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Project-Team NACHOS

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

IN COLLABORATION WITH: Laboratoire Jean-Alexandre Dieudonné (JAD)

RESEARCH CENTER
Sophia Antipolis - Méditerranée

THEME
Computational models and simulation

Table of contents

1. Members	1
2. Overall Objectives	1
3. Scientific Foundations	2
3.1. High order discretization methods	2
3.2. Domain decomposition methods	4
3.3. High performance numerical computing	5
4. Application Domains	6
4.1. Computational electromagnetics	6
4.2. Computational geoseismics	6
5. Software	8
5.1. MAXW-DGTD	8
5.2. MAXW-DGFD	8
5.3. SISMO-DGTD	9
5.4. NUM3SIS	9
5.5. Medical Image Extractor	9
6. New Results	10
6.1. Discontinuous Galerkin methods for Maxwell's equations	10
6.1.1. DGTD- \mathbb{P}_p method based on hierarchical polynomial interpolation	10
6.1.2. DGTD- $\mathbb{P}_p\mathbb{Q}_k$ method on multi-element meshes	11
6.1.3. DGTD- \mathbb{P}_p method for dispersive materials	11
6.1.4. DGFD- \mathbb{P}_p method for the frequency domain Maxwell equations	12
6.1.5. Hybridized DGFD- \mathbb{P}_p method	12
6.1.6. Exact transparent condition in a DGFD- \mathbb{P}_p method	12
6.2. Discontinuous Galerkin methods for the elastodynamic equations	13
6.3. Time integration strategies and resolution algorithms	13
6.3.1. Hybrid explicit-implicit DGTD- \mathbb{P}_p method	13
6.3.2. Explicit local time stepping DGTD- \mathbb{P}_p method	14
6.3.3. Optimized Schwarz algorithms for the frequency domain Maxwell equations	14
6.4. High performance computing	14
7. Contracts and Grants with Industry	14
7.1. High order DGTD- \mathbb{P}_p Maxwell solver for electric vulnerability studies	14
7.2. High order DGTD- \mathbb{P}_p Maxwell solver for numerical dosimetry studies	14
7.3. Volumic, automatic, industrial and generic mesh generation (MIEL3D-MESHER)	15
7.4. Seismic risk assessment by a discontinuous Galerkin method	15
7.5. Ultra-wideband microwave imaging and inversion (MAXWELL)	15
7.6. Analysis of children exposure to electromagnetic waves (KidPocket)	15
7.7. Statistical numerical dosimetry (DONUT)	15
8. Partnerships and Cooperations	16
8.1. Regional Initiatives	16
8.2. European Initiatives	16
8.3. Teaching	16
8.4. Ongoing PhD theses	16
9. Bibliography	17

Project-Team NACHOS

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2. Overall Objectives

2.1. Overall objectives

The overall objectives of the NACHOS project-team are the formulation, analysis and evaluation of numerical methods and high performance algorithms for the solution of first order linear systems of partial differential equations (PDEs) with variable coefficients pertaining to electrodynamics and elastodynamics with applications to computational electromagnetics and computational geoseismics. In both domains, the applications targeted by the team 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

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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, the 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 exploits 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 [43] 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 [49] 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 exist 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 [39] 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 [48] 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 are available 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 putting the emphasis on several 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 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). A second, more classical approach is to devise a local time strategy in the context of a fully explicit time integration scheme. Stability and accuracy are still important challenges in this case.

On the other hand, when considering time harmonic wave propagation problems, numerical efficiency is mainly linked to the solution of the system of algebraic equations resulting from the discretization in space of the underlying PDE model. Various strategies exist ranging from the more robust and efficient sparse direct solvers to the more flexible and cheaper (in terms of memory resources) iterative methods. Current trends tend to show that the ideal candidate will be a judicious mix of both approaches by relying on domain decomposition principles.

- Computational efficiency. 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). Besides, appropriate parallelization strategies need to be designed that combine SIMD and MIMD 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 [36]- [37]- [38]- [42]:

- 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 proven 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 DGTD (Discontinuous Galerkin Time Domain) method working on unstructured conforming simplicial meshes [14]-[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 by the team deal with the extension of these methods towards non-conforming meshes and *hp*-adaptivity [12]-[13], their coupling with hybrid explicit/implicit time integration schemes in order to improve their efficiency in the context of locally refined meshes [6]. A high order DG method has also been proposed for the numerical resolution of the elastodynamic equations modeling the propagation of seismic waves [5]-[11]. For the numerical treatment of the time harmonic Maxwell equations, we have studied similar DG methods [7]-[16] and more recently, HDG (Hybridized Discontinuous Galerkin) methods [33].

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 [45], 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 can generally distinguish three kinds of DD methods:

- Overlapping methods use a decomposition of the computational domain in overlapping pieces. The so-called Schwarz method belongs to this class. Schwarz initially introduced this method for proving the existence of a solution to a Poisson problem. In the Schwarz method applied to the numerical resolution of elliptic PDEs, the transmission conditions at artificial subdomain boundaries are simple Dirichlet conditions. Depending on the way the solution procedure is performed, the iterative process is called a Schwarz multiplicative method (the subdomains are treated 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 [45]- [44]- [47].

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 [9]. 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 [10].

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 demonstrating 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

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 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. Although the principles of electromagnetics are well understood, their application to practical configurations of current interest 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 technology that have taken place over the last two decades have been such that numerical modeling and computer simulation is nowadays ubiquitous in the study of electromagnetic interactions. The team is actively contributing to the design of advanced numerical methodologies for the solution of the PDE models of electromagnetism with a focus on problems relevant to computational bioelectromagnetics i.e. which require the simulation of the interaction of electromagnetic waves with biological tissues. Applications are concerned with the evaluation of potential sanitary effects of human exposure to electromagnetic waves (see Fig. 1), or with the design of biomedical devices and systems (i.e. imaging systems, implantable antennas, etc.).

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. The team is before all considering the first of these topics. Indeed, 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 hazards. 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

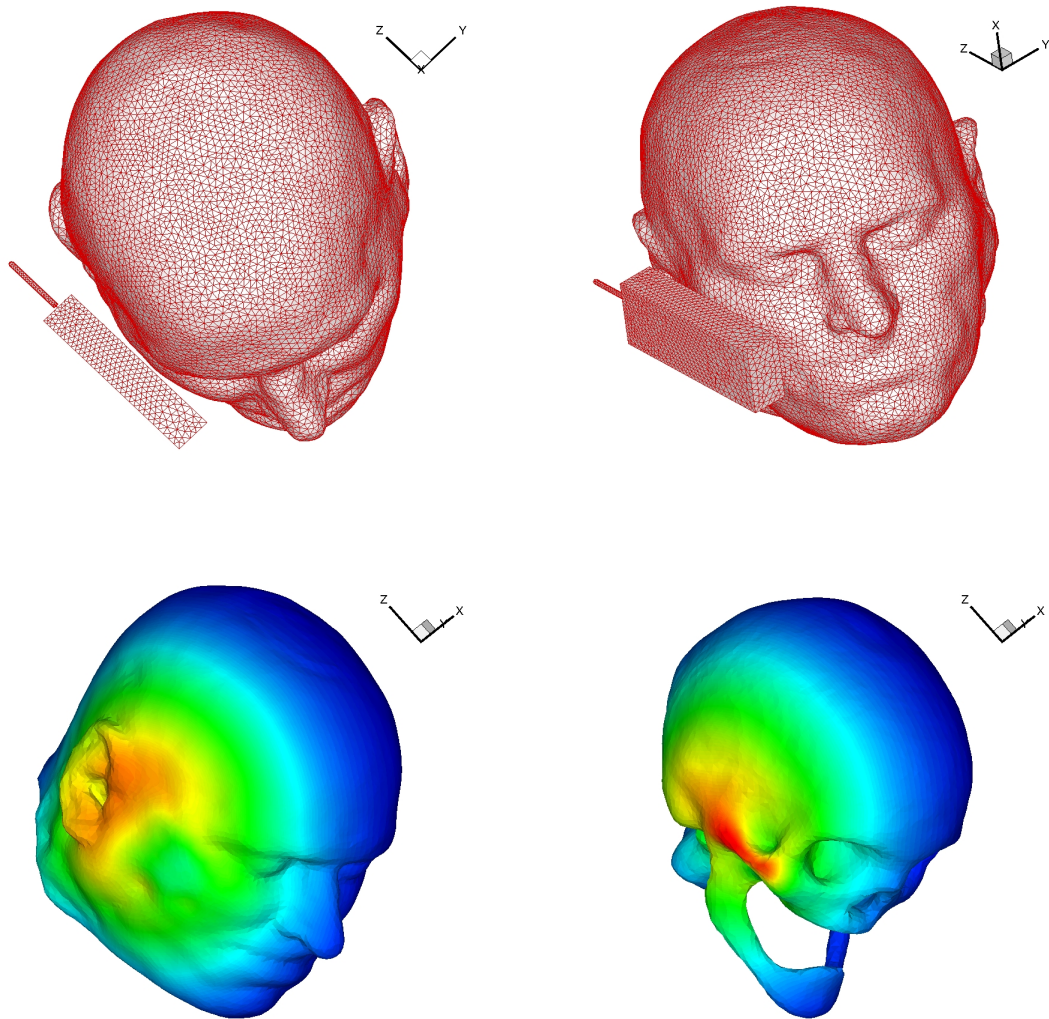


Figure 1. Exposure of head tissues to an electromagnetic wave emitted by a localized source Top figures: surface triangulations of the skin and the skull. Bottom figures: contour lines of the amplitude of the electric field.

heterogeneous. And fifth, geology and source parameters are observable only indirectly and thus introduce uncertainty in the modeling process. In this context, the team undertakes research and development activities aiming at the design of numerical modeling strategies for accurately and efficiently handling the interaction of seismic waves generated by an earthquake source with complex geological media. These activities are conducted in the framework of a collaboration with CETE Méditerranée <http://www.cete-mediterranee.fr/gb> which is a regional technical and engineering centre whose activities are concerned with seismic risk assessment studies.

5. Software

5.1. MAXW-DGTD

Participants: Joseph Charles, Tristan Cabel, Stéphane Lanteri [correspondant], Loula Fezoui.

MAXW-DGTD is a software suite for the simulation of time domain electromagnetic wave propagation. It implements a solution method for the Maxwell equations in the time domain. MAXW-DGTD is based on a discontinuous Galerkin method formulated on unstructured triangular (2D case) or tetrahedral (3D case) meshes [14]. Within each element of the mesh, the components of the electromagnetic field are approximated by a arbitrary high order nodal polynomial interpolation method. This discontinuous Galerkin method combines a centered scheme for the evaluation of numerical fluxes at a face shared by two neighboring elements, with an explicit Leap-Frog time scheme. The software and the underlying algorithms are adapted to distributed memory parallel computing platforms thanks to a parallelization strategy that combines a partitioning of the computational domain with message passing programming using the MPI standard. Besides, a peripheral version of the software has been recently developed which is able to exploit the processing capabilities of a hybrid parallel computing system comprising multicore CPU and GPU nodes [20]. Moreover, a recent methodological achievement has been the extension of the implemented DGTD method to deal with a Debye type dispersive propagation medium [35].

- 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), CUDA
- Programming language: Fortran 77/95

5.2. MAXW-DGFD

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

MAXW-DGFD is a software suite for the simulation of time harmonic electromagnetic wave propagation. It implements a solution method for the Maxwell equations in the frequency domain. MAXW-DGFD is based on a discontinuous Galerkin method formulated on unstructured triangular (2D case) or tetrahedral (3D case) meshes. Within each element of the mesh, the components of the electromagnetic field are approximated by a arbitrary high order nodal polynomial interpolation method. 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. The software and the underlying algorithms are adapted to distributed memory parallel computing platforms thanks to a parallelization strategy that combines a partitioning of the computational domain with message passing programming using the MPI standard. Some recent achievements have been the implementation of non-uniform order DG method in the 2D case [17] and of a new hybridizable discontinuous Galerkin (HDG) formulation also in the 2D case [33].

- 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. SISMO-DGTD

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

SISMO-DGTD is a software for the simulation of time domain seismic wave propagation. It implements a solution method for the velocity-stress equations in the time domain. SISMO-DGTD is based on a discontinuous Galerkin method formulated on unstructured triangular (2D case) or tetrahedral (3D case) meshes [5]. Within each element of the mesh, the components of the electromagnetic field are approximated by an arbitrary high order nodal polynomial interpolation method. This discontinuous Galerkin method combines a centered scheme for the evaluation of numerical fluxes at a face shared by two neighboring elements, with an explicit Leap-Frog time scheme. The software and the underlying algorithms are adapted to distributed memory parallel computing platforms thanks to a parallelization strategy that combines a partitioning of the computational domain with message passing programming using the MPI standard.

- 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

5.4. NUM3SIS

Participants: Nora Aissiouene, Tristan Cabel, Thibaud Kloczko [SED³ team], Régis Duvigneau [OPALE project-team], Thibaud Kloczko [SED team], Stéphane Lanteri, Julien Wintz [SED team].

NUM3SIS <http://num3sis.inria.fr> is a modular platform devoted to scientific computing and numerical simulation. It is designed to handle complex multidisciplinary simulations involving several fields such as Computational Fluid Dynamics (CFD), Computational Structural Mechanic (CSM) and Computational ElectroMagnetics (CEM). In this context, the platform provides a comprehensive framework for engineers and researchers that speeds up implementation of new models and algorithms. From a software engineering point of view, num3sis specializes and extends some layers of the meta-platform dtk, especially its core and composition layers. The core layer enables the user to define generic concepts used for numerical simulation such as mesh or finite-volume schemes which are then implemented through a set of plugins. The composition layer provides a visual programming framework that wraps these concepts inside graphical items, nodes. These nodes can then be connected to each other to define data flows (or compositions) corresponding to the solution of scientific problems. NUM3SIS provides a highly flexible, re-usable and efficient approach to develop new computational scenarios and takes advantage of existing tools. The team participates to the development of the NUM3SIS platform through the adaptation and integration of the MAXW-DGTD simulation software. This work is being carried out with the support of two engineers in the framework of an ADT (Action de Développement Technologique) program.

5.5. Medical Image Extractor

Participants: Stéphane Lanteri, Julien Wintz [SED team].

³Service d'Experimentation et de Développement

Medical Image Extractor <http://num3sis.inria.fr/software/apps/numMedicalImageExtractor> provides functionalities needed to extract meshes from labeled MR or PET-CT medical images. It puts the emphasis on consistency, by generating both boundary surfaces, and volume meshes for each label (ideally identifying a tissue) of the input image, using the very same tetrahedrization. As this process requires user interaction, images and meshes are visualized together with tools allowing navigation and both easy and accurate refinement of the generated meshes, that can then be exported to serve as an input for other tools, within a multidisciplinary software toolchain. Using both DTK <http://dtk.inria.fr> and NUM3SIS SDKs, Medical Image Extractor comes within NUM3SIS' framework. Using cutting edge research algorithms developed by different teams at Inria, spread among different research topics, namely, visualization algorithms from medical image processing, meshing algorithms from algorithmic geometry, it illustrates the possibility to bridge the gap between software that come from different communities, in an innovative and highly non invasive development fashion.

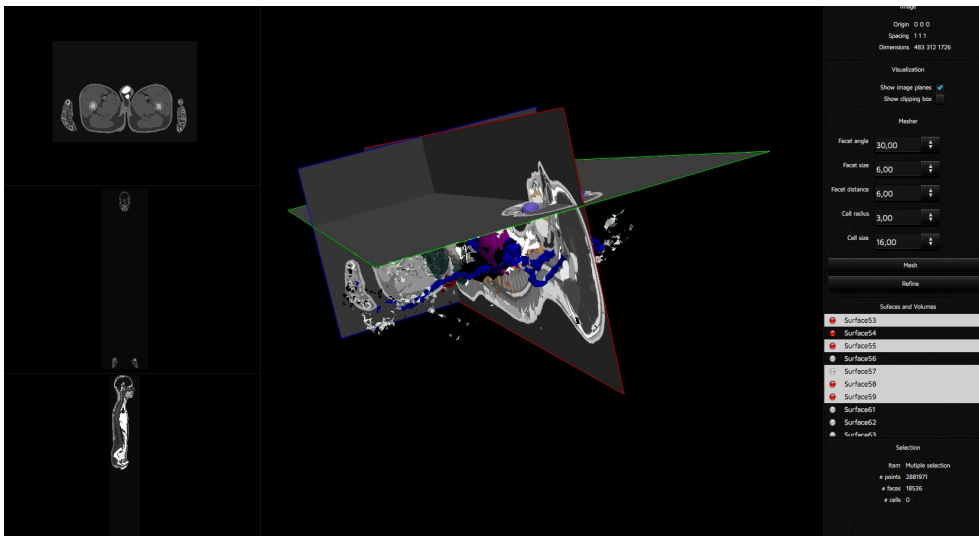


Figure 2. Medical Image Extractor tool graphical user interface.

6. New Results

6.1. Discontinuous Galerkin methods for Maxwell's equations

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

Participants: Loula Fezoui, Joseph Charles, Stéphane Lanteri.

The DGTD (Discontinuous Galerkin Time Domain) method originally proposed by the team for the solution of the time domain Maxwell's equations [14] relies on an arbitrary high order polynomial interpolation of the component of the electromagnetic field, and its computer implementation makes use of nodal (Lagrange) basis expansions on simplicial elements. The resulting method is often denoted by DGTD- \mathbb{P}_p where p refers to the interpolation degree that can be defined locally i.e. at the element level. In view of the design of a hp -adaptive DGTD method, i.e. a solution strategy allowing an automatic adaptation of the interpolation degree p and the discretization step h , we now investigate alternative polynomial interpolation and in particular those which lead to hierarchical or/and orthogonal basis expansions. Such basis expansions on simplicial elements have been extensively studied in the context of continuous finite element formulations (e.g. [46]) and have thus been designed with global conformity requirements (i.e. H_1 , $H(\text{rot})$ or (div)) whose role in the context of a discontinuous Galerkin formulation has to be clarified. This represents one of the objectives of this study.

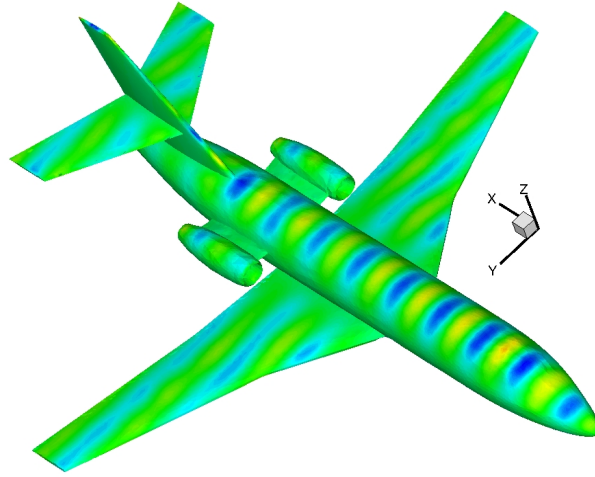


Figure 3. Scattering of a plane wave by a business aircraft geometry computed by $DGTD-\mathbb{P}_1$ method on a tetrahedral mesh. Contour lines of the amplitude of the electric field.

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

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

In this work, we study a multi-element DGTD method formulated on a hybrid mesh which combines a structured (orthogonal) quadrangulation of the regular zones of the computational domain with an unstructured triangulation for the discretization of the irregularly shaped objects. The general objective is to enhance the flexibility and the efficiency of DGTD methods for large-scale time domain electromagnetic wave propagation problems with regards to the discretization process of complex propagation scenes. As a first step, we have designed and analyzed a $DGTD-\mathbb{P}_p\mathbb{Q}_k$ method formulated on conforming hybrid quadrangular/triangular meshes for the solution of the 2D Maxwell's equations.

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

Participants: Claire Scheid, Maciej Klemm [Communication Systems & Networks Laboratory, Centre for Communications Research, University of Bristol, UK], Stéphane Lanteri.

This work is undertaken in the context of a collaboration with the Communication Systems & Networks Laboratory, Centre for Communications Research, University of Bristol (UK). This laboratory is studying imaging modalities based on microwaves with applications to dynamic imaging of the brain activity (Dynamic Microwave Imaging) on one hand, and to cancerology (imaging of breast tumors) on the other hand. The design of imaging systems for these applications is extensively based on computer simulation, in particular to assess the performances of the antenna arrays which are at the heart of these systems. In practice, one has to model the propagation of electromagnetic waves emitted from complex sources and which propagate and interact with biological tissues. In relation with these issues, we study the extension of the $DGTD-\mathbb{P}_p$ method originally proposed in [14] to the numerical treatment of electromagnetic wave propagation in dispersive media. We consider an approach based on an auxiliary differential equation modeling the time evolution of the electric polarization for a dispersive medium of Debye type (other dispersive media will be considered subsequently). 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 [35].

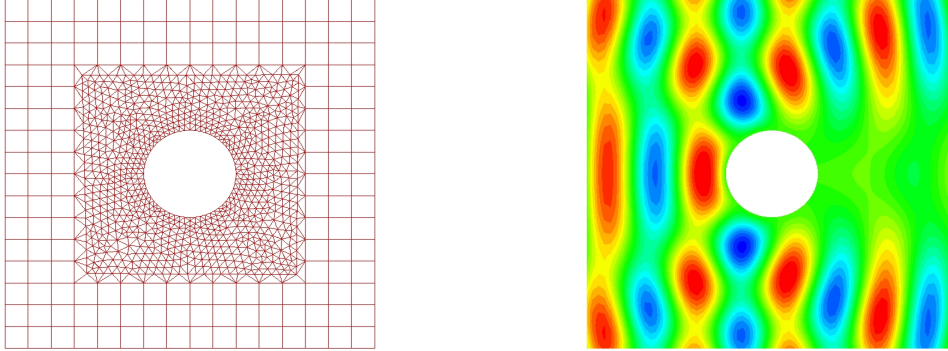


Figure 4. Scattering of a plane wave by a perfectly conducting cylinder computed by a $DGTD-\mathbb{P}_2\mathbb{Q}_4$ method on a hybrid triangular-quadrangular mesh.

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

Participants: Victorita Dolean, Mohamed El Bouajaji, Stéphane Lanteri, Ronan Perrussel [Laplace Laboratory, INP/ENSEEIH/UPS, Toulouse].

For certain types of problems, a time harmonic evolution can be assumed leading to the formulation of the frequency domain Maxwell equations, and solving these equations may be more efficient than considering the time domain variant. We are studying a high order Discontinuous Galerkin Frequency Domain ($DGFD-\mathbb{P}_p$) method formulated on triangular meshes for solving the 2D time harmonic Maxwell equations [16]. This work is undertaken in the context of the ANR MAXWELL project whose objective is the development of an ultra wideband georadar system for imaging the subsurface. In this context, the $DGFD-\mathbb{P}_p$ method that we have proposed is used as the forward solver in an inversion process for the electric permittivity [17].

6.1.5. Hybridized $DGFD-\mathbb{P}_p$ method

Participants: Stéphane Lanteri, Liang Li, Ronan Perrussel [Laplace Laboratory, INP/ENSEEIH/UPS, Toulouse].

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.* [40] 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. This work is concerned with the study of such Hybridizable Discontinuous Galerkin (HDG) 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. As a first step, HDGTD and HDGFD [33] methods have been developed for the solution of the 2D propagation problems.

6.1.6. Exact transparent condition in a $DGFD-\mathbb{P}_p$ method

Participants: Mohamed El Bouajaji, Nabil Gmati [ENIT-LAMSIN, Tunisia], Stéphane Lanteri, Jamil Salhi [ENIT-LAMSIN, Tunisia].

In the numerical treatment of propagation problems theoretically posed in unbounded domains, an artificial boundary is introduced on which an absorbing condition is imposed. For the frequency domain Maxwell equations, one generally use the Silver-Müller condition which is a first order approximation of the exact radiation condition. Then, the accuracy of the numerical treatment greatly depends on the position of the artificial boundary with regards to the scattering object. In this work, we have conducted a preliminary study aiming at improving this situation by using an exact transparent condition in place of the Silver-Müller condition. Promising results have been obtained in the 2D case and call for an extension of this work to the more challenging 3D case.

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 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. Recent results concern two particular points.

The first novelty is the extension of the DGTD- \mathbb{P}_p method initially introduced in [5] to the numerical treatment of viscoelastic attenuation. For this, the velocity-stress first order system is completed by additional equations for the anelastic functions describing the strain history of the material. These additional equations result from the rheological model of the generalized Maxwell body and permit the incorporation of realistic attenuation properties of viscoelastic material accounting for the behaviour of elastic solids and viscous fluids. In practice, one needs to add $3L$ additional equations in 2D and $6L$ in 3D, where L is the number of relaxation mechanisms of the generalized Maxwell body. This method has been implemented in 2D and validated thanks to comparisons with a FDTD method.

The second contribution is concerned with 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. Moreover, the results obtained on several homogeneous and heterogeneous configurations prove the influence of the medium in-depth geometry on the amplifications measures at the surface [26], [25].

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.

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 [14], we have proposed the use of a Crank-Nicolson scheme in place of the explicit leap-frog scheme adopted in this method [4]. 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. Such an approach, combining a leap-frog scheme and a Crank-Nicolson scheme, has been studied numerically in [6], showing promising results which have motivated further investigations on theoretical issues (especially, convergence in the ODE and PDE senses) [28].

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 [41] 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 [Laplace Laboratory, INP/ENSEEIH/UPS, Toulouse].

We continued with the design of optimized Schwarz algorithms for the solution of the frequency domain Maxwell equations. In particular, we have analyzed a family of methods adapted to the case of conductive media [21]. Besides, we have also proposed discrete variants of these algorithms in the framework of a high order discontinuous Galerkin discretization method formulated on unstructured triangular meshes for the solution of the 2D time harmonic Maxwell equations.

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 polynomial 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 IFSTTAR <http://www.ifsttar.fr> (French institute of sciences and technology for transport, development and networks) 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. 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 <http://leat.unice.fr/pages/anr-maxwell/anr-maxwell.html>

7.6. 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 <http://whist.institut-telecom.fr/kidpocket>

7.7. Statistical numerical dosimetry (DONUT)

Participants: Amine Drissou [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. Partnerships and Cooperations

8.1. Regional Initiatives

The team is collaborating with CETE Méditerranée <http://www.cete-mediterranee.fr/gb> which is a regional technical and engineering centre whose activities are concerned with seismic risk assessment studies. The PhD thesis of Fabien Peyrusse is co-funded by a fellowship from the PACA regional council and a research grant with IFSTTAR <http://www.ifsttar.fr> (French institute of sciences and technology for transport, development and networks) and CETE Méditerranée.

8.2. European Initiatives

Prof. Martin Gander: University of Geneva, Mathematics section (Switzerland)

Domain decomposition methods (optimized Schwarz algorithms) for the solution of the frequency domain Maxwell equations

Dr. Maciej Klemm: University of Bristol, Communication Systems & Networks Laboratory, Centre for Communications Research (United Kingdom)

Numerical modeling of the propagation of electromagnetic waves in biological tissues with biomedical applications

8.3. Teaching

Claire Scheid and Stéphane Lanteri, *Introduction to scientific computing*, MathMods - Erasmus Mundus MSc Course, 30 h, University of Nice-Sophia Antipolis.

Claire Scheid, *Practical works on differential equations*, 36 h, L3, University of Nice-Sophia Antipolis.

Victorita Dolean and Stéphane Lanteri, *Computational electromagnetics*, MAM5, 30 h, Polytech Nice.

Victorita Dolean, Ecole thématique CNRS *Decomposition de domaine*, Frejus 14-18 Novembre, *Introductions aux méthodes de Schwarz*, doctoral level, 6h.

8.4. Ongoing PhD theses

PhD in progress : Joseph Charles, *Arbitrarily high-order discontinuous Galerkin methods on simplicial meshes for time domain electromagnetics*, University of Nice-Sophia Antipolis, 01/10/2008, Stéphane Lanteri.

PhD in progress : Clément Durochat, *Discontinuous Galerkin methods on hybrid meshes for time domain electromagnetics*, University of Nice-Sophia Antipolis, 01/10/2009, Stéphane Lanteri.

PhD in progress : Mohamed El Bouajaji, *Optimized Schwarz algorithms for the time harmonic Maxwell equations discretized by discontinuous Galerkin methods*, University of Nice-Sophia Antipolis, 01/20/2008, Victorita Dolean and Stéphane Lanteri.

PhD in progress : Caroline Girard, *Numerical modeling of the electromagnetic susceptibility of innovative planar circuits*, Stéphane Lanteri, Ronan Perrussel and Nathalie Raveu (Laplace Laboratory, INP/ENSEEIH/UPS, Toulouse).

PhD in progress : Ludovic Moya, *Numerical modeling of electromagnetic wave propagation in biological tissues*, University of Nice-Sophia Antipolis, 01/10/2010, Stéphane Descombes and Stéphane Lanteri.

PhD in progress : Fabien Peyrusse, *Numerical simulation of strong earthquakes by a discontinuous Galerkin method*, University of Nice-Sophia Antipolis, 01/10/2010, Nathalie Glinsky and Stéphane Lanteri.

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