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Activity Report 2013

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
Numerical schemes and simulations

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Project-Team NACHOS

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Creation of the Project-Team: 2007 July 01.

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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 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 structured/unstructured) 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 [53] 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 [63] 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. 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 [46] 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 [62] 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 five 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) numerical treatment of complex propagation media models (i.e. physical dispersion models), (d) 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 (e) 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. Research Program

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 relies 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 [43]- [44]- [45]- [52]:

- 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 [16]-[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 [13]-[14], their coupling with hybrid explicit/implicit time integration schemes in order to improve their efficiency in the context of locally refined meshes [7]. A high order DG method has also been proposed for the numerical resolution of the elastodynamic equations modeling the propagation of seismic waves [6]-[12]. For the numerical treatment of the time harmonic Maxwell equations, we have studied similar DG methods [8]-[24] and more recently, HDG (Hybridized Discontinuous Galerkin) methods [26].

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 [58], 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 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 [58]- [57]- [61].

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 [10]. 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 [11]. Recent contributions are concerned with the design and anlysis of such optimized Schwarz algorithm for the solution of the time harmonic Maxwell equations with non-zero conductivity [4].

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

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 (e.g microwave imaging, micro-antenna design for telemedecine, 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 defence 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.).

Part of the activities of the NACHOS project-team aim at the development of high performance, high order, unstructured mesh based solvers for the full system of Maxwell equations, in the time domain and frequency domain regimes. Although many of the above-mentioned electromagnetic wave propagation problems can potentially benefit from the proposed numerical methodologies, the team concentrates its efforts on the following two situations.

4.1.1. Interaction of electromagnetic waves with biological tissues at microwave frequencies.

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 identified previously 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 is of interest to several 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 both in terms of heterogeneity and geometrical features of tissues, the great majority of numerical studies so far have been conducted using variants of the widely known FDTD (Finite Difference Time Domain) method due to Yee [63]. 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 contributions 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 biological tissues with emphasis on applications related to numerical dosimetry. Since the creation of the team, our works on this topic have mainly been focussed on the study of the exposure of humans to radiations from mobile phones or wireless communication systems (see Fig. 1). This activity has been conducted in close collaboration with the team of Joe Wiart at Orange Labs/Whist Laboratory http://whist.institut-telecom.fr/en/index.html (formerly, France Telecom Research & Development) in Issy-les-Moulineaux [15].

4.1.2. Interaction of electromagnetic waves with nanoparticles at optical frequencies (nanophotonics).

Nanostructuring of materials has opened up a number of new possibilities for manipulating and enhancing light-matter interactions, thereby improving fundamental device properties. Low-dimensional semiconductors, like quantum dots, enable one to catch the electrons and control the electronic properties of a material, while photonic crystal structures allow to synthesize the electromagnetic properties. These technologies may, e.g., be employed to make smaller and better lasers, sources that generate only one photon at a time, for applications in quantum information technology, or miniature sensors with high sensitivity. The incorporation of metallic structures into the medium add further possibilities for manipulating the propagation of electromagnetic waves. In particular, this allows subwavelength localisation of the electromagnetic field and, by subwavelength structuring of the material, novel effects like negative refraction, e.g. enabling super lenses, may be realized. Nanophotonics is the recently emerged, but already well defined, field of science and technology aimed at establishing and using the peculiar properties of light and light-matter interaction in various nanostructures. Nanophotonics includes all the phenomena that are used in optical sciences for the development of optical devices. Therefore, nanophotonics finds numerous applications such as in optical microscopy, the design of optical switches and electromagnetic chips circuits, transistor filaments, etc. Because of its numerous scientific and technological applications (e.g. in relation to telecommunication, energy production and biomedicine), nanophotonics represents an active field of research increasingly relying on numerical modeling beside experimental studies.

Plasmonics is a related field to nanophotonics. Nanostructures whose optical scattering is dominated by the response of the conduction electrons are considered as plasmomic media. If the structure presents an interface with e.g. a dielectric with a positive permittivity, collective oscillations of surface electrons create surface-plasmons-polaritons (SPPs) that propagate along the interface. SPPs are guided along metal-dielectric interfaces much in the same way light can be guided by an optical fiber, with the unique characteristic of subwavelength-scale confinement perpendicular to the interface. Nanofabricated systems that exploit SPPs offer fascinating opportunities for crafting and controlling the propagation of light in matter. In particular, SPPs can be used to channel light efficiently into nanometer-scale volumes, leading to direct modification of mode dispersion properties (substantially shrinking the wavelength of light and the speed of light pulses for example), as well as huge field enhancements suitable for enabling strong interactions with nonlinear

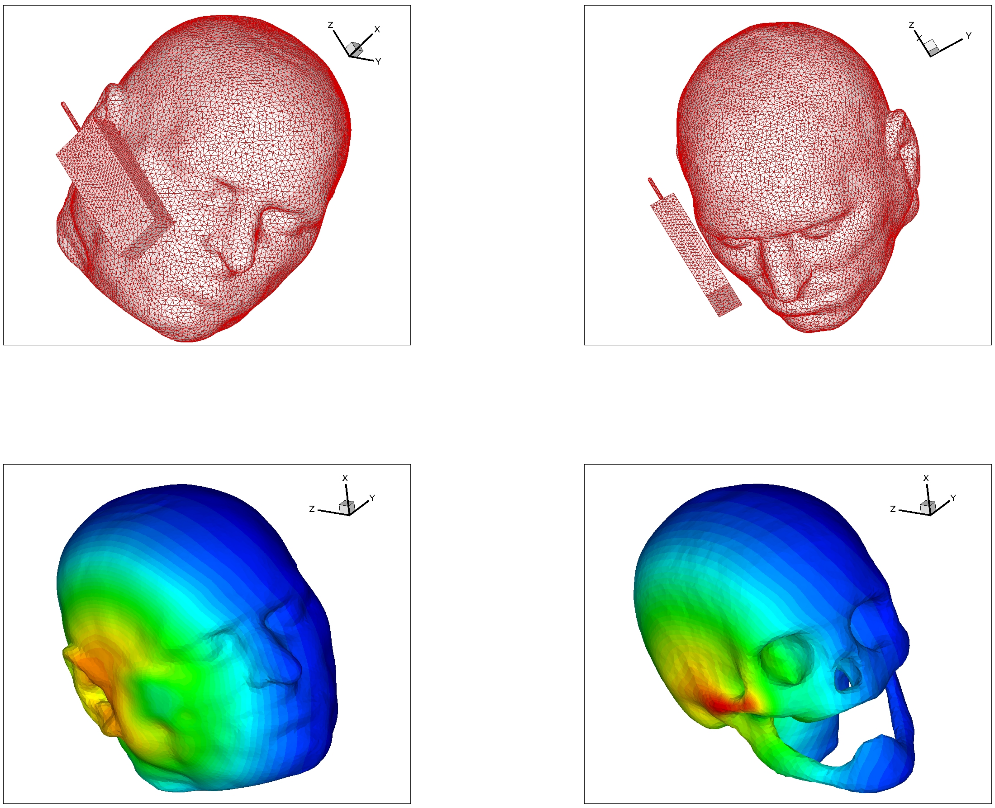

Figure 1. Exposure of head tissues to an electromagnetic wave emitted by a localized source. Top figures: surface triangulations of the skin and the skull. Bottom figures: contour lines of the amplitude of the electric field.

materials. The resulting enhanced sensitivity of light to external parameters (for example, an applied electric field or the dielectric constant of an adsorbed molecular layer) shows great promise for applications in sensing and switching. In particular, very promising applications are foreseen in the medical domain [49]- [64].

Numerical modeling of electromagnetic wave propagation in interaction with metallic nanostructures at optical frequencies requires to solve the system of Maxwell equations coupled to appropriate models of physical dispersion in the metal, such the Drude and Drude-Lorentz models. Her again, the FDTD method is a widely used approach for solving the resulting system of PDEs [60]. However, for nanophotonic applications, the space and time scales, in addition to the geometrical characteristics of the considered nanostructures (or structured layouts of the latter), are particularly challenging for an accurate and efficient application of the FDTD method. Recently, unstructured mesh based methods have been developed and have demonstrated their potentialities for being considered as viable alternatives to the FDTD method [54]- [56]- [47]. The activities of the NACHOS project-team towards the development of accurate and efficient unstructured mesh based methods for nanophotonic applications have started in 2012 and are conducted in collaboration with Dr. Maciej Klemm at University of Bristol who is designing nanoantennas for medical applications [55].

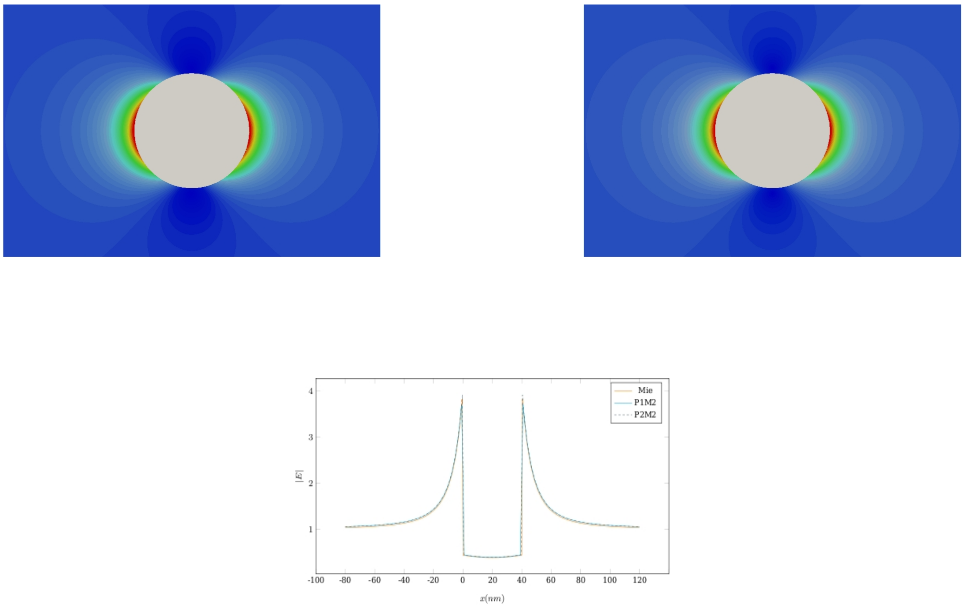

Figure 2. Scattering of a 20 nanometer radius gold nanosphere by a plane wave. The gold properties are described by a Drude dispersion model. Modulus of the electric field in the frequency domain. Top left figure: Mie solution. Top right figure: numerical solution. Bottom figure: 1D plot of the electric field modulus for various orders of approximation (PhD thesis of Jonathan Viquerat).

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 research activities of the NACHOS project-team in this domain before all focus on the development of numerical methodologies and simulation tools for seismic hazard assessment, while the involvement on the second topic has been been intiated recently.

4.2.1. Seismic hazard assessment.

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 hazard 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 the physical understanding of the earthquake rupture processes and seismic wave propagation. Large scale simulations of earthquake rupture dynamics and wave propagation 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 hundredths 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, 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 difference type methods. Among the most popular schemes, one can cite the staggered grid finite difference scheme proposed by Virieux [62] and based on the first order velocity-stress hyperbolic system of elastic waves equations, which is an extension of the scheme derived by Yee [63] for the solution of the Maxwell equations. Many improvements of this method have been proposed, in particular, higher order schemes in space or rotated staggered-grids allowing strong fluctuations of the elastic parameters. Despite these improvements, the use of cartesian grids is a limitation for such numerical methods especially when it is necessary to incorporate surface topography or curved interface. Moreover, in presence of a non planar topography, the free surface condition needs very fine grids (about 60 points by minimal Rayleigh wavelength) to be approximated. In this context, our objective is to develop high order unstructured mesh based methods for the numerical solution of the system of elastodynamic equations for elastic media in a first step, and then to extend these methods to a more accurate treatment of the heterogeneities of the medium or to more complex propagation materials such as viscoelastic media which take into account the intrinsic attenuation. Initially, the team has considered in detail the necessary methodological developments for the large-scale simulation of earthquake dynamics [2]-[1]. More recently, the team has initiated a close collaboration with CETE Méditerranée http://www.cete-mediterranee.fr/gb which is a regional technical and engineering centre whose activities are concerned with seismic hazard assessment studies, and IFSTTAR http://www.ifsttar.fr/en/welcome which is the French institute of science and technology for transport, development and networks, conducting research studies on control over aging, risks and nuisances.

4.2.2. Imperfect interfaces.

A long term scientific collaboration (at least 5 years long) has been recently set up between the NACHOS project-team and LMA (Laboratoire de Mécanique et Acoustique) http://www.lma.cnrs-mrs.fr with the arrival of Marie-Hélène Lallemand who joigned NACHOS in October 2012. That collaboration has been motivated by common scientific interests concerning both geodynamics (seismic wave propagation) and seismology (Non Destructive Control by wave propagation). The goal is to contribute in the area of both fracture dynamics modelings and the setting of adequate constitutive laws for interfaces separating two continuous media. Since the whole medium under study is heterogeneous in term of both materials and geometries, the study of

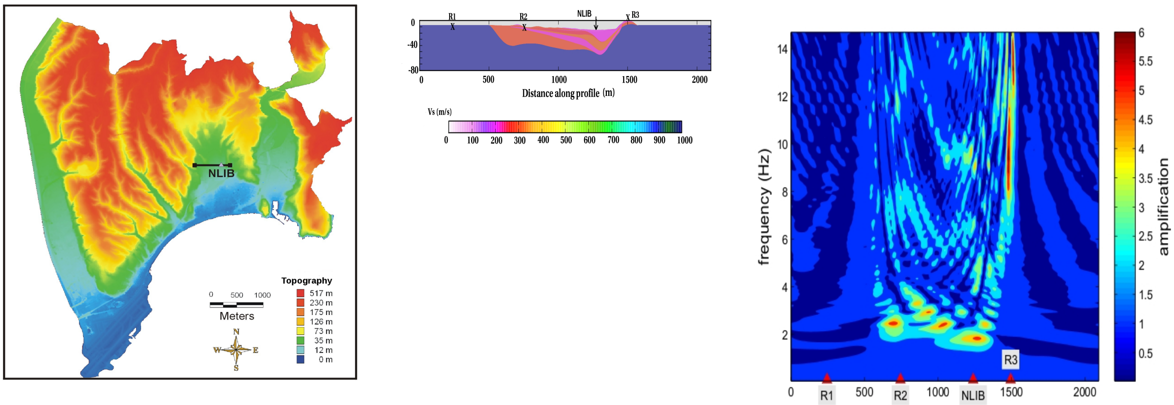

Figure 3. Propagation of a plane wave in a heterogeneous model of Nice area (provided by CETE Méditerranée). Left figure: topography of Nice and location of the cross-section used for numerical simulations (black line). Middle figure: S-wave velocity distribution along the cross-section in the Nice basin. Right figure: transfer functions (amplification) for a vertically incident plane wave ; receivers every 5 m at the surface. This numerical simulation was performed using a numerical method for the solution of the elastodynamics equations coupled to a Generalized Maxwell Body (GMB) model of viscoelasticity (PhD thesis of Fabien Peyrusse).

equivalent homogeneous representation/modellings is crucial to get a suitable reduced model which can be used for numerical simulations. In the particular example of rock-type soils near mountain areas, the medium may be viewed from the geologist, at the macro-scale, for example, as large layers of continuous materials separated by interfacial areas through which discontinuities (of displacements, velocities, stress components ...) may occur. Even if the so-called interfaces may have a depth which may attain many times ten meters and a length of many times hundred meters, they are assimilated as interfaces, from the geologist point of view. Inside those *thin* layers, there are usually some mixture of multiphase materials (water, sand, gas, etc.), and the exact composition is not known in advance. While perfect interfaces are usually assumed in inverse problems in sismology, the question is to qualify and to quantify the errors if we do not take those assumptions for granted. When soil rheology is requested, assuming perfect interfaces or imperfect interfaces greatly influence the physical parameters obtained in reversing the data collected in the captors. Interface modelling is one of the expertise area of LMA, and the project-team is interested in taking that opportunity to improve its knowledge in multi-scale modelling while ready to help answering the numerical implementation of such resulting models. That collaboration is not restricted to that aspect though. Well-posedness of the resulting models, numerical solvers are also domains which are also addressed.

4.2.3. Seismic exploration.

This application topic has been considered recently by the NACHOS project-team and this is done in close collaboration with the MAGIQUE-3D project-team at Inria Bordeaux - Sud-Ouest which is coordinating the Depth Imaging Partnership (DIP) http://dip.inria.fr between Inria and TOTAL. The research program of DIP includes different aspects of the modeling and numerical simulation of sesimic wave propagation that must be considered to construct an efficient software suites for producing accurate images of the subsurface. Our common objective with the MAGIQUE-3D project-team is to design high order unstructured mesh based methods for the numerical solution of the system of elastodynamic equations in the time domain and in the frequency domain, that will be used as forward modelers in appropriate inversion procedures.

5. Software and Platforms

5.1. MAXW-DGTD

Participants: Stéphane Lanteri [correspondant], Loula Fezoui, Ludovic Moya, Raphaël Léger, Jonathan Viquerat.

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 [16]. 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 muticore CPU and GPU nodes.

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

5.2. MAXW-DGFD

Participants: Stéphane Lanteri [correspondant], Ronan Perrussel.

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 paralleization strategy that combines a partitioning of the computational domain with a message passing programming using the MPI standard. Some recent achievements have been the implementation of non-uniform order DG method in the 2D case and of a new hybridizable discontinuous Galerkin (HDG) formulation also in the 2D and 3D cases.

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

5.3. SISMO-DGTD

Participants: 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 [6]. 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 paralleization strategy that combines a partitioning of the computational domain with a 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/Middelware: Linux
- Required library or software: MPI (Message Passing Interface)
- Programming language: Fortran 77/95

5.4. NUM3SIS

Participants: Nora Aissiouene, Thibaud Kloczko [SED [1] 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].

Medical Image Extractor http://num3sis.inria.fr/software/apps/extractor provides functionalities needed to extract meshes from labeled MR or PET-CT medical images. It puts the emphasis on consistence, by generating both boundary surfaces, and volume meshes for each label (ideally identifying a tissue) of the input image, using the very same tetreahedrization. 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 multidisciplinar software toolchain. Using both DTK http://dtk.inria.fr and NUM3SIS SDKs, Medical Image Extractor comes within NUM3SIS'framework. Using cutting edge research algorithms developped 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.

[1] Service d'Experimentation et de Développement

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, Stéphane Lanteri.

The DGTD (Discontinuous Galerkin Time Domain) method originally proposed by the team for the solution of the time domain Maxwell's equations [16] 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. [59]) 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. This year, we have started the development of a new software platform in Fortran 95 implementing DGTD-$\mathbb{P}_p$ able to deal with different polynomial basis expansions on a tetrahedral element, for the solution of the 3D time domain Maxwell equations.

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

Participants: Clément Durochat, Stéphane Lanteri, Raphael Léger, Claire Scheid, Mark Loriot [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) discretization of the regular zones of the computational domain with an unstructured 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. With this objective in mind, we have designed and analyzed a DGTD-$\mathbb{P}_p\mathbb{Q}_k$ method formulated on non-conforming hybrid quadrangular/triangular meshes (2D case) or non-conforming hexahedral/tetrahedral meshes (3D case) for the solution of the time domain Maxwell's equations [23]-[22].

6.1.3. DGTD-$\mathbb{P}_p$ method for Debye media and applications to biolectromagnetics

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 [16] 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). The stability and a priori convergence analysis of the resulting DGTD-$\mathbb{P}_p$ method has been studied [25], and its application to the simulation of the propagation in realistic geometrical models of head tissues is underway in the context of our participation to the DEEP-ER FP7 project.

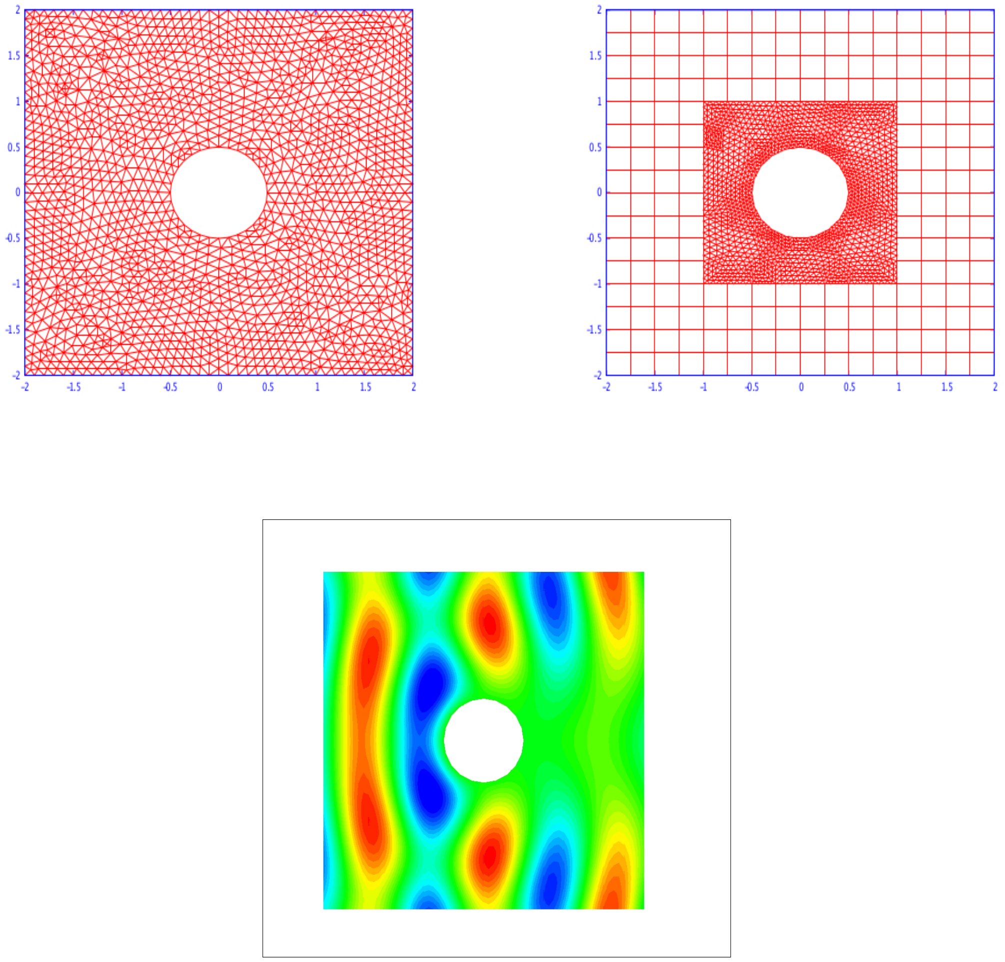

Figure 4. Scattering of a plane wave by a disk. Conforming triangular mesh (top left) and non-conforming quadrangular/triangular mesh (top right). Contour lines of electrical field component E_z from a simulation with a DGTD-$\mathbb{P}_2\mathbb{Q}_4$ method (bottom).

6.1.4. DGTD-$\mathbb{P}_p$ method for nanophotonics

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

Modelling and numerical simulation aspects are crucial for a better understanding of nanophotonics. Media that one encounters are complex and the geometries quite involved, so that while a FDTD method failed to be accurate enough, a non conforming discretisation method seems to be well adapted. In this direction, since the end of 2012, we are actively studying the numerical modeling of electromagnetic wave interaction with nanoscale metallic structures. In this context, one has to take into account the dispersive characteristics of metals in the frequency range of interest to nanophotonics. As a first step in this direction, we have considered an auxiliary differential equation approach for the numerical treatment of a Drude, Drude-Lorentz and a generalized dispersion models in the framework of a DGTD-$\mathbb{P}_p$ method [20]-[36]. We performed the corresponding numerical analysis as well as numerical validation tests cases. Some methodological improvements, such as curvilinear elements and higher order time discretization schemes are also underway.

6.1.5. Frequency domain hybridized DGFD-$\mathbb{P}_p$ methods

Participants: Stéphane Lanteri, Liang Li [Faculty Member, School of Mathematical Sciences, Institute of Computational Science, University of Electronic Science and Technology of China Chengdu, China], Ronan Perrussel [Laplace Laboratory, INP/ENSEEIHT/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 unstructured meshes for solving the 2D and 3D time harmonic Maxwell equations. However, 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.* [48] 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. We have been one of the first groups to study HDGFD-$\mathbb{P}_p$ methods based on nodal interpolation methods for the solution of the 2D and 3D frequency domain Maxwell equations [26]-[27].

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 [30].

6.2. Discontinuous Galerkin methods for the elastodynamic equations

6.2.1. DGTD-$\mathbb{P}_p$ method for viscoelastic media

Participants: Nathalie Glinsky, Stéphane Lanteri, 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. 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 numerical dispersion.

A recent novel contribution is the extension of the DGTD method to include viscoelastic attenuation. For this, the velocity-stress first-order hyperbolic system is completed by additional equations for the anelastic functions including 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, we need solving 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 by comparison to results obtained by a finite-difference method, in particular for wave propagation in a realistic basin of the area of Nice (south of France)

6.2.2. DGTD-$\mathbb{P}_p$ method for the assessment of topographic effects

Participants: Etienne Bertrand [CETE Méditerranée], Nathalie Glinsky.

This study addresses 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 occured 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 .

6.2.3. DGTD-$\mathbb{P}_p$ method for arbitrary heterogeneous media

Participants: Nathalie Glinsky, Diego Mercerat [CETE Méditerranée].

We have recently devised an extension of the DGTD method for elastic wave propagation in arbitrary heterogeneous media. In realistic geological media (sedimentary basins for example), one has to include strong variations in the material properties. Then, the classical hypothesis that these properties are constant within each element of the mesh can be a severe limitation of the method, since we need to discretize the medium with very fine meshes resulting in very small time steps. For these reasons, we propose an improvement of the DGTD method allowing non-constant material properties within the mesh elements. A change of variables on the stress components allows writing the elastodynamic system in a pseudo-conservative form. Then, the introduction of non-constant material properties inside an element is simply treated by the calculation, via convenient quadrature formulae, of a modified local mass matrix depending on these properties. This new extension has been validated for a smoothly varying medium or a strong jump between two media, which can be accurately approximated by the method, independently of the mesh .

6.2.4. DGFD-$\mathbb{P}_p$ method for frequency domain elastodynamics

Participants: Hélène Barucq [MAGIQUE3D project-team, Inria Bordeaux - Sud-Ouest], Marie Bonnasse, Julien Diaz [MAGIQUE3D project-team, Inria Bordeaux - Sud-Ouest], Stéphane Lanteri.

We have started this year a research direction aiming at the development of high order discontinuous Galerkin methods on unstructured meshes for the simulation of frequency domain elastodynamic and viscelastic wave propagation. This study is part of the Depth Imaging Partnership (DIP) between Inria and TOTAL. The PhD thesis of Marie Bonnasse is at the heart of this study which is funded by TOTAL.

6.3. Multiscale finite element methods for time-domain wave models

Participants: Marie-Helene Lallemand Tenkes, Stéphane Lanteri, Claire Scheid, Frédéric Valentin [LNCC, Petrópolis, Brazil].

Mathematical (partial differential equation) models embedding multiscale features occur in a wide range of natural situations and industrial applications involving wave propagation. This is for instance the case of electromagnetic or seismic wave propagation in heterogenous media. Although the related applications take place at the macro-scale, it is well known that the parameters describing the macro-scale processes are eventually determined by the solution behavior at the micro-sacle. As a result, each stage of the modeling of the underlying problem is driven by distinct sets of PDEs with highly heterogeneous coefficients and embedded high-contrast interfaces. Because of the huge difference in physical scales in heterogenous media it is not computationally feasible to fully resolve the micro-scale features directly. Macroscopic models or upscaling techniques have therefore to be developed that are able to accurately capture the macroscopic behavior while significantly reducing the computational cost. In this context, researchers at LNCC have recently proposed a new family of finite element methods [51]- [50], called Multiscale Hybrid-Mixed methods (MHM), which is particularly adapted to be used in high-contrast or heterogeneous coefficients problems. Particularly, they constructed a family of novel finite element methods sharing the following properties: (i) stable and high-order convergent; (ii) accurate on coarse meshes; (iii) naturally adapted to high-performance parallel computing; (iv) induce a face-based a posteriori error estimator (to drive mesh adaptativity); (v) locally conservative. We have started this year a new reserach direction aiming at the design of similar MHM methods for solving PDE models of time-domain electromagnetic and seismic wave propagation.

6.4. Time integration strategies and resolution algorithms

6.4.1. 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 [16], we have proposed the use of Crank-Nicolson scheme in place of the explicit leap-frog scheme adopted in this method [5]. 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. In [7], we conducted a preliminary numerical study of a hyrbid explicit-implicit DGTD-$\mathbb{P}_p$ method, combining a leap-frog scheme and a Crank-Nicolson scheme, and obtained promising results. More recently, we further investigated two such strategies, both theoretically (especially, convergence in the ODE and PDE senses) [17] and numerically in the 2D case [28]. A last topic is to propose higher order time integration techniques based on the second-order locally implicit method to fully exploit the attractive features of this approach combined with a DG discretisation which allows to easily increase the spatial convergence order. Promising results in 2D reaching high order in time, between $3, 5$ and 4, have been obtained in [29] by applying Richardson extrapolation and composition methods.

6.4.2. Optimized Schwarz algorithms for the frequency domain Maxwell equations

Participants: Victorita Dolean, Martin Gander [Mathematics Section, University of Geneva], Stéphane Lanteri, Ronan Perrussel [Laplace Laboratory, INP/ENSEEIHT/UPS, Toulouse].

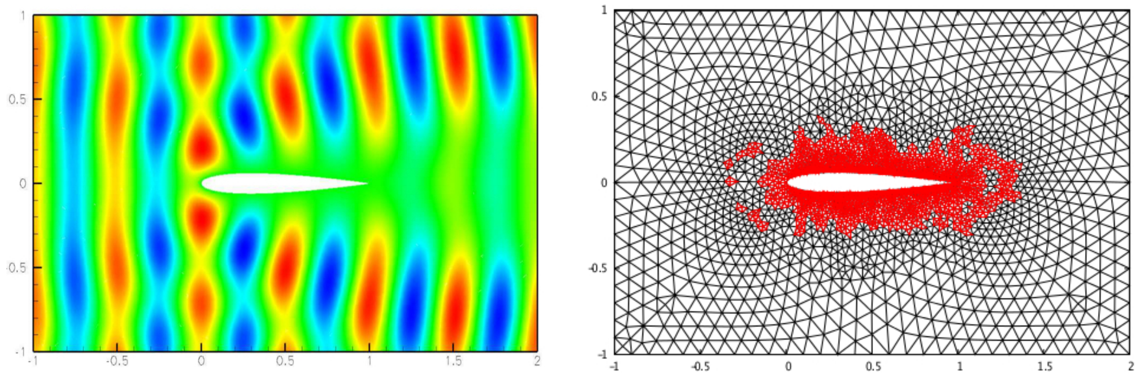

Figure 5. Scattering of a plane wave by an airfoil profile. Contour lines of electrical field component E_z (left) and locally refined triangular mesh with partitioning in explicit/implicit zones (right).

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 developement 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 Schwartz 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 studied in [9]. The optimized interface conditions proposed in [9] were devised for the case of non-conducting propagation media. We have recently studied the formulation of such conditions for conducting media [4]. Besides, we have also proposed an appropriate discretization strategy of these optimized Schwarz algorithms in the context of a high order DGFD-$\mathbb{P}_p$ method formulated on unstructured triangular meshes for the solution of the 2D frequency domain Maxwell equations [42].

7. Bilateral Contracts and Grants with Industry

7.1. 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 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.

8. Partnerships and Cooperations

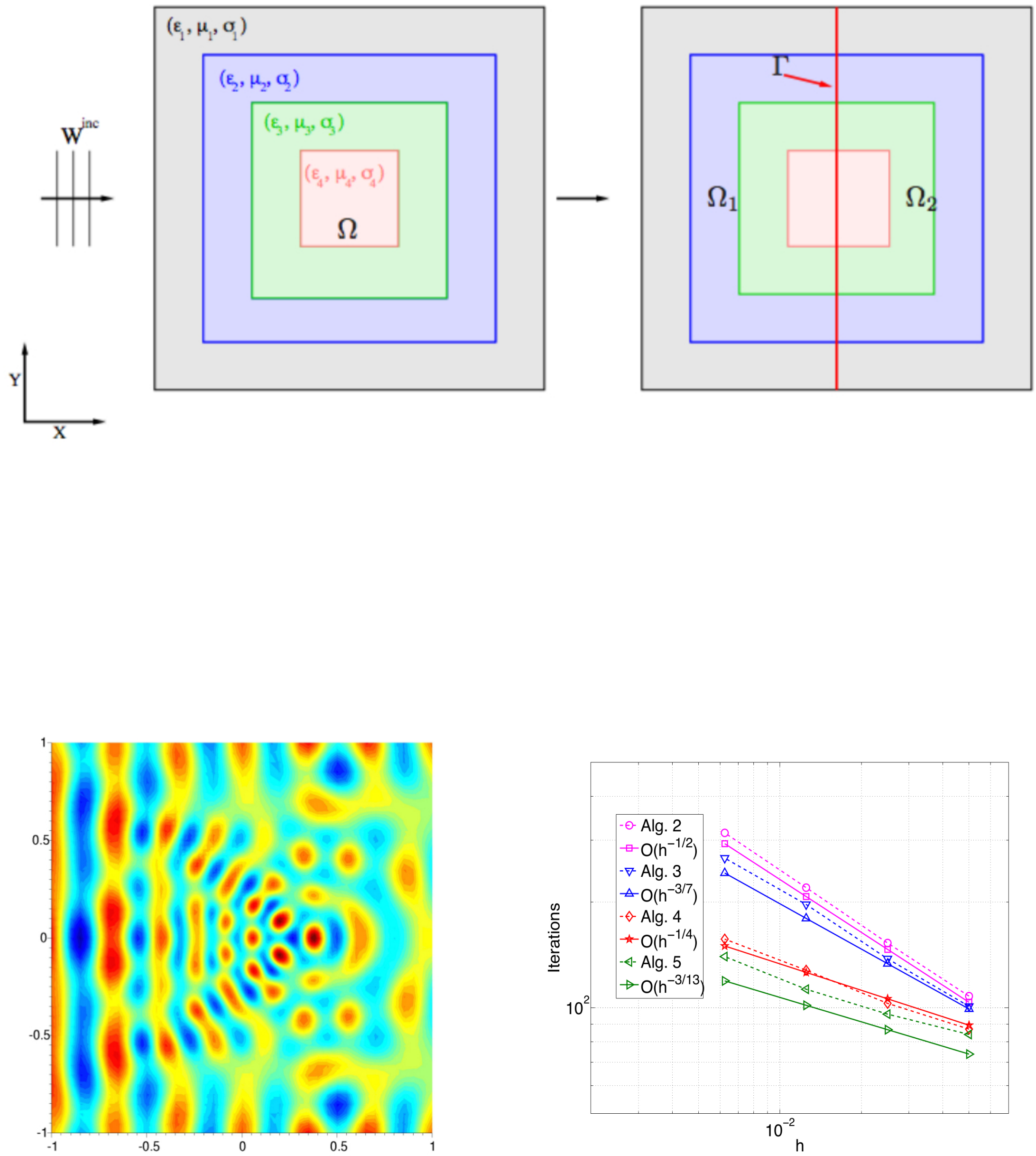

Figure 6. Propagation of a plane wave in a multilayered heterogeneous medium. Problem setting and two-subdomain decompositin (top). Contour lines of the real part of the E_z component of the electrical field (bottom left) and asymptotic convergence of the optimized Schwarz algorithms (bottom right).

8.1. National Initiatives

8.1.1. Inria Project Lab

8.1.1.1. C2S@Exa - Computer and Computational Scienecs at Exascale

Participants: Olivier Aumage [RUNTIME project-team, Inria Bordeaux - Sud-Ouest], Jocelyne Erhel [SAGE project-team, Inria Rennes - Bretagne Atlantique], Philippe Helluy [TONUS project-team, Inria Nancy - Grand-Est], Laura Grigori [ALPINE project-team, Inria Saclay - Île-de-France], Jean-Yves L'excellent [ROMA project-team, Inria Grenoble - Rhône-Alpes], Thierry Gautier [MOAIS project-team, Inria Grenoble - Rhône-Alpes], Luc Giraud [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Michel Kern [POMDAPI project-team, Inria Paris - Rocquencourt], Stéphane Lanteri [Coordinator of the project], François Pellegrini [BACCHUS project-team, Inria Bordeaux - Sud-Ouest], Christian Perez [AVALON project-team, Inria Grenoble - Rhône-Alpes], Frédéric Vivien [ROMA project-team, Inria Grenoble - Rhône-Alpes].

Since January 2013, the team is coordinating the C2S@Exa http://www-sop.inria.fr/c2s_at_exa Inria Project Lab (IPL). This national initiative aims at the development of numerical modeling methodologies that fully exploit the processing capabilities of modern massively parallel architectures in the context of a number of selected applications related to important scientific and technological challenges for the quality and the security of life in our society. At the current state of the art in technologies and methodologies, a multidisciplinary approach is required to overcome the challenges raised by the development of highly scalable numerical simulation software that can exploit computing platforms offering several hundreds of thousands of cores. Hence, the main objective of C2S@Exa is the establishment of a continuum of expertise in the computer science and numerical mathematics domains, by gathering researchers from Inria project-teams whose research and development activities are tightly linked to high performance computing issues in these domains. More precisely, this collaborative effort involves computer scientists that are experts of programming models, environments and tools for harnessing massively parallel systems, algorithmists that propose algorithms and contribute to generic libraries and core solvers in order to take benefit from all the parallelism levels with the main goal of optimal scaling on very large numbers of computing entities and, numerical mathematicians that are studying numerical schemes and scalable solvers for systems of partial differential equations in view of the simulation of very large-scale problems.

8.2. European Initiatives

8.2.1. FP7 Projects

8.2.1.1. DEEP-ER

Type: COOPERATION

Defi: Exascale computing platforms, software and applications

Instrument: Integrated Project

Objectif: Dynamic Exascale Entry Platform - Extended Reach

Duration: October 2013 - September 2016

Coordinator: Forschungszentrum Juelich Gmbh (Germany)

Partner: Intel Gmbh (Germany), Bayerische Akademie der Wissenschaften (Germany), Ruprecht-Karls-Universitaet Heidelberg (Germany), Universitaet Regensburg (Germany), Fraunhofer-Gesellschaft zur Foerderung der Angewandten Forschung E.V (Germany), Eurotech Spa (Italy), Consorzio Interuniversitario Cineca (Italy), Barcelona Supercomputing Center - Centro Nacional de Supercomputacion (Spain), Xyratex Technology Limited (United Kingdom), Katholieke Universiteit Leuven (Belgium), Stichting Astronomisch Onderzoek in Nederland (The Netherlands) and Inria (France).

Inria contact: Stephane Lanteri

Abstract: the DEEP-ER project aims at extending the Cluster-Booster Architecture that has been developed within the DEEP project with a highly scalable, efficient, easy-to-use parallel I/O system and resiliency mechanisms. A Prototype will be constructed leveraging advances in hardware components and integrate new storage technologies. They will be the basis to develop a highly scalable, efficient and user-friendly parallel I/O system tailored to HPC applications. Building on this I/O functionality a unified user-level checkpointing system with reduced overhead will be developed, exploiting multiple levels of storage. The DEEP programming model will be extended to introduce easy-to-use annotations to control checkpointing, and to combine automatic re-execution of failed tasks and recovery of long-running tasks from multi-level checkpoint. The requirements of HPC codes with regards to I/O and resiliency will guide the design of the DEEP-ER hardware and software components. Seven applications will be optimised for the DEEP-ER Prototype to demonstrate and validate the benefits of the DEEP-ER extensions to the Cluster-Booster Architecture.

8.2.2. Collaborations with Major European Organizations

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 at the nanoscale for biomedical applications

8.3. International Initiatives

8.3.1. Participation In other International Programs

8.3.1.1. CNPq-Inria HOSCAR project

Participants: Reza Akbarinia [ZENITH project-team, Inria Sophia Antipolis - Méditerranée], Rossana Andrade [CSD/UFC], Hélène Barucq [MAGIQUE3D project-team, Inria Bordeaux - Sud-Ouest], Alvaro Coutinho [COPPE/UFR], Juklien Diaz [MAGIQUE3D project-team, Inria Bordeaux - Sud-Ouest], Thierry Gautier [MOAIS project-team, Inria Grenoble - Rhone-Alpes], Antônio Tadeu Gomes [LNCC], Pedroedro Leite Da Silva Dias [LNCC, Coordinator of the project on the Brazilian side], Luc Giraud [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Stéphane Lanteri [Coordinator of the project on the French side], Alexandre Madureira [LNCC], Nicolas Maillard [INF/UFRG], Florent Masseglia [ZENITH project-team, Inria Sophia Antipolis - Méditerranée], Marta Mattoso [COPPE/UFR], Philippe Navaux [INF/UFRG], Esther Pacitti [ZENITH project-team, Inria Sophia Antipolis - Méditerranée], François Pellegrini [BACCHUS project-team, Inria Bordeaux - Sud-Ouest], Fabio Porto [LNCC], Bruno Raffin [MOAIS project-team, Inria Grenoble - Rhone-Alpes], Pierre Ramet [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Jean-Louis Roch [MOAIS project-team, Inria Grenoble - Rhone-Alpes], Patrick Valduriez [ZENITH project-team, Inria Sophia Antipolis - Méditerranée], Frédéric Valentin [LNCC].

Since July 2012, the team is coordinating the HOSCAR http://www-sop.inria.fr/hoscar Brazil-France collaborative project. he HOSCAR project is a CNPq - Inria collaborative project between Brazilian and French researchers, in the field of computational sciences. The project is also sponsored by the French Embassy in Brazil.

The general objective of the project is to setup a multidisciplinary Brazil-France collaborative effort for taking full benefits of future high-performance massively parallel architectures. The targets are the very large-scale datasets and numerical simulations relevant to a selected set of applications in natural sciences: (i) resource prospection, (ii) reservoir simulation, (iii) ecological modeling, (iv) astronomy data management, and (v) simulation data management. The project involves computer scientists and numerical mathematicians divided in 3 fundamental research groups: (i) numerical schemes for PDE models (Group 1), (ii) scientific data management (Group 2), and (iii) high-performance software systems (Group 3). Several Brazilian institutions are participating to the project among which: LNCC (Laboratório Nacional de Computação Científica), COPPE/UFRJ (Instituto Alberto Luiz Coimbra de Pós-Graduação e Pesquisa de Engenharia/Alberto Luiz Coimbra Institute for Grad<uate Studies and Research in Engineering, Universidade Federal do Rio de Janeiro), INF/UFRGS (Instituto de Informática, Universidade Federal do Rio Grande do Sul) and LIA/UFC (Laboratórios de Pesquisa em Ciência da Computação Departamento de Computação, Universidade Federal do Ceará). The French partners are research teams from several Inria research centers.

8.4. International Research Visitors

8.4.1. Visits of International Scientists

Prof. Kurt Busch, Theoretical Optics & Photonics, Humboldt-Universität zu Berlin, July 4-5

Prof. Martin Gander, University of Geneva, Switzerland, July 1-12

Prof. Jay Gopalakrishnan, Portland University, USA, July 15-19

Dr. Maciej Klemm, University of Bristol, UK, July 29-August 2

Dr. Antoine Moreau, Institut Pascal, Université Blaise Pascal, June 11-12

8.4.1.1. Internships

Anis Ben El Haj Midani Mohamed, ENIT-LAMSIN, Tunisia, April 30-July 31

Nicole Olivares, Mathematics Department, Portland University, Oregon, USA, JUne 11-Auguts 21

8.4.2. Visits to International Teams

Stéphane Lanteri, School of Mathematical Sciences, Institute of Computational Sciences, University of Electronic Science and Technology of China Chengdu, June 2-7

Stéphane Lanteri, Laboratory for Computational Mathematics, Center of Mathematics, and Institute for Biomedical Imaging and Life Sciences, Coimbra University, Portugal, October 27-November 1

9. Dissemination

9.1. Teaching - Supervision - Juries

9.1.1. Teaching

Victorita Dolean, *Scilab*, MAM3, 24 h, Polytech Nice.

Victorita Dolean, *Partial differential equations*, MAM4, 66 h, Polytech Nice.

Victorita Dolean, *Computational electromagnetics*, MAM5, 40 h, Polytech Nice.

Victorita Dolean, *Numerical analysis*, L2, 30 h, University of Nice-Sophia Antipolis.

Victorita Dolean, *Mathematics and statistics*, M1 Erasmus Mundus EuroAquae, 34 h, University of Nice-Sophia Antipolis.

Claire Scheid and Stéphane Lanteri, *Introduction to scientific computing*, M2 Erasmus Mundus MathMods, 30 h, University of Nice-Sophia Antipolis.

Claire Scheid, *Practical works on differential calculus*, 26 h, L2, University of Nice-Sophia Antipolis.

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

Stéphane Descombes, *Analyse numérique et applications en finances*, M2, 30 h, University of Nice-Sophia Antipolis.

9.1.2. Supervision

PhD in progress : Caroline Girard, *Numerical modeling of the electromagnetic susceptibility of innovative planar circuits*, October 2011, Stéphane Lanteri, Ronan Perrussel and Nathalie Raveu (Laplace Laboratory, INP/ENSEEIHT/UPS, Toulouse).

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

PhD in progress : Marie Bonnasse, *Numerical simulation of frequency domain elastic and viscoelastic wave propagation using discontinuous Galerkin methods*, University of Nice-Sophia Antipolis, October 2012, Julien Diaz (MAGIQUE3D project-team, Inria Bordeaux - Sud-Ouest) and Stéphane Lanteri.

PhD in progress : Jonathan Viquerat, *Discontinuous Galerkin time domain methods for nanophotonics*, October 2012, Stéphane Lanteri and Claire Scheid.

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