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Activity Report 2019

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 [55] 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 [61] 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 [50] 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 [59] 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 [47]- [48]- [49]- [54]:

- 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]-[14]-[13]. 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.*[52] 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[12].
- **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]-[14]-[13] 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 [11]. 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 [17]. In the context of seismic wave propagation, we are interested by the intrinsic attenuation of the medium [15]. 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 [61]. 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

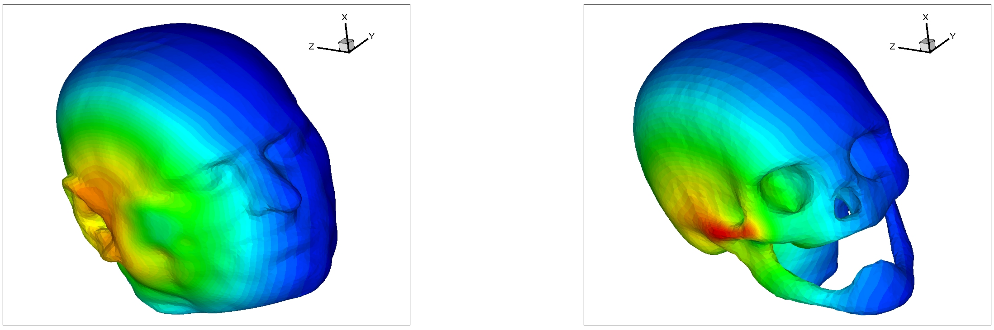

Figure 1. Exposure of head tissues to an electromagnetic wave emitted by a localized source. Top figures: surface triangulations of the skin and the skull. Bottom figures: contour lines of the amplitude of the electric field.

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 [53]- [62].

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 [58]. 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 [56]- [57]- [51]. 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.

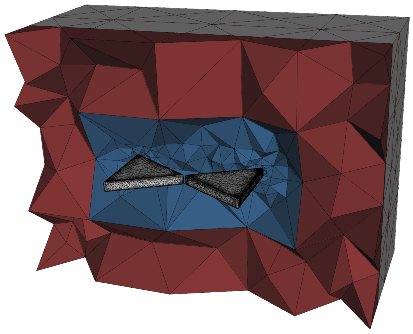

Figure 2. Simulation of the field enhancement at the tip of a gold bowtie nanoantenna (PhD thesis of Jonathan Viquerat).

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

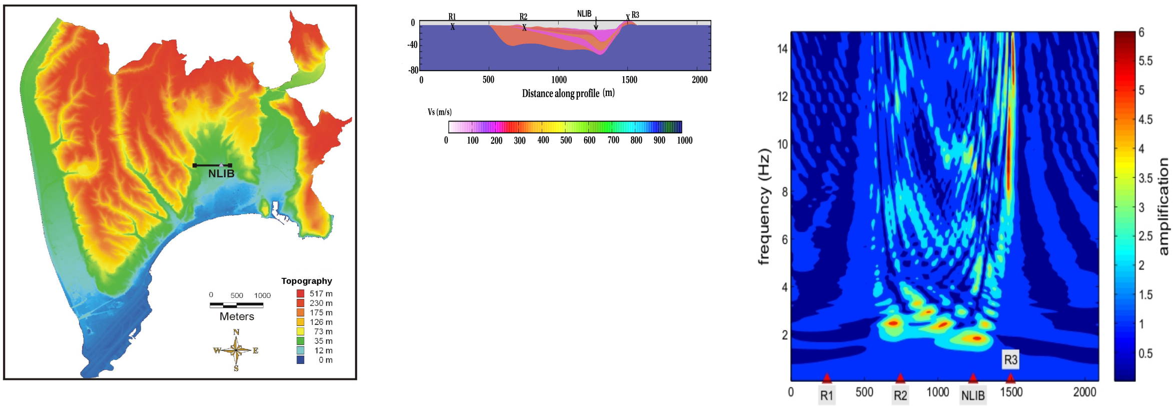

Figure 3. Propagation of a plane wave in a heterogeneous model of Nice area (provided by CETE Méditerranée). Left figure: topography of Nice and location of the cross-section used for numerical simulations (black line). Middle figure: S-wave velocity distribution along the cross-section in the Nice basin. 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 Gobé 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.

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- 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.

- Authors: Ludovic Moya and Alexis Gobé
- 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. Study of 3D periodic structures at oblique incidences

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 has been accepted for publication in 2019.

6.1.3. Stability and asymptotic properties of the linearized Hydrodynamic Drude model

Participants: Serge Nicaise [Université de Valenciennes], Claire Scheid.

We go a step further toward a better understanding of the fundamental properties of the linearized hydrodynamical model studied in the PhD of Nikolai Schmitt [16]. This model is especially relevant for small nanoplasmonic structures (below 10nm). Using a hydrodynamical description of the electron cloud, both retardation effects and non local spatial response are taken into account. This results in a coupled PDE system for which we study the linear response. In [45] (submitted, under revision), we concentrate on establishing well posedness results combined to a theoretical and numerical stability analysis. We especially prove polynomial stability and provide optimal energy decay rate. Finally, we investigate the question of numerical stability of several explicit time integration strategies combined to a Discontinuous Galerkin spatial discretization.

6.1.4. Toward thermoplasmonics

Participants: Yves d'Angelo, 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.

6.1.5. Corner effects in nanoplasmonics

Participants: Camille Carvalho [Applied Mathematics Department, University of California Merced, USA], Claire Scheid.

In this work, we study nanoplasmonic structures with corners (typically a diedral/triangular structure); a situation that raises a lot of issues. We focus on a lossles Drude dispersion model and propose to investigate the range of validity of the amplitude limit principle. The latter predicts the asymptotic harmonic regime of a structure that is monochromatically illuminated, which makes a frequency domain approach relevant. However, in frequency domain, several well posedness problems arise due to the presence of corners (addressed in the PhD thesis of Camille Carvalho). This should impact the validity of the limit amplitude principle and has not yet been addressed in the literature in this precise setting. Here, we combine frequency-domain and time-domain viewpoints to give a numerical answer to this question in two dimensions. We show that the limit amplitude principle does not hold for whole interval of frequencies, that are explicited using the well-posedness analysis. This work is now being finalized.

6.1.6. 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.

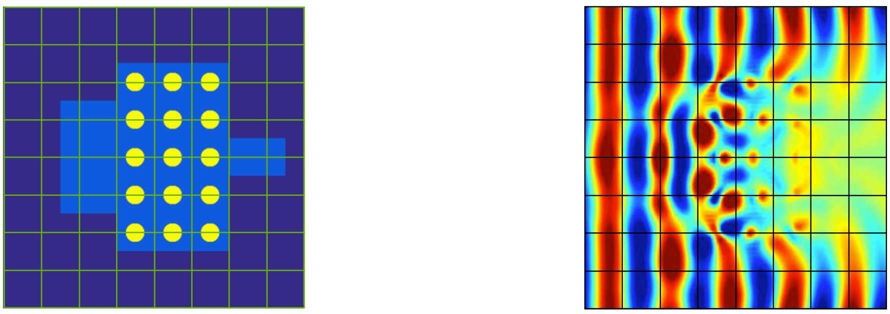

Figure 4. Light propagation in a photonic crystal structure using a MHM-DGTD method for solving the 2D Maxwell's equations. Left: quadrangular mesh. Right: contour lines of the amplitude of the electric field.

6.1.7. HDG methods for the time-domain Maxwell equations

Participants: Théophile Chaumont-Frelet, Stéphane Descombes, Stéphane Lanteri, Georges Nehmetallah.

Hybridizable discontinuous Galerkin (HDG) methods have been investigated in the team since 2012. This family of method employs face-based degrees of freedom that can be viewed as a fine grain domain decomposition technique. We originally focused on frequency-domain applications, for which HDG methods enable the use of static condensation, leading to drastic reduction in computational time and memory consumption. More recently, we have investigated the use of HDG discretization to solve time-dependent problems. Specifically, in the context of the PhD thesis of Georges Nehmetallah, we focused on two particular aspects. On the one hand, HDG methods exhibit a superconvergence property that allows, by means of local postprocessing, to obtain new improved approximations of the unknowns. Our first contribution is to apply this methodology to time-dependent Maxwell's equations, where the post-processed approximation converges with order $k+1$ instead of k in the $H(curl)$-norm, when using polynomial of degree $k \geq 1$. The proposed method has been implemented for dealing with general 3D problems. Fig. 5 highlights the improved accuracy of the post-processed approximation on a cavity benchmark.

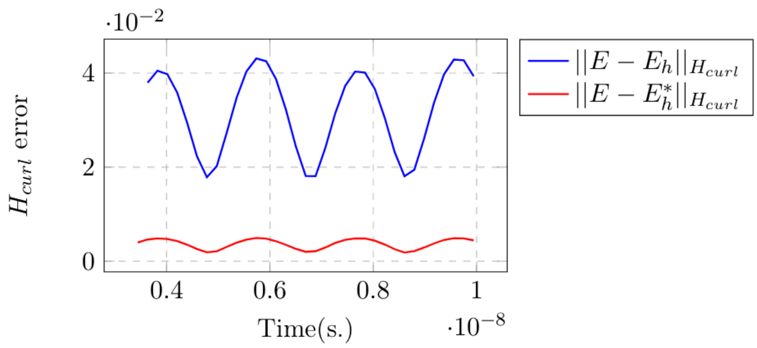

Figure 5. Time evolution of the $H(curl)$-error before and after postprocessing for P_2 interpolation and a fixed mesh constituted by 3072 elements

Another interesting aspect of the HDG method is that it can be conveniently employed to blend different time-integration schemes in different regions of the mesh. This is especially useful to efficiently handle locally refined space grids, that are required to take into account geometrical details. These ideas have already been explored for standard discontinuous Galerkin discretization in the context of the PhD thesis of Ludovic Moya [13], [14]. Here, we focused on HDG methods and we introduced a family of coupled implicit-explicit (IMEX) time integration methods for solving time-dependent Maxwell's equations. We established stability conditions that are independent of the size of the small elements in the mesh, and are only constrained by the coarse part. Numerical experiments on two-dimensional benchmarks illustrate the theory and the usefulness of the approach.

6.1.8. A posteriori error estimators

Participants: Théophile Chaumont-Frelet, Alexandre Ern [SERENA project-team], Patrick Vega, Martin Vohralík [SERENA project-team].

The development of *a posteriori* error estimators and is a new topic of interest for the team. Concerning *a posteriori* estimators, a collaboration with the SERENA project-team has been initiated. We mainly focus on a technique called equilibrated fluxes, which has the advantage to produce p-robust error estimators together with guaranteed error estimates. This means in particular that these estimators are particularly suited for high-order discretization schemes. Our first results deal with the Helmholtz equation, and have been recently submitted [39] and presented at the Enumath international conference [29]. Fig. 6 depicts the ability of the estimators to accurately describe the error distribution in a realistic application. Future works in this line will include the treatment of Maxwell's equations. The recently hired postdoctoral fellow Patrick Vega will actively participate in these developments.

6.1.9. hp-adaptivity

Participants: Théophile Chaumont-Frelet, David Pardo [Basque Center for Applied Mathematics, Bilbao, Spain].

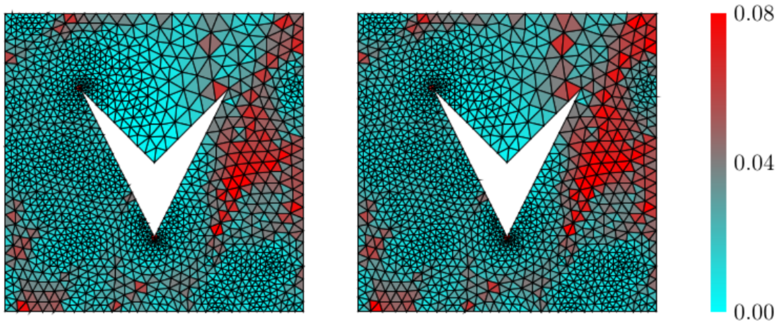

Figure 6. Estimators η_K (left) and elementwise errors $\|u-u_h\|_K$ (right) for a scattering problem discretized with $\mathcal{P}_3$ elements

Together with the development of a posteriori estimators, a novel activity in the team is the design of efficient hp-adpative strategy. In this regard, we propose a multi-level hierarchical data structure imposing Dirichlet nodes to manage the so-called hanging nodes. Our hp-adaptive strategy is based on performing quasi-optimal unrefinements. Taking advantage of the hierarchical structure of the basis functions both in terms of the element size h and the polynomial order of approximation p, we mark those with the lowest contributions to the energy of the solution and remove them. This straightforward unrefinement strategy does not require from a fine grid or complex data structures, making the algorithm flexible to many practical situations and existing implementations. Our first contribution has been recently submitted [42], and deals with the Poisson equation. Fig. 7 shows how the algorithm is able to correctly refine the computational grid to capture a shock wave.

6.1.10. Multiscale methods for frequency-domain wave propagation

Participants: Théophile Chaumont-Frelet, Zakaria Kassali, Stéphane Lanteri, Frédéric Valentin.

The design and analysis of multiscale methods for wave propagation is an important research line for team. The team actually mainly specializes in one family of multiscale methods, called multiscale hybrid-mixed (MHM). These developments started thanks to the close collaboration with Frédéric Valentin, who has recently been awarded an Inria international chair. Previous investigations in the context of this collaboration focused on time-dependent Maxwell's equations [10]. Recent efforts have been guided towards the realization of a MHM method for time-harmonic Maxwell's equations. We first focused on the Helmholtz equation, that modelizes the particular case of polarized waves. Our first results include the implementation of the method for two-dimensional problems as well as rigorous, frequency-explicit, stability and convergence analysis. These findings have recently been accepted for publication [40]. In the context of the internship of Zakaria Kassali, the method has been further adapted for the propagation of polarized waves in solar cells. Specifically, it is required in this case to take into account "quasi-periodic" boundary conditions that deserve a special treatment. We are currently undertaking further developments guided toward full three-dimensional Maxwell's equations with the PhD of Zakaria Kassali, which started in November 2019.

6.2. High performance numerical computing

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

Participants: Emmanuel Agullo [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Théophile Chaumont-Frelet, Luc Giraud [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Stéphane Lanteri.

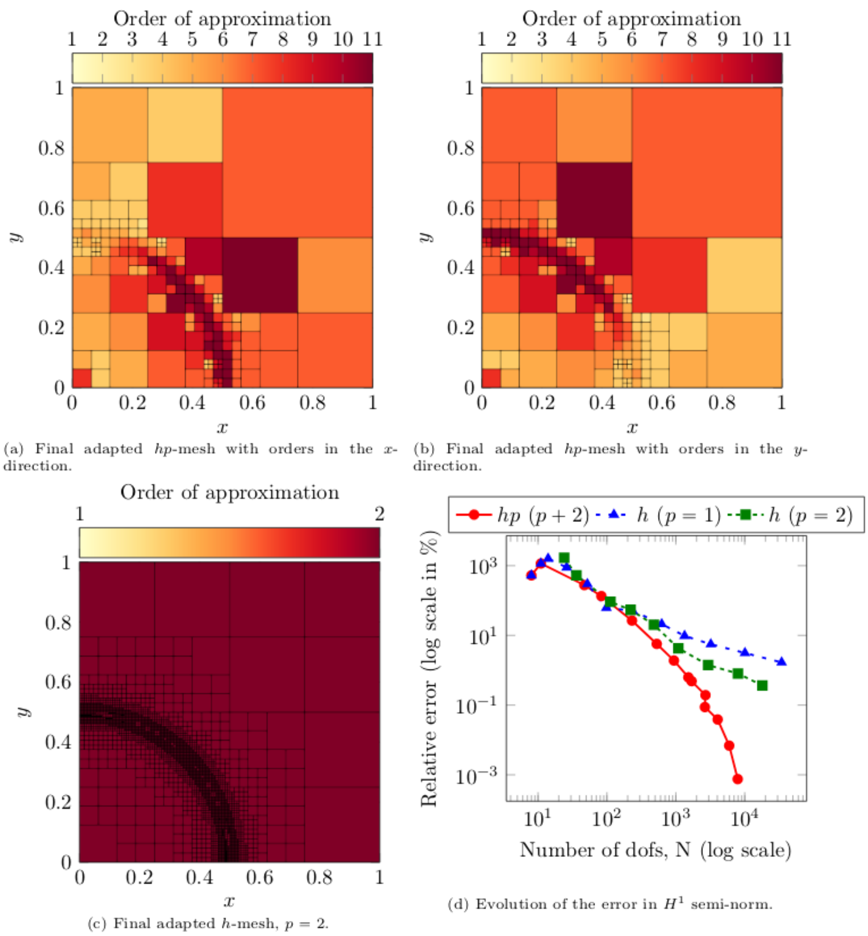

Figure 7. Different hp-adptive strategies for capturing a shock wave

This work is undertaken in the context of PRACE 6IP project and aims at the development of scalable frequency-domain electromagnetic wave propagation solvers, in the framework of the DIOGENeS software suite. This solver 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 dispersive 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.

6.3. Applications

6.3.1. Inverse design of metasurfaces using statistical learning methods

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

Metasurfaces are flat optical nanocomponents, that are the basis of several more complicated optical devices. The optimization of their performance is thus a crucial concern, as they impact a wide range of applications. Yet, current design techniques are mostly based on *engineering knowledge*, and may potentially be improved by a rigorous analysis based on accurate simulation of Maxwell's equations. The goal of this study is to optimize phase gradient metasurfaces by taking advantage of our fullwave high order Discontinuous Galerkin time-Domain solver implemented in DIOGENeS, coupled with two advanced optimization techniques based on statistical learning and evolutionary strategies. Our key findings are novel designs for Gan semiconductor phase gradient metasurfaces operating at visible wavelengths. Our numerical results reveal that rectangular and cylindrical nanopillar arrays can achieve more than respectively 88% and 85% of diffraction efficiency for TM polarization and both TM and TE polarization respectively, using only 150 fullwave simulations. To the best of our knowledge, this is the highest blazed diffraction efficiency reported so far at visible wavelength using such metasurface architectures. Fig. 8 depicts the superiority of the proposed statistical learning approaches over standard gradient-based optimization strategies. This work has been recently published [22].

6.3.2. Optimization of 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 [60]. In the present study, we adopt the nanocone grating considered in [60]. 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. We use two efficient global optimization techniques based on statistical learning to adpat the geometrical characteristics of the nanocones in order the maximize the light absorption properties of this type of solr cells.

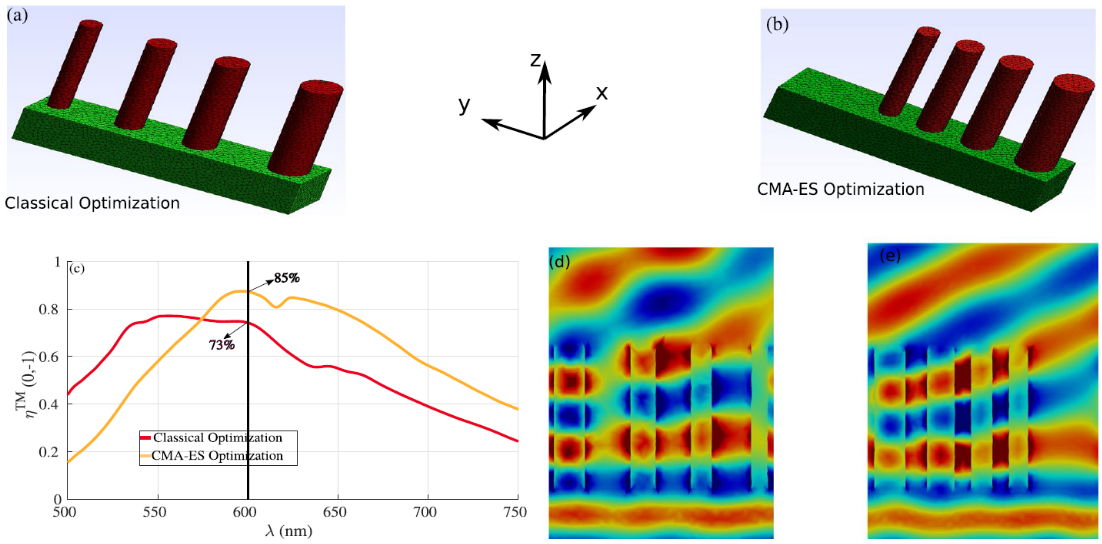

Figure 8. Comparison between the classical approach to phase gradient metasurface design and our optimized geometries for the cylindrical nanopillars with $h = 800$ nm. (a,b) The geometry obtained using the classical approach in which each nanopillar is optimized manually by changing the diameter and finally placed together in order to obtain the desired phase shift needed to maximize the light deflection for the first order mode at $\lambda = 600$ nm with period 1500 nm in y-direction. (c) Results obtained using the CMA-ES for the cylindrical nanopillars (see Table 3) for the corresponding parameters. (c) Comparison between the deflection efficiency for the first order mode obtained using the classical (red curve) and the CMA-ES (orange curve). (d,e) Represent field maps of $Re(E_y)$ obtained using the classical optimization design and the CMA-ES results, respectively

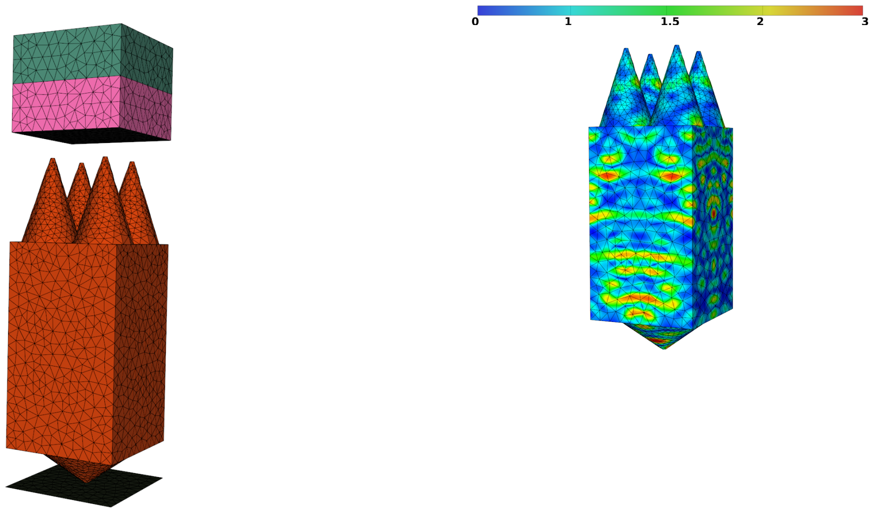

Figure 9. Simulation of light trapping in a solar cell based on nanocone gratings. Geometrical model (left) and contour lines of the module of the DFT of $\mathbf{E}$ *for a wavelength* $\lambda = 857$ *nm (right).*

6.3.3. Influence of spatial dispersion on surface plasmons and grating couplers

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

Recent experiments have shown that spatial dispersion may have a conspicuous impact on the response of plasmonic structures. This suggests that in some cases the Drude model should be replaced by more advanced descriptions that take spatial dispersion into account, like the hydrodynamic model. Here we show that nonlocality in the metallic response affects surface plasmons propagating at the interface between a metal and a dielectric with high permittivity. As a direct consequence, any nanoparticle with a radius larger than 20 nm can be expected to be sensitive to spatial dispersion whatever its size. The same behavior is expected for a simple metallic grating allowing the excitation of surface plasmons, just as in Woods famous experiment. Finally, we carefully set up a procedure to measure the signature of spatial dispersion precisely, leading the way for future experiments. Importantly, our work suggests that for any plasmonic structure in a high permittivity dielectric, nonlocality should be taken into account.

6.3.4. Optimization and uncertainty quantification of gradient index metasurfaces

Participants: Gauthier Brière [CRHEA laboratory, Sophia Antipolis], Herbert de Gersem [TEMF institute, TU Darmstadt, Germany], Patrice Genevet [CRHEA laboratory, Sophia Antipolis], Niklas Georg [TEMF institute, TU Darmstadt, Germany], Stéphane Lanteri, Dimitrios Loukrezis [TEMF institute, TU Darmstadt, Germany], Ulrich Römer [TEMF institute, TU Darmstadt, Germany], Nikolai Schmitt.

The design of intrinsically flat two-dimensional optical components, i.e., metasurfaces, generally requires an extensive parameter search to target the appropriate scattering properties of their constituting building blocks. Such design methodologies neglect important near-field interaction effects, playing an essential role in limiting the device performance. Optimization of transmission, phase-addressing and broadband performances of metasurfaces require new numerical tools. Additionally, uncertainties and systematic fabrication errors should be analysed. These estimations, of critical importance in the case of large production of metaoptics components, are useful to further project their deployment in industrial applications. Here, we report on a computational methodology to optimize metasurface designs. We complement this computational methodology by quantifying the impact of fabrication uncertainties on the experimentally characterized components. This analysis provides general perspectives on the overall metaoptics performances, giving an idea of the expected average behavior of a large number of devices.

7. Bilateral Contracts and Grants with Industry

7.1. Bilateral Contracts with Industry

7.1.1. DGTD solver for time-domain elecromagnetics with application to geoseismics

Participants: Andreas Atle [TOTAL], Henri Calandra [TOTAL], Karim El Maarouf [TOTAL], Alexis Gobé, Stéphane Lanteri, Michael Sekachev [TOTAL].

This contract with TOTAL CSE (Computational Science and Engineering) division in Houston, Texas, is concerned with the development of a DGTD solver for applications in geoseismics. The R&D division of the EP (Oil, Gas Exploration & Production) branch of TOTAL has been interested in DG type methods since many years. It acquired a know-how on these methods and developed internally software tools integrating DG methods as solvers of the direct problem (forward propagators) in different seismic imaging processes (RTM - Reverse Time Migration, and FWI - Full Waveform Inversion). These solvers are concerned with the numerical resolution of PDE systems of acoustics and elastodynamics. TOTAL is now interested in having a similar DGTD solver for the numerical resolution of the system of time-domain Maxwell equations, in view of the development of an electromagnetic imaging process to identify conductivity of a medium. This electromagnetic imaging process would then be coupled to the existing seismic imaging ones.

8. Partnerships and Cooperations

8.1. National Initiatives

8.1.1. ANR project

8.1.1.1. OPERA (Adpative planar optics)

Participants: Emmanuel Agullo [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Régis Duvigneau [ACUMES project-team], Mahmoud Elsawy, Patrice Genevet [CRHEA laboratory, Sophia Antipolis], Luc Giraud [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Stéphane Lanteri.

Type: ANR ASTRID Maturation

See also: http://www-sop.inria.fr/nachos/opera/

Duration: Avril 2019 - March 2022

Coordinator: Inria

Partner: CRHEA laboratory in Sophia Antipolis and NAPA Technologies in Archamps

Inria contact: Stéphane Lanteri

Abstract: In the OPERA project, we are investigating and optimizing the properties of planar photonic devices based on metasurfaces using numerical modelling. The scientific and technical activities that constitute the project work programme are organized around 4 main workpackages. The numerical characterization of the optical properties of planar devices based on metasurfaces, as well as their optimization are at the heart of the activities and objectives of two horizontal (transversal) workpackages. These numerical methodologies will be integrated into the DIOGENeS software framework that will eventually integrates (1) discontinuous Galerkin-type methods that have been tested over the past 10 years for the discretization of Maxwell equations in time and frequency regimes, mainly for applications in the microwave band, (2) parallel resolution algorithms for sparse linear systems based on the latest developments in numerical linear algebra, (3) modern optimization techniques based on learning and metamodeling methods and (4) software components adapted to modern high performance computing architectures. Two vertical workpackages complete this program. One of them aims to demonstrate the contributions of methodological developments and numerical tools resulting from transversal workpackages through their application to diffusion/radiation control by passive planar devices. The other, more prospective, concerns the study of basic building blocks for the realization of adaptive planar devices.

8.2. European Initiatives

8.2.1. H2020 Projects

8.2.1.1. PRACE 6IP

Title: PRACE Sixth Implementation Phase (PRACE-6IP) project

See also: https://cordis.europa.eu/project/id/823767

Duration: May 2019 - December 2021

Partners: see https://cordis.europa.eu/project/id/823767

Inria contact: Luc Giraud

PRACE, the Partnership for Advanced Computing is the permanent pan-European High Performance Computing service providing world-class systems for world-class science. Systems at the highest performance level (Tier-0) are deployed by Germany, France, Italy, Spain and Switzerland, providing researchers with more than 17 billion core hours of compute time. HPC experts from 25 member states enabled users from academia and industry to ascertain leadership and remain competitive in the Global Race. Currently PRACE is finalizing the transition to PRACE 2, the successor of the initial five year period. The objectives of PRACE-6IP 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 development of PRACE 2; strengthening the internationally recognised PRACE brand; continuing and extend advanced training which so far provided more than 36 400 person·training days; preparing strategies and best practices towards Exascale computing, work on forward-looking SW solutions; coordinating and enhancing the operation of the multi-tier HPC systems and services; and supporting users to exploit massively parallel systems and novel architectures. A high level Service Catalogue is provided. The proven project structure will be used to achieve each of the objectives in 7 dedicated work packages. The activities are designed to increase Europe's research and innovation potential especially through: seamless and efficient Tier-0 services and a pan-European HPC ecosystem including national capabilities; promoting take-up by industry and new communities and special offers to SMEs; assistance to PRACE 2 development; proposing strategies for deployment of leadership systems; collaborating with the ETP4HPC, CoEs and other European and international organisations on future architectures, training, application support and policies. This will be monitored through a set of KPIs.

8.2.1.2. 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.

8.3. International Initiatives

8.3.1. Participation in Other International Programs

8.3.1.1. 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
Instito de Matemáticas, PUCV (Chile), Diego Paredes

Duration: 2018 - 2020

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.

8.3.1.2. Informal International Partners

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

8.3.1.3. Inria International Chairs

IIC VALENTIN Frédéric

Title: Innovative multiscale numerical algorithms for wave-matter interaction models at the nanoscale

International Partner (Institution - Laboratory - Researcher):

Laboratório Nacional de Computação Científica (Brazil), Frédéric Valentin

Duration: 2018 - 2022

Start year: 2018

See also: https://www.lncc.br/~valentin/

The project addresses complex three-dimensional nanoscale wave-matter interaction models, which are relevant to the nanophotonics and nanophononics fields, and aims at devising innovative multiscale numerical methods, named Multiscale Hybrid-Mixed methods (MHM for short), to solve them with high accuracy and high performance.

8.4. International Research Visitors

8.4.1. Visits of International Scientists

- David Pardo (Basque Center for Applied Mathematics, Spain) at Inria, France, April 2-5, 2019.
- Christophe Geuzaine (University of Liège, Belgium) at Inria, France, April 29-30, 2019.
- Jean-Francois Remacle (Ecole Polytechnique de Louvain, Belgium) at Inria, France, April 29-30, 2019.
- Jay Gopalakrishnan (University of Portland, USA) at Inria, France, June 4-5, 2019.

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 PHOTOM (PHOTOvoltaic solar devices in Multiscale computational simulations) project that took place at Inria Sophia Antipolis-Méditerranée, France, Jan 28-Feb 01, 2019.
- Stéphane Lanteri has chaired the third workshop of the CLIPhTON (advanCed numericaL modelIng for multiscale and multiphysics nanoPhoTONics) network that took place ati Inria Sophia Antipolis-Méditerranée, France, October 24-25, 2019.

9.1.2. Journal

9.1.2.1. Reviewer - Reviewing Activities

- Théophile Chaumont-Frelet: ESAIM Math. Model. Numer. Anal., NUMA, NME
- Yves D'Angelo: Nanotechnology, Journal of Geophysical & Astrophysical Fluid Dynamics
- Claire Scheid: SIAM J. Numer. Anal., SIAM J. Sci. Comput.
- Stéphane Lanteri: J. Comput. Phys., Comp. Meth. Appl. Mech. Engrg.

9.1.3. Invited Talks

- Théophile Chaumont-Frelet, Journées Ondes Sud-Ouest, MIOS, France , January 2019.
- Théophile Chaumont-Frelet, Séminaire LJAD, Nice, France , November 2019.
- Théophile Chaumont-Frelet at University of Basel, Switzerland, December 11-13, 2019.
- Théophile Chaumont-Frelet at University of Bath, UK, November 11-15, 2019.
- Théophile Chaumont-Frelet at the Basque Center for Applied Mathematics, Spain, May 1-3, 2019.

9.1.4. Scientific Expertise

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

9.1.5. Research Administration

- Yves D'Angelo is the head of the "Laboratoire J.A. Dieudonné" (LJAD, UMR 7351).
- Stéphane Descombes is the head of the "Maison de la Modélisation, de la Simulation et des Interactions" (MSI) of Université Côte d'Azur
- Stéphane Lanteri is a member of the Project-team Committee's Bureau of the Inria Sophia Antipolis-Méditerranée research center.

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

License: Yves D'Angelo, *Analyse des Séries de Fourier* , 30 h, L3, Univ. Côte d'Azur

Lisence: Claire Scheid, *Fondements 2* , 24 h, L1, Univ. Côte d'Azur

Master: Yves D'Angelo, *Modélisation et Simulation Numérique* , 48 h, M1, Univ. Côte d'Azur

Master: Yves D'Angelo, *Modélisation de la Turbulence fluid* , 30 h, M2, Univ. Côte d'Azur

Master: Claire Scheid, *Analyse, Lecture and practical works* , 27 h, M2, Univ. Côte d'Azur

Master: Claire Scheid, *Méthodes numériques en EDP, Lectures and practical works* , 63 h, M1, Univ. Côte d'Azur

Master: Claire Scheid, *Option Modélisation, Lectures and practical works* , 48 h, M2, Univ. Côte d'Azur

Master: Claire Scheid, *Soutien Analyse Fonctionnelle et Esepacde de Hilbert* , 18 h, M1, Univ. Côte d'Azur

Master: Stéphane Descombes, *Introduction aux EDP* , 30 h, M1, Univ. Côte d'Azur

Master: Stéphane Descombes, *ACP et reconnaissance de caractères* , 9 h, M2, Univ. Côte d'Azur

License: Stéphane Descombes, *Travaux dirigés de mathématiques pour l'économie*, 18 h, L1, Univ. Côte d'Azur

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

9.2.2. Supervision

PhD in progress: Alexis Gobé, Multiscale hybrid-mixed methods for time-domain nanophotonics, vNovember 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 in progress: Zakaria Kassali, Multiscale finite element simulations applied to the design of photovoltaic cells, November 2019, Théophile Chaumont-Frelet and Stéphane Lanteri

PhD in progress: Massimiliano Montone, High order finite element type solvers for the coupled Maxwell-semiconductor equations in the time-domain, December 2019, Stéphane Lanteri and Claire Scheid

9.2.3. Juries

Yves D'Angelo: Basile Radisson, IRPHE Marseille, France, Avril 2019, Rapporteur.

Claire Scheid: Pierre Mennuni, Lille, France, November 2019, Examinatrice.

Claire Scheid: Weslley Da Silva Peireira, LNCC, Petropolis, Brazil, September 2019, Examinatrice.

Stéphane Lanteri: Aurélien Citrain, Inria Pau, December 2019, Rapporteur.

Stéphane Lanteri: Nicolas Lebbe, CEA LETI, Grenoble, Novembre 2019, Examinateur.

Stéphane Lanteri: Matthieu Patrizio, ISAE, Toulouse, Mai 2019: Examinateur.

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Major publications by the team in recent years

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