RESEARCH CENTRE

Inria Centre
at Université Côte d’Azur

IN PARTNERSHIP WITH:
CNRS, Université Côte d’Azur

2023
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

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Project-Team ATLANTIS

Creation of the Project-Team: 2020 February 01

Keywords

Computer sciences and digital sciences

A6. – Modeling, simulation and control

A6.2. – Scientific computing, Numerical Analysis & Optimization

A6.2.1. – Numerical analysis of PDE and ODE

A6.2.7. – High performance computing

Other research topics and application domains

B4. – Energy

B4.3.4. – Solar Energy

B5.3. – Nanotechnology

B5.5. – Materials

B8. – Smart Cities and Territories

B8.2. – Connected city

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2 Overall objectives

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* [55], 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 [60] 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 dielectric permittivity, 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 promises for applications in sensing and switching.

In ATLANTIS, our research activities aim at studying and impacting some scientific and technological challenges raised by physical problems involving optical 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. Driven by a number of nanophotonics-related physical drivers, our overall objectives are to design and develop innovative numerical methodologies for the simulation of nanoscale light-matter interactions and to demonstrate their capabilities by studying challenging applications in close collaboration with our physicist partners. On the methodological side, the Discontinous Galerkin (DG) family of methods is a cornerstone of our contributions. In particular, we study various variants of DG methods that can deal with complex material models and coupled PDE systems that are relevant to the study of nanoscale light-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. Novel methodological contributions on these topics in the context of the physical problems studied in ATLANTIS are eventually implemented in the DIOGENeS software suite, which is a unique software plaform dedicated to computational nanophotonics.

3 Research program

3.1 Driving physical fields

Our research activities eventually materialize as innovative computational techniques for studying concrete questions and applications that are tightly linked to specific physical fields (driving physical fields) related to nanophotonics and plasmonics. In most cases, these scientific topics and applications are addressed in close collaboration with physicists.

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 [48]. These advances have also allowed to achieve spatial separation between metallic elements of only few nanometers [47]. 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. In ATLANTIS, we study novel numerical modeling methods for solving some semi-classical models of quantum plasmonic effects such as in the context of the PhD work of Nikolkai Schmitt [69]-[18].

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 [56]-[46]-[51]. 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. Our first contributions on this topic have been obtained in the context of the ANR OPERA project (completed in September 2022) and are concerned with numerical modeling methods for the inverge design of metasurfaces [9]-[7] and metalenses [8].

Thermoplasmonics. Plasmonic resonances can be exploited for many applications [60]. 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 [44]. 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).

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 [61], 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.

High order DG methods. Designing numerical schemes that are high order accurate on general meshes, i.e., unstructured or hybrid structured/unstructured meshes, is a major objective of our core research activities in ATLANTIS. We focus on the family of Discontinuous Galerkin (DG) methods that has been extensively developed for wave propagation problems during the last 15 years. We investigate several variants, namely nodal DGTD for time-domain problems, and HDG (Hybridized DG) for frequency-domain problems, with the general goal of devising, analyzing and developing extensions of these methods in order to deal with the above-mentioned physical drivers: 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. Our methodological contributions of these methods eventually materialize in the DIOGENeS software suite.

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 designing 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 are designed in the framework of MHM (Multiscale Hybrid-Mixed) formulations that we study in the context of a long-term collaboration with the research group of 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.

Time integration for multiscale problems. Multiscale physical problems with complex geometries or heterogeneous 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 consider 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.

Reduced-order and surrogate modeling. Reduced-order modeling aims at reducing the computational requirements of costly high-fidelity solution methods while maintaining an acceptable level of accuracy. One of the most studied methods for establishing the reduced-order model is the Proper Orthogonal Decomposition (POD), also known as Karhunen-Loéve decomposition, principal component analysis, or singular value decomposition, which uses the solutions of high fidelity numerical simulations or experiments at certain time instants, typically called *snapshots*, to compute a set of POD basis vectors spanning a low-dimensional space. POD is very popular in the computational fluid dynamics field. However, the development of POD for time-domain electromagnetics has been more scarce. We study POD-based reduced-order modeling strategies in the context of a long-term collaboration with the research group of Liang Li at the School of Mathematical Sciences of the University of Electronic Science and Technology of China in Chengdu [13]-[11]-[12]. Alternatively, several works in the recent years have promoted highly efficient surrogate modeling approaches based on Deep Neural Networks (DNNs) but most of these approaches rely on the availability of large data set of solutions for training. We initiated in 2022 a new research direction on a particular family of DNNs referred as Physics-Informed Neural Networks (PINNs) [67] that we plan to investigate for PDE models that are relevant to nanophotonics with the goal of designing non-intrusive surrogate modeling approaches that require a minimal amount of data.

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 direction consists in refining classical linear dispersion models and we 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, nonlinear quantum hydrodynamic theory models, etc.). One possible approach relies on an accurate description of the Hamiltonian dynamics with intricate kinetic and exchange correlation energies, for different modeling purposes. A second direction is 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, that could in all generality be nonlinear. Assessing these two directions requires efficient dedicated numerical algorithms that are 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's 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 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 in the framework of the DIOGENeS software suite.

3.2.2 Complementary topics

Beside the above-discussed core research 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.

Numerical optimization. Inverse design has emerged rather recently in nanophotonics, and is currently the subject of intense research as witnessed by several reviews [62]. Artificial Intelligence (AI) techniques are also increasingly investigated within this context [71]. 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 [52]-[53] and fluid-structure interaction problems [68].

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 [57]. We study this topic in close collaboration with researchers of the ACUMES project-team one on hand, and researchers at TU Braunschweig in Germany.

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 [16]. 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 [43], or low-rank compression techniques [66]. 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 CONCACE (Inria center at Université de Bordeaux) industrial 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 [70] 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 [65].

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 [64]-[72]. The recently-introduced concept of hybrid photoconductive antennas leveraging plasmonic effects is even more challenging [59]. So far, existing simulation approaches are based on the Finite Difference Time-Domain (FDTD) method, and are only able to deal with classical PCAs. In relation with the design of photonic devices for THz waves generation and manipulation, we intend to develop a multiscale numerical modeling strategy for solving the system of Maxwell equations coupled to various models of charge carrier dynamics in semiconductors.

4.4 Plasmonic nanostructures 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 [50] 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 [49], which materializes as a system of PDEs coupled to Maxwell's equations [18]-[17]. 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 effects

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 [58]. Also, bio-functionalized gold nanorods are promising candidates for light-induced hyperthermia [63], 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 [45], 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 Social and environmental responsibility

5.1 Impact of research results

The parts of our research activities that are addressing the design of nanostructures for sunlight harvesting on one hand, and of nanostructures for photothermal effects on the other hand, target applications concerned with production of renewable energy and biomedical engineering (ranging from light controlled drug-release to the ongoing battle against Covid-19).

6 New software, platforms, open data

6.1 New software

6.1.1 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 nano-plasmonics (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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7 New results

7.1 High order methods for coupled problems

In this section, we present ongoing studies aiming at designing, analyzing and developing novel high order methods for solving electromagnetic wave propagation problems in general on one hand, and for differential systems modeling nanoscale light-matter interactions with complex media on the other hand. We focus on the family of Discontinuous Galerkin (DG) methods. In the time-domain setting, the starting point of these works is the DGTD (Discontinuous Galerkin Time-Domain) method introduced in [10]. In the frequency-domain setting, the HDGFD (Hybridized Discontinuous Galerkin Frequency-Domain) method [1] is considered as the basis of our works.

7.1.1 Time-domain numerical modeling of gain media

Participants: Stéphane Descombes, Stéphane Lanteri, Cédric Legrand, Gian Luca Lippi *(INPHYNI laboratory, Sophia Antipolis)*.

In laser physics, gain or amplification is a process where the medium transfers part of its energy to an incident electromagnetic radiation, resulting in an increase in optical power. This is the basic principle of all lasers. Quantitatively, gain is a measure of the ability of a laser medium to increase optical power. Modeling optical gain requires to study the interaction of the atomic structure of the medium with the incident electromagnetic wave. Indeed, electrons and their interactions with electromagnetic fields are important in our understanding of chemistry and physics. In the classical view, the energy of an electron orbiting an atomic nucleus is larger for orbits further from the nucleus of an atom. However, quantum mechanical effects force electrons to take on discrete positions in orbitals. Thus, electrons are found in specific energy levels of an atom. In a semiclassical setting, such transitions between atomic energy levels are generally described by the so-called *rate equations*. These rate equations model the behavior of a gain material, and they need to be solved self-consistently with the system of Maxwell equations. So far, the resulting coupled system of Maxwell-rate equations has mostly been considered in a time-domain setting using the FDTD method for which several extensions have been proposed. In the context of the PhD of Cédric Legrand, we study an alternative numerical modeling approach based on a high order DGTD method. This year, we have proposed a first variant that extends the DGTD method introduced in [54]. This novel DGTD method has been formulated and analyzed in the three-dimensional case. A fully discrete stability analysis has been conducted and a computer implementation has been finalized. Numerical validations are underway before proceeding to a concrete application in the field of random lasing in collaboration with Gian Luca Lippi at INPHYNI laboratory.

7.1.2 Time-domain numerical modeling of semiconductor devices

Participants: Eric Guichard *(Silvaco Inc., Santa Clars, CA, USA)*, Stéphane Lanteri, Massimiliano Montone, Claire Scheid.

In the field of semiconductor physics modeling, charge carrier 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. Charge carrier transport is generally described by a drift-diffusion model. This yields a system of coupled partial differential equations which can be solved at two levels: (1) 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); (2) 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 (defended in March 2023 [35]) we have a designed a DGTD method for solving the coupled system of Maxwell equations and drift-diffusion equations in the fullwave setting. The method has been formulated in the general three-dimensional case, and a computer implementation has been realized in a one dimensional and two-dimensional setting. Furthermore a first 1D theoretical stability study has been completed. A preprint is in finalization.

7.1.3 A posteriori error estimates for time-dependant wave propagation problems

Participants: Théophile Chaumont-Frelet.

The goal of this research line is to rigorously estimate the error incured by numerical approximation for time-dependent wave propagation problems.

In [2], we derive an equilibrated a posteriori error estimator for the space (semi) discretization of the scalar wave equation by finite elements. In the idealized setting where time discretization is ignored and the simulation time is large, we provide fully-guaranteed upper bounds that are asymptotically constant-free and show that the proposed estimator is efficient and polynomial-degree-robust, meaning that the efficiency constant does not deteriorate as the approximation order is increased. To the best of our knowledge, this work is the first to propose an estimator for the wave equation that is provably reliable and efficient in the same norm. We also explain, without analysis, how the estimator is adapted to cover time discretization by an explicit time integration scheme. Numerical examples illustrate the theory and suggest that it is sharp.

The work published in [2] is also the starting point of the ANR project APOWA, where other aspects of the a posteriori error estimation for time-dependent wave propagation problems will be be studied in depth.

7.1.4 Efficient approximation of high-frequency Helmholtz problems

Participants: Théophile Chaumont-Frelet, Victorita Dolean *(LJAD, Université Côte d'Azur)*, Maxime Ingremeau *(LJAD, Université Côte d'Azur)*, Florentin Proust.

Helmholtz problems describe the time-harmonic solutions of the wave equation (possibly in a heterogeneous medium, in a bounded medium, with boundary conditions, ...). In general, there is no explicit solution to such an equation, and an approximate solution of the equation must be computed numerically. All the existing methods (finite elements, finite differences...) have in common that they are more and more expensive when the frequency of the waves increases. In [37], we study new finite-dimensional spaces specifically designed to approximate the solutions to high-frequency Helmholtz problems with smooth variable coefficients. These discretization spaces are spanned by Gaussian coherent states, that have the key property to be localized in phase space. We carefully select the Gaussian coherent states spanning the approximation space by exploiting the (known) micro-localization properties of the solution. This work is conducted in the context of the POPEG Exploratory Research Action and the topic is also at the heart of the PhD thesis of Florentin Proust.

In the beginning of this thesis, such a method had been implemented for a simple one-dimensional problem. Even in this very simple case, it became clear that Gaussian coherent states could not be used in practice because they were strongly ill-conditioned. However, if the discretization spaces are now spanned by some particular linear combinations of Gaussian coherent states forming a so-called Wilson basis, then this problem disappears. In [3], it had been mathematically proved that using Gaussian coherent states to solve high-frequency Helmholtz problems had some advantages. In 2023, we started to prove similar - and even broader - results about Wilson basis.

7.2 Data-driven reduced-order modeling

In short, reduced order modeling (ROM) allows to construct simplifications of high fidelity, complex models. The resulting lower fidelity (also referred as surrogate) models capture the salient features of the source models so that one can quickly study a system's dominant effects using minimal computational resources. In collaboration with researchers at the University of Electronic Science and Technology of China (UESTC) and the Southwestern University of Finance (SUFEC) and Economics, which are both located in Chengdu, we study ROM for time-domain electromagnetics and nanophotonics. More precisely, we have considered the applicability of the proper orthogonal decomposition (POD) technique for the system of 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. Our first contributions are described in [11]-[13] where we have proposed POD approach for building a reduced subspace with a significantly smaller dimension given a set of space-time snapshots that are extracted from simulations with a high order DGTD method. Then, a POD-based ROM is established by projecting (Galerkin projection) the global semi-discrete DG scheme onto the low-dimensional space spanned by the POD basis functions.

7.2.1 Non-intrusive ROM for parameterized electromagnetic problems

Participants: Stéphane Lanteri, Kun Li *(SUFEC, Chengdu, China)*, Liang Li *(UESTC, Chengdu, China)*, Ying Zhao *(UESTC, Chengdu, China)*.

In [12], we have introduced a non-intrusive variant of the POD-based ROM initially introduced in [11]-[13], in the context of parameterized time-domain electromagnetic scattering problems. The considered parameters are the dielctric electric permittivity and the temporal variable. The snapshot vectors are produced by a high order DGTD method formulated on an unstructured simplicial mesh. Because the second dimension of the snapshots matrix is large, a two-step or nested POD method is employed to extract time- and parameter-independent POD basis functions. By using the singular value decomposition (SVD) method, the principal components of the projection coefficient matrices (also referred to as the reduced coefficient matrices) of full-order solutions onto the reduced-basis (RB) subspace are extracted. A cubic spline interpolation-based (CSI) approach is proposed to approximate the dominating time- and parameter-modes of the reduced coefficient matrices without resorting to Galerkin projection. The generation of snapshot vectors, the construction of POD basis functions and the approximation of reduced coefficient matrices based on the CSI method are completed during the offline stage. The RB solutions for new time and parameter values can be rapidly recovered via outputs from the interpolation models in the online stage. In particular, the offline and online stages of the proposed POD-CSI method are completely decoupled, which ensures the computational validity of the method. Moreover, a surrogate error model is constructed as an efficient error estimator for the POD-CSI method.

More recently, in [24]-[14], we have designed an improved versions of the POD-CSI method [12]. During the offline stage, the training parameters are chosen by using a Smolyak sparse grid method with a fixed approximation level L over a target parameterized space. For each selected parameter, the snapshot vectors are first produced by a high order DGTD method. In order to minimize the overall computational cost in the offline stage and to improve the accuracy of the Non-Intrusive MOR (NIMOR) method, a radial basis function (RBF) interpolation method is then used to construct more snapshot vectors at the sparse grid with approximation level L+1, which includes the sparse grids from approximation level L. Moreover, a Gaussian process regression (GPR) method is proposed to approximate the dominating time- and parameter-modes of the reduced coefficient matrices. During the online stage, the reduced-order solutions for new time and parameter values can be rapidly recovered via outputs from the regression models without using the DGTD method.

Finally, in [15], we study the simulation of the interaction of light with 3D metallic nanostructures using an adapted version of the method initially introduced in [11]-[13].

7.2.2 ROM using matrix decomposition and deep neural networks

Participants: Xiao-Feng He *(UESTC, Chengdu, China)*, Stéphane Lanteri, Kun Li *(SUFEC, Chengdu, China)*, Liang Li *(UESTC, Chengdu, China)*.

In [23], we propose a non-intrusive ROM method for solving parameterized electromagnetic scattering problems. A database collecting snapshots of high-fidelity solutions is built by solving the parameterized time-domain Maxwell equations for some values of the material parameters using a fullwave solver based on a high order discontinuous Galerkin time-domain (DGTD) method. To perform a prior dimensionality reduction, a set of reduced basis (RB) functions are extracted from the database via a two-step proper orthogonal decomposition (POD) method. Intrinsic coordinates of the high-fidelity solutions are further compressed through a convolutional autoencoder (CAE) network. Singular value decomposition (SVD) is then used to extract the principal components of the low dimensional coding matrices generated by CAE, and a cubic spline interpolation-based (CSI) approach is employed for approximating the dominating time- and parameter-modes of these matrices. The generation of the reduced basis and the training of the CAE and CSI are accomplished in the offline stage, thus the RB solution for given time/parameter values can be quickly recovered via outputs of the interpolation model and decoder network. In particular, the offline and online stages of the proposed RB method are completely decoupled, which ensures the validity of the method. The performance of the proposed CAE-CSI ROM is illustrated with numerical experiments for scattering of a plane wave by a 2-D dielectric disk and a multi-layer heterogeneous medium.

7.2.3 ROM via dynamic mode decomposition and radial basis functions

Participants: Stéphane Lanteri, Kun Li *(SUFEC, Chengdu, China)*, Liang Li *(UESTC, Chengdu, China)*, Yixin Li *(UESTC, Chengdu, China)*.

In [25], we study another variant of a non-intrusive model order reduction (NIMOR) method for surrogate modeling of time-domain electromagnetic wave propagation. The nested POD method, as a prior dimensionality reduction technique, is employed to extract the time- and parameter-independent reduced basis (RB) functions from a collection of high-fidelity solutions (or snapshots) on a properly chosen training parameter set. A dynamic mode decomposition (DMD) method, resulting in a further dimension reduction of the NIMOR method, is then used to predict the reduced-order coefficient vectors for future time instants on the previous training parameter set. The radial basis function (RBF) is employed for approximating the reduced-order coefficient vectors at a given untrained parameter in the future time instants, leading to the applicability of DMD method to parameterized problems. A main advantage of the proposed method is the use of a multi-step procedure consisting of the POD, DMD and RBF techniques to accurately and quickly recover field solutions from a few large-scale simulations. Numerical experiments for the scattering of a plane wave by a dielectric disk, by a multi-layer disk, and by a 3-D dielectric sphere nicely illustrate the performance of the NIMOR method.

7.2.4 Nonlinear ROM with Graph Convolutional Autoencoder

Participants: Carlotta Filippin, Stéphane Lanteri, Federico Pichi *(EPFL, Switzerland)*, Maria Strazzullo *(Politecnico di Torino, Italy)*.

Although this POD-CSI method introduced in [12] provides encouraging results, it is not as efficient and robust as one would expect from a ROM perspective. Indeed, the hyperbolic nature of the underlying PDE system, i.e., the system of time-domain Maxwell equations, is known to represent a challenging issue for linear reduction methods such as POD. In practice, a large number of modes is required therefore hampering the obtention of an efficient ROM strategy. One possible path to address this problem which is currently investigated by several groups worldwide relies on nonlinear reduction techniques. We initiated this year a study on nonlinear ROM for the time-domain Maxwell quations. More precisely, we study the approach recently proposed in [42], which proposes a nonlinear model order reduction based on a Graph Convolutional Autoencoder (GCA-ROM). This preliminary study aims at realizing a first adaptation and evaluation of the GCA-ROM in the modeling context of time-domain electromagnetics. This study is at the heart of the Master thesis of Carlotta Filippin, and it is conducted in collaboration with Federico Pichi (EPFL, Switzerland) and Maria Strazzullo (Politecnico di Torino, Italy).

7.3 Dealing with complex models

7.3.1 Toward thermoplasmonics

Participants: Yves D'Angelo, 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 (or parabolic) 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 in October 2020, 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). We first especially targeted the hyperbolic version of the model and proposed an implementation in 2D, based on a Discontinuous Galerkin approximation in space. We used specific strategies for time integration to account for the multiple time scales of the problem. This has been validated on academical test cases, but also on more concrete cases. For the latter, we began an interdisciplinary collaboration with Stefan Dilhaire (Professor, Laboratoire Ondes et matières d'Aquitaine, Bordeaux, France). A preprint with these first results is in preparation. Moreover, to make the picture complete and investigate the parabolic limit of the hyperbolic approximation, we also considered the numerical modeling of the parabolic version of the model in a similar discrete framework. This will in particular allow us to assess the potential of an hyperbolic approach. Finally a theoretical stability study is also in progress.

7.4 Deep Learning methods

We initiated in 2022 a prospective research direction on alternative numerical modeling methods based on Neural Networks (NN). We investigate both data-driven and model-driven approaches for dealing with the system of Maxwell equations possibly coupled with various material models of interest to nanophotonics. One first question that we want to address is wether DL methods can yield highly efficient surrogate models of 3D time-domain electromagnetic wave propagation problems. Beside, we are also interested in devising DL-based methods for dealing with problems which are more difficult to handle with traditional numerical methods such as electromagnetic wave interaction with space-time adaptive materials or nonlinear media.

7.4.1 Physics-Informed Neural Networks for Maxwell equations

Participants: Oussama Hajji, Stéphane Lanteri, Alexandre Pugin.

Numerical simulations of electromagnetic wave propagation problems primarily rely on discretization of the system of time-domain Maxwell equations using finite difference or finite element type methods. For complex and realistic three-dimensional situations, such a process can be computationally prohibitive, especially in view of many-query analyses (e.g., optimization design and uncertainty quantification). Therefore, developing cost-effective surrogate models is of great practical significance. Among the different possible approaches for building a surrogate model of a given PDE system in a non-intrusive way (i.e., with minimal modifications to an existing discretization-based simulation methodology), approaches based on neural networks and Deep Learning (DL) has recently shown new promises due to their capability of handling nonlinear or/and high dimensional problems. In the present study, we propose to focus on the particular case of Physics-Informed Neural Networks (PINNs) introduced in [67]. PINNs are neural networks trained to solve supervised learning tasks while respecting any given laws of physics described by a general (possibly nonlinear) PDE system. They seamlessly integrate the information from both the measurements and partial differential equations (PDEs) by embedding the PDEs into the loss function of a neural network using automatic differentiation. In 2022, we have initiated a study dedicated to the applicability of PINNs for building efficient surrogate models of the system Maxwell equations. We have continued this study this year in the context of the internships of Oussama Hajji (frequency-domain Maxwell equations) and Alexandre Pugin (time-domain Maxwell equations).

7.4.2 Interplay of Physics-Informed Neural Networks and multiscale numerical methods

Participants: Antonio Tadeu Gomes *(LNCC, Petropolis, Brazil)*, Stéphane Lanteri, Larissa Miguez Da Silva *(LNCC, Petropolis, Brazil)*, Frédéric Valentin *(LNCC, Petropolis, Brazil)*.

This study is concerned with multiscale modeling using the family of Multiscale Hybrid-Mixed (MHM) algorithms. and aims at improving the accuracy and computational efficiency of MHM methods for wave propagation PDE models. For that purpose, we adopted numerical analysis tools based on hybridization techniques as usual, and in a more innovative way investigating the interaction between multiscale methods and the new field of Scientific Artificial Intelligence (SciIA). Specifically, we investigate alternatives to the current computational cost of the MHM method, notably associated with the calculation of multiscale basis functions. In fact, it can become particularly prohibitive in time-dependent or nonlinear 3D problems. We foresee the strategies to resolve such a drawback by proposing a hybrid strategy to adapt the MHM methodology to incorporate scientific physics-driven machine learning techniques (PINNs-Physical-Informed Neural Network, for example). We believe that such a methodology will be at the forefront of the next wave of data-driven scientific discoveries in the physical and engineering sciences.

7.4.3 Back-propagation optimization and multi-valued artificial neural networks for highly vivid structural color filter metasurfaces

Participants: Hugo Enirique Hernández-Figueroa *(Laboratory of Applied and Computational Electromagnetism (LEMAC), University of Campinas, Sao Paulo, Brazil)*, , David Grosso *(CNRS-IM2NP, Université Aix Marseille, France)*, Badre Kerzabi *(Solnil, Marseille, France)*, Marco Abbarchi *()*, Arthur Clini de Souza, Mahmoud Elsawy, Stéphane Lanteri.

In this work, we introduce a novel technique for designing color filter metasurfaces using a data-driven approach based on deep learning. Our innovative approach employs inverse design principles to identify highly efficient designs that outperform all the configurations in the dataset in terms of color filtering properties, which consists of 585 distinct geometries solely. By combining Multi-Valued Artificial Neural Networks and back-propagation optimization, we overcome the limitations of previous approaches, such as poor performance due to extrapolation and undesired local minima. The numerical tool developed in this study enables the cost-effective fabrication of structural color filters by exploring a wide range of narrow line shapes that exhibit high-quality resonances, aligning with desired spectral reflection responses. Notably, our methodology expands the color gamut beyond the conventional RGB colors, offering unprecedented versatility in color generation (see Fig. 1). Furthermore, our Deep Learning approach successfully respects fabrication constraints, ensuring practical feasibility. The achievements of our research significantly contribute to the field of optical device design. By pushing the boundaries of metasurface optimization, we open up new possibilities for the development of advanced optical devices. The proposed methodology holds promise for various applications, such as display technologies, data encoding, and artistic expression. These notable advancements not only enhance the understanding of metasurface design principles but also provide valuable insights for future research endeavors. The paper has been published recently in Scientific Reports journal [21]

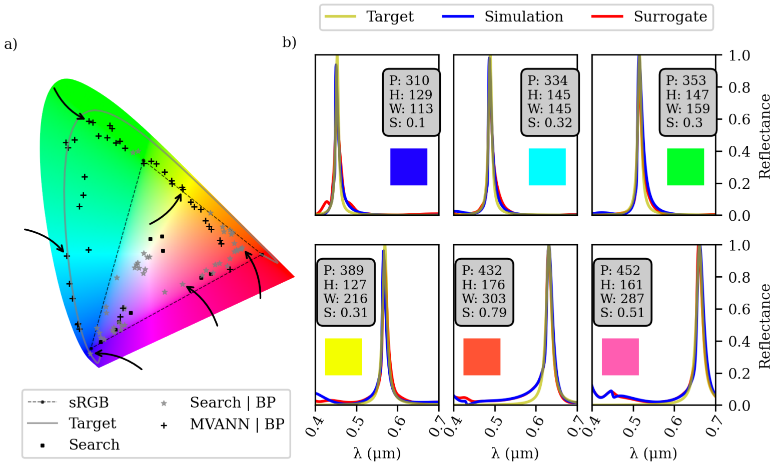

Figure 1: (a) Chromaticity diagram depicting the outcomes of the 100 optimization results. The arrows in the diagram indicate the corresponding designs showcased in (b). The gray line represents the calculated perceived color corresponding to the target spectrum. (b) Detailed examination of 6 different optimizations, displaying their dimensions (in nm) of each geometrical parameter and the corresponding sRGB color representation of the simulated spectrum.

7.5 Discovering novel nanoscale structures

At the creation of the team in February 2020, our collaborations with physicists from the nanophotonics domain aimed at leveraging our developed numerical modeling methodologies in order to study specific topics in relation with concrete applications (see Section 7.7 for more details). An evolution that started in 2022 was our will to adapt and exploit these numerical methodologies to discover nanostructure organizations exhibiting behaviors and performances opening the road to new application perspectives.

7.5.1 Universal active metasurfaces for ultimate wavefront molding by manipulating the reflection singularities

Participants: Patrice Genevet *(CRHEA laboratory, Sophia Antipolis)*, Rémi Colom *(CRHEA laboratory, Sophia Antipolis)*, Christina Kyrou *(CRHEA laboratory, Sophia Antipolis)*, Elena Mikheeva *(CRHEA laboratory, Sophia Antipolis)*, Jean-Yves Duboz *(CRHEA laboratory, Sophia Antipolis)*, Mahmoud Elsawy, Stéphane Lanteri.

Optical metasurfaces have become increasingly prevalent as key components for manipulating light properties. Nevertheless, the majority of these devices remain passive and lack the capability to adapt to changing environmental conditions. Here, we propose an innovative design approach using asymmetric Gires–Tournois resonators to achieve comprehensive phase modulation of light with near-unity efficiency. The active metasurface resonators filled with either silicon or hetero-structured materials. These choices allow for the utilization of thermo-optical or electro-optical effects, respectively. Remarkably, in both cases, complete phase modulation, combined with a 100% reflection amplitude, is observed, even when dealing with exceedingly low refractive index changes on the order of 0.01. To account for the strong nonlocal effect and enhance deflection efficiencies for each deflection angle, a sophisticated statistical learning optimization methodology is employed to optimize the refractive index modulation profile within the extended unit cell. As a result, active beam steering designs, leveraging the active thermo-optical effect, have been optimized to achieve exceptional performance exceeding 90% (see Fig. 2). Additionally, optimization efforts have been directed towards active wavefront splitting using electro-optic materials, leading to ultimate modulation performance levels with nearly 92% efficiency. The realization of highly efficient active beam shaping at high frequencies holds the potential for significant applications in areas such as imaging microscopy and three-dimensional light detection and ranging (LiDAR). The paper is published in Laser and Photonics Review [22].

7.5.2 Advancing wavefront shaping with resonant nonlocal metasurfaces: beyond the limitations of lookup tables

Participants: Sébastien Héron *(Thales Research & Technology, Palaiseau, France)*, Enzo Isnard, Mahmoud Elsawy, Stéphane Lanteri.

Resonant metasurfaces are of paramount importance in addressing the growing demand for reduced thickness and complexity, while ensuring high optical efficiency. This becomes particularly crucial in overcoming fabrication challenges associated with high aspect ratio structures, thereby enabling seamless integration of metasurfaces with electronic components at an advanced level. However, traditional design approaches relying on lookup tables and local field approximations often fail to achieve optimal performance, especially for nonlocal resonant metasurfaces. In this study, we investigate the use of statistical learning optimization techniques for nonlocal resonant metasurfaces, with a specific emphasis on the role of near-field coupling in wavefront shaping beyond single unit cell simulations. Indeed, state-of-the art optimization algorithms as evolutionary algorithm and local gradient can be utilized, but to the extent of requiring prohibitive number of simulations, getting stuck in a local design or requiring a careful starting point. Three different resonant metasurfaces were considered in this study (see Fig. 3). The first one operates in transmission and utilizes the properties of resonant Huygens metasurfaces. Numerical results indicate that a beam steering metasurface achieved an efficiency of 80%, surpassing the classical design with only 23% efficiency. Additionally, an extended depth-of-focus (EDOF) metalens was optimized, resulting in a five-fold increase in focal depth and a four-fold enhancement in focusing power compared to classical designs. Furthermore, the performance of wavelength-selected metagratings in reflection was investigated based on asymmetric cavity considerations. Notably, non-intuitive designs were obtained, surpassing 85% efficiency, which far exceeds the efficiency achieved with classical gradient phase distribution. The presence of nonlocal effects arising from the interaction between neighboring unit cells significantly alters the behavior of the fields. A comprehensive understanding of this phenomenon is crucial for designing high-performance resonant metasurfaces. This knowledge empowers researchers and engineers to create metasurfaces with enhanced performance, opening avenues for novel

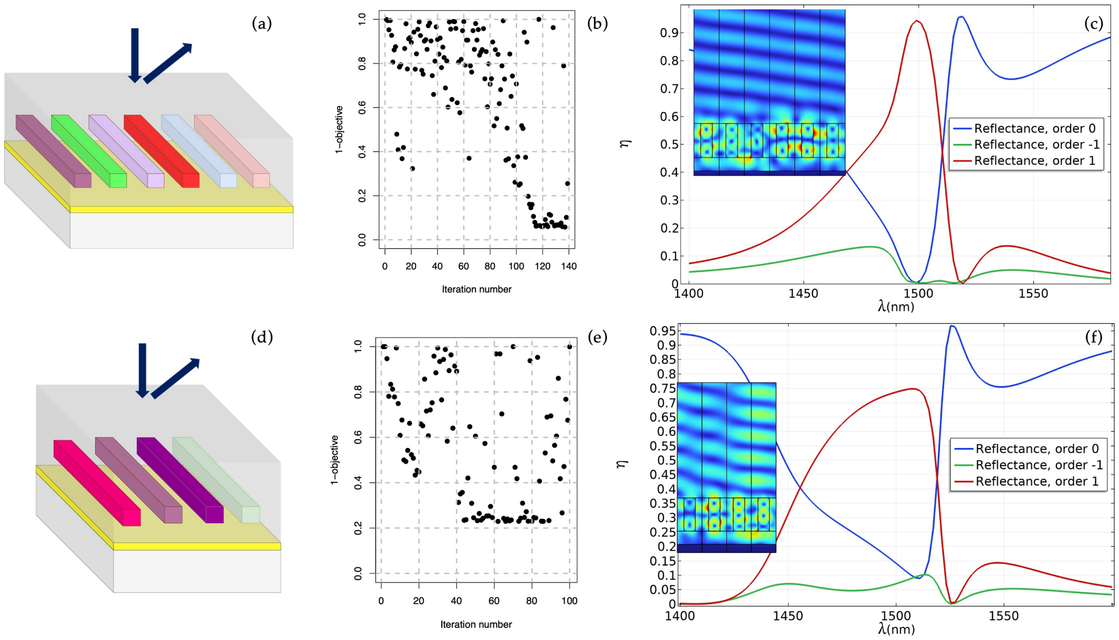

Figure 2: Active beam steering using an array of active G-T Si nanoresonators. Periodic electrical activation of six (a) and four (d) unit cells with pixel-by-pixel refractive index modulation. The optimization results for each case are depicted in (b) and (e), respectively. The beam steering responses after the optimized refractive index distribution in the sequential pixels are shown in panels (c) and (f) for six- and four- pixels configuration, respectively, with the corresponding field map at the design wavelength $\lambda = 1500$ nm. The optimization parameters represent the refractive index distribution in each pixel represented by different colors in (a) and (d).

applications in various domains. This work has been accepted for publication in Scientific Reports early 2024.

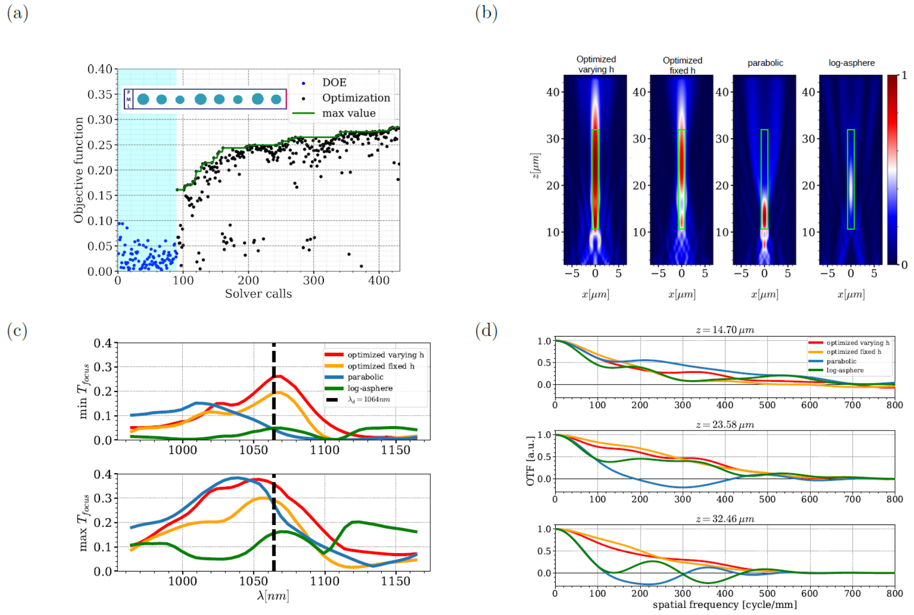

Figure 3: Optimization results for the EDOF nonlocal metalens. (a) Objective function values as a function of the number of simulations. The insight represents the geometry of half of the metalens in the x direction. (b) Field maps of $\|\mathbf{E}\|^2$ at 1064 nm of the optimized design with fixed and varying h, the parabolic designs and of the log-asphere design. The green rectangle represents the region in which we try to increase the DOF (c) Plot of the minimum and maximum focus efficiency over 20 equally spaced rectangles in the target region. The focus efficiency is defined as the part the incident power that is transmitted in a focus plane. The focus efficiency for the optimized design with a varying h varies from 26% to 35% while for the parabolic designs it varies between 0.05% and 27%. (d) Optical Transfer Functions (OTFs) of each designs at f, $f + 2.5$ DOF and $f + 5$ DOF. Optimized designs preserve spatial frequencies up to 600 cycle/mm at the three locations whereas the classical ones both fail at $f + 5$ DOF.

7.6 Software developments in DIOGENeS

Participants: Alexis Gobé, Guillaume Leroy, Stéphane Lanteri.

In order to maximize the impact of our research activities described in section 3, a modern software platform is necessary. For that purpose, the team develops the DIOGENeS (DIscOntinuous GalErkin Nanoscale Solvers) software suite, which is dedicated to the numerical modeling of nanoscale wave-matter interactions in the 3D case. The initial (and current) version of this software concentrates on light-matter interactions with nanometer scale structures, for applications to nanophotonics and nanoplasmonics. DIOGENeS is a unique numerical framework leveraging the capabilities of discontinuous Galerkin methods for the simulation of multiscale problems relevant to nanophotonics and nanoplasmonics. DIOGENeS is a major asset in our strategy to demonstrate that the methodological contributions that we produce can be successfully applied to problems addressed by physicists and engineers trying to exploit specific features of nanoscale wave-matter interactions for scientific and technological applications.

This suite is organized around the following components:

- A core library containing all the basic building blocks for the construction of high order discontinuous Galerkin methods formulated on tetrahedral, orthogonal hexahedral and hybrid tetrahedral-hexahedral meshes;

- Fullwave solvers implementing high order discontinuous Galerkin methods for the discretization of time domain (DGTD - Discontinuous Galerkin Time-Domain) and in frequency domain (HDGFD - Hybridized Discontinuous Galerkin Frequency-Domain) coupled to a generalized model of physical dispersion in metallic or semiconductor materials;
- A library of geometric modeling modules for the definition of simulation configurations involving nanostructures or nanostructured materials. This library exploits the Python API of the GMSH solver;
- A bridge component between fullwave solvers, geometric modeling modules and numerical optimization algorithms for the inverse design of nanostructures. This component integrates shape parameterization modules, but also scripts defining optimization workflows driving the use of statistical learning-based global optimization algorithms from the Triese toolbox, which is built on TensorFlow and is dedicated to Bayesian optimization;
- A library of core modules for allowing users to define their own physical observables, e.g., total transmittance, volumic absorptance, scattering parameters, etc., from results of fullwave simulations.

The core library and the fullwave solvers are based on an object-oriented architecture implemented in Fortran 2008. The DGTD and HDGFD solvers are adapted to high performance computing platforms. Two levels of parallelization are currently exploited: a coarse-grained parallelization in distributed memory (between SMP computation nodes) combining a partitioning of the computation mesh and a parallel programming based on the message exchange model using the MPI standard.

This year several novel features have been developed that are concerned with the GFactory and Observer components (see Fig. 4).

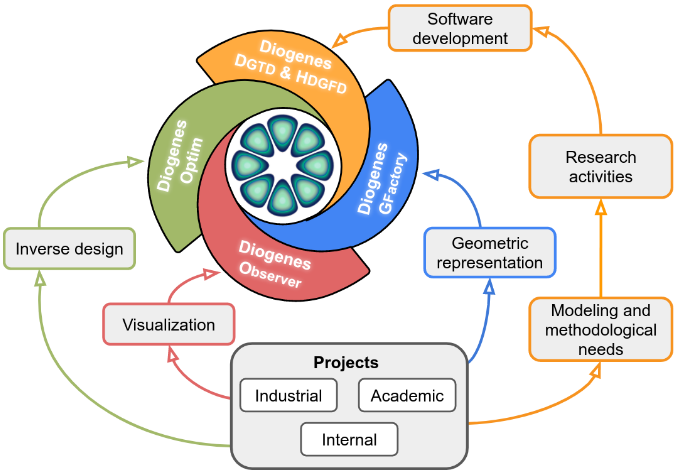

Figure 4: Architecture of the DIOGENeS software suite. DGTD and HDGFD are the high order DG-based fullwave solvers for time-domain and frequency-domain modeling settings. GFactory is the geometrical modeling component that exploits the Python API of the GMSH mesh generation tool. Observer is the base component for developing post-processing scripts of simulation results. Optim is the base component for developing inverse design workflows in Python by using statistical learning global optimization algorithms from external frameworks such as Trieste.

7.7 Applications

7.7.1 Advanced modeling of nanostructured CMOS imagers based on DG methods

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

The exploitation of nanostructuring to improve the performance of CMOS imagers based on microlens grids is a very promising avenue. In this perspective, numerical modeling is a key component to accurately characterize the absorption properties of these complex imaging structures, which are intrinsically multiscale (from the micrometer scale of the lenses to the nanometric characteristics of the nanostructured material layers). The FDTD (Finite Difference Time-Domain) method is the solution adopted in the first instance for the simulation of the interaction of light with this type of structure. However, because FDTD is based on a Cartesian mesh, this method shows limitations when it comes to accurately account for complex geometric features such as the curvature of microlenses or the texturing of material layer surfaces. In this context of the PhD of Jérémy Grebot, our main objectives are (1) to leverage locally refined meshes with a high order DGTD method for modeling the propagation of light in a nanostructured CMOS imager and, (2) to study and optimize the impact of nanostructuring for improving light absorption. In particular, for what concern the second objective, an inverse design methodology combining a high order DGTD method with a statistical learning-based global optimization algorithm is developed for studying various nanostructuring patterns of the surface of the absorbing semiconductor material such as one- and two-dimensional gratings.

7.7.2 Nanoimprint color filter metasurface for imaging devices

Participants: David Grosso *(Institut Matériaux Microélectronique Nanosciences de Provence (IM2NP) Aix-Marseille Université and Solnil)*, Marco Abbarchi *(Institut Matériaux Microélectronique Nanosciences de Provence (IM2NP) Aix-Marseille Université and Solnil)*, Badre Kerzabi *(Solnil)*, Mahmoud Elsawy, Alexis Gobé, Stéphane Lanteri.

Due to the rapid growth of metasurface applications, several manufacturing techniques have been developed in the past few years. Among them, NanoImprint Lithography (NIL) has been considered as a promising fabrication possibility for metasurface. NIL can achieve features below 100 nm without the need for complex and expensive optics and light sources needed to achieve similar resolutions in advanced photolithography. Yet, despite the advantages of this fabrication procedure, it has some limitations related to the dimensions of the single nanoresonators. In other words, the fabrication constraints related to the aspect ratio (ratio between height and width) is important. Typically, a maximum aspect ratio of 2 can be considered in such a technique. In this work, together with our collaborators from IM2NP, Aix-Marseille Université and the Solnil startup who are specialists in nanoimprint technology, we aim at optimizing a low cost color filtering metasurface for imaging applications taking into account all the fabrication constraints. The main goal of this study is to deploy our optimization methodology to maximize the efficiency of such metasurface configuration. Various shapes with different physical mechanisms have been investigated. It is worth mentioning that in this study various shapes have been optimized and studied numerically, yet, as a starting point for the fabrication, the cylindrical pillars will be considered as a first illustration for the nanoimprint fabrication.

7.7.3 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 spectrum as illustrated in Fig. 5. 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).

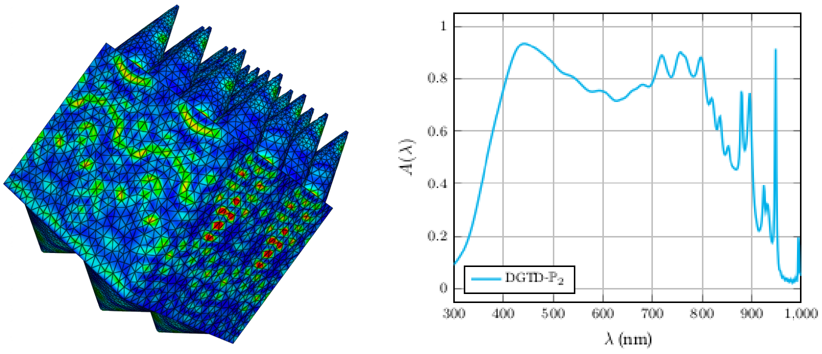

Figure 5: Optimization of light absorption in a solar cell based on a nanocone grating.

7.7.4 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 (see Fig. 6). This study is conducted in collaboration with Antoine Moreau at Institut Pascal (CNRS). Starting in January 2024, we will continue this study in the context of the ANR SWAG-P, which is coordinated by Antoine Moreau.

7.7.5 Multiple scattering in random media

Participants: Stéphane Descombes, Stéphane Lanteri, Guillaume Leroy, Cédric Legrand, 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

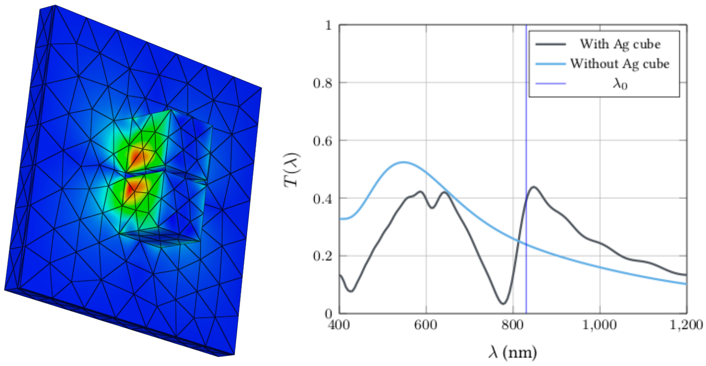

Figure 6: Optimization of a plasmonic nanocube dimer setting for the generation of Fano resonances.

from strengthening the signal, since electronic post-amplification raises the noise floor as well. Molecule-specific biochemical processes are being developed for this purpose, and 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 an 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 (see Fig. 7). 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.

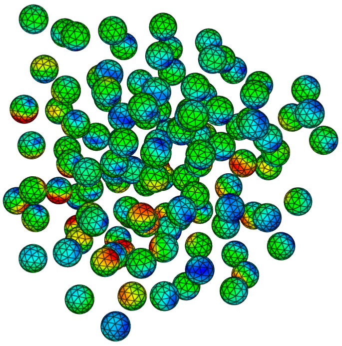

Figure 7: Multiple scattering by randomly distributed nanospheres in a bulk medium.

7.7.6 Nonlinear wavefront shaping with optical metasurfaces

Participants: Giuseppe Leo *(CNRS-MPQ, Université Paris Cité, France)*, Jean-Michel Gerard *(PHELIQS, CEA and Université Grenoble Alpes, France)*, Mahmoud Elsawy, Stéphane Lanteri.

In recent years, the control of sub-wavelength light-matter interactions has enabled the observation of new linear optical phenomena, further establishing a new class of ultra-thin devices for real-world applications. To extend metasurface functionality and implement nonlinear manipulations, the scientific community has considered optical metasurfaces for harmonic emission field control. However, the performance of nonlinear metasurfaces is still modest. Flat optics have also shown their potential in the nonlinear optics with wavefront shaping in far-harmonic fields. There is currently a related effort by the nonlinear nanophotonics community to seek higher conversion efficiencies across narrow resonances of the quasi-bound states of the continuum (qBIC) associated with strong near-field coupling and nonlocal resonance modes. However, the overall performance is relatively weak as most of the current studies ignore the strong near-field coupling between neighboring cells. In this collaboration, we exploit the specific advantages of 'thin' resonators that behave like phased-array antennas, unlike photonic crystals with strong localized energies, to develop highly efficient nonlinear metasurfaces for nonlinear wavefront shaping. Within this strategy, we improve the performance of nonlinear wavefront shaping by inverse design optimization of both meta-atoms and meta-molecules. In addition, we consider long-term design options for nonlinear metasurfaces based on perfect nonlocal responses and long-range near-field coupling, and rigorous computational methods to address nonlinearities in terms of nonlocal configurations. Our preliminary results (see Fig. 8)show the ability to improve the second harmonic generation signal by almost a factor of seven. Fabrication and characterization of the structure is currently underway, and the results will be published in a prominent journal.

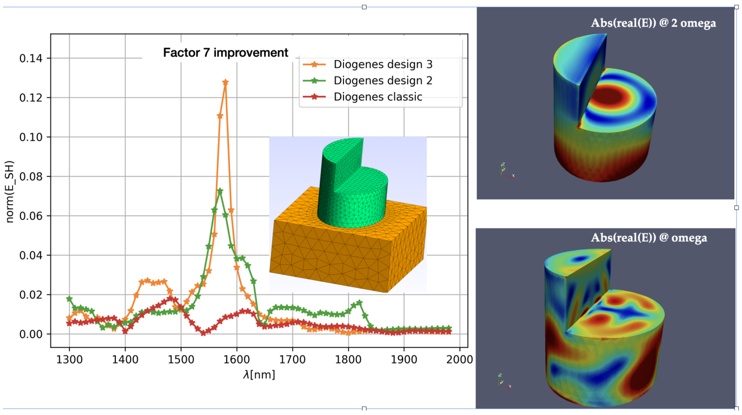

Figure 8: Optimized second-harmonic generation (SHG) from an asymmetric nanochair (inset). The left column represent the comparison of SHG response as a function of the pump wavelength for three different designs (classical denote the design without optimization). The right column refers to the field profiles at the two frequencies 2ω and ω for the optimal design.

7.7.7 Biosensor metasurface

Participants: Haogang Cai *(Department of Biomedical Engineering, New York University, USA)*, Mahmoud Elsawy, Stéphane Lanteri.

Over the last decades, the domain of nanophotonic biosensors has witnessed an expansion from extensively investigated plasmonic platforms to dielectric metasurfaces. In contrast to plasmonic resonance, dielectric metasurfaces operate on the basis of Mie resonances, yielding sensitivity comparable to plasmonic counterparts while exhibiting superior resonance bandwidth, Q factor among others figures of merit. While the plasmonic photothermal effect has proven advantageous in various biomedical applications, it presents an inherent constraint in biosensing. Dielectric metasurfaces address issues associated with ohmic loss and heating, thereby enhancing repeatability, stability, and biocompatibility. However the overall performance is less than the plasmoic counterparts. In this collaboration, we exploit innovative metasurface configurations characterized by high-Q resonances, providing insight into a range of physical phenomena customized through the geometric designs of meta-atoms. Specifically, we engineer a single-unit cell based on trimmer silicon meta-atoms, capitalizing on robust near-field coupling by introducing symmetry breaking to the unit cell. This novel design facilitates the creation of a highly efficient biosensor dielectric metasurface that surpasses the performance of conventional configurations. The structure has been successfully fabricated and is presently undergoing characterization.

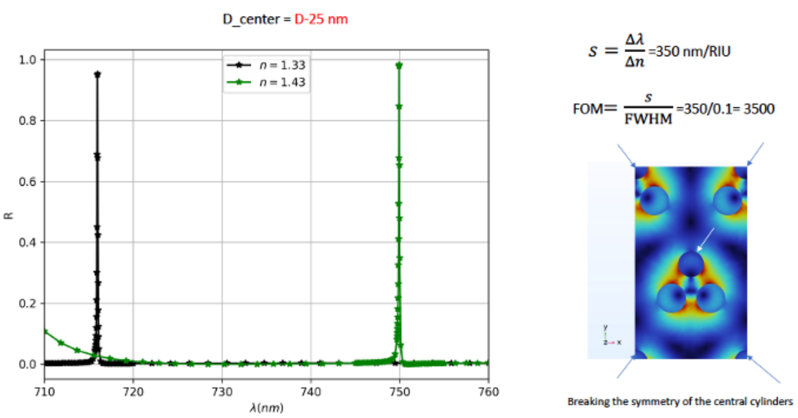

Figure 9: Optimized biosensor metasurface based on trimmer silicon meta-atoms.

8 Bilateral contracts and grants with industry

8.1 Bilateral contracts with industry

Nom: Simulation of photonic pigments

Participants: Alexis Gobé, Stéphane Lanteri.

- Duration: Jun 2023 - Dec 2023
- Local coordinator: Stéphane Lanteri
- Participants: Valérie Alard [LVMH], Nicolas Benoot [LVMH]
- To manufacture a colored material, one normally use a dye or pigment. But another approach to producing color is to fabricate a nanostructure that reflects or scatters light so that waves of certain frequencies can interfere constructively. These nanostructured materials are said to have structural colors. Unlike traditional traditional colors, which comes from light-absorbing dyes or pigments that absorb light, structural colors can be made resistant to fading. In this context, it is desirable to obtain a structural color that is independent of angle, i.e., the color is the same regardless of the orientation of the material, and whatever the angle between the light source and the eyes. There are many structurally colored materials that, like an opal stone, are iridescent, which means that the color changes depending on viewing angle and orientation. The reason for this is that the nanostructure of these materials is well-ordered (or crystalline), as in photonic crystals. To manufacture materials whose color is independent of angle, we need to create disordered nanostructures. These materials are called photonic glasses. The aim is to study how the optical properties of these glasses are linked to their structure and the particles. This type of study is primarily based on experiment. In this project, we relied on numerical modeling to study the optical properties of photonic pigments.

Nom: SEASIDE - numerical Study of mEtasurfAceS by Inverse DEsign

Participants: Mahmoud Elsawy, Alexis Gobé, Guillaume Leroy, Stéphane Lanteri.

- Duration: Sep 2022 - Aug 2023
- Local coordinator: Stéphane Lanteri
- Participants: Abbarchi, David Grosso and Badre Kerzabi [Solnil, Marseille]
- Solnil is a startup company launched in 2020. Its activities are concerned with the design, development, operation and provision of products, hardware, software services, automatons or complex machines, implementing innovative technologies resulting from research on processes for the nano-fabrication of sol-gel materials and in particular, the direct nano-printing of such materials for various applications in the fields of optics and optoelectronics. Solnil carries out research and development operations, as well as scientific and technical studies. The company's ambition is to exploit and industrialize a low-cost nano-fabrication process for optical applications. This process is an evolution of an existing technology, referred as nanoimprinting, which can be described as a molding process at sub-micrometer resolutions. The industrial applications of nanoimprinting are numerous today numerous: 3D measurements for recognition, DNA sequencing augmented reality glasses, anti-reflection films, LED sources etc. In the present project, which is a first step toward a longer term partnership, we resort to numerical modeling for the optimal design of metasurface-based multispectral sensors.

Nom: DGTD solvers for semiconductor device modeling

Participants: Stéphane Lanteri, Massimiliano Montone, Claire Scheid.

- 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.

8.2 Grants with industry

Nom: DGTD solvers for modeling light absorption in CMOS imagers

Participants: Alexis Gobé, Jérémy Grebot, Guillaume Leroy, Stéphane Lanteri.

- Duration: Jan 2019-Jun 2023
- Local coordinator: Stéphane Lanteri

- Participants: 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.

9 Partnerships and cooperations

9.1 International initiatives

9.1.1 STIC/MATH/CLIMAT AmSud projects

- Claire Scheid is member of the MatAmSud (between Chile, Uruguay, Argentina and France) project entitled NoLoCE (Nonlocal and Local Coupled Equations: Analysis, Computation, and Probability), PI: Juan Pablo Borthagaray (Associate Professor at the Instituto de Matemática y Estadística, Facultad de Ingeniería, Universidad de la República, Uruguay).

9.2 International research visitors

9.2.1 Visits of international scientists

Inria International Chair

- Frédéric Valentin from LNCC, Petropolis, Brasil, is holding an Inria International Chair from January 2018 until May 2023. He has visited the team between January and February 2023.

Other international visits to the team

- Haogang Cai from the Health Technology and Engineering Institute (Tech4Health) at New York University Grossman School of Medicine, USA, has visited the team on July 24-25 2023.

- Hugo Hernandez Figueroa who is the head of the Laboratory of Applied and Computational Electromagnetism (LEMAC) at Universidade Estadual de Campinas, Brasil, has visited the team on November 2nd-3rd 2023.

9.3 European initiatives

9.3.1 H2020 projects

RISC2 (A network for supporting the coordination of High-Performance Computing research between Europe and Latin America)

Participants: Luc Giraud *(HIEPACS project-team, Inria Bordeaux - Sud-Ouest)*, Stéphane Lanteri, Patrick Valduriez *(ZENITH project-team)*.

- Type: H2020 (Coordinated Support Action)
- Link.
- Duration: Jan 2021 - Jun 2023
- Coordinator: Barcelona Supercomputing Center
- Partners:
    - Forschungzentrum Julich GMBH (Germany)
    - Inria (France)
    - Bull SAS (France)
    - INESC TEC (Portugal)
    - Universidade de Coimbra (Portugal)
    - CIEMAT (Spain)
    - CINECA (Italy)
    - Universidad de Buenos Aires (Argentina)
    - Universidad Industrial de Santander (Columbia)
    - Universidad de le Republica (Uruguay)
    - Laboratorio Nacional de Computacao Cientifica (Brazil)
    - Centro de Investigacion y de Estudios Avanzados del Instituto Politecnico Nacional (Mexico)
    - Universidad de Chile (Chile)
    - Fundacao Coordenacao de Projetos Pesquisas e Estudos Tecnologicos COPPETEC (Brazil)
    - Fundacion Centro de Alta Tecnologia (Costa Rica)
- Inria contact: Stéphane Lanteri
- Recent advances in AI and the Internet of things allow high performance computing (HPC) to surpass its limited use in science and defence and extend its benefits to industry, healthcare and the economy. Since all regions intensely invest in HPC, coordination and capacity sharing are needed. The EU-funded RISC2 project connects eight important European HPC actors with the main HPC actors from Argentina, Brazil, Chile, Colombia, Costa Rica, Mexico and Uruguay to enhance cooperation between their research and industrial communities on HPC application and infrastructure development. The project will deliver a cooperation roadmap addressing policymakers and the scientific and industrial communities to identify central application areas, HPC infrastructure and policy needs.

9.4 National initiatives

9.4.1 ANR project

SWEET (Sub-WavelEngth Electro-optic sysTems)

Participants: Henri Camon *(CNRS-LAAS)*, Jean-Yves Duboz *(CNRS-CRHEA)*, Mahmoud Elsawy, Olivier Gauthier-Lafaye *(CNRS-LAAS)*, Samira Khadir *(CNRS-CRHEA)*, Stéphane Lanteri, Daniel Turover *(NAPA Technologies)*.

- Type: ANR
- Duration: Jan 2023 to Dec 2026
- Coordinator: CNRS-LAAS (Toulouse)
- Partner: Inria (ATLANTIS project-team), CNRS-CRHEA (Sophia Atipolis), NAPA Technologies (Archamps)
- Inria contact: Stéphane Lanteri
- Beam steering is a key enabling photonic technology that would improve the performance of light detection and ranging modules (LiDAR). A typical LiDAR component consists of a light source for illumination, a light modulating device to scan the scene and finally a fast detection system to recover the optical information received from the scene. The operation principle of conventional LiDARs relies on the Time-of-Flight (ToF) measurement, where a pulsed laser directed toward a distant reflective object measures the propagation round-trip time (ToF) of light pulses propagating from the laser to the scene and back to the detection module. The LiDAR sector is currently ongoing important research and development efforts to enable real-time sensing of the distance of fast-moving objects, with applications in robotics, autonomous vehicles and future augmented reality devices. Dynamic beam steering with competitive performances requires the deflection of a light beam along any arbitrary direction to spatially scan a large angular field-of-view (FoV) with high speed and high efficiency. SWEET addresses several drawbacks of current LiDAR technologies by proposing innovative ultrafast beam steering systems, their combinations and integration into demonstrator. We propose to realize an ultrafast 2D beam steering system using innovative transparent tunable MS using LC and III-nitride materials. Our motivation is to develop a generic technology to meet the market needs of LiDAR applications in terms of operation speed, FoV, angular resolution, manufacturability. As indicators, we consider the most stringent requirements for LiDAR integration in the automotive industry. In this context, the general objective of our contribution to the SWEET project is to design active metasurface components for synamic beam steering.

9.4.2 DGA/AID RAPID project

AEROCOM (Ultra-flat and low-cost antennas)

Participants: Ayoub Bellouch, Guillaume Bouchet, Guillaume de Calan *(NANOE)*, Mahmoud Elsawy, Van Hoang *(Thales Research & Technology)*, Guillaume Leroy, Stéphane Lanteri, Julien Sourice *(NANOE)*, Erika Vandelle *(Thales Research & Technology)*.

- Type: RAPID
- Duration: Jan 2023 to Dec 2024
- Coordinator: NANOE (Palaiseau)
- Partner: Inria (ATLANTIS project-team), Thales Research & Technology (Palaiseau)
- Inria contact: Stéphane Lanteri
- The development of agile, ultra-flat and low-cost Ka-band antennas is a major challenge to enable Internet accessibility in mobility, in particular on board of public land and air transport (trains, buses, airliners), and to secure communication servers (for combat aircraft, military vehicles, etc.). A possible antenna architecture to address this challenge is composed of a radiating source and a deflection system consisting of two deflectors. The compactness and the moderate cost of the de-pointing system could be obtained thanks to the sub-wavelength structuring technique, and to the shaping by additive manufacturing. Indeed, the sub-wavelength patterning technique has

recently shown the possibility to realize antenna components much thinner than a homogeneous bulk material, with equivalent or even better radio frequency performance. In this context, the general objective of our contribution to the AEROCOM project is to develop an advanced numerical methodology for the virtual design of subwavelength structured deflectors and their cascading to achieve an ultra-flat Ka-band antenna system consisting of two such metadeflectors.

10 Dissemination

Participants: Stéphane Descombes, Mahmoud Elsawy, Stéphane Lanteri, Claire Scheid.

10.1 Promoting scientific activities

10.1.1 Scientific events: organisation

General chair, scientific chair

- Stéphane Lanteri was a member of the Scientific Committee of the 3rd Inria-DFKI European Summer School on AI (IDESSAI 2023), Sophia Antipolis, Setember 4-8, 2023.

Member of the organizing committees

- Stéphane Descombes was a member of the steering committee of the 6th edition of the SophI.A Summit, 22-24 November, Sophia Antipolis.
- Claire Scheid and Stéphane Lanteri have co-organized a minisymposium on "Advances in numerical methods for nonlinear optics", at the ICIAM 2023 conference, Tokyo, Japan, August 20-25, 2023, with Camille Carvalho (Université de Lyon, INSA Lyon, UJM, UCBL, ECL, CNRS) and Vrushali A. Bokil (Department of Mathematics, College of Science, Oregon State University, USA).

10.1.2 Scientific expertise

- Claire Scheid was a member of the Maître de Conférence selection committee for Centrale Méditerranée (spring 2023).
- Since July 2023, Claire Scheid is a member of the Scientific Committee of the "Maison de la simulation et des interactions" of Université Côte d'Azur (https ://msi.univ-cotedazur.fr/).

10.1.3 Research administration

- Stéphane Lanteri: member of the Project-team Committee's Bureau of the Inria research center at Université Côte d'Azur
- Stéphane Lanteri: Deputy Head of Science of Inria Research Center at Université Côte d'Azur (since September 2022)
- Stéphane Lanteri: member of Evaluation Committee of Inria (since September 2022)
- Stéphane Lanteri: member of the "Comité de Chercheurs Calculant au CINES"

10.2 Teaching - Supervision - Juries

10.2.1 Teaching

- Claire Scheid, *EDP et Différences finies, Practical works*, Master 1 MPA, 18h, Université Côte d'Azur

- Claire Scheid, *Optimisation et éléments finis. Lecture, practical works*, M1 MPA and IM, 72h eq.TD, Université Côte d'Azur
- Claire Scheid, *Option modélisation. Lectures and practical works*, M2 Agrégation, 45h eq.TD, Université Côte d'Azur
- Claire Scheid, *Approximation Numérique des fonctions, intégrales et équations différentielles. Lecture*, L3, 56h, 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, *Mathematics practical works*, L1 Eco, 40 h, Université Côte d'Azur,
- Engineering: Stéphane Descombes, *Scientific Machine Learning*, 12 h, MAM5, Polytech Nice Sophia - Université Côte d'Azur,
- Stéphane Descombes, *Approximation Numérique des fonctions, intégrales et équations différentielles, practical works*, L3, 28h, Université Côte d'Azur,
- Engineering: Stéphane Lanteri, *High performance scientific computing*, 24 h, MAM5, Polytech Nice Sophia - Université Côte d'Azur

10.2.2 Supervision

- PhD defended: Théophile Chaumont-Frelet and Stéphane Lanteri have co-supervised the PhD of Zakaria Kassali, Multiscale finite element simulations applied to the design of photovoltaic cells, defended in January 2023
- PhD defended: Stéphane Lanteri and Claire Scheid have co-supervised the PhD of Massimiliano Montone, High order finite element type solvers for the coupled Maxwell-semiconductor equations in the time-domain, defended in March 2023
- PhD in progress: Arthur Clini De Souza, Deep neural networks for the design of large-scale photonic devices for active beam steering, Mahmoud Elsawy and Stéphane Lanteri
- PhD in progress: Jérémy Grebot, Advanced modeling of nanostructured CMOS imagers, Stéphane Lanteri and Claire Scheid
- PhD in progress: Enzo Isnard, Modeling and optimization of freeform optical metasurfaces integrated to an imaging system, Mahmoud Elsawy and Stéphane Lanteri
- PhD in progress: Thibault Laufroy, High order finite element type solvers for thermoplamonics, Yves d'Angelo and Claire Scheid
- PhD in progress: Cédric Legrand, High order finite element type solvers for modeling gain media, Stéphane Descombes and Stéphane Lanteri
- PhD in progress: Martin Leppers, Microlenses based on metasurfaces for image sensor pixels, Patrice Genevet (CRHEA, Sophia Antipolis) and Stéphane Lanteri
- PhD in progress: Florentin Proust, Novel finite element methods for dealing with high frequency wave propagation problems, Maxime Ingremeau (Université Côte d'Azur, LJAD) and Théophile Chaumont-Frelet

10.2.3 Juries

- Claire Scheid was a reviewer of the PhD and a member of the PhD committee of Maria Cabrera Calvo, Sorbonne University, France, March 20, 2023
- Stéphane Lanteri was a reviewer of the PhD and a member of the PhD committee of Jayeeta Amboli, Université d'Aix-Marseille, Institut Fresnel, France, December 18, 2023
- Stéphane Lanteri was a member of the PhD committee of Victoriya Kashtanova, Université Côte d'Azur, Inria, Sophia Antipolis, June 14, 2023

11 Scientific production

11.1 Major publications

[1] E. Agullo, L. Giraud, A. Gobé, M. Kuhn, S. Lanteri and L. Moya. 'High order HDG method and domain decomposition solvers for frequency-domain electromagnetics'. In: *International Journal of Numerical Modelling: Electronic Networks, Devices and Fields* (17th Oct. 2019). DOI: `10.1002/jnm.2678`. URL: `https://hal.inria.fr/hal-02327982`.

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