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# Optimal design of all-dielectric 3D gradient metasurfaces

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## Abstract

Metasurfaces are flat surfaces consisting of sub-wavelength nanoresonators, made of plasmonic or high dielectric refractive index materials patterned in a specific way. These flat surfaces provide nearly full control of the light properties in a very short propagation distance with high resolution [1]. By changing the dimensions, shapes, and orientation of these nanoresonators, different functionalities can be obtained [2, 3]. The complexity of the problem and the wide parameter space, make the direct modelling problem insufficient. Recently, several optimization techniques have been applied to the field of nanophotonics (including metasurfaces) [4] by solving an inverse design problem. Generally speaking, there are two classes of optimization techniques that have been used in the metasurface designs; local and global techniques. The local methods depend on the initial guess and most of them require the computation of the gradient, which might be challenging. On the other hand, global optimization techniques are easier to use because the solver is considered as a black box moreover, they do not get stuck in a local minima/maxima like the local methods [4]. However, most of the global techniques used in the metasurface designs require costly simulations (for large parameter space), which make them inapplicable for modelling 3D real-life designs that require 3D solvers.

In our work, we use two efficient global optimization techniques based respectively on advanced evolution strategies and statistical learning. The first one is the covariance matrix adaptation evolution strategy (CMA-ES) [5]. The CMA-ES has been gaining a lot of attention since it requires fewer cost function evaluations compared to the other evolutionary algorithms like genetic algorithms (GA) [6] especially for 3D real designs that require expensive simulations even with the high-performance computational resources. The second method is the Efficient Global Optimization (EGO) algorithm [7]. The EGO algorithm is based on the surrogate modelling, that is to say, replacing the complex or costly evaluation process by a simpler and cheaper model [7] to reduce dramatically the computational cost (number of calls for the electromagnetic simulations).

We use our rigorous Discontinuous Galerkin Time Domain (DGTD) solver from the Diogenes-suite [8] together with the optimization algorithms, in order to optimize 3D meta-gratings (periodic in two directions) in the visible regime. The proposed metasurfaces are based on GaN due to its negligible losses and due to its high refractive index in the visible regime, which make it ideal nanoresonator (phase-shifters) for metasurface designs [1]. As a first design, we aim to maximize the total transmission at a desired wavelength  $\lambda = 600$  nm using CMA-ES and EGO methods by optimizing 6 parameters. A comparison between the results obtained from the two methods will be presented. Our results reveal that CMA-ES and EGO seem to be more efficient than GA [6]. Based on the above methods together with our 3D solver, different metasurface designs will be presented with different functionalities including theoretical and experimental study of enhancing the diffraction efficiency of 3D real-life gradient metasurface designs.

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