

Fraunhofer-Institut für Integrierte Systeme und Bauelementetechnologie IISB

Physics-informed Neural Networks for quasi-static Maxwell's Equations

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- Quasi-static Maxwell Equation
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Introduction



Motivation

- Applications in Power-Electronics require accurate simulation of the underlying Physics in order to optimize Devices or Processes
- accurate numerical Schemes and Softwares (FEM, FD, etc.) usually exist but can be:
 → computationally demanding
 → even more demanding at scale for optimization purposes with many degrees of freedom
- traditional ML-Approaches:
 - \rightarrow quick inference times on trained Models
 - ightarrow limited possibility to include physics
 - \rightarrow "black-box"





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→ Physics-Informed Neural Networks





Physics-Informed Neural Networks

- notion first introduced by Raissi et al. in 2017 [4]
- Conceptual Difference in how Neural Networks are trained:
 - <u>classical Neural Network</u>:
 - "data-supervised Learning"
 - e.g.: Input-Image \rightarrow Output-Image
 - Loss-Function: e.g. MSE over all pixels
 - Physics-Informed Neural Network:
 - "physics-supervised" Learning
 - e.g.: $(x, y, t) \rightarrow u(x,y,t) \rightarrow (du/dx, du/dy, du/dt, ...)$
 - Loss-Function: Residuals on PDE, BCs, ICs







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 - Loss-Function: Residuals on PDE, BCs, ICs
- Benefits
 - no data required \rightarrow explicit supervision by Physics
 - implicit meshing \rightarrow adaptive strategies can be applied
 - generalization \rightarrow additional Inputs e.g. for different Geometries







Parametrization of Heat Sink Geometries [6]



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 - generalization \rightarrow additional Inputs e.g. for different Geometries
- Increasing Amounts of Publications and (Open-Source) Software [5]



Temperature Simulation in Fluids & Solids [7]







Parametrization of Heat Sink Geometries [6]



Blood flow simulation in an Aneurysm [7]



Simulation of aircraft cabin panel stress [7]



A Use-Case from Power-Electronics Topology-Optimization of a Power Converter







Goals

- 1. Approximation of magnetic Fields by solving quasi-static Maxwell's Equation
- 2. Calculation of relevant Quantities like Inductivities and Coupling k
- 3. Optimization of Topology with respect to those Quantities

$$k = \frac{M}{\sqrt{L_{11}L_{22}}}.$$

$$M \coloneqq L_{12} = L_{21}.$$







Modeling



Modeling Quasi-static Maxwell Equation

K.Angermeier: "Topology-Optimization of inductive Components" [8]

$$\nabla \times \boldsymbol{H} = \boldsymbol{J} + \frac{\partial \boldsymbol{D}}{\partial t} \quad (1)$$
$$\nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t} \quad (2)$$
$$\nabla \cdot \boldsymbol{B} = 0 \quad (3)$$
$$\nabla \cdot \boldsymbol{D} = \rho \quad (4)$$
$$\boldsymbol{B} = \mu \boldsymbol{H}$$
$$\boldsymbol{J} = \sigma \boldsymbol{E} \quad (5)$$
$$\boldsymbol{D} = \varepsilon \boldsymbol{E}.$$





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- no free electric charges/currents
- Existence of magnetic Vector Potential A, s.t.

 $\boldsymbol{B} =
abla imes \boldsymbol{A}$

Coulomb Gauging for Uniqueness of A

$$\nabla \cdot \boldsymbol{A} = 0$$

 rotational symmetry, current J only in zdirection







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$$\sigma \frac{\partial \boldsymbol{A}}{\partial \boldsymbol{\iota}} + \nabla \times \frac{1}{\mu} \nabla \times \boldsymbol{A} = \boldsymbol{J}$$

time-dependence on J and A

$$J_z(x, y; t) = e^{i\omega t} \overline{J_z}(x, y)$$
$$A_z(x, y; t) = e^{i\omega t} \overline{A_z}(x, y)$$

$$\sigma i \omega \overline{A}_z(x,y) + \frac{1}{\mu} \left(-\frac{\partial^2 \overline{A}_z(x,y)}{\partial x^2} - \frac{\partial^2 \overline{A}_z(x,y)}{\partial y^2} \right) = \overline{J}_z(x,y)$$



Modeling Boundary Conditions





 anti-symmetric Mirroring of source currents by enforcing zero magnetic flux across Boundary, cf. Harlander, 2002 [9]:

 $\boldsymbol{n}\cdot\boldsymbol{B}=0$

 Biro, Preis, 1989 [10]: equivalence to homogeneous dirichlet conditions on magnetic Vector Potential A

$$A_z n_x = 0, \ A_z n_y = 0$$



Modeling Interface Conditions



$H(\operatorname{div};\Omega) \coloneqq \left\{ v \in L^2(\Omega)^3 : \nabla \cdot v \in L^2(\Omega) \right\}$	}
$H(\operatorname{rot};\Omega) \coloneqq \left\{ v \in L^2(\Omega)^3 : \nabla \times v \in L^2(\Omega)^3 \right\}$	'}

$\boldsymbol{H}(\cdot,t)\in$	$H(\mathrm{rot};\Omega),$	$\boldsymbol{E}(\cdot,t)$	e	$H(\operatorname{rot};\Omega)$
$\boldsymbol{B}(\cdot,t)\in$	$H(\operatorname{div}; \Omega),$	$oldsymbol{J}(\cdot,t)$	e	$H(\operatorname{div};\Omega)$

• For L2-Regularity, we require continuity across interfaces [11]:

• normal component of magnetic flux
$$\rightarrow$$
 B₁·n = B₂·n

 $oldsymbol{B} =
abla imes oldsymbol{A}$

$$(A_{z2} - A_{z1})n_y = 0, \ (A_{z2} - A_{z1})n_x = 0$$



Modeling Interface Conditions



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$$\nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t}$$
$$\boldsymbol{J} = \sigma \boldsymbol{E}$$

$$\sigma_1 n_z \overline{A}_{z1} - \sigma_2 n_z \overline{A}_{z2} = 0$$



■ normal component of current \rightarrow J₁·n = J₂·n

Modeling Interface Conditions



$H(\operatorname{div}; \Omega) \coloneqq$	${v \in L^2(\Omega)^3}$:	$\nabla \cdot v \in L^2(\Omega) \Big\}$
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$\boldsymbol{H}(\cdot,t)\in H(\mathrm{re}$	\mathbf{D} t; Ω), $\boldsymbol{E}(\cdot, t)$	\in	$H(\mathrm{rot};\Omega)$
$\boldsymbol{B}(\cdot,t)\in H(\mathrm{d}t)$	iv; Ω), $\boldsymbol{J}(\cdot, t)$	\in	$H(\operatorname{div};\Omega)$

- For L2-Regularity, we require continuity across interfaces [11]:
 - normal component of magnetic flux \rightarrow B₁·n = B₂·n

$$oldsymbol{B} =
abla imes oldsymbol{A}.$$

$$(A_{z2} - A_{z1})n_y = 0, \ (A_{z2} - A_{z1})n_x = 0$$

• normal component of current
$$\rightarrow J_1 \cdot n = J_2 \cdot n$$



$$\sigma_1 n_z \overline{A}_{z1} - \sigma_2 n_z \overline{A}_{z2} = 0$$

• tangential component of magnetic field intensity
$$\rightarrow$$
 H₁·t = H₂·t



$$\left(\frac{1}{\mu_1}\frac{\partial A_{z1}}{\partial x} - \frac{1}{\mu_2}\frac{\partial A_{z2}}{\partial x}\right)n_z = 0, \ \left(\frac{1}{\mu_1}\frac{\partial A_{z1}}{\partial y} - \frac{1}{\mu_2}\frac{\partial A_{z2}}{\partial y}\right)n_z = 0, \\ \left(\frac{1}{\mu_2}\frac{\partial A_{z2}}{\partial x} - \frac{1}{\mu_1}\frac{\partial A_{z1}}{\partial x}\right)n_x + \left(\frac{1}{\mu_2}\frac{\partial A_{z2}}{\partial y} - \frac{1}{\mu_1}\frac{\partial A_{z1}}{\partial y}\right)n_y = 0.$$



Modeling Summary







$$\begin{split} \sigma i\omega \overline{A}_z(x,y) + \frac{1}{\mu} \left(-\frac{\partial^2 \overline{A}_z(x,y)}{\partial x^2} - \frac{\partial^2 \overline{A}_z(x,y)}{\partial y^2} \right) &= \overline{J}_z(x,y) \\ \text{Randbedingungen:} \\ A_z n_x &= 0, \ A_z n_y = 0 \ \text{auf } \Gamma \\ \text{Interfacebedingungen:} \\ (A_{z2} - A_{z1})n_y &= 0, \ (A_{z2} - A_{z1})n_x = 0 \ \text{auf } \Sigma_{12} \\ \left(\frac{1}{\mu_1} \frac{\partial A_{z1}}{\partial x} - \frac{1}{\mu_2} \frac{\partial A_{z2}}{\partial x} \right) n_z &= 0, \ \left(\frac{1}{\mu_1} \frac{\partial A_{z1}}{\partial y} - \frac{1}{\mu_2} \frac{\partial A_{z2}}{\partial y} \right) n_z = 0, \\ \left(\frac{1}{\mu_2} \frac{\partial A_{z2}}{\partial x} - \frac{1}{\mu_1} \frac{\partial A_{z1}}{\partial x} \right) n_x + \left(\frac{1}{\mu_2} \frac{\partial A_{z2}}{\partial y} - \frac{1}{\mu_1} \frac{\partial A_{z1}}{\partial y} \right) n_y = 0 \ \text{auf } \Sigma_{12} \\ \sigma_1 n_z \overline{A}_{z1} - \sigma_2 n_z \overline{A}_{z2} = 0 \ \text{auf } \Sigma_{12}. \end{split}$$





Modeling Main Challenges





- Main Issues (presumably):
 - numerically small material parameters
 - permeability jumps by a factor of 2000 across interfaces

Property	Ferrit	Air
Permeability $\mu \; [H/m]$	2.704e-3	1.255e-6
Conductivity $\sigma\left[1/(\Omega^*m)\right]$	5.8e-7	0.0

- Beltran-Pulido et. al, 2022 [12]
 - "... help to alleviate the effects of sharp changes of material properties across interfaces between materials"







introducing rescaled, non-dimensionalized variables and parameters:

$$\sigma i \omega A + \nabla (\frac{1}{\mu} (-\nabla A)) = J$$





$$\overline{\sigma}\overline{A} + \overline{\nabla}(\frac{1}{\overline{\mu}}(-\overline{\nabla}\ \overline{A})) = \overline{J}$$



introducing rescaled, non-dimensionalized variables and parameters:

$$\sigma i \omega A + \nabla (\frac{1}{\mu} (-\nabla A)) = J$$

$$\overline{x} = \frac{x}{x^*}$$
$$\overline{A} = \frac{A}{A^*}$$
$$\overline{J} = \frac{J}{J^*}$$
$$\overline{\mu} = \frac{\mu}{\mu^*}$$
$$\overline{\sigma} = \frac{\sigma}{\sigma^*}$$

$$\mu^* = \frac{A^*}{(x^*)^2 J^*}$$
$$\sigma^* = \frac{J^*}{i\omega A^*}$$

$$\overline{\sigma}\overline{A} + \overline{\nabla}(\frac{1}{\overline{\mu}}(-\overline{\nabla}\ \overline{A})) = \overline{J}$$

• choice of constants, cf. [12], s.t.:

 $rac{1}{\overline{\mu}} \in [0.05, 100]$

$$x^* = 7.0 \text{ cm}$$

$$A^* = 4.9 \frac{\text{mWb}}{\text{m}}$$

$$\mu^* = 1.352 \cdot 10^{-4} \frac{\text{H}}{\text{m}}$$

$$\int J^* = 1.352 \cdot 10^4 \frac{\Lambda}{\text{m}^2}$$

$$\sigma^* = 0.2759 \cdot 10^4$$



 (so far only) empirical evidence that even really simple use-cases behave a lot more stable in the nondimensionalized setting









Implementation



Implementation PINN-Frameworks

- technical simplicity of the approach:
 - many open-source implementations available:
 - stand-alone Code for highly specific Problems
 - more general Frameworks with active development and maintenance
- Nvidia Modulus [6]:
 - formerly known as SimNet[™] [13]
 - more advanced, professionally maintained
 - more demanding/difficult to setup, especially in HPC-Environments
- DeepXDE [14]:
 - Python-based Framework
 - support for all common Machine-Learning Libraries (TensorFlow, PyTorch, ...)
 - active online-community with many Publications connected to it
 - \rightarrow currently Framework of Choice for our work:
 - ightarrow introduction of several Use-Cases to reflect different Complexity-Aspects



DeepXDE-Flowchart[14]



Implementation

Use-Cases & Reference Solutions





Implementation Reference Solutions





open-source Software FEMM: Finite-Element-Method Magnetics [15]



Implementation **Reference Solutions**

Need for Reference Solutions in Practice

Losses:

- numerically depend on weights
- might be misbalanced and misleading
- evaluation via relative L2-Error more helpful, e.g. to determine good Hyperparameters







Chapter 04

PINNs in Practice



PINNs in Practice (Adaptive) Loss-Weighting

- Different Types and Numbers of Loss-Terms depending on Problem Formulation
 - PDE-Loss(es)
 - Loss for PDE-Residual
 - Loss for B = rot(A)



- Boundary Condition Losses
 - Dirichlet-Type Conditions can be enforced directly via Network-Structure
 - all other Types lead to additional Loss-Terms
- Interface Condition Losses
 - additional Terms for any Interfaces
 - amount increasing with complexity of topology
- Mathematically Advanced Strategies exist based on:
 - Neural Tangent Kernel [16] \rightarrow Spectral Bias of Neural Networks
 - augmented Lagrangian Method $[17] \rightarrow$ adaptive Imitation of Lagrange-Multipliers





PINNs in Practice (Adaptive) Loss-Weighting

Example: Weighting of Interface Condition Loss



Output

- 0.0025

- 0.0000

-0.0025

IC-Residual

0.0035

0.0030

PINNs in Practice Adaptive Sampling

- uniform sampling does not resolve the most dynamic areas sufficiently:
 - interfaces where material properties change
 - conductive parts of the material



- Residual-based adaptive Refinement (RAR)
 - based on the highest Residuals (PDE, BC, IC,..) new points in the domain are selected for Training
 - leads to new Hyperparameters
 - how many points to add?
 - at which point during training should this be done?
 - how often and how long (# epochs) should a Refinement-Step be done?







Chapter 05

Results & Outlook



Intermediate Results Use-Case a1



early Trials without Interface Conditions:



Residual-based Adaptive Refinement

To be continued...









Intermediate Results Use-Case b1







early Trials without Interface Conditions:







Residual-based Adaptive Refinement

To be continued...



Intermediate Results Effect of Interface Conditions

$(A_{z2} - A_{z1})n_y = 0, (A_{z2} - A_{z1})n_x = 0 \text{ auf } \Sigma_{12}$
$\left(\frac{1}{\mu_1}\frac{\partial A_{z1}}{\partial x} - \frac{1}{\mu_2}\frac{\partial A_{z2}}{\partial x}\right)n_z = 0, \\ \left(\frac{1}{\mu_1}\frac{\partial A_{z1}}{\partial y} - \frac{1}{\mu_2}\frac{\partial A_{z2}}{\partial y}\right)n_z = 0,$
$\left(\frac{1}{\mu_2}\frac{\partial A_{z2}}{\partial x} - \frac{1}{\mu_1}\frac{\partial A_{z1}}{\partial x}\right)n_x + \left(\frac{1}{\mu_2}\frac{\partial A_{z2}}{\partial y} - \frac{1}{\mu_1}\frac{\partial A_{z1}}{\partial y}\right)n_y = 0 \text{ auf } \Sigma_{12}$
$\sigma_1 n_z \overline{A}_{z1} - \sigma_2 n_z \overline{A}_{z2} = 0 \text{ auf } \Sigma_{12}.$



0 1 2 3 4 5 6 7

0.08 0.06 0.04 0.02 0.00 - 0.08

0.06

- 0.04

- 0.02

- 0.00

0

1 2 3 without Interface Conditions









Outlook

- Implementation & Evaluation of more advanced PINN-Specific Methods
 - Augmented Lagrangian Method for Loss-Balancing
 - Good Strategies for adaptive Sampling
- Tuning of Hyperparameters:
 - choice of optimizer (ADAM, L-BFGS,
 - activation functions, learning rate(-decay)
 - neural network size and structure
 - Parameter related to training schemes \rightarrow Residual-based Refinement, Lagrange-Method
 - ...there are many!
- Parametrization of Topologies \rightarrow Generalization of PINN for arbitrary Topologies
- Further Read → Recent Survey on PINNs for Scientific Machine Learning [18]







References

Images:

- [1] <u>Planar Inductor</u>
- [2] <u>Ferrit-Cores</u>
- [3] <u>Lithography</u>

Publications & Software:

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Thank you for your Attention!