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Advanced computational design of complex nanophotonic devices using high-fidelity fullwave solvers and statistical learning global optimization algorithms

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Abstract. We report on our recent achievements on the development of a suite of innovative computational tools for the study of light-matter interactions at the nanoscale and in particular for the inverse design of nanophotonic devices. Our software suite, named DIOGENeS (<https://diogenes.inria.fr/>), is organized around high-order accurate finite element type fullwave solvers and statistical learning global optimization algorithms. We present several applications of these computational tools for the design of optical metasurfaces, nanostructured solar cells and plasmonic nanostructures.

1 Introduction

Nanostructuring of materials has paved the way for manipulating and enhancing light-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, 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. We present our recent efforts and achievements toward the development of innovative numerical methodologies for the design of nanoscale photonic devices. Numerical modeling plays a crucial role in this context, in particular for discovering non-intuitive nanostructures or material nanostructuring for harvesting and tailoring the interaction of light with matter at the nanoscale. In our works, we combine two main numerical ingredients: (1) high order Discontinuous Galerkin (DG) methods for solving the system of time-domain [1] or frequency-domain [2] Maxwell equations in 3D coupled to appropriate differential mod-

els of physical dispersion in photonic materials and (2) one of the most advanced optimization techniques that belongs to the class of Bayesian optimization and is known as Efficient Global Optimization (EGO) [3]. The capabilities of the resulting numerical methodology have been first demonstrated for the inverse design of phase-gradient metasurfaces [4, 5] and RGB metalenses [6]. Here, we will also report on recent extensions and applications of this methodology to deal with other nanophotonic devices.

2 Fullwave solver

Our high-fidelity fullwave solvers adopt the DG discretization framework. In the last ten years, we have developed two DG-based fullwave solvers that are high order accurate and able to deal with unstructured meshes for a detailed representation of irregular geometrical features: a high order DGTD (Discontinuous Galerkin Time-Domain) solver of the time-domain Maxwell equations coupled to a Generalized dispersion Model [1] and a high order HDGFD (Hybridized Discontinuous Galerkin Frequency-Domain) solver of the frequency-domain Maxwell equation [2].

3 Numerical optimization

In our works, we use one of the most advanced optimization techniques based on a statistical learning-based approach, which is known as Efficient Global Optimization (EGO) [3]. The EGO algorithm is a global optimization algorithm that substitutes the complex and costly iterative electromagnetic evaluation process with a simpler and cheaper metamodel. EGO is related to the class of Bayesian optimization. Contrary to the traditional common global optimization strategies like genetic algorithms,

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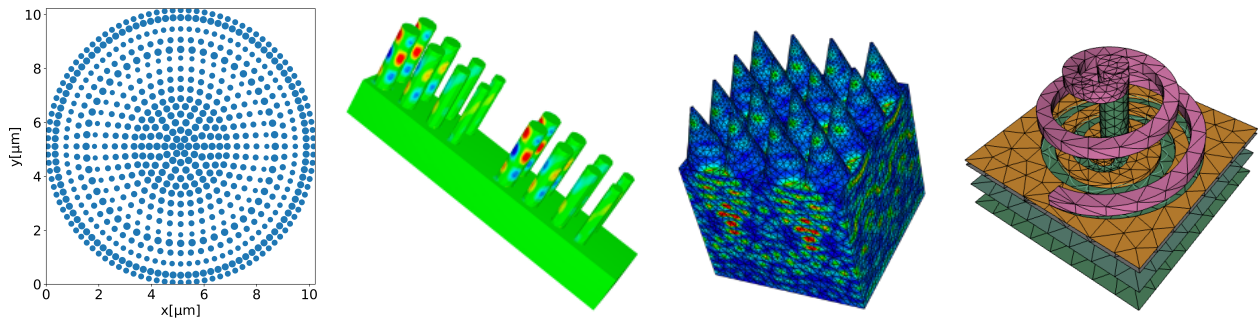


Figure 1. Left: 3D achromatic metalens for light for shaping. Middle left: phase gradient metasurfaces for deflecting light. Middle right: nanostructured solar cell for solar light trapping. Right: chiral plasmonic nanostructures.

EGO is not based on adaptive sampling but on a surrogate model, which is constructed on the basis of available objective function evaluations. This surrogate model utilizes a statistical learning criterion related to the optimization target (usually called *merit function*) in order to identify which design (set of parameters) should be tested in the next iteration that would provide better results close to the predefined goal.

4 Inverse design methodology

We have developed an inverse design methodology that combines two ingredients: the DGTD and HDGFD full-wave solvers for the numerical characterization of a given design, and the EGO [3] algorithm for the optimization of the geometrical characteristics of nanostructures or nanophotonic devices. The capabilities of this methodology have been first demonstrated in the context of the design of optical metasurfaces. More precisely, in [4], we have optimized GaN (Gallium Nitride) semiconductor phase gradient metasurfaces operating at visible wavelengths, and we have clarified the importance of near-field coupling for a simple supercell made of four nanopillars. In [6], we presented for the first time to the metasurface community a multiobjective inverse design approach leveraging the EGO statistical learning-based global optimization method, in order to optimize 3D achromatic metalens with numerical aperture NA above 0.5 (see figure 1 left). Our metalens attempts to focus the RGB colours at the same focal plane with the maximum feasible focusing efficiency. In other words, we seek to get the most suitable compromise between the chromatic dispersion and the focusing efficiency for a given fixed focal distance. It is worth mentioning that the optimized designs have been fabricated and experimentally characterized by our physics collaborators at CRHEA in Sophia Antipolis. Finally, in [5], we addressed the optimization of metasurface designs taking into account uncertainties due to fabrication

errors. This time, we formulate a multiobjective optimization problem that aims at minimizing two statistical robustness measures defined on the parameterized metasurface geometry. We apply this technique to optimize and design realistic phase gradient metasurfaces in the visible regime. Our preliminary results reveal that we obtain robust designs, which are less sensitive to the geometrical fabrication errors as compared to the one optimized without considering uncertainties.

5 Closure

We have developed an innovative software suite dedicated to computational nanophotonics, which is named DIOGENeS (<https://diogenes.inria.fr/>). The numerical tools from this software suite are utilized for conducting concrete studies in close collaboration with physicists from laboratories at the national and international levels. We will present several applications of these computational tools for the design of optical metasurfaces, nanostructured solar cells and plasmonic nanostructures (see figure 1).

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