PINNs for the time-domain Maxwell equations - Preliminary results

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Preliminary results

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Plan

Motivations

- Surrogate models : ultra-fast electromagnetic solvers
- Include physical and geometrical parameters in addition to space and time/frequency ones
- Main target : inverse design of large-scale photonic devices

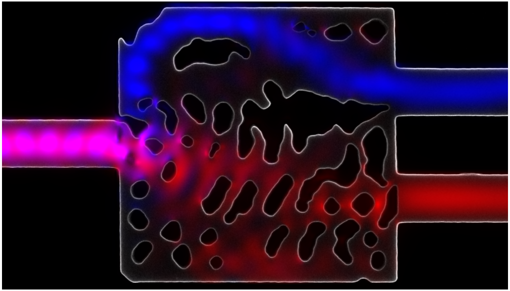


Figure: A compact demultiplexer for telecommunications wavelengths.[1]

[1] Source: https://nqp.stanford.edu/inverse-design-photonics

Objectives

Roadmap

1. Evaluate PINN approach for electromagnetic wave propagation (Maxwell equations)
   - Time-domain formulation
   - Frequency-domain formulation
2. Identify possible directions of methodological improvement
   - Training point sampling strategy
   - Activation function formulation
   - Network topology
   - Other routes : transfer learning, tensor-compressed training, adaptive strategies, etc.
3. Extend PINN models to the nanophotonics setting

Model and IBV problem: the 3D case

Maxwell equations, $\mathbf{x} \in \Omega$, $t > 0$

$$\begin{cases} \varepsilon \partial_t \mathbf{E} - \nabla \times \mathbf{H} = 0 \\ \\ \mu \partial_t \mathbf{H} + \nabla \times \mathbf{E} = 0 \end{cases}$$

$$\mathbf{E} = \mathbf{E}(\mathbf{x}, t) \quad \text{and} \quad \mathbf{H} = \mathbf{H}(\mathbf{x}, t)$$

Boundary conditions: $\partial\Omega = \Gamma_a \cup \Gamma_m$

$$\begin{cases} \mathbf{n} \times \mathbf{E} = 0 \text{ on } \Gamma_m \text{ (metallic boundary)} \\ \mathbf{n} \times \mathbf{E} - \sqrt{\dfrac{\mu}{\varepsilon}} \mathbf{n} \times (\mathbf{H} \times \mathbf{n}) = \mathbf{n} \times \mathbf{E}_{\text{inc}} - \sqrt{\dfrac{\mu}{\varepsilon}} \mathbf{n} \times (\mathbf{H}_{\text{inc}} \times \mathbf{n}) \text{ on } \Gamma_a \text{ (absorbing boundary)} \end{cases}$$

where $(\mathbf{E}_{\text{inc}}, \mathbf{H}_{\text{inc}})$ is a given incident field.

Initial conditions

$$\mathbf{E}_0 = \mathbf{E}(\mathbf{x}, 0) \quad \text{and} \quad \mathbf{H}_0 = \mathbf{H}(\mathbf{x}, 0)$$

Transverse Magnetic mode (TM_z)

$\mathbf{H} = {}^t\left(H_x, H_y, 0\right), \mathbf{E} = {}^t\left(0, 0, E_z\right)$

$$\begin{cases} \varepsilon \dfrac{\partial E_z}{\partial t} & - & \dfrac{\partial H_y}{\partial x} + \dfrac{\partial H_x}{\partial y} = 0, \\ \mu \dfrac{\partial H_x}{\partial t} & + & \dfrac{\partial E_z}{\partial y} = 0 \\ \mu \dfrac{\partial H_y}{\partial t} & - & \dfrac{\partial E_z}{\partial x} = 0 \end{cases}$$

General framework

$$\begin{cases} \dfrac{\partial u(\mathbf{x},t)}{\partial t} + \mathcal{N}[u(\mathbf{x},t);\lambda] & = & 0, \quad \mathbf{x} \in \Omega \subset \mathbb{R}^d, \quad t \in [0,T] \\ u(\mathbf{x},t) & = & g(\mathbf{x},t), \quad \mathbf{x} \in \partial\Omega, \quad t \in [0,T] \\ u(\mathbf{x},0) & = & h(\mathbf{x}), \quad \mathbf{x} \in \Omega, \quad t = 0 \end{cases}$$

where $\mathcal{N}[u(\mathbf{x},t);\lambda]$ is a differential operator parametrized by λ;[a] and $u(\mathbf{x},t)$ is the solution.

Let u_θ be the NN prediction for u and $f(\mathbf{x},t;\theta,\lambda) := \dfrac{\partial}{\partial t} u_\theta(\mathbf{x},t) + \mathcal{N}[u_\theta(\mathbf{x},t);\lambda]$.

Let also $\{\mathbf{x}_i, t_i\}_{i=1}^{N_f} \in \Omega \times [0,T]$.

- Residual part of the loss function : $\mathcal{L}_f(\theta,\lambda) = \dfrac{1}{N_f} \displaystyle\sum_{i=1}^{N_f} |f(\mathbf{x}_i, t_i;\theta,\lambda)|^2$
- Data loss for initial and boundary conditions : $\mathcal{L}_u(\theta) = \dfrac{1}{N_u} \displaystyle\sum_{i=1}^{N_u} |u_\theta(\mathbf{x}_i, t_i) - u_i^*|^2$

  where $\left\{\mathbf{x}_i, t_i, u_i^*\right\}_{i=1}^{N_u}$ denotes the initial and boundary training data on $u(\mathbf{x},t)$.

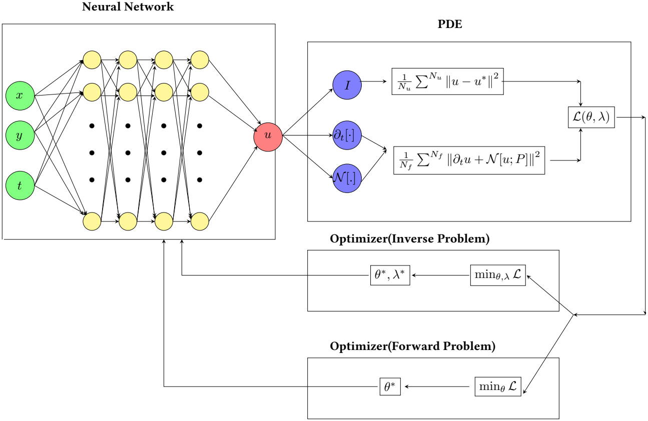
[a] For direct problems λ is (in general) specified.

General framework: problem statement (NN training)

Find the parameters θ (and λ in the inverse case) which minimizes the loss function

$$\mathcal{L}(\theta, \lambda) = w_f \mathcal{L}_f(\theta, \lambda) + w_u \mathcal{L}_u(\theta)$$

where w_f and w_u are loss weights.



Standing wave in a metallic cavity : homogeneous material case

- Material is taken to be the vacuum, i.e., $\varepsilon = \mu = 1$[a]
- The computational domain is defined by $\Omega = [0,1] \times [0,1]$
- Time window for the training is $[0\ ,\ 2\mathrm{m}]$[b]
- Exact time-domain solution

$$\begin{cases} H_x = \dfrac{-\pi}{\omega} \sin(\pi x) \cos(\pi y) \sin(\omega t) \\ H_y = \dfrac{\pi}{\omega} \cos(\pi x) \sin(\pi y) \sin(\omega t) \\ E_z = \sin(\pi x) \sin(\pi y) \cos(\omega t) \end{cases}$$

with $\omega = \pi\sqrt{2}$.

- Boundary condition: $E_z = 0$
- Electromagnetic field at the time $t = 0$ for $(x, y) \in [0,1] \times [0,1]$

$$H_x = H_y = 0, \quad E_z = \sin(\pi x) \sin(\pi y)$$

[a] Relative quantities.
[b] Renormalized units.

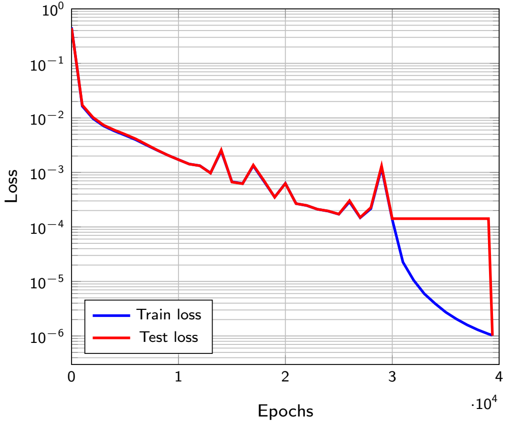
Results using DeepXDE

Standing wave in a metallic cavity (homogeneous material case)

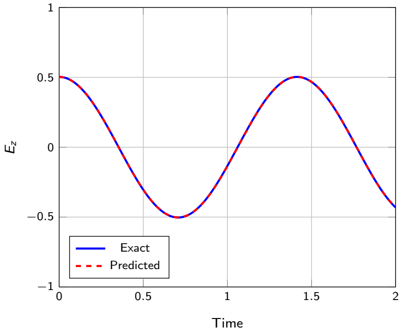
- Numbers of random sample points are $N_0 = 400$, $N_b = 400$ and $N_f = 2000$
- Network structure: 3 inputs (x, y, t), 3 outputs (E_z, H_x, H_y), 4 hidden layers and 50 neurons per layer
- Nonlinear activation function: hyperbolic tangent *tanh*
- The model is first trained for 10 000 iterations using Adam optimizer with learning rate set to 0.001
- L-BFGS optimizer is then used to improve the convergence

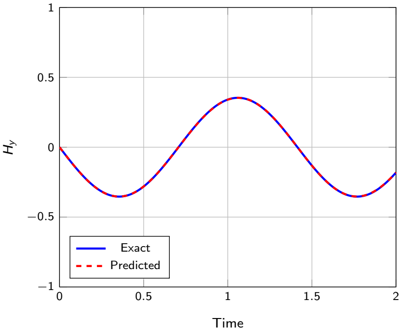
Results using DeepXDE

Standing wave in a metallic cavity (homogeneous material case)



Results using DeepXDE
Standing wave in a metallic cavity (homogeneous material case)





Solutions at $x = 0.75$ m and $y = 0.75$

Results using DeepXDE

Standing wave in a metallic cavity (homogeneous material case)

	L_2 errors	4×20	4×50
$t_0 = 0.25$	$\mathcal{L}_{2,E_z}(t_0)$	$7.6 \cdot 10^{-3}$	$2.2 \cdot 10^{-3}$
	$\mathcal{L}_{2,H_x}(t_0)$	$5.8 \cdot 10^{-3}$	$1.6 \cdot 10^{-3}$
	$\mathcal{L}_{2,H_y}(t_0)$	$5.3 \cdot 10^{-3}$	$1.4 \cdot 10^{-3}$
$t_1 = 1$	$\mathcal{L}_{2,E_z}(t_1)$	$2.3 \cdot 10^{-2}$	$7.2 \cdot 10^{-3}$
	$\mathcal{L}_{2,H_x}(t_1)$	$1.1 \cdot 10^{-2}$	$5.5 \cdot 10^{-3}$
	$\mathcal{L}_{2,H_y}(t_1)$	$1.2 \cdot 10^{-2}$	$3.2 \cdot 10^{-3}$

Relative L_2 errors of E_z, H_x and H_y for two network configurations (4×20 and 4×50)

Standing wave in a metallic cavity : heterogeneous material case

- The computational domain is defined by $\Omega = [0, \frac{5}{4}] \times [0, 1]$
- $\varepsilon = \varepsilon_2$ if $0 \leqslant x \leqslant \frac{1}{2}$ and $0 \leqslant y \leqslant 1$, and $\varepsilon = \varepsilon_1$ if $\frac{1}{2} \leqslant x \leqslant \frac{5}{4}$ and $0 \leqslant y \leqslant 1$
- Exact time-domain solution

$$E_z = \begin{cases} \sin(a_1 x)\sin(by)\sin(\omega t), & 0 \leqslant x \leqslant \frac{1}{2} \quad 0 \leqslant y \leqslant 1 \\ \cos(a_2 x)\sin(by)\sin(\omega t), & \frac{1}{2} \leqslant x \leqslant \frac{5}{4} \quad 0 \leqslant y \leqslant 1 \end{cases}$$

$$H_y = \begin{cases} -\frac{a_1}{\omega}\cos(a_1 x)\sin(by)\cos(\omega t), & 0 \leqslant x \leqslant \frac{1}{2} \quad 0 \leqslant y \leqslant 1 \\ \frac{a_2}{\omega}\sin(a_2 x)\sin(by)\cos(\omega t), & \frac{1}{2} \leqslant x \leqslant \frac{5}{4} \quad 0 \leqslant y \leqslant 1 \end{cases}$$

$$H_x = \begin{cases} \frac{b}{\omega}\sin(a_1 x)\cos(by)\cos(\omega t), & 0 \leqslant x \leqslant \frac{1}{2} \quad 0 \leqslant y \leqslant 1 \\ \frac{b}{\omega}\cos(a_2 x)\cos(by)\cos(\omega t), & \frac{1}{2} \leqslant x \leqslant \frac{5}{4} \quad 0 \leqslant y \leqslant 1 \end{cases}$$

where $\varepsilon_1 = 1, \varepsilon_2 = 2, a_1 = 3\pi, a_2 = 2\pi, b = \pi$, and $\omega = \sqrt{5}\pi$.

Standing wave in a metallic cavity : heterogeneous material case

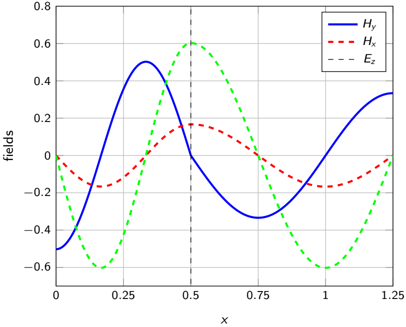
- The computational domain is defined by $\Omega = [0, \frac{5}{4}] \times [0, 1]$
- $\varepsilon = \varepsilon_2$ if $0 \leqslant x \leqslant \frac{1}{2}$ and $0 \leqslant y \leqslant 1$, and $\varepsilon = \varepsilon_1$ if $\frac{1}{2} \leqslant x \leqslant \frac{5}{4}$ and $0 \leqslant y \leqslant 1$
- Time window for the training is [0 , 2m][a]
- Boundary condition: $E_z = 0$
- Electromagnetic field at the time $t = 0$ for $(x, y) \in \Omega$ computed from exact solution

[a] Renormalized units.

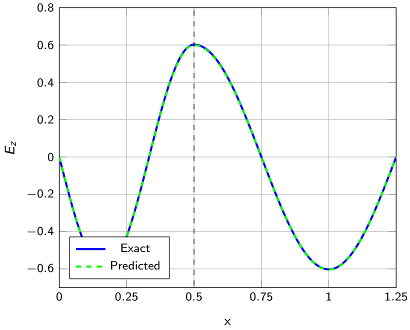
Results using DeepXDE

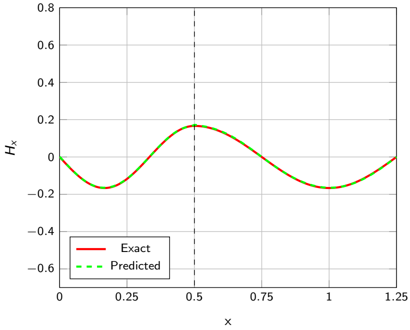
Standing wave in a metallic cavity (heterogeneous material case)

- Numbers of random sample points are $N_0 = 1000$, $N_b = 500$ and $N_f = 5000$
- Network structure: 3 inputs (x, y, t), 3 outputs (E_z, H_x, H_y), 4 hidden layers and 80 neurons per layer
- Nonlinear activation function: hyperbolic tangent *tanh*
- The model is first trained for 30 000 iterations using Adam optimizer with learning rate set to 0.001
- L-BFGS optimizer is then used to improve the convergence

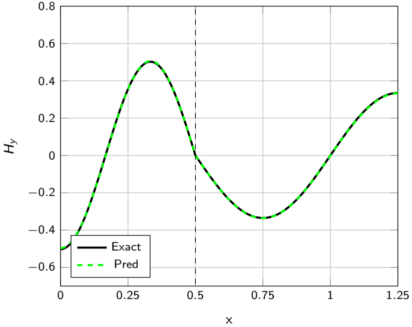


Plots of the analytical solution along the line $y = 0.75$ at time $t = 0.75$ m





Solutions at $t = 0.75$ m and $y = 0.75$.



Solutions at $t = 0.75$ m and $y = 0.75$.

Number of training points	Error on E_z	Error on H_x	Error on H_y	CPU (mn)
1000	$1.38 \cdot 10^{-2}$	$2.08 \cdot 10^{-2}$	$1.33 \cdot 10^{-2}$	19
2500	$7.73 \cdot 10^{-3}$	$1.53 \cdot 10^{-2}$	$9.37 \cdot 10^{-3}$	28
4000	$7.43 \cdot 10^{-3}$	$1.14 \cdot 10^{-2}$	$7.48 \cdot 10^{-3}$	35
5000	$4.88 \cdot 10^{-3}$	$8.60 \cdot 10^{-3}$	$5.35 \cdot 10^{-3}$	40

Relative L_2 errors of E_z,H_x and H_y with different training points

Ongoing works

- Extension to 3D case
- PINNs formulation for parameterized problems
- Interpolation versus extrapolation in output predictions
- Detailed performance study
- CPU versus GPU acceleration

Thank you!

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