

INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Project-Team caiman

Calcul scientifique, modélisation et analyse numérique

Sophia Antipolis



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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, Informatique et Calcul Scientifique", Teaching and Research Center on Mathematics, Computer Science and Scientific Computing), with 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

The project aims at proposing new and efficient solutions for the numerical simulation of physical phenomena related to electromagnetics and complex flows in interaction (fluid-structure interactions, epitaxy, etc.). Scientific activities sweep a large range from physical modelling to design and analysis of numerical methods. A particular emphasis is put on their validation on realistic configurations and their algorithmic - possibly parallel - implementation.

Research themes

Electromagnetics:

- In the frequency domain, we investigate several aspects of integral equations (fast multipole method, multi-layer models, coupling with volumic discretizations). The designed applications are RCS and near-field computations of large bodies or antennas.
- In the time domain, we construct numerical methods based on discontinuous finite element or finite volume methods, including coupling schemes with time and space multi-scale approaches. We also study the coupling of the Maxwell equations with the transport of charges in rarefied gases. The main application is the spatial environment of satellites.

Complex fluid dynamics:

- In aeroacoustics, we adapt the numerical methods developed for the heterogeneous Maxwell equations, in order to propagate acoustic waves in a continuously varying steady flow, with no numerical dissipation added.
- In fluid structure interaction, we study the coupling between algorithms for solving the
 fluid and the structure, aiming at constructing new, stable and efficient coupling algorithms
 (new applications with incompressible fluids: wind in civil engineering and blood or air in
 biomedical engineering).
- We intend to simulate epitaxy (cristal growth) on complex geometries via unstructured finite elements grids. This also requires the treatment of complex state laws formulated.

International and industrial relations

- Industrial contracts with EADS CCR, Alcatel Space, France Telecom R&D, Centre d'Études de Gramat.
- Collaborations with Dassault-Aviation, Cerfacs, ENST, Ecole Polytechnique, universities of Nice, Provence, Paris VI.

3. Scientific Foundations

3.1. Conservation laws and finite volume methods

Key words: finite volume, discontinuous Galerkin finite element, unstructured mesh, electromagnetics, computational fluid dynamics, Riemann problem, monotonicity, ALE formulation, moving variable mesh.

Participants: Serge Piperno, Stéphane Lanteri, Loula Fezoui, Nathalie Glinsky-Olivier, Alexandre Ern, Marc Bernacki, Nicolas Canouet, Hugo Fol, Maud Meriaux-Poret, Saïd El Kasmi, Stéphanie Lohrengel [Laboratoire Dieudonné, UNSA-CNRS].

Glossary

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.

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.

Many different PDEs are considered by team members. However, they are 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 [73] 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 into control volumes and the numerical unknowns are approximates for the mean value of the fields inside the control volumes (it is different from finite differences methods, where unknowns are approximates for 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. They can simply lead to conservative method (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 to distinct field average values on the two control volumes). The construction of these numerical flux functions is itself based on approximate Riemann solvers [7] and interpolation and slope limitation can yield higher accuracy (outside discontinuity zones) [61].

These methods can be used in many application fields: complex CFD (with several species or phases), wave propagation in the time-domain in heterogeneous media [65] (acoustics, electromagnetics, etc). In wave propagation fields, the finite volume methods based on local Riemann solvers induce a numerical diffusion which pollutes the simulation results (the diffusion is necessary for CFD, 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 the FDTD [9] in terms of numerical properties [64] and computational efficiency. This method is currently extended to higher orders of accuracy with discontinuous Galerkin approaches [2].

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 form, allowing the use of deforming meshes past a deforming structure). We currently make some effort to propose finite volume extensions on variable meshes (both the coordinates and the topology of the unstructured mesh vary), excluding classical remeshings of mesh adaptation [40].

3.2. High-performance parallel and distributed computing

Key words: parallel computing, distributed computing, grid computing, domain partitioning, message passing, object oriented programming, scientific visualization.

Participants: Stéphane Lanteri, Loula Fezoui, Guillaume Sylvand, Nathalie Bartoli, Zhongze Li, Saïd El Kasmi, Jessy Aipert, Victorita Dolean [CMAP, Ecole Polytechnique], Frédéric Nataf [CMAP, Ecole Polytechnique].

The efficient use of modern parallel computing platforms implies a careful adaptation of the underlying numerical algorithms. In practice, this translates into two main types of activities: most often, existing methods are parallelized with no modification to the numerical ingredients; however, in certain situations, new numerical methods have to be designed in order to fully benefit from the capabilities of these computers. 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 [72][67]. Project team Caiman

is currently contributing to both of these 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 general sparse linear systems.

Moreover, the popularity of the Internet as well as the availability of powerful computers and highspeed 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 [52]. 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 multilocalization. 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, project team Caiman is collaborating with project team Oasis (also located at INRIA Sophia Antipolis) with the common aim of developing a problem solving environment that will allow an effective use of a heterogeneous, distributed, computing platform for the simulation of large-scale electromagnetics phenomena.

3.3. Coupling of models and methods

Key words: coupling, modelling, electromagnetics, computational fluid dynamics, fluid-structure interaction, numerical analysis, finite element, finite volume, unstructured mesh.

Participants: Serge Piperno, Frédéric Poupaud, Nicolas Canouet, Martine Chane-Yook, Hugo Fol, Nathalie Bartoli, Emmanuel Briand.

Glossary

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

coupling algorithm: 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).

Research themes in the team are widely spread: wave propagation, field-plasma coupling, fluid-structure interaction. All these research directions have in common the efficient, accurate coupling of different partial differential equations like the Maxwell system, the Vlasov and Poisson equations, the Navier-Stokes equations and equations for structural dynamics...

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, where 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 [8].

3.4. Boundary element methods and Fast Multipole Methods

Key words: *Maxwell system, acoustics, electromagnetics, frequency domain, boundary finite element, integral equation, fast multipole method, high performance computing.*

Participants: Serge Piperno, Guillaume Sylvand, Hugo Fol, Nathalie Bartoli, Christel Luquet-Piperno, Jessy Aipert, Guillaume Alléon [Centre Commun de Recherche Louis Blériot, EADS].

Glossary

sparse matrix, dense matrix: a sparse matrix is almost only filled with zero (for example, a large tridiagonal matrix is sparse). On the contrary, a dense matrix is only filled with *a priori* non-zero terms

integral equation: functional equation in which the functional unknown appears under the integration sign; in scientific computing, they play an important role in wave propagation in the frequency domain (acoustics, electromagnetics). The three-dimensional partial differential equations can be transformed into an integral equation on the boundary of the scattering object. This allows to reduce the space dimension of the problem and the mesh (from three to two). However, the induced linear systems are not sparse (like for volumic finite elements), but dense and complex.

multipole method: recursive algorithm based on a octree which fastens and approximates the matrix-vector products appearing in surface discretizations of integral equations. The solution of linear systems are therefore solved using iterative algorithms.

One elementary problem in electromagnetics is the computation of the field scattered by an object. For a perfectly conducting object $(\Omega, \text{ with } \Gamma \text{ its boundary})$ and a known incident field E_{inc} , the problem, in the frequency domain, reduces to the computation of induced electric currents on Γ (and the scattered field in the whole domain outside the object is simply expressed in terms of the currents). The variational form of the equation on the currents writes: $find \ \phi \in X \ such \ that \ \forall \phi^t \in X$,:

$$\int_{\Gamma} \int_{\Gamma} (\phi(x).\phi^t(x') - \frac{1}{k^2} div\phi(x).div\phi^t(x')).K(x,x').dx.dx' = - \langle E_{inc}, \phi^t \rangle,$$

where ϕ denotes the unknown current field on Γ , ϕ^t is a test-function, X is some space of test-functions, and K(x,x') denotes the Green elementary solution of Helmholtz equation: $K(x,x') = \frac{e^{ik\|x-x'\|}}{\|x-x'\|}$.

This variational equation is solved using boundary finite elements. This leads to solving a dense (because of the Green's kernel), complex, linear system. This can be done directly for small systems (cpu time growing like n^3 , where n is the number of unknowns - itself growing like the size of the object in wavelengths or like the frequency). For large systems, this must be done using an iterative method (the QMR method for instance). However, the necessary matrix-vector products require cpu time and storage growing like n^2 . For high frequencies (GigaHertz) and large objects (airplanes), n goes far beyond 10^6 [4] and these matrix-vector products must be accelerated.

The fast multipole method [6] allows the fast but approximate computation of matrix-vector products resulting from boundary element discretizations of integral equations (see [3] for a complete introduction). The algorithm can be single-level (complexity in $n^{3/2}$) or multi-level (theoretical complexity in $n \log n$ (where Γ is recursively decomposed through an octree, whose smallest cell usually has a size of $\lambda/2$). The matrix-vector products are then computed, separating close and far interactions and grouping contributions of currents located at neighboring cells on Γ .

4. Application Domains

4.1. Wave propagation in electromagnetics

Key words: telecommunications, biomedical engineering, plasma, satellites, electromagnetic compatibility, furtivity, acoustics, antenna.

We develop numerical methods and algorithms for the numerical solution (in the time or frequency domain) of electromagnetic wave propagation. They can be applied to many different physical settings and several very rich application domains, like telecommunications, biomedical and transportation 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 thought for the solution of compressible fluid dynamics on unstructured grids. Their upwind nature [62] lead to numerical dissipation of the electromagnetic energy. We then went on with dissipation-free finite volume methods based on centered fluxes [64]. For the Maxwell system, they compared well with commonly-used finite difference methods [9]) in terms of accuracy and efficiency on regular meshes, but with spurious propagations on highly distorted meshes for example. At the same time, these methods could be coupled with Yee's FDTD method, in order to use different numerical methods in the context where they are the most efficient [69]. Finally, we are now developing software based on discontinuous element methods, which can be seen as high-order extensions of finite volume methods [2]. These methods can easily and accurately deal with highly heterogeneous materials, 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 (for example for applications in biomedical engineering), based on explicit, time and space domain-decomposed schemes.

In the frequency domain, we consider several developments of boundary element methods for the numerical solution for integral equations. We solve large problems (in terms of the size of the scattering object in wavelengths) using a multilevel, parallel, out-of-core fast multipole method [6]. This formulation (first in the frequency domain, subsequently in the time domain) could also be coupled with volumic methods (for instance in cases where the volumic discretization of heterogeneous materials leads to cheaper algorithms than boundary formulations). Finally, following a long tradition in the team, initiated by A. de La Bourdonnaye (on microlocal analysis [47]), we still study some particular cases of integral methods, like the coupling of several axisymmetric integral formulations [29] or like the integral formulation of multi-layered patches on antennas (this could lead to interesting comparisons between approximate integral methods and volumic methods inside multi-layered materials).

In the field of plasmas, we are highly interested in the study of the plasmic and electromagnetic environment of artificial satellites. Satellites receive and emit high energy electromagnetic waves, have many different potential levels on different parts and are evolving in a cloud of charged particles (which may induce electric discharges and other severe problems). Although the physical context is rather electrostatic (the Vlasov-Poisson equations), we use our own experience on the Vlasov-Maxwell system to couple a finite element approach with particle methods, in order to provide meaningful numerical simulations of the plasmic environment of satellites, in the framework of a continuous collaboration with an industrial partner, which pays attention to the physical meaning of both available experimental and numerical results.

4.2. Computational fluid dynamics and related problems

Key words: biomedical engineering, telecommunications, coupling algorithm, fluid-structure interaction, multiphase flow, combustion, real gas, finite volume, finite element, unstructured mesh, civil engineering.

We are interested in several physical problems where fluids dynamics are coupled to other phenomena: fluid-structure interactions, flows of real gases, aeroacoustics, etc.

In the field of fluid-structure interactions, many different application domains appear, like aerospace engineering, biomedical engineering, civil engineering. In aerospace engineering, the fluid flow is compressible and light compared with the structure. The stability properties of recent (both military and civil) airplanes is strongly dependent on the coupled behavior of the structure and the flow past itself. We have proposed with Charbel Farhat (Colorado university at Boulder, Colorado) criteria for the design of efficient, accurate and stable coupling algorithms in this context [8]. Ideas driving from these criteria are currently reformulated for the domain decomposed solution of wave propagation in the time domain with different time-steps for each subdomain. Concerning cases with incompressible flows, we have participated in common efforts at INRIA in two different fields. In civil engineering, we proposed a prototype software platform for the stability analysis of elementary bridge sections in uniform prescribed winds [60] (in collaboration with Laboratoire Central des Ponts et Chaussées, Centre Scientifique et Technique du Bâtiment, Service d'Études Techniques des Routes et Autoroutes, and INRIA). In biomedical engineering (the flow is considered as Newtonian, incompressible, but not light compared to blood vessels), we participated to the joint effort "ARC VitesV" [78] for the realistic simulation of highly deformable vessels (collapsible vessels, aneurisms). These works are continued in other project teams (see the MACS and M3N projects).

We are also interested in realistic flows (reactive flows of multiphase flows). For vapor phase epitaxy (industrial process of high importance for growing of single crystals in which chemical reactions produce thin layers of materials whose lattice structures are identical to that of the substrate on which they are deposited), we have developed a unstructured two-dimensional basic reactor simulator [51], where the flow cannot be considered as polytropic (there is no more linear relation between the internal energy and the temperature) because of very high temperatures and a energy relaxation method [45] has been extended to the Navier-Stokes equations. This allows the use of a lightly modified version of a classical "perfect gas" solver.

Finally, in connection with the general problem of the simulation of wave propagation, we have started a new research direction on aeroacoustics. We have chosen to limit our investigations to a context (validated by industrials) 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 DNS or turbulent models for example). This requires numerical methods able to deal with heterogeneous propagation properties and producing very few numerical dissipation. The method developed in the framework of electromagnetics and classical acoustics are being extended to this context.

5. Software

5.1. AS_ELFIP_FMM - ACTI3S_TMM

Key words: Helmholtz equations, frequency domain, time domain, finite elements, integral equations, multipole method, parallel computation.

Participants: Guillaume Sylvand, Guillaume Alléon [Corporate research center, EADS].

AS_ELFIP is a software developed internally by EADS for solving Helmholtz equations in both the frequency domain and the time domain using integral equations. It is used to simulate acoustic waves propagations around aircrafts and engines. In the frequency domain, the EADS software AS_ELFIP_FMM we strongly contributed to is based on a full multilevel Fast Multipole Method and allows the solution of very large problems (up to 25,6 million of degrees of freedom, solved in 18 hours on a 64-processor IBM/SP3). In the time domain, it uses a time-marching solver and classical sparse matrices. We are in the process of implementing a multipole algorithm in this code in order to treat much larger problems in shorter execution times. The resulting software is for the moment called AS_ELFIP_TMM (TMM stands for "Time domain Multipole Method").

5.2. NS3IFS/COUPLEUR

Key words: *fluid-structure interaction, incompressible viscous fluid, moving mesh, finite element, shell finite element, modulef, civil engineering, blood flow.*

Participants: Serge Piperno, Marina Vidrascu [project team MACS], Marc Thiriet [project team M3N], Jean-Frédéric Gerbeau [project team M3N].

The platform NS3IFS allows the coupled simulation of a viscous incompressible unsteady flow in a moving mesh and a deforming structure (simple structural dynamics solver). Coupled in the framework of the software COUPLEUR [41] developed within INRIA collaborative action "Simulations numériques d'interactions fluide-structure en Génie Civil et ingénierie biomédicale" [63], we can handle structures modeled as shells using the public domain MODULEF library [42]. This has been used to obtain simulations of blood flows in deforming blood vessels within INRIA collaborative action Vitesv [78], where coupling algorithms including iterative subcycling and relaxation have been implemented in the COUPLEUR.

5.3. EM3D/VFC

Key words: electromagnetics, Maxwell system, time domain, finite volume, heterogeneous medium, parallel computing.

Participants: Loula Fezoui, Stéphane Lanteri, Serge Piperno.

The team has developed a new version of the software EM3D/VFC [55] for the numerical simulation of the three-dimensional Maxwell equations in time domain, for heterogeneous media and on tetrahedral unstructured grids. The software is based on a finite volume method (cells centered on tetrahedra) with centered fluxes and a leap-frog explicit time-scheme [68]. The parallelization is based on mesh partitioning and message passing using standard MPI. Many test-cases and post-processing developments have been recently added.

5.4. EM3D/GLK

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

Participants: Loula Fezoui, Stéphane Lanteri, Serge Piperno.

The team has developed a discontinuous Galerkin version of the software EM3D/VFC for the numerical simulation of the three-dimensional Maxwell equations in time domain, for heterogeneous media and on tetrahedral unstructured grids. The software EM3D/GLK is based on a complete P1 discontinuous Galerkin discretization (cells centered on tetrahedra) with centered fluxes and a leap-frog explicit time-scheme [36]. The parallelization is based on mesh partitioning and message passing using standard MPI. Test-cases and post-processing capabilities are the same as EM3D/VFC.

6. New Results

6.1. Electromagnetics and wave propagation

6.1.1. Accelerating the retarded potentials for acoustics through Time domain Multipole Method

Key words: Helmholtz equations, acoustics, time domain, boundary finite elements, integral equations, multipole method, parallel computations, retarded potentials.

Participant: Guillaume Sylvand.

The retarded potentials [50][53] method belongs to the state-of-the-art in time domain integral equation methods in acoustics. It is very accurate and unconditionally stable. Our aim is to use our expertise in fast multipole algorithms to speed-up this time marching solver and allow the treatment of much larger case. Basically, the TMM (Time domain Multipole Method) is a method to speed-up the computation of the influence of surfacic potentials on the surface. A large part of the method is similar to what has been done in the frequency domain during the last years. A prototype of an effective implementation of this algorithm is to be delivered before the end of the year.

6.1.2. Coupling of axisymmetric integral formulations

Key words: *Maxwell system, frequency domain, integral equation, multi-axisymmetric geometry, near field, multipole algorithm parallel computing.*

Participants: Nathalie Bartoli, Serge Piperno, Christelle Jamonac [Alcatel Space], Denis Pogarieloff [Alcatel Space].

In a joint work with Alcatel, we have proposed ways to accelerate the software Echo-light for the electromagnetic scattering of several axisymmetric objects with different symmetry axes. The basic shell script has been optimized and validated. The post processing was accelerated using the multipole method [28]. More precisely, the computation of the near field is done by integral equations and only axisymmetric objects are considered. From the knowledge of the currents at the surface of the object, we are interested in evaluating the fields in the vicinity of this object. Our approach is based on the multipole method, well known to compute very quickly some matrix-vector products in the Maxwell equations. Its efficiency is validated on numerical examples compared to some classical methods. The improvement is particularly interesting for the software Echo-light of Alcatel Space requiring a large amount of computation for the interaction between obstacles.

6.1.3. DGTD methods for the Maxwell equations on unstructured meshes

Key words: Maxwell system, time domain, structured mesh, locally refined mesh, conforming mesh, non-conforming mesh, finite volume method, discontinuous Galerkin method, stability.

Participants: Loula Fezoui, 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 [36] a Discontinuous Galerkin method for the numerical solution of the time-domain Maxwell equations on 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.

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

Key words: Maxwell system, time domain, structured mesh, locally refined mesh, conforming mesh, non-conforming mesh, finite volume method, discontinuous Galerkin method, stability.

Participants: Nicolas Canouet, Loula Fezoui, Serge Piperno, Stéphane Lanteri, 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-conforming meshes.

We have proposed [34] an explicit scheme based on a classical Discontinuous Galerkin formulation which is able to deal with structured non-conforming grids. We use a leap-frog time scheme coupled with a centered flux formula depending on a parameter α . Although the refinement rate is high between the coarse and the refined zones, the dispersion is very small. This method provides the conservation of a discrete energy on non-conforming grids ensuring the stability of the scheme.

We have also proposed [33] a hp-type Discontinuous Galerkin method (for the time domain solution of the Maxwell equations on conforming or non-conforming orthogonal grids. 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. We also analyze the dispersion error in the uniform mesh case.

6.1.5. Finite volume and discontinuous Galerkin type methods for frequency domain electromagnetics

Key words: Maxwell equations, frequency domain, unstructured mesh, finite volume, discontinuous Galerkin, cell centered scheme.

Participants: Hugo Fol, Stéphane Lanteri, Serge Piperno.

The goal of this study, that has started in October 2003 with the doctoral thesis of Hugo Fol, is to extend the finite volume [64] and discontinuous Galerkin [36] methods, previously designed for the numerical simulation of time domain problems, to the solution of the frequency domain Maxwell equations. As for time domain applications, we are interested in numerical methods that work with unstructured (tetrahedral) meshes. Such frequency domain finite volume and finite element methods lead to the inversion of a sparse (complex) linear system whose matrix operator may exhibit scale discrepancies in the coefficients due to the heterogeneity of the underlying medium as in the study of head tissues exposure to a radio-frequency field. Then, if an iterative solution method is preferred, it is necessary to devise appropriate preconditioners that take care of the matrix stiffness. This is an important component of our study that will lead us to investigate various strategies including domain decomposition based and algebraic multigrid preconditioning methods among others.

6.1.6. Computational bioelectromagnetics

Key words: mobile-phone, numerical dosimetry, thermal effects, MRI, image processing, Maxwell equations, structured mesh, finite difference time domain, unstructured mesh, finite volume time domain, finite element time domain.

Participants: Nicholas Ayache [project team Epidaure], Isabelle Bloch [ENST Paris], Jasmin Burguet [ENST Paris], Olivier Clatz [project team Epidaure], Maureen Clerc [project team Odyssée], Garry Cohen [project team Ondes], René De Seze [INERIS, center of Verneuil-en-Halatte], Claude Dedeban [France Télécom R&D, center of La Turbie], Hervé Delingette [project team Epidaure], Patrick Joly [project team Ondes], Stéphane Lanteri, Theodore Papadopoulo [project team Odyssée], Serge Piperno, Joe Wiart [France Télécom R&D, center of Issy-les-Moulineaux].

Project team Caiman is the coordinator of the HEADEXP [56] (realistic numerical modelling of human HEAD tissues EXPosure to electromagnetic waves from mobile phones) cooperative research initiative started in January 2003 for a duration of two years. The ever-rising diffusion of mobile phones has determined an increased concern for possible consequences of electromagnetic radiation on human health. In fact, when a cellular phone is in use, the transmitting antenna is placed very close to the user's head where a substantial part of the radiated power is absorbed. In the last decade, several research projects have been conducted in order to evaluate the biological effects resulting from human exposure to electromagnetic radiation. In this context, it is widely accepted that a distinction must be made between thermal and non-thermal biological effects. Thermal effects such as headaches have been reported by numerous users. Unfortunately, despite the high level of scientific activities undertaken in the recent years, one must recognize that, today, it is not yet possible to give a clear answer to the existence of non-thermal effects. Meanwhile, the number of mobile phone users raises continually and includes now representatives of all the age classes from children to the elderly.

Biological effects of microwave radiation have been investigated both from the experimental and numerical viewpoints. Concerning numerical modelling, the power absorption in a user head is computed using discretized models built from clinical MRI data. The great majority of such numerical studies have been conducted using the widely known FDTD (Finite Difference Time Domain) method due to Yee [9]. In this method, the whole computational domain is discretized using a structured (Cartesian) grid. Due to the possible straightforward implementation of the algorithm and the availability of computational power, FDTD is currently the leading method for numerical assessment of human exposure to electromagnetic waves. However, limitations are still seen, due to the rather difficult departure from the commonly used rectilinear grid and cell size limitations regarding very detailed structures of head tissues as well as of a handset which might be essential for reliable compliance testing. So far, little attention has been put to the application of numerical methods able

to deal with unstructured grids that is, FETD (Finite Element Time Domain) and FVTD (Finite Volume Time Domain) methods.

The HEADEXP project aims at filling the gap between human head MRI images and the efficient and accurate numerical modelling of the interaction of electromagnetic waves emitted by mobile phones on biological tissues. This is made possible by the development of appropriate image analysis tools and automated unstructured mesh generation tools for the construction of realistic discretized human head models. Then, the numerical simulation of the propagation of electromagnetic waves throughout the head tissues calls for modern unstructured mesh solvers of the time domain Maxwell equations. A particular emphasis is put on the ability of the solvers to take into account the heterogeneity of the electromagnetic characteristics (conductivity, permittivity, permeability tensors) of the underlying media.

6.1.7. Finite volume method for seismic wave propagation

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

Participants: Nathalie Glinsky-Olivier, Jean Virieux [Géosciences Azur].

Numerical methods for the propagation of seismic waves have been studied for many years. Most of these numerical codes rely on the finite-element or the finite-difference methods. Among the most popular schemes, we can cite the staggered-grid-finite-difference scheme proposed by J. Virieux [76] 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 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. Then, our objective is to solve these equations by finite volume methods on unstructured triangular meshes. This work is done in close collaboration with J. Virieux (Géosciences Azur, CNRS, Sophia Antipolis).

To study the P-SV wave propagation in an heterogeneous medium, we solve the first-order hyperbolic system of elastic wave equations (Virieux, 1986) in a vertical 2D medium, supposed linearly elastic and isotropic

$$\begin{cases}
\rho \frac{\partial v_x}{\partial t} = \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xz}}{\partial z}, \\
\rho \frac{\partial v_z}{\partial t} = \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{zz}}{\partial zz}, \\
\frac{\partial \tau_{xx}}{\partial t} = (\lambda + 2\mu) \frac{\partial v_x}{\partial x} + \lambda \frac{\partial v_z}{\partial z}, \\
\frac{\partial \tau_{zz}}{\partial t} = (\lambda + 2\mu) \frac{\partial v_z}{\partial z} + \lambda \frac{\partial v_x}{\partial x}, \\
\frac{\partial \tau_{xz}}{\partial t} = \mu \left(\frac{\partial v_x}{\partial z} + \frac{\partial v_z}{\partial x} \right)
\end{cases} (1)$$

where (v_x, v_z) are the two components of the velocity, $(\tau_{xx}, \tau_{zz}, \tau_{xz})$ are the components of the stress tensor, ρ is the density, λ and μ are the Lamé coefficients. This system having the same characteristics the Maxwell equations, we solve it using an adaptation of the second-order centered leap-frog scheme initially developed by M. Remaki [69]. The finite volumes are the elements of the triangular mesh.

The validation of this method is actually done on academic test cases. Firstly, we study the radial numerical displacement produced by an explosive source. This solution is compared to the analytical solution (provided by Géosciences Azur) of the propagation of a P-wave in an infinite medium. A second-test case, is the P-SV wave propagation in an homogeneous medium with an horizontal free surface. Solutions are compared to analytical seismograms for horizontal and vertical velocities [58]. Absorbing boundary conditions of PML type have also been implemented.

6.2. Computational fluid dynamics and related problems

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

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

Participants: Marc Bernacki, Serge Piperno, Gilbert Rogé [Dassault-Aviation].

We are currently studying the propagation of acoustic waves in a steady inviscid flow. This subject is directly related to many research themes of the project. Starting from a steady solution of 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.

We have proved in [31] a sufficient CFL-like stability condition for the L^2 stability of a second-order accurate finite volume scheme with centered fluxes for the solution of linearized Euler equations around an uniform flow in two or three space dimensions, with absorbing or reflecting boundary conditions. Some tests cases illustrate the potential of our scheme and we have widened our study with another test case within the framework of small perturbations around a non uniform steady flow.

Similarly, a discontinuous Galerkin method was applied [30]. We have used a centered mean approximation for the surface integrals and a leap-frog scheme for advancing in time. We have extended an absorbing boundary condition and a perfectly reflecting boundary condition. We have proved within the framework of an uniform flow a sufficient CFL-type L^2 stability condition. Some tests cases illustrate the large potential of our scheme. They are being compared with other numerical schemes in collaboration with Dassault-Aviation.

6.2.2. Auto-adaptive moving meshes

Key words: computational fluid dynamics, hyperbolic conservation laws, finite volume, unstructured dynamic mesh, mesh adaptation, variable topology, arbitrary Lagrangian-Eulerian formulation, arbitrary explicitimplicit scheme, monotonicity, TVD property.

Participants: Maud Mériaux-Poret, Serge Piperno.

We have developed a dynamic self-adaptative mesh method for solving hyperbolic linear or non-linear equations in one space dimension [35]. This method is based on two approaches: the first relies on a moving mesh process without changing mesh topology, the second consists in local and dynamical grid refinement-coarsening. We employ a finite volume scheme based on variable grids (moving and refined) with numerical Godunov-type flows. The main originality consists in writing a finite volume method on a variable topology, hence introducing appearing or disappearing finite volumes (and writing finite volume formulations on possibly void control volumes).

The solutions adopted in one-dimensional problems were chosen for their natural extension to more than one space dimension (for example, working on mesh vortices rather than on control volumes interfaces, which is quite equivalent in one dimension, but strongly different in more than one dimension). The one-dimensional work is now being extended in two space dimensions. The main difficulties are the handling of an unstructured topology with appearing and disappearing elements, and the application of constraints on mesh adaptation and motion ensuring that control volume do not get strictly negative (leading to more than one approximate value for some portions of the space).

6.2.3. Relaxation methods for the compressible Navier-Stokes equations

Key words: Navier-Stokes equations, relaxation method, entropy, Enskog-Chapman development, real gas, finite volume.

Participants: Nathalie Glinsky-Olivier, Alexandre Ern [CERMICS].

Gas flows arising in many engineering applications may be modeled using the compressible Navier-Stokes equations. These equations express the conservation of mass, momentum and energy and must be completed by a thermodynamic model providing the pressure and the temperature as a function of the conservative variables. The simplest model is that of a thermically perfect and calorifically perfect gas (TPCP, also referred to as polytropic ideal gas) in which, firstly, the pressure p is bilinear in the density ρ and the specific internal energy ε , $p = (\gamma - 1)\rho\varepsilon$, where $\gamma > 1$ is a constant (which is also the ratio between calorific capacities

at constant pressure and volume) and secondly, the temperature T is linear in ε and does not depend on the density : ε : $T = (\gamma - 1) \varepsilon / R$, where R is a constant given by the universal gas constant divided by the molecular mass of the gas. Because of its relative simplicity, the TPCP gas model has often been considered in applications. Many robust Navier-Stokes solvers based on this assumption exist; some of them involve finite volume discretizations in which the Riemann solver explicitly relies upon the TPCP gas model.

Many gas flows require a more elaborate thermodynamic model (for instance, polyatomic gas flows or high pressure flows). The pressure and the temperature are then nonlinear functions of the specific internal energy, while the pressure is still bilinear in the density and the temperature. Such gases will be referred to as thermically perfect (TP).

An attractive approach to incorporate complex pressure and temperature laws in the numerical simulation of gas flows is to consider a relaxation method. For the Euler equations, a relaxation method has been derived recently by Coquel and Perthame [45]. The authors consider an internal energy decomposition of the form $\varepsilon = \varepsilon_1 + \varepsilon_2$, where ε_1 is the internal energy of a fictitious gas (typically TPCP) and ε_2 a nonlinear perturbation. The relaxed Euler equations consist of the Euler equations for the fictitious gas coupled to a transport equation with a relaxation source term for ε_2 . From a theoretical viewpoint, the main result is that under some subcharacteristic conditions, the stability of the relaxation process is guaranteed via the positivity of a suitable entropy production. From a practical viewpoint, the key advantage of the relaxation method is that it provides a very effective means of extending TPCP solvers to tackle real gas flows. Numerical simulations using finite volume and WENO schemes have shown that the relaxation method can produce accurate solutions of inviscid real flows.

We have developed a relaxation method for the compressible Navier-Stokes equations. The main difference with the Euler equations is that because of the presence of diffusive fluxes, it is necessary to account not only for pressure relaxation but also for temperature relaxation. Keeping the internal energy splitting and the same sub-characteristic conditions as for the Euler equations, we introduce a weighted decomposition of the diffusive flux contribution to the energy balance of both the real and the fictitious gas as well as a global temperature for the relaxation system. We have first specified general consistency conditions guaranteeing that the original Navier-Stokes system is recovered at equilibrium. We have then addressed the stability of the relaxation system and obtained an estimate for the entropy production under certain conditions on the weighting coefficients and the global temperature. A first-order asymptotic analysis around equilibrium states has confirmed the stability results.

The new system is solved using a mixed finite volume/finite element method applicable to unstructured triangular meshes. The convective fluxes are evaluated using a Roe scheme of order 3, thanks to a combination of the MUSCL method and a β -scheme. For most complex test cases, a recent more robust limiter designed for the Euler equations [61] to yield fourth-order accuracy has also been implemented. The scheme is explicit in time and based on a four step Runge-Kutta method. The diffusive fluxes and the additional terms coming from the relaxation method are approximated by a P1 finite element interpolation technique.

Recently, two test cases have been studied thoroughly allowing publication of this work: the interaction of a temperature spot with a weak shock for high temperatures (for a TPCP gas and two different real gas) and the interaction of a reflected shock wave with the incident boundary layer in a shock tube for a Reynolds number Re = 200, with comparison with pushlished results [46][71].

6.3. Domain decomposition and coupling algorithms

6.3.1. Convergence analysis of additive Schwarz for the Euler equations

Key words: Euler equations, domain decomposition, finite volume, additive Schwarz, interface conditions.

Participants: Victorita Dolean [Université d'Evry et CMAP, École Polytechnique], Stéphane Lanteri, Frédéric Nataf [CMAP, École Polytechnique].

We are interested here in the design, analysis and evaluation of domain decomposition methods for the solution of algebraic systems resulting from the discretization of hyperbolic or mixed hyperbolic/parabolic systems of

partial differential equations such as those modelling compressible fluid mechanics problems. This activity is carried out in the context of a collaboration that was initiated during the doctoral thesis of Victorita Dolean [48]. This study is concerned with the convergence analysis of a domain decomposition method applied to the solution of the system of Euler equations. This method has previously been the subject of a numerical investigation in the context of the calculation of steady, 2D, compressible inviscid flows using a finite volume formulation on unstructured triangular meshes [49]. We recall that the proposed domain decomposition method relies on the formulation of a non-overlapping additive Schwarz algorithm which involves interface conditions that are Dirichlet conditions for the characteristic variables corresponding to incoming waves (often referred to as *natural* or *classical* interface conditions), thus taking into account the hyperbolic nature of the Euler equations. Here (see also [17]), the convergence of the additive Schwarz algorithm is first analyzed in the two- and three-dimensional continuous cases by considering the linearized equations and applying a Fourier analysis. We limit ourselves to the cases of two and three-subdomain decompositions with or without overlap and we obtain analytical expressions of the convergence rate of the Schwarz algorithm. Besides the fact that the algorithm is always convergent, surprisingly, there exist flow conditions for which the asymptotic convergence rate is equal to zero. Moreover, this behavior is independent of the space dimension. In a second step, we study the discrete counterpart of the non-overlapping additive Schwarz algorithm based on the implementation adopted [49] but assuming a finite volume formulation on a quadrangular mesh. We find out that the expression of the convergence rate is actually more characteristic of an overlapping additive Schwarz algorithm. Finally, updated numerical results confirm qualitatively the convergence behavior found analytically.

6.3.2. Hybrid multiplicative-additive preconditioning for general sparse linear systems

Key words: sparse linear system, domain decomposition, multiplicative Schwarz, additive Schwarz.

Participants: Stéphane Lanteri, Zhongze Li [Institute of Computational Mathematics, Chinese Academy of Sciences], Yousef Saad [University of Minnesota, USA].

This study has been initiated during the postdoctoral stay of Zhongze Li in the project team Caiman. The objective is to define an effective strategy to benefit from both the numerical efficiency of a multiplicative Schwarz algorithm and the parallel efficiency of an additive Schwarz variant. Let M_1 and M_2 be two preconditioners for the general sparse linear system Ax = b. Then, a composite preconditioner M can be obtained from M_1 and M_2 by combining them in a multiplicative way. The new preconditioner M is never generated explicitly. To apply M^{-1} to a vector z within a Krylov method iteration, the following procedure can be used [72]:

$$\begin{array}{rcl} y & \leftarrow & M_1^{-1}z \\ w & \leftarrow & z-Ay \\ y & \leftarrow & y+M_2^{-1}w \end{array}$$

Finding a combination that works somewhat optimally is not an easy task since, even when a combined preconditioner leads to fewer iterations for the convergence of the Krylov method than a standard preconditioner alone, it may be the case that the additional cost of computing r = z - Ay will outweigh the gain in iteration count. However, by exploiting features of distributed data structures for parallel sparse linear algebra [70], it is possible to significantly reduce the cost of the preconditioner through the use of an approximation of A for computing the residual r. This is the basis of the strategy that we are investigating and for which preliminary results have been presented to the Preconditioning 2003 conference [22].

6.3.3. Time and space multi-scale approaches for the 1D Maxwell equations

Key words: one-dimensional Maxwell system, time domain, finite volume method, discontinuous Galerkin method, centered flux, leap-frog time scheme, coupling algorithm, subcycling, stability, locally refined mesh.

Participant: Serge Piperno.

Aiming at solving the Maxwell equations in the time domain with locally refined grids (structured or unstructured), we study the possibility of using both space and time locally refined subdomains. We first

reviewed in [37] available numerical methods for the simulation of wave propagation (electromagnetics, acoustics) in one space dimension. We only deal with methods that can easily be extended to three space dimensions and unstructured grids (we compare them in one dimension with Yee's FDTD though) and which do conserve a discrete energy (they are genuinely non dissipative): like finite volumes and Galerkin Discontinuous methods. We investigate in details their properties and show it is possible to couple them on locally refined grids, both in time and space, and preserve their totally explicit nature. More precisely, this means that no implicit solution is required, which couples values of the unknowns at the interface between subdomains in the future (this is an additional constraint compared to the work of Fouquet [44]). The ideal coupling algorithm is still to be found, since some spurious reflections appear at the fictitious interface between subdomains (they get smaller as the number of discretization points per wavelength increases).

6.3.4. Plasmic environment of satellites

Key words: plasma, plasmic propulsion, magnetosphere, ionization, Vlasov-Poisson equations model coupling.

Participants: Martine Chane-Yook, Anne Nouri [LATP, CMI, Université de Provence], Frédéric Poupaud, Serge Piperno, Sébastien Clerc [Alcatel Space].

In collaboration with Alcatel Space, we study problems related to the electrostatic charge of satellites. These charges are received periodically from the sun and from the plasmic propulsors (which will be more used in a near future). The presence of these charged particles can lead to undesired potential gaps and eventually to electrostatic discharges (able to destroy some parts of solar energy generators). Following the pioneering work of Olivier Chanrion, which provided a software for the pseudo-transient two-dimensional axisymmetric Vlasov-Poisson equations, Martine Chane-Yook is aiming at developing a three-dimensional code, including the same features and starting from a basis developed by Sébastien Clerc at Alcatel. During the last year, the use of infinite elements at the outside boundary for the Poisson equation has been validated in three space dimensions. At the same time, the spatial volumic discharge was everywhere taken into account and computed (the currents as well), in order to determine a boundary layer thickness. Finally, an algorithm for the determination of the electric potential of conductors (starting from magnetospheric currents, themselves evaluated using back-trajectories) has been proposed.

6.3.5. Validation of NSI3FS on turbulent flows around an elementary bridge deck

Key words: *fluid-structure interaction, Navier-Stokes equations, incompressible fluid, vortex shedding, turbulence, k-\epsilon models, finite element.*

Participants: Emmanuel Briand, Serge Piperno.

The NSI3FS software has been used to study the wind effect on bridge decks and aeroelastic instabilities. In the continuity of validation works on elementary geometries which have shown a good aeroelastic coefficients prediction on laminar forced oscillation, we went on with turbulent flows [32]. On turbulent flows and fixed structure, the k- ϵ model used previously disclosed discrepancies in the recirculation zones, which cast shadows on the ability of the NSI3FS software to predict correct aeroelastic instability domains for high Reynolds structures. Simulations were launched to quantify this bad behavior and a two-layer model was proposed and tested. When the bridge deck is fixed (not moving), the obtained flows were encouraging and best recirculations were produced. Nevertheless the arising of low frequency vortex events imposed the use of big meshes and long time runs, even more for forced oscillations studies. In fact to correctly predict the aeroelastic coefficients, it seems necessary to describe very precisely the vortex dynamic and it is not sure that the averaged turbulence models are sufficiently accurate for such a description.

6.4. High performance parallel and distributed computing

6.4.1. Large-scale three-dimensional electromagnetics calculations

Key words: Maxwell equations, time domain, unstructured mesh, finite volume, discontinuous Galerkin, cell centered scheme, parallel computing, domain partitioning, message passing, MPI.

Participants: Loula Fezoui, Stéphane Lanteri, Serge Piperno.

The numerical simulation of realistic three-dimensional electromagnetics problems typically translates into the processing of very large amounts of data, especially for external problems. This is essentially the result of two antagonistic parameters: the characteristic space step of the mesh and the computational domain size. For high frequency phenomena, 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 partially cure this problem such as, for instance, the reduction of the computational domain size through the use of perfectly matched layers. 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 [64] and discontinuous Galerkin[36] methods for the solution of the time domain Maxwell equations on unstructured tetrahedral meshes, 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).

6.4.2. Parallel computing for medical image applications

Key words: cardiac activity, electro-mechanical model, neurosurgery, MRI, non-rigid registration, finite element, sparse linear system, additive Schwarz.

Participants: Nicholas Ayache [project team Epidaure], Olivier Clatz [project team Epidaure], Hervé Delingette [project team Epidaure], Stéphane Lanteri, Zhongze Li [Institute of Computational Mathematics, Chinese Academy of Sciences], Maxime Sermesant [project team Epidaure].

This year, we have initiated a collaboration with the project team Epidaure on various aspects of parallel computing for medical image applications. These studies are carried out in the framework of Yav++ [79] which is a generic platform for the visualization and processing of volumetric medical images. Project team Caiman has been involved in the ICEMA-2 [43] (Images of the Cardiac Electro-Mechanical Activity) cooperative research initiative. In ICEMA-2, Yav++ is the central platform for the development of an interactive deformable model used to simulate the cardiac electro-mechanical activity. During the postdoctoral stay of Zhongze Li in the project team Caiman, we have worked on the parallelization of this coupled electromechanical model. In this model, the heart is discretized using a tetrahedral mesh and its deformation calls for a finite element discretization method coupled to an implicit time integration scheme. As classically observed in similar situations, the solution of the sparse linear system obtained at each time step can exceed 80% of the total computing time of a beating heart cycle. Since the resulting coupled electro-mechanical problem aims at being used in a clinical environment, simulation time should be reduced as far as possible, especially when the discrete heart model relies on a high resolution tetrahedral mesh. This objective has been achieved, on one hand, through the parallelization of the underlying numerical kernels and, on the other hand, by using efficient linear algebra solvers. Both aspects have been considered using the PETSc [59] environment. In particular, the (restricted) additive Schwarz method of PETSc has been shown to be an effective preconditioning method for the linear systems characterizing the mechanical part of the beating-heart model.

Parallel computing can also benefit to other aspects of medical image processing. This is for instance the case for certain aspects of neurosurgery. Because of the accuracy required by a neurosurgical procedure, tracking intra-operative deformations is a challenging task. Therefore, clinical environment demand for fast non-rigid registration have to be met in a very near future. With regards to this need, we have been involved in a study whose general objective was to combine a patient-specific biomechanical model with block-matching features to register two MRI images of the same patient in a parallel implementation [24]. Compared to other intra-operative registration techniques, the proposed strategy puts in competition a viscoelastic mechanical regularization and block-matching features directly in a non-linear dynamic deformation process. Similarly to what has been discussed above, a notable reduction of the computing time can only be obtained by working both on the parallelization of the underlying image processing algorithms and on the improvement of the efficiency of numerical kernels.

6.4.3. Grid computing for the simulation of large-scale electromagnetic problems

Key words: Grid computing, high performance computing, parallel and distributed computing, ProActive java library, time-domain Maxwell equations.

Participants: Françoise Baude [project team Oasis], Denis Caromel [project team Oasis], Christian Delbe [project team Oasis], Nicolas Gama [project team Oasis], Saïd El Kasmi, Stéphane Lanteri, Romain Quilici [project team Oasis].

For scientific applications such as those considered in project team Caiman, the effective use of a heterogeneous, distributed, computing platform (i.e. a grid computing platform) requires new studies that must address several topics ranging from computer science concerns to more application related issues. This is for example the case for the development of numerical simulation tools that will be able to exploit several high performance computers (clusters of PCs, SMPs) geographically distributed. Indeed, 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. This characteristic could also be considered at the numerical modelling level through the design of hierarchical PDE solvers based on domain decomposition principles. However, grid computing also motivates the development of new generation collaborative tools that will allow several people located in different sites, to follow or even act on a running numerical simulation. Such a tool will ideally be based on different modules (PDE solver, visualization server, geometric modeler, etc.) that will be coupled and distributed on special purpose computers (clusters of PCs, SMPs, high performance graphical server).

Both of the applications discussed above could be designed as component based distributed applications and, in order to do so, it is necessary to adopt an appropriate programming paradigm. In 2002, we have initiated a collaboration with computer scientists from the project team Oasis at INRIA Sophia Antipolis whose general objective is to apply distributed object-oriented programming principles in the context of computational electromagnetism applications. Two main activities are considered so far.

For what concerns numerical simulation tools, we have developed JEM3D [57], an object-oriented time domain finite volume solver for the 3D Maxwell equations. This solver is built on top of a library of general classes for the development of numerical methods that rely on finite volume or finite element formulations on unstructured meshes. The underlying object-oriented model is able to deal with two-dimensional (2D) or three-dimensional (3D) problems, different types of discretization element (triangle, quadrangle, tetrahedron and hexahedron), the two main families of finite volume formulations (vertex centered and element or cell centered formulations), etc. For the implementation of JEM3D, the Java language has been selected. Several reasons have motivated this choice but the intrinsic distributed computing features of Java was the most important one. However, the practical use of such features is not an easy task for the non specialist. This is where the collaboration with the project team Oasis is particularly important due to the availability of the ProActive Java library [66] that greatly facilitates distributed programming (among other aspects) through the concept of active objects.

Beside this activity, we are also working on the development of a collaborative tool for the interactive visualization of three-dimensional numerical simulation results. Here, the objective is to define a framework that allows for the coupling of a parallel PDE solver with a visualization server. The visualization server is based on the VTK [77] (Visualization ToolKit). Ideally, this environment should be as generic as possible with regards to the characteristics of the parallel PDE solver. In practice, a client/server based paradigm is selected and implemented using a component based model. As previously, the development of this collaborative tool relies on the ProActive library.

6.4.4. Grid Computing for the solution of linear systems: application to integral equations

Key words: Maxwell equations, integral equations, fast multipole method, grid computing.

Participants: Guillaume Sylvand, Jessy Aipert.

We compute the scattering of an electromagnetic wave by an object using integral equations. The solution algorithm involves the inversion of a dense linear system. The starting point of this study is provided by a

software library (developed by EADS, CERFACS and the team) making it possible to solve linear systems on traditional parallel machines by direct methods (LU, LDL factorizations), iterative methods (CG, GMRES) and iterative multipole methods. The goal of this study is to adapt these various methods to the concept of computational grids, aiming at exploiting the idle periods of a great number of unused machines without being concerned by their heterogeneity of their dispersion. We show in [26] how this approach was considered and based on various existing works, and how it is possible to undertake the solution of large industrial computations on such computational grids. The resulting prototype software, AS_GRID, based on the EADS integral equation software AS_ELFIP, solves the Maxwell equations in the frequency domain using either direct, iterative or multipole solvers. The various matrix operations required for these three kind of algorithms have been implemented in a common framework to be treated on a computation grid. The idea it to cut the process into small sequential jobs, and to submit them on a grid. The first tests run on INRIA's cluster demonstrate the software's validity. Further tests should be done on a "real" grid managed by a specialized grid software.

7. Contracts and Grants with Industry

7.1. Electromagnetic vulnerability (INRIA-BERTIN)

Participants: Stéphane Lanteri, Serge Piperno, Loula Fezoui.

The team has taken an active part in the answer proposed by the group GERAC-BERTIN-INRIA to the open call of CEG (Centre d'Etudes de Gramat) on method hybridation solutions for the numerical solution of the three-dimensional Maxwell equations in the time-domain. Within this framework, the team was partially funded to promote the use of discontinuous finite volume and element methods, and show that complex computations (on possibly million-vertex unstructured tetrahedral meshes) on realistic configurations (electromagnetic vulnerability of metallic boxes designed to receive electronic devices). The final answer could lead to an important contract with CEG, including an actual industrialization of some of our softwares.

7.2. Fast multipole methods (INRIA-ENPC-EADS)

Participants: Guillaume Sylvand, Guillaume Alléon [Centre Commun de Recherche Louis Blériot, EADS].

EADS (CCR) has been supporting our research and development effort for many years, mainly concerning the Fast Multipole Methods and their multiple extensions. This year, a new extension to FMM in the time domain has been considered. The goal is to obtain the well known acceleration factor of the fast multipole methods to boundary element formulations of integral equations in the time domain.

7.3. Fast multipole method and acoustics (ENPC-Renault)

Participants: Guillaume Sylvand, Éric Duceau [Centre Commun de Recherche Louis Blériot, EADS], Sébastien Chaigne [Renault, Technocentre].

This short study aims at evaluating the possibility to include fast multiple methodology in the development process of Renault vehicles. Renault is interested in simulating acoustics in parts of vehicles (motor compartment, passenger space) with complex geometries and materials. The commercial code they use is limited in terms of number if degrees of freedom. The fast multipole method is currently the unique solution towards the solution of large integral equation systems.

7.4. Coupling axisymmetric integral formulations (INRIA-Alcatel)

Participants: Nathalie Bartoli, Serge Piperno, Christelle Jamonac [Alcatel Space], Denis Pogarieloff [Alcatel Space].

Alcatel Space has developed its own software for the solution of integral equations for electromagnetics in the frequency domain, for special configurations where only axisymmetric elements (with possibly non parallel

symmetry axes) are considered. These kind of simulations are mainly relevant for example for antennas and structures used on artificial satellites. In this study, ended at the beginning of the year, Nathalie Bartoli proposed an algorithm optimization for the iterative solution of coupled integral equations and, at the same time, provided an evaluation of possible gains given by the fast multipole methods for the computation of close and far fields and the interactions between objects (a multipole library developed at Cerfacs was used in that context).

7.5. Electrostatic charge of satellites (INRIA-Alcatel)

Participants: Martine Chane-Yook, Frédéric Poupaud, Serge Piperno, Sébastien Clerc [Alcatel Space], Thierry Dargent [Alcatel Space].

In collaboration with Alcatel, we continue our effort on the numerical simulation of electrostatic charges and discharges of artificial satellites. After the PhD thesis of Olivier Chanrion, Alcatel partially supports the PhD thesis of Martine Chane-Yook, on the three-dimensional simulation of the Vlasov-Poisson equations around realistic satellites, starting from an Alcatel software basis from Sébastien Clerc.

7.6. Multilayer modelling and integral equations (INRIA-FT R&D)

Participants: Serge Piperno, Christel Luquet-Piperno, Claude Dedeban [France Télécom R&D, center of La Turbie].

France Télécom R&D (center of La Turbie) has developed an internal software for the numerical solution of three-dimensional electromagnetics in the frequency domain by integral equations. In this context, they have developed but not yet validated an approach allowing the simulation of multi-layered patch antennas, without any discretization of all interfaces between different media. This software is being validated, extended to magnetic currents and will help us to make accurate numerical comparisons between integral equation solutions and our discontinuous finite element solutions based on volumic formulations.

8. Other Grants and Activities

8.1. Regional collaborations (Géosciences Azur)

8.1.1. Finite volume method for seismic wave propagation

Numerical methods for the propagation of seismic waves have been studied for many years. Most of these numerical codes relies on the finite-element or the finite-difference methods. Among the most popular schemes, we can cite the staggered-grid-finite-difference scheme proposed by J. Virieux [76] 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 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. Then, our objective is to solve these equations by finite volume methods on unstructured triangular meshes. This work is done in close collaboration with J. Virieux (Géosciences Azur, CNRS, Sophia Antipolis).

8.1.2. Plasmic environment of satellites (University of Provence)

In collaboration with Alcatel Space, we study the problems related to the electrostatic charge of satellites. These charges are received periodically from the sun and from the plasmic propulsors (which will be more used in a near future). The presence of these charged particles can lead to undesired potentials gaps and eventually to electrostatic discharges (able to destroy some parts of solar energy generators). Following the pioneering work of Olivier Chanrion, Martine Chane-Yook is aiming at developing a three-dimensional code, including the same features and starting from a basis developed by Sébastien Clerc at Alcatel. This PhD thesis work is advised by Anne Nouri (LATP, CMI, Université de Provence).

8.2. National collaborations (Cerfacs)

8.2.1. Parallel solution algorithms of integral equations

Participants: Guillaume Sylvand, Luc Giraud [Cerfacs], Bruno Carpentieri [Cerfacs], Francis Collino [Cerfacs], Florence Millot [Cerfacs].

We maintain an active collaboration with the team "parallel computing" of Cerfacs on iterative solvers (flexible GMRES and multiple solution with several right-hand-sides) and preconditioners (SPAI and LRU) using the fast multipole method we have developed.

8.2.2. Numerical simulation of wind effects on Civil Engineering structures (LCPC)

Participants: Serge Piperno, Emmanuel Briand, Dominique Chapelle [projet MACS], Frédéric Bourquin [LCPC].

In the framework of a LCPC (Laboratoire Central des Ponts et Chaussées) research theme on "Wind effects on Civil Engineering flexible structures" (this work also concerns CSTB - scientific and technical centre for buildings, and SETRA - service for technical studies on highways), Emmanuel Briand (technical engineer) went on with turbulent flows [32]. On turbulent flows and fixed structure, the k- ϵ model used previously disclosed discrepancies in the recirculation zones, which cast shadows on the ability of the NSI3FS software to predict correct aeroelastic instability domains for high Reynolds structures. Simulations were launched to quantify this erroneous behavior and a two-layer model was proposed and tested. When the bridge deck is fixed (not moving), the obtained flowfield computations were encouraging and best recirculations were produced. Nevertheless the arising of low frequency vortex events imposed the use of large meshes and long time runs, even more for forced oscillations studies. In fact to predict correctly the aeroelastic coefficients, it seems necessary to describe very precisely the vortex dynamic and it is not sure that the averaged turbulence models are able to do that. He also made a synthetic website reporting numerical simulations based on the software NS3IFS (cf. 5.2).

8.2.3. Biological fluid dynamics (RNRT RMOD)

Participants: Stéphane Lanteri, Serge Piperno, Marc Thiriet [project team Bang].

The working group on "biological fluid dynamics" [74] created by Marc Thiriet in year 2000 (including also researchers from project teams Bang, Gamma, Macs and Laboratoire Jacques-Louis Lions) has found an extension as an Ercim working group [75] globally named "Informatics and mathematics applied to interventional medicine". In this context, we take an small part of the RMOD RNRT project, coordinated by Air Liquide CRCD (Centre of Research Claude Delorme) which aims at developing a numerical morpho-functional simulator for the respiratory tract, more particularly for evaluation of performances of suspension inhalations. The main contribution of the team deals with actual three-dimensional parallel gas flow simulations (at small Mach numbers) on unstructured geometries provided by the group, which are to be compared with other numerical results (yielded by NS3IFS and commercial softwares - FIDAP/FLUENT - for instance).

8.2.4. Parallel computing for medical image applications (INRIA ARC ICEMA-2)

Key words: cardiac activity, electro-mechanical model, neurosurgery, MRI, non-rigid registration, finite element, sparse linear system, additive Schwarz.

Participants: Nicholas Ayache [project team Epidaure], Olivier Clatz [project team Epidaure], Hervé Delingette [project team Epidaure], Stéphane Lanteri, Zhongze Li [Institute of Computational Mathematics, Chinese Academy of Sciences], Maxime Sermesant [project team Epidaure].

Project team Caiman has been involved in the cooperative research initiative "ICEMA-2" [43], aiming at developing an interactive deformable model used to simulate the cardiac electro-mechanical activity. During the postdoctoral stay of Zhongze Li in the project team Caiman, we have worked on the parallelization of this coupled electro-mechanical model. In this model, the heart is discretized using a tetrahedral mesh and its deformation calls for a finite element discretization method coupled to an implicit time integration scheme. As classically observed in similar situations, the solution of the sparse linear system obtained at each time

step can exceeds 80% of the total computing time of a beating heart cycle. Since the resulting coupled electromechanical problem aims at being used in a clinical environment, simulation time should be reduced as far as possible, especially when the discrete heart model relies on a high resolution tetrahedral mesh. This objective has been achieved, on one hand, through the parallelization of the underlying numerical kernels and, on the other hand, by using efficient linear algebra solvers. Both aspects have been considered using the PETSc [59] environment. In particular, the (restricted) additive Schwarz method of PETSc has been shown to be an effective preconditioning method for the linear systems characterizing the mechanical part of the beating-heart model.

8.2.5. Computational bioelectromagnetics (INRIA ARC HEADEXP)

Key words: mobile-phone, numerical dosimetry, thermal effects, MRI, image processing, Maxwell equations, structured mesh, finite difference time domain, unstructured mesh, finite volume time domain, finite element time domain.

Participants: Nicholas Ayache [project team Epidaure], Isabelle Bloch [ENST Paris], Jasmin Burguet [ENST Paris], Olivier Clatz [project team Epidaure], Maureen Clerc [project team Odyssée], Garry Cohen [project team Ondes], René De Seze [INERIS, center of Verneuil-en-Halatte], Claude Dedeban [France Télécom R&D, center of La Turbie], Hervé Delingette [project team Epidaure], Patrick Joly [project team Ondes], Stéphane Lanteri, Theodore Papadopoulo [project team Odyssée], Serge Piperno, Joe Wiart [France Télécom R&D, center of Issy-les-Moulineaux].

Stéphane Lanteri is the coordinator of the HEADEXP [56] (realistic numerical modelling of human HEAD tissues EXPosure to electromagnetic waves from mobile phones) cooperative research initiative that has started in January 2003 and will last two years. The ever-rising diffusion of mobile phones has determined an increased concern for possible consequences of electromagnetic radiation on human health. In fact, when a cellular phone is in use, the transmitting antenna is placed very close to the user's head where a substantial part of the radiated power is absorbed. In the last decade, several research projects have been conducted in order to evaluate the biological effects resulting from human exposure to electromagnetic radiation. In this context, it is widely accepted that a distinction must be made between thermal and non-thermal biological effects. Thermal effects such as headaches have been reported by numerous users. Unfortunately, despite the high level of scientific activities undertaken in the recent years, one must recognize that, today, it is not yet possible to give a clear answer to the existence of non-thermal effects. Meanwhile, the number of mobile phone users raises continually and includes now representatives of all the age classes from children to elderly people.

The HEADEXP project aims at filling the gap between human head MRI images and the efficient and accurate numerical modelling of the interaction of electromagnetic waves emitted by mobile phones on biological tissues. This is made possible by the development of appropriate image analysis tools and automated unstructured mesh generation tools for the construction of realistic discretized human head models. Then, the numerical simulation of the propagation of electromagnetic waves throughout the head tissues calls for modern unstructured mesh solvers of the time domain Maxwell equations. A particular emphasis is put on the ability of the solvers to take into account the heterogeneity of the electromagnetic characteristics (conductivity, permittivity, permeability tensors) of the underlying media.

9. Dissemination

9.1. Scientific animation

9.1.1. Sophia Antipolis Club of parallel computing users

Stéphane Lanteri is co-chairing the local club of parallel computing users in Sophia Antipolis and PACA region [54].

9.1.2. Editing, scientific committees

Stéphane Lanteri is a nominated member of CNU 26th section at University Claude Bernard Lyon 1.

Serge Piperno is a supplementary elected member of INRIA's evaluation board and participated to CR2 local admissibility boards at Rocquencourt and Sophia Antipolis, to CR1 and DR2 national admissibility boards.

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

Serge Piperno is a member of the steering scientific committee of ONERA's federative research project "Couplage de Codes de Calcul Scientifique".

9.2. Teaching

- *Introduction au calcul parallèle*, Stéphane Lanteri, "Mastère de Mécanique Numérique", École Nationale Supérieure des Mines de Paris (18h).
- Calcul numérique parallèle, Stéphane Lanteri, École Supérieure des Sciences Informatiques, filière Calcul Scientifique pour l'Ingénieur (31h).
- Équations intégrales, Interactions fluide-structure, Électromagnétisme, Serge Piperno, "Mastère de Mécanique Numérique", École Nationale Supérieure des Mines de Paris (18h).
- Aéroélasticité, Serge Piperno, Ecole de Printemps de Mécanique des Fluides Numérique, CNRS (4h).
- Organization by Serge Piperno of an opening week at INRIA Sophia Antipolis pour ENPC students.
- Organization by Anne Nouri, Frédéric Poupaud and Serge Piperno of "Journée simulation numérique pour les plasmas", CIRM, May 23-24.

9.3. Master and PhD students supervision

9.3.1. PhD theses defended in 2003 in the project team

- Nicolas Canouet, Schémas multi-échelles pour la résolution numérique des équations de Maxwell, Thèse de l'ENPC, soutenue le 15 décembre. Jury : Loula Fezoui et Serge Piperno (codirecteurs), Peter Monk (rapporteur), Éliane Bécache (rapporteur), Claude Dedeban, Isabelle Terrasse, Jean-Michel Ghidaglia.
- Stéphane Lanteri, Méthodes numériques performantes en maillages non-structurés et applications en mécanique des fluides compressibles, Habilitation à Diriger des Recherches, Université de Nice-Sophia Antipolis, soutenue le 5 décembre. Jury : Olivier Pironneau (rapporteur), David Keyes (rapporteur), Frédéric Poupaud, Jacques Blum, Rémi Abgrall, Frédéric Desprez.

9.3.2. Ongoing PhD theses in the project team

- 1. Marc Bernacki, Schémas en volumes finis avec flux centrés appliqués à l'aéroacoustique, ENPC
- 2. Martine Chane-Yook, Modélisation et simulation 3D de la charge d'un satellite en environnement plasmique, université de Provence.
- 3. Maud Mériaux-Poret, Méthodes en maillages mobiles auto-adaptatifs pour des systèmes hyperboliques en une et deux dimensions d'espace Application aux interactions fluide-structure, ENPC
- 4. Hugo Fol, Couplage de schémas en volumes finis et de méthodes intégrales pour la propagation d ondes électromagnétiques, acoustiques et sismiques, Université de Nice-Sophia Antipolis.

9.3.3. Supervision activity

- 1. Loula Fezoui has supervised the PhD of Nicolas Canouet.
- Serge Piperno was second advisor for the thesis of Nicolas Canouet. He is supervising the theses of Marc Bernacki and Maud Poret, and co-supervising the one of Hugo Fol.
- 3. Stéphane Lanteri has supervised the post-doctoral research of Zhongze Li. He is supervising the action of Saïd El Kasmi and is co-supervisor of the thesis of Hugo Fol.

9.3.4. Training in the project team

 Jessy Aipert, "GRID Computing pour la résolution de systèmes linéaires: Application aux calculs de diffraction électromagnétique", DESS "Calcul Scientifique et Applications", University of Bordeaux 1.

9.4. Post-doctoral assistants, technical staff

- Nathalie Bartoli, in a financially supported collaboration with Alcatel Space, in post-doctoral
 position till 2/1. Her contribution concerned the optimization and the validation of an Alcatel Space
 software of electromagnetic wave scattering past several axisymmetric objects. The study also dealt
 with the investigation on the possibility to accelerate computations using fast multipole methods
 (also in collaboration with Cerfacs).
- Emmanuel Briand, as technical staff, in the framework of the LCPC research theme « Wind Effects on Civil Engineering Structures », till 2/1. Emmanuel Briand made a browsable synthesis of numerical results obtained with the NS3IFS software.
- Zhongze Li, in postdoctoral position, within ARC ICEMA-2, till 9/1. He contributed to the acceleration of the software Yav++ developed at INRIA for the numerical simulation of the electromechanical cardiac activity, through parallelization of numerical methods and use of efficient solution algorithms.
- Saïd El Kasmi, as junior technical staff, is contributing to our effort on Grid Computing for the simulation of large-scale electromagnetic problems, in strong collaboration with the Oasis project team.

9.5. Invitations, seminars, communications

- Communications of Nicolas Canouet and Guillaume Sylvand at Waves 2003.
- Posters of Nicolas Canouet, Serge Piperno, Stéphane Lanteri, Loula Fezoui at NUMELEC 2003, 4th Conference on Numerical Methods in Electromagnetism, Octobre 28-30.
- Invited lecture of Serge Piperno at the colloquium "Fluid-structure coupling problems and non-linear PDEs", University of Haute Alsace, Mulhouse, october 9-10.
- Seminars of Saïd El Kasmi and Jessy Aipert at INRIA Sophia Antipolis in a "Day on use of INRIA's cluster", July, 9.
- Seminar of Martine Chane-Yook in a "Tropics/Caiman crossed seminar" at INRIA Sophia Antipolis, July 1.
- Presentation of Marc Bernacki in a closed "Computational Aeroacoustics Seminar" with Dassault-Aviation, October 29.

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