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ACTIVITY REPORT

Project-Team
ATLANTIS

modeling and numerical methods for computATionaL wave-mAtter iNteracTIons at the nanoScale

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

DOMAIN

Applied Mathematics, Computation and Simulation

THEME

Numerical schemes and simulations

Contents

Project-Team ATLANTIS 1

1 Team members, visitors, external collaborators 2

2 Overall objectives 3

3 Research program 4
3.1 Driving physical fields . . . 4
3.2 Research agenda . . . 5
3.2.1 Core research topics . . . 5
3.2.2 Complementary topics . . . 7

4 Application domains 7
4.1 Nanostructures for sunlight harvesting . . . 8
4.2 Metasurfaces for light shaping . . . 8
4.3 THz wave generation . . . 8
4.4 Metallic nanocubes for nanoscale sensing . . . 9
4.5 Plasmonic nanostructures for photothermal effect . . . 9

5 New software and platforms 9
5.1 New software . . . 9
5.1.1 DIOGENeS . . . 9

6 New results 10
6.1 Time-domain problems . . . 10
6.1.1 Explicit and IMEX Hybridizable DG methods . . . 10
6.1.2 Reduced-order modeling for time-domain electromagnetics . . . 10
6.1.3 Stability and asymptotic properties of the linearized Hydrodynamic Drude model . 11
6.1.4 Toward thermoplasmonics . . . 11
6.1.5 Corner effects in nanoplasmonics . . . 11
6.1.6 DG methods for semiconductor device modeling . . . 12
6.1.7 Advanced modeling of nanostructured CMOS imagers based on DG methods . . . 12
6.2 Frequency-domain problems . . . 13
6.2.1 Homogenization theory for metasurfaces . . . 13
6.2.2 Equilibrated error estimators for high-order methods . . . 14
6.2.3 Residual error estimators for high frequency problems . . . 14
6.2.4 Analysis of quasi-periodic boundary conditions . . . 15
6.3 Applications . . . 15
6.3.1 Inverse design of metasurfaces using statistical learning methods . . . 15
6.3.2 Multiobjective optimization for large-scale achromatic metalenses . . . 16
6.3.3 Optimization of metasurfaces accounting for fabrication uncertainties . . . 17
6.3.4 Simulation of 3D conformal metasurfaces using GSTCs . . . 17
6.3.5 3D metamaterial mode converter for integrated optics . . . 18
6.3.6 Optimization of light-trapping in nanostructured solar cells . . . 18
6.3.7 Plasmonic sensing with nanocubes . . . 19
6.3.8 Multiple scattering in randon media . . . 20

7 Bilateral contracts and grants with industry 20
7.1 Bilateral contracts with industry . . . 20
7.2 Grants with industry . . . 22

8 Partnerships and cooperations **22**
8.1 European initiatives 22
8.1.1 FP7 & H2020 Projects 22
8.2 National initiatives 24
8.2.1 ANR project 24

9 Dissemination **24**
9.1 Promoting scientific activities 24
9.1.1 Journal 24
9.1.2 Leadership within the scientific community 25
9.2 Teaching - Supervision - Juries 25
9.2.1 Teaching 25
9.2.2 Supervision 25
9.2.3 Juries 26

10 Scientific production **26**
10.1 Major publications 26
10.2 Publications of the year 27
10.3 Cited publications 28

Project-Team ATLANTIS

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B5.5. – Materials

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B8.2. – Connected city

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2 Overall objectives

ATLANTIS is a joint project-team between Inria, CNRS and Université Côte d'Azur thanks to its association with the J.A. Dieudonné Mathematics Laboratory (UMR 7351). It is a follow-up of the NACHOS project-team from which it inherits a well identified expertise on theoretical and methodological aspects of the solution of PDE (Partial Differential Equation) systems modeling electromagnetic and elastodynamic wave propagation. Relying on this expertise, our research activities in Atlantis will aim at studying and impacting more deeply some scientific and technological challenges raised by physical problems involving waves in interaction with nanostructured matter. A crucial component in the implementation of this scientific endeavor lies in a close networking with physicists who bring the experimental counterpart of the proposed research.

Nanostructuring of materials has paved the way for manipulating and enhancing wave-matter interactions, thereby opening the door for the full control of these interactions at the nanoscale. In particular, the interaction of *light waves* (or more general *optical waves*) with matter is a subject of rapidly increasing scientific importance and technological relevance. Indeed, the corresponding science, referred to as *nanophotonics* [37], aims at using nanoscale light-matter interactions to achieve an unprecedented level of control on light. Nanophotonics encompasses a wide variety of topics, including metamaterials, plasmonics, high resolution imaging, quantum nanophotonics and functional photonic materials. Previously viewed as a largely academic field, nanophotonics is now entering the mainstream, and will play a major role in the development of exciting new products, ranging from high efficiency solar cells, to personalized health monitoring devices able to detect the chemical composition of molecules at ultralow concentrations. Plasmonics [42] is a field closely related to nanophotonics. Metallic nanostructures whose optical scattering is dominated by the response of the conduction electrons are considered as plasmonic media. If the metallic structure presents an interface with a positive permittivity dielectric, collective oscillations of surface electrons create waves (called surface plasmons) that are guided along the interface, with the unique characteristic of subwavelength-scale confinement. Nanofabricated systems that exploit these plasmon waves offer fascinating opportunities for crafting and controlling the propagation of light in matter. In particular, it can be used to channel light efficiently into nanometer-scale volumes. As light is squeezed down into nanoscale volumes, field enhancement effects occur resulting in new optical phenomena that can be exploited to challenge existing technological limits and deliver superior photonic devices. 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 also great promise for applications in sensing and switching.

In ATLANTIS, our short-term and medium-term activities mainly focus on research fields related to nanophotonics. Driven by a number of nanophotonics-related physical drivers, our overall objectives are on one hand to design and develop innovative numerical methodologies for the simulation of nanaoscale light-matter interactions and to demonstrate their capabilities by studying challenging applications in close collaboration with physicist partners. On the methodological side, the Discontinous Galerkin (DG) family of methods is a cornerstone of our contributions, and our research directions in ATLANTIS aim at extending our former achievements on these methods in order to deal with more complex PDEs, including nonlinear problems and coupled systems stemming from multiphysics problems, relevant to the study of nanoscale wave-matter interactions. Moreover, mathematical modeling is a central activity of the team, in particular for shaping initial and boundary value problems in view of devising accurate, efficient and robust numerical methods in the presence of multiple space and time scales or/and geometrical singularities. Additional methodological topics that are considered in close collaboration with colleagues from other Inria teams or external applied mathematics research groups are model order reduction, inverse design, uncertainty analysis and high order geometry approximation. New contributions on these topics in the context of the physical problems studied in ATLANTIS will ultimately be implemented in the DIOGENeS software suite, which is a unique software plaform dedicated to computationl nanophotonics.

As a more prospective and longer term objective, we will also explore the possibility of exporting our methodological contributions to the much more recent scientific field of nanophononics that exploit the dynamics of phonons (quanta of lattice vibrations) at the nanoscale. These vibrations, occuring in a large variety of material systems, solids or liquids, can manifest as sound or heat. In contrast with electrons and photons, the launched efforts to achieve control of phonons are quite recent and the physics (and subsequent mathematical modeling) are not completely understood yet. These efforts came, as for nanophotonics, from the reduction of the size of electronic devices that opened up new possibilities for phonon propagation and interaction. By way of consequences, new thrilling perspectives to enhance the properties of nanodevices have appeared with technological applications encompassing nanoelectronics, renewable energy harvesting, nano- and optomechanics, quantum technologies, as well as medical therapy, imaging and diagnostics. The mathematical modeling of nanoscale sound and heat transport control raises several questions and it is not clear so far that it can rely on classical physics (mechanics) differential models as it is the case with nanophotonics, although the study of microscale phononic devices relies on PDE models that are relevant to our research activities.

3 Research program

3.1 Driving physical fields

Our activities ultimately materialize as innovative computational techniques for studying concrete questions and applications that are tightly linked to specific physical fields related to nanophotonics and plasmonics, and which will be considered in collaboration with physicists. These driving physical fields aim at exploiting the peculiarities of nanoscale light-matter interactions.

Quantum plasmonics. The physical phenomena involved in the deep confinement of light when interacting with matter opens a major route for novel nanoscale devices design. Indeed, the recent progress of fabrication at the nanoscale makes it possible to conceive metallic structures with increasingly large size mismatch, in which microscale devices can be characterized by sub-nanometer features [31]. These advances have also allowed to achieve spatial separation between metallic elements of only few nanometers [30]. At such sizes *quantum* effects become non-negligible, producing huge variations in the macroscopic optical response. Following this evolution, the quantum plasmonics field has emerged, and with it the possibility of building quantum-controled devices, such as single photon sources, transistors and ultra-compact circuitry at the nanoscale.

Thermoplasmonics. Plasmonic resonances can be exploited for many applications [42]. In particular, the strong local field enhancement associated with the plasmonic resonances of a metallic nanostructure, together with the absorption properties of the metal, induce a photo-thermal energy conversion. Thus, in the vicinity of the nanostructure, the temperature increases. These effects, viewed as ohmic losses, have been for a long time considered as a severe drawback for the realization of efficient devices. However, the possibility to control this temperature rise with the illumination wavelength or polarization has gathered strong interest in the nano-optics community, establishing the basis of thermoplasmonics [27]. By increasing temperature in their surroundings, metal nanostructures can be used as integrated heat nanosources. Decisive advances are foreseen in nanomedicine with applications in photothermal cancer therapy, nano-surgery, drug delivery, photothermal imaging, protein tracking, photoacoustic imaging, but also in nano-chemistry, optofluidics, solar and thermal energy harvesting (thermophotovoltaics).

Planar optics. Nanostructuring of matter can be tailored to shape, control wavefront and achieve unusual device operations. Recent years have seen tremendous advances in the fabrication and understanding of two-dimensional (2D) materials, giving rise to the field of planar optics. In particular, the concept of quasi-2D metasurfaces has started to develop into an exciting research area, where nanostructured surfaces are designed for novel functionalities [38]-[29]-[34]. Metasurfaces are planar metamaterials with subwavelength thickness, consisting of single-layer or few-layer stacks of nanostructures. They 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 (e.g. scattering amplitude, phase, and polarization). They 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.

Optoelectronics and nanoelectronics. Semiconductors also play a major role in leveraging nanoscale light-matter interactions. Emission or absorption of light by a semiconductor is at the heart of optoelectronics, which is concerned with devices that source, detect or control light. Photodiodes, solar cells, light emitting diodes (LEDs), optical fibers and semiconductor lasers are some typical examples of optoelectronic devices. The attractive properties of these devices is based on their efficiency in converting light into electrical signals (or vice versa). Using a structuration with low dimensional materials and carrier-photons interaction, optoelectronics aims at improving the quality of these systems. A closeby field is nanoelectronics [43], i.e., the physical field that, while incorporating manufacturing constraints, tries to describe and understand the influence of the nanostructuration of electronic devices on their electronic properties. This area has quickly evolved with the increasing fabrication capabilities. One striking motivating example is the drastic increase of the number of transistors (of a few nanometer size) per chip on integrated circuits. At the achieved nanostructuration scales, inter-atomic forces, tunneling or quantum mechanical properties have a non-negligible impact. A full understanding of these effects is mandatory for exploiting them in the design of electronic components, thereby improving their characteristics.

3.2 Research agenda

The processes that underly the above-described physical fields raise a number of modeling challenges that motivate our research agenda:

- They exhibit multiple space and time scales;
- They are highly sensitive to exquisite geometrical features of nanostructures and matter nanostructuring;
- They impose dealing with unconventional material models;
- They may require to leave the comfortable setting of linear differential models;
- Some of them are inherently multiphysics processes.

3.2.1 Core research topics

Our research activities are organized around core theoretical and methodological topics to address the above-listed modeling challenges.

Multiscale modeling. The physical models that we consider may feature three different space scales. First, the size of the computational domain is fixed by the nanostructure under consideration and the required observables. Second, the solution wavelength depends on the operating frequency and on the light velocity in the constitutive materials. Finally, the finest scale involved corresponds to the nanostructuring length. These three space scales can differ by orders of magnitude, leading to unaffordable computational costs, if the discretization scheme must resolve the nanostructure details. We thus aim at providing multiscale numerical schemes, that can embed fine scale information into a coarser mesh. Such methodologies lead to embarrassingly parallel two-level algorithms, that are especially suited for HPC environments and produce accurate numerical approximations. These multiscale schemes will in particular be designed in the framework of MHM (Multiscale Hybrid-Mixed) formulations recently introduced in collaboration with Frédéric Valentin at LNCC, Petropolis, Brazil. In the MHM framework, the inherent upscaling procedure that is at the heart of the approach, allows to incorporate more physics in the numerical schemes themselves, as the upscaling principle is used to construct physical basis functions that resolve the fine scales. At the second level, one defines a set of boundary value problems, whose solutions call for adapted versions of classical finite element or DG methods, and yield the upscaled basis functions.

High order DG methods. Designing numerical schemes that are high order accurate on general meshes, i.e., unstructured or hybrid structured/unstructured meshes, will still represent a major objective of our core research activities in ATLANTIS. We will focus on the family of Discontinuous Galerkin (DG) methods that has been extensively developed for wave propagation problems during the last 15 years. We will investigate several variants, namely nodal DGTD for time-domain problems, and HDG (Hybridized DG) for time-domain and frequency-domain problems, with the general goal of devising, analyzing and developing extensions of these methods, in order to deal with the physical drivers described in section 3.1: nonlinear features, in particular in relation with generation of higher order harmonics in electromagnetic wave interaction with nonlinear materials, and nonlinear models of electronic response in metallic and semiconductor materials; multiphysic couplings such as for instance when considering PDE models relevant to thermoplasmonics, optoelectronics and nanoelectronics. There are to date very few works promoting DG-type methods for these situations. Concerning nonlinear effects, it is worth notice that DG methods have already proved to be attractive and have been extensively developed for computational fluid dynamics, and in particular for gas dynamics. The development of a high order DG method for situations involving nonlinear materials require to address several issues such as the construction approximate Riemann solvers for the evaluation of numerical traces associated with the evaluation of boundary integral terms in DG weak forms, the formulation of positivity-preserving schemes as continuous solutions may develop nonlinear discontinuities and the definition of linearization strategies in conjunction with time-integration schemes.

Error estimation and adaptivity. While standard theory ensures the convergence of the discrete approximation to the correct solution, it does not permit to quantitatively estimate the discretization error in actual applications. As a result, the selection of the discretization parameters is often carried out by the practitioners themselves, based on their experience and hence manual approaches to guarantee a sufficient accuracy level. We aim at providing reliable measurements of the discretization error and devising a more systematic and rigorous procedure to select and adapt discretization parameters — in particular the mesh size and the discretization order — through the use of a posteriori estimators. On the one hand, we propose to design a posteriori error estimators for the wave-matter interaction problems we consider in ATLANTIS, able to provide a fully reliable error estimation. On the other hand, such estimators can be employed to drive hp-adaptive algorithms, where the mesh and discretization order are iteratively improved to fit the complicated structure of the solution.

Time integration for multiscale problems. Multiscale physical problems with complex geometries or het- erogeneous media are extremely challenging for conventional numerical simulations. Adaptive mesh refinement is an attractive technique for treating such problems and will be developed in our research activities in Atlantis. Local mesh refinement imposes a severe stability condition on explicit time integration since the allowed maximal time step size is constrained by the smallest element in the mesh. We will focus on different ways to overcome this stability condition, especially by using implicit-explicit (IMEX) methods where a time implicit scheme is used only for the refined part of the mesh, and a time explicit scheme is used for the other part. Optimizing the CPU time requires coupling IMEX methods with hybridized DG (HDG) methods and non-conforming meshes and will be one of the main objectives of our research activities in ATLANTIS.

Dealing with complex materials. Physically relevant simulations deal with increasing levels of complexity in the geometrical and/or physical characteristics of nanostructures, as well as their interaction with light. Standard simulation methods may fail to reproduce the underlying physical phenomena, therefore motivating the search for more sophisticated light-matter interaction numerical modeling strategies. A first decisive direction consists in refining classical linear dispersion models and we shall put a special focus on deriving a complete hierarchy of models, that will encompass standard linear models to more complex and nonlinear ones (such as Kerr-type materials, non- linear quantuum hydrodynamic theory models, etc.). One approach will rely on an accurate description of the Hamiltonian dynamics with intricate kinetic and exchange correlation energies, for different modeling purposes. A second direction will be motivated by the study of 2D materials. A major concern is centered around the choice of the modeling approach between a full costly 3D modeling and the use of equivalent boundary conditions (the so-called GSTC), that could in all generality be completely nonlinear. Assessing these two directions will require efficient dedicated numerical algorithms that will especially be able to tackle several types of nonlinearities and scales.

Dealing with coupled models. Several of our target physical fields are multiphysics in essence and require going beyond the sole description of the electromagnetic response. In thermoplasmonics, the various phenomena (heat transfer through light concentration, bubbles formation and dynamics) call for different kinds of governing PDEs (Maxwell, conduction, fluid dynamics). Since, in addition, these phenomena can occur in significatively different space and time scales, drawing a quite complete picture of the underlying physics is a challenging task, both in terms of modeling and numerical treatment. In the nanoelectronics field, an accurate description of the electronic properties involves including quantum effects. A coupling between Maxwell's and Schrödinger equations (again at significantly different time and space scales) is a possible relevant scenario. In the optoelectronics field, the accurate prediction of semiconductors optical properties is a major concern. A possible strategy may require to solve both the electromagnetic and the drift-diffusion equations. In all these aforementioned examples, difficulties mainly arise both from the differences in physical nature as well as in the time/space scales at which each physical phenomenon occurs. Accurately modeling/solving their coupled interactions remains a formidable challenge.

High performance computing (HPC). HPC is transversal to almost all the other research topics considered in the team, and is concerned with both numerical algorithm design and software development. We will work toward taking advantage of fine grain massively parallel processing offered by GPUs in modern exascale architectures, by revisiting the algorithmic structure of the computationally intensive numerical kernels of the high order DG-based solvers that we develop. We will mostly rely on the lastest features of the OpenMP standard for implementing these numerical algorithms in the DIOGENeS software suite, which already offers a coarse grain parallelization based on MPI. We will also investigate task-based fine grain parallelization for dealing with load balancing issues inherent to realistic wave-matter interaction problems and that are sourced by both numerical (e.g., locally adapted interpolation order, PML layers, volumic observables, etc.) and physical (e.g., multiple material models) characteristics.

3.2.2 Complementary topics

Beside the above-discussed core reserach topics, we have also identified additional topics that are important or compulsory in view of maximizing the impact in nanophotonics or nanophononics of our core activities and methodological contributions.

Inverse design. Inverse design has emerged rather recently in nanophotonics, and is currently the subject of intense research as witnessed by several reviews [44]. Artificial Intelligence (AI) techniques are also increasingly investigated within this context [51]. In ATLANTIS, we will extend the modeling capabilities of the DIOGENeS software suite by using *statistical learning* techniques for the inverse design of nanophotonic devices. When it is linked to the simulation of a realistic 3D problem making use of one of the high order DG and HDG solvers we develop, the evaluation of a figure of merit is a costly process. Since a sufficiently large input data set of candidate designs, as required by using Deep Learning (DL), is generally not available, global optimization strategies relying on Gaussian Process (GP) models are considered in the first place. This activity will be conducted in close collaboration with researchers of the ACUMES project-team. In particular, we investigate GP-based inverse design strategies that were initially developed for optimization studies in relation with fluid flow problems [35]-[36] and fluid-structure interaction problems [49].

Uncertainty analysis and quantification. The automatic inverse design of nanophotonic devices enables scientists and engineers to explore a wide design space and to maximize a device performance. However, due to the large uncertainty in the nanofabrication process, one may not be able to obtain a deterministic value of the objective, and the objective may vary dramatically with respect to a small variation in uncertain parameters. Therefore, one has to take into account the uncertainty in simulations and adopt a robust design model [39]. We study this topic in close collaboration with researchers of the ACUMES project-team.

Numerical linear algebra. Sparse linear systems routinely appear when discretizing frequency-domain wave-matter interaction PDE problems. In the past, we have considered direct methods, as well as domain decomposition preconditioning coupled with iterative algorithms to solve such linear systems [7] In the future, we would like to further enhance the efficiency of our solvers by considering state-of-the-art linear algebra techniques such as block Krylov subspace methods [26], or low-rank compression techniques [48]. We will also focus on multi-incidence problems in periodic structures, that are relevant to metagrating or metasurface design. Indeed, such problems lead to the resolution of several sparse linear systems that slightly differ from one another and could benefit from dedicated solution algorithms. We will collaborate with researchers of the HIEPACS (Inria Bordeaux-Sud Ouest) project-team to develop efficient and scalable solution strategies for such questions.

4 Application domains

Nanoscale wave-matter interactions find many applications of industrial and societal relevance. The applications discussed in this section are those that we address in the first place in the short- to medium-term. Our general goal is to impact scientific discovery and technological development in these application topics by leveraging our methodological contributions for the numerical modeling of nanoscale wave-matter interactions, and working in close collaboration with external partners either from the academic or the industrial world. Each of these applications is linked to one or more of the driving physical fields described in section 3.1 except nanoelectronics that we consider as a more prospective, hence long-term application.

4.1 Nanostructures for sunlight harvesting

Photovoltaics (PV) converts photon energy from the sun into electric energy. One of the major challenges of the PV sector is to achieve high conversion efficiencies at low cost. Indeed, the ultimate success of PV cell technology requires substantial progress in both cost reduction and efficiency improvement. An actively studied approach to simultaneously achieve both objectives is to exploit light trapping schemes. Light trapping enables solar cells absorption using an active material layer much thinner than the material intrinsic absorption length. This then reduces the amount of materials used in PV cells, cuts cell cost, facilitates mass production of these cells that are based on less abundant material and moreover can improve cell efficiency (due to 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 costs. Our activities in relation with this application field aim at precisely studying light absorption in nanostructured solar cell structures with the help of an adapted numerical procedure. We consider both the characterization of light trapping for a given texturing of material layers, and the goal-oriented inverse design of the nanostructuring.

4.2 Metasurfaces for light shaping

Metasurfaces produce abrupt changes over the scale of the free-space wavelength in the phase, amplitude and/or polarization of a light beam. Metasurfaces are generally created by assembling arrays of miniature, anisotropic light scatterers (i.e. resonators such as optical antennas). The spacing between antennas and their dimensions are much smaller than the wavelength. As a result the metasurfaces, on account of Huygens principle, are able to mould optical wavefronts into arbitrary shapes with subwavelength resolution by introducing spatial variations in the optical response of the light scatterers. Designing metasurfaces for realistic applications such as metalenses [50] is a challenging inverse problem. In this context, the ultimate goal of our activities is to develop numerical methodologies for the inverse design of large-area metasurfaces [47].

4.3 THz wave generation

Recent research on the interaction of short optical pulses with semiconductors has stimulated the development of low power terahertz (THz) radiation transmitters. The THz spectral range of electromagnetic waves (0.1 to 10 THz) is of great interest. In particular, it includes the excitation frequencies of semiconductors and dielectrics, as well as rotational and vibrational resonances of complex molecules. As a result, THz waves have many applications in areas ranging from the detection of dangerous or illicit substances and biological sensing to diagnosis and diseases treatment in medicine. The most common mecanism of THz generation is based on the use of THz photoconductive antennas (PCA), consisting of two electrodes spaced by a given gap and placed onto a semiconductor surface. The excitation of the gap by a femtosecond optical pulse induces a sharp increase of the concentration of charge carriers for a short period of time, and a THz pulse is generated. Computer simulation plays a central role in understanding and mastering these phenomena in order to improve the design of PCA devices. The numerical modeling of a general 3D PCA configuration is a challenging task. Indeed, it requires the simultaneous solution of charge transport in the semiconductor substrate and the electromagnetic wave radiation from the antenna [46]-[52]. The recently-introduced concept of hybrid photoconductive antennas leveraging plasmonic effects is even more challenging [41]. So far, existing simulation approaches are based on the FDTD method, and are only able to deal with classical PCAs. In relation with the design of photonic devices for THz waves generation and manioulation, we intend to a multiscale numerical modeling strategy for solving the system of Maxwell equations coupled to various models of charge carrier dynamics in semiconductors.

4.4 Metallic nanocubes for nanoscale sensing

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. Nanocubes are extensively studied in this context and have been shown to support such gap plasmon modes. 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. Such metallic nanocubes can be used for a broad range of applications including plasmonic sensing, surface enhanced Raman scattering (SERS), metamaterials, catalysis, and bionanotechnology. We aim at devising a numerical methodology for characterizing the impact of geometrical parameters such as the dimensions of the cube, the rounding of nanocube corners or the size of the slit separating the cube and the substrate, on the overall performance of these absorbers. In practice, this leads us to address two main modeling issues. First, as the size of the slit is decreased, spatial dispersion effects [33] have to be taken into account when dealing with plasmonic structures. For this purpose, we consider a fluid model in the form of a nonlocal hydrodynamic Drude model [32], which materializes as a system of PDEs coupled to Maxwell's equations [9]-[8]. The second issue is concerned with the assessment of geometrical uncertainties and their role in the development of spatial dispersion effects.

4.5 Plasmonic nanostructures for photothermal effect

The field of thermoplasmonics has developed an extensive toolbox to produce, control and monitor heat at the nanometer scale. Nanoparticles are promising nano-sensing and nano-manipulating tools, and recent studies yielded remarkable advances in design, synthesis, and implementation of luminescent nanoparticles. Some applications deal with bio-imaging and bio-sensing, like e.g. luminescent nanothermometers, nanoparticles capable of providing contactless thermal reading through their light emission properties [40]. Also, bio-functionalized gold nanorods are promising candidates for light-induced hyperthermia [45], to cause local and selective damage in malignant tissue. At the same time, laser pulse interaction with plasmonic nanostructures can also be exploited for cell nanosurgery [28], including plasmonic enhanced cell transfection, molecular surgery and drug delivery. In parallel to all these bio-oriented applications, plasmonic nanoparticles can also be thought of as prototypic systems for understanding *fundamental aspects* of nanoscale material as well as light-matter interaction. Specific numerical modeling tools are essential to provide a good insight in this understanding.

5 New software and platforms

5.1 New software

5.1.1 DIOGENeS

Name: 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 nanoplasmonics (interaction with metals). A parallel implementation allows to consider large problems on dedicated cluster-like architectures.

URL: `https://diogenes.inria.fr/`

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6 New results

6.1 Time-domain problems

6.1.1 Explicit and IMEX Hybridizable DG methods

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

Hybridizable discontinuous Galerkin (HDG) methods were first studied in the team for frequency domain applications for which they 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 greater than 1. The proposed method has been implemented for dealing with general 3D problems.

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 [3]-[2]. 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 elements in the fine part of 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.

6.1.2 Reduced-order modeling for time-domain electromagnetics

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 [6]-[5] have been confirmed by extending the proposed POD-based ROM to the simulation of 3D nanophotonic problems.

6.1.3 Stability and asymptotic properties of the linearized Hydrodynamic Drude model

Participants Serge Nicaise *(Université de Valenciennes)*, Claire Scheid.

We go one step further toward a better understanding of the fundamental properties of the linearized hydrodynamical model studied in [9]. This model is especially relevant for small nanoplasmonic structures (below 10 nm). Using a hydrodynamical description of the electron cloud, both retardation effects and nonlocal spatial response are taken into account. This results in a coupled PDE system for which we study the linear response. In [16], 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, Thibault Laufroy, Claire Scheid.

Although losses in metal are 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 temperature increase 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. Due to the various scales and phenomena that come into play, accurate numerical modeling is challenging. Laser illumination first excites a plasmon oscillation (reaction of the electrons of the metal) that relaxes to a thermal equilibrium and in turn excites the metal lattice (phonons). The latter is then responsible for heating the surroundings. A relevant modeling approach thus consists in describing the electron-phonon coupling through the evolution of their respective temperature. Maxwell's equations are then coupled to a set of coupled nonlinear hyperbolic equations for the temperatures of respectively 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. In the context of the PhD of Thibault Laufroy, which has started this year, we propose to develop a suitable numerical framework for studying thermoplasmonics. As a first step, we have reviewed the models used in thermoplasmonics that are most often based on strong or weak (nonlinear) couplings of Maxwell's equations with nonlinear equations modeling heat transfer (hyperbolic or parabolic), in order to lay the foundations of the numerical approximation framework that we will consider in the sequel. This activity is planed to be carried out in close collaboration with physicists or chemists specialized in the field, in particular from the Fresnel Institute in Marseilles (Guillaume Baffou).

6.1.5 Corner effects in nanoplasmonics

Participants Camille Carvalho *(Applied Mathematics Department, University of California Merced, USA)*, Patrick Ciarlet *(Inria POEMS project-team and ENSTA, Paris)*, 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 (studied 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 will be submitted in 2021.

6.1.6 DG methods for semiconductor device modeling

Participants Stéphane Lanteri, Massimiliano Montone, Claire Scheid.

Semiconductors constitute the heart and soul of integrated electronic systems, thus of modern technology. The extraordinary progress in circuit integration, since Moore's prediction from the early seventies, can certainly be majorly credited to the concurrent refinement of computer-aided design tools. Indeed, a higher scale of integration has punctually demanded a deeper understanding of semiconductor physics and more accurate mathematical models of devices to be numerically implemented and simulated. Charge transport is the starring phenomenon that needs to be predicted in order to build a mathematical model, based on higher-level quantities (e.g. electric current and voltage), that can be practically used for device simulation. A rigorous description demands statistics and quantum mechanics of electron/hole ensembles in crystal lattices, an approach that eventually leads to the Boltzmann transport equation, which solves for a state density function in the position-momentum space. The Boltzmann transport equation is extremely complex to deal with. In most applications, it is licit to call for simplifying assumptions to the degree where electron and hole ensembles are seen as gases of classical particles having an effective mass, which accounts for them being subjected to the electrostatic field produced by the atomic lattice. As a result, charge carrier transport is eventually described by a drift-diffusion model. This yields a system of partial differential equations (PDEs) which can be solved at two levels:

- Quasistatic approximation - The external force applied to the crystal is electrostatic, and drift-diffusion equations are coupled to a Poisson equation for the electrostatic potential. The goal is to determine the spatial distribution of carrier concentrations and the electric field (deduced from the potential).
- Fullwave model - The crystal is subject to an applied electromagnetic field, and Maxwell equations are coupled with transport equations for carrier dynamics. The goal is to determine the space-time evolution of carrier concentrations and the electromagnetic field.

The quasistatic approximation is rigorous when the steady state of the semiconductor has to be calculated. For example, this could be a preliminary step to the fullwave simulation of a device that is biased prior to responding to a (time-varying) electromagnetic excitation. The fullwave model is particularly relevant to electro-optics, i.e. when light-matter interaction is investigated. Indeed, such study is essential to understanding and accurately modeling the operation of photonic devices for light generation, modulation, absorption. In the context of the PhD of Massimiliano Montone that started thsi year, we study the formulation, analysis and development of a DGTD method for solving the coupled system of Maxwell equatiosn and drift-diffusion equations in the fullwave setting.

6.1.7 Advanced modeling of nanostructured CMOS imagers based on DG methods

Participants Jérémy Grebot, Stéphane Lanteri, Denis Rideau *(STMicroelectronics, Crolles)*, Claire Scheid.

In the context of the PhD of Jérémy Grebot that started this year, we study the photo-conversion process in CMOS imagers at micrometric wavelengths. If the majority of sensors operate on visible light, their modeling remains a difficult task. Indeed, part of the complexity of the modeling results from the very different shape and size factors between the whole pixel, the micrometric lenses and the nanometric structuring of the surface of the absorbing semiconductor. Moreover, an accurate estimation of light absorption is delicate because it depends on the absorbing material but also on the temperature of the latter and the density of free carriers. Finally, the transport of the photo-generated carriers can be tricky to simulate when they are in limited number. This last step requires, for example, a Monte-Carlo algorithm dedicated to stochastic phenomena. All in all, the ideal simulation chain will therefore have to deal with light transport, photon absorption in the SiGe (Germanium-doped Silicon) semiconductor material and the transport of the induced carriers to the electrodes. In this study, a true multiscale methodology will be set up to analyze several optimization strategies for imagers under development at STMicroelectronics. In particular, our goals are investigate, model and optimize the quantum efficiency and SNR (Signal-to-Noise Ratio) for infrared light in an image sensor. The impact of the absorbing material (SiGe or Ge possibly mechanically stressed) as well as the complex structuring of the surfaces will be systematically studied. For this purpose a modeling of the light absorption in the whole device, from curved and micrometric lenses to the pyramidal and nanometric texturing of the doped silicon, is necessary. This modeling of the absorption of photons is carried out with the help of a high order DGTD method. A preliminary task, which is underway, is to define an appropriate dispersion model of the SiGe for different doping rates, and taking into account the dependence to the temperature.

6.2 Frequency-domain problems

6.2.1 Homogenization theory for metasurfaces

Participants Agnès Maurel *(ESPCI, Paris)*, Kim Pham *(ENSTA, Paris)*, Nicolas Lebbe.

We applied the (surfacic) quasi-periodic homogeneization theory to derive equivalent transmission condition of deeply subwavelength microstructured metasurfaces. The resulting conditions are closely related to the so-called GSTC (Generalized Sheet Transition Conditions) that were originally derived in the 90s from physicial principles. Our approach provides a direct link between the coefficients of the susceptibility tensors driving surfacic polarization fields and the structural design of a microstructured metasurface. These equivalent boundary conditions are useful for numerical simulations since they reduce the complexity of the meshes at the interfaces and thus the number of degrees of freedom to be solved (see Fig. 1 (a)). The numerical implementation of these GSTCs was done both in 2D and 3D using the finite element method (FEM) in the frequency domain (see Fig. 1 (b)).

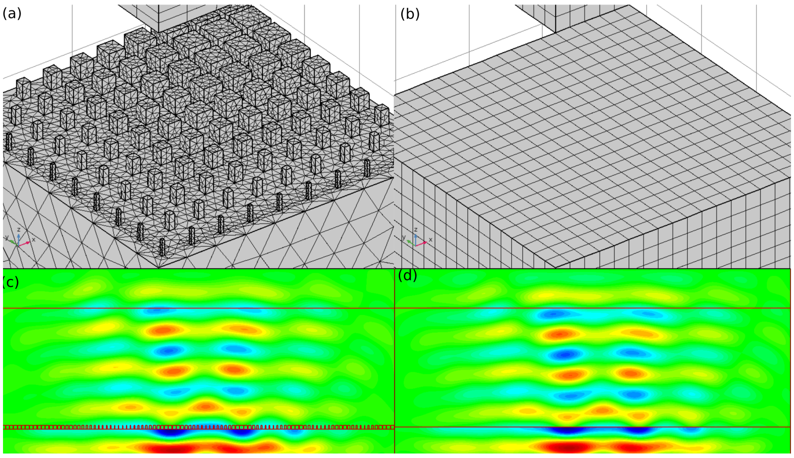

Figure 1: (a) Mesh with a microstructure. (b) Cartesian mesh used for the simulation with the GSTCs. (c) reference solution computed on a nanostructured mesh. (d) Simulation with homogeneization-based equivalent boundary conditions.

6.2.2 Equilibrated error estimators for high-order methods

Participants Théohpile Chaumont-Frelet, Alexandre Ern *(SERENA project-team, Inria Paris)*, Patrick Vega, Martin Vohralík *(SERENA project-team, Inria Paris)*.

Error estimators are an important tool in the discretization of PDE poblems. On the one hand, they permit to estimate the accuracy of the discrete model. In addition, estimators typically provide local information about the error in parts of the discretization mesh, enabling local refinement algorithms.

A now well-established and widely used family of error estimators is called "residual-based". These estimators have the advatange to be relatively easy to implement, and very efficient. Unfortunately, they become less accurate as the discretization order is increased. This leads in general to large error over-estimation, and decreased performance of adaptive algorithms.

In this collaboration with the SERENA project-team, we are interested in a modern family of error estimators, called "equilibrated-fluxes". These estimators are slightly more costly to compute than residual-based ones, but they are much more efficient when combined with high-order discretization schemes. A key properties of such estimators is that they are p-robust, meaning that they do not suffer from an increase in the polynomial degree p employed in the discretization method.

A first contribution in this context is the work [1] already mentioned in the activity report of the last year. It is concerned with high-frequency Helmholtz problems, and that has just been accepted for publication in February 2021.

In 2020, we have focused on Maxwell's equations in the low-frequency limit. While the low-frequency limit is not directly of interest to the applications considered in the Atlantis project-team, it is mathematically interesting as a simplified foundation for later extension to the high-frequency case. Part of our work, presenting crucial abstract mathematical results as been published this year [10]. We also submitted our main results [20], where the novel estimator is presented and analyzed, and its efficiency is numerically assessed.

A novel research direction we have started in 2020 in the context of the post-doctoral fellowship of Patrick Vega, concerns the use of equilibrated-fluxes for the Helmholtz equation combined with high-order absorbing boundary conditions. These boundary conditions are of great interest in applications as they lead to improved approximations of radiation conditions and more efficient domain-decomposition preconditioners. They are also challenging to deal with from the numerical point of view, since they combine "volume" PDEs with "surface" PDEs.

6.2.3 Residual error estimators for high frequency problems

Participants Théohpile Chaumont-Frelet, Stéphane Lanteri, Patrick Vega.

Residual error estimators are widely employed in applications to drive adaptive mesh refinement algorithms. However, most of the work available in the literature deals with coercive problems and unfortunately, this setting does not cover high-frequency wave problems, which are of central interest in the Atlantis project-team.

The postdoctoral subject of Patrick Vega is to adapt, analyze and implement residual error estimators for high-frequency wave problems, and in particular, Maxwell's equations. So far, a rigorous analysis of high-frequency Maxwell's equations discretized with Nédélec finite elements or a hybridizable discontinuous Galerkin method have been performed in 3D [22]. This theoretical analysis is also backed up by 2D numerical experiments, showing the ability of the estimator to efficiently drive adaptive mesh refinements.

We also started to investigate the use of residual error estimator for Maxwell's equations coupled with a linearized hydrodynamic Drude model. We covered the theoretical analysis and our first numerical experiments are promising. We are currently finalizing a publication on the subject, which is to be submitted in 2021.

6.2.4 Analysis of quasi-periodic boundary conditions

Participants Théohpile Chaumont-Frelet, Zakaria Kassali, Stéphane Lanteri.

Quasi-perodidc boundary conditions arise in a number of applications considered in the team. Important examples are the simulations of solar cells and photonic crystals. These “unusual” boundary conditions correspond to an incident wave with an oblique incidence, and can strongly impact the stability and accuracy of numerical discretizations. We investigate these boundary conditions in the PhD of Zakaria Kassali. We have been able to derive sharp stability estimates for finite element discretizations involving quasi-periodicity. In particular, we have shown that a drastic accuracy loss can appear at certain angle of incidence, that mathematically correspond to “parabolically trapped” rays (see Fig. 2, blue curve). We propose to remedy this problem by using a multiscale hybrid-mixed (MHM) method (see Fig. 2, red curve). Our numerical investigations are rather promising, and current efforts are guided toward a rigorous error analysis for the MHM method, showing its robustness with respect to parabolically trapped rays.

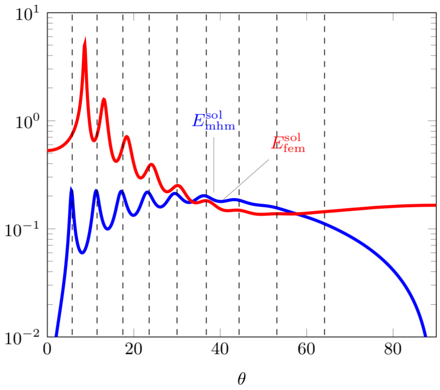

Figure 2: Errors of FEM (red) and MHM (blue) discretizations in a solar cell experiment as a function of the angle of incidence.1

6.3 Applications

6.3.1 Inverse design of metasurfaces using statistical learning methods

Participants Mickael Binois *(ACUMES project-team, Inria Sophia Antipolis-Méditerranée)*, Régis Duvigneau *(ACUMES project-team, Inria Sophia Antipolis-Méditerranée)*, Mahmoud Elsawy, Patrice Genevet *(CRHEA laboratory, Sophia Antipolis)*, Stéphane Lanteri.

Metasurfaces are flat optical nanocomponents, which 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 resorting to inverse design. In this work, which is conducted in close collaboration with the group of Patrice Genevet at the Research Center for Heteroepitaxy and its Applications (CRHEA, CNRS), we study phase gradient metasurfaces. More precisely, we leverage a computational modeling strategy that combines a high order discontinuous Galerkin time-domain solver implemented in the DIOGENeS software suite with a statistical learning-based global optimization technique developed by researchers from the ACUMES project-team, to discover novel metasurface designs with high efficiency. 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 less than 200 fullwave simulations. This year we extended our former work in [4] by considering multiobjective optimization settings as illustrated in Fig. 3.

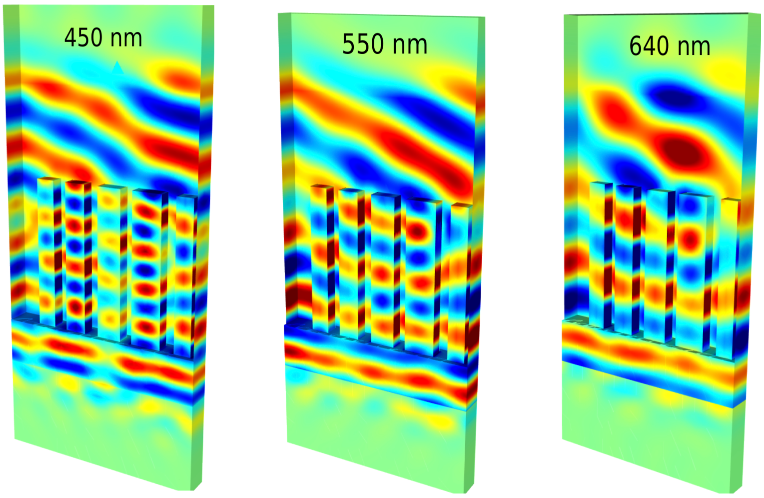

Figure 3: Optimization of a phase gradient metasurface made of rectangular GaN (Gallium Nitride) nanopillars. In this example, a multiobjective optimization is conducted for maximizing a particular diffraction efficiency order at three wavelengths.

6.3.2 Multiobjective optimization for large-scale achromatic metalenses

Participants Mickaël Binois *(ACUMES project-team, Inria Sophia Antipolis-Méditerranée)*, Régis Duvigneau *(ACUMES project-team, Inria Sophia Antipolis-Méditerranée)*, Mahmoud Elsawy, Patrice Genevet *(CRHEA laboratory, Sophia Antipolis)*, Stéphane Lanteri.

In this work, we present for the first time to the metasurface community a multiobjective optimization approach based on statistical learning. This method is based on a surrogate modeling, which replaces the high fidelity electromagnetic evaluation process with a simpler and cheaper model for the prediction of the new designs during the optimization process. Even though it converges to the global set of solutions, it requires fewer iterations compared to the classical global evolutionary strategies. We combine this approach with our in-house developed 3D electromagnetic solver based on the Discontinuous Galerkin Time-Domain (DGTD) method in order to optimize 3D achromatic metalens with numerical aperture NA above 0.5. Our metalens attempts to focus the RGB colours at the same focal plane with the maximum feasible focusing efficiency (see Fig. 4 (a)). In other words, we seek to get the most suitable compromise between the chromatic dispersion and the focusing efficiency for a given fixed focal distance. Our 3D lens is composed of concentric rings of cylindrical nanopillars represented by the red colour in Fig. 4 (b). In order to reduce the computational cost, we assume that the cylinders in each ring share the same diameter. In Fig. 4 (c), we present the intensity profile along the propagation direction z for one of the optimized designs, where the NA=0.56. As can be seen, the three colours are focused nearly at the predefined focal plane (represented by the vertical black line). The average focal error for the three wavelengths is less than 6%.

It is worth mentioning that the optimized designs have already been fabricated by our physical partners from CRHEA as depicted in Figs. 4 (d-f). The experimental characterization will be performed in the next weeks. In addition, the manuscript for our joint paper will be submitted soon to one of the prestigious scientific journals in the field of metasurfaces.

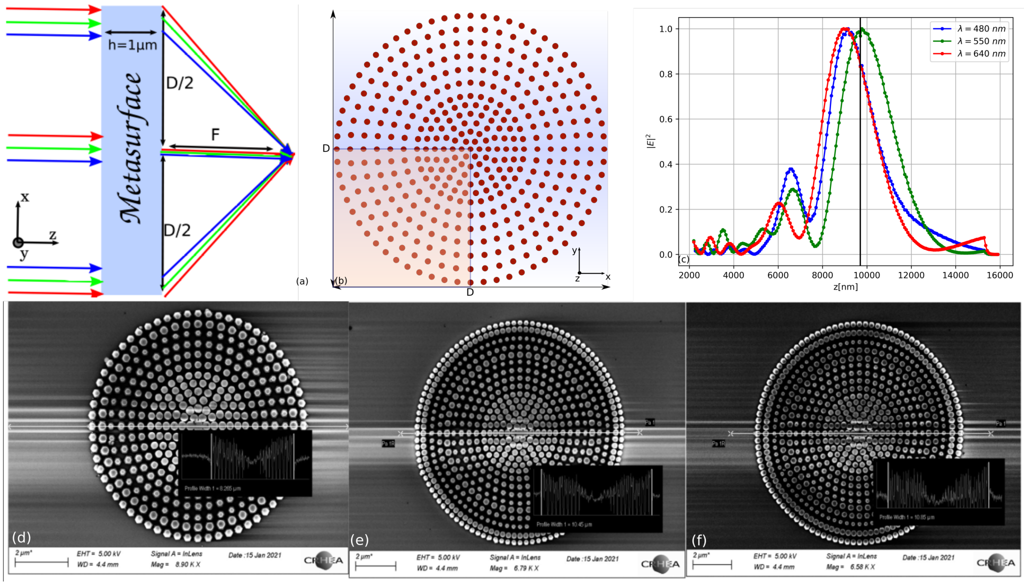

Figure 4: a) schematic view of the 3D achromatic metalens in the x-z plane. The metalens aims at focusing the three colours at the same focal distance F. The diameter of the metasurface is D and the thickness is fixed as h=1000 nm. (b) Details of the geometry at the x-y plane (shadow region represents the one quarter of the structure after imposing the symmetry properties). The optimization parameters are the diameters of the cylinders and the distances between them (16 parameters in general). (c) refers to the intensity profile cut along the propagation direction z for one of the optimized designs with NA=0.56. (d-f) Fabricated designs at CRHEA, CNRS, the experimental characterization will be performed in the next weeks.

6.3.3 Optimization of metasurfaces accounting for fabrication uncertainties

Participants Mickaël Binois *(ACUMES project-team, Inria Sophia Antipolis-Méditerranée)*, , Régis Duvigneau *(ACUMES project-team, Inria Sophia Antipolis-Méditerranée)*, , Mahmoud Elsawy, Patrice Genevet *(CRHEA laboratory, Sophia Antipolis)*, Stéphane Lanteri.

Fabrication processes of metasurface components require dealing with geometrical features in the nanometer scale. Despite the advances of nanofabrication facilities developed during the past few years, uncertainties and systematic fabrication errors are usually non-negligible, and are the source of efficiency degradation compared to modeling and simulation results. In this study, we consider the optimization of metasurface designs taking into account uncertainties due to fabrication errors. Our approach is based on statistical learning optimization, where robust statistical metamodels replace expensive high fidelity numerical simulations. We apply this technique to optimize and design realistic phase gradient metasurfaces in the visible regime. Our preliminary results reveal that we obtain robust designs. which are less sensitivity to the geometrical fabrication errors as compared to the one optimized without considering uncertainties.

6.3.4 Simulation of 3D conformal metasurfaces using GSTCs

Participants Sandeep Yadav Golla *(CRHEA laboratory, Sophia Antipolis)*, Patrice Genevet *(CRHEA laboratory, Sophia Antipolis)*, Nicolas Lebbe.

The development of metamaterials and the associated technologies have exploited transformation optics and its analogy with light propagation in curved space to manipulate light in arbitrary ways. In this collaboration, we addressed the problem of metasurface tranmission conditions at conformal interfaces using Generalized Sheet Transitions Conditions (C-GSTCs) derived following pioneering works of Idemen for planar interfaces using surfacic Dirac distributions. We also adapted the classical inversion procedure used in planar GSTCs to retrieve the susceptibilities to the conformal case by restricting the tensors values to their sole tangential components. These C-GSTCs were first implemented in both 2D and 3D using the FEM (see Fig. 15) and then used to study the impact of the interface geometry on different types of aberrations for metalenses.

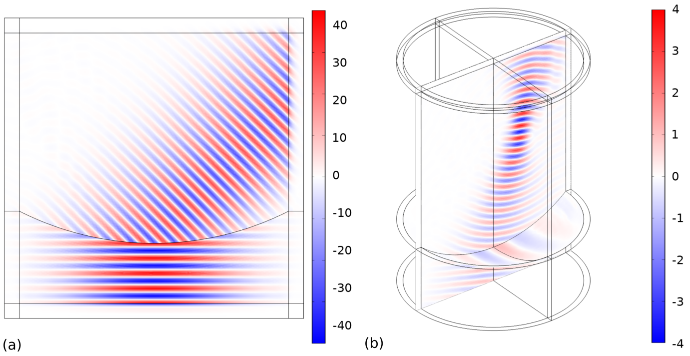

Figure 5: (a) 2D simulation of a diffraction conformal metasurface. (b) 3D simulation of a conformal metalens.

6.3.5 3D metamaterial mode converter for integrated optics

Participants Karim Hassan *(CEA-LETI, Grenoble)*, Salim Boutami *(CEA-LETI, Grenoble)*, Mahmoud Elsawy, Stéphane Lanteri.

In this study, we combined a statistical learning-based global optimization strategy with a high order 3D DGTD asolver to design a compact and highly efficient graded index photonic metalens. The metalens is composed of silicon (Si) strips of varying widths (in the transverse direction) and lengths (in the propagation direction) and operates at the telecommunication wavelength (see Fig.6 (a)) In our work [14], we tackled the challenging Transverse Electric case (TE) where the incident electric field is polarized perpendicular to strips direction. We reveal that the focusing efficiency approaches 80% for the traditional design with fixed strip lengths and varying widths. Nevertheless, we demonstrate numerically that the efficiency is as high as 87% for a design with varying strip lengths along the propagation direction. Our findings open numerous fascinating paths towards the realization of compact and highly efficient integrated photonic components.

6.3.6 Optimization of light-trapping in nanostructured solar cells

Participants Stéphane Collin *(Sunlit team, C2N-CNRS, Paris-Saclay)*, Alexis Gobé, 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 exploit statistical learning methods for the inverse design of material nanostructuring with the goal of optimizing light trapping properties of ultraphin solar cells. This objective is challenging because the underlying electromagnetic wave problems exhibit multiple resonances, while the geometrical settings are non-trivial. Such multi-resonant solar cell structures are attractive for maximizing light absorption for the full solar light

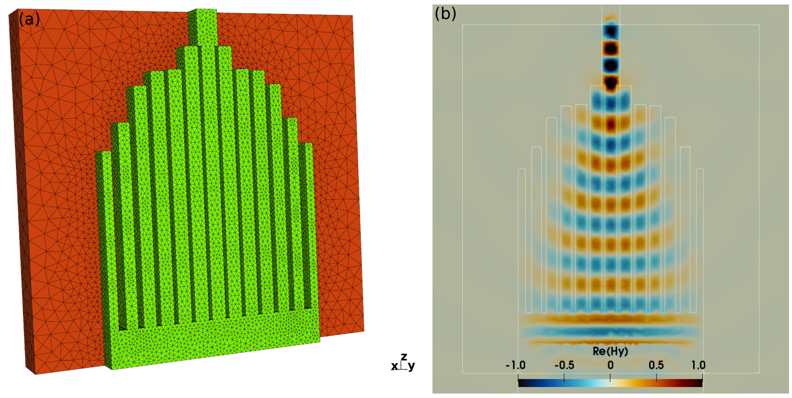

Figure 6: (a): 3D mesh for the optimized design with different lengths for the strips. (b): Field map of $\Re e(H_y)$ for the optimized design with changing length in the $x-z$ plane obtained from our DGTD solver using $\mathbb{P}_4$ interpolation and mesh with 334 000 cells.

spectrum as illustrated in Fig. 7. We exploit statistical learning methods for the inverse design of material nanostructuring with the goal of optimizing light trapping properties of ultraphin solar cells. This study is conducted in collaboration with the Sunlit headed by Stéphane Collin at the Center for Nanoscience and Nanotechnology (C2N, CNRS).

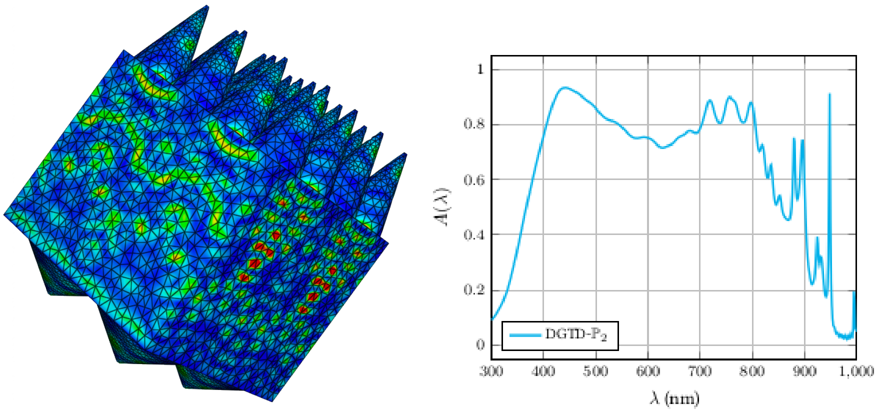

Figure 7: Optimization of light absorption in a solar cell based on a nanocone grating.

6.3.7 Plasmonic sensing with nanocubes

Participants Antoine Moreau *(Institut Pascal, Clermont-Ferrand)*, Stéphane Lanteri, Guillaume Leroy, Claire Scheid.

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. We study the generation of gap plasmons by various configurations of silver nanocubes separated from a gold substrate by a dielectric layer, 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. We exploit statistical learning methods for the goal-oriented inverse design of cube size, dielectric and gold layer thickness, as well as gap size between cubes in a dimer configuration. This study is conducted in collaboration with Antoine Moreau at Institut Pascal (CNRS).

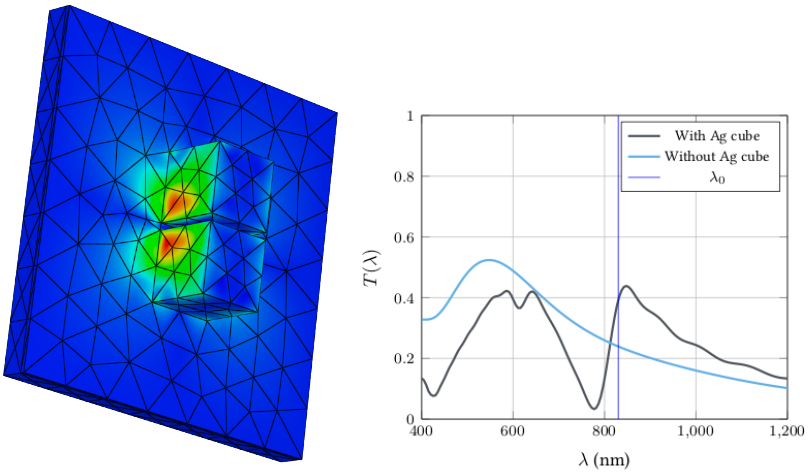

Figure 8: Optimization of a plasmonic nanocube dimer setting for the generation of Fano resonances.

6.3.8 Multiple scattering in randon media

Participants Stéphane Lanteri, Guillaume Leroy, Gian Luca Lippi *(INPHYNI laboratory, Sophia Antipolis)*.

Fluorescence signals emitted by probes, used to characterize the expression of biological markers in tissues or cells, can be very hard to detect due to a small amount of molecules of interest (proteins, nucleic sequences), to specific genes expressed at the cellular level, or to the limited number of cells expressing these markers in an organ or a tissue. Access to information coming from weaker emitters can only come from strengthening the signal, since electronic post-amplification raises the noise floor as well. While costly and molecule-specific biochemical processes are being developed for this purpose, a new mechanism based on the simultaneous action of stimulated emission and multiple scattering, induced by nanoparticles suspended in the sample, has been recently demonstrated to effectively amplify weak fluorescence signals. A precise assessment of the signal fluorescence amplification that can be achieved by such a scattering medium requires a electromagnetic wave propagation modeling approach capable of accurately and efficiently coping with multiple space and time scales, as well as with non-trivial geometrical features (shape and topological organization of scatterers in the medium). In the context of a collaboration with physicists from the Institut de Physique de Nice INPHYNI (Gian Luca Lippi from the complex photonic systems and materials group), we initiated this year a study on the simultaneous action of stimulated emission and multiple scattering by randomly distributed nanospheres in a bulk medium. From the numerical modeling point of view, or short term goal is to develop a time-domain numerical methodology for the simulation of random lasing in a gain medium.

7 Bilateral contracts and grants with industry

7.1 Bilateral contracts with industry

Nom: DGTD solvers for time-domain elecromagnetics with application to photovoltaics

- Duration: Jan 2019-Dec 2020

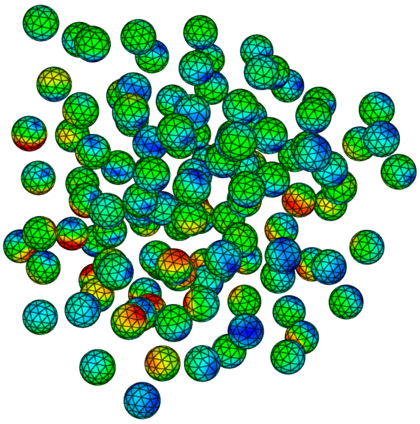

Figure 9: Multiple scattering by randomly distributed nanospheres in a bulk medium.

- Local coordinator: Stéphane Lanteri
- Participants: Andreas Atle [TOTAL, Houston, USA], Henri Calandra [TOTAL, Pau], Alexis, Gobé, Michael Sekachev [TOTAL, Hoiuston, USA]
- This contract with TOTAL CSE (Computational Science and Engineering) division in Houston, Texas, is concerned with the development of DGTD solvers for time-domain elecromagnetics with application to photovoltaics. In the field of photovoltaics, modeling and simulation is considered by the R&D division of the GRP (Gas, Renewables & Power) branch in the context of the involvement of TOTAL in the IPVF (Institut Photovoltaïque d'Île-de-France) for dealing with two subjects: on the one hand, for the study of laser-matter interaction in order to optimize the nanostructuring process of materials in the design of solar cell structures; on the other hand, for the characterization of the light absorption properties of complex solar cell structures. The latter is the subject considered in thsi contract. A numerical study of the absorption of light in nanostructured solar cells is conducted. The goal is to demonstrate the capabilities of DG type methods for dealing accurately and efficiently with the multiscale nature of the considered problem (in particular with regard to the nanostructuring of the different material layers).

Nom: DGTD solvers for semiconductor device modeling

- Duration: Nov 2019-Jan 2023
- Local coordinator: Stéphane Lanteri
- Participants: Eric Guichard [Silvaco Inc., Santa Clara, USA], Massimiliano Montone, Claire Scheid, Slim Chourou [Silvaco Inc., Santa Clara, USA], Mark Townsend [Silvaco Inc., Santa Clara, USA]
- This contract with the TCAD division of Silvaco Inc. is closely linked to the PhD project of Massimiliano Montone and is concerned with the numerical modeling of semiconductor-based photonic devices using high order DGTD methods. More precisely, the main methodological objective of the PhD project is to design, analyze and develop DG-based approaches for solving the system of time-domain Maxwell equations coupled to the unsteady drift-diffusion equations in 3D. On the application side, in close collaboration with Silvaco Inc., microLEDs and CMOS image sensors will constitute the driving technologies for the application of the methodological developments achieved in the PhD work; moreover, Nanostructured solar cells and photoconductive antennas (including hybrid photoconductive antennas leveraging plasmonic effects) will serve as more prospective applications that will possibly be considered in collaboration with physicists from academic groups, which are partners of the ATLANTIS project-team.

7.2 Grants with industry

Nom: DGTD solvers for modeling light absorption in CMOS imagers

- Duration: Jan 2019-Dec 2022
- Local coordinator: Stéphane Lanteri
- Participants: Marios Barlas [STMicroelectronics, Crolles], Alexis Gobé, Valentin Goblot [STMicroelectronics, Crolles], Jérémy Grebot, Denis Rideau [STMicroelectronics, Crolles], Guillaume Leroy, Claire Scheid
- This grant is part of the Nano 2022 IPCEI (Important Projects of Common European Interest) program, which involves several european industrial groups and companies in the microelectronics field. The team is involved in a subproject conducted in close collaboration with STMicrolectronics (CMOS Imagers division of the Technology for Optical Sensors department) in Crolles. The exploitation of nanostructuring to improve the performance of CMOS imagers based on microlens grids is a very promising path. In this perspective, numerical modeling is a key component to accurately characterize the absorption properties of these complex imager structures that are intrinsically multiscale (from the micrometer scale of lenses to the nanometric characteristics of nanostructured layers of materials). The FDTD method (for Finite Difference Time-Domain) is the solution adopted in the first instance for the numerical simulation of the interaction of light with this type of structure. However, because it is based on a Cartesian mesh (mostly uniform structured mesh), this method has limitations when it comes to accurately account for complex geometrical features such as microlens curvature or texturing of material layer surfaces. In this context, the main objective of our study is to take advantage of the possibilities offered by the DGTD method with realistic geometric models of complex imager structures based on locally refined tetrahedral meshes.

8 Partnerships and cooperations

8.1 European initiatives

8.1.1 FP7 & H2020 Projects

EPEEC (European joint effort toward a highly productive programming environment for heterogeneous exascale computing)

Participants Alexis Gobé, Stéphane Lanteri.

- Type: H2020
- See also: `https://epeec-project.eu`
- Duration: Oct 2018 - Sep 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.

PRACE 6IP (PRACE Sixth Implementation Phase)

Participants Emmanuel Agullo *(HIEPACS project-team, Inria Bordeaux - Sud-Ouest)*, Alexis Gobé, Luc Giraud *(HIEPACS project-team, Inria Bordeaux - Sud-Ouest)*, Stéphane Lanteri.

- Type: H2020

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

- Duration: May 2019 - Dec 2021

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

- 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-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. 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.

8.2 National initiatives

8.2.1 ANR project

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: Apr 2019 to Sep 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.

9 Dissemination

9.1 Promoting scientific activities

9.1.1 Journal

Reviewer - reviewing activities

- Mahmoud Elsawy: ACS Nano, Optics Letters, Applied Physics A
- Stéphane Lanteri: Journal of Computational Physics, Computer Methods in Applied Mechanics and Engineering, Optica

9.1.2 Leadership within the scientific community

Review on numerical optimization methods for metasurfaces

Participants Jonathan A. Fan *(Stanford University, California, United States)*, Régis Duvigneau *(ACUMES project-team, Inria Sophia Antipolis-Méditerranée)*, Patrice Genevet *(CRHEA laboratory, Sophia Antipolis)*, Mahmoud Elsawy, Stéphane Lanteri.

We have produced a review of recent optimization techniques used in the inverse design of high performance metasurfaces. We believe that this review will push this exciting field towards realistic and practical applications, ranging from laser wavefront engineering to innovative facial recognition and motion detection devices, including augmented reality retro-reflectors and related complex light field engineering. This review has been published in Laser & Photonics Review [13].

9.2 Teaching - Supervision - Juries

9.2.1 Teaching

- Claire Scheid, *Analyse Fonctionnelle, Practical works*, Master 1 MPA, 18 h, Université Côte d'Azur
- Claire Scheid, *Optimisation et éléments finis*, Master 1 MPA and IM, 54 h, Université Côte d'Azur
- Claire Scheid, *Option Modélisation, Lectures and practical works*, Master 2 Agrégation, 43 h, Université Côte d'Azur
- Yves D'Angelo, *Modélisation Simulation Numérique*, Master 1 IM/MPA, 50 h, Université Côte d'Azur
- Yves D'Angelo, *Modélisation de la Turbulence dans l'Industrie*, Master 1 MPA and IM, 16 h, Université Côte d'Azur
- Stéphane Descombes, *Introduction to partial differential equations* Master 1 MPA and IM, 30 h, Université Côte d'Azur
- Stéphane Descombes, *Principal component analysis and supervised analysis*, Master 2 SIRIS, Université Côte d'Azur
- Stéphane Descombes, *Mathematics practical works*, L1 SocioEco, 18 h, Université Côte d'Azur
- Engineering: Stéphane Lanteri, *High performance scientific computing*, 24 h, MAM5, Polytech Nice Sophia - Université Côte d'Azur

9.2.2 Supervision

- PhD defended: Alexis Gobé, Discontinuous Galerkin methods for the simulation of multiscale nanophotonic problems with application to light trapping in solar cells, February 2020, Stéphane Lanteri
- PhD defended: Georges Nehmetallah, Hybridized discontinuous Galerkin methods coupled with hybrid explicit/implicit schemes for the unsteady maxwell equations, December 2020, Stéphane Descombes and Stéphane Lanteri
- PhD in progress: Zakaria Kassali, Multiscale finite element simulations applied to the design of photovoltaic cells, 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, Stéphane Lanteri and Claire Scheid
- PhD in progress: Jérémy Grebot, Advanced modeling of nanostructured CMOS imagers, Stéphane Lanteri and Claire Scheid

9.2.3 Juries

- Stéphane Lanteri, reviewer: Minh Duy Truong, Aix-Marseille Univ., October 2020
- Stéphane Lanteri, examiner: Léo Martire, ISAE-Supaero, October 2020

10 Scientific production

10.1 Major publications

[1] T. Chaumont-Frelet, A. Ern and M. Vohralík. 'On the derivation of guaranteed and p-robust a posteriori error estimates for the Helmholtz equation'. working paper or preprint. Aug. 2020. URL: `https://hal.inria.fr/hal-02202233`.

[2] S. Descombes, S. Lanteri and L. Moya. 'Locally implicit discontinuous Galerkin time domain method for electromagnetic wave propagation in dispersive media applied to numerical dosimetry in biological tissues'. In: *SIAM Journal on Scientific Computing* 38.5 (2016), A2611–A2633. DOI: `10.1137/15M1010282`. URL: `https://hal.inria.fr/hal-01133694`.

[3] S. Descombes, S. Lanteri and L. Moya. 'Temporal convergence analysis of a locally implicit discontinuous galerkin time domain method for electromagnetic wave propagation in dispersive media'. In: *Journal of Computational and Applied Mathematics* 316 (May 2017), pp. 122–132. DOI: `10.1016/j.cam.2016.09.038`. URL: `https://hal.archives-ouvertes.fr/hal-01244237`.

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[5] K. Li, T.-Z. Huang, L. Li and S. Lanteri. 'A reduced-order discontinuous Galerkin method based on a Krylov subspace technique in nanophotonics'. In: *Applied Mathematics and Computation* 358 (Oct. 2019), pp. 128–145. DOI: `10.1016/j.amc.2019.04.031`. URL: `https://hal.inria.fr/hal-02433050`.

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10.2 Publications of the year

International journals

[10] T. Chaumont-Frelet, A. Ern and M. Vohralík. 'Polynomial-degree-robust H(curl)-stability of discrete minimization in a tetrahedron'. In: *Comptes Rendus Mathématique* 358.9-10 (24th Dec. 2020), pp. 1101–1110. DOI: `10.5802/crmath.133`. URL: `https://hal.inria.fr/hal-02631319`.

[11] T. Chaumont-Frelet, S. Nicaise and J. Tomezyk. 'Uniform a priori estimates for elliptic problems with impedance boundary conditions'. In: *Communications on Pure and Applied Analysis* (2020). DOI: `10.3934/cpaa.2020107`. URL: `https://hal.archives-ouvertes.fr/hal-01887269`.

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[17] M. M. R. Elsawy, S. Lanteri, R. Duvigneau and P. Genevet. 'Statistical Learning Optimization for Highly Efficient Metasurface Designs'. In: SIAM Conference on Computational Science and Engineering 2021. Texas, United States, 1st Mar. 2021. URL: `https://www.hal.inserm.fr/inserm-03070707`.

Doctoral dissertations and habilitation theses

[18] A. Gobé. 'Discontinuous Galerkin methods for the simulation of multiscale nanophotonic problems with application to light trapping in solar cells'. Université Côte d'Azur, 17th Feb. 2020. URL: `https://tel.archives-ouvertes.fr/tel-03000583`.

Reports & preprints

[19] C. Carvalho, P. Ciarlet and C. Scheid. *Limiting amplitude principle and resonances in plasmonic structures with corners: numerical investigation.* 5th Mar. 2021. URL: `https://hal.archives-ouvertes.fr/hal-03160574`.

[20] T. Chaumont-Frelet, A. Ern and M. Vohralík. *Stable broken H(curl) polynomial extensions and p-robust quasi-equilibrated a posteriori estimators for Maxwell's equations.* 28th May 2020. URL: `https://hal.inria.fr/hal-02644173`.

[21] T. Chaumont-Frelet, S. Lanteri and P. Vega. *A posteriori error estimates for finite element discretizations of time-harmonic Maxwell's equations coupled with a non-local hydrodynamic Drude model.* 9th Mar. 2021. URL: `https://hal.inria.fr/hal-03164225`.

[22] T. Chaumont-Frelet and P. Vega. *Frequency-explicit a posteriori error estimates for finite element discretizations of Maxwell's equations.* 19th Sept. 2020. URL: https://hal.inria.fr/hal-02943386.

[23] T. Chaumont-Frelet and B. Verfürth. *A generalized finite element method for problems with sign-changing coefficients.* 27th Aug. 2020. URL: https://hal.inria.fr/hal-02496832.

[24] T. Chaumont-Frelet and M. Vohralík. *Equivalence of local-best and global-best approximations in H(curl).* 2nd June 2020. URL: https://hal.inria.fr/hal-02736200.

[25] G. Nehmetallah, T. Chaumont-Frelet, S. Descombes and S. Lanteri. *A postprocessing technique for a discontinuous Galerkin discretization of time-dependent Maxwell's equations.* 3rd Oct. 2020. URL: https://hal.inria.fr/hal-02956882.

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