Predicting Long- and Variable-Distance Coupling Effects in Metasurface Optics

Li, Xinhao; Kojima, Keisuke; Brand, Matthew

TR2021-140 December 08, 2021

Abstract

A novel deep learning neural network architecture is proposed to predict the near electrical field produced by metasurface devices with long-distance coupling effects in large neighborhoods of nano-pillars. This reduces LPA-FDTD error by 60%.

IEEE Photonics Conference (IPC) 2021

Predicting Long- and Variable-Distance Coupling Effects in Metasurface Optics

Xinhao Li
Dept. Mechanical Engineering, MIT
Cambridge, MA, USA
xinhaoli@mit.edu

Keisuke Kojima Matt Brand
Mitsubishi Electric Research Labs
Cambridge, MA, USA
kojima, brand@merl.com

Abstract

A novel deep learning neural network architecture is proposed to predict the near electrical field produced by metasurface devices with long-distance coupling effects in large neighborhoods of nano-pillars. This reduces LPA-FDTD error by 60%.

I. Introduction

Automated design of large-scale metasurfaces is usually done under the principle of domain decomposition [1]: The near field generated by the whole metasurface is approximated by stitching together near-field responses of individual unit cells, each simulated separately under the local periodic assumption (LPA). However, the LPA does not hold when there is a strong coupling between adjacent unit cells, which has been documented in several settings [2]–[4]. Available methods to capture the coupling effects are costly on the simulation side and ultimately require exponentially larger dictionaries for design [2], [3]. Consequently, coupling effects are seldom incorporated in design algorithms, due to the cost of simulating multi-unit cells with many degrees of design freedom. Here, we introduce an efficient deep neural network (DNN) architecture for predicting the near fields of metasurfaces with significant long-range inter-cell coupling effects.

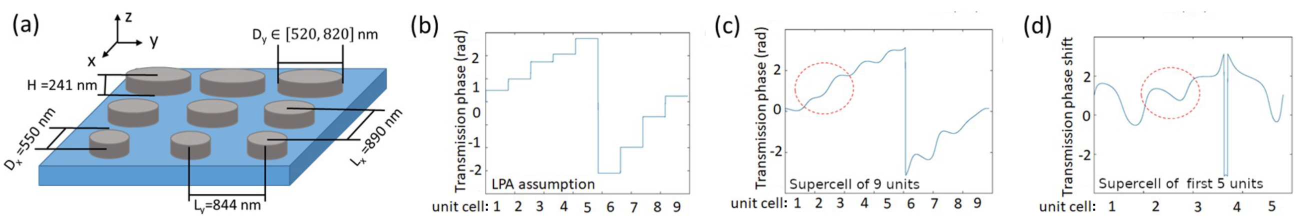

Fig. 1. (a) A 3x3 supercell of Si nanopillars with identical Dx and variable Dy, with PDMS cladding on a SiO_2 substrate. (b) FTDT-LPA prediction of phase shifting provided by a 9x1-unit neighborhood of varied nanopillars, tessellated on the plane. (c) "gold standard" FDTD 9x1 supercell simulation of the same design reveals that the LPA-predicted shifts are inaccurate. (d) Simulation of supercells containing only the first 5 nanopillars indicates that the difference in the red circle is due to coupling effects across distances > 2 unit cells.

II. Recurrent Neural Network for variable-range couplings

As illustrated in Fig. 1, FDTD simulations in the $\lambda = 1550$ nm band indicate that elliptical nano-pillars on a 890-nm unit cell pitch have significant shape-dependent coupling effects beyond 2 unit cell widths. More subtle effects can be observed over 3x that distance. To capture these effects, we seek to design and train a modular recurrent DNN that mimics the Schwarz alternating method (SAM) [7], which solves large scale PDEs by overlapped domain decomposition, as shown in Figure 2(a) and (b). Each module of the DNN is a U-Net [8] that takes as input the unit cell physical parameters and rough estimates of the electrical fields in the X,Y and Z planes around the cell, then outputs revised estimates of these fields. The DNN has (a) 3 encoding blocks that use 2D convolutional layers, leaky ReLu units, and max-pooling to compress the descriptions of the real and imaginary components of the input fields; (b) a convolutional block to model the coupling effects; and (c) 3 decoding layers to generate the predicted the output fields. There are shortcut connections between the encoding and decoding blocks. Virtual copies of this DNN are assigned to each unit cell, each taking the X- and Y-plane field estimates output by its neighbors as input. The entire array of modules is then run recurrently, so that the coupling information travels one unit cell laterally per iteration. We trained the network to predict the residual coupling effects that are not captured in low-cost simulations of each unit cell under LPA, by unrolling it in time and minimizing squared-error loss via stochastic gradient descent.

III. Results and Conclusions

The method was tested on elliptical nano-pillar metasurfaces designed for $\lambda = 1550$-nm plane waves with square lattice and $\lambda/4$ unit cell pitch. For proof-of-concept, the training data consisted of 10-nm-grid FDTD simulations of 100 randomly generated supercells containing 13 unit cells arrayed in the X direction, with y-axis diameter of the nano-pillar increasing by random increments to provide a phase delay $\geq 2\pi$ across the supercell. The supercells are periodically tiled in both the X and Y direction.The DNN was trained for 600 iteration, 7 recurrences/iteration, to predict the coupling effects that are neglected by FDTD/LPA simulation of the central unit cell. The DNN was then tested on both 13- and 20-unit supercells, where it

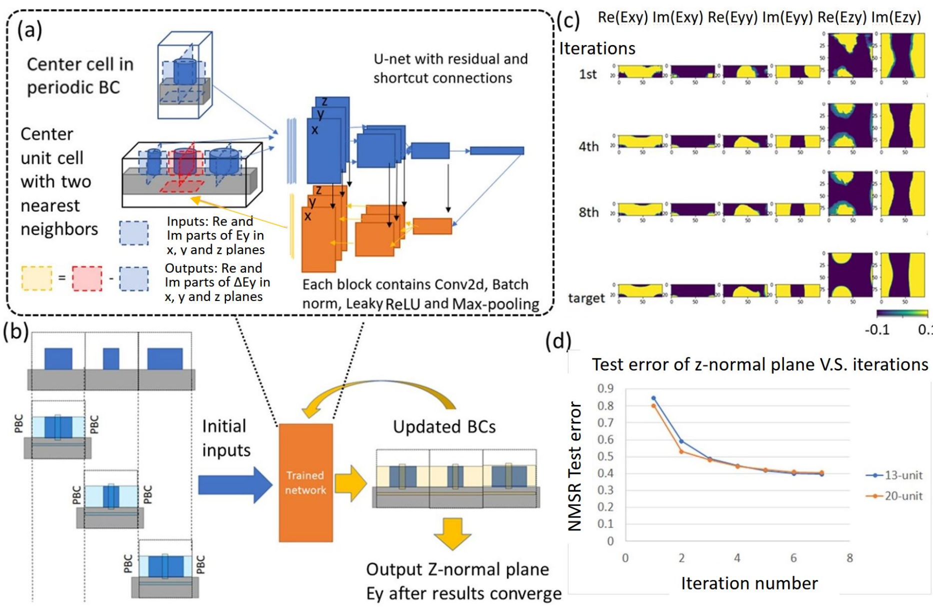

Fig. 2. (a) and (b) Architecture of the U-Net module as in the recurrent DNN. (c) Example of the evolution of output fields in x, y and z planes around a single unit cell through the iterations. (d) Each iteration of the DNN (trained with 13-unit supercells) approaches the actual differential field, stabilizing at a 60% error reduction after 7 iterations, compared to LPA results.

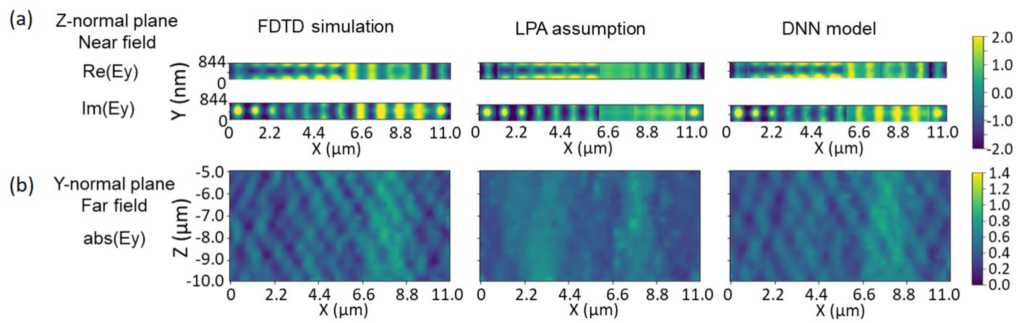

Fig. 3. (a) Z-normal plane near fields of Ey calculated by FDTD simulation, LPA and the DNN model on a 13-unit super cell. (b) Far field projection of Ey in Y-normal plane, obtained based on the near fields in (a). The DNN model improves the estimation accuracy in both near and far fields.

exhibited an average reduction of error of $> 60\%$ in the Z-plane electrical field, as shown in Figure 2(c) and (d). The DNN predictions also support more accurate far-field estimation: Figure 3 contrasts near-to-far-field projection [1] calculated from (a) gold-standard full-supercell FDTD simulation; (b) LPA simulation; and (c) DNN prediction, which closely approximates (a). The model improves the accuracy and efficiency of near-field estimation, as shown in Fig 3(a). Further incorporating with the near-to-far-field projection [1], as shown in Fig 3(b), the DNN model shows potential to serve as an efficient and accurate forward estimator for metasurface design considering the near-field coupling effects.

We have demonstrated that long-distance couplings in metasurfaces have significant effects on both near and far fields. Modeling this effect in FDTD can be prohibitively expensive, so we developed a recurrent DNN that captures $> 60\%$ of the coupling effect over variable-sized spans of the metasurface up to 20 unit cells in width. Future work will expand this approach to broader classes of metasurfaces and deploy it in an automated metasurface inverse design algorithm. These should enable higher density metasurface designs, leading to higher efficiency.

References

[1] R. Pestourie,et al. "*Inverse design of large-area metasurfaces*," Opt. Express 26, 33732-33747 (2018)
[2] Z. Lin and S.G. Johnson, "*Overlapping domains for topology optimization of large-area metasurfaces*," Opt. Express 27, 32445-32453 (2019)
[3] S.J. Byrnes, et al. "*Designing large, high-efficiency, high-NA, transmissive meta-lenses for visible light*," Opt. Express 24, 5110-5124 (2016)
[4] Y. Yang, et al. "*All-dielectric metasurface analogue of electromagnetically induced transparency*," Nat Commun 5, 5753 (2014).
[5] S. Lepeshov and Y. Kivshar. "*Near-field coupling effects in Mie-resonant photonic structures and all-dielectric metasurfaces*," Acs Photonics 5, no. 7 (2018): 2888-2894.
[6] Z. Liu, et al. "*Compounding meta-atoms into metamolecules with hybrid artificial intelligence techniques*," Advanced Materials 32.6 (2020): 1904790.
[7] H.A. Schwarz(1869), "*Über einige Abbildungsaufgaben*," J. Reine Angew. Math., 1869 (70): 105–120, doi:10.1515/crll.1869.70.105.
[8] P.R. Wiecha and O.L. Muskens, "*Deep learning nanophotonics: A generalized accurate predictor for near fields and far fiels of arbitrary 3D nanosstructures*," ACS Nano Letters 20, 329-338 (2020).