Physics-guided hierarchical Neural Networks for Maxwell's equations in metamaterials

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Abstract:
We develop a hierarchical approach to building a Physics-guided neural network (PGNN) for scalable solutions of Maxwell equations with high spatial resolution and illustrate the developed formalism on a metamaterial photonic funnel example.

Composite materials with engineered optical properties, metamaterials and metasurfaces, are rapidly advancing as platforms for optical communications, sensing, imaging, and computing [1]. Light interaction with metamaterials is often analyzed by computational science, where numerical algorithms are used to solve Maxwell's equations [2]. Here we develop an approach to the design of physics-guided neural networks (PGNNs)[3] that are capable of analyzing the complex structure of electromagnetic fields within metamaterials, with significantly higher accuracy and lower training sets than conventional physics-agnostic neural networks [4].

The approach is illustrated on photonic funnels [5]: conical structures with hyperbolic metamaterials cores that are capable of concentrating light to deep subwavelength areas. Photonic funnels (Fig.1a) reflect fundamental challenges facing NN-computational science interface: composite nature of the core and its hyperbolic dispersion [6] yield highly oscillatory fields, with local wavelength changing by an order of magnitude within the simulation domain (Fig.1b...e). Finite-element based solutions require $\sim$10 Gb of RAM and $\sim$ 30s of time to calculate the field distribution around an individual funnel at a specific frequency, virtually preventing large scale or optimization studies.

A neural network (NN, Fig.1f) can learn the field distributions across the metamaterials, drastically speeding up such large scale studies. Recently, NN efforts [4] found wide use in predicting the few-parameter macroscopic responses of the complex electromagnetic systems (reflection/transmission spectra) based on the structure or properties of the composite. However, extending these 'black-box' NNs to the domain of solving for complex field distributions requires extremely large (of the order of 10^4 elements) training sets. Generation of such training sets would by itself be a resource-costly process that would severely limit practical benefits of black box NN tools.

Physics-guided neural nets (PGNN) are known to require smaller training sets than their physics-agnostic counterparts. Previously, PGNNs have been demonstrated on relatively small "toy models" [3]. Here we utilize PGNN formalism to solve for field distribution within wavelength-scale domain with deep subwavelength resolution.

To generate the datasets used in the study, the electromagnetic response of photonic funnels with metamaterial cores was calculated with the commercial finite-element solver, COMSOL Multiphysics [7]. To analyze generalizability of the resulting model, optical response of funnels with five plasma frequencies (6 µm, 7 µm, 8.5 µm, 10 µm and 11 µm) was analyzed. The original FEM-generated datasets have been re-sampled into three separate datasets, 60×20, 300×100, and 600×200 pixels with resolution of 250 nm $\times$ 200 nm, 40 nm $\times$ 50 nm, and 20 nm $\times$ 25 nm, respectively. We refer to these datasets as low, medium, and high-resolution.

The convolutional neural net (CNN) is designed to learn the distribution of the ϕ components of the electric and magnetic fields. As seen in Fig.1f, the network's core remains the same, independent of the data set resolution, with the outer structure producing encoding/decoding from/to a higher resolution. It's inner structure (layer dimensionality and filter size) was optimized using a low-resolution dataset. The medium and high-resolution networks build upon this geometry by adding "hierarchical" downsampling and upsampling layers. The physics-agnostic portion of the CNN is followed by the physics-informed "field-expanding" layer that produces distributions of H_r, H_z components based on Maxwell's equations.

The CNN is trained with a "hybrid" loss function $L = w_\phi L_\phi + w_{rz} L_{rz} + w_{ph} L_{ph}$ where $L_\phi = \left\langle w(r)\left[\left(H_\phi^Y - H_\phi^T\right)^2 + \left(E_\phi^Y - E_\phi^T\right)^2\right]\right\rangle$ describes the radially-weighted MSE for the field components directly produced by the CNN, $L_{rz} = \left\langle w(r)R^2\left[\left(H_r^Y - H_r^T\right)^2 + \left(H_z^Y - H_z^T\right)^2\right]\right\rangle$ represents the regularized radially-weighted MSE for components that are produced by the physics-informed layer, and the physics loss is $L_{ph} = \left\langle\left|\frac{\partial(H_z^Y R^2)}{\partial r} - \frac{\partial(H_r^Y R^2)}{\partial z} + i\frac{\omega}{c}\varepsilon\, E_\phi^Y R^2 - 2\left(H_z^Y R\frac{\partial R}{\partial r} - H_r^Y R\frac{\partial R}{\partial z}\right)\right|\right\rangle/\max\left|H_\phi^Y\right|$. In the expressions above, R is

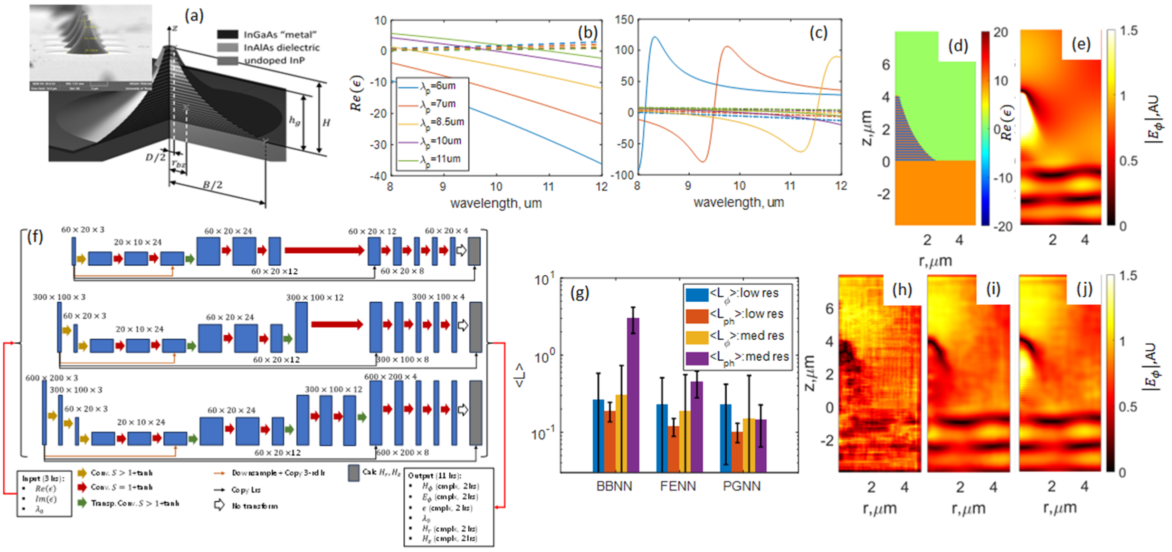

Fig. 1. (a) schematics and the SEM image of a photonic funnel; panels (b,c) illustrate permittivity of the doped layers and effective medium theory permittivity of the metamaterial core, respectively; (d,f) representative distribution of permittivity (d) and intensity (e) within the structure; (f) NN configuration; (g) averaged prediction accuracy (characterized by Loss) for black box (BBNN), field-expanced (FENN), and physics-guided (PGNN) models; panels (h..j) illustrate predictions of BBNN, FENN, and PGNN for the same input/training parameters

a function regularizing the rz fields, superscripts Y and T represent NN outputs and targets, and hyperparameters $w(r), w_\phi, w_{rz}, w_{ph}$ control the relative weight of the components of the loss function [3]. Combinations $(w_\phi = 1, w_{rz} = w_{ph} = 0)$, $(w_\phi = w_{rz} = 1, w_{ph} = 0)$, and $(w_\phi = w_{rz} = 1, w_{ph} \neq 0)$ represent black-box (BB), field-expanded (FE) and Physics-Guided (PG) NNs, respectively. The latter setup can take advantage of unlabeled data to expand the training set without needing to solve the PDEs. All models were trained on ~ 60 labeled points; the PGNN was trained on an additional ~ 30 unlabeled points. Other hyperparameters (learning rate, max epochs, etc) were hand-tuned.

Fig.1(g...j) summarize the main results of our study: the performance of physics-agnostic NNs is significantly below that of field-expanded and physics-informed models, especially when deployed for medium and high-resolution data. Importantly, the field expanded and physics-guided models are not just closer to FEM-based targets but are more consistent with Maxwell equations as compared with "black box" NNs. produce the fields Our results suggest that incorporation of physics constraints into learning process allows for relatively small ($\sim$100 elements) training sets. The approach presented here can be straightforwardly extended to other composite geometries, potentially leading to hybrid FEM-NN computing.

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