and accuracy).

Many recent research themes in the project-team Caiman (wave propagation, fluid-structure interaction) have a connection with the same goal: the efficient and accurate coupling of different partial differential equations (domain decomposition for the Maxwell system or CFD, the Vlasov/Poisson system, etc).

The coupled transient solution of different PDEs is still an open problem (from the theoretical and numerical points of view). The general approach is based on staggered algorithm (problems are solved separately and one after each other). This allows the use of existing codes and procedures. This kind of staggered partitioned procedure allows also the iterative solution of difficult coupled problems, when time scales are similar in different subsystems. Finally, one more and more important aspect of coupling is the transient coupling of numerical methods (the question of coupling the same method on several subdomains is still very interesting).

All these works are motivated by the fact that the attention paid to the coupling algorithm can prevent numerical efficiency, stability, and accuracy breakdowns [5].

In the domain of wave propagation (reversible equations where a global electromagnetic energy should be conserved), we have obtained very promising results in time subcycling by using symplectic algorithms [21].

3.3. High-performance parallel and distributed computing

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

Participants: Marc Bernacki, Victorita Dolean, Loula Fezoui, Stéphane Lanteri.

The development of numerical simulation software adapted to modern parallel computing platforms is generally realized following two complementary paths: in general, the numerical methods used in the sequential case are parallelized by choosing a suitable parallel programming paradigm; additionally, new numerical methods have to be designed in order to fully exploit the capabilities of these computing platforms. For example, the solution of the algebraic systems resulting from the discretization of partial differential equations is a classical context which is witnessing a large number of research activities worldwide that aim at developing new parallel solvers. These are for a great part based on domain decomposition principles [39], [37]. The Caiman project-team is currently contributing to both of the above aspects. On one hand, the finite volume and discontinuous Galerkin methods on unstructured tetrahedral meshes are parallelized 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). On the other hand, we develop domain decomposition algorithms for the solution of Maxwell equations modelling electromagnetic waves propagation.

Moreover, the popularity of the Internet as well as the availability of powerful computers and high-speed network technologies as low-cost commodity components is changing the way we use computers today. These technological opportunities have led to the possibility of using distributed computing platforms as a single, unified resource, leading to what is popularly known as grid computing [25]. Grids enable the sharing, selection and aggregation of a wide variety of resources including supercomputers, storage systems and specialized devices that are geographically distributed and owned by different organizations, for solving large-scale computational and data intensive problems in science, engineering and commerce. However this emerging grid computing concept also brings additional constraints on the development of scientific applications such as, heterogeneity (both in terms of CPUs and interconnection networks) and multi-localization. The development of scientific applications that fully exploit such distributed and heterogeneous computing platforms requires to bring together computer scientists from the grid computing community and computational mathematicians. The former are currently developing languages and tools relying on new programming paradigms, such as distributed oriented programming, that offer new perspectives of scientific applications. Since 2002, Caiman is collaborating with researchers from the Oasis project-team (also located at INRIA Sophia Antipolis) with the common aim of developing parallel and distributed finite element simulation software adapted to grid computing platforms.

4. Application Domains

4.1. Computational electromagnetics for engineering design

Keywords: *antenna design*, *electromagnetic compatibility*, *furtivity*, *telecommunications*, *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 FDTD method [42], in order to use different numerical methods in the context where they are the most efficient [38]. Finally, we are now developing methods based on the discontinuous Galerkin setting, which can be seen as high-order extensions of finite volume methods [24]. These methods can easily and accurately deal with highly heterogeneous materials [14], highly distorted meshes and non-conform 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 conform or non-conform decomposition of the computational domain combined to hybrid explicit/implicit time integration schemes.

We are 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 in view of applying the resulting DGEM/BEM methodology to radar furtivity investigations.

4.2. Bioelectromagnetics

Keywords: *Maxwell equations*, *geometrical modelling*, *medical image processing*, *mobile phone*, *numerical dosimetry*, *segmentation*, *thermal effects*.

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 [27] 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: *P-SV wave propagation*, *centered scheme*, *finite volume*, *velocity-stress system*.

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, we can cite the staggered grid finite difference scheme proposed by Virieux [41] and based on the first order velocity-stress hyperbolic system of elastic waves equations, which is an extension of the scheme derived by K.S. Yee [42] for the solution of the Maxwell equations. The use of quadrangular meshes is a limitation for such codes especially when it is necessary to incorporate surface topography or curved interface. In this

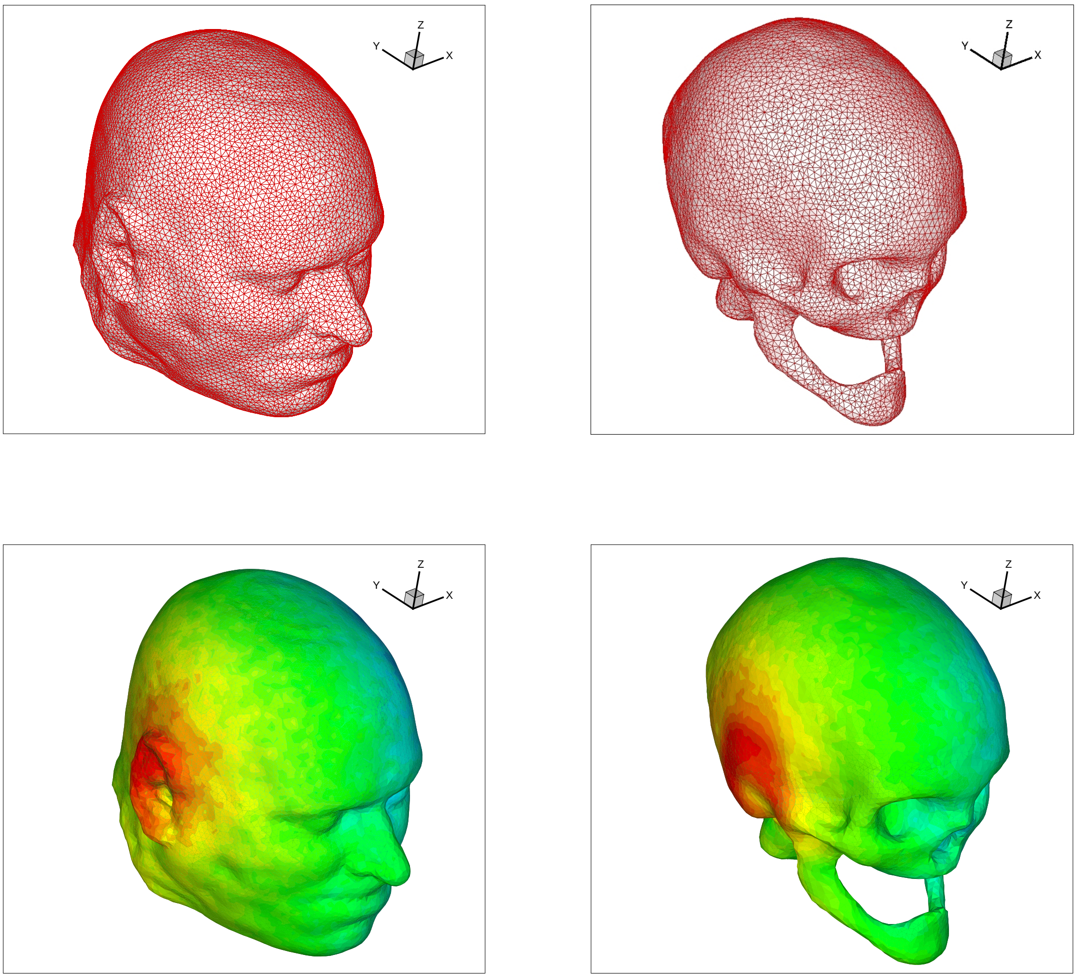

Figure 1. Triangulated surfaces for meshes of the skin and the skull (top figures)

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 project-team (launched in mid-2004), which is conducted in close collaboration with the team of J. Virieux at the Géosciences Azur CNRS laboratory in Sophia Antipolis. Our first achievement in this domain is a centered finite volume software on unstructured triangular meshes 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.

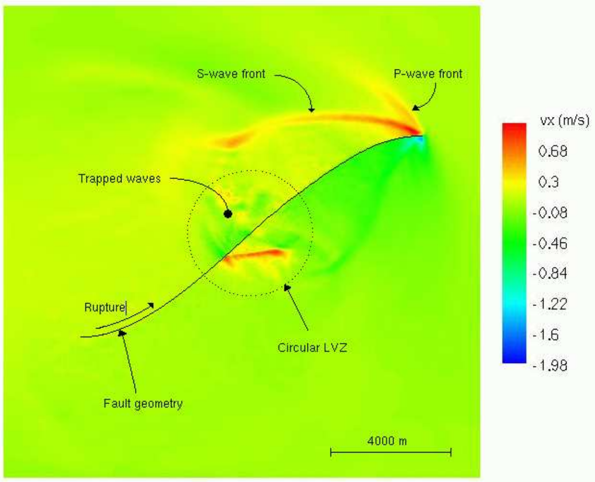

Figure 2. Propagation of a non-planar fault in an heterogeneous medium

4.4. Computational aeroacoustics

Keywords: *aeroacoustics*, *noise reduction*, *non-uniform flow*.

In connection with the general problem of the simulation of wave propagation, we consider aeroacoustics as a challenging domain of application of the unstructured mesh numerical methods that we design for time domain problems. We have here chosen to limit our investigations to a context (validated through discussions with industrials interested by the subject) where the steady flow is known and the goal is to propagate acoustic waves in a non-uniform flow (then, we do not consider the modelling of noise generation, using Direct Numerical Simulation or turbulent models for example). This requires numerical methods able to deal with heterogeneous propagation properties and producing very few numerical dissipation. The Finite Volume and discontinuous Galerkin methods that we have developed in the framework of electromagnetics and classical acoustics are being extended to this context.

As an illustration of our achievements in this domain, we consider the propagation of waves emitted by an acoustic mono-polar source located on the nose of an aircraft, in a steady subsonic flow computed for a free stream Mach number $M_\infty = 0.5$. The surfacic mesh and the contour lines of the Mach number for the steady flow are shown on Fig. 3. Contour lines of the pressure perturbation δp at different times on the surface of the aircraft are shown on the bottom figures.

5. Software

5.1. MAXDGk

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

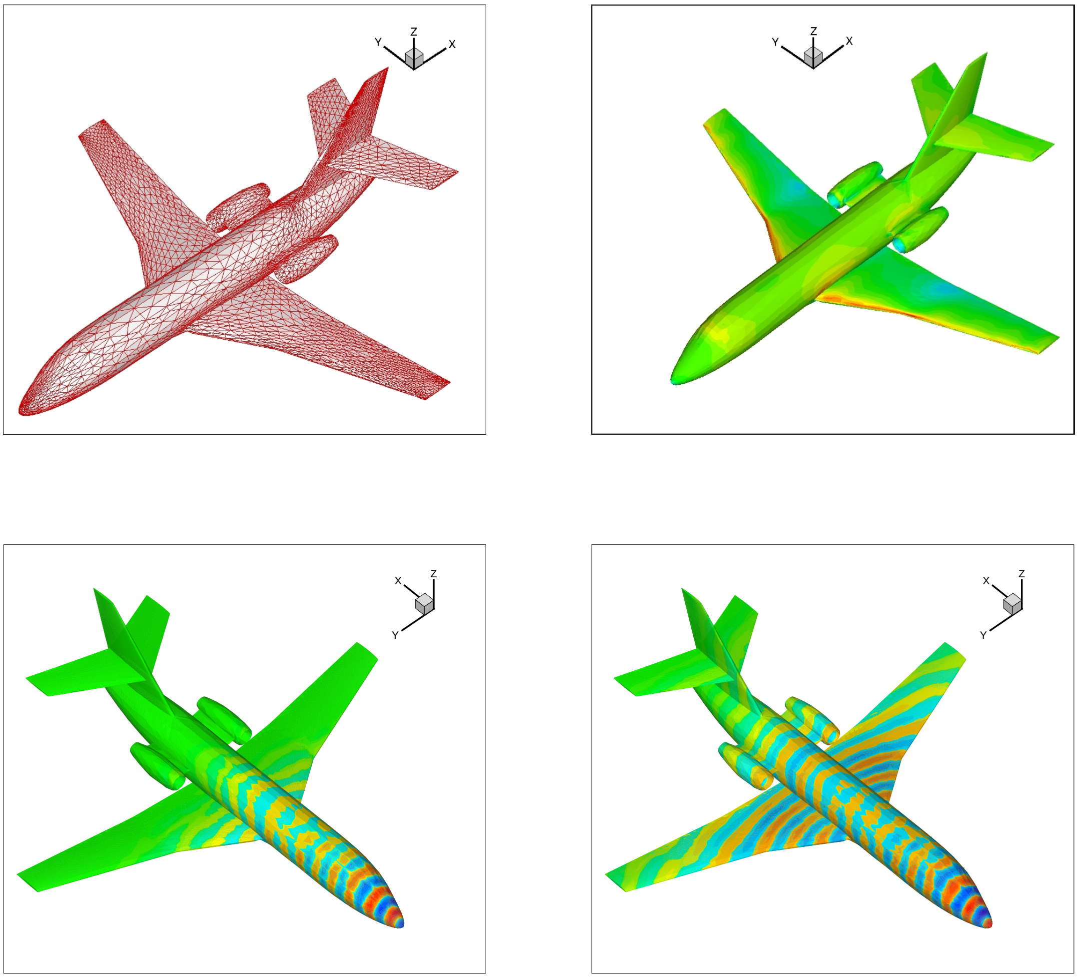

Figure 3. Aeroacoustic propagation past a Falcon aircraft

Participants: Loula Fezoui, Stéphane Lanteri, Serge Piperno.

The team develops the MAXDGk [30] software suite for the numerical simulation of the three-dimensional Maxwell equations in the time domain, for heterogeneous media and using tetrahedral unstructured grids. MADXGk currently consists of two components (MAXDG0 and MAXDG1) that are respectively based on a Finite Volume method (cells centered on tetrahedra) and on a P1 discontinuous Galerkin method, both with centered fluxes and a leap-frog explicit time-scheme. A third component based on a discontinuous Galerkin method with P2 interpolation (MAXDG2) is under development. The parallelization of the MAXDGk solvers is based on mesh partitioning and message passing using standard MPI.

5.2. MAXDGHk

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

Participants: Hugo Fol, Stéphane Lanteri, Serge Piperno.

The team has started this year the development of the MAXDGHk software suite for the numerical simulation of the three-dimensional Maxwell equations in the frequency domain, for heterogeneous media and using tetrahedral unstructured grids. MADXGHk currently consists of two components (MAXDGH0 and MAXDGH1) that are respectively based on a finite volume method (cells centered on tetrahedra) and on a P1 discontinuous Galerkin method, both with centered fluxes. The parallelization of the MAXDGHk solvers is based on mesh partitioning and message passing using standard MPI.

5.3. AERODG1

Keywords: *Euler equations*, *aeroacoustics*, *discontinuous Galerkin*, *parallel computing*, *time domain*.

Participants: Marc Bernacki, Stéphane Lanteri, Serge Piperno.

The team has developed the AERODG1 [23] software for the numerical simulation in the time domain of the three-dimensional propagation of waves inside a steady inviscid flow, using tetrahedral unstructured grids. The equations solved are the linearized Euler equations around a steady-state solution provided by an Euler equation solver developed at INRIA Sophia Antipolis. Then, the wave propagation (which is massively, yet smoothly heterogeneous) is modelled using a P1 discontinuous Galerkin method (also with centered fluxes and a leap-frog explicit time-scheme). The parallelization is based on mesh partitioning and message passing using standard MPI.

5.4. JEM3D

Keywords: *Grid computing*, *ProActive Java library*, *high performance computing*, *parallel and distributed computing*, *time-domain Maxwell equations*.

Participants: Françoise Baude [project-team Oasis], Denis Caromel [project-team Oasis], Christian Delbe [project-team Oasis], Fabrice Huet [project-team Oasis], Stéphane Lanteri, Romain Quilici [project-team Oasis].

As a first step towards the development of a finite element numerical simulation tool that fully exploit a grid computing platform, project-team Caiman is currently involved in the co-development with computer scientists from the Oasis project-team, of JEM3D [29], an object-oriented (exclusively written in Java) time domain finite volume solver for the 3D Maxwell equations. The Java language has been selected, mainly because of its intrinsic distributed computing features. In the present case, these features are exploited through the use of the ProActive library developed by the Oasis project-team. This library [31] greatly facilitates distributed programming through the concept of active objects. In order to improve the communication performances of the JEM3D software, the Ibis [28] has been interfaced with the ProActive library. Ibis is an efficient and flexible Java-based programming environment for Grid computing, in particular for distributed supercomputing applications, developed at the department of computer science of Vrije University. JEM3D is currently used for two main purposes: on one hand, it is a realistic, non-embarrassingly parallel test-bed for the ProActive library; on the other hand, it serves as a basis for the development of high performance numerical simulation software adapted to grid computing platforms. With regards to the second point, the Caiman and Oasis project-teams currently investigate the use of component based models with the aim of encapsulating existing MPI-based solvers in a distributed Proactive-based framework.

6. New Results

6.1. Electromagnetics and wave propagation

6.1.1. DGTD methods for the Maxwell equations on unstructured meshes

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

Participants: Loula Fezoui, Stéphane Lanteri, Serge Piperno.

Electromagnetic problems often involve objects with complex geometries. Therefore, the use of unstructured tetrahedral meshes is mandatory for many applications. We have proposed [14] a discontinuous Galerkin method for the numerical solution of the time-domain Maxwell equations over unstructured meshes (DGTD method). The method relies on the choice of a local basis of functions (for standard applications, P1 elements yield very satisfactory results), a centered mean approximation for the surface integrals 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 [14]. A proof for the convergence has been established for arbitrary orders of accuracy on tetrahedral meshes, as well as a weak divergence preservation property [14]. We are now considering possible implementations of discontinuous Galerkin methods on tetrahedra beyond P1 elements. Fruitful discussions with Jan Hesthaven (Brown University) in summer lead us to a first extension to the P2-Lagrange nodal elements which is almost validated. We are currently investigating the possibility to consider modal elements, for which the local mass matrix is ill-conditioned, but with a well-known inverse.

6.1.2. DGTD methods for the Maxwell equations on locally refined meshes

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

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

Electromagnetic 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 locally refined, possibly non-conform meshes. We had proposed an explicit scheme based on a classical discontinuous Galerkin formulation which is able to deal with structured non-conform grids [13]. The method relies on a set of local basis functions whose degree may vary at subgrid interfaces. We still use a centered mean approximation for the surface integrals and a second-order leap-frog scheme for advancing in time. We prove that the resulting scheme is stable and that it conserves a discrete analog of the electromagnetic energy.

The method is currently being re-implemented in a cartesian grid setting and numerical parallel acceleration of this implementation will be a part of the PhD thesis subject of Antoine Bouquet (completely funded by France Telecom R&D). We also consider returning to full $P1$ elements rather than only the $P1_{div}$ proposed by Nicolas Canouet in his PhD thesis [33]. Other interesting directions (which are under investigation) are the possibilities to enhance the accuracy and to couple with fictitious domain methods.

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

Keywords: *acoustics, discontinuous Galerkin, local time-stepping, mass matrix condition number, 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 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 [22]. Locally implicit time integration schemes have also been proposed [21]. Still, modal or nodal local basis functions have to be chosen carefully to obtain actual numerical accuracy. We have proposed original polynomial function bases, which have many interesting properties in this context [21].

6.1.4. Implicit DGTD methods for the Maxwell equations

Keywords: *Maxwell system, discontinuous Galerkin, finite volume, implicit time integration, stability, time domain.*

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 tetrahedral meshes. The present study aims at investigating the applicability of implicit time integration schemes in conjunction with discontinuous Galerkin methods for the solution of the time domain Maxwell equations. The ultimate goal is to design hybrid time integration strategies, coupling an implicit scheme which is applied locally in regions where the mesh is highly refined and an explicit scheme is applied elsewhere. The important questions to be studied are concerned with the stability of the overall scheme, its accuracy properties (in particular, the numerical dispersion) and the algorithms used to solve the linear systems resulting from the implicit scheme.

6.1.5. Discontinuous Galerkin methods for the frequency domain Maxwell equations

Keywords: *Maxwell equations, cell centered scheme, discontinuous Galerkin, finite volume, frequency domain, time harmonic, unstructured mesh.*

Participants: Victorita Dolean, Hassan Fahs, Hugo Fol, Stéphane Lanteri, Ronan Perrussel, Serge Piperno.

A large number of electromagnetic wave propagation problems require to solve the time harmonic (or frequency domain) Maxwell equations. In view of solving time harmonic propagation problems in heterogeneous media, we investigate the applicability of discontinuous Galerkin methods based on centered fluxes to the frequency domain Maxwell equations. As for time domain applications, we are interested in numerical methods that can handle unstructured tetrahedral meshes. Such discontinuous Galerkin in the 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 as in the case of head tissues exposure to a radio-frequency field. From the theoretical point of view, we study the inversibility of the resulting matrix operators (or the well-posedness of the discrete problem). 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 multigrid preconditioning methods among others.

6.2. Seismic wave propagation

6.2.1. Seismic wave propagation with faults

Keywords: *P-SV wave propagation, centered scheme, finite volume, velocity-stress system.*

Participants: Mondher Benjemaa, Nathalie Glinsky-Olivier, Serge Piperno, Jean Virieux [Géosciences Azur].

As a first step, we study the two-dimensional P-SV wave propagation in an heterogeneous medium and we consider the first order hyperbolic system of elastic wave equations in a vertical medium, supposed linearly elastic and isotropic (parameters for the medium are the density ρ and the Lamé coefficients λ and μ). After a change of variables, this new system has the same characteristics as the Maxwell equations (hyperbolicity, linearity, conservation of an energy). Then, we solve this system using an adaptation of the centered finite volume scheme initially developed by M. Remaki [38], 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 complexities (heterogeneities, nonlinearities of the 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 [35]. 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, dynamic or preexistent. 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. Using Finite Volume methods, two techniques can be proposed. The first one considers the fault as a set of triangles 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 a set of (infinitely thin) segments instead of elements. A study of the conservation of the total energy of the system provides a flux condition in the fault which is stable and accurate. 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 cracks 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.

We are now considering the application of discontinuous Galerkin methods to the solution of these equations as well as the extension to the three-dimensional case.

6.3. Acoustic wave propagation

6.3.1. Acoustic waves propagation in a steady non-uniform flow

Keywords: *L2 stability*, *absorbing boundary condition*, *centered fluxes*, *discontinuous Galerkin*, *finite volume*, *leap-frog time scheme*, *linearized Euler equations*, *reflecting boundary condition*, *steady non-uniform flow*, *unstructured meshes*.

Participants: Marc Bernacki, Stéphane Lanteri, Serge Piperno.

We are studying the propagation of acoustic waves in a steady inviscid flow. Starting from a steady solution of the Euler equations in a given configuration (geometry, mesh, flow), we aim at propagating acoustic waves in this continuously heterogeneous medium. This is done by simulating the propagation of very small perturbations, following the linearized Euler equations. We then apply in this context of wave-advection equations the same kind of dissipation-free numerical methods which were developed by the team for electromagnetics in the time domain.

A general discontinuous Galerkin framework has been introduced for the propagation of aeroacoustic perturbations of either uniform or non uniform, steady solution of the three-dimensional Euler equations [9]. An explicit leap-frog time integration scheme along with centered numerical fluxes are used into the proposed discontinuous Galerkin time domain method. We have developed slip and absorbing boundary conditions. Stability is proved, under CFL-like stability condition on the time step for steady uniform flow. For steady non uniform flow, we dispose of energy estimations depending of the regularity of the flow. Tests cases illustrate the potentialities of our scheme [12]. We have shown the possibility to stabilize Kelvin-Helmholtz instabilities in a controlled way, i.e. without using overall numerical dissipation [11]. A possible follow-up for this study is to introduce a more accurate description for the supporting flow (it is currently constant over tetrahedra, and could simply be piecewise linear and continuous).

6.4. Domain decomposition and coupling algorithms

6.4.1. Additive Schwarz algorithms for the frequency domain Maxwell equations

Keywords: *Maxwell equations, additive Schwarz, domain decomposition, frequency domain, interface conditions*.

Participants: Victorita Dolean, Hugo Fol, Stéphane Lanteri.

The linear systems resulting from the discretization of the frequency domain Maxwell equations using Finite Element methods on unstructured meshes are known to be very ill conditioned. A standard approach for solving these systems is to use sparse direct solvers. However, such an approach is not feasible for reasonably large systems due to the memory requirements of direct solvers. Then, parallel computing is a mandatory route for the design of solution algorithms capable of solving problems of realistic importance. Parallel direct solvers are developed by several teams worldwide. In France, two such sparse direct solvers are MUMPS (co-developed by the Cerfacs, Enseeiht and ENS Lyon) and PastiX (co-developed by the LABRi and the Scalapplix project-team at INRIA Futurs in Bordeaux). Even if these solvers efficiently exploit distributed memory parallel computing platforms and allow to tackle very large problems, there is still room for improvements of the situation. In this context, domain decomposition algorithms can be used as parallel preconditioning techniques for Krylov type iterative methods or as coordination methods for subdomain based parallel direct solvers.

We have started this year a new study aiming at the design of domain decomposition algorithms for the solution of the frequency domain Maxwell equations. We are interested in additive Schwarz algorithms, considering variants for both overlapping and non-overlapping partitionings of the computational domain. We begin with algorithms based on first order absorbing interface conditions and we study the convergence of overlapping and non-overlapping variants in the continuous and discrete cases as a preliminary necessary step prior to investigating the possibility of using optimized interface conditions following the strategy previously adopted for the Euler equations modelling inviscid compressible flows [3].

6.4.2. DGTD methods on non-conform tetrahedral meshes for Maxwell equations

Keywords: *Maxwell equations, discontinuous Galerkin, domain decomposition, locally refined meshes, non-conform meshes, time domain, unstructured meshes*.

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

This study has been launched in fall 2005 with the PhD thesis of Hassan Fahs. It is complementary to the research activity of the project-team on discontinuous Galerkin methods on non-conform hexahedral meshes in the context of the PhD thesis of Nicolas Canouet (defended in 2004) and Antoine Bouquet (started in fall 2004). In theory, discontinuous Galerkin methods are applicable to conform meshes and non-conform discretizations as well. The non-conformity can be due to local refinements with hanging nodes on edges and faces, or/and the result of subregion (or subdomain) based meshing strategies. We first concentrate on the two-dimensional cases (triangular meshes) and investigate questions concerning the stability of discontinuous Galerkin methods on non-conform meshes (one goal being to produce appropriate CFL criteria) and the link with Mortar Finite Element methods.

6.5. High performance parallel and distributed computing

6.5.1. Distributed memory parallelization of unstructured mesh solvers

Keywords: *MPI, aeroacoustics, discontinuous Galerkin, domain partitioning, electromagnetics, finite volume, message passing, parallel computing, unstructured mesh*.

Participants: Marc Bernacki, Loula Fezoui, Stéphane Lanteri, Serge Piperno.

The numerical simulation of realistic three-dimensional electromagnetics and aeroacoustics problems typically translates into the processing of very large amounts of data. This is essentially the result of two antagonistic parameters: the characteristic space step of the mesh and the computational domain size. For example, for high frequency electromagnetic wave propagation, the space step can be very small while the artificial boundaries of the computational domain are located near the scattering object whereas an opposite situation is obtained for low frequency phenomena. Several numerical techniques can be considered in order to handle this problem to some extent such as, for instance, the reduction of the computational domain size through the use of PML. However, these numerical modelling adaptations are generally not sufficient and the computational power and memory capacity that are required for the simulation of realistic problems are such that the use of parallel computing platforms becomes essential. With respect to this need, we have developed parallel versions of our finite volume and discontinuous Galerkin methods for the solution of electromagnetic and aeroacoustic wave propagation problems on unstructured tetrahedral meshes [12], using a 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).

6.5.2. *Development of grid-aware simulation software for the GRID'5000 test-bed*

Keywords: *Grid computing*, *ProActive Java library*, *component programming*, *distributed object-oriented programming*, *high performance computing*, *message passing programming*, *parallel and distributed computing*.

Participants: Françoise Baude [project-team Oasis], Denis Caromel [project-team Oasis], Christian Delbe [project-team Oasis], Fabrice Huet [project-team Oasis], Stéphane Lanteri, Stéphane Mariani [project-team Oasis], Romain Quilici [project-team Oasis].

A grid computing platform such as the GRID'5000 experimental test-bed can be viewed as a two level architecture: the lower level consists of a set of clusters with between a few hundreds to one thousand processors eventually interconnected by one or several high performance networks; at the higher level, these clusters are interconnected by a wide area network. Ideally, this hierarchical structure should impact the design of numerical algorithms. More importantly, the programming of the simulation software should rely on hierarchical principles and methodologies. Thus, the development of high performance parallel and distributed scientific applications that efficiently exploit grid computing platforms requires to address several topics ranging from applied mathematics to computer science in close interaction. On one hand, from the computer science viewpoint, it is necessary to devise new parallelization strategies that will take into account the heterogeneity of the computational nodes (CPUs) and the interconnection networks. On the other hand, from the numerical algorithms viewpoint, one could for instance design hierarchical PDE solvers based on domain decomposition principles. Theoretically, the development of grid-aware simulation software can rely on a message passing programming paradigm; as a matter of fact, several implementations of MPI have been specifically designed for grid computing platforms, the most popular being MPICH-G2 which is linked to the Globus toolkit. However, other alternatives exist that seem to be better suited to such developments. Building on a collaboration with computer scientists from the Oasis project-team, we investigate the use of distributed object-oriented and component programming with the ProActive Java library, for the development of grid-aware simulation software based on finite volume and discontinuous Galerkin methods on unstructured tetrahedral meshes.

7. Contracts and Grants with Industry

7.1. Expertise in the parallelization of structured grid schemes on clusters (INRIA-FT R&D)

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

France Télécom R&D (center of La Turbie) is developing its own FDTD-based software and exploits them on internal parallel machines. We help FT R&D with the transfer of time domain software from shared to distributed memory parallel platforms. This collaboration also deals with some parallel and structured reprogramming of the experimental software developed by N. Canouet during his thesis.

7.2. Evaluation of MAXDGk for a coupled Vlasov/Maxwell software (INRIA-CEA/CESTA)

Participants: Stéphane Lanteri, Serge Piperno, Loula Fezoui.

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 Caiman project-team, as a basis for the development of a Vlasov/Maxwell software.

7.3. Numerical methods for the frequency domain solution of Maxwell equations (INRIA-EADS)

Participants: Stéphane Lanteri, Serge Piperno, Hugo Fol.

EADS (CCR) has been supporting our research and development efforts for many years, mainly concerning the Fast Multipole Method and its numerous extensions. This ongoing collaboration allows the partial funding of a PhD thesis on the development of frequency domain versions of our finite volume and discontinuous Galerkin methods in view of the coupling with a BEM/FMM method of EADS.

7.4. Coupled DGEM/BEM solution of the frequency domain Maxwell equations (INRIA-FT R&D)

Participants: Stéphane Lanteri, Serge Piperno, Hugo Fol.

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. It is complementary to the previous grant as, in this study, we concentrate on the design of domain decomposed based solution algorithms for the linear systems resulting from the time harmonic finite volume and discontinuous Galerkin methods.

8. Other Grants and Activities

8.1. Regional collaborations

8.1.1. FVTD and DGTD methods for seismic wave propagation (Géosciences Azur)

The work described in section 6.2 concerning the development of finite volume and discontinuous Galerkin methods for the seismic wave propagation is done in close collaboration with the team of J. Virieux at the Géosciences Azur CNRS laboratory in Sophia Antipolis, who is partially funding the PhD thesis of Mondher Benjemaa.

8.2. National collaborations

8.2.1. FVTD and DGTD methods for electromagnetic wave propagation in head tissues (FT R&D Issy-les-Moulineaux)

Keywords: *Maxwell equations, geometrical modelling, medical image processing, mobile phone, numerical dosimetry, segmentation, thermal effects.*

Participants: Olivier Clatz [project-team Epidaure], Stéphane Lanteri, Steve Oudot [project-team Geometrica], Jean-Philippe Pons [project-team Odyssée], Serge Piperno, Gilles Scarella, Joe Wiart [France Télécom R&D, center of Issy-les-Moulineaux].

The work described in section 4.2 concerning the numerical modelling of the propagation of an electromagnetic wave emitted from a cellular phone in head tissues, using finite volume and discontinuous Galerkin methods on unstructured tetrahedral meshes, is done in close collaboration with the team of Joe Wiart at France Télécom R&D in Issy-les-Moulineaux.

8.2.2. Quantitative Seismic Hazard Assessment (QSHA)

Keywords: *numerical methods*, *seismic hazard*, *seismicity*, *seismology*, *wave propagation*.

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: BRGM (Service Aménagement et Risques Naturels), CNRS/Géosciences Azur, INRIA Sophia Antipolis (project-team Caiman), ENPC (Champs-sur-Marne), CEREGE (Centre Européen de Recherche et d'Enseignement des Géosciences de l'Environnement, Aix en Provence), CNRS/LGIT (Laboratoire de Géophysique Interne et Tectonique, Observatoire de Grenoble), CETE Méditerranée, LAM (Laboratoire de Mécanique, Université Marne la Vallée) and LMS (Laboratoire de Mécanique des Solides, Ecole Polytechnique).

Goals of this project focus on better description of crustal structures (in a more quantitative way for extracting rheological parameters for wave propagation), better constraints in characteristic earthquakes one may expect and more precise modelling of waves emitted by these expected earthquakes and quantitative estimation of ground motion based on previous informations.

Quantitative seismic hazard assessment will be investigated around Western Mediterranean Sea with three coastal densely populated zones (Naples zone, French Riviera-Ligurian Sea zone and the Algiers area). Data analysis will focus on 3D information: seismograms, seismic profiles, seismicity, geological information, geotechnical data, gravimetry and so on. Both construction of 3D structures and characterization of earthquakes including uncertainties will be oriented for wave modelling purposes. Up-to-date numerical modelling based on boundary integral equations, finite element method (including spectral element method), finite difference method, finite volume method and discrete element method will be improved in order to achieve a frequency content above 1Hz.

9. Dissemination

9.1. Scientific animation

9.1.1. Grid5000@Sophia project

Stéphane Lanteri is the scientific coordinator of the Grid5000@Sophia project [26]. The INRIA Sophia Antipolis research unit has been selected by the French Ministry of Research, in the framework of the ACI GRID program, to be one of the main nodes of the GRID'5000 computing infrastructure. The GRID'5000 initiative aims at building an experimental grid platform gathering less than a dozen of geographically distributed sites in France combining up to 5000 processors with a certain level of heterogeneity both in terms of processor and network types. The current plans are to assemble a physical platform featuring 8 clusters, each with between 100 to 1000 PCs connected by the Renater education and research national network. All clusters will be connected to Renater at 1 Gb/s (10 Gb/s is expected in a near future). This highly collaborative effort is funded by the French Ministry of Research, INRIA, CNRS and several regional councils. The Grid5000@Sophia project is built around scientific contributions from the Caiman, Coprin, Epidaure, Oasis and Smash project-teams that are concerned with object oriented middleware for distributed computing, algorithms for high performance computing on the grid (computational electromagnetics, computational fluid dynamics, optimal design of complex systems) and grid computing for medical applications.

9.1.2. Editing, scientific committees

Stéphane Lanteri is a member of the scientific committee of the ANR program "Calcul Intensif et Grilles de Calcul".

Stéphane Lanteri is a member of the scientific committee of the VECPAR'2006 International Conference on High Performance Computing and Computational Science.

Serge Piperno was a supplementary elected member of INRIA's evaluation board till september. He participated to INRIA's CR2 local admissibility board at Rennes and Rocquencourt, and to INRIA's DR2 admissibility board.

Serge Piperno is member of the editing committee of "Progress in computational fluid dynamics" (Inderscience).

Serge Piperno was an invited member of the evaluation and orientation committee of the Information Processing and Modeling Department of ONERA (the French national aerospace research establishment).

9.2. Teaching

- *Calcul numérique parallèle*, Stéphane Lanteri, "Mastère de Mécanique Numérique", École Nationale Supérieure des Mines de Paris (18h).
- *Équations intégrales*, *Interactions fluide-structure*, Serge Piperno, "Mastère de Mécanique Numérique", École Nationale Supérieure des Mines de Paris (12h).
- Organization by Serge Piperno of an "opening week" at INRIA Sophia Antipolis for “Maths-Info” students, École Nationale des Ponts et Chaussées.

9.3. Master and PhD students supervision

9.3.1. PhD thesis defended in 2005 in the project-team

1. Maud Poret, “Méthodes en maillages mobiles auto-adaptatifs pour des systèmes hyperboliques en une et deux dimensions d'espace”, ENPC. Jury : Alain Dervieux (reviewer), Frédéric Hecht (reviewer), Thierry Coupez, Bruno Koobus, Stéphane Lanteri, Serge Piperno (advisor).
2. Marc Bernacki, “Schémas en volumes finis avec flux centrés : application à l'áeroacoustique”, ENPC. Jury : Christophe Bailly (reviewer), Olivier Pironneau (reviewer), Alexandre Ern, Uwe Ehrenstein, Isabelle Terrasse, Serge Piperno (advisor).

9.3.2. Ongoing PhD theses in the project-team

1. Mondher Benjemaa, “Simulation numérique de la rupture dynamique des séismes par des méthodes volumes finis en maillages non structurés”, Université de Nice-Sophia Antipolis.
2. Antoine Bouquet, “Adaptation de méthodes des domaines fictifs au schémas de type Galerkin discontinu avec sous-maillage”, Université de Nice-Sophia Antipolis.
3. Hugo Fol, “Méthodes de type Galerkin discontinu en maillages tétraédriques pour la résolution des équations de Maxwell en régime harmonique”, Université de Nice-Sophia Antipolis.
4. Adrien Catella, “Méthode de type Galerkin discontinu d'ordre élevé en maillages tétraédriques non-structurés pour la résolution des équations de Maxwell en domaine temporel - Schémas d'intégration en temps implicites et résolution itérative”, Université de Nice-Sophia Antipolis.
5. Hassan Fahs, “Méthodes de type Galerkin discontinu en maillages tétraédriques non-conformes pour la résolution des équations de Maxwell en domaine temporel”, Université de Nice-Sophia Antipolis.

9.3.3. Supervision activity

1. Serge Piperno has been supervising the thesis of Marc Bernacki and Maud Poret. He is advisor for the thesis of Antoine Bouquet, and co-advisor for the theses of Mondher Benjemaa and Pierre Sochala (ENPC).
2. Nathalie Glinsky-Olivier is co-advisor for the thesis of Mondher Benjemaa.
3. Stéphane Lanteri has been supervising the post-doctoral research of Gilles Scarella and is supervising the one of Ronan Perrussel.
4. Stéphane Lanteri is supervising the thesis of Adrien Catella (co-supervision by Victorita Dolean), Hassan Fahs (co-supervision by Francesca Rapetti) and Hugo Fol.
5. Victorita Dolean is co-advisor for the thesis of Adrien Catella.
6. Francesca Rapetti is co-advisor for the thesis of Hassan Fahs.

9.3.4. Thesis reviewing activity

- Serge Piperno was reviewer for the PhD Thesis of Pierre Crispel (Supaero Toulouse) and Yoann Ventribout (Supaero Toulouse) and took part to the jury of Olivier Marsden (EC Lyon).
- Stéphane Lanteri was reviewer for the PhD theses of Vincent Garonne (Université de la Méditerranée, Aix-Marseille II), Olga Karaseva (École Nationale Supérieure des Mines de Paris and Cemef) and Emeric Martin (Institut National Polytechnique de Toulouse and Cerfacs).

9.4. Invitations, seminars, communications

- Seminar of Stéphane Lanteri on "Bibliothèques d'algèbre linéaire" during the short course "Méthodes performantes en algèbre linéaire pour la résolution de systèmes et le calcul de valeurs propres", Collège de Polytechnique, March 15th-17th 2005.
- Seminars of Serge Piperno at INRIA-Industry Meeting at INRIA Rocquencourt and at France Telecom R&D in Issy-les-Moulineaux.
- Short course of Serge Piperno on "Interactions fluide-structure : couplages et algorithmiques de résolution" at Forum IPSI (Formation et Information en Analyse des Structures)
- Communications of Serge Piperno and of Marc Bernacki at Waves 2005, of Stéphane Lanteri at the DCABES and ICPACE joint Conference on Distributed Algorithms for Science and Engineering, University of Greenwich (UK), August 25th-27th 2005.

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