Simulation of large-area metasurfaces with a distributed transition matrix method

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Abstract: We present a method to accurately compute simulations and gradients of large-area metasurfaces. Our distribution strategy gives a linear simulation time reduction proportional to number of compute nodes, opening the door to accurate large-scale inverse-design. © 2022 The Author(s)

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Fig. 1: Simulation and optimization of large-area metasurfaces with distributed T-matrix method. (a) Diagram of applying the Nyquist sampling theorem to the propagating, and thus bandlimited, incident field. (b) Simulation distribution technique, enabled by the spatial-locality of the Nyquist samples. (c) Total simulation vs number of GPU’s used to simulate metasurfaces at $\lambda = 1.55\mu m$ with linear dimension 50 $\mu m$ (black), 100 $\mu m$ (blue), and 300 $\mu m$ (green). (d) Gradient-based optimization improvement of a 15 $\times$ 15 $\mu m$ Huygens metalens with NA = 0.996. (Top) Lens efficiency versus optimization iteration. (Bottom) Electric field distribution at the focal plane of the metalens before and after optimization (left and right, respectively).

Metasurface-based optical elements provide a potential compact and integrable solution to the central challenge of optical phase shaping in important application spaces including sensing, augmented and virtual reality, and imaging.
Although metasurfaces typically span thousands of wavelengths in linear dimension, the full parameter space is rarely explored during design because traditional electromagnetic simulation techniques (e.g. FDTD, FDFD, FEM) become prohibitively slow at these size scales. Instead, most current methods for designing 3D metasurfaces rely on approximating a full electromagnetic simulation of the metasurface with local simulations using either periodic or radiation boundary conditions [3–5]. This approach does not fully account for interactions between the unit-cells and restricts the design degrees of freedom. In this talk, we present a scalable method to compute accurate simulations and gradients of large-area metasurfaces without making a locally-periodic approximation.

To simulate arbitrarily-large metasurfaces, our approach relies on a simulation distribution strategy that allows a linear reduction in simulation time with number of compute nodes. Since the incident field is propagating, it is bandlimited in k-space and can thus be represented by its Nyquist samples [6] as:

\[ E_{\text{inc}}^T(x,y,z) = \sum_{i,j} E_{\text{inc}}^T(x_i,y_j,z)f_{i,j}(x,y), \]

where \( x_i, y_j = i\lambda/2, j\lambda/2 \) with \( \lambda \) being the wavelength in the background medium, and \( f_{i,j}(x,y) \) is a jinc function [7] centered at \( (x_i,y_j) \). As shown in Fig. 1a, the electric field corresponding to each Nyquist sample is spatially limited and, consequently, the response of the metasurface to this sample can be accurately locally simulated. The parallelization scheme that we employ, shown in Fig. 1b, divides the full metasurface simulation into smaller metasurface subregion simulations, which are each performed on an individual GPU node, based on groupings of the incident field samples. Each individual GPU node performs a fast Transition-matrix based simulation using vector spherical wavefunctions. Fig. 1c shows that this distributed transition-matrix approach allows the total simulation time to scale as approximately \( 1/N_{\text{nodes}} \), allowing simulation of a \( 200\lambda \times 200\lambda \) metasurface in about 3.25 hours with 24 GPU nodes.

Our simulation method can also be used for efficient computation of gradients based on adjoint-sensitivity analysis [8, 9], enabling inverse-design of the full metasurface. Importantly, although optimization of scatterer position is very challenging under a locally-periodic approximation, our method allows optimization of both the scatterer shapes and the scatterer positions. Fig. 1d demonstrates a gradient-based optimization improvement of a very high NA Huygens metalens, resulting in an efficiency improvement of about \( 2\times \).

The scalability and accuracy of our distributed transition-matrix simulation method finally opens the door to full inverse-design of large-area metasurfaces, which may unlock new metasurface designs with unprecedented efficiency and functionality.

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