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Activity Report 2015

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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2. Overall Objectives

2.1. Overall Objectives

The overall objectives of the NACHOS project-team are the design, mathematical analysis and actual leveraging of numerical methods for the solution of first order linear systems of partial differential equations (PDEs) with variable coefficients modeling wave propagation problems. The two main physical contexts considered by the team are electrodynamics and elastodynamics. The corresponding applications lead to the simulation of electromagnetic or seismic wave interaction with media exhibiting space and time heterogeneities. Moreover, in most of the situations of practical relevance, the propagation settings involve structures or/and material interfaces with complex shapes. Both the heterogeneity of the media and the complex geometrical features of the propagation domains motivate the use of numerical methods that can deal with non-uniform discretization meshes. In this context, the research efforts of the team concentrate on numerical methods formulated on unstructured or hybrid structured/unstructured meshes for the solution of the systems of PDEs of electrodynamics and elastodynamics. Our activities include the implementation of these numerical methods in advanced 3d simulation software that efficiently exploit the capabilities of modern high performance computing platforms. In this respect, our research efforts are also concerned with algorithmic issues related to the design of numerical algorithms that perfectly fit to the hardware characteristics of petascale class supercomputers.

In the case of electrodynamics, the mathematical model of interest is the full system of unsteady Maxwell equations [57] 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 [62] in 1996 is the most popular and which often serves as a reference method for the works of the team. 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, Drude model, Drude-Lorentz model, etc.).

In the case of elastodynamics, the mathematical model of interest is the system of elastodynamic equations [52] 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 [61] 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.

3. Research Program

3.1. Scientific foundations

The research activities undertaken by the team aim at developing innovative numerical methodologies putting the emphasis on several features:

- **Accuracy**. The foreseen numerical methods should rely on discretization techniques that best fit to the geometrical characteristics of the problems at hand. Methods based on unstructured, locally refined, even non-conforming, simplicial meshes are particularly attractive in this regard. In addition, the proposed numerical methods should also be capable to accurately describe the underlying physical phenomena that may involve highly variable space and time scales. Both objectives are generally addressed by studying so-called hp-adaptive solution strategies which combine h-adaptivity using local refinement/coarsening of the mesh and p-adaptivity using adaptive local variation of the interpolation order for approximating the solution variables. However, for physical problems involving strongly heterogeneous or high contrast propagation media, such a solution strategy may not be sufficient. Then, for dealing accurately with these situations, one has to design numerical methods that specifically address the multiscale nature of the underlying physical phenomena.
- **Numerical efficiency**. The simulation of unsteady problems most often relies on explicit time integration schemes. Such schemes are constrained by a stability criterion, linking some 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. One possible overcoming solution consists in resorting to an implicit time scheme in regions of the computational domain where the underlying mesh size is very small, while an explicit time scheme is applied elsewhere in the computational 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, often considered approach is to devise a local time stepping strategy. Beside, when considering time-harmonic (frequency-domain) 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 involve 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). In addition, appropriate parallelization strategies need to be designed that combine SIMD and MIMD programming paradigms.

From the methodological point of view, the research activities of the team are concerned with four main topics: (1) high order finite element type methods on unstructured or hybrid structured/unstructured meshes for the discretization of the considered systems of PDEs, (2) efficient time integration strategies for dealing with grid induced stiffness when using non-uniform (locally refined) meshes, (3) numerical treatment of complex propagation media models (e.g. physical dispersion models), (4) algorithmic adaptation to modern high performance computing platforms.

3.2. High order discretization methods

3.2.1. The Discontinuous Galerkin method

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 (FV) 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 and conservation law systems. The success of the FV 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 FV methods this property since a first order FV scheme may be viewed as a 0th order DG scheme. However a DG method may also be considered as a Finite Element (FE) one where the continuity constraint at an element interface is released. While keeping almost all the advantages of the FE 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 [49]- [50]- [51]- [56]:

- 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 space discretization is coupled to an explicit time integration scheme, the DG method leads to a block diagonal mass matrix whatever the form of the local approximation (e.g. the type of polynomial interpolation). This is a striking difference with classical, continuous FE formulations. Moreover, the mass matrix may be diagonal if the basis functions are orthogonal.
- It easily handles complex meshes. The grid may be a classical conforming FE 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 (and flexible) to the design of some hp-adaptive solution strategy.
- It is also 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 FE 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 locally, 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 FV 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.

3.2.2. High order DG methods for wave propagation models

DG methods are at the heart of the activities of the team regarding the development of high order discretization schemes for the PDE systems modeling electromagnetic and elatsodynamic wave propagation.

- **Nodal DG methods for time-domain problems**. 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 [13]. This DG method combines a central numerical flux function for the approximation of the integral term at the interface of 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 unstructured [10]-[11] and hybrid structured/unstructured meshes [6], their coupling with hybrid explicit/implicit time integration schemes in order to improve their efficiency in the context of locally refined meshes [4]-[19]-[18]. A high order DG method has also been proposed for the numerical resolution of the elastodynamic equations modeling the propagation of seismic waves [2]-[9].

- **Hybridizable DG (HDG) method for time-domain and time-harmonic problems**. For the numerical treatment of the time-harmonic Maxwell equations, nodal DG methods can also be considered [8]. However, such DG formulations are highly expensive, especially for the discretization of 3d problems, because they lead to a large sparse and undefinite linear system of equations coupling all the degrees of freedom of the unknown physical fields. 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.*[54] 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. The team has been a precursor in the development of HDG methods for the frequency-domain Maxwell equations [15]-[16].
- **Multiscale DG methods for time-domain problems**. More recently, in collaboration with LNCC in Petropolis (Frédéric Valentin) the framework of the HOMAR assoacite team, we have started to investigate a family of methods specifically designed for an accurate and efficient numerical treatment of multiscale wave propagation problems. These methods, referred to as Multiscale Hybrid Mixed (MHM) methods, are currently studied in the team for both time-domain electromagnetic and elastodynamic PDE models. They consist in reformulating the mixed variational form of each system into a global (arbitrarily coarse) problem related to a weak formulation of the boundary condition (carried by a Lagrange multiplier that represents e.g. the normal stress tensor in elastodynamic sytems), and a series of small, element-wise, fully decoupled problems resembling to the initial one and related to some well chosen partition of the solution variables on each element. By construction, that methodology is fully parallelizable and recursivity may be used in each local problem as well, making MHM methods belonging to multi-level highly parallelizable methods. Each local problem may be solved using DG or classical Galerkin FE approximations combined with some appropriate time integration scheme (θ-scheme or leap-frog scheme).

3.3. Efficient time integration strategies

The use of unstructured meshes (based on triangles in two space dimensions and tetrahedra in three space dimensions) is an important feature of the DGTD methods developed in the team which can thus easily deal with complex geometries and heterogeneous propagation media. Moreover, DG discretization methods are naturally adapted to local, conforming as well as non-conforming, refinement of the underlying mesh. Most of the existing DGTD methods rely on explicit time integration schemes and lead to block diagonal mass matrices which is often recognized as one of the main advantages with regards to continuous finite element methods. However, explicit DGTD methods are also constrained by a stability condition that can be very restrictive on highly refined meshes and when the local approximation relies on high order polynomial interpolation. There are basically three strategies that can be considered to cure this computational efficiency problem. The first approach is to use an unconditionally stable implicit time integration scheme to overcome the restrictive constraint on the time step for locally refined meshes. In a second approach, a local time stepping strategy is combined with an explicit time integration scheme. In the third approach, the time step size restriction is overcome by using a hybrid explicit-implicit procedure. In this case, one blends a time implicit and a time explicit schemes where only the solution variables defined on the smallest elements are treated implicitly. The first and third options are considered in the team in the framework of DG [4]-[19]-[18] and HDG discretization methods.

3.4. Numerical treatment of complex material models

Towards the general aim of being able to consider concrete physical situations, we are interested in taking into account in the numerical methodologies that we study, a better description of the propagation of waves in realistic media. In the case of electromagnetics, a typical physical phenomenon that one has to consider is *dispersion*. It is present in almost all media and expresses the way the material reacts to an electromagnetic field. In the presence of an electric field a medium does not react instantaneously and thus presents an electric polarization of the molecules or electrons that itself influences the electric displacement. In the case of a linear homogeneous isotropic media, there is a linear relation between the applied electric field and the polarization. However, above some range of frequencies (depending on the considered material), the dispersion phenomenon cannot be neglected and the relation between the polarization and the applied electric field becomes complex. This is rendered via a frequency-dependent complex permittivity. Several models of complex permittivity exist. Concerning biological media, the Debye model is commonly adopted in the presence of water, biological tissues and polymers, so that it already covers a wide range of applications [14]. In the context of nanoplasmonics, one is interested in modeling the dispersion effects on metals on the nanometer scale and at optical frequencies. In this case, the Drude or the Drude-Lorentz models are generally chosen [21]. In the context of seismic wave propagation, we are interested by the intrinsic attenuation of the medium [20]. In realistic configurations, for instance in sedimentary basins where the waves are trapped, we can observe site effects due to local geological and geotechnical conditions which result in a strong increase in amplification and duration of the ground motion at some particular locations. During the wave propagation in such media, a part of the seismic energy is dissipated because of anelastic losses relied to the internal friction of the medium. For these reasons, numerical simulations based on the basic assumption of linear elasticity are no more valid since this assumption results in a severe overestimation of amplitude and duration of the ground motion, even when we are not in presence of a site effect, since intrinsic attenuation is not taken into account.

3.5. 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 computational 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. Electromagnetic wave propagation

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.).

Although many of the above-mentioned application contexts can potentially benefit from numerical modeling studies, the team currently concentrates its efforts on two physical situations.

4.1.1. *Microwave interaction with biological tissues*

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 [62]. 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 [12].

4.1.2. *Light/matter interaction on the nanoscale*

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

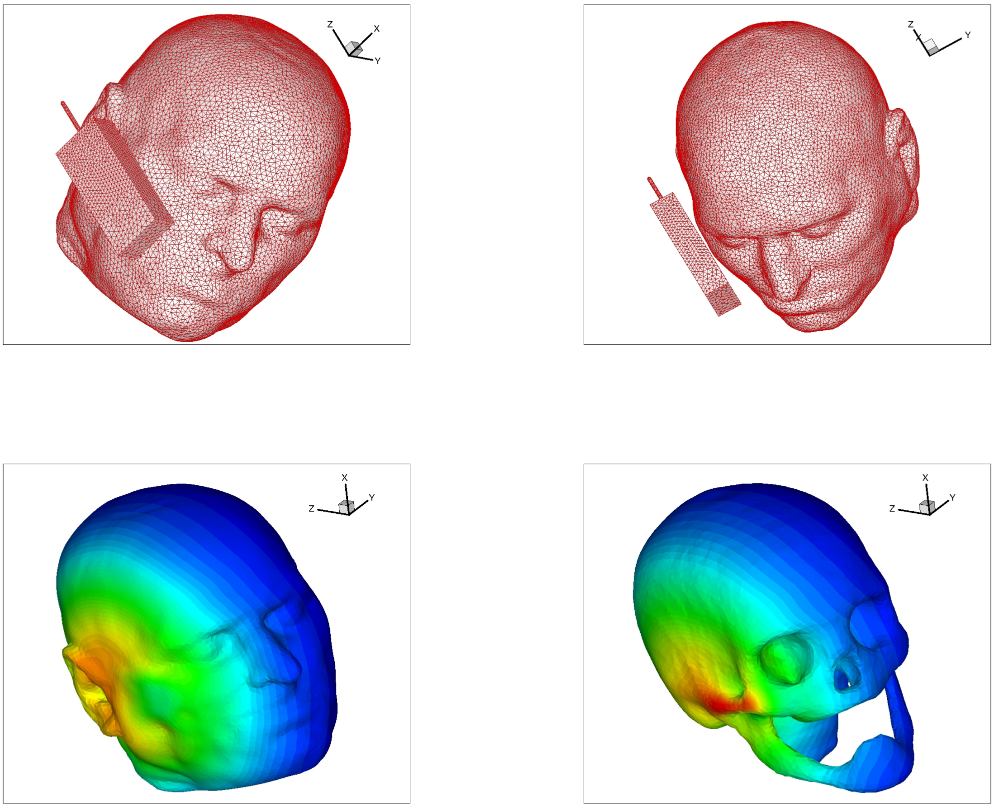


Figure 1. Exposure of head tissues to an electromagnetic wave emitted by a localized source. Top figures: surface triangulations of the skin and the skull. Bottom figures: contour lines of the amplitude of the electric field.

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. Metallic 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 non-linear 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 [55]- [63].

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 as the Drude and Drude-Lorentz models. Here 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 [58]- [59]- [53]. Since the end of 2012, nanophotonics/plasmonics is increasingly becoming a focused application domain in the research activities of the team in close collaboration with physicists from CNRS laboratories, and also with researchers from international institutions.

4.2. Elastodynamic wave propagation

Elastic wave propagation in interaction with solids are encountered in a lot of scientific and engineering contexts. One typical example is geoseismic wave propagation, in particular in the context of earthquake dynamics or resource prospection.

4.2.1. Earthquake dynamics

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 buildings 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 multiscale physics together with data assimilation and inversion.

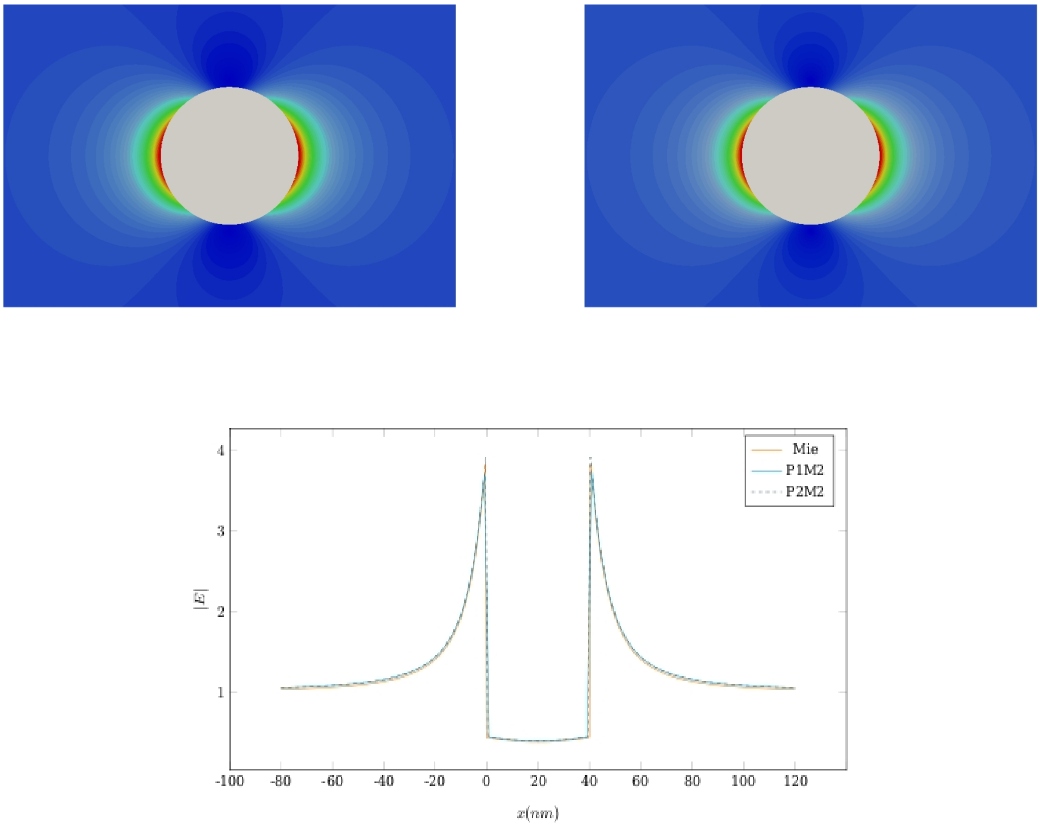


Figure 2. Scattering of a 20 nanometer radius gold nanosphere by a plane wave. The gold properties are described by a Drude dispersion model. Modulus of the electric field in the frequency domain. Top left figure: Mie solution. Top right figure: numerical solution. Bottom figure: 1d plot of the electric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

High resolution models are also required to develop and assess fast operational analysis tools for real time seismology and early warning systems.

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 [61] and based on the first order velocity-stress hyperbolic system of elastic waves equations, which is an extension of the scheme derived by Yee [62] 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 [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.

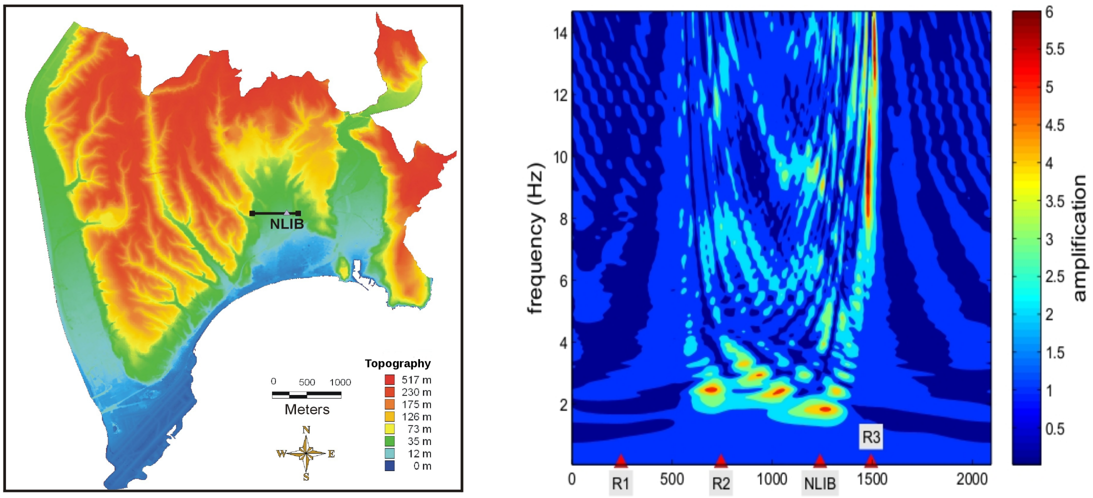


Figure 3. Propagation of a plane wave in a heterogeneous model of Nice area (provided by CETE Méditerranée). Left figure: topography of Nice and location of the cross-section used for numerical simulations (black line). Right figure: transfer functions (amplification) for a vertically incident plane 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.

4.2.2. 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. New Software and Platforms

5.1. MAXW-DGTD

- Participants: Alexandra Christophe-Argenvillier, Loula Fezoui, Stéphane Lanteri, Raphaël Léger, Jonathan Viquerat
- Contact: Stéphane Lanteri
- 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

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 [13]. 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. 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.

5.2. MAXW-DGFD

- Participants: Thomas Frachon, Stéphane Lanteri, Ludovic Moya
- Contact: Stéphane Lanteri
- 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

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 an 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 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.

5.3. SISMO-DGTD

- Participants: Nathalie Glinsky, Stéphane Lanteri
- Contact: 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 [2]. 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 a message passing programming using the MPI standard.

6. New Results

6.1. Electromagnetic wave propagation

6.1.1. Numerical study of the non-linear Maxwell equations for Kerr media

Participants: Loula Fezoui, Stéphane Lanteri.

The system of Maxwell equations describes the evolution of the interaction of an electromagnetic field with a propagation medium. The different properties of the medium, such as isotropy, homogeneity, linearity, among others, are introduced through *constitutive laws* linking fields and inductions. In the present study, we focus on non-linear effects and address non-linear Kerr materials specifically. In this model, any dielectric may become non-linear provided the electric field in the material is strong enough. As a first setp, we considered the one-dimensional case and study the numerical solution of the non-linear Maxwell equations thanks to DG methods. In particular, we make use of an upwind scheme and limitation techniques because they have a proven ability to capture shocks and other kinds of singularities in the fluid dynamics framework. The numerical results obtained in this preliminary study gave us confidence towards extending them to higher spatial dimensions. As a matter of fact, we recently started to work on the three-dimensional case and have initiated the development of a parallel simulation software based on our past contributions on DGTD methods for the case of linear propagation media.

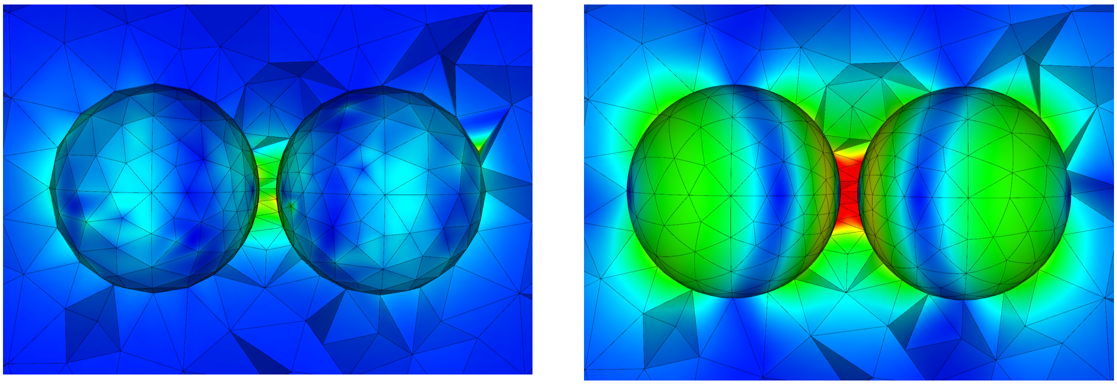
6.1.2. High order geometry conforming DGTD method for nanophotonics

Participants: Stéphane Lanteri, Claire Scheid, Jonathan Viquerat.

Usually, unstructured mesh based methods rely on tessellations composed of straight-edged elements mapped linearly from a reference element, on domains which physical boundaries are indifferently straight or curved. Such meshes represent a serious hindrance for high order finite element (FE) methods since they limit the accuracy to second order in the spatial discretization. Thus, exploiting an enhanced representation of physical geometries is in agreement with the natural procedure of high order FE methods, such as the DG method. There are several ways to account for curved geometries. One could choose to incorporate the knowledge coming from CAD in the method to design the geometry and the approximation. These methods are called *isogeometric*, and have received a lot of attention recently. This naturally implies to have access to CAD models of the geometry. On the other hand, *isoparametric* usually rely on a polynomial approximation of both the boundary and the solution. This can be added fairly easily on top of existing implementations. In the present study we focus on the latter type of method, since our goal is first to envisage the benefit of curvilinear meshes for light/matter interaction with nanoscale structures.

6.1.3. Local approximation order DGTD method for nanophotonics

Participants: Stéphane Lanteri, Jonathan Viquerat.



Mesh with affine elements Mesh with curvilinear elements

Figure 4. Near-field visualization of the amplitude of the electric field Fourier transformed for a gold nanosphere dimer. Surface-to-surface distance is set to 4 nm. Calculations are based on a DGTD-$\mathbb{P}_4$ method.

High order DGTD methods for the numerical modeling of light/matter interactions on the nanoscale often assume a uniform distribution of the polynomial order to the cells of the underlying mesh. However, in the case of a mesh showing large variations in cell size, the time step imposed by the smallest cells can be a serious hindrance when trying to exploit high approximation orders. Indeed, a potentially large part of the CPU time is spent in the update of the physical field inside small cells where high polynomial orders might not be essential, while they are necessary in the larger cells. In this study, we consider the possibility of using a non-uniform distribution of the polynomial order in the framework of a global time step DGDT method. By imposing low orders in small cells and high orders in large cells, it is possible to significantly alleviate both the global number of degrees of freedom and the time step restriction with a minimal impact on the method accuracy. Strategies exploiting locally adaptive (LA) formulations usually combine both h- and p-adaptivity (where h denotes the discretization parameter in space and p the degree of the interpolation of the field components) in order to concentrate the computational effort in the areas of high field variations. Here, the adopted point of view is quite different: starting from a given mesh and a uniform distribution of the polynomial order k, the LA strategy exploits all the polynomial orders p with $p \leq k$ to obtain a solution of similar accuracy with a reduced computational cost.

6.1.4. Numerical treatment of non-local dispersion for nanoplasmonics

Participants: Stéphane Lanteri, Claire Scheid, Colin Vo Cong Tri.

When metallic nanostructures have sub-wavelength sizes and the illuminating frequencies are in the regime of metal's plasma frequency, electron interaction with the exciting fields have to be taken into account. Due to these interactions, plasmonic surface waves can be excited and cause extreme local field enhancements (surface plasmon polariton electromagnetic waves). Exploiting such field enhancements in applications of interest requires a detailed knowledge about the occurring fields which can generally not be obtained analytically. For the numerical modeling of light/matter interaction on the nanoscale, the choice of an appropriate model is a crucial point. Approaches that are adopted in a first instance are based on local (no interaction between electrons) dispersion models e.g. Drude or Drude-Lorentz. From the mathematical point of view, these models lead to an additional ordinary differential equation in time that is coupled to Maxwell's equations. When it comes to very small structures in a regime of 2 nm to 25 nm, non-local effects due to electron collisions have to be taken into account. Non-locality leads to additional, in general non-linear, partial differential equations and is significantly more difficult to treat, though. In this work, we study a DGTD method able to solve the system of Maxwell equations coupled to a linearized non-local dispersion model relevant to nanoplasmonics.

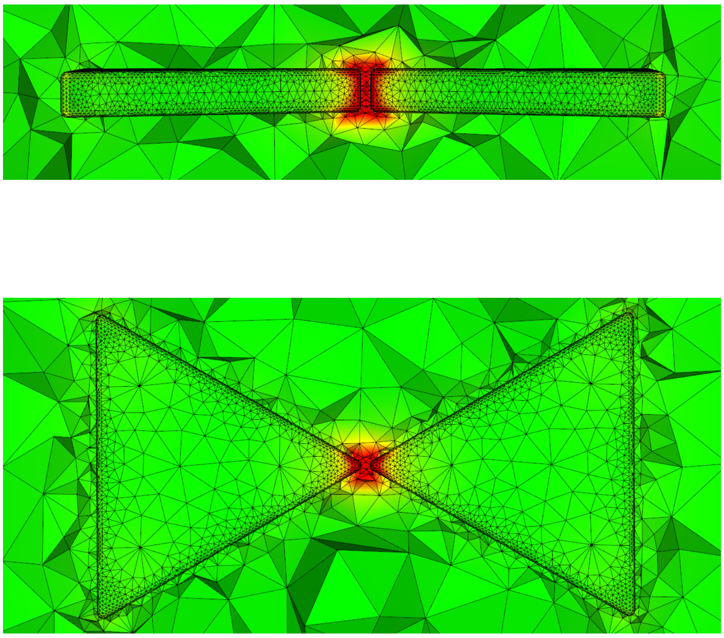


Figure 5. Near-field plasmonic interaction with a bowtie nanoantenns: contour line the amplitude of the discrete Fourier transform of the electric field.

While the method is presented in the general 3d case, in this preliminary stdudy, numerical results are given for 2d simulation settings.

6.1.5. Corner effects in nanoplasmonics

Participants: Camille Carvalho [ENSTA, POEMS project-team], Patrick Ciarlet [ENSTA, POEMS project-team], Claire Scheid.

The starting point of this ongoing work is the theoretical and numerical study of nanoplasmonic structures with corners. This is the central subject of the PhD thesis of Camille Carvalho. In the latter, the focus is made on a lossles Drude dispersion model with a frequency domain approach. Several well posedness problems arise due to the presence of corners and are addressed in the PhD thesis. A time domain approach in this context can also be investigated with the techniques developed in our project-team. Even if both approaches (time domain and frequency domain) represent similar physical phenomena, problems that arise are different and they appear as complementary; it is thus worth bridging the gap between the two frameworks. We propose to perform a thorough comparison in the case of structures with corners. Several extensions to other models are also envisaged, especially concerning the non local dispersion model.

6.1.6. DGTD method for nanoplasmonics based on generalized dispersion model

Participants: Stéphane Lanteri, Claire Scheid, Jonathan Viquerat.

In this work, we are concerned with the numerical modelling of the propagation of electromagnetic waves in dispersive materials for nanophotonics applications. We focus on a generalized model that allows for the description of a wide range of dispersive media. The underlying differential equations are recast into a generic form and we establish an existence and uniqueness result. We then turn to the numerical treatment and propose an appropriate DGTD framework. We obtain the semi-discrete convergence and prove the stability (and to a large extent, the convergence) in the fully discrete case when time integration is achieved with a 4 steps low storage Runge-Kutta scheme, *via* a technique relying on energy principles. Finally, we validate our results through the numerical simulation of two nanophotonics test cases.

6.1.7. Travelling waves for the non-linear Schrödinger equation in 2d

Participants: David Chiron [J.A. Dieudonné Laboratory, University of Nice-Sophia Antipolis], Claire Scheid.

We are interested in the numerical study of the two-dimensional travelling waves of the non-linear Schrödinger equation for a general non-linearity and with nonzero condition at infinity that can appear in optics. The equation has a variational structure that we propose to exploit to design a numerical method. We characterize the saddle points of the action as minimizers of another functional, allowing us to use a gradient flow. Combining this approach with a continuation method in the speed of the wave, we obtain the numerical solution for the full range of velocities. We plot the energy-momentum diagrams for different type of non-linearities. Through various examples, we show that even though the non-linearity has the same behaviour as the well-known Gross-Pitaevskii (GP) non-linearity, the qualitative properties of the travelling waves may be extremely different. For instance, we observe cusps, a modified Kadomtsev-Petviashvili I (KP-I) asymptotic in the transonic limit (as the speed of the wave approaches the speed of sound), various multiplicity results.

6.1.8. Multiscale DG methods for the time-domain Maxwell equations

Participants: Stéphane Lanteri, Raphaël Léger, Diego Paredes Concha [Instituto de Matemáticas, Universidad Católica de Valparaiso, Chile], Claire Scheid, Frédéric Valentin [LNCC, Petropolis, Brazil].

Although the DGTD method has already been successfully applied to complex electromagnetic wave propagation problems, its accuracy may seriously deteriorate on coarse meshes when the solution presents multiscale or high contrast features. In other physical contexts, such an issue has led to the concept of multiscale basis functions as a way to overcome such a drawback and allow numerical methods to be accurate on coarse meshes. The present work, which has been initiated in the context of the visit of Frédéric Valentin in the team, is concerned with the study of a particular family of multiscale methods, named Multiscale Hybrid-Mixed (MHM) methods. Initially proposed for fluid flow problems, MHM methods are a consequence of a hybridization procedure which caracterize the unknowns as a direct sum of a coarse (global) solution and the solutions to (local) problems with Neumann boundary conditions driven by the purposely introduced hybrid (dual) variable. As a result, the MHM method becomes a strategy that naturally incorporates multiple scales while providing solutions with high order accuracy for the primal and dual variables. The completely independent local problems are embedded in the upscaling procedure, and computational approximations may be naturally obtained in a parallel computing environment. In this study, a family of MHM methods is proposed for the solution of the time-domain Maxwell equations where the local problems are discretized either with a continuous FE method or a DG method (that can be viewed as a multiscale DGTD method). Preliminary results have been obtained in the 2d case for models problems.

6.1.9. HDG methods for the time-domain Maxwell equations

Participants: Alexandra Christophe-Argenvillier, Stéphane Descombes, Stéphane Lanteri.

This study is concerned with the development of accurate and efficient solution strategies for the system of 3d time-domain Maxwell equations coupled to local dispersion models (e.g. Debye, Drude or Drude-Lorentz models) in the presence of locally refined meshes. Such meshes impose a constraint on the allowable time step for explicit time integration schemes that can be very restrictive for the simulation of 3d problems. We consider here the possibility of using an unconditionally stable implicit time or a locally implicit time integration scheme combined to a HDG discretization method. In doing so, we extend our former study which was dealing with the 2d time-domain Maxwell equations for non-dispersive media.

6.1.10. HDG methods for the frequency-domain Maxwell equations

Participants: Thomas Frachon, Stéphane Lanteri, Liang Li [UESTC, Chengdu, China], Ludovic Moya, Ronan Perrussel [Laplace Laboratory, Toulouse].

In the context of the ANR TECSER project, we continue our efforts towards the development of scalable high order HDG methods for the solution of the system of 3d frequency-domain Maxwell equations. We aim at fully exploiting the flexibiity of the HDG discretization framework with regards to the adaptation of the interpolation order (p-adaptivity) and the mesh (h-adaptivity). In particular, we study the formulation of HDG methods on a locally refined non-conforming tetrahedral mesh and on a non-confoming hybrid cubic/tetrahedral mesh. We also investigate the coupling between the HDG formulation and a BEM (Boundary Element Method) discretization of an integral representation of the electromagnetic field in the case of propagation problems theoretically defined in unbounded domains.

6.2. Elastodynamic wave propagation

6.2.1. Sesimic wave interaction with viscoelastic media

Participants: Nathalie Glinsky, Stéphane Lanteri, Fabien Peyrusse [Department of Mathematics, Purdue University].

This work is concerned with the development of high order DGTD methods formulated on unstructured simplicial meshes for the numerical solution of the system of time-domain elastodynamic equations. These methods share some ingredients of the DGTD 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. A recent novel contribution is the numerical treatment of 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 3d.

6.2.2. DG 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.

6.2.3. HDG method for the frequency-domain elastodynamic equations

Participants: Hélène Barucq [MAGIQUE-3D project-team, Inria Bordeaux - Sud-Ouest], Marie Bonnasse, Julien Diaz [MAGIQUE-3D project-team, Inria Bordeaux - Sud-Ouest], Stéphane Lanteri.

One of the most used seismic imaging methods is the full waveform inversion (FWI) method which is an iterative procedure whose algorithm is the following. Starting from an initial velocity model, (1) compute the solution of the wave equation for the N sources of the seismic acquisition campaign, (2) evaluate, for each source, a residual defined as the difference between the wavefields recorded at receivers on the top of the subsurface during the acquisition campaign and the numerical wavefields, (3) compute the solution of the wave equation using the residuals as sources, and (4) update the velocity model by cross correlation of images produced at steps (1) and (3). Steps (1)-(4) are repeated until convergence of the velocity model is achieved. We then have to solve $2N$ wave equations at each iteration. The number of sources, N, is usually large (about 1000) and the efficiency of the inverse solver is thus directly related to the efficiency of the numerical method used to solve the wave equation. Seismic imaging can be performed in the time-domain or in the frequency-domain regime. In this work which is conducted in the framework of the Depth Imaging Partnership (DIP) between Inria and TOTAL, we adopt the second setting. The main difficulty with frequency-domain inversion lies in the solution of large sparse linear systems which is a challenging task for realistic 3d elastic media, even with the progress of high performance computing. In this context, we study novel high order HDG methods formulated on unstructured meshes for the solution of the frency-domain elastodynamic equations. Instead of solving a linear system involving the degrees of freedom of all volumic cells of the mesh, the principle of a HDG formulation is to introduce a new unknown in the form of Lagrange multiplier representing the trace of the numerical solution on each face of the mesh. As a result, a HDG formulation yields a global linear system in terms of the new (surfacic) unknown while the volumic solution is recovered thanks to a local computation on each element.

6.2.4. Multiscale DG methods for the time-domain elastodynamic equations

Participants: Marie-Hélène Lallemand, Frédéric Valentin [LNCC, Petropolis, Brazil].

In the context of the visit of Frédéric Valentin in the team, we have initiated a study aiming at the design of novel multiscale methods for the solution of the time-domain elastodynamic equations, in the spirit of MHM (Multiscale Hybrid-Mixed) methods previously proposed for fluid flow problems. Motivation in that direction naturally came when dealing with non homogeneous anisotropic elastic media as those encountered in geodynamics related applications, since multiple scales are naturally present when high contrast elasticity parameters define the propagation medium. Instead of solving the usual system expressed in terms of displacement or displacement velocity, and stress tensor variables, a hybrid mixed-form is derived in which an additional variable, the Lagrange multiplier, is sought as representing the (opposite) of the surface tension defined at each face of the elements of a given discretization mesh. We consider the velocity/stress formulation of the elastodynamic equations, and study a MHM method defined for a heterogeneous medium where each elastic material is considered as isotropic to begin with. If the source term (the applied given force on the medium) is time independent, and if we are given an arbitrarily coarse conforming mesh (triangulation in 2d, tetrahedrization in 3d), the proposed MHM method consists in first solving a series of fully decoupled (therefore parallelizable) local (element-wise) problems defining parts of the full solution variables which are directly related to the source term, followed by the solution of a global (coarse) problem, which yields the degrees of freedom of both the Lagrange multiplier dependent part of the full solution variables and the Lagrange multiplier itself. Finally, the updating of the full solution variables is obtained by adding each splitted solution variables, before going on the next time step of a leap-frog time integration scheme. Theoretical analysis and implementation of this MHM method where the local problems are discretized with a DG method, are underway.

6.3. High performance numerical computing

6.3.1. Porting a DGTD solver for bioelectromagnetics to the DEEP-ER architecture

Participants: Alejandro Duran [Barcelona Supercomputing Center, Spain], Stéphane Lanteri, Raphaël Léger, Damian A. Mallón [Juelich Supercomputing Center, Germany].

We are concerned here with the porting of a Discontinuous Galerkin Time-Domain solver for computational bioelectromagnetics to the novel heterogeneous architecture proposed in the DEEP-ER european project on exascale computing. This architecture is based on a Cluster/Booster division concept (see Fig. 6). The Booster nodes are based on the Intel Many Integrated Core (MIC) architecture. Therfore, one objective of our efforts is the algorithmic adaptation of the DG kernels in order to leverage the vectorizing capabilities of the MIC processor. The other activities that are undertaken in the context of our contribution to this project aim at exploiting the software environments and tools proposed by DEEP-ER partners for implementing resiliency strategies and high performance I/O operations. In particular, the Cluster nodes are used for running some parts of the pre- and post-processing phases of the DGTD solver which do not lend themselves well to multithreading, as well as I/O intensive routines. One possibility to achieve this is to consider a model in which these less scalable and I/O phases are reverse-offloaded from Booster processes to Cluster processes in a one-to-one mapping. This is achieved by exploiting the OmpSs offload functionality, developed at Barcelona Supercomputing Center for the DEEP-ER platform. In future work, the OmpSs framework will also be leveraged to expose task-based parallelism and exploit task-based resilience.

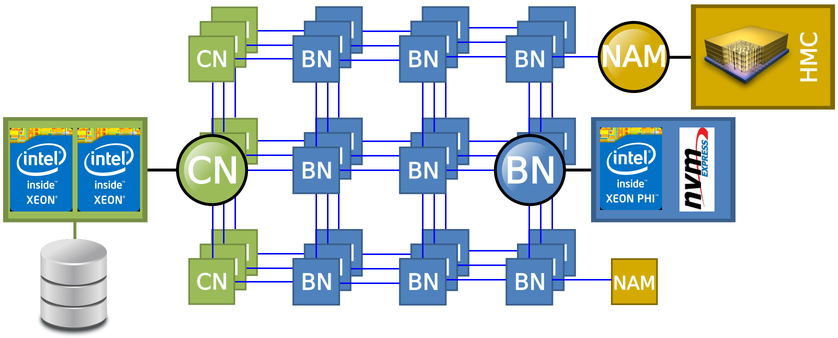


Figure 6. DEEP-ER hardware architecture sketch.

6.3.2. Hybrid MIMD/SIMD high order DGTD solver for nanophotonics

Participants: Tristan Cabel, Gabriel Hautreux [CINES, Montpellier], Stéphane Lanteri, Raphaël Léger, Claire Scheid, Jonathan Viquerat.

This work is concerned with the development of a scalable high order finite element type solver for the numerical modeling of light interaction with nanometer scale structures. From the mathematical modeling point of view, one has to deal with the differential system of Maxwell equations in the time domain, coupled to an appropriate differential model of the behavior of the underlying material (which can be a dielectric and/or a metal) at optical frequencies. For the numerical solution of the resulting system of differential equations, we adopt the high order DGTD (Discontinuous Galerkin Time-Domain) solver described in [21]. A hybrid MIMD/SIMD parallelization of this DGTD solver has been developed by combining the MPI and OpenMP parallel programming models. The performances of the resulting parallel DGTD solver have been assessed on the Curie system of the PRACE research infrastructure. For that purpose, we selected a use case typical of optical guiding applications. A Y-shaped waveguide is considered which consists in nanosphere embedded in vacuum (see Fig. 7). The constructed tetrahedral mesh consists of 520,704 vertices and 2,988,103 elements. The high order discontinuous finite element method designed for the solution of the system of time-domain Maxwell equations coupled to a Drude model for the dispersion of noble metals at optical frequencies is formulated on a tetrahedral mesh.

6.4. Applications

6.4.1. Light diffusion in nanostructured optical fibers

Participants: Wilfried Blanc [Optical Fibers team, LPMC, Nice], Stéphane Lanteri, Paul Loriot, Claire Scheid.

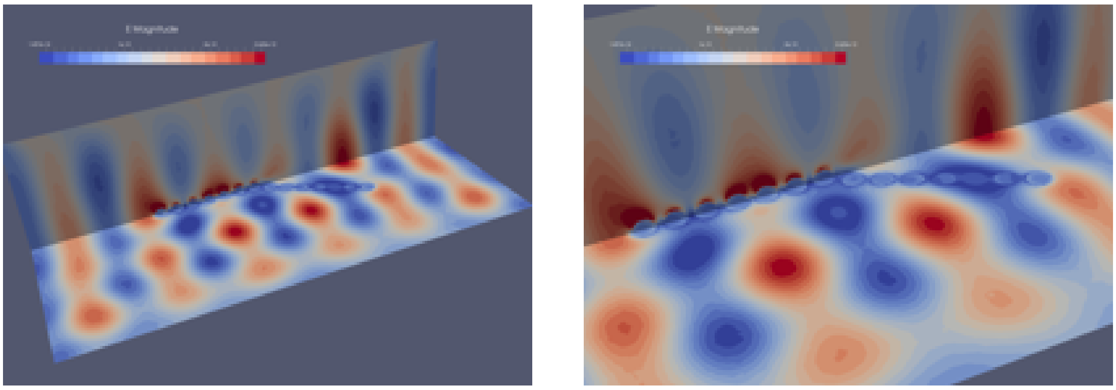


Figure 7. Y-shaped waveguide: contour lines of the amplitude of the discrete Fourier transform of the electric field.

Optical fibers are the basis for applications that have grown considerably in recent years (telecommunications, sensors, fiber lasers, etc.). Despite these undeniable successes, it is necessary to develop new generations of amplifying optical fibers that will overcome some limitations typical of silica. In this sense, the amplifying Transparent Glass Ceramics (TGC), and particularly the fibers based on this technology, open new perspectives that combine the mechanical and chemical properties of a glass host and the augmented spectroscopic properties of embedded nanoparticles, particularly rare earth-doped oxide nanoparticles. Such rare earth-doped silica-based optical fibers with transparent glass ceramic (TGC) core are fabricated by the Optical Fibers team of the Laboratory of Condensed Matter (LPMC) in Nice. The obejctive of this collaboration with Wilfried Blanc at LPMC is the study of optical transmission terms of loss due to scattering through the numerical simulation of light propagation in a nanostructured optical fiber core using a high order DGTD method developed in the team.

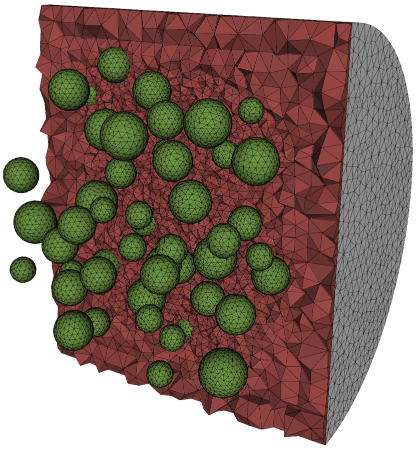


Figure 8. Unstructured tetrahdral mesh of a nanostructured optical fiber core.

6.4.2. Gap-plasmon confinement with gold nanocubes

Participants: Stéphane Lanteri, Antoine Moreau [Institut Pascal, Université Blaise Pascal], Claire Scheid, Jonathan Viquerat.

The propagation of light in a slit between metals is known to give rise to guided modes. When the slit is of nanometric size, plasmonic effects must be taken into account, since most of the mode propagates inside the metal. Indeed, light experiences an important slowing-down in the slit, the resulting mode being called *gap-plasmon*. Hence, a metallic structure presenting a nanometric slit can act as a light trap, i.e. light will accumulate in a reduced space and lead to very intense, localized fields. Recently, the chemical production of random arrangements of nanocubes on gold films at low cost was proved possible by Antoine Moreau and colleagues at Institut Pascal. Nanocubes are separated from the gold substrate by a dielectric spacer of variable thickness, thus forming a narrow slit under the cube. When excited from above, this configuration is able to support gap-plasmon modes which, once trapped, will keep bouncing back and forth inside the cavity. At visible frequencies, the lossy behavior of metals will cause the progressive absorption of the trapped electromagnetic field, turning the metallic nanocubes into efficient absorbers. The frequencies at which this absorption occurs can be tuned by adjusting the dimensions of the nanocube and the spacer. In collaboration with Antoine Moreau, we propose to study numerically the impact of the geometric parameters of the problem on the behaviour of a single nanocube placed over a metallic slab (see Fig. 9). The behavior of single nanocubes on metallic plates has been simulated, for lateral sizes c ranging from 50 to 80 nm, and spacer thicknesses δ from 3 to 22 nm. The absorption efficiency in the cube Q_{cube} at the resonance frequency is retrieved from the results of each computation (see Fig. 10).

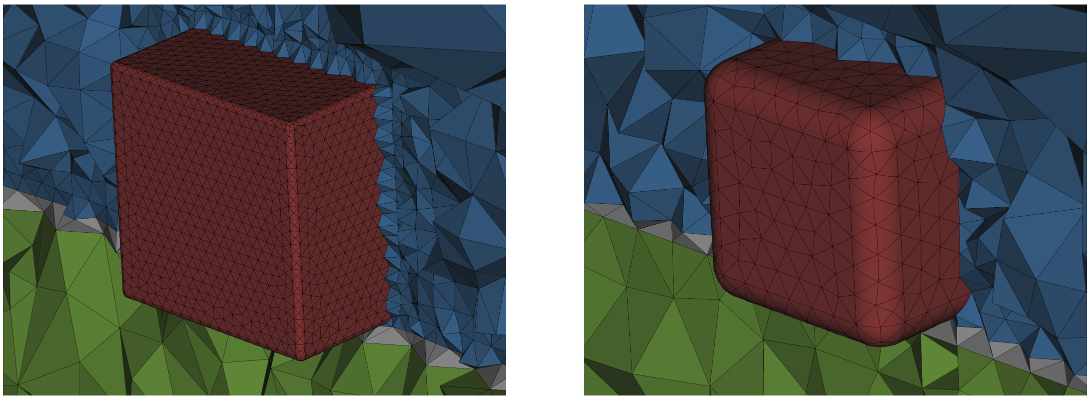
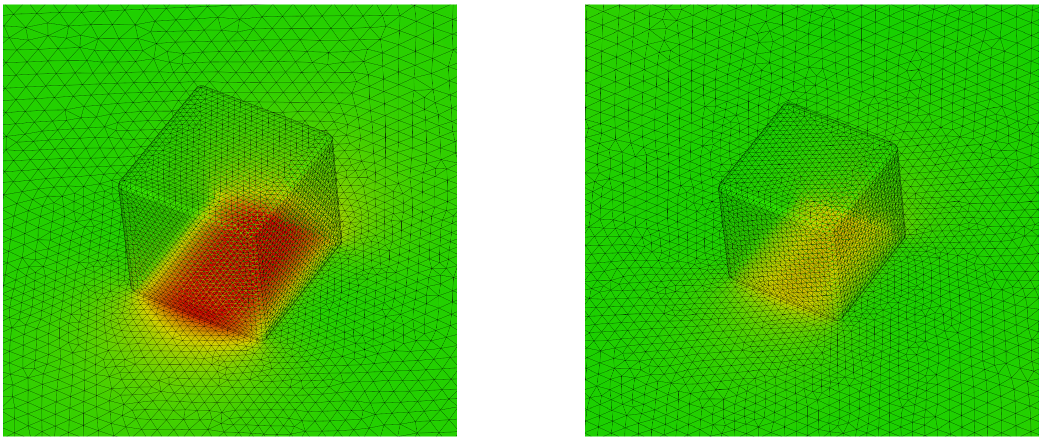


Figure 9. Meshes of rounded nanocubes with rounding radii ranging from 2 to 10 nm. Red cells correspond to the cube. The latter lies on the dielectric spacer (gray cells) and the metallic plate (green). Blue cells represent the air surrounding the device.

6.4.3. Light propagation in power splitters

Participants: Julien Coulet, Carlos Henrique Da Silva Santos [Instituto Federal de Educaçäo, Ciência e Tecnologia de Säo Paulo, Brazil], Hugo Enrique Hernandez Figueroa [Universidade Estadual de Campinas, Faculdade de Engenharia Elétrica e de Computaçäo, Säo Paulo, Brazil], Stéphane Lanteri, Frédéric Valentin [LNCC, Petropolis, Brazil].

Power splitters are passive devices widely used in signal processing, which splits an input signal into two or more output signals. The repartition of the input power over each output is specifc to the required usage. Even if power splitters are common in classical electronics, designing them at the micrometric scale is quietly recent and is an active field of research. The purpose of this study initiated in the framework of a collaboration with



$c = 70$ nm, $\delta = 12$ nm

$c = 60$ nm, $\delta = 18$ nm

Figure 10. Amplitude of the discrete Fourier transform of the magnetic field for different nanocube configurations. All field maps are scaled identically for better comparison. The obtained field is more intense for configurations that yield high Q_{cube} values.

researchers at Unicamp in Säo Paulo is to study the electromagnetic wave propagation is such a power splitter geometry using a high order DGTD method developed in the team, see Fig. 11.

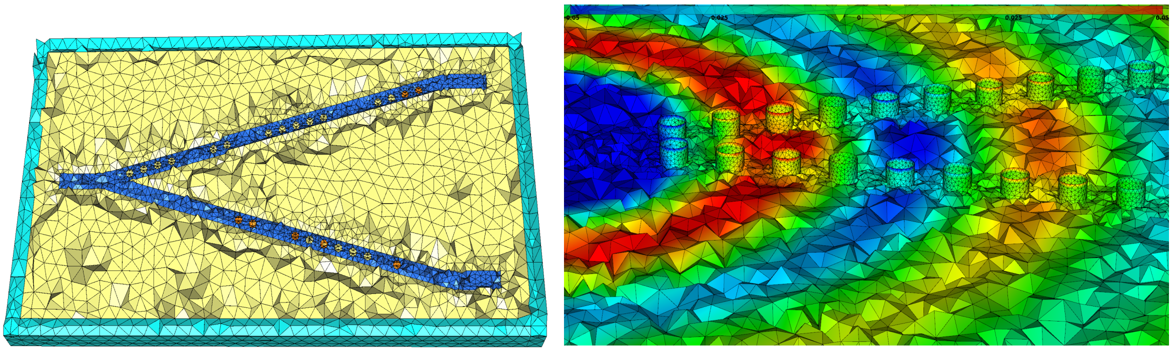
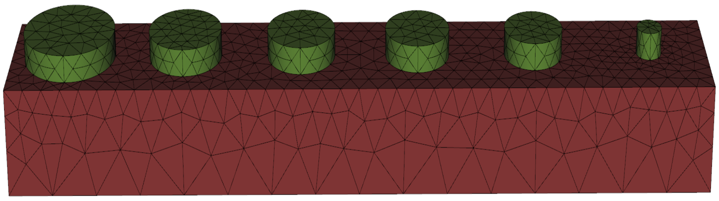


Figure 11. Geomtry of Y-shaped power splitter (left) and contour lines of the amplitude of the electric field (right).

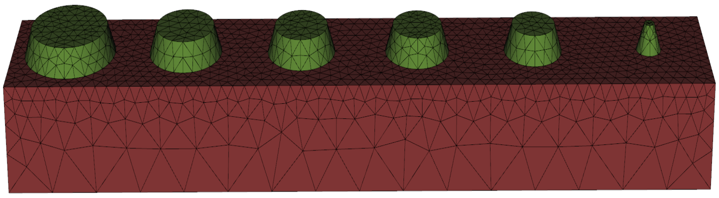
6.4.4. Dielectric reflectarrays

Participants: Maciej Klemm [Centre for Communications Research, University of Bristol], Stéphane Lanteri, Claire Scheid, Jonathan Viquerat.

In the past few years, important efforts have been deployed to find alternatives to on-chip, low-performance metal interconnects between devices. Because of the ever-increasing density of integrated components, intra- and inter-chip data communications have become a major bottleneck in the improvement of information processing. Given the compactness and the simple implantation of the devices, communications *via* free-space optics between nanoantenna-based arrays have recently drawn more attention. Here, we focus on a specific low-loss design of dielectric reflectarray (DRA), whose geometry is based on a periodic repartition of dielectric cylinders on a metallic plate. When illuminated in normal incidence, specific patterns of such resonators provide a constant phase gradient along the dielectric/metal interface, thus altering the phase of the incident wavefront. The gradient of phase shift generates an effective wavevector along the interface, which is able to deflect light from specular reflection. However, the flaws of the lithographic production process can lead to discrepancies between the ideal device and the actual resonator array. Here, we propose to exploit our DGTD solver to study the impact of the lithographic flaws on the performance of a 1D reflectarray (see Fig. 12). Efficient computations are obtained by combining high-order polynomial approximation with curvilinear meshing of the resonators, yielding accurate results on very coarse meshes (see Fig. 13). The study is continued with the computation of the reflection of a 2D reflectarray. This work constitutes the base of a wider study in collaboration with Maciej Klemm at the Centre for Communications Research, University of Bristol.



Ideal reflectarray



Realistic reflectarray

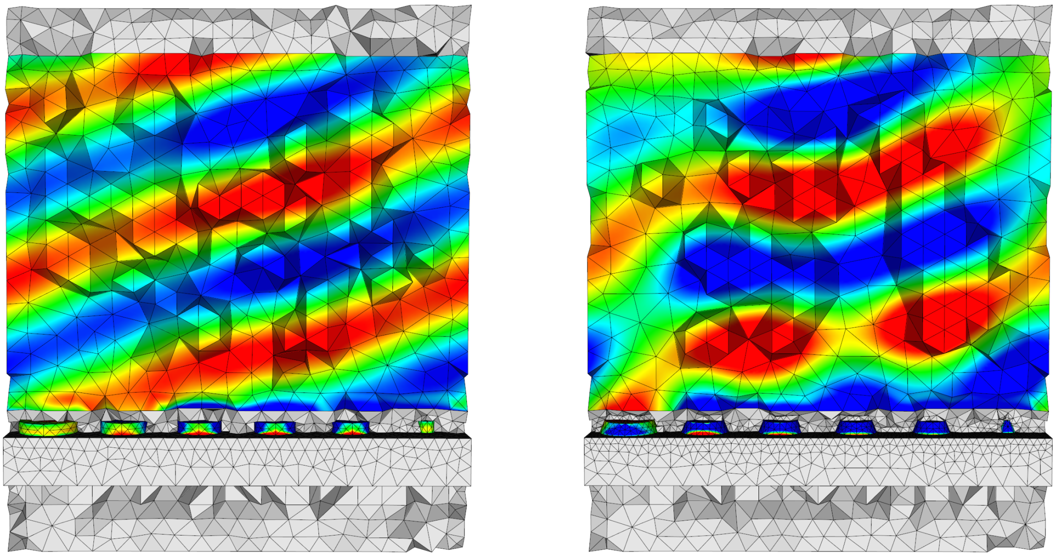
Figure 12. Ideal and realistic 1D dielectric reflectarray meshes. The red tetrahedra correspond to silver, while the green ones are made of an anisotropic dielectric material. The device is surrounded by air and terminated by a PML above and below, and by periodic boundary conditions on the lateral sides.

7. Partnerships and Cooperations

7.1. National Initiatives

7.1.1. Inria Project Lab

7.1.1.1. C2S@Exa (Computer and Computational Sciences at Exascale)



Ideal reflectarray Realistic reflectarray

Figure 13. Time-domain snapshot of E_y component for ideal and realistic 1D dielectric reflectarrays. Solution is obtained in established regime at $t = 0.1$ ps. Fields are scaled to $[-1, 1]$.

Participants: Olivier Aumage [STORM project-team, Inria Bordeaux - Sud-Ouest], Philippe Helluy [TONUS project-team, Inria Nancy - Grand-Est], Luc Giraud [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Stéphane Lanteri [Coordinator of the project], Jean-François Méhaut [CORSE project-team, Inria Grenoble - Rhône-Alpes], Christian Perez [AVALON 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.

7.1.2. ANR project

7.1.2.1. TECSER

Participants: Emmanuel Agullo [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Xavier Antoine [CORIDA project-team, Inria Nancy - Grand-Est], Patrick Breuil [Nuclétudes, Les Ulis], Thomas Frachon, Luc Giraud [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Stéphane Lanteri, Ludovic Moya, Guillaume Sylvand [Airbus Group Innovations].

Type: ANR ASTRID

Duration: May 2014 - April 2017

Coordinator: Inria

Partner: Airbus Group Innovations, Inria, Nuclétudes

Inria contact: Stéphane Lanteri

Abstract: the objective of the TECSER project is to develop an innovative high performance numerical methodology for frequency-domain electromagnetics with applications to RCS (Radar Cross Section) calculation of complicated structures. This numerical methodology combines a high order hybridized DG method for the discretization of the frequency-domain Maxwell in heterogeneous media with a BEM (Boundary Element Method) discretization of an integral representation of Maxwell's equations in order to obtain the most accurate treatment of boundary truncation in the case of theoretically unbounded propagation domain. Beside, scalable hybrid iterative/direct domain decomposition based algorithms are used for the solution of the resulting algebraic system of equations.

7.2. European Initiatives

7.2.1. FP7 & H2020 Projects

7.2.1.1. DEEP-ER

Title: Dynamic Exascale Entry Platform - Extended Reach

Program: FP7

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: Stéphane 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.

7.2.1.2. HPC4E

Title: HPC for Energy

Programm: H2020
Duration: December 2015 - November 2017
Coordinator: Barcelona Supercomputing Center
Partner: Barcelona Supercomputing Center (Spain), Centro de Investigaciones Energeticas, Medioambientales y Tecnologicas - CIEMAT (Spain), REPSOL SA (Spain), Iberdrola Renovables Energia SA (spain), Lancaster University (United Kingdom), COPPE/UFRJ - Universidade Federal do Rio de Janeiro (Brazil), LNCC (Brazil), INF/UFRGS - Universidade Federal do Rio Grande do Sul (Brazil), CER/UFPE - Universidade Federal de Pernambuco (Brazil), PETROBRAS (Brazil), TOTAL SA (France), and Inria (France).
Inria contact: Stéphane Lanteri
Abstract: This project aims to apply the new exascale HPC techniques to energy industry simulations, customizing them, and going beyond the state-of-the-art in the required HPC exascale simulations for different energy sources: wind energy production and design, efficient combustion systems for biomass-derived fuels (biogas), and exploration geophysics for hydrocarbon reservoirs. For wind energy industry HPC is a must. The competitiveness of wind farms can be guaranteed only with accurate wind resource assessment, farm design and short-term micro-scale wind simulations to forecast the daily power production. The use of CFD LES models to analyse atmospheric flow in a wind farm capturing turbine wakes and array effects requires exascale HPC systems. Biogas, i.e. biomass-derived fuels by anaerobic digestion of organic wastes, is attractive because of its wide availability, renewability and reduction of CO2 emissions, contribution to diversification of energy supply, rural development, and it does not compete with feed and food feedstock. However, its use in practical systems is still limited since the complex fuel composition might lead to unpredictable combustion performance and instabilities in industrial combustors. The next generation of exascale HPC systems will be able to run combustion simulations in parameter regimes relevant to industrial applications using alternative fuels, which is required to design efficient furnaces, engines, clean burning vehicles and power plants. One of the main HPC consumers is the oil & gas (O&G) industry. The computational requirements arising from full wave-form modelling and inversion of seismic and electromagnetic data is ensuring that the O&G industry will be an early adopter of exascale computing technologies. By taking into account the complete physics of waves in the subsurface, imaging tools are able to reveal information about the Earth's interior with unprecedented quality.

7.3. International Initiatives

7.3.1. Inria Associate Teams not involved in an Inria International Labs

7.3.1.1. HOMAR

Title: High performance Multiscale Algorithms for wave pRopagation problems
International Partner (Institution - Laboratory - Researcher):

Laboratório Nacional de Computação Científica (Brazil) - Coordenação de Matemática Aplicada e Computaciona - Frédéric Valentin

Start year: 2015
See also: http://www-sop.inria.fr/nachos/index.php/Main/HOMAR

The general scientific context of the collaboration proposed in the HOMAR project is the study of time dependent wave propagation problems presenting multiscale features (in space and time). The general goal is the design, analysis and implementation of a family of innovative high performance numerical methods particularly well suited to the simulation of such multiscale wave propagation problems. Mathematical models based on partial differential equations (PDE) embedding multiscale features occur in a wide range of scientific and technological applications involving wave propagation in heterogeneous media. Electromagnetic wave propagation and seismic wave propagation are two relevant physical settings that will be considered in the project. Indeed, the present collaborative project will focus on two particular application contexts: the interaction of light (i.e. optical wave) with nanometer scale structure (i.e. nanophotonics) and, the interaction of seismic wave propagation with geological media for quantitative and non destructive evaluation of imperfect interfaces.

7.3.2. Inria International Partners

7.3.2.1. Informal International Partners

Prof. Liang Li, School of Mathematical Sciences, University of Electronic Science and Technology of China, Chengdu.

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

Prof. Hugo Enrique Hernandez Figueroa, Universidade Estadual de Campinas, Faculdade de Engenharia Elétrica e de Computação, Säo Paulo, and Prof. Carlos Henrique da Silva Santos, Instituto Federal de Educação, Ciência e Tecnologia de São Paulo, Brazil

Dr. Urs Aeberhard and Dr. Markus Ermes, Theory and Multiscale Simulation, IEK-5 Photovoltaik, Forschungszentrum Jülich, Germany

7.3.3. Participation In other International Programs

7.3.3.1. CNPq-Inria HOSCAR project

Participants: Reza Akbarinia [ZENITH project-team, Inria Sophia Antipolis - Méditerranée], Rossana Andrade [CSD/UFC], Hélène Barucq [MAGIQUE-3D project-team, Inria Bordeaux - Sud-Ouest], Alvaro Coutinho [COPPE/UFR], Julien Diaz [MAGIQUE-3D 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 Graduate 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. Dissemination

8.1. Promoting Scientific Activities

8.1.1. Scientific events organisation

8.1.1.1. Member of the organizing committees

Claire Scheid and David Chiron (University of Nice - Sophia Antipolis) co-organized of the conference entitled "IDTPsi: Theory and Numerics" around Schrödinger equations, J.A. Dieudonné Laboratory, University of Nice - Sophia Antipolis, January 12-14, 2015.

Peter Bastian (Interdisziplinäres Zentrum für Wissenschaftliches Rechnen Universität Heidelberg) and Stéphane Lanteri have co-organized a mini-symposium on "Recent advances on scalable high order finite element type schemes for PDEs" in the framework of the Platform for Advanced Scientific Computing (PASC15), ETH Zurich, Switzerland, June 1-3, 2015.

Marcus Grote (Mathematisches Institut - Universität Basel) and Stéphane Lanteri have co-organized a mini-symposium on "Advanced time-stepping methods for wave propagation" in the framework of the International Conference on Scientific Computation And Differential Equations (SciCADE 2015), University of Potsdam, Germany, September 14-18, 2015.

8.1.2. Invited talks

Claire Scheid, “Etude numérique de modèles milieux dispersifs et application en nanophotonique”, Analyse Numérique et EDP seminar, Laboratoire de Mathématiques d’Orsay, March 12, 2015.

Claire Scheid, “Numerical study of dispersive media and application to nanophotonics”, KIT Seminar, Karlsruhe, Germany, Frebruary 9, 2015

Stéphane Descombes, “Locally implicit and implicit discontinuous Galerkin time domain method for electromagnetic wave propagation in dispersive media”, Numerical Solution of Differential and Differential-Algebraic Equations (Numdiff-14), Martin Luther University Halle-Wittenberg, Germany, September 7-11, 2015.

Stéphane Lanteri, “Numerical modeling of light/matter interaction on the nanoscale with a high order finite element type time-domain solver”, Annual meeting of GDR PMSE (Plasmonique Moléculaire et Spectroscopies Exaltées), Inria Paris-Rocquencourt, November 25-27, 2015.

8.2. Teaching - Supervision - Juries

8.2.1. Teaching

Stéphane Descombes is the head of the mathematical department of the faculty of sciences at the University of Nice-Sophia Antipolis. He is responsible of the managment of all mathematical courses (around 13 000 hours/year), and especially of the M2 *Computational Biology*.

Stéphane Descombes, *Scientific computing*, M1, 18 h, University of Nice-Sophia Antipolis.

Stéphane Descombes, *Principal components analysis*, M2, 30 h, University of Nice-Sophia Antipolis.

Stéphane Descombes, *Statistics*, M2, 30 h, University of Nice-Sophia Antipolis.

Stéphane Lanteri, *Computational electromagnetics*, MAM5, 20 h, Polytech Nice.

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

Claire Scheid, *Lectures and practical works, Analysis*, "Agrégation", 22h, University of Nice Sophia Antipolis.

Claire Scheid, *Lectures and practical works in Numerical Analysis*, 36 h, M1, Mathematics engineering, University of Nice-Sophia Antipolis.

Claire Scheid, *Lectures and practical works, Option*, "Agrégation", 16h, University of Nice Sophia Antipolis.

8.2.2. Supervision

PhD defended in December 2015: 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 defended in December 2015: Jonathan Viquerat, *Discontinuous Galerkin Time-Domain methods for nanophotonics applications*, October 2012, Stéphane Lanteri and Claire Scheid.

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: Colin Vo Cing Tri, *Numerical modeling of non-local dispersion for plasmonic nanostructures*, November 2014, Stéphane Lanteri and Claire Scheid.

PhD in progress: Nikolai Schmitt, *Numerical modeling of electron beam interaction with nanostructures*, October 2015, Stéphane Lanteri.

PhD in progress: Van Hieu Nguyen, *SMART-RATS: Small Animals RFID Integrated Antenna Tracking System*, october 2015, Philippe Lethuc (University of Nice-Sophia Antipolis and LEAT) and Stéphane Lanteri.

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