IN PARTNERSHIP WITH:
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Université Nice - Sophia Antipolis

Activity Report 2018

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

Creation of the Project-Team: 2007 July 01

Keywords:

Computer Science and Digital Science:

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A6.2.6. - Optimization
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Other Research Topics and Application Domains:

B4.3. - Renewable energy production
B4.3.4. - Solar Energy
B5.3. - Nanotechnology
B5.5. - Materials

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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 [42] 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 [48] 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 [37] 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 [46] 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 [34]- [35]- [36]- [41]:

- 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 [9]. 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 [6]-[7] and hybrid structured/unstructured meshes [4], their coupling with hybrid explicit/implicit time integration schemes in order to improve their efficiency in the context of locally refined meshes [3]-[13]-[12]. A high order DG method has also been proposed for the numerical resolution of the elastodynamic equations modeling the propagation of seismic waves [2].

- **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 [5]. 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.*[39] 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[11].
- **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 are investigating 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 [3]-[13]-[12] 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 [10]. 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 [15]. In the context of seismic wave propagation, we are interested by the intrinsic attenuation of the medium [14]. 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 method due to Yee [48]. 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 [8].

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

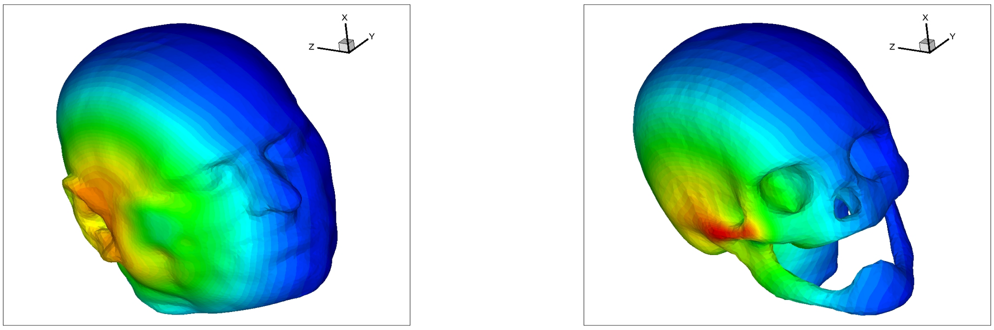

Figure 1. Exposure of head tissues to an electromagnetic wave emitted by a localized source. Top figures: surface triangulations of the skin and the skull. Bottom figures: contour lines of the amplitude of the electric field.

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 [40]- [49].

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 [45]. 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 [43]- [44]- [38]. 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.

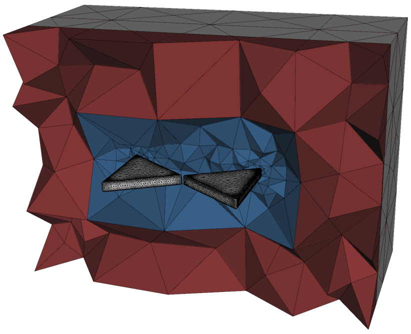

Figure 2. Simulation of the field enhancement at the tip of a gold bowtie nanoantenna (PhD thesis of Jonathan Viquerat).

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 for 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. 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 [46] and based on the first order velocity-stress hyperbolic system of elastic waves equations, which is an extension of the scheme derived by Yee [48] 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 collaborated with CETE

Méditerranée which is a regional technical and engineering centre whose activities are concerned with seismic hazard assessment studies, and IFSTTAR (https://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.

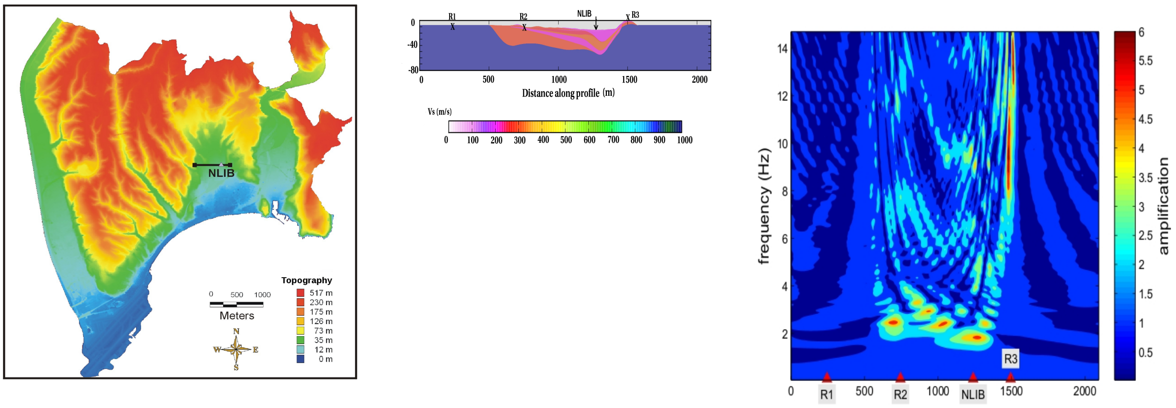

Figure 3. Propagation of a plane wave in a heterogeneous model of Nice area (provided by CETE Méditerranée). Left figure: topography of Nice and location of the cross-section used for numerical simulations (black line). Middle figure: S-wave velocity distribution along the cross-section in the Nice basin.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

4.2.2. Seismic exploration

This application topic is considered 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. DIOGENeS

DIscOntinuous GalErkin Nanoscale Solvers

KEYWORDS: High-Performance Computing - Computational electromagnetics - Discontinuous Galerkin - Computational nanophotonics

FUNCTIONAL DESCRIPTION: The DIOGENeS software suite provides several tools and solvers for the numerical resolution of light-matter interactions at nanometer scales. A choice can be made between time-domain (DGTD solver) and frequency-domain (HDGFD solver) depending on the problem. The available sources, material laws and observables are very well suited to nano-optics and nano-plasmonics (interaction with metals). A parallel implementation allows to consider large problems on dedicated cluster-like architectures.

- Authors: Stéphane Lanteri, Nikolai Schmitt, Alexis Gobe and Jonathan Viquerat
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- URL: https://diogenes.inria.fr/

5.2. GERShWIN

discontinuous GalERkin Solver for microWave INteraction with biological tissues
KEYWORDS: High-Performance Computing - Computational electromagnetics - Discontinuous Galerkin - Computational bioelectromagnetics
FUNCTIONAL DESCRIPTION: GERShWIN is based on a high order DG method formulated on unstructured tetrahedral meshes for solving the 3D system of time-domain Maxwell equations coupled to a Debye dispersion model.

- Contact: Stéphane Lanteri
- URL: http://www-sop.inria.fr/nachos/index.php/Software/GERShWIN

5.3. HORSE

High Order solver for Radar cross Section Evaluation
KEYWORDS: High-Performance Computing - Computational electromagnetics - Discontinuous Galerkin
FUNCTIONAL DESCRIPTION: HORSE is based on a high order HDG (Hybridizable Discontinuous Galerkin) method formulated on unstructured tetrahedral and hybrid structured/unstructured (cubic/tetrahedral) meshes for the discretization of the 3D system of frequency-domain Maxwell equations, coupled to domain decomposition solvers.

- Contact: Stéphane Lanteri
- URL: http://www-sop.inria.fr/nachos/index.php/Software/HORSE

6. New Results

6.1. Electromagnetic wave propagation

6.1.1. POD-based reduced-order DGTD method

Participants: Stéphane Lanteri, Kun Li [UESTC, Chengdu, China], Liang Li [UESTC, Chengdu, China].

This study is concerned with reduced-order modeling for time-domain electromagnetics and nanophotonics. More precisely, we consider the applicability of the proper orthogonal decomposition (POD) technique for the system of 3D time-domain Maxwell equations, possibly coupled to a Drude dispersion model, which is employed to describe the interaction of light with nanometer scale metallic structures. We introduce a discontinuous Galerkin (DG) approach for the discretization of the problem in space based on an unstructured tetrahedral mesh. A reduced subspace with a significantly smaller dimension is constructed by a set of POD basis vectors extracted offline from snapshots that are obtained by the global DGTD scheme with a second order leap-frog method for time integration at a number of time levels. POD-based ROM is established by projecting (Galerkin projection) the global semi-discrete DG scheme onto the low-dimensional space. The stability of the POD-based ROM equipped with the second order leap-frog time scheme has been analysed through an energy method. Numerical experiments have allowed to verify the accuracy, and demonstrate the capabilities of the POD-based ROM. These very promising preliminary results are currently consolidated by assessing the efficiency of the proposed POD-based ROM when applied to the simulation of 3D nanophotonic problems.

6.1.2. Numerical treatment of non-local dispersion for nanoplasmonics

Participants: Herbert de Gersem [TEMF, Technische Universität Darmstadt, Germany], Stéphane Lanteri, Antoine Moreau [Université Clermont Auvergne], Claire Scheid, Dimitrios Loukrezis [TEMF, Technische Universität Darmstadt, Germany], Serge Nicaise [Université de Valenciennes et du Hainaut-Cambresis], Armel Pitelet [Université Clermont Auvergne], Nikolai Schmitt, Jonathan Viquerat.

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 (called plasmons) can be excited and cause extreme local field enhancements. 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 response due to electron collisions have to be taken into account. This leads to additional, in general non-linear, partial differential equations and is significantly more difficult to treat, though. The classical model is based on a hydrodynamical approach that takes non-local response of the electrons into account. We in particular focus our attention on the linearized version of this model called Linearized Hydrodynamical Drude model. We conducted numerical studies in 2D (published in 2016) and 3D on a linearized hydrodynamic model (published in 2018). However differences between local and nonlocal response are still small. Especially for today's fabrication precision, it remains a challenging task to find reliable structures where non-locality is dominant over e.g. geometrical errors. Motivated by trying to find experimental setups where non-locality is clearly distinguishable from other effects, we studied two promising structures, in close collaboration with physicists. First, in collaboration with A. Pitelet and A. Moreau from Université Clermont Auvergne, and D. Loukrezis and H. De Gersem from Technische Universität Darmstadt, we studied the impact of non-locality on gratings and showed that non-locality can affect surface plasmons propagating at the interface between a metal and a dielectric with a sufficiently high permittivity. We then design a grating coupler that should allow to experimentally observe this influence. Finally, we carefully set up a procedure to measure the signature of spatial dispersion precisely, paving the way for future experiments. Indeed, to ensure that the impact of non-locality exceeds geometric fabrication uncertainties, we proposed a post-fabrication characterization of the grating coupler. Based on the solution of inverse problems leading to the actually fabricated geometry and an uncertainty quantification (UQ) analysis, we conclude that non-locality should clearly be measurable in the grating coupler setting. This work has been submitted in a physics journal. Secondly in collaboration with A. Moreau we considered a nanocube setup that consists of an infinite gold ground layer plus a dielectric spacer of a given height above which a silver nanocube is chemically deposited. Due to this particular setting, the illumination of such a device is creating inside the gap between the nanocube and the ground layer (i.e. inside the dielectric layer) a gap plasmon that is very sensitive to non-locality. We proposed a surrogate-model based telemetry strategy in order to obtain the fabricated cube dimension (inverse problem). Based on this geometric characterization, we decreased the gap-size between the gold substrate and the silver cube and have compared local and non-local numerical simulations. We showed that the influence of non-locality exceeds the experimental error-bars for gap-sizes below 3.1 nm. Additionally, our nonlocal simulations are able to explain the discrepancy between the experiment and local simulations for very small gap-sizes. This project is still ongoing, since we are waiting for another set of experimental results.

On a theoretical side, we pursue the collaboration with S. Nicaise (Université de Valenciennes et du Hainaut-Cambresis) and proved well-posedness of the linearized non-local Drude model for various boundary conditions. We furthermore focused on establishing polynomial stability with optimal energy decay rate. We conducted a thorough study of energy stability for various numerical schemes and DG formulation using a general framework and finally numerically investigate the discrete polynomial stability. This work is almost finalized.

6.1.3. Study of 3D periodic structures at oblique incidences

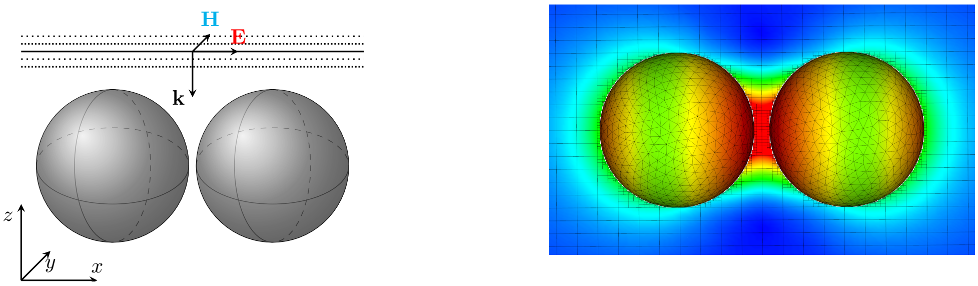

Figure 4. Nanosphere dimer system. Left figure sketches the dimer setup with an $\mathbf{e}_x$ polarized incident plane wave. Right figure shows the 3D field distribution of the electric field on the dimer surface and on a cutting plane and along the dimer axis (PhD thesis of Nikolai Schmitt).

Participants: Claire Scheid, Nikolai Schmitt, Jonathan Viquerat.

In this work, we focus on the development of the use of periodic boundary conditions with sources at oblique incidence in a DGTD framework. Whereas in the context of the Finite Difference Time Domain (FDTD) methods, an abundant literature can be found, for DGTD, the amount of contributions reporting on such methods is remarkably low. In this work, we supplement the existing references using the field transform technique with an analysis of the continuous system using the method of characteristics and provide an energy estimate. Furthermore, we also study the numerical stability of the resulting DGTD scheme. After numerical validations, two realistic test problems have been considered in the context of nanophotonics with our DIOGENeS DGTD solver. This work is under review.

6.1.4. Toward thermoplasmonics

Participants: Yves d'Angelo, Guillaume Baffou [Fresnel Institute, Marseille], Stéphane Lanteri, Claire Scheid.

Although losses in metal is viewed as a serious drawback in many plasmonics experiments, thermoplasmonics is the field of physics that tries to take advantage of the latter. Indeed, the strong field enhancement obtained in nanometallic structures lead to a localized raise of the temperature in its vicinity leading to interesting photothermal effects. Therefore, metallic nanoparticles may be used as heat sources that can be easily integrated in various environments. This is especially appealing in the field of nanomedecine and can for example be used for diagnosis purposes or nanosurgery to cite but just a few. This year, we initiated a preliminary work towards this new field in collaboration with Y. D'Angelo (Université Côte d'Azur) and G. Baffou (Fresnel Institute, Marseille) who is an expert in this field. Due to the various scales and phenomena that come into play, the numerical modeling present great challenges. The laser illumination first excite a plasmon oscillation (reaction of the electrons of the metal) that relaxes in a thermal equilibrium and in turn excite the metal lattice (phonons). The latter is then responsible for heating the environment. A relevant modeling approach thus consists in describing the electron-phonon coupling through the evolution of their respective temperature. Maxwell's equations is then coupled to a set of coupled nonlinear hyperbolic equations describing the evolution of the temperatures of electrons, phonons and environment. The nonlinearities and the different time scales at which each thermalization occurs make the numerical approximation of these equations quite challenging.

6.1.4.1. Numerical modeling of metasurfaces

Participants: Loula Fezoui, Patrice Genevet [CRHEA laboratory, Sophia Antipolis], Stéphane Lanteri, Liang Li [UESTC, Chengdu, China], Ronan Perrussel [Laplace laboratory, Toulouse].

Metamaterials are composed of periodic subwavelength metal/dielectric structures that resonantly couple to the electric and/or magnetic components of the incident electromagnetic fields, exhibiting properties that are not found in nature. Planar metamaterials with subwavelength thickness, or metasurfaces, consisting of a layer of dielectric or plasmonic nanostructures, can be readily fabricated using lithography and nanoprinting methods, and the ultrathin thickness in the wave propagation direction can greatly suppress the undesirable losses. Metasurfaces enable a spatially varying optical response, mold optical wavefronts into shapes that can be designed at will, and facilitate the integration of functional materials to accomplish active control and greatly enhanced nonlinear response. Designing metasurfaces is generally a challenging inverse problem. A recently introduced synthesis techniques is based on so-called General Sheet Transition Conditions (GSTC) that can be leveraged to define the components of general bianisotropic surface susceptibility tensors characterizing the metasurface. A GSTC-based design technique has several advantages: 1) it is exact; 2) it is general, transforming arbitrary incident waves into arbitrary reflected and transmitted waves, 3) it often admits closed-form solutions, 4) it provides deep insight into the physics of the transformations, 5) it allows multiple (at least up to 4) simultaneous and independent transformations. We study the numerical treatment of GSTC in the time-domain and frequency-domain regimes in the DG and HDG settings respectively.

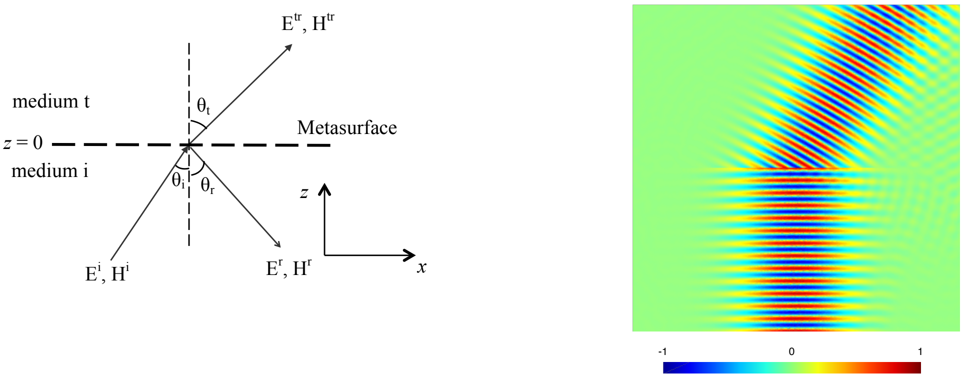

Figure 5. Simulation of a generalized refracting metasurface: problem formulation (left) and real part of H_y, refraction at $\theta = \pi/6$ (right).

6.1.4.2. Corner effects in nanoplasmonics

Participants: Camille Carvalho [Applied Mathematics Department, University of California Merced, USA], Patrick Ciarlet [ENSTA, POEMS project-team], Claire Scheid.

In this work, we study nanoplasmonic structures with corners (typically a diedral/triangular structure). This is the central subject considered in 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 is also relevant and we propose to use the techniques developed in the team in this prospect. Even if both approaches (time-domain and frequency-domain) represent similar physical phenomena, problems that arise are different. These two approaches appear as complementary; it is thus worth bridging the gap between the two frameworks. We are currently performing a thorough comparison in the case of theses 2D structures with corners and we especially focus on the amplitude principle limit that raises a lot of questions.

6.1.4.3. MHM methods for the time-domain Maxwell equations

Participants: Alexis Gobé, Stéphane Lanteri, 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 is conducted in the context of the HOMAR Associate 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 two-dimensional case.

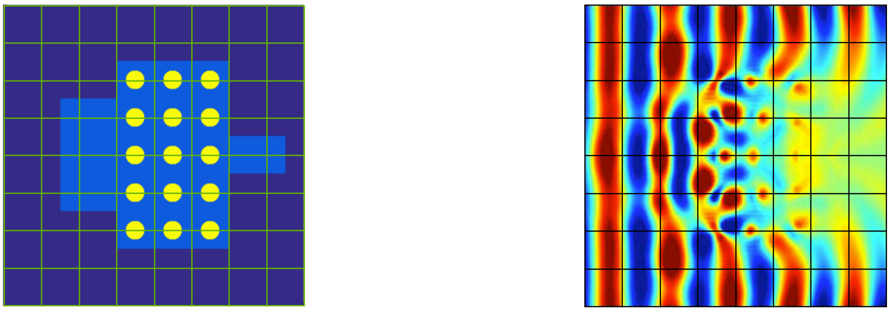

Figure 6. Light propagation in a photonic crystal structure using a MHM-DGTD method for solving the 2D Maxwell's equations. Left: quadrangular mesh. Right: contour lines of the amplitude of the electric field.

6.1.4.4. MHM methods for the frequency-domain Maxwell equations

Participants: Théophile Chaumont-Frelet, Zakaria Kassali, Stéphane Lanteri, Frédéric Valentin [LNCC, Petropolis, Brazil].

We have initiated this year a study of MHM methods for the system of frequency-domain Maxwell equations based on very promising results recently obtained by T. Chaumont-Frelet and F. Valentin for the Helmholtz equation. The design principles are very similar to those underlying MHM methods for the system of time-domain Maxwell equations however we expect to achieve more convincing results for highly multiscale problems since we do not have to deal with the time dimension in the present case. Part of this study is conducted in the context of the PHOTOM (PHOTOvoltaic solar devices in Multiscale computational simulations) Math-Amsud project.

6.1.4.5. HDG methods for the time-domain Maxwell equations

Participants: Stéphane Descombes, Stéphane Lanteri, Georges Nehmetallah.

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. As a preliminary step, we have investigated a fully explicit HDG method generalizing the classical upwind flux-based DG method for the system of time-domain Maxwell equations. We have studied the stability of this new HDG method and in particular, the influence of the stabilization parameter on the CFL condition. We are now progressing toward the design of a new family of high order in time hybrid explicit-implicit HDG methods to deal efficiently with CFL restriction due to grid-induced stiffness.

6.1.4.6. HDG methods for frequency-domain plasmonics

Participants: Stéphane Lanteri, Mostafa Javadzadeh Moghtader, Liang Li [UESTC, Chengdu, China].

HDG method is a new class of DG family with significantly less globally coupled unknowns, and can leverage a post-processing step to gain super-convergence. Its features make HDG a possible candidate for computational electromagnetics applications, especially in the frequency-domain. The HDG method introduces an hybrid variable, which represents an additional unknown on each face of the mesh, and leads to a sparse linear system in terms of the degrees of freedom of the hybrid variable only. Our HDG method had been first introduced for the system of 3D time-harmonic Maxwell's, combined to an iterative Schwarz domain decomposition (DD) algorithm to allow for an efficient parallel hybrid iterative-direct solver. The resulting DD-HDG solver has been applied to classical applications of electromagnetics in the microwave regime. In the present study we further focus on this particular physical context and propose a arbitrary high order HDG method for solving the system of 3D frequency-domain Maxwell equations coupled to a generalized model of physical dispersion in metallic nanostructures at optical frequencies. Such a generalized dispersion model unifies most common dispersion models, like Drude and Drude-Lorentz models, and it permits to fit large range of experimental data. The resulting DD-HDG solver is capable of using different element types and orders of approximation, hence enabling the possibilities of p-adaptivity and non-conforming meshing, and proves to have interesting potentials for modeling of complex nanophotonic and nanoplasmonic problems.

6.2. Elastodynamic wave propagation

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

Participants: Marie-Hélène Lallemand, Claire Scheid, Weslley Da Silva Pereira [LNCC, Petropolis, Brazil], 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.

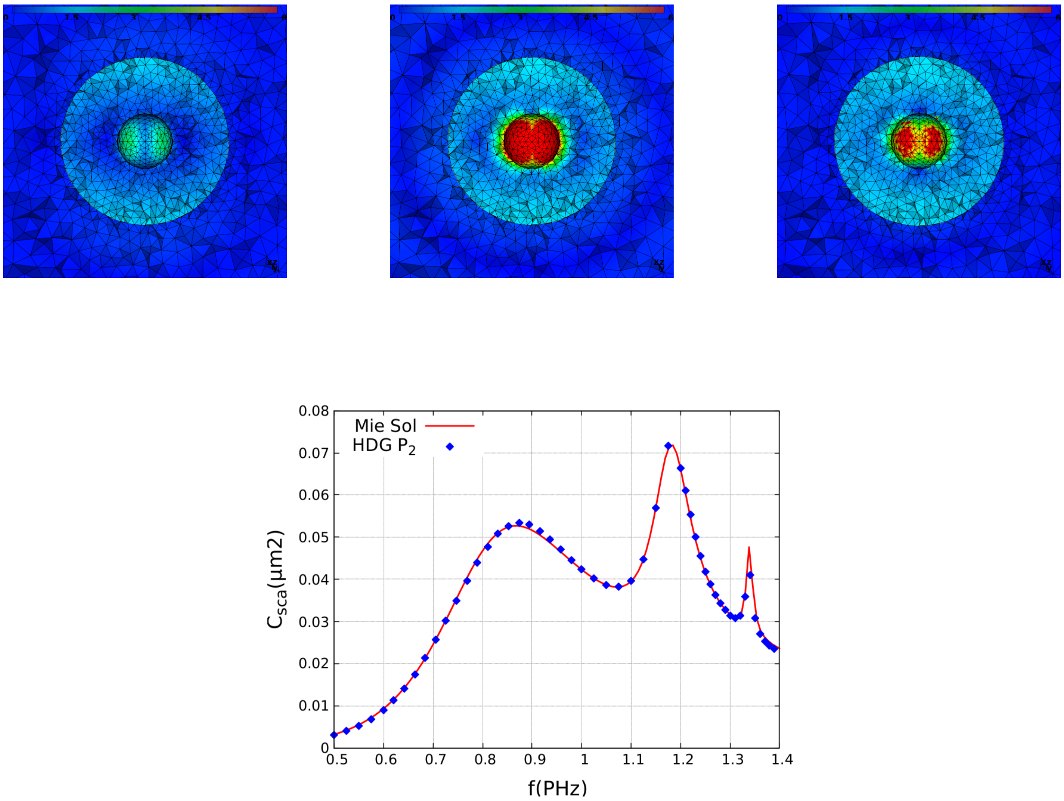

Figure 7. Top figures: scattering of a plane wave by a 50 nm gold nanosphere: magnitude of $\mathbf{E}$ *field at frequencies 1070 THz (left), 1185 THz (middle) and 1300 THz (right). Simulations based on a HDG-*$\mathbb{P}_2$ *method. Bottom figure: Scattering cross section.*

6.3. High performance numerical computing

6.3.1. High order HDG schemes and domain decomposition solvers for frequency-domain electromagnetics

Participants: Emmanuel Agullo [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Cristobal Samaniego Alvarado [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Mathieu Faverge [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Luc Giraud [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Matthieu Kuhn [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Stéphane Lanteri, Grégoire Pichon [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Pierre Ramet [HIEPACS project-team, Inria Bordeaux - Sud-Ouest].

This work is undertaken in the context of PRACE 5IP (http://www.prace-ri.eu/prace-5ip/) project and aims at the development of scalable frequency-domain electromagnetic wave propagation solvers, in the framework of the HORSE simulation software. HORSE is based on a high order HDG scheme formulated on an unstructured tetrahedral grid for the discretization of the system of three-dimensional Maxwell equations in heterogeneous media, leading to the formulation of large sparse undefinite linear system for the hybrid variable unknowns. This system is solved with domain decomposition strategies that can be either a purely algebraic algorithm working at the matrix operator level (i.e. a black-box solver), or a tailored algorithm designed at the continuous PDE level (i.e. a PDE-based solver). In the former case, we collaborate with the HIEPACS project-team at Inria Bordeaux - Sud-Ouest in view of adapting and exploiting the MaPHyS (Massively Parallel Hybrid Solver - https://gitlab.inria.fr/solverstack/maphys) algebraic hybrid iterative-direct domain decomposition solver. More precisely, this collaboration is concerned with two topics: one one hand, the improvement of the iterative convergence of MaPHyS for the HDG hybrid variable linear system and, on the other hand, the leveraging of low rank compression techniques for reducing the memory footprint of the factorization of subdomain problems using the PaStiX (Parallel Sparse matriX package - http://pastix.gforge.inria.fr/) package.

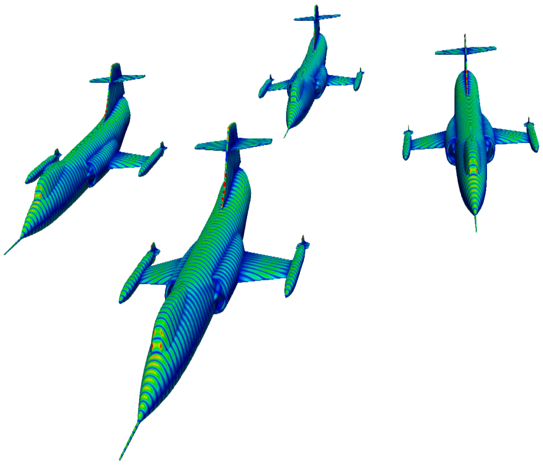

Figure 8. Scattering of a plane wave by a squadron Lockheed F-104 Starfighter. Contour lines of the amplitude of **E** *field. Simulations are performed with a HDG scheme based on a cubic interpolation of the electric and magnetic field unknowns, combined with a PDE-based domain decomposition solver.*

6.3.2. High order HDG schemes and domain decomposition solvers for frequency-domain electromagnetics

Participants: Stéphane Lanteri, Laércio Lima Pilla [CORSE project-team, Inria Grenoble - Rhône Alpes], Jean-François Méhaut [CORSE project-team, Inria Grenoble - Rhône Alpes].

This work is undertaken in the context of PRACE 5IP (http://www.prace-ri.eu/prace-5ip/) project and aims at the development of a hybrid MPI/OpenMP parallellization of the DGTD solver of the DIOGENeS software suite. In practice, we concentrated our efforts on identifying and evaluating the best approaches for implementing fine grain parallism of the main DG numerical kernels, based on OpenMP features for loop-based parallelism on one hand, and task-based parallelism on the other hand.

6.4. Applications

6.4.1. Gap-plasmon confinement with gold nanocubes

Participants: Stéphane Lanteri, Antoine Moreau [Institut Pascal, Université Blaise Pascal], Armel Pitelet [Institut Pascal, Université Blaise Pascal], Claire Scheid, Nikolai Schmitt, 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).

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.

6.4.2. Photovoltaics

The ultimate success of photovoltaic (PV) cell technology requires substantial progress in both cost reduction and efficiency improvement. An actively studied approach to simultaneously achieve these two objectives is to leverage *light trapping* schemes. Light trapping allows solar cells to absorb sunlight using an active material layer that is much thinner than the material's intrinsic absorption length. This then reduces the amount of materials used in PV cells, which cuts cell cost in general, and moreover facilitates mass production of PV cells that are based on less abundant materials. In addition, light trapping can improve cell efficiency, since thinner cells provide better collection of photo-generated charge carriers. Enhancing the light absorption in ultrathin film silicon solar cells is thus of paramount importance for improving efficiency and reducing cost. We are involved in several studies in collaboration with physicists that aim at simulating light trapping in complex solar cell structures using high order DG and HDG solvers developed in our core research activities.

6.4.2.1. Light-trapping in texturized thin film solar cells

Participants: Urs Aeberhard [IEK5 - Photovoltaik, Forschungszentrum Juelich GmbH, German], Karsten Bittkau [IEK5 - Photovoltaik, Forschungszentrum Juelich GmbH, German], Alexis Gobé, Stéphane Lanteri.

This work is undertaken in the context of the EoCoE Center of Excellence in collaboration with researchers from IEK5 - Photovoltaik, Forschungszentrum Juelich GmbH, Germany. The objective is to design a scalable high order DGTD solver for the simulation of light trapping in a multi-layer solar cell with surface texture. For that purpose, we rely on the DIOGENeS software suite from which we extract a high order DGTD solver for the problem under consideration, taking into account its specificities (in particular, with regards to material models and boundary conditions). We also need to specify and develop a dedicated preprocessing tool for building topography conforming geometrical models. Simulations are performed on the Occigen PRACE system at CINES.

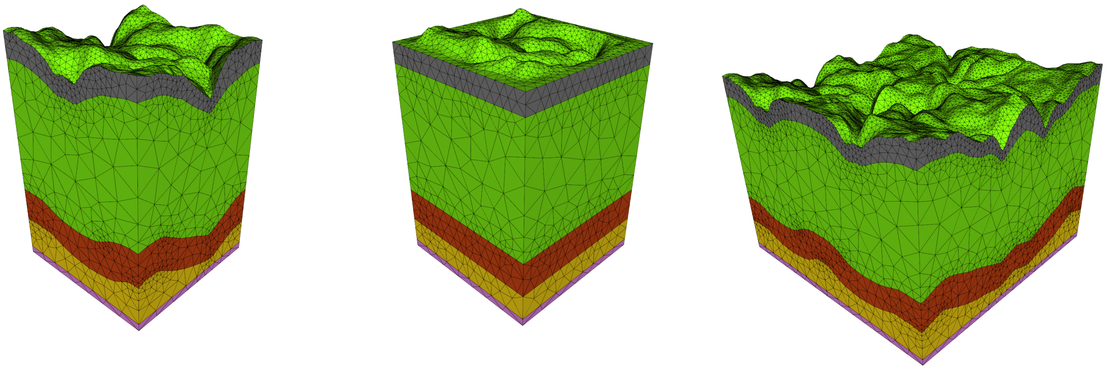

Figure 10. Simulation of light trapping in a multi-layer solar cell with surface texture using a high order DGTD fullwave solver and topography conforming geometrical models.

6.4.2.2. Light-trapping in nanocone gratings

Participants: Stéphane Collin [Sunlit team, C2N-CNRS, Marcoussi], Alexis Gobé, Julie Goffard [Sunlit team, C2N-CNRS, Marcoussi], Stéphane Lanteri.

There is significant recent interest in designing ultrathin crystalline silicon solar cells with active layer thickness of a few micrometers. Efficient light absorption in such thin films requires both broadband antireflection coatings and effective light trapping techniques, which often have different design considerations. In collaboration with physicists from the Sunlit team at C2N-CNRS, we conduct a numerical study of solar cells based on nanocone gratings. Indeed, it has been previously shown that by employing a double-sided grating design, one can separately optimize the geometries for antireflection and light trapping purposes to achieve broadband light absorption enhancement [47]. In the present study, we adopt the nanocone grating considered in [47]. This structure contains a crystalline silicon thin film with nanocone gratings also made of silicon. The circular nanocones form two-dimensional square lattices on both the front and the back surfaces. The film is placed on a perfect electric conductor (PEC) mirror. The ultimate objective of this study is to devise a numerical optimization strategy to infer optimal values of the geometrical characteristics of the nanocone grating on each side of the crystalline silicon thin film. Absorption characteristics are here evaluated using the high order DGTD solver from the DIOGENeS software suite.

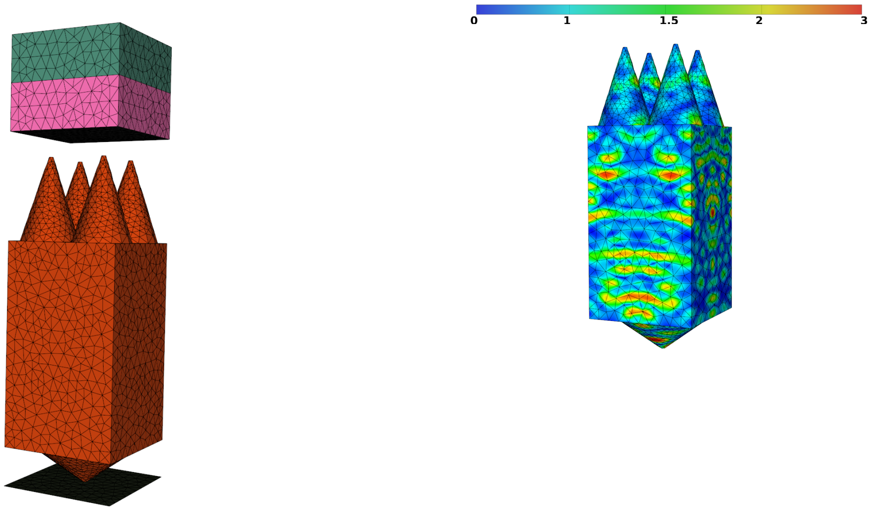

Figure 11. Simulation of light trapping in a solar cell based on nanocone gratings. Geometrical model (left) and contour lines of the module of the DFT of $\mathbf{E}$ *for a wavelength* $\lambda = 857$ *nm (right).*

6.4.3. Inver design of metasurfaces

Participants: Régis Duvigneau [ACUMES project-team, Inria Sophia Antipolis-Méditerranée], Mahmoud Elsawy, Patrice Genevet [CRHEA laboratory, Sophia Antipolis], Stéphane Lanteri.

Metasurfaces are flat surfaces consisting of sub-wavelength nanoresonators, made of plasmonic or high dielectric refractive index materials patterned in a specific way. These flat surfaces provide nearly full control of the light properties in a very short propagation distance with high resolution. By changing the dimensions, shapes, and orientation of these nanoresonators, different functionalities can be obtained. The complexity of the problem and the wide parameter space, make the direct modelling problem insufficient. Recently, several optimization techniques have been applied to the field of nanophotonics (including metasurfaces) by solving an inverse design problem. Generally speaking, there are two classes of optimization techniques that have been used in the metasurface designs; local and global techniques. The local methods depend on the initial guess and most of them require the computation of the gradient, which might be challenging. In addition, they are limited to small parameter space. On the other hand, global optimization techniques are suitable for optimizing several parameters moreover, they do not stuck in a local minima/maxima like the local methods. However, most of the global techniques used in the metasurface designs require costly simulations (for large parameter space), which make them inapplicable for modeling real-life designs that require 3D fullwave solvers. In this study conducted in collaboration with physicists at CRHEA, we use two efficient global optimization techniques based on statistical learning in order to overcome the disadvantageous of usual global optimization methods. The first one is the covariance matrix adaptation evolutionary strategy (CMA-ES). The CMA-ES has been gaining a lot of attention since it requires fewer cost function evaluations compared to the other evolutionary algorithms like genetic algorithms especially for 3D problems that require expensive simulations even with the high-performance computational resources. The second method is the Efficient Global Optimization (EGO) algorithm. The EGO algorithm is based on the surrogate modelling, that is to say, replacing the complex or costly evaluation process by a simpler and cheaper model to reduce dramatically the computational cost (number of calls for the electromagnetic simulations). Both techniques are offered by the Famosa library (http://famosa.gforge.inria.fr), which is developed by R. Duvigneau and colleagues in the ACUMES project-team.

7. Bilateral Contracts and Grants with Industry

7.1. Bilateral Contracts with Industry

7.1.1. Numerical study of light absorption in a photovoltaic glass

Participants: Alexis Gobé, Badre Kerzabi [Sunpartner Technologies, Rousset], Stéphane Lanteri.

Sunpartner Technologies is a company in the field of novel technologies for a sustainable environment, which develops innovative photovoltaic solutions dedicated to the connected object, building and transport markets. In particular, the company is designing devices using solar energy to improve the autonomy of connected objects such as smartphones. Supartner Technologies also offers glass modules that can be integrated on the screen of a watch or a smart e-reader, for example. These glass modules are transparent and integrate photovoltaic cells to recover solar energy in order to recharge the batteries. In all these products, nanostructuring of constituent materials is an exploited strategy to maximize the absorption of sunlight. In addition to measurement, the simulation of the interaction between light and nanostructured matter is an important ingredient in the implementation of this strategy. As an extension of the simulation, the optimization of nanostructuring makes it possible to explore many solutions before the design stage. In the context of this partnership that has started this year, we aim at adapting and applying a DGTD solver from the DIOGENeS software suite to characterize and further optimize the nanostructuring of a photovoltaic glass.

8. Partnerships and Cooperations

8.1. European Initiatives

8.1.1. FP7 & H2020 Projects

8.1.1.1. EoCoE

Title: Energy oriented Centre of Excellence for computer applications

Program: H2020

See also: https://www.eocoe.eu

Duration: October 2015 - October 2018

Coordinator: CEA

Partners:

- Barcelona Supercomputing Center (Spain)
- CEA (France)
- CERFACS (France)
- CNR (Italy)
- The Cyprus Institute (Cyprus)
- ENEA (Italy)
- Fraunhofer–Gesellschaft (Germany)
- Instytut Chemii Bioorganicznej Polskiej Akademii Nauk (Poland)
- Forschungszentrum Julich (Germany)
- Max-Planck-Gesellschaft (Germany)

University of Bath (United Kingdom)
Universite Libre de Bruxelles (Belgium)
Universita Degli Studi di Trento (Italy)

Inria contact: Michel Kern

The aim of the present proposal is to establish an Energy Oriented Centre of Excellence for computing applications, (EoCoE). EoCoE (pronounce “Echo”) will use the prodigious potential offered by the ever-growing computing infrastructure to foster and accelerate the European transition to a reliable and low carbon energy supply. To achieve this goal, we believe that the present revolution in hardware technology calls for a similar paradigm change in the way application codes are designed. EoCoE will assist the energy transition via targeted support to four renewable energy pillars: Meteo, Materials, Water and Fusion, each with a heavy reliance on numerical modelling. These four pillars will be anchored within a strong transversal multidisciplinary basis providing high-end expertise in applied mathematics and HPC. EoCoE is structured around a central Franco-German hub coordinating a pan-European network, gathering a total of 8 countries and 23 teams. Its partners are strongly engaged in both the HPC and energy fields; a prerequisite for the long-term sustainability of EoCoE and also ensuring that it is deeply integrated in the overall European strategy for HPC. The primary goal of EoCoE is to create a new, long lasting and sustainable community around computational energy science. At the same time, EoCoE is committed to deliver high-impact results within the first three years. It will resolve current bottlenecks in application codes, leading to new modelling capabilities and scientific advances among the four user communities; it will develop cutting-edge mathematical and numerical methods, and tools to foster the usage of Exascale computing. Dedicated services for laboratories and industries will be established to leverage this expertise and to foster an ecosystem around HPC for energy. EoCoE will give birth to new collaborations and working methods and will encourage widely spread best practices.

8.1.1.2. PRACE 5IP

Title: PRACE Fifth Implementation Phase (PRACE-5IP) project

See also: http://www.prace-ri.eu/prace-5ip

Duration: January 2017 - April 2019

Partners: see http://www.prace-ri.eu/member-systems

Inria contact: Stéphane Lanteri

The mission of PRACE (Partnership for Advanced Computing in Europe) is to enable high-impact scientific discovery and engineering research and development across all disciplines to enhance European competitiveness for the benefit of society. PRACE seeks to realise this mission by offering world class computing and data management resources and services through a peer review process. PRACE also seeks to strengthen the European users of HPC in industry through various initiatives. PRACE has a strong interest in improving energy efficiency of computing systems and reducing their environmental impact. The objectives of PRACE-5IP are to build on and seamlessly continue the successes of PRACE and start new innovative and collaborative activities proposed by the consortium. These include: assisting the transition to PRACE2 including ananalysis of TransNational Access; strengthening the internationally recognised PRACE brand; continuing and extend advanced training which so far provided more than 18 800 persontraining days; preparing strategies and best practices towards Exascale computing; coordinating and enhancing the operation of the multi-tier HPC systems and services; supporting users to exploit massively parallel systems and novel architectures.

8.1.1.3. EPEEC

Title: European joint effort toward a highly productive programming environment for heterogeneous exascale computing

Program: H2020

See also: https://epeec-project.eu

Duration: October 2018 - September 2021

Coordinator: Barcelona Supercomputing Center

Partner: Barcelona Supercomputing Center (Spain)

Coordinator: CEA

Partners:

- Fraunhofer–Gesellschaft (Germany)
- CINECA (Italy)
- IMEC (Blegium)
- INESC ID (Portugal)
- Appentra Solutions (Spain)
- Eta Scale (Sweden)
- Uppsala University (Sweden)
- Inria (France)
- Cerfacs (France)

Inria contact: Stéphane Lanteri

EPEEC's main goal is to develop and deploy a production-ready parallel programming environment that turns upcoming overwhelmingly-heterogeneous exascale supercomputers into manageable platforms for domain application developers. The consortium will significantly advance and integrate existing state-of-the-art components based on European technology (programming models, runtime systems, and tools) with key features enabling 3 overarching objectives: high coding productivity, high performance, and energy awareness. An automatic generator of compiler directives will provide outstanding coding productivity from the very beginning of the application developing/porting process. Developers will be able to leverage either shared memory or distributed-shared memory programming flavours, and code in their preferred language: C, Fortran, or C++. EPEEC will ensure the composability and interoperability of its programming models and runtimes, which will incorporate specific features to handle data-intensive and extreme-data applications. Enhanced leading-edge performance tools will offer integral profiling, performance prediction, and visualisation of traces. Five applications representative of different relevant scientific domains will serve as part of a strong inter-disciplinary co-design approach and as technology demonstrators. EPEEC exploits results from past FET projects that led to the cutting-edge software components it builds upon, and pursues influencing the most relevant parallel programming standardisation bodies.

8.2. International Initiatives

8.2.1. Participation in Other International Programs

8.2.1.1. International Initiatives

PHOTOM

Title: PHOTOvoltaic solar devices in Multiscale computational simulations

International Partners:

- Center for Research in Mathematical Engineering, Universidad de Concepcion (Chile), Rodolfo Araya
- Laboratório Nacional de Computação Científica (Brazil), Frédéric Valentin
- Instituto de Matemáticas, PUCV (Chile), Diego Paredes

Duration: 2018 - 2019

Start year: 2018

See also: http://www.photom.lncc.br

The work consists of devising, analyzing and implementing new multiscale finite element methods, called Multiscale Hybrid-Mixed (MHM) method, for the Helmholtz and the Maxwell equations in the frequency domain. The physical coefficients involved in the models contain highly heterogeneous and/or high contrast features. The goal is to propose numerical algorithms to simulate wave propagation in complex geometries as found in photovoltaic devices, which are naturally prompt to be used in massively parallel computers. We demonstrate the well-posedness and establish the optimal convergence of the MHM methods. Also, the MHM methods are shown to induce a new face-based a posteriori error estimator to drive space adaptivity. An efficient parallel implementation of the new multiscale algorithm assesses theoretical results and is shown to scale on a petaflop parallel computer through academic and realistic two and three-dimensional solar cells problems.

8.2.2. Inria International Partners

8.2.2.1. Informal International Partners

Prof. Kurt Busch, Humboldt-Universität zu Berlin, Institut für Physik, Theoretical Optics & Photonics

Prof. Martijn Wubs, Technical University of Denmark (DTU), Structured Electromagnetic Materials Theory group

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

8.3. International Research Visitors

8.3.1. Visits of International Scientists

Prof. Liang Li, School of Mathematical Sciences, University of Electronic Science and Technology of China, Chengdu. From July to August 2018.

Stéphane Lanteri and Théophile Chaumont-Frelet at LNCC, Petropolis, Brazil, March 12-16, 2018.

Stéphane Lanteri and Claire Scheid at UAM and CSIC, Spain, May 29-30, 2018.

Stéphane Lanteri and Claire Scheid at Humboldt-Universität zu Berlin, Berlin, Germany, July 12-13, 2018.

Stéphane Lanteri at Barcelona Supercomputing Center, Barcelona, Spain, July 23-24, 2018.

9. Dissemination

9.1. Promoting Scientific Activities

9.1.1. Scientific Events Organisation

9.1.1.1. General Chair, Scientific Chair

Stéphane Lanteri has chaired the second workshop of the CLIPhTON (advanCed numericaL modelIng for multiscale and multiphysics nanoPhoTONics) network that took place at Humboldt-Universität zu Berlin, Berlin, Germany, July 12-13, 2018.

9.1.2. *Invited Talks*

Claire Scheid, "A Discontinuous Galerkin Time-Domain framework for nanoplasmonics", Topical Workshop "Computational Aspects of Time Dependent Electromagnetic Wave Problems in Complex Materials", ICERM, Brown University, Providence, USA, June 25-29, 2018

Stéphane Lanteri, "Discontinuous Galerkin solvers for the numerical modeling of nanoscale light-matter interactions", MATHIAS 2018 - Computational Science Engineering & Data Science by TOTAL, Paris, October 22-24, 2018

Stéphane Lanteri, "Rigorous modeling of light absorption in nanostructured materials using a parallel high order finite element time-domain technique", Research Center for Advanced Science and Technology, The University of Tokyo, Japan, July, 30 2018

Stéphane Lanteri, "An upscaled DGTD method for time-domain electromagnetics", Special Session "Multiscale and multiphysics computation and applications", Progress In Electromagnetics Research Symposium - PIERS 2018, Toyama, Japan, August 1-4, 2018

9.1.3. *Scientific Expertise*

Stéphane Lanteri is a member of the Scientific Committee of CERFACS.

9.1.4. *Research Administration*

Stéphane Lanteri is a member of the Project-team Committee's Bureau of the Inria Sophia Antipolis-Méditerranée research center.

Stéphane Lanteri is a member of the Sciences Fondamentales et Appliquées Doctoral School Committee (until December 2018).

9.2. Teaching - Supervision - Juries

9.2.1. *Teaching*

Stéphane Descombes, *Scientific computing*, M1, 36 h, Université Côte d'Azur.

Stéphane Descombes, *Principal components analysis*, M2, 30 h, Université Côte d'Azur.

Stéphane Lanteri, *High performance scientific computing*, MAM5, 24 h, Polytech Nice Sophia.

Claire Scheid, *Analyse Hibertienne et analyse de Fourier, Practical works*, Master 1 MPA, 36h, Université Côte d'Azur.

Claire Scheid, *Option Math 2*, Licence 1, 20h, Université Côte d'Azur.

Claire Scheid, *Méthodes numériques en EDP, Lectures and practical works*, Master 1 MPA and IM, 63h, Université Côte d'Azur.

Claire Scheid, *Option Modélisation, Lectures and practical works*, Master 2 Agrégation, 48h, Université Côte d'Azur.

Claire Scheid, *Analyse, Lecture and practical works*, Master 2 Agrégation, 27h, Université Côte d'Azur.

Claire Scheid, *EDP et Différences Finies, Lectures and practical works*, Master 1 MPA and IM, 72h, Université Côte d'Azur.

9.2.2. *Supervision*

PhD in progress: Alexis Gobé, *Multiscale hybrid-mixed methods for time-domain nanophotonics*, November 2016, Stéphane Lanteri.

PhD in progress: Georges Nehmetallah, *Efficient finite element type solvers for the numerical modeling of light transmission in nanostructured waveguides and cavities*, November 2017, Stéphane Descombes and Stéphane Lanteri.

PhD defened in September 2018: Nikolai Schmitt, *High-order simulation and calibration strategies for spatially dispersive metals in nanophotonics*, Stéphane Lanteri and Claire Scheid.

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