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## **PINNs for the time-domain Maxwell equations - Preliminary results**

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# PINNs for the time-domain Maxwell equations

## Preliminary results

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- 1 Objectives of the study
- 2 Mathematical model
- 3 PINN formulation
- 4 Results using DeepXDE  
CHECK OUR TUTORIAL “A Short Introduction to Physics-Informed Neural Networks” TOMORROW!
  - Standing wave in a metallic cavity : homogeneous material case
  - Standing wave in a metallic cavity : heterogeneous material case
- 5 Closure

## 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

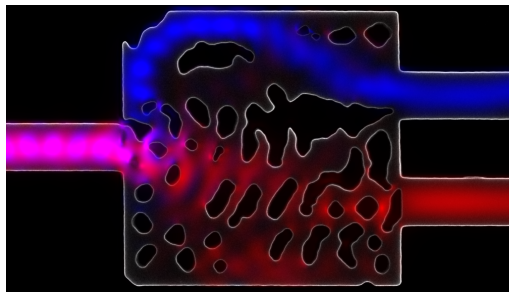


Figure: A compact demultiplexer for telecommunications wavelengths.<sup>1</sup>

<sup>1</sup>Source: <https://nqp.stanford.edu/inverse-design-photonics>

## 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:  $\partial\Omega = \Gamma_a \cup \Gamma_m$

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

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 ( $\text{TM}_z$ )

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

$$\left\{ \begin{array}{l} \epsilon \frac{\partial E_z}{\partial t} - \frac{\partial H_y}{\partial x} + \frac{\partial H_x}{\partial y} = 0, \\ \mu \frac{\partial H_x}{\partial t} + \frac{\partial E_z}{\partial y} = 0 \\ \mu \frac{\partial H_y}{\partial t} - \frac{\partial E_z}{\partial x} = 0 \end{array} \right.$$

## General framework

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

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

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

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

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

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

<sup>a</sup>For direct problems  $\lambda$  is (in general) specified.

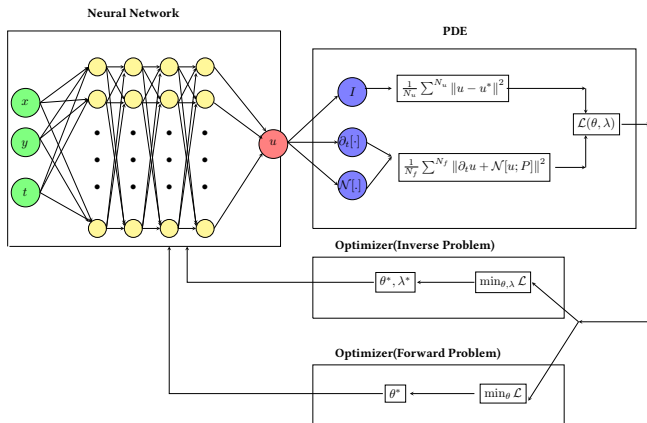


## General framework: problem statement (NN training)

Find the parameters  $\theta$  (and  $\lambda$  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  $[0, 2\pi]^b$
- Exact time-domain solution

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

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

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

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

<sup>a</sup>Relative quantities.

<sup>b</sup>Renormalized units.

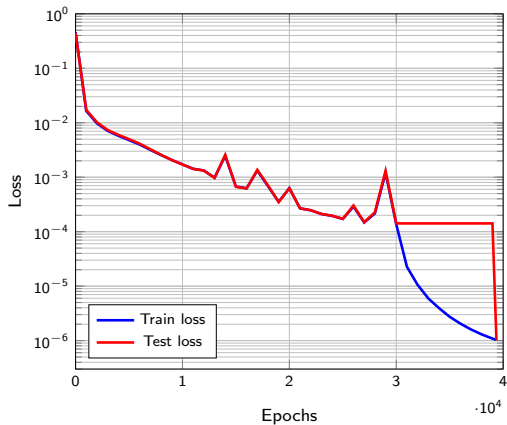
# Results using DeepXDE

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

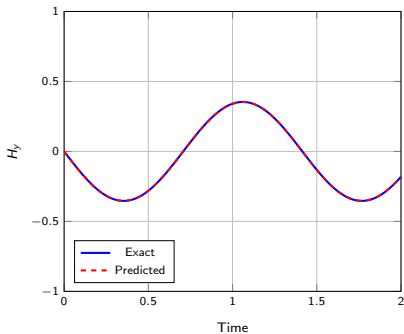
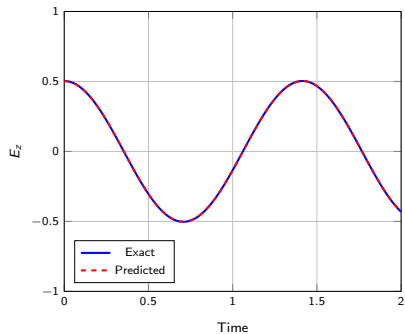
# Results using DeepXDE

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

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

## 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  $0 \leq x \leq \frac{1}{2}$  and  $0 \leq y \leq 1$ , and  $\varepsilon = \varepsilon_1$  if  $\frac{1}{2} \leq x \leq \frac{5}{4}$  and  $0 \leq y \leq 1$
- Exact time-domain solution

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

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

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

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  $0 \leq x \leq \frac{1}{2}$  and  $0 \leq y \leq 1$ , and  $\varepsilon = \varepsilon_1$  if  $\frac{1}{2} \leq x \leq \frac{5}{4}$  and  $0 \leq y \leq 1$
- Time window for the training is  $[0, 2\pi]^a$
- Boundary condition:  $E_z = 0$
- Electromagnetic field at the time  $t = 0$  for  $(x, y) \in \Omega$  computed from exact solution

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<sup>a</sup>Renormalized units.



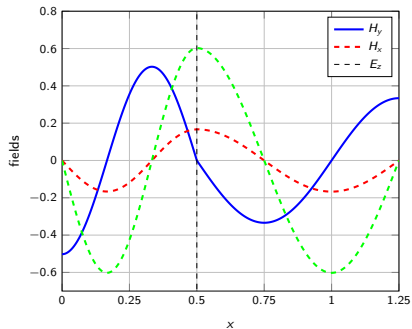
# Results using DeepXDE

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

# Results using DeepXDE

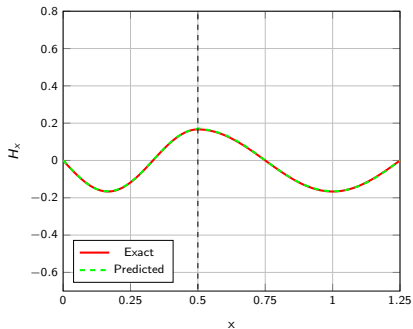
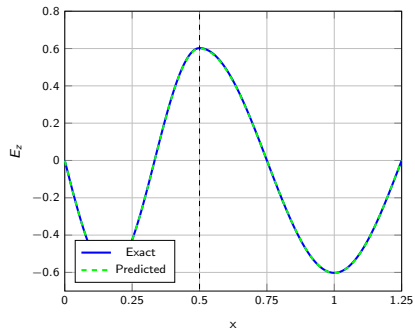
Standing wave in a metallic cavity (heterogeneous material case)



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

# Results using DeepXDE

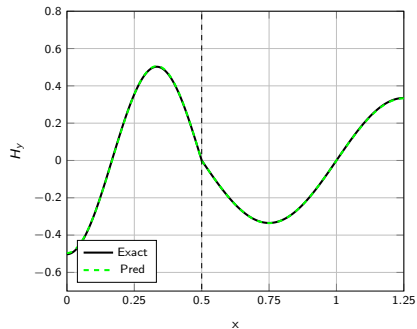
Standing wave in a metallic cavity (heterogeneous material case)



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

# Results using DeepXDE

Standing wave in a metallic cavity (heterogeneous material case)



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

# Results using DeepXDE

Standing wave in a metallic cavity (heterogeneous material case)

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

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

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