ANALYSIS AND DESIGN OF LARGE METASURFACES

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Metasurfaces are collections of interacting subwavelength scatterers, typically operating near resonance. They are also versatile in shaping and manipulating electromagnetic waves for various applications, including biosensing, imaging, and analog and quantum computing. Metalenses are one common class of metasurfaces, in which the unit cells are designed to impart a specific, position-dependent phase shift to transmitted light, resulting in a global focusing effect. Accurate simulation of metasurfaces and metalenses, with efficient use of time and memory, is crucial for understanding their fundamental properties and optimizing their performance.

Integral formulations of electromagnetic scattering are appealing for the analysis of metasurfaces because they define the unknowns only within the objects' volumes or on their boundaries if the objects are spatially piecewise homogeneous and naturally satisfy radiation conditions at infinity. However, they usually involve dense matrices, which are computationally demanding to invert, even with acceleration techniques like the fast multipole method [1,2]. A brute-force strategy for scaling full-wave simulations involves adapting general-purpose computational electromagnetic algorithms to massive parallelization for CPU-based or GPU-based computing platforms. However, it is more efficient to tailor existing methods to the specific characteristics of the problem of electromagnetic scattering from metasurfaces, which generally consist of repeated particle shapes arranged in aperiodic positions and arbitrary orientations, typically subwavelength.

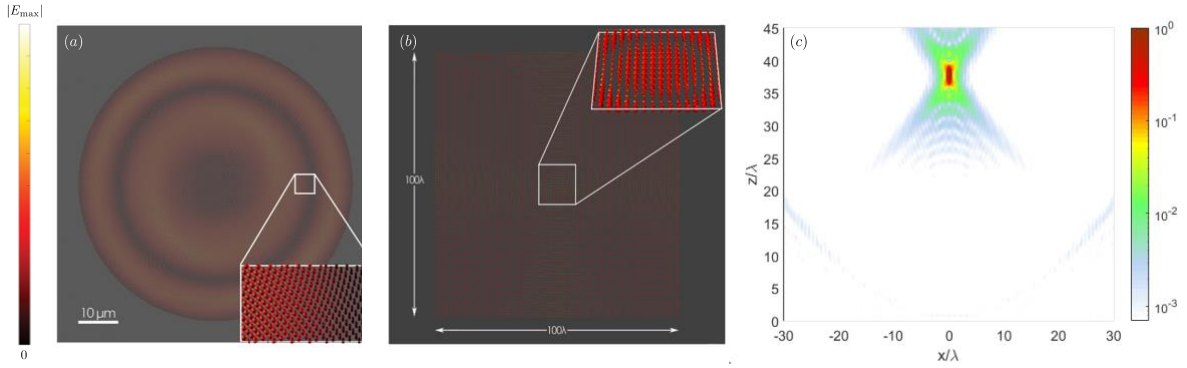

Fig. 1. (a) Electric field magnitude on the particles' surface of a Vogel spiral of size 115λ composed of 40·103 gold bricks of dimension 200×200×100 nm excited by a linearly polarized plane wave at wavelength λ = 600 nm. (b) Electric field magnitude on the particles' surface of a metalens of size 100λ, lying on the xy plane, and composed of 104 TiO2 nanofins of dimension 410 × 85 × 600 nm excited by a circularly polarized plane wave at wavelength λ = 660 nm. (c) Electric field normalized intensity on the x-z cross-sectional plane. The achieved focal length is consistent with the prescribed value f = 37.5λ.

In References [3,4] we introduce a fast boundary integral method specifically tailored for large arrays of subwavelength scatterers, leveraging the Poggio-Miller-Chang-Harrington-Wu-Tsai (PMCHWT) formulation. We combined the Multilevel Fast Multiple Method with the boundary integral equation method employing an expansion of the unknowns of the Poggio-Miller-Chang-Harrington-Wu-Tsai (PMCHWT) equation in terms of a particular class of entire-domain basis functions, defined on the individual meta-atom, and denoted as static modes. As demonstrated in Reference [3], static modes drastically reduce the total number of unknowns in scattering problems involving arrays of penetrable particles compared to discretization based on sub-domain basis functions, such as RWG.

The design of large-area metasurfaces is very challenging because of the large number of degrees of freedom involved and for the time-consuming multiple solutions of the direct scattering problem. From an engineering perspective, the design of a metasurface is recast in terms of the search for several parameters that optimize one or multiple proper figures of merit. Typical *figures of merit* include the near-field enhancement at a single or multiple hot-spots; the far-field focusing efficiency; the emission enhancement of nearby quantum emitters; the distance of the metasurface phase profile from a prescribed one; minimization of chromatic/achromatic aberrations. The optimization problem may also be subject to several *constraints* arising from fabrication and technological limitations.

As *target problem*, we are considering the design of large-area three-dimensional achromatic metalenses with high numerical aperture and optimal focusing efficiency. This is a prototypical problem that allows one to compare our results with the theoretical and experimental literature. We then consider the planar metasurface constituted by a collection of N elementary scatterers (e.g. nanopillars, nanofins, ...) of prescribed permittivity. Then, we search for the individual position, orientation, and size of each elementary meta-atom that optimize the figures of merit of interest. This approach, if compared to the competing philosophy of the Topological Design where the metalens is obtained by properly shaping a dielectric material of constant thickness, is interesting because it requires a lower computational cost in solving the direct problem.

Evolutionary algorithms and AI-based approaches, require numerous evaluations of the forward problem, making them computationally expensive and prone to missing local optima. Instead, we consider *gradient-based methods*, which are more efficient for large numbers of unknowns. We propose the adjoint equation method, which enables rapid gradient computation of an objective function through a corresponding "adjoint" problem. Unlike traditional methods that require multiple forward problem solutions to compute gradients, the adjoint method needs only a single forward problem solution, making it computationally efficient.

References

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