Computational Nanophotonics Engineering

Simulation and Inverse Design of Nonlinear Nanostructured Materials

Johannes Gedeon, Izzatjon Allayarov, Antonio Calà Lesina,
Hannover Centre for Optical Technologies,
Institute of Transport and Automation Technology
(Faculty of Mechanical Engineering), and
Cluster of Excellence PhoenixD,
Leibniz University Hannover, Hannover, Germany.

In Short

- Fast and accurate simulations to engineer the nonlinear emission from complex nanostructured materials
- Discovery and engineering of new conceptual designs for nanophotonic devices via topology optimization
- Implementation of advanced algorithms for the simulation and design of nanophotonic materials on supercomputers

The last decade witnessed an exponential rise in research in nanophotonics, which studies the interaction of light with metallic and dielectric objects of nanoscale dimension. Nanostructures arranged in a 3D lattice form a metamaterial (matasurface for 2D lattice). Due to plasmonic and Mie-type resonances, metal and dielectric nanostructures can be designed to engineer light-matter interaction [1]. This allows us to achieve optical properties not available in the bulk counterpart. Such nano-engineered materials are being investigated to manipulate and dynamically tune the properties of light in the linear and nonlinear regimes for applications in imaging, biosensing, communications, security, autonomous driving, and quantum technologies. This is made possible by advances in nanofabrication techniques, such as e-beam lithography, focused ion beam and two-photon polymerization, that offer unprecedented control at the nanoscale and support the growth of this research field by allowing the realization of nanostructured materials with complex designs.

In this project, we tackle modelling and design challenges. This includes the modelling of nonlinear processes in nanostructures (see Fig. 1 [2]), and the automatic discovery and design of complex nanostructured devices via topology optimization techniques (see Figs. 2 and 3 [3]).

1. Fast and accurate nonlinear simulations

Nonlinear simulation techniques for nanophotonic devices are not as established as their linear counterpart, and only marginally available in commercial software. Within a collaboration with the University of Ottawa, a hydrodynamic model was recently developed for the simulation of the electric current density induced in the nanostructured material by the incoming light and the interaction with the boundaries (spill-out effects). This model automatically takes into account the nonlocal effects (arising because of the nanometric sizes of the nanostructures), allowing us to approach the limit of a quantum simulation with a classical electrodynamics technique [4]; the model also produces all the harmonics and is a viable tool for nonlinear generation simulations.

Although we could match experimental nonlinear measurements [5], this model is computationally expensive because high-resolution simulations are required to describe the physics correctly, due to large gradients in electron density near nanoparticles. The model is also complex, and thus hard to use for the design of nonlinear nanophotonic devices. We are currently working on the development of alternative numerical approaches that are computationally simpler while preserving accuracy, and can speed-up the design process.

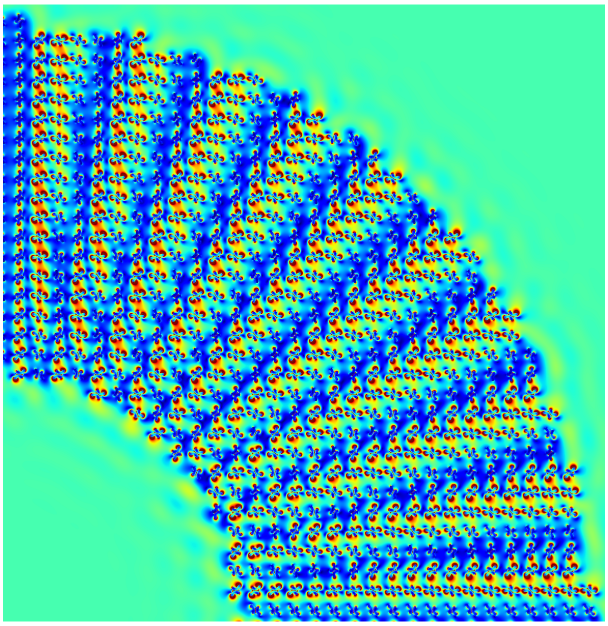

Figure 1: *Large-scale simulation of a hybrid plasmonic/dielectric metasurface for nonlinear generation and control (light structuring) via parallel 3D-FDTD [2].*

2. Inverse design of nanophotonic devices

Exploring large design spaces has the potential not only to find solutions to complex optimization problems but also to offer new conceptual designs for nanophotonic structures. While metaheuristic meth-

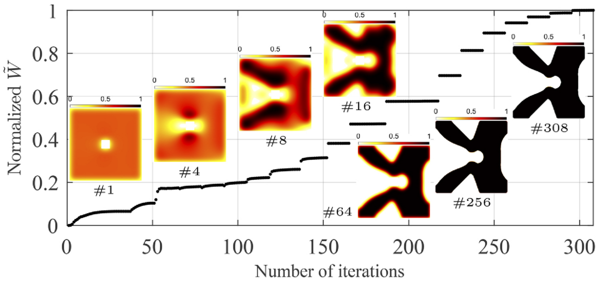

__Figure 2:__ Development of the objective function $\tilde{W}$ (electric energy enhancement in the gap) and snapshots showing the topology evolution of a metallic nanoantenna. Black is metal, and white is vacuum [3].

ods have been used for design problems with a few number of design variables, they are computationally prohibitive for large-scale optimisation problems, and therefore only useful when a good initial design is known. Gradient-based optimization methods can efficiently handle large-scale optimization problems when access to the gradient information is feasible, for example, by using the adjoint method.

Topology optimization based on the material distribution approach has been developed for a broad range of applications and is currently used in many fields, e.g., to optimize load-carrying elastic structures (a full airplane wing was designed [6]), and various electromagnetic problems covering the microwaves, millimeter waves, and optical frequencies [7,8]. For electromagnetic problems, however, most of the reported work in the literature focused on problems that can be decomposed by symmetry into 2D problems, or 3D problems with the design space only consisting of planar sheets. At optical frequencies, various classes of problems require full-wave simulations using the 3D Maxwell's equations. We developed an algorithm for the topology optimization of dispersive metallic nanoantennas at optical frequencies [3]. We will extend this method to handle large-scale design volumes for the optimization of realistic optical devices, as preliminarily shown in Fig. 3 for silver nanoantennas optimized in 3D to provide field enhancement in the gap [3].

__Figure 3:__ Topology optimization of silver nanoantennas in 3D [3].

The computational complexity of the problems that our group is tackling requires access to high-performance computing. Our problems are large-scale for at least three reasons: (i) we are interested in realistic devices, so we need to simulate full metasurfaces/metamaterials in 3D, (ii) plasmonic and nonlinear nanostructures require a fine discretization to accurately describe fields that vary over nano-scale dimensions [4,9], and (iii) topology optimization requires hundreds of iterations to find the optimal design solution. Optical simulations in this project will be conducted using parallel in-house codes based on the finite-difference time-domain (FDTD) method [9].

WWW

`https://www.hot.uni-hannover.de/en/research-groups/computational-photonics/`

More Information

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Project Partners

Prof. L. Ramunno (University of Ottawa, Canada);
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