



INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

*Project-Team nachos*

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

*Sophia Antipolis - Méditerranée*

Theme : Computational models and simulation

*Activity*  
*R* *eport*

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## 2. Overall Objectives

### 2.1. Overall objectives

The research activities of the NACHOS project-team are concerned with the formulation, analysis and evaluation of numerical methods and high performance resolution algorithms for the computer simulation of evolution problems in complex domains and heterogeneous media. The team concentrates its activities on mathematical models that rely on first order linear systems of partial differential equations (PDEs) with

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

In the case of electrodynamics, the mathematical model of interest is the full system of unsteady Maxwell equations [38] which is a first-order hyperbolic linear system of PDEs (if the underlying propagation media is assumed to be linear). This system can be numerically solved using so-called time domain methods among which the Finite Difference Time Domain (FDTD) method introduced by K.S. Yee [45] in 1996 is the most popular and which often serves as a reference method for the works of the team. In the vast majority of existing time domain methods, time advancing relies on an explicit time scheme. For certain types of problems, a time harmonic evolution can be assumed leading to the formulation of the frequency domain Maxwell equations whose numerical resolution requires the solution of a linear system of equations (i.e in that case, the numerical method is naturally implicit). Heterogeneity of the propagation media is taken into account in the Maxwell equations through the electrical permittivity, the magnetic permeability and the electric conductivity coefficients. In the general case, the electrical permittivity and the magnetic permeability are tensors whose entries depend on space (i.e heterogeneity in space) and frequency (i.e physical dispersion and dissipation). In the latter case, the time domain numerical modeling of such materials requires specific techniques in order to switch from the frequency evolution of the electromagnetic coefficients to a time dependency. Moreover, there exists several mathematical models for the frequency evolution of these coefficients (Debye model, Lorentz model, etc.).

In the case of elastodynamics, the mathematical model of interest is the system of elastodynamic equations [34] for which several formulations can be considered such as the velocity-stress system. For this system, as with Yee's scheme for time domain electromagnetics, one of the most popular numerical method is the finite difference method proposed by J. Virieux [44] in 1986. Heterogeneity of the propagation media is taken into account in the elastodynamic equations through the Lamé and mass density coefficients. A frequency dependence of the Lamé coefficients allows to take into account physical attenuation of the wave fields and characterizes a viscoelastic material. Again, several mathematical models exist for expressing the frequency evolution of the Lamé coefficients.

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

## 3. Scientific Foundations

### 3.1. High order discretization methods

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

- Accuracy. The foreseen numerical methods should ideally rely on discretization techniques that best fit to the geometrical characteristics of the problems at hand. For this reason, the team focuses on methods working on unstructured, locally refined, even non-conforming, simplicial meshes. These methods should also be capable to accurately describe the underlying physical phenomena that may involve highly variable space and time scales. With reference to this characteristic, two main strategies are possible: adaptive local refinement/coarsening of the mesh (i.e  $h$ -adaptivity) and adaptive local variation of the interpolation order (i.e  $p$ -adaptivity). Ideally, these two strategies are combined leading to the so-called  $hp$ -adaptive methods.
- Numerical efficiency. The simulation of unsteady problems most often rely on explicit time integration schemes. Such schemes are constrained by a stability criteria linking the space and time discretization parameters that can be very restrictive when the underlying mesh is highly non-uniform (especially for locally refined meshes). For realistic 3D problems, this can represent a severe limitation with regards to the overall computing time. In order to improve this situation, one possible approach which is considered by the team consists in resorting to an implicit time scheme in regions of the computational domain where the underlying mesh is refined while an explicit time scheme is applied to the remaining part of the domain. The resulting hybrid explicit-implicit time integration strategy raises several challenging questions concerning both the mathematical analysis (stability and accuracy, especially for what concern numerical dispersion), and the computer implementation on modern high performance systems (data structures, parallel computing aspects). On the other hand, for implicit time integration schemes on one hand, and for the numerical treatment of time harmonic problems on the other hand, numerical efficiency also refers to a foreseen property of linear system solvers.
- Computational efficiency. Despite the ever increasing performances of microprocessors, the numerical simulation of realistic 3D problems is hardly performed on a high-end workstation and parallel computing is a mandatory path. Realistic 3D wave propagation problems lead to the processing of very large volumes of data. The latter results from two combined parameters: the size of the mesh i.e the number of mesh elements, and the number of degrees of freedom per mesh element which is itself linked to the degree of interpolation and to the number of physical variables (for systems of partial differential equations). Hence, numerical methods must be adapted to the characteristics of modern parallel computing platforms taking into account their hierarchical nature (e.g multiple processors and multiple core systems with complex cache and memory hierarchies). Appropriate parallelization strategies need to be designed that combine distributed memory and shared memory programming paradigms. Moreover, maximizing the effective floating point performances will require the design of numerical algorithms that can benefit from the optimized BLAS linear algebra kernels.

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

geometries, etc.), the DG method has other nice properties which explain the renewed interest it gains in various domains in scientific computing as witnessed by books or special issues of journals dedicated to this method [31]- [32]- [33]- [37]:

- it is naturally adapted to a high order approximation of the unknown field. Moreover, one may increase the degree of the approximation in the whole mesh as easily as for spectral methods but, with a DG method, this can also be done very locally. In most cases, the approximation relies on a polynomial interpolation method but the DG method also offers the flexibility of applying local approximation strategies that best fit to the intrinsic features of the modeled physical phenomena.
- When the discretization in space is coupled to an explicit time integration method, the DG method leads to a block diagonal mass matrix independently of the form of the local approximation (e.g. the type of polynomial interpolation). This is a striking difference with classical, continuous finite element formulations. Moreover, the mass matrix is diagonal if an orthogonal basis is chosen.
- It easily handles complex meshes. The grid may be a classical conforming finite element mesh, a non-conforming one or even a hybrid mesh made of various elements (tetrahedra, prisms, hexahedra, etc.). The DG method has been proved to work well with highly locally refined meshes. This property makes the DG method more suitable to the design of a  $hp$ -adaptive solution strategy (i.e. where the characteristic mesh size  $h$  and the interpolation degree  $p$  changes locally wherever it is needed).
- It is flexible with regards to the choice of the time stepping scheme. One may combine the DG spatial discretization with any global or local explicit time integration scheme, or even implicit, provided the resulting scheme is stable,
- it is naturally adapted to parallel computing. As long as an explicit time integration scheme is used, the DG method is easily parallelized. Moreover, the compact nature of DG discretization schemes is in favor of high computation to communication ratio especially when the interpolation order is increased.

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

For the numerical solution of the time domain Maxwell equations, we have first proposed a non-dissipative high order DG method working on unstructured conforming simplicial meshes [11]-[3]. This DG method combines a central numerical flux function for the approximation of the integral term at an interface between two neighboring elements with a second order leap-frog time integration scheme. Moreover, the local approximation of the electromagnetic field relies on a nodal (Lagrange type) polynomial interpolation method. Recent achievements in the framework of the team deal with the extension of these methods towards non-conforming meshes and  $hp$ -adaptivity [9]-[10], their coupling with hybrid explicit/implicit time integration schemes in order to improve their efficiency in the context of locally refined meshes [14], and their extension to the numerical resolution of the elastodynamic equations modeling the propagation of seismic waves [4].

## 3.2. Domain decomposition methods

Domain Decomposition (DD) methods are flexible and powerful techniques for the parallel numerical solution of systems of PDEs. As clearly described in [41], they can be used as a process of distributing a computational domain among a set of interconnected processors or, for the coupling of different physical models applied in different regions of a computational domain (together with the numerical methods best adapted to each model) and, finally as a process of subdividing the solution of a large linear system resulting from the discretization



of a system of PDEs into smaller problems whose solutions can be used to devise a parallel preconditioner or a parallel solver. In all cases, DD methods (1) rely on a partitioning of the computational domain into subdomains, (2) solve in parallel the local problems using a direct or iterative solver and, (3) call for an iterative procedure to collect the local solutions in order to get the global solution of the original problem. Subdomain solutions are connected by means of suitable transmission conditions at the artificial interfaces between the subdomains. The choice of these transmission conditions greatly influences the convergence rate of the DD method. One generally distinguishes three kinds of DD methods:

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

Schwarz algorithms have enjoyed a second youth over the last decades, as parallel computers became more and more powerful and available. Fundamental convergence results for the classical Schwarz methods were derived for many partial differential equations, and can now be found in several books [41]- [40]- [43].

The research activities of the team on this topic aim at the formulation, analysis and evaluation of Schwarz type domain decomposition methods in conjunction with discontinuous Galerkin approximation methods on unstructured simplicial meshes for the solution of time domain and time harmonic wave propagation problems. Ongoing works in this direction are concerned with the design of non-overlapping Schwarz algorithms for the solution of the time harmonic Maxwell equations. A first achievement has been a Schwarz algorithm for the time harmonic Maxwell equations, where a first order absorbing condition is imposed at the interfaces between neighboring subdomains [7]. This interface condition is equivalent to a Dirichlet condition for characteristic variables associated to incoming waves. For this reason, it is often referred as a natural interface condition. Beside Schwarz algorithms based on natural interface conditions, the team also investigates algorithms that make use of more effective transmission conditions [8]. From the theoretical point of view, this represents a much more challenging goal since most of the existing results on optimized Schwarz algorithms have been obtained for scalar partial differential equations. For the considered systems of PDEs, the team plan to extend the techniques for obtaining optimized Schwarz methods previously developed for the scalar PDEs to systems of PDEs. This can be done by using appropriate relationships between systems and equivalent scalar problems [6].

### 3.3. High performance numerical computing

Beside basic research activities related to the design of numerical methods and resolution algorithms for the wave propagation models at hand, the team is also committed to demonstrate the benefits of the proposed numerical methodologies in the simulation of challenging three-dimensional problems pertaining to computational electromagnetics and computation geoseismics. For such applications, parallel computing is a mandatory path. Nowadays, modern parallel computers most often take the form of clusters of heterogeneous

multiprocessor systems, combining multiple core CPUs with accelerator cards (e.g Graphical Processing Units - GPUs), with complex hierarchical distributed-shared memory systems. Developing numerical algorithms that efficiently exploit such high performance computing architectures raises several challenges, especially in the context of a massive parallelism. In this context, current efforts of the team are towards the exploitation of multiple levels of parallelism (computing systems combining CPUs and GPUs) through the study of hierarchical SPMD (Single Program Multiple Data) strategies for the parallelization of unstructured mesh based solvers.

## 4. Application Domains

### 4.1. Computational electromagnetics and bioelectromagnetics

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

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

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

- first, from the numerical modeling point of view, the interaction between electromagnetic waves and biological tissues exhibit the three sources of complexity listed above and are thus particularly challenging for pushing one step forward the state-of-the art of numerical methods for computational electromagnetics. The propagation media is strongly heterogeneous and the electromagnetic characteristics of the tissues are frequency dependent. Interfaces between tissues have rather complicated shapes that cannot be accurately discretized using Cartesian meshes. Finally, the source of the signal often takes the form of a complicated device (e.g a mobile phone or an antenna array).

- second, the study of the interaction between electromagnetic waves and living tissues finds applications of societal relevance such as the assessment of potential adverse effects of electromagnetic fields or the utilization of electromagnetic waves for therapeutic or diagnostic purposes. It is widely recognized nowadays that numerical modeling and computer simulation of electromagnetic wave propagation in biological tissues is a mandatory path for improving the scientific knowledge of the complex physical mechanisms that characterize these applications.

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

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

PIC codes have become a major research tool in different areas of physics involving self-consistent interaction of charged particles, in particular in plasma and beam physics. Two-dimensional simulations have now become very reliable and can be used as well for qualitative as for quantitative results that can be compared to experiments with good accuracy. As the power of supercomputers was increasing three dimensional codes have been developed in the recent years. However, even in order to just make qualitative 3D simulations, an enormous computing power is required. Today's and future massively parallel supercomputers allow to envision the simulation of realistic problems involving complex geometries and multiple scales. In order to achieve this efficiently, new numerical methods need to be designed. This includes the investigation of high order Maxwell solvers, the use of hybrid grids with several homogeneous zones having their own structured or unstructured mesh type and size, and a fine analysis of load balancing issues. These issues are studied in details in the team in the context of discontinuous Galerkin discretization methods on simplicial meshes. Indeed, the team is one of the few groups worldwide [39] considering the development of parallel unstructured mesh PIC solvers for the three-dimensional Vlasov-Maxwell equations.

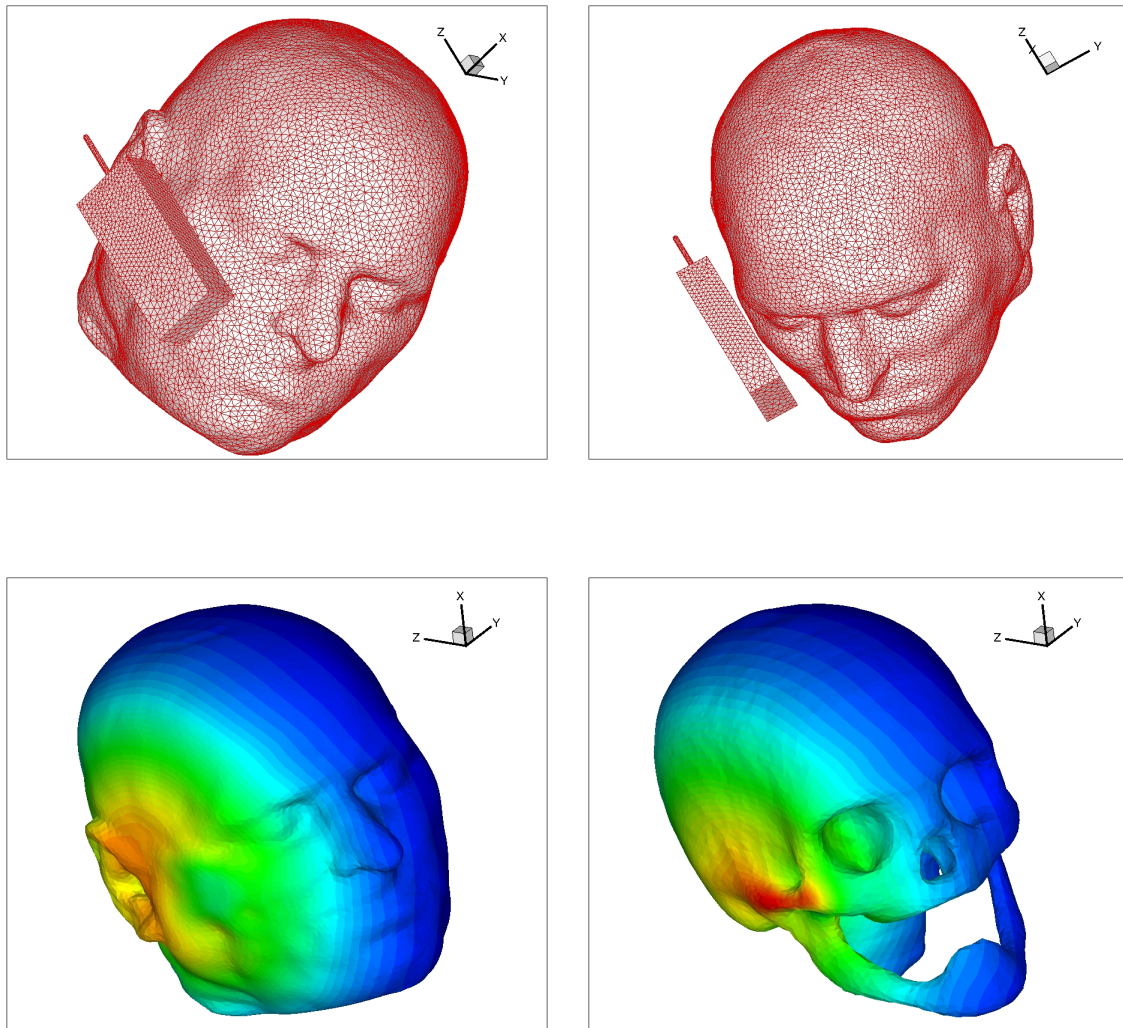


Figure 1. Exposure of head tissues to an electromagnetic wave emitted by a localized source Top figures: surface triangulations of the skin and the skull. Bottom figures: contour lines of the amplitude of the electric field.

## 4.2. Computational geoseismics

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

To understand the basic science of earthquakes and to help engineers better prepare for such an event, scientists want to identify which regions are likely to experience the most intense shaking, particularly in populated sediment-filled basins. This understanding can be used to improve building codes in high risk areas and to help engineers design safer structures, potentially saving lives and property. In the absence of deterministic earthquake prediction, forecasting of earthquake ground motion based on simulation of scenarios is one of the most promising tools to mitigate earthquake related hazard. This requires intense modeling that meets the spatial and temporal resolution scales of the continuously increasing density and resolution of the seismic instrumentation, which record dynamic shaking at the surface, as well as of the basin models. Another important issue is to improve our physical understanding of the earthquake rupture processes and seismicity. Large scale simulations of earthquake rupture dynamics, and of fault interactions, are currently the only means to investigate these multi-scale physics together with data assimilation and inversion. High resolution models are also required to develop and assess fast operational analysis tools for real time seismology and early warning systems. Modeling and forecasting earthquake ground motion in large basins is a challenging and complex task. The complexity arises from several sources. First, multiple scales characterize the earthquake source and basin response: the shortest wavelengths are measured in tens of meters, whereas the longest measure in kilometers; basin dimensions are on the order of tens of kilometers, and earthquake sources up to hundreds of kilometers. Second, temporal scales vary from the hundredth of a second necessary to resolve the highest frequencies of the earthquake source up to as much as several minutes of shaking within the basin. Third, many basins have a highly irregular geometry. Fourth, the soil's material properties are highly heterogeneous. And fifth, geology and source parameters are observable only indirectly and thus introduce uncertainty in the modeling process. Because of its modeling and computational complexity and its importance to hazard mitigation, earthquake simulation is currently recognized as a grand challenge problem.

Numerical methods for the propagation of seismic waves have been studied for many years. Most of existing numerical software rely on finite element or finite difference methods. Among the most popular schemes, one can cite the staggered grid finite difference scheme proposed by Virieux [44] 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 [45] for the solution of the Maxwell equations. The use of cartesian meshes is a limitation for such codes especially when it is necessary to incorporate surface topography or curved interface. In this context, our objective is to solve these equations by finite volume or discontinuous Galerkin methods on unstructured triangular (2D case) or tetrahedral (3D case) meshes. Our first achievement in this domain has been a centered finite volume method on unstructured simplicial meshes [2]-[1] for the simulation of dynamic fault rupture, which has been validated and evaluated on various problems, ranging from academic test cases to realistic situations. More recently, a high order discontinuous Galerkin method has been proposed for the resolution of the systems of 2D and 3D elastodynamic equations[4].

## 5. Software

## 5.1. MAXW-DGTD

**Participants:** Stéphane Lanteri [correspondant], Loula Fezoui.

MAXW-DGTD is a software suite for the solution of the 2D and 3D Maxwell equations in the time domain, modeling electromagnetic wave propagation in heterogeneous, possibly lossy media. MAXW-DGTD implements a high order discontinuous Galerkin method on unstructured triangular (2D case) or tetrahedral (3D case) meshes based on nodal polynomial interpolation. This discontinuous Galerkin method combines a centered scheme for the evaluation of numerical fluxes at a face common to neighboring elements, with an explicit Leap-Frog time scheme. The 3D software and the underlying algorithms are adapted to distributed memory parallel computing platforms.

- AMS: AMS 35L50, AMS 35Q60, AMS 35Q61, AMS 65N08, AMS 65N30, AMS 65M60
- Keywords: Computational electromagnetics, Maxwell equations, discontinuous Galerkin, tetrahedral mesh.
- OS/Middleware: Linux
- Required library or software: MPI (Message Passing Interface)
- Programming language: Fortran 77/95

## 5.2. MAXW-DGFD

**Participants:** Mohamed El Bouajaji, Stéphane Lanteri [correspondant].

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

- AMS: AMS 35L50, AMS 35Q60, AMS 35Q61, AMS 65N08, AMS 65N30, AMS 65M60
- Keywords: Computational electromagnetics, Maxwell equations, discontinuous Galerkin, tetrahedral mesh.
- OS/Middleware: Linux
- Required library or software: MPI (Message Passing Interface)
- Programming language: Fortran 77/95

## 5.3. MAXWPIC-DGTD

**Participants:** Loula Fezoui [correspondant], Stéphane Lanteri.

MAXWPIC-DGTD is a software for for the solution of the 2D and 3D systems of coupled Maxwell-Vlasov equations in the time domain. This software is based on the MAXW-DGTD software and a Particle-In-Cell (PIC) method for the solution of the Vlasov equation. The underlying algorithms are adapted to distributed memory parallel computing platforms.

- AMS: AMS 35L50, AMS 35Q60, AMS 35Q61, AMS 35Q70, AMS 65N08, AMS 65N30, AMS 65M60
- Keywords: Computational electromagnetics, Maxwell equations, discontinuous Galerkin, tetrahedral mesh.
- OS/Middleware: Linux
- Required library or software: MPI (Message Passing Interface)
- Programming language: Fortran 77/95

## 5.4. SISMO-DGTD

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

SISMO-DGTD is a software for the solution of the 2D and 3D velocity-stress equations in the time domain. This software implements a high order discontinuous Galerkin method on unstructured triangular (2D case) or tetrahedral (3D case) meshes. The local approximation of the velocity and stress components currently relies on a nodal (Lagrange type) polynomial interpolation method. The underlying algorithms are adapted to distributed memory parallel computing platforms.

- AMS: AMS 35L50, AMS 35Q74, AMS 35Q86, AMS 65N08, AMS 65N30, AMS 65M60
- Keywords: Computational geoseismics, elastodynamic equations, discontinuous Galerkin, tetrahedral mesh.
- OS/Middleware: Linux
- Required library or software: MPI (Message Passing Interface)
- Programming language: Fortran 77/95

## 6. New Results

### 6.1. Discontinuous Galerkin methods for the Maxwell equations

#### 6.1.1. DGTD- $\mathbb{P}_p$ method based on hierarchical polynomial interpolation

**Participants:** Loula Fezoui, Joseph Charles, Stéphane Lanteri.

The goal of this study is to design a high order DGTD- $\mathbb{P}_p$  method based on hierarchical polynomial basis expansions on simplicial elements in view of the development of a  $p$ -adaptive solution strategy. As a first step, we consider using the conforming hierarchical polynomial basis expansions described in [42].

#### 6.1.2. DGTD- $\mathbb{P}_p\mathbb{Q}_k$ method on multi-element meshes

**Participants:** Clément Durochat, Stéphane Lanteri, Mark Lorient [Distene, Pôle Teratec, Bruyères-le-Chatel].

In this work we have designed a DGTD- $\mathbb{P}_p\mathbb{Q}_k$  method formulated on conforming hybrid quadrangular/triangular meshes [29]-[23]. This is part of an ongoing effort which aims at developing a flexible DGTD- $\mathbb{P}_p\mathbb{Q}_k$  method on non-conforming hybrid hexahedral/tetrahedral meshes for the numerical simulation of 3D time domain electromagnetic wave propagation problems.

#### 6.1.3. DGTD- $\mathbb{P}_p$ method for dispersive materials

**Participants:** Claire Scheid, Maciej Klemm [Electromagnetics Group, University of Bristol, UK], Stéphane Lanteri.

We have started the development of a numerical methodology combining a high order DGTD- $\mathbb{P}_p$  method on triangular meshes with an auxiliary differential equation modeling the time evolution of the electric polarization for a dispersive medium of Debye type. This work comprises both theoretical aspects (stability and convergence analysis) of the resulting DGTD- $\mathbb{P}_p$  method for the time domain Maxwell equations for dispersive media, and application aspects.

#### 6.1.4. DGFD- $\mathbb{P}_p$ method for the frequency domain Maxwell equations

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

This study is concerned with the development of an arbitrary high order discontinuous Galerkin frequency domain DGFD- $\mathbb{P}_p$  method on triangular or tetrahedral meshes for solving the 2D and 3D time harmonic Maxwell equations. Moreover, as a first step towards the development of a  $p$ -adaptive DGFD- $\mathbb{P}_p$  method, the approximation order is allowed to be defined at the element level based on a local geometrical criterion.

### 6.1.5. Hybridizable DGTD- $\mathbb{P}_p$ and DGFD- $\mathbb{P}_p$ methods

**Participants:** Stéphane Lanteri, Liang Li, Ronan Perrussel [Ampère Laboratory, Ecole Centrale de Lyon].

One major drawback of DG methods is their intrinsic cost due to the very large number of globally coupled degrees of freedom as compared to classical high order conforming finite element methods. Different attempts have been made in the recent past to improve this situation and one promising strategy has been recently proposed by Cockburn *et al.* [35] in the form of so-called hybridizable DG formulations. The distinctive feature of these methods is that the only globally coupled degrees of freedom are those of an approximation of the solution defined only on the boundaries of the elements. The present work is concerned with the study of such hybridizable DG methods for the solution of the system of Maxwell equations in the time domain when the time integration relies on an implicit scheme, or in the frequency domain. Preliminary results have been presented in [27].

## 6.2. Discontinuous Galerkin methods for the elastodynamic equations

### 6.2.1. DGTD- $\mathbb{P}_p$ method for the elastodynamic equations

**Participants:** Nathalie Glinsky, Fabien Peyrusse.

We continue developing high order non-dissipative discontinuous Galerkin methods on simplicial meshes (triangles in the 2D case and tetrahedra in the 3D case) for the numerical solution of the first order hyperbolic linear system of elastodynamic equations. These methods share some ingredients of the DGTD- $\mathbb{P}_p$  methods developed by the team for the time domain Maxwell equations among which, the use of nodal polynomial (Lagrange type) basis functions, a second order leap-frog time integration scheme and a centered scheme for the evaluation of the numerical flux at the interface between neighboring elements. The resulting DGTD- $\mathbb{P}_p$  methods have been validated and evaluated in detail in the context of propagation problems in both homogeneous and heterogeneous media including problems for which analytical solutions can be computed. Particular attention was given to the study of the mathematical properties of these schemes such as stability, convergence and dispersion. Recent results concern the numerical assessment of site effects especially topographic effects. The study of measurements and experimental records proved that seismic waves can be amplified at some particular locations of a topography. Numerical simulations are exploited here to understand further and explain this phenomenon. The DGTD- $\mathbb{P}_p$  method has been applied to a realistic topography of Rognes area (where the Provence earthquake occurred in 1909) to model the observed amplification and the associated frequency [26].

## 6.3. Time integration strategies and resolution algorithms

### 6.3.1. Hybrid explicit-implicit DGTD- $\mathbb{P}_p$ method

**Participants:** Stéphane Descombes, Stéphane Lanteri, Ludovic Moya, Jan Verwer [Modeling, Analysis and Simulation Department, CWI, Amsterdam].

Existing numerical methods for the solution of the time domain Maxwell equations often rely on explicit time integration schemes and are therefore constrained by a stability condition that can be very restrictive on highly refined meshes. An implicit time integration scheme is a natural way to obtain a time domain method which is unconditionally stable. Starting from the explicit, non-dissipative, DGTD- $\mathbb{P}_p$  method introduced in [11], we have proposed to use of Crank-Nicolson scheme in place of the explicit leap-frog scheme adopted in this method [13]. As a result, we obtain an unconditionally stable, non-dissipative, implicit DGTD- $\mathbb{P}_p$  method, but at the expense of the inversion of a global linear system at each time step, thus obliterating one of the attractive features of discontinuous Galerkin formulations. A more viable approach for 3D simulations consists in applying an implicit time integration scheme locally i.e in the refined regions of the mesh, while preserving an explicit time scheme in the complementary part, resulting in an hybrid explicit-implicit (or locally implicit) time integration strategy. We have recently started a study in this direction and preliminar results are presented in [14] for a second order hybrid explicit-implicit DGTD- $\mathbb{P}_p$  method.



### 6.3.2. *Explicit local time stepping DGTD- $\mathbb{P}_p$ method*

**Participants:** Joseph Charles, Julien Diaz [MAGIQUE-3D project-team, INRIA Bordeaux - Sud-Ouest], Stéphane Descombes, Stéphane Lanteri.

We have initiated this year a collaboration with the MAGIQUE-3D project-team aiming at the design of local time stepping strategies inspired from [36] for the time integration of the system of ordinary differential equations resulting from the discretization of the time domain Maxwell equations in first order form by a DGTD- $\mathbb{P}_p$  method. A numerical study in one- and two-space dimensions is underway.

### 6.3.3. *Optimized Schwarz algorithms for the frequency domain Maxwell equations*

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

Even if they have been introduced for the first time two centuries ago, over the last two decades, classical Schwarz methods have regained a lot of popularity with the development of parallel computers. First developed for the elliptic problems, they have been recently extended to systems of hyperbolic partial differential equations, and it was observed that the classical Schwarz method can be convergent even without overlap in certain cases. This is in strong contrast to the behavior of classical Schwarz methods applied to elliptic problems, for which overlap is essential for convergence. Over the last decade, optimized versions of Schwarz methods have been developed for elliptic partial differential equations. These methods use more effective transmission conditions between subdomains, and are also convergent without overlap for elliptic problems. The extension of such methods to systems of equations and more precisely to Maxwell's system (time harmonic and time discretized equations) has been done recently in [6]. The optimized interface conditions proposed in [6] were devised for the case of non-conducting propagation media. We are now studying the formulation of such conditions for conducting media [21].

### 6.3.4. *Algebraic preconditioning techniques for a high order DGFD- $\mathbb{P}_p$ method*

**Participants:** Matthias Bollhoefer [Institute of Computational Mathematics, TU Braunschweig], Luc Giraud [HiePACS project-team, INRIA Bordeaux - Sud-Ouest], Stéphane Lanteri, Jean Roman [HiePACS project-team, INRIA Bordeaux - Sud-Ouest].

For large 3D problems, the use of a sparse direct method for solving the algebraic sparse system resulting from the discretization of the frequency domain Maxwell equations by a high order DGFD- $\mathbb{P}_p$  method is simply not feasible because of the memory overhead, even if these systems are associated to subdomain problems in a domain decomposition setting. A possible alternative is to replace the sparse direct method by a preconditioned iterative method for which an appropriate preconditioning technique has to be designed. For this purpose, we are investigating incomplete factorization methods that exploit the block structure of the underlying matrices which is directly related to the approximation order of the physical quantities within each mesh element in the DGFD- $\mathbb{P}_p$  method [18].

## 6.4. High performance computing

### 6.4.1. *High order DGTD- $\mathbb{P}_p$ method on hybrid CPU/GPU parallel systems*

**Participants:** Tristan Cabel, Stéphane Lanteri.

Modern massively parallel computing platforms most often take the form of hybrid shared memory/distributed memory heterogeneous systems combining multi-core processing units with accelerator cards. In particular, graphical processing units (GPU) are increasingly adopted in these systems because they offer the potential for a very high floating point performance at a low purchase cost. DG methods are particularly appealing for exploiting the processing capabilities of a GPU because they involve local linear algebra operations (mainly matrix/matrix products) on relatively dense matrices whose size is directly related to the approximation order of the physical quantities within each mesh element. We have initiated this year a technological development project aiming at the adaptation to hybrid CPU/GPU parallel systems of a high order DGTD- $\mathbb{P}_p$  method for the numerical solution of the 3D Maxwell equations.

## 7. Contracts and Grants with Industry

### 7.1. High order DGTD- $\mathbb{P}_p$ Maxwell solver for electric vulnerability studies

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

The objective of this research grant with CEA/CESTA in Bordeaux is the development of a coupled Vlasov-Maxwell solver combining the high order DGTD- $\mathbb{P}_p$  method on tetrahedral meshes developed in the team and a Particle-In-Cell method. The resulting DGTD- $\mathbb{P}_p$ /PIC solver is used for electrical vulnerability assessment of the experimental chamber of the *Laser Mégajoule* system.

### 7.2. High order DGTD- $\mathbb{P}_p$ Maxwell solver for numerical dosimetry studies

**Participants:** Stéphane Lanteri, Joe Wiart [WHIST Laboratory, Orange Labs, Issy-les-Moulineaux].

The objective of this research grant with the WHIST (Wave Human Interactions and Telecommunications) Laboratory at Orange Labs in Issy-les-Moulineaux is the adaptation of a high order DGTD- $\mathbb{P}_p$  method on tetrahedral meshes developed in the team and its application to numerical dosimetry studies in the context of human exposure to electromagnetic waves emitted from wireless systems. These studies involve realistic geometrical models of human tissues built from medical images.

### 7.3. Volumic, automatic, industrial and generic mesh generation (MIEL3D-MESHER)

**Participants:** Clément Durochat, Paul-Louis Georges [GAMMA project-team, INRIA Paris - Rocquencourt], Stéphane Lanteri, Mark Lorient [Distene, Pôle Teratec, Bruyères-le-Chatel], Philippe Pasquet [Samtech France].

MIEL3D-MESHER is a national project of the SYSTEM@TIC Paris-Région cluster which aims at the development of automatic hexahedral mesh generation tools and their application to the finite element analysis of some physical problems. One task of this project is concerned with the definition of a toolbox for the construction of non-conforming, hybrid hexahedral/tetrahedral meshes. In this context, the contribution of the team to this project aims at the development of a DGTD- $\mathbb{P}_p\mathbb{Q}_k$  method formulated on such hybrid meshes. Here,  $\mathbb{P}_p$  stands for the polynomial interpolation method on tetrahedral elements while  $\mathbb{Q}_k$  denotes the polyomial interpolation method on hexahedral elements.

### 7.4. Seismic risk assessment by a discontinuous Galerkin method

**Participants:** Nathalie Glinsky, Stéphane Lanteri, Fabien Peyrusse.

The objective of this research grant with LCPC and CETE Méditerranée is concerned with the numerical modeling of earthquake dynamics taking into account realistic physical models of geological media relevant to this context. In particular, a discontinuous Galerkin method will be designed for the solution of the elastodynamic equations coupled to an appropriate model of physical attenuation of the wave fields for the characterization of a viscoelastic material.

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

**Participants:** Loula Fezoui, Stéphane Lanteri, Muriel Sesques [CEA/CESTA, Bordeaux], Eric Sonnendrücker [IRMA and CALVI project-team, INRIA Nancy - Grand Est].

The project-team is a partner of the HOUPIC project which is funded by ANR in the framework of the *Calcul Intensif et Simulations* program (this project has started in January 2007 for a duration of 3.5 years). The main objective of this project is to develop and compare Finite Element Time Domain (FETD) solvers based on high order Hcurl conforming elements and high order Discontinuous Galerkin (DG) finite elements and investigate their coupling to a PIC method.

## 7.6. Ultra-wideband microwave imaging and inversion (MAXWELL)

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

The project-team is a partner of the MAXWELL project (Novel, ultra-wideband, bistatic, multipolarization, wide offset, microwave data acquisition, microwave imaging, and inversion for permittivity) which is funded by ANR under the non-thematic program (this project has started in January 2008 for a duration of 4 years). See also the web page <http://leat.unice.fr/pages/anr-maxwell/anr-maxwell.html>

## 7.7. Analysis of children exposure to electromagnetic waves (KidPocket)

**Participants:** Stéphane Lanteri, Joe Wiart [WHIST Laboratory, Orange Labs, Issy-les-Moulineaux].

The project-team is a partner of the KidPocket project (Analysis of RF children exposure linked to the use of new networks or usages) which is funded by ANR in the framework of the *Réseaux du Futur et Services* program and has started in October 2009 for a duration of 3 years. See also the ewb page <http://whist.institut-telecom.fr/kidpocket>

## 7.8. Statistical numerical dosimetry (DONUT)

**Participants:** Amine Drissaoui [Ampère Laboratory, Ecole Centrale de Lyon], Stéphane Lanteri, Philippe Leveque [XLIM Laboratory, Limoges], Ronan Perrussel [Ampère Laboratory, Ecole Centrale de Lyon], Damien Voyer [Ampère Laboratory, Ecole Centrale de Lyon].

The objectives of the DONUT project are to develop and validate a new numerical dosimetry approach for dealing with the variability of human exposure to electromagnetic fields, in order to directly deduce a statistical analysis of the effects of the exposure. The proposed numerical methodology which is based on a stochastic finite element method and can exploit in a non intrusive way existing Maxwell solvers for the calculation of the Specific Absorption Rate in biological tissues. This feature is demonstrated in the project by considering both finite difference, finite element and discontinuous Galerkin Maxwell solvers.

# 8. Other Grants and Activities

## 8.1. Regional Initiatives

We have initiated this year a partnership with the Provence-Alpes-Côte d'Azur (PACA) regional council in the framework of our collaboration with CETE Méditerranée concerning the numerical modeling of earthquake dynamics. The PhD thesis of Fabien Peyrusse is co-funded by a fellowship from the PACA regional council and a research grant with LCPC and CETE Méditerranée.

## 8.2. International Initiatives

Since 2008, the team is collaborating with the Mathematics section of the University of Geneva (Prof. Martin Gander) on the design of domain decomposition methods (optimized Schwarz algorithms) for the solution of the frequency domain Maxwell equations [22]-[21]. This collaboration involves Victorita Dolean, Mohamed El Bouajaji (PhD Student in the NACHOS project-team) and Stéphane Lanteri, and also Ronan Perrussel for the Ampère Laboratory, Ecole Centrale de Lyon. This year, Martin Gander has visited the team for one week in February and two weeks in August.

Since 2010, the team is collaborating with the Modeling, Analysis and Simulation Department, CWI, Amsterdam, (Prof. Jan Verwer) on the design of hybrid explicit-implicit time integration schemes for the the systems of ordinary differential equations resulting from the discretization of the time domain Maxwell equations by discontinuous Galerkin methods. This collaboration involves Stéphane Descombes, Stéphane Lanteri and Ludovic Moya (PhD Student in the NACHOS project-team). Jan Verwer has visited the team for three days in January while Ludovic Moya has visited the CWI for one week in December.

Since 2010, the team is collaborating with the Electromagnetics Group at the University of Bristol (Dr. Maciej Klemm) on the design of a discontinuous Galerkin time domain method for the numerical modeling of the propagation of electromagnetic waves in biological tissues. The resulting numerical methodology will be used in the context of a radar based imaging system of breast tumors which is under development at the University of Bristol. This collaboration involves Claire Scheid and Stéphane Lanteri. This year, Maciej Klemm has visited the team for one week in October.

Since 2009, the team is collaborating with the Institute of Computational Mathematics at TU Braunschweig (Prof. Matthias Bollhoefer) on the design of algebraic preconditioning techniques for the linear systems of equations resulting from the discretization of the frequency domain Maxwell equations by a high order discontinuous Galerkin method[18]. This collaboration involves Stéphane Lanteri, and also Luc Giraud and Jean Roman from the HiePACS project-team, INRIA Bordeaux - Sud-Ouest. This year, Matthias Bollhoefer has visited the team for two weeks in September.

## 9. Dissemination

### 9.1. Animation of the scientific community

Lecture of Stéphane Lanteri at the Médiathèque of Antibes in the framework of the *Conférence-débat Média Sciences* series, entitled *Peut-on évaluer l'impact des rayonnements des téléphones mobiles sur notre santé?*

### 9.2. Ongoing PhD theses

Joseph Charles, *Arbitrarily high-order discontinuous Galerkin methods on simplicial meshes for time domain electromagnetics*, University of Nice-Sophia Antipolis.

Amine Drissauoui, *Stochastic finite element methods for uncertainty analysis in the numerical dosimetry of human exposure to electromagnetic waves*, Ecole Centrale de Lyon<sup>3</sup>.

Clément Durochat, *Discontinuous Galerkin methods on hybrid meshes for time domain electromagnetics*, University of Nice-Sophia Antipolis.

Mohamed El Bouajaji, *Optimized Schwarz algorithms for the time harmonic Maxwell equations discretized by discontinuous Galerkin methods*, University of Nice-Sophia Antipolis.

Ludovic Moya, *Numerical modeling of electromagnetic wave propagation in biological tissues*, University of Nice-Sophia Antipolis.

Fabien Peyrusse, *Numerical simulation of strong earthquakes by a discontinuous Galerkin method*, University of Nice-Sophia Antipolis.

### 9.3. Teaching

Claire Scheid and Stéphane Lanteri, *Introduction to scientific computing*, MathMods - Erasmus Mundus MSc Course, University of Nice-Sophia Antipolis, 50 h.

Victorita Dolean, *Méthodes numériques pour les équations évolutives paraboliques*, Master 2 IMEA and Master Mathématiques, University of Nice-Sophia Antipolis, 24 h.

Victorita Dolean, *Atelier méthodes numériques pour les équations Black-Scholes: implémentation en C++*, Master 2 IMEA, University of Nice-Sophia Antipolis, 15 h.

Victorita Dolean, *Eléments finis*, Master 2 Pro MQM, University of Nice-Sophia Antipolis, 12 h.

Victorita Dolean, *Electromagnétisme numérique*, MAM5, EPU, 20 h.

<sup>3</sup>Under joint supervision between INRIA, Ampère Laboratory (in Lyon) and XLIM Laboratory (in Limoges).

## 9.4. Participation to PhD and HDR defense committees

Stéphane Lanteri has been a reviewer of the PhD thesis of Fabrice Dupros (University of Bordeaux I) and has been a member of the PhD defense committee of Elton Mathias (University of Nice-Sophia Antipolis).

# 10. Bibliography

## Major publications by the team in recent years

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## Publications of the year

### Articles in International Peer-Reviewed Journal

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