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Towards Physics-Informed Graph Neural Network-based Computational Electromagnetics

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***Abstract*—This paper presents a generalizable data-driven computational electromagnetics (CEM) framework leveraging graph neural networks (GNNs). The proposed model supports training and inference for CEM scenarios with different simulation domain sizes and electromagnetic properties, while exploiting the locality of GNNs to achieve reduced complexity and enhanced accuracy. Our results indicate that GNNs can successfully infer the electromagnetic field spatiotemporal evolution for arbitrary simulation domain setups, paving the way for fully-fledged data-driven CEM models.**

I. Introduction

Computational electromagnetics (CEM) provides numerical transient or steady-state solutions to the governing laws of electromagnetism, and they constitute a principal component of multiple scientific disciplines. Transient CEM approaches, such as the finite-difference time-domain (FDTD) method [1], enable the emulation of electromagnetic (EM) field evolution in space and time by solving numerically Maxwell's differential equations; however, their fundamental drawback is that they are computationally demanding. To overcome this limitation, several data-driven frameworks have been proposed recently, aspiring to extract knowledge from synthetic data generated by asymptotic or full-wave CEM solvers [2]–[5]. A major bottleneck in existing approaches is their generalizability, *i.e.*, how a data-driven model can be employed to infer the EM field strength for new scenarios with unknown EM characteristics and arbitrary computational domain size and structure. Specifically, most of the current frameworks leverage convolutional neural networks (CNNs) along with recurrent neural networks and multilayer perceptrons (MLPs) that necessitate that the physical domain assumes a predefined size. On the contrary, CEM is employed to solve problems of varied size and complexity.

To satisfy the essential generalizability requirement, in this paper, we propose a physics-informed graph neural network (GNN)–based CEM framework. The use of shared linear transformations in GNNs enables accruing knowledge simultaneously from and generalizing to transient CEM simulations with varying computational domain sizes and properties. More importantly, unlike approaches exploiting MLPs, or CNNs in conjunction with MLPs, [4], [5], the use of GNNs enables updating the neuron values exploiting information only from some selected adjacent and important nodes, *i.e.*, the EM field inference benefits from *locality*. To further enhance the performance of our framework, we design a physics-based input tensor conveying information related to the EM field evolution, the EM properties of the environment, and the source excitation, as well as a loss function that is appropriate for the problem and related to the EM field values. Ultimately, the proposed framework is trained with FDTD-simulated data and learns to infer the spatial distribution of the electric field over time.

II. Problem Formulation

A. Physics-Informed GNN-based CEM Framework

The implementation of the proposed data-driven framework building on FDTD simulated data is shown in Fig. 1, treating each FDTD cell as a graph node. The input data are represented as an $W \times H \times M$ tensor, where W and H are the numbers of nodes, *i.e.*, FDTD cells, in the horizontal and vertical direction, respectively, and $M = 3 + T_m$ is the number of input features. Specifically, the node input features used are (i) the relative permittivity, ϵ_r, (ii) the conductivity, σ, (iii) the source excitation, J_s, and (iv) the values of the electric field at the previous T_m time steps, E^t to E^{t-T_m}, for each cell of the simulated domain. As shown in Fig. 1, the FDTD cells/nodes form an undirected (unweighted $\&$ bidirectional) graph, where each cell is connected to the surrounding first-hop cells. Then, a two-layer graph attention (GAT) network processes the node input information, updating the node feature values based on their own and their neighbor feature values and eventually transforming them to the target tensor, which is the electric field at the next time step, E^{t+1}.

B. Graph Attention Network

A graph, $\mathcal{G}$, is represented by a set of n_v vertices or nodes, $\mathcal{V}$, and a set of n_e edges, $\mathcal{E}$, connecting the graph nodes, *i.e.*, $\mathcal{G} = (\mathcal{V}, \mathcal{E})$. An edge $e_{i,j} = (v_i, v_j) \in \mathcal{E}$ designates that there is a connection between the nodes v_i and $v_j \in \mathcal{V}$. The set of edges emanating from a node v is called neighborhood and is formally defined as $N(v) = \{v' \in \mathcal{V} | (v, v') \in \mathcal{E}\}$. Each node is associated with a node feature matrix, $\mathbf{X}^v \in \mathcal{R}^{n_v \times M}$, including the features discussed in Section II-A. For a GNN with l cascaded GAT layers, let $\mathbf{H}^{(l)} = [\mathbf{h_1}^{(l)}, \mathbf{h_2}^{(l)}, ..., \mathbf{h_n}^{(l)}] \in \mathcal{R}^{n_v \times M_h^{(l)}}$ be the $M_h^{(l)}$-th dimensional hidden state feature matrix at the l-th layer, with $\mathbf{H}^{(0)} = \mathbf{X}^v$. Then, the updated hidden states of the i-th node, h_i, at the $l+1$ GAT layer with K independent attention heads are computed as [6]:

$$\mathbf{h_i}^{(l+1)} = g\left(\frac{1}{K}\sum_{k}^{K}\sum_{j \in N(v_i)} a_{i,j}^{k,(l)} \mathbf{\Theta}^{(l)} \mathbf{h_j}^{(l)}\right), \tag{1}$$

where g is a non-linear acitvation function, $\mathbf{\Theta}^{(l)}$ applies a shared linear transformation to all nodes, and $a_{i,j}^{k,(l)}$ are the attention coefficients between the i-th and the j-th node for the k-th attention head, computed as in [6] and indicating the importance of the j-th node features to i-th node hidden state.

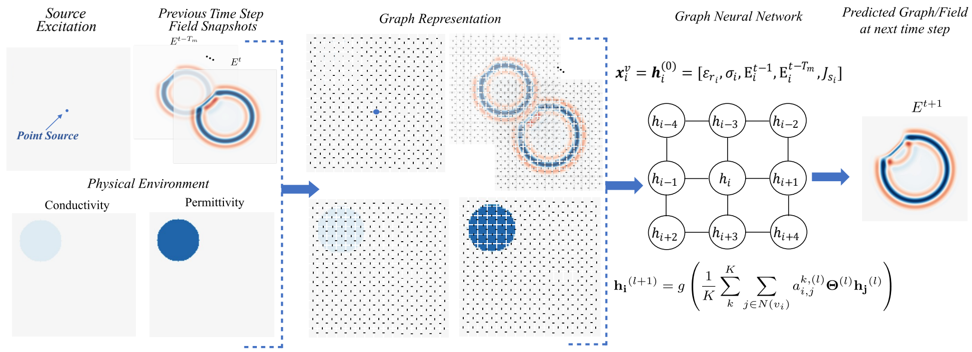


Fig. 1: Proposed physics-informed GNN-based CEM framework.

C. Physcis-based Loss Function

The loss function to be minimized is a mixed mean absolute percentage error (mMAPE), defined as:

$$L(E^{t+1}, \hat{E}^{t+1}) = \begin{cases} |E^{t+1} - \hat{E}^{t+1}|/E^{t+1} & E^{t+1} \geq A/10^2 \\ |E^{t+1} - \hat{E}^{t+1}| & E^{t+1} \leq A/10^2 \end{cases} \quad (2)$$

where A is the amplitude of the EM field, whilst E^{t+1} and $\hat{E}^{t+1}$ depict the ground truth and predict field strength. Using a relative measure as MAPE supports training with different amplitude EM field data, while the use of a simple absolute difference when the target variable assumes small values eliminates biased errors that are innate in MAPE.

III. Numerical Results

The proposed data-driven framework relies on data derived from two-dimensional FDTD simulations assuming a transverse electric polarization and using a perfectly matched layer [1]. The spatial grid is discretized using 20 points per the shortest wavelength of the structure and the Courant number is set to 0.95 [1]. We conduct 1,000 simulations for which the simulation domain contains one or more non-magnetic objects (cylinders, triangles, rectangles, walls) with randomly sampled electric parameters; $\epsilon_r \sim \mathcal{U}(0, 12)$, $\sigma \sim \mathcal{U}(0, 0.5)$. A Gaussian source is placed at a random position within a rectangular grid with a side size equal to 100, 200, 300, or 400 cells, and the EM fields are probed until they decay. For each simulation timestep, we derive an input and target graph, and we use 70% of the simulations to train our model, 10% to select the best-performing instance during training, and 20% to assess its generalizability.

After parameter fine-tuning, the final GNN configuration comprises two GAT layers with $M_h = 32$ and $K = 8$ attention heads each. The data-driven framework is implemented in PyTorch Geometric using an NVIDIA A100 with 80GB of memory, and its weights are computed using the Adam optimization algorithm with the learning rate set to 10^{-4}. Fig. 2 shows the performance of the GNN-based framework for different values of T_m, while inferring the EM field evolution over time using its own predictions. As can be seen, for all T_m values the field strength at the next FDTD iteration is inferred faithfully, however, as the model uses its predictions to infer the field values the error accumulates quickly, and only for $T_m = 16$ we can observe high accuracy predictions, yielding a mMAPE close to 10%. The fidelity of the predictions is further

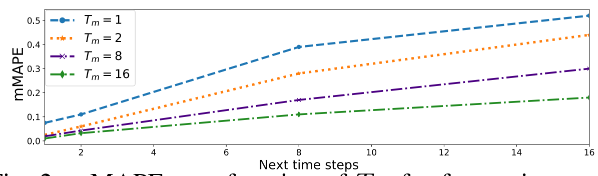
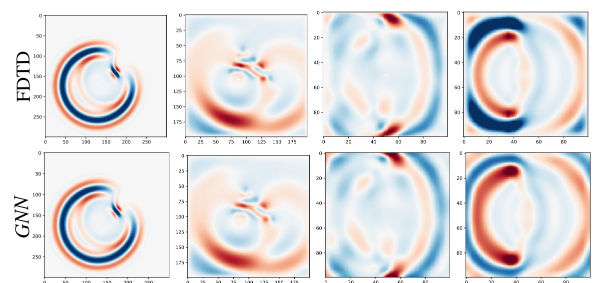


Fig. 2: mMAPE as a function of T_m for future time steps.



(a) $T_n = 1$. (b) $T_n = 2$. (c) $T_n = 8$. (d) $T_n = 16$.

Fig. 3: Electric field snapshots at next iterations, T_n, emulated with FDTD (top) and the GNN with $T_m = 16$ (bottom).

corroborated in Fig. 3 which juxtaposes the simulated electric field via FDTD and the GNN. Overall, the results evince that GNNs can accrue knowledge from different simulation setups and infer reliably the spatiotemporal EM wave propagation for unknown scenarios.

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