Internship proposition - Year 2018

Optimal design of nanostructured devices driven by specific resonant and scattering properties

Inria Sophia Antipolis - Méditerranée research center
ACUMES project-team, NACHOS project-team
2004 Route des Lucioles, BP 92, 06902 Sophia Antipolis Cedex, France

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Supervisors: Regis Duvigneau (ACUMES project-team) and Stéphane Lanteri (NACHOS project-team)
Contact: Regis.Duvigneau@inria.fr/Stephane.Lanteri@inria.fr
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1 Scientific context

1.1 Nanoscale light-matter interactions

Nanostructuring of materials has opened up a number of new possibilities for manipulating and enhancing light-matter interactions, thereby improving fundamental device properties. Low-dimensional semiconductors, like quantum dots, enable one to catch the electrons and control the electronic properties of a material, while photonic crystal structures allow to synthesize the electromagnetic properties. These technologies may, e.g., be employed to make smaller and better lasers, sources that generate only one photon at a time, for applications in quantum information technology, or miniature sensors with high sensitivity. The incorporation of metallic structures into the medium add further possibilities for manipulating the propagation of electromagnetic waves. In particular, this allows subwavelength localisation of the electromagnetic field and, by subwavelength structuring of the material, novel effects like negative refraction, e.g. enabling super lenses, may be realized. Nanophotonics [Gap10] is the science which is concerned with the study and leveraging of nanoscale light-matter interactions. Nanophotonics has become a quickly evolving field of research and applications ranging from fundamental studies to applied science. High-tech nanoscale fabrication processes for dielectric and metal structures, as well as for semi-conductors and composite materials, have paved the way to tailored nano-devices. Such devices may range from light-guiding applications [BYPD+17] over metasurfaces [GC15] and single molecule sensing [MMT+17] to cancer treatment [SSD+14].

1.2 High order DGTD methods for time-domain nanophotonics

Numerical modeling of nanoscale light-matter interaction requires to solve the system of Maxwell equations possibly coupled to appropriate models of physical dispersion such as the Drude and Drude-Lorentz models. The Finite Difference Time-Domain (FDTD) method introduced by K.S. Yee in 1996 is a widely used approach for solving the resulting system of partial differential equations (PDEs). In this method, the whole computational domain is discretized using a structured (cartesian) grid. Due to the possible straightforward implementation of the algorithm and the availability of computational power, FDTD is often the method of choice for the simulation of time-domain nanoscale light-matter interaction problems. However, the space and time scales that characterize the underlying physical phenomena, in addition to the geometrical characteristics of the considered nanostructures, are particularly challenging for an accurate and efficient application of the FDTD method. During the last twenty years, numerical methods formulated on unstructured meshes have drawn a lot of attention in computational electromagnetics with the aim of dealing with irregularly shaped structures and heterogeneous media. In particular, the discontinuous Galerkin time-domain (DGTD) method [HW08] has progressively emerged as a viable alternative to the well established FDTD method. Busch et al. have intensively pushed the development of DGTD methods purposely tailored to nanophotonics [BKN11] and have also demonstrated the advantages of DGTD in comparison to Finite Difference Time-Domain (FDTD) methods [Nie09].

1.3 Numerical optimization algorithms for systems governed by PDEs

Design optimization for PDE systems consists in searching for parameter values that allow to maximize an objective function depending on the PDE solution, for a set of user-defined design parameters. According to the characteristics of the design space (discrete / continuous, dimension, constrained, etc.) and the objective function (uni- / multi-modal, differentiable, noisy, computationally expensive, etc.), a selected optimization algorithm is thus coupled to a PDE solver in an iterative design loop, until convergence to the set of optimal design parameters [BS12, HM03, KN05]. The choice of the optimization algorithm is usually critical for realistic design problems, because of the computational burden related to high-fidelity PDE solvers and the presence of several local optima. Therefore, modern design approaches are based on iterative learning strategies, involving expensive and accurate high-fidelity PDE solvers to construct low-cost surrogate models, that are exploited to drive the search for the optimum in a statistical framework [Jon01]. The most advanced methods allow to account for uncertainties in performance evaluations, arising from a lack of knowledge in some physical parameters [PWG13], and may rely on multi-fidelity simulations, mixing high- and low-accurate models in an adaptive fashion to reduce the computational time [GG14].

2 Description of the hosting teams

2.1 Acumes project-team

Acumes is a joint project-team from Inria Sophia Antipolis Méditerranée Center and Jean-Alexandre Dieudonné Mathematics Laboratory at University Nice Sophia Antipolis. The team focuses on the analysis and optimization of classical and non-classical systems of evolutionary partial differential equations arising in a variety of applications, ranging from fluid-dynamics and structural mechanics to traffic flow and biology. The complexity of the involved dynamical systems is expressed by multi-scale, time-dependent phenomena subject to uncertainty, which can hardly be tackled using classical approaches, and require the development of unconventional techniques for analysis as well as optimization. In this context, the team has developed an expertise in shape optimization procedures, based on various geometrical parameterization (surface-based or volume-based) and optimization algorithms, ranging from descent methods which necessitate sensitivity analysis to black-box algorithms, like evolution strategies and response surface methodologies, implemented in the FAMOSA software toolbox.

2.2 Nachos project-team

Nachos is a joint project-team between Inria and the Jean-Alexandre Dieudonné Mathematics Laboratory at University Nice Sophia Antipolis. The team gathers applied mathematicians and computational scientists who are collaboratively undertaking research activities aiming at the design, analysis, development and application of innovative numerical methods for systems of partial differential equations (PDEs) modeling nanoscale light-matter interaction problems. In this context, the team is developing the DIOGENeS software suite (https://diogenes.inria.fr/), which implements several Discontinuous Galerkin (DG) type methods tailored to the systems of time- and frequency-domain Maxwell equations possibly coupled to differential equations modeling the behaviour of propagation media at optical frequencies. The DGTD method is a discontinuous finite element type that relies on a high order interpolation of the electromagnetic field components within each cell of discretization mesh. This piecewise polynomial numerical approximation is allowed to be discontinuous from one mesh cell to another, and the consistency of the global approximation is obtained thanks to the definition of appropriate numerical traces for imposing the continuity of the tangential fields on faces shared by two neighboring cells. Time integration is achieved using an explicit scheme and, as a result of the discontinuity of the approximation, no global mass matrix inversion is required to advance the solution at each time step. Such a DGTD method, which is formulated on an unstructured tetrahedral mesh, has been designed in the context of the Ph.D thesis of Jonathan Viquerat for the simulation of nanoscale light-matter interaction problems [Viq16]. This DGTD method has been recently refactored and implemented in the object-oriented framework of the DIOGENeS software suite.

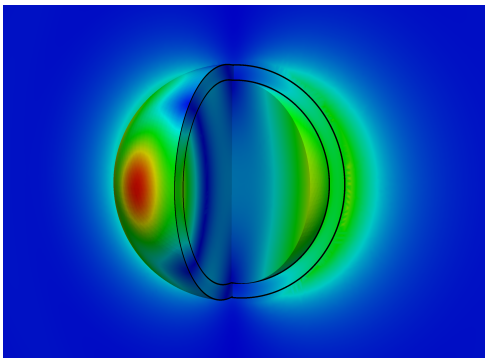
3 Objectives of the study

The recent numerous discoveries in nanophotonics, driven by the advancements in nanofabrication and characterization techniques, require to revisit the traditional electromagnetic design paradigm. Specific and rigorous strategies for the design of nanostructures are not yet fully established. The geometries that have beed studied and designed so far require additional refinements by a full-wave electromagnetic simulation, carried out by sweeping the relevant geometrical parameters through a given range. This time-consuming design process exacerbates the delay between proof of concept plasmonic devices and marketable technology. On the other hand, the automation of the design of nanostructures by rigorous inverse design strategies [MARC+12, FHW+16] could make very large search spaces easily accessible, where the user could look for a specific nanostructure meeting specific needs with unparalleled accuracy. Contrary to the solution of a direct problem, which simply aims at determining the electromagnetic field scattered by a given nanostructure of prescribed shape, size and composition, under assigned excitation conditions, the inverse design problem consists of determining the characteristics of the scattering object, based on the desired properties of the scattered electromagnetic field.

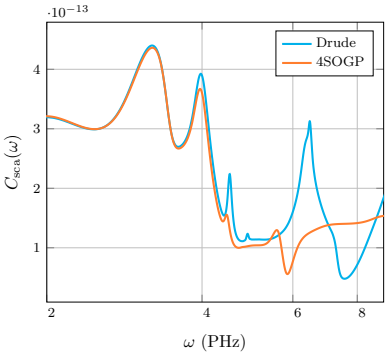
The objective of the present study will be to develop a methodology for the rigorous inverse design of the shape of three-dimensional (3D) nanophotonic devices, aiming at the maximization of an assigned objective function in a continuous parameter space. In order to do so, we will bridge the expertise of the ACUMES and NACHOS project-team to tackle the inverse problem by coupling efficient global optimization stretagies with a high order full wave timed-domain Maxwell solver for the optimal design of 3D nanophotonic devices. The following three topics will have to be addressed:

1. Problem parametrization: the influence of the parameterization of nanophotonic device geometries will be investigated, by comparing ad-hoc representations (Gielis' formula) to generic geometrical models (B-Spline based free-form deformation).
2. Direct electromagnetic solver: we will leverage a parallel high order DGTD solver of the system of 3D time-domain Maxwell equations coupled to a generalized model for taking into account the disperion of metallic nanostructures at optical frequencies [LSV17].
3. Optimization algorithm: we will couple the electromagnetic solver to a surrogate-based optimization strategy.

In the spirit of recently published studies [MARC+12, FHW+16], we will apply the resulting inverse design methodology to the optimization of nanoshells by maximimizing a figure of merit such as the scattering cross-section (see Figure 1). Geometrical parameters that will have to be considered are the nanostructure shape (nanosphere, nanoellispoid, nanorod, etc.) and the thickness of the coating. Other parameters that will be studies are the material characteristics and the target resonant wavelength.



(a) Modulus of the electric field in the vicinity of the nanoshell. A 4SOGP dispersion model is used to describe the gold shell



(b) Computed scattering cross-sections of the nanoshell for various gold dispersion models

Figure 1: Near-field solution and scattering cross-section of a silica/gold nanoshell device. $\mathbb{P}_4$ polynomial approximation is used for the spatial DG discretization, along with curvilinear element for an enhanced geometrical description of the shell.

Required background:

- Master in applied mathematics or scientific computing;
- Knowledge of finite element type methods for solving PDE;
- Software development skills, preferably in Fortran 200x.

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