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ADVANCED COMPUTATIONAL DESIGN OF COMPLEX  
NANOSTRUCTURED PHOTONIC DEVICES USING  
HIGH ORDER DISCONTINUOUS GALERKIN METHODS  
AND STATISTICAL LEARNING GLOBAL OPTIMIZATION

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**ABSTRACT**

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. In this talk, we will 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 [1] for solving the system of time-domain [1] or frequency-domain [2] Maxwell equations in 3D coupled to appropriate differential models 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 has been first demonstrated for the inverse design of phase-gradient metasurfaces [4]-[5] and RGB metalenses [6] (see Fig. 2). In the present talk, we will also report on recent extensions and applications of this methodology to deal with improving the light absorption in ultra-thin solar cells and nanostructured CMOS imager pixels (see Fig. 1). In the context of the Atlantis research group at Inria, we are developing an innovative software suite dedicated to computational nanophotonics that integrates the above-mentioned numerical ingredients (see Fig. 3).

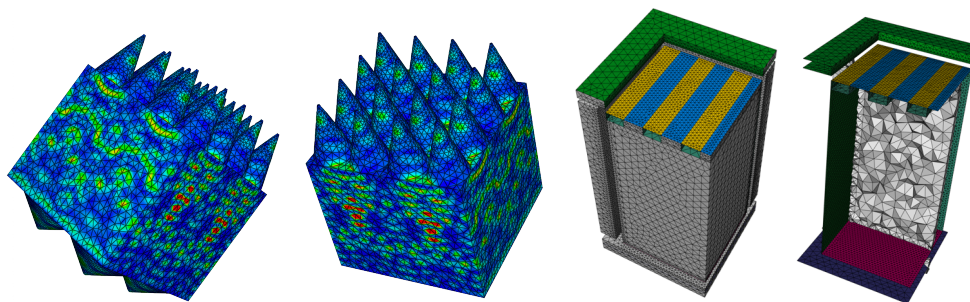


Fig 1. Optimization of nanostructuring for improving light trapping in ultra-thin solar cells (left) and light absorption in nanostructured CMOS imager pixel.

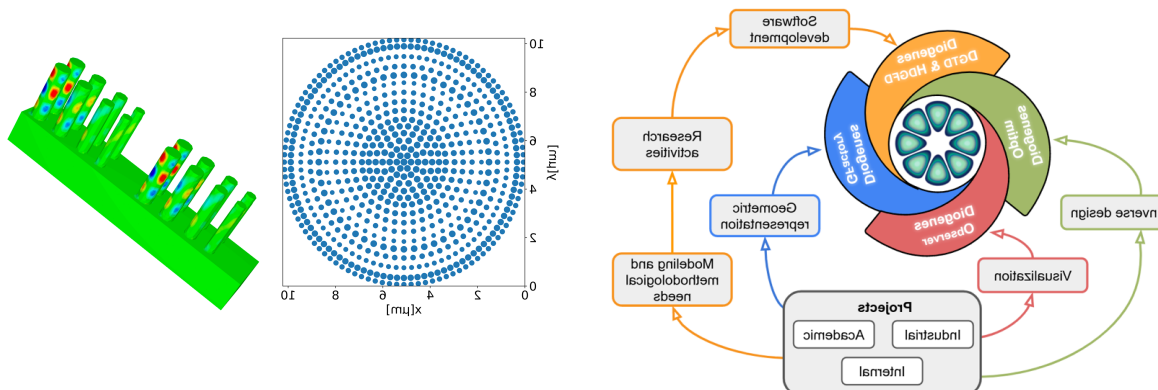


Fig 2. Optimization of phase gradient metasurface (left) and of a RGB metalens (middle) for the design of planar photonic devices (right). Architecture of the DIOGENeS software suite. DGTD and HDGFD are the high order DG-based fullwave solvers for time-domain and frequency-domain modeling settings. GFactory 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 [DIOGENeS: <https://diogenes.inria.fr/>].

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