Physics-Informed Neural Networks

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Group Exl at MMM (Uni Vie) ”Math. Machine Learning”

- MMM: Development of innovative resource-saving / environmentally friendly (magnetic) materials and materials in biology/medicine. (4 Faculties involved)
- Synergy with FWF projects like P31140 and P35413
- Development of num. Methods in „Computational & Data Science“
- Esp. data-driven Reduced Order Approaches in Micromagnetism
- Efficient solution of PDEs (with ML)

Partial Differential Equations

- fluid dynamic
- heat diffusion
- electromagnetism
- celestial mechanics
- quantum mechanics
- etc.

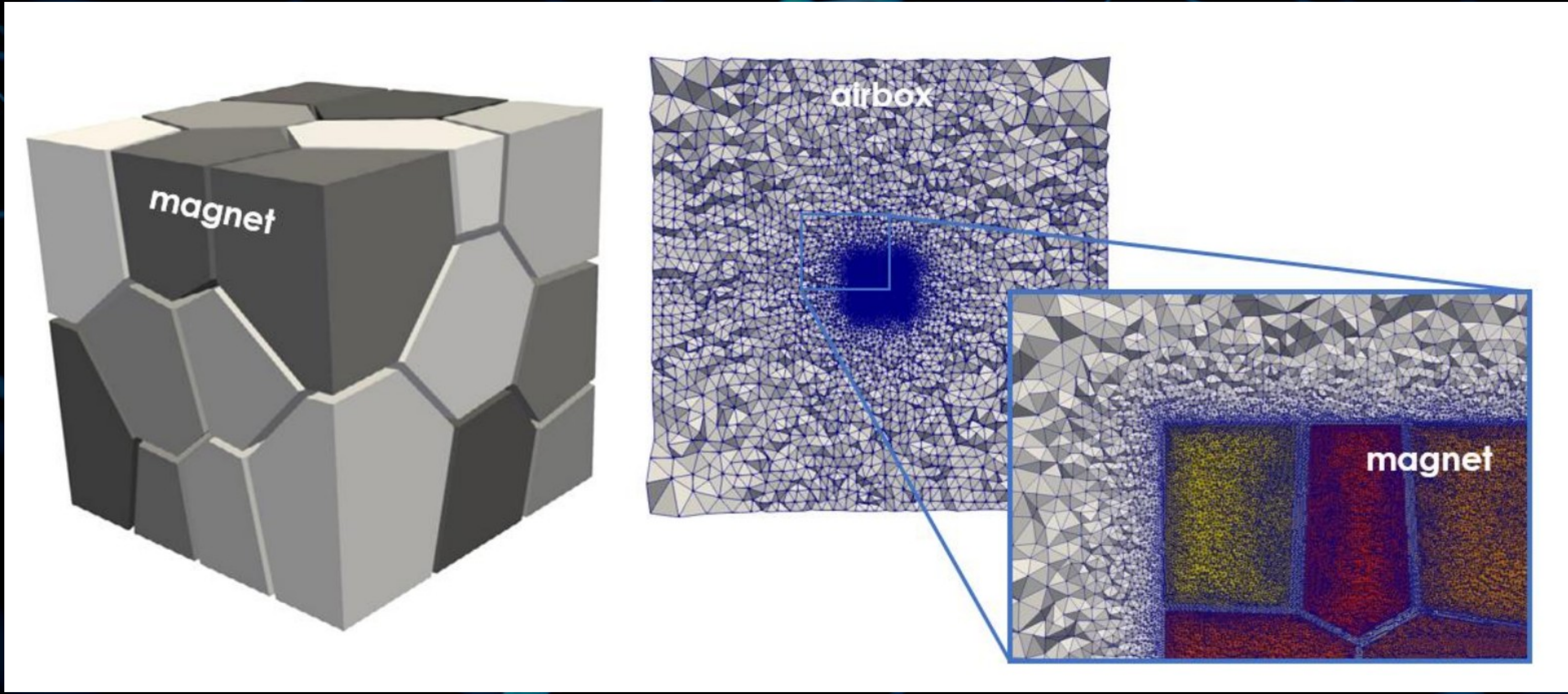
$$\rho(\frac{\partial \boldsymbol{u}}{\partial t}+\boldsymbol{u}\cdot\nabla\,\boldsymbol{u})=\nabla\,p+\rho g+\mu\Delta\boldsymbol{u}$$

$$\frac{\partial u}{\partial t}=c\,\Delta u$$

$$\nabla\cdot\boldsymbol{D}=\rho_v$$
$$\nabla\cdot\boldsymbol{B}=0$$
$$\nabla\times\boldsymbol{E}=-\frac{\partial\,\boldsymbol{B}}{\partial t}$$
$$\nabla\times\boldsymbol{H}=\frac{\partial\,\boldsymbol{D}}{\partial t}+\boldsymbol{J}$$

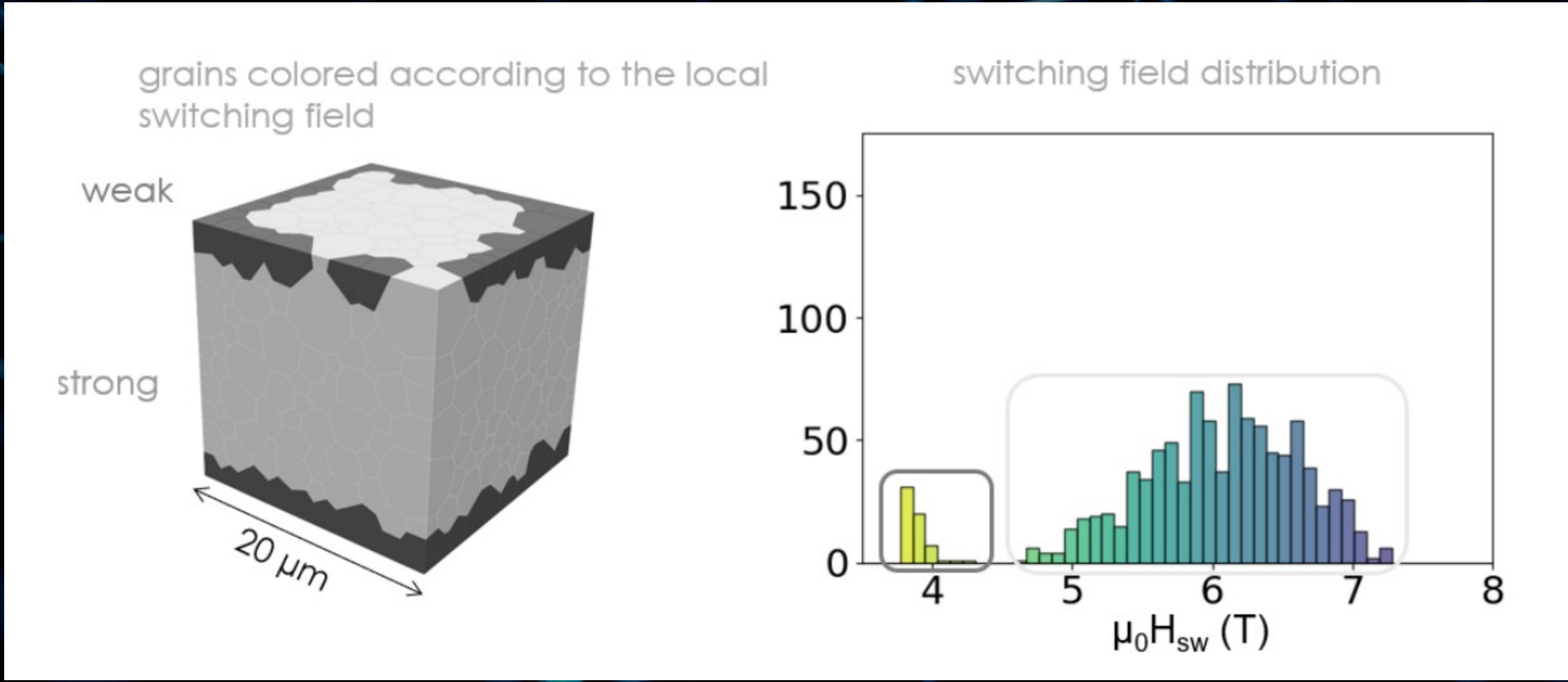
$$i\hbar\frac{\partial\boldsymbol{\Psi}}{\partial t}=\hat{H}\,\boldsymbol{\Psi}$$

Numerical Magnetism



Exl, Lukas, et al. "Magnetic microstructure machine learning analysis." Journal of Physics: Materials 2.1 (2018): 014001.

Numerical Magnetism



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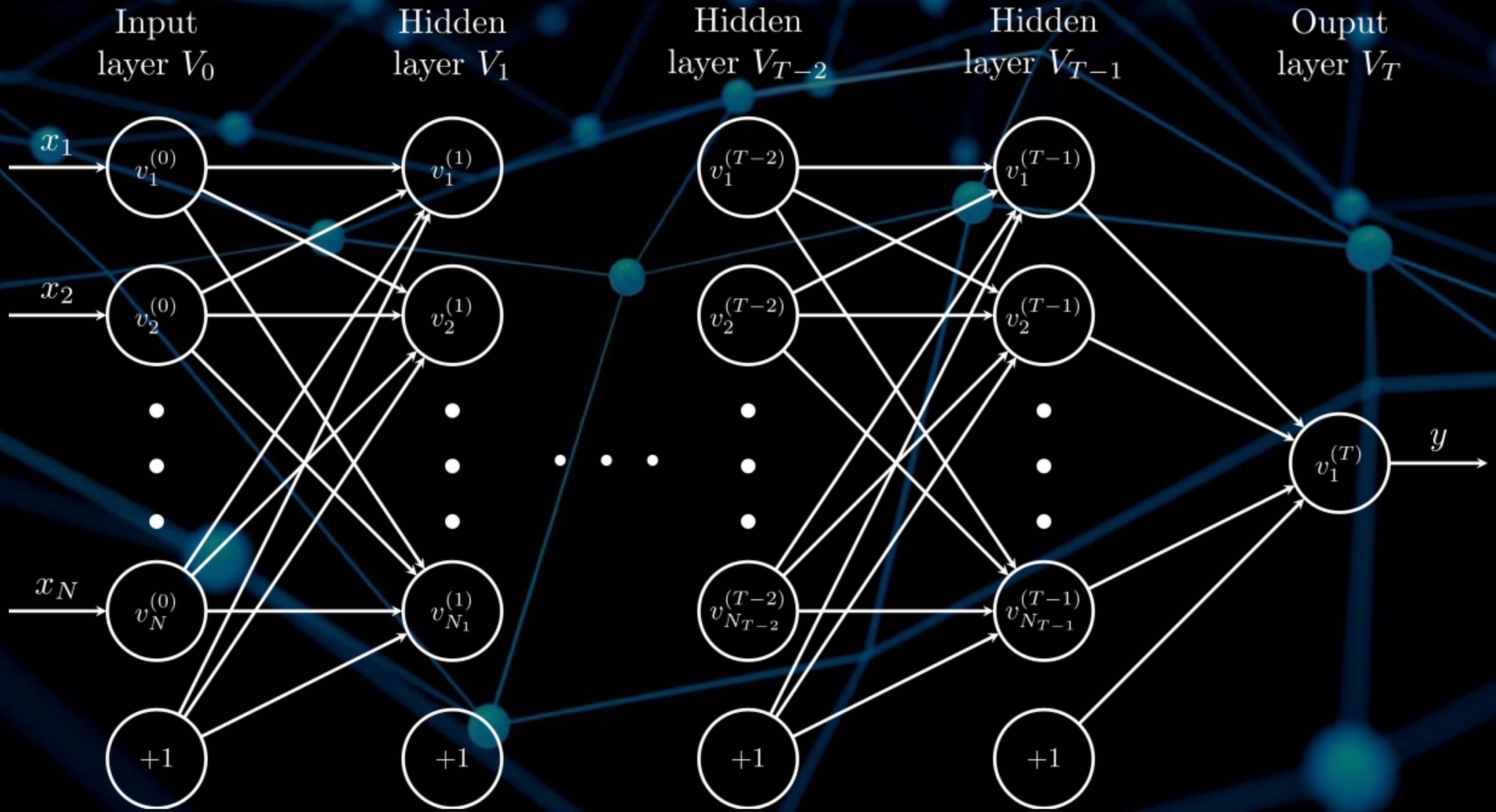
Neural Networks



Supervised

- Training samples

$\{x_1, \ldots, x_n\} \quad \{y_1, \ldots, y_n\}$

- Minimize objective

$$MSE(\omega) = \frac{1}{n}\sum_{i=1}^{n}(\mathcal{N}(\mathbf{x}_i;\omega) - y_i)^2 \rightarrow min_\omega!$$

Physics-Informed (unsupervised)

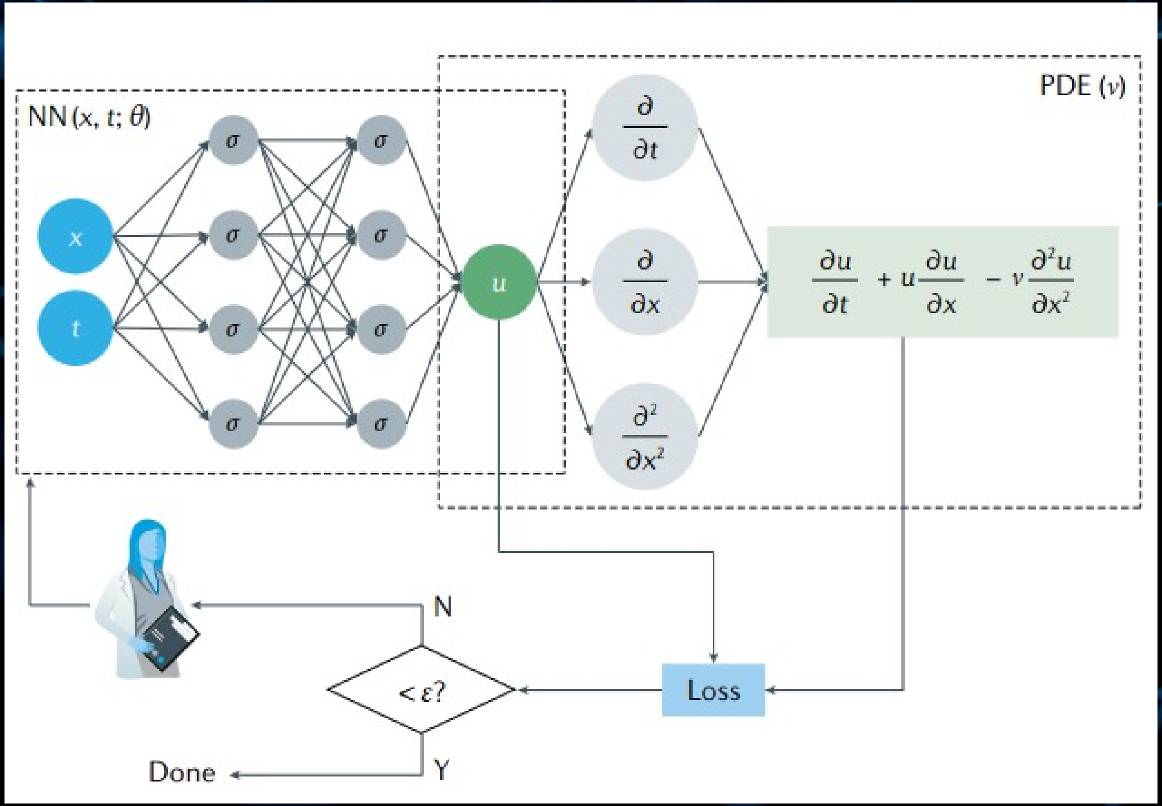
- Training samples

$\{x_1, \ldots, x_n\}$

- Minimize physics informed objective

$$\frac{1}{n}\sum_{i=1}^{n} L(\mathcal{N}(\mathbf{x}_i;\omega)) + \mathrm{Penalty}(\omega) \rightarrow min_\omega!$$

Physics-Informed Neural Networks



$$u^* = \arg\min_u \Big(\underbrace{\sum_i L(u(x_i), y_i)}_{\text{label-based}} + \underbrace{\lambda_r R(u)}_{\text{regularization}} + \underbrace{\lambda_k L_k(u(x_i), x_i)}_{\text{knowledge-based}} \Big)$$

Karniadakis, George Em, et al. "Physics-informed machine learning." Nature Reviews Physics 3.6 (2021): 422-440.

Stray Field Problem

$$
\begin{aligned}
-\Delta\phi &= -\nabla\cdot\boldsymbol{m} \quad \text{in } \Omega\subset\mathbb{R}^3,\\
-\Delta\phi &= 0 \quad \text{in } \overline{\Omega}^c,\\
[\phi] &= 0 \quad \text{in } \partial\Omega,\\
\left[\frac{\partial\phi}{\partial\boldsymbol{n}}\right] &= -\boldsymbol{m}\cdot\boldsymbol{n} \quad \text{in } \partial\Omega,\\
\phi(\boldsymbol{x}) &= \mathcal{O}\left(\frac{1}{\|\boldsymbol{x}\|_2}\right) \quad \text{as } \|\boldsymbol{x}\|_2\to\infty.
\end{aligned}
$$

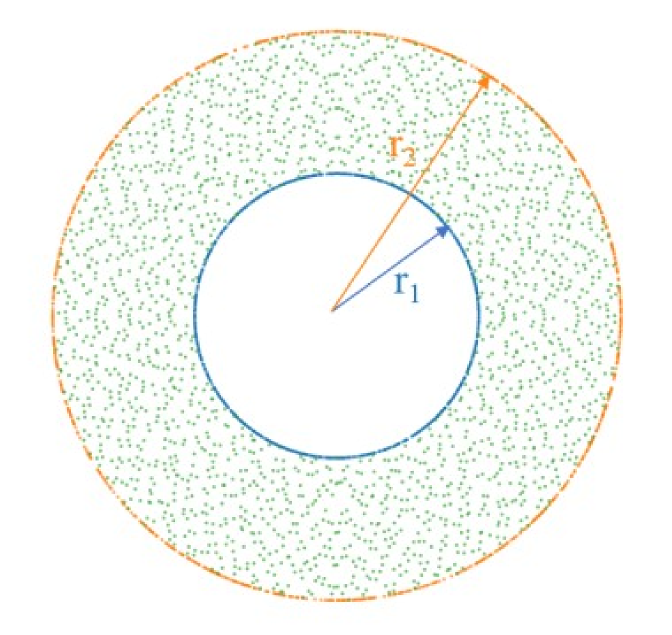
$$
\begin{aligned}
-\Delta\phi_1 &= -\nabla\cdot\boldsymbol{m} \quad \text{in } \Omega,\\
\phi_1 &= 0 \quad \text{on } \partial\Omega,
\end{aligned}
$$

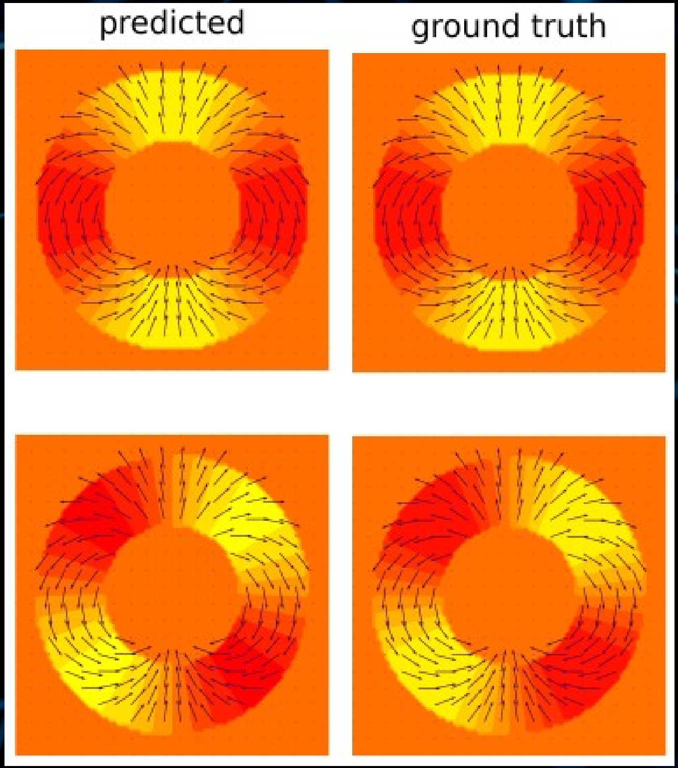
$$
-\Delta\phi_2 = 0 \quad \text{in } \Omega,
$$

$$
\phi_2^*(\boldsymbol{x}) = \int_{\partial\Omega}\left(\frac{(\boldsymbol{m}\cdot\boldsymbol{n}-\frac{\partial}{\partial_{\boldsymbol{n}}}\phi_1)(\boldsymbol{y})}{4\pi\|\boldsymbol{x}-\boldsymbol{y}\|_2}\right)d\sigma(\boldsymbol{y})
$$

Exl, Lukas, and Thomas Schrefl. "Non-uniform FFT for the finite element computation of the micromagnetic scalar potential." Journal of Computational Physics 270 (2014): 490-505.

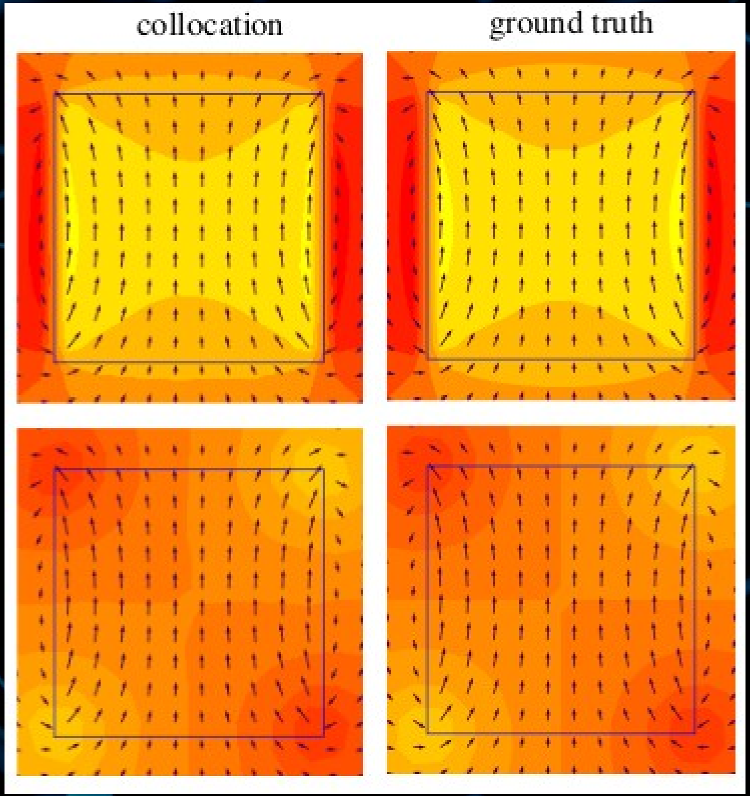
Physics-Informed Neural Networks





Schrefl, Thomas, et al. "Magnetostatics and micromagnetics with physics informed neural networks." Journal of Magnetism and Magnetic Materials 548 (2022): 168951.

Physics-Informed Neural Networks



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Constraints

- Soft constraints
  - minimize the initial and/or boundary error of the model
- Hard constraints
  - initial/boundary conditions are enforced on the model

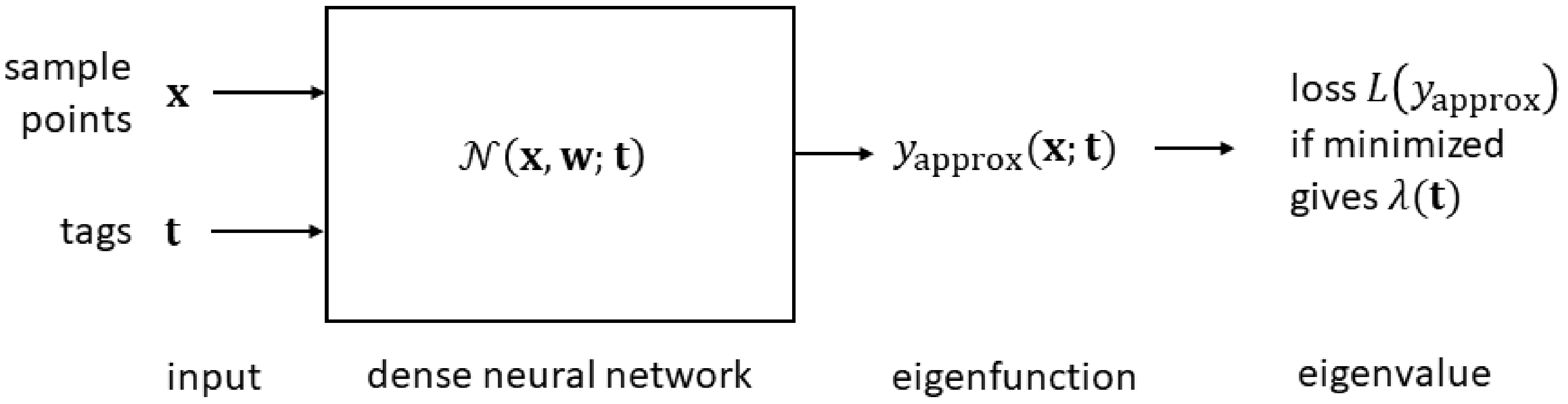
$$tu(x,t) = 0 \quad \text{at} \quad t = 0$$

Conditional Physics-Informed Neural Networks

eigenvalue problem

$$\nabla(p(\mathbf{x};\mathbf{t})\nabla y(\mathbf{x};\mathbf{t})) + q(\mathbf{x};\mathbf{t})y(\mathbf{x};\mathbf{t}) = -\lambda(\mathbf{t})r(\mathbf{x};\mathbf{t})y(\mathbf{x};\mathbf{t})$$

conditional physics informed neural network



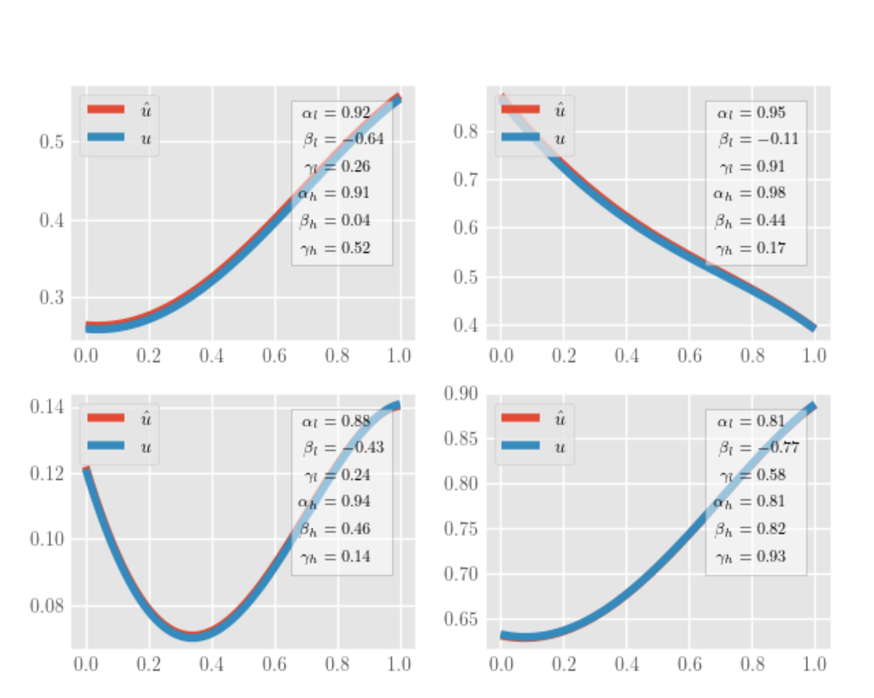
Kovacs, Alexander, et al. "Conditional physics informed neural networks." Communications in Nonlinear Science and Numerical Simulation 104 (2022): 106041.

Conditional Physics-Informed Neural Networks

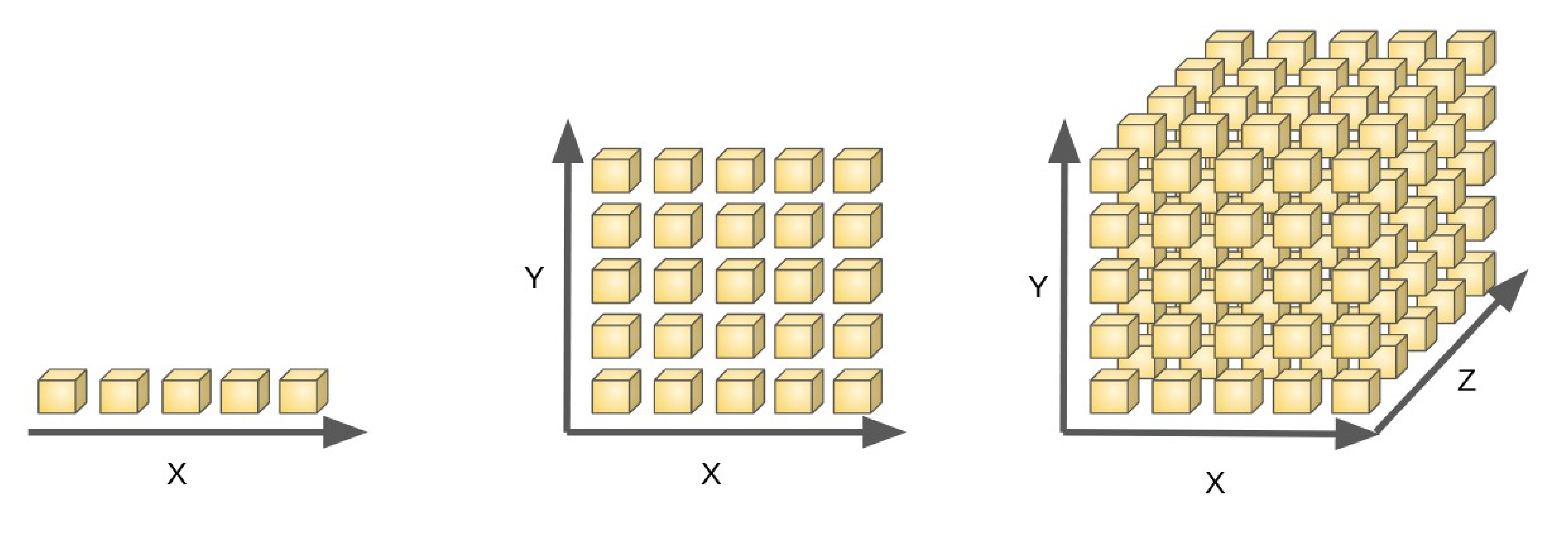
$$\frac{d^2u(x)}{dx^2} = 1 - 2x^2$$

$$\alpha_l u(x) + \beta_l \frac{d^2u(x)}{dx^2} = \gamma_l \quad \text{at } x = 0,$$
$$\alpha_h u(x) + \beta_h \frac{d^2u(x)}{dx^2} = \gamma_h \quad \text{at } x = 1,$$

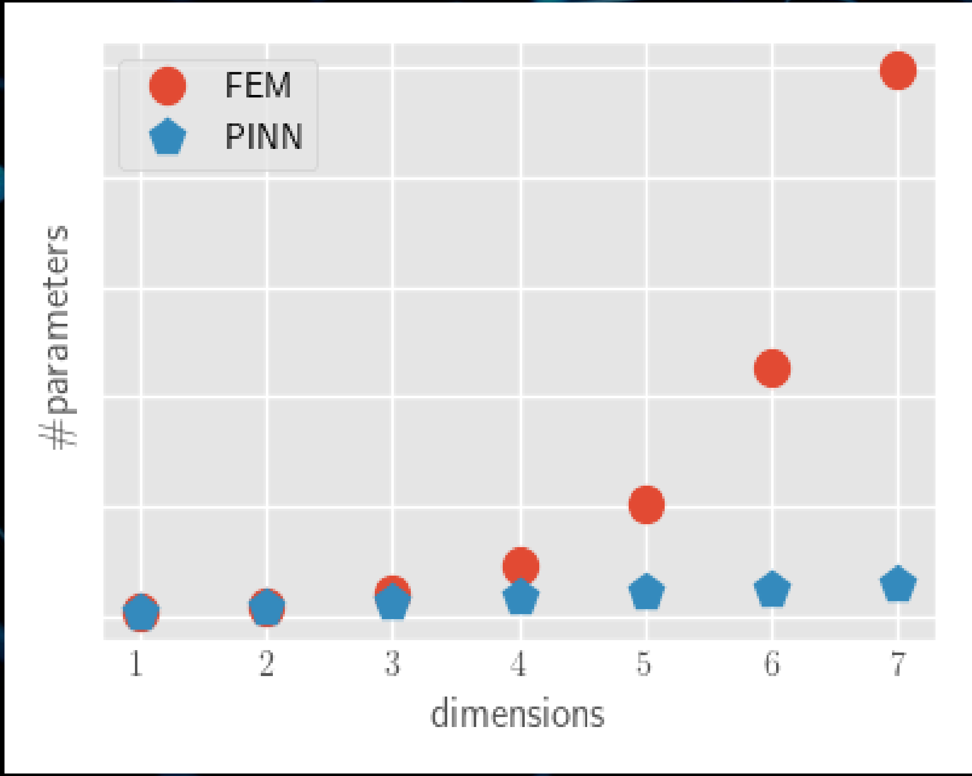
for $x \in [0, 1]$, $\alpha_l \in [0.8, 1]$, $\beta_l \in [-1, 0]$, $\gamma_l \in [0, 1]$, $\alpha_h \in [0.8, 1]$, $\beta_h \in [0, 1]$ and $\gamma_h \in [0, 1]$



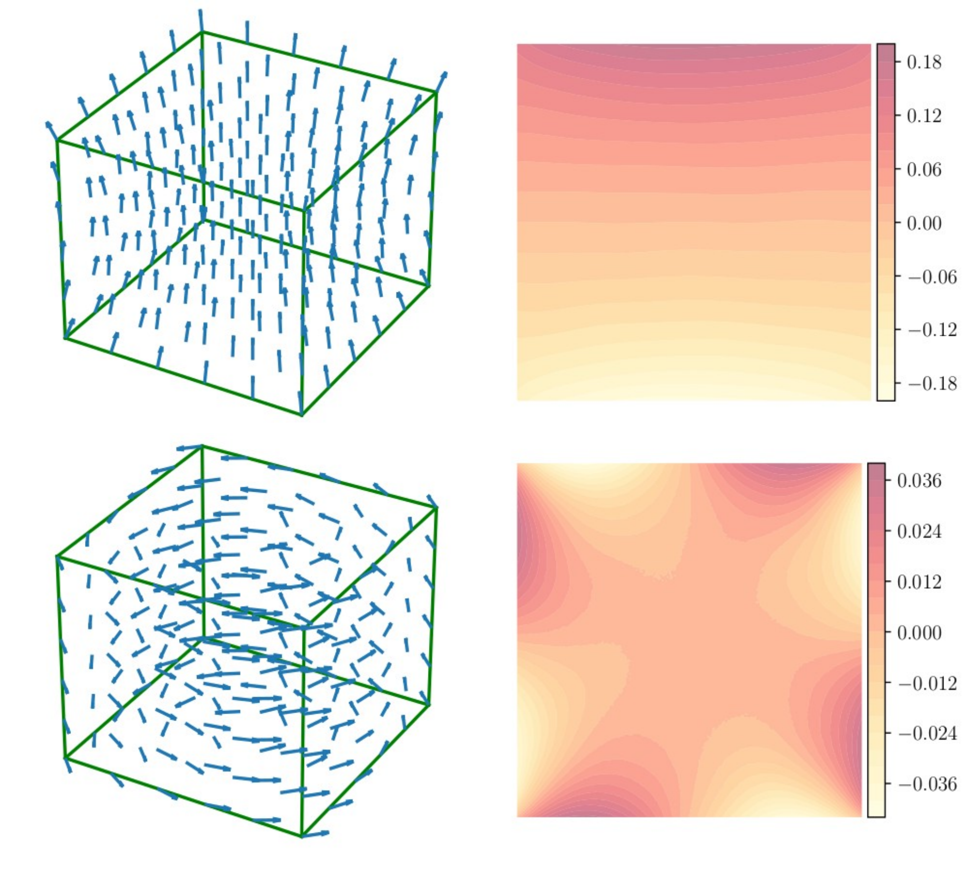
Curse of Dimensionality

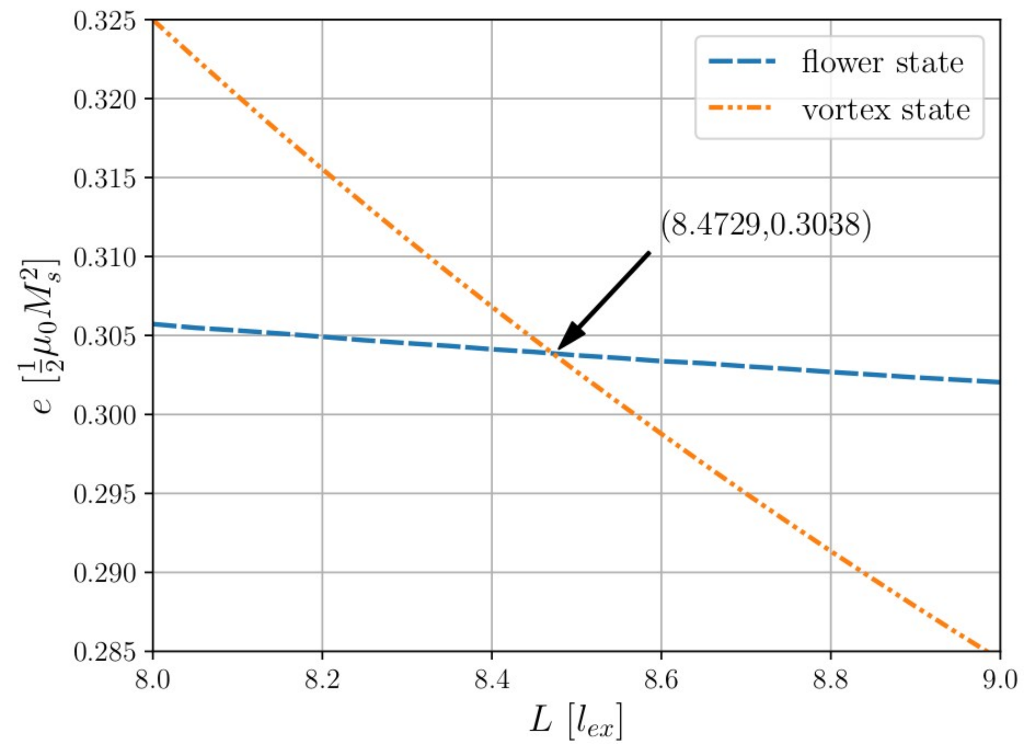


Curse of Dimensionality



PINNs in Micromagnetism





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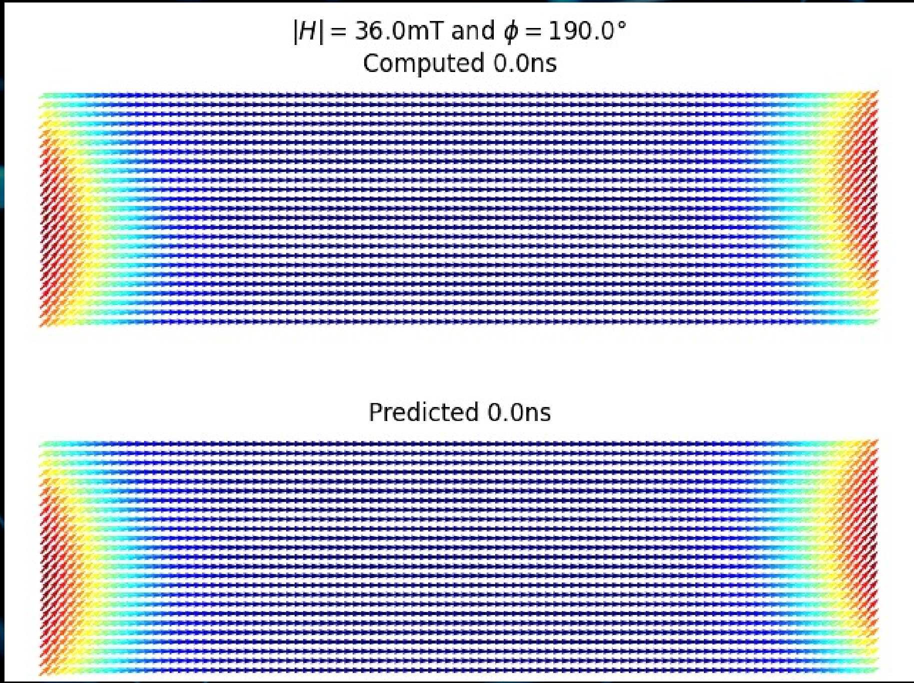
PINNs in Micromagnetism



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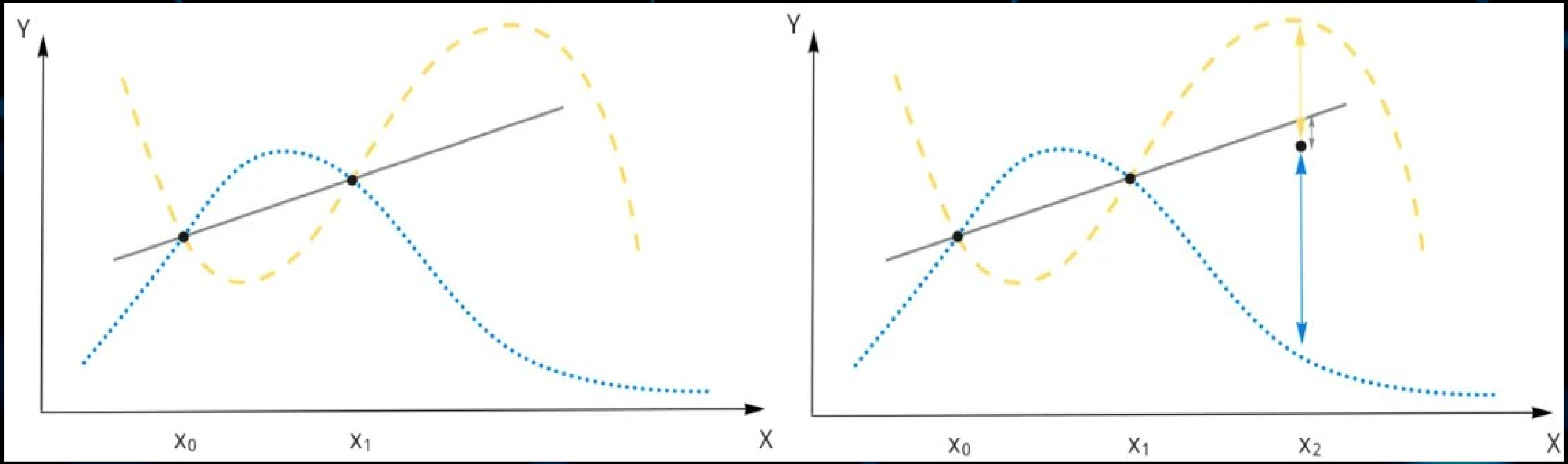
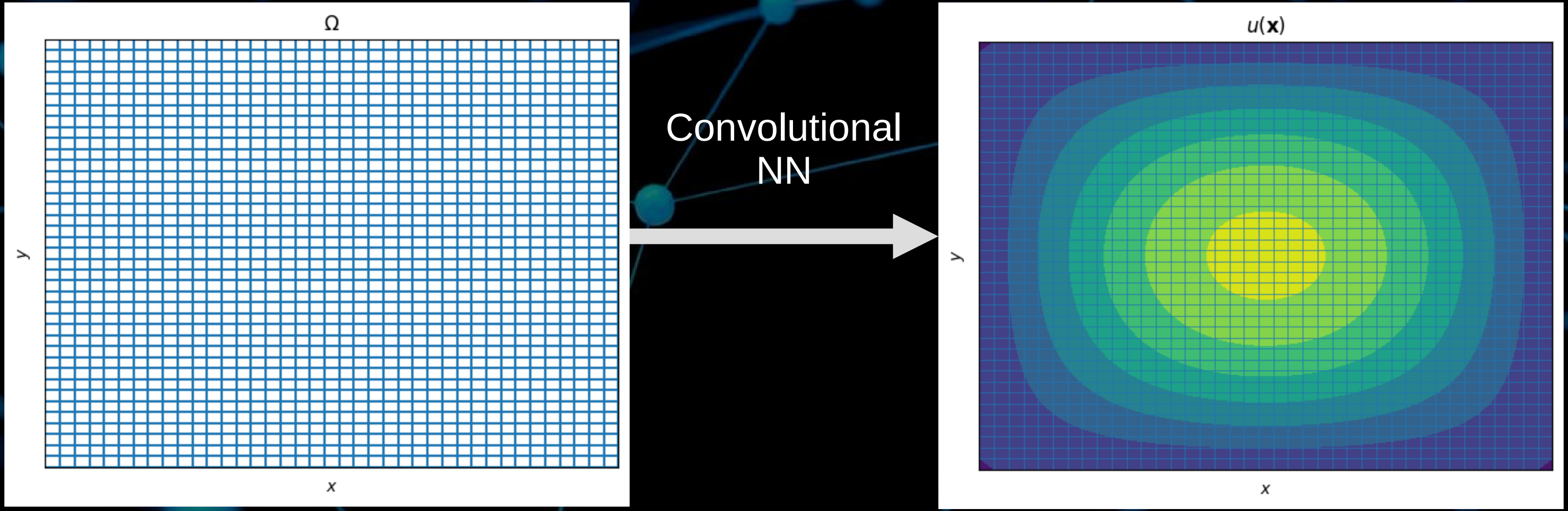
Inductive Bias

- Inductive reasoning refers to generalization from specific observations to a conclusion.
- The less training data we have, the stronger inductive bias should be to help the model to generalize well.
- Choosing a model with the right bias boosts chances of finding a better generalization with less data



https://towardsdatascience.com/the-inductive-bias-of-ml-models-and-why-you-should-care-about-it-979fe02a1a56

Physics-Informed Convolutional Networks



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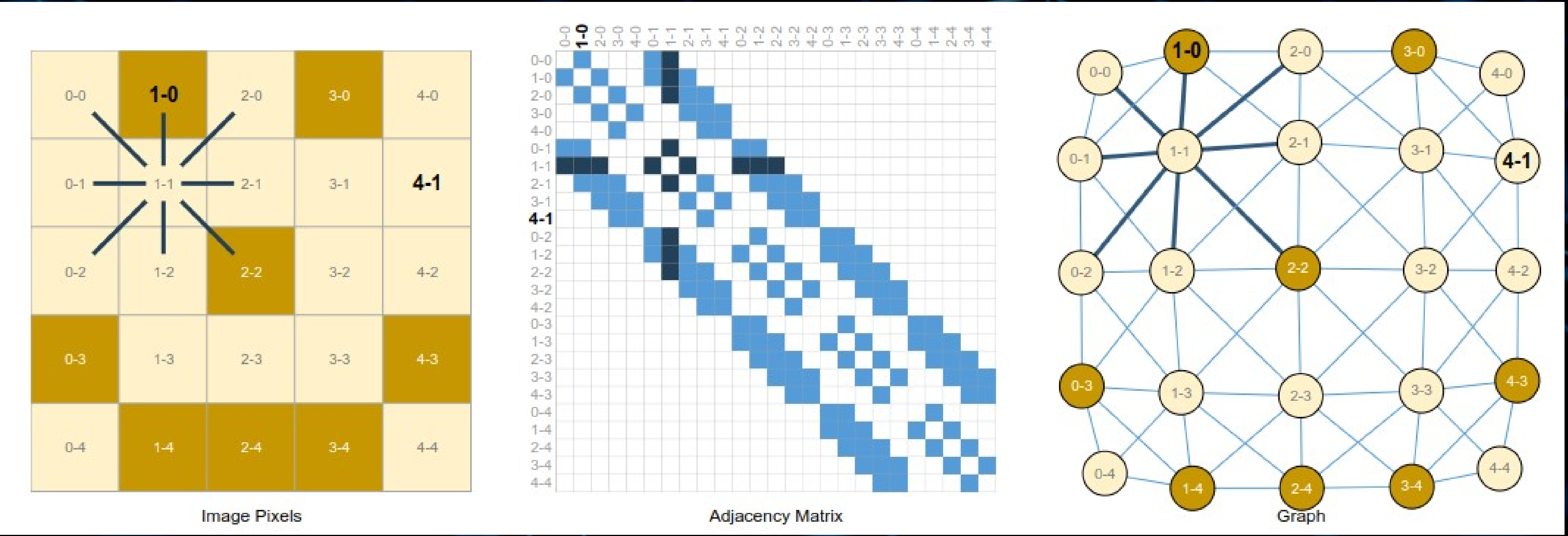
Gao, Han, Matthew J. Zahr, and Jian-Xun Wang. "Physics-informed graph neural galerkin networks: A unified framework for solving pde-governed forward and inverse problems." Computer Methods in Applied Mechanics and Engineering 390 (2022): 114502.

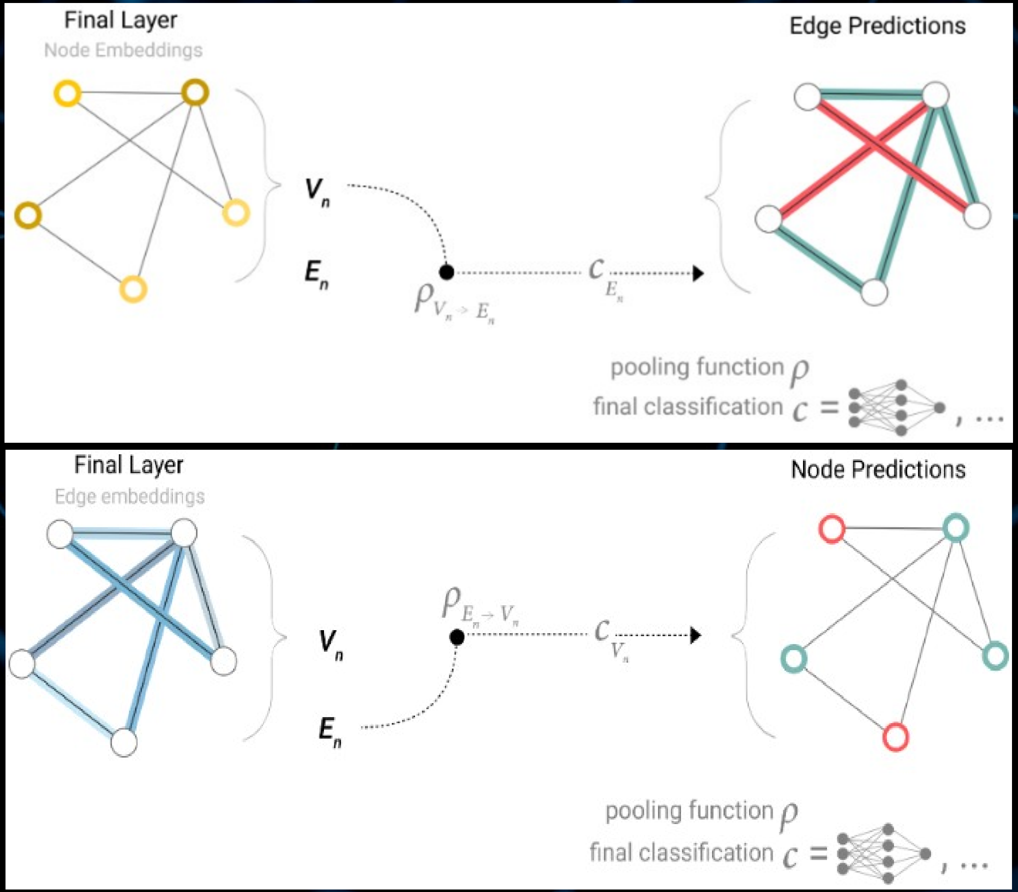
Fang, Zhiwei. "A high-efficient hybrid physics-informed neural networks based on convolutional neural network." IEEE Transactions on Neural Networks and Learning Systems 33.10 (2021): 5514-5526.

Graph Neural Networks



Sanchez-Lengeling, et al., "A Gentle Introduction to Graph Neural Networks", Distill, 2021.

Graph Neural Networks



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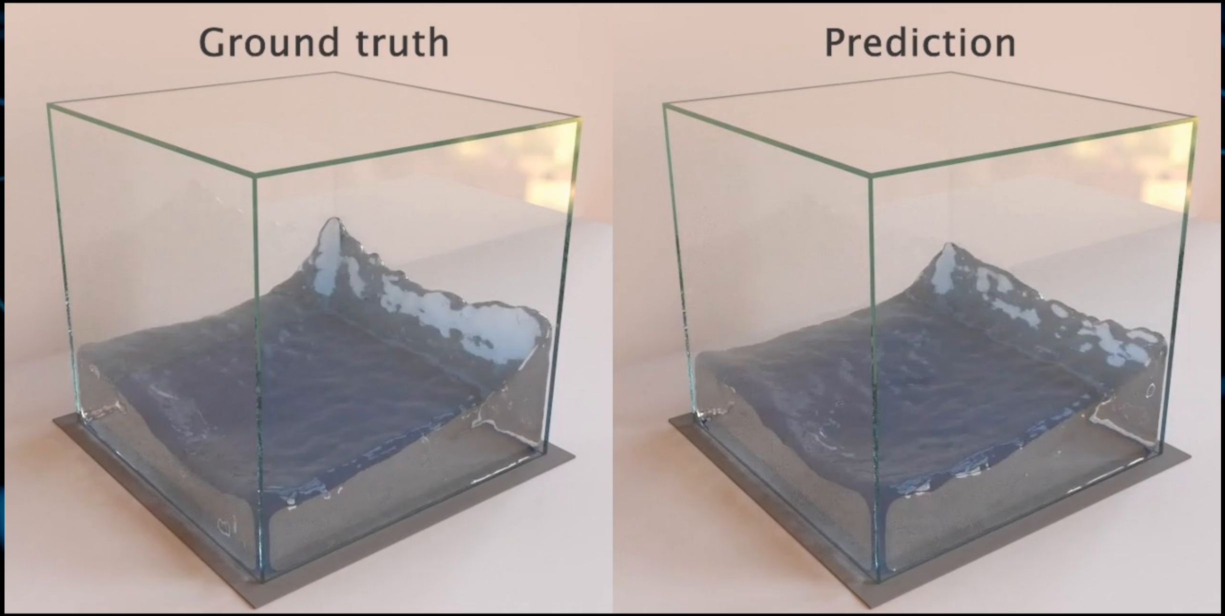

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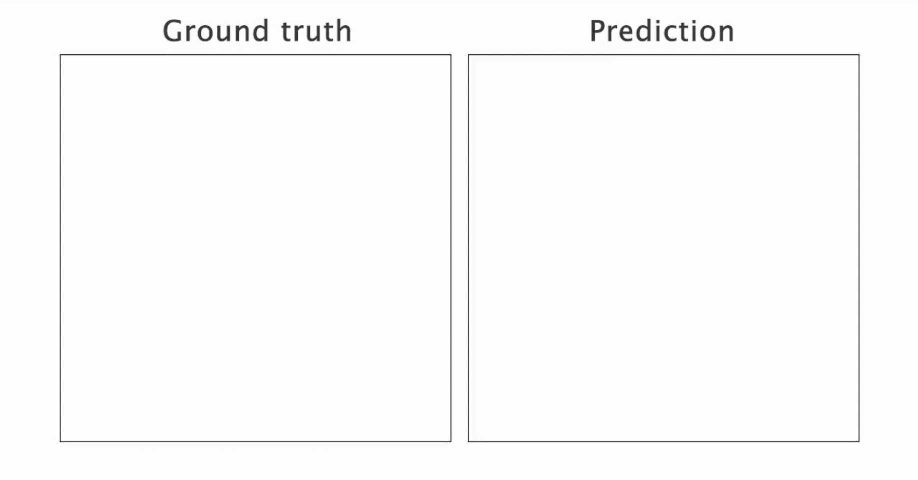
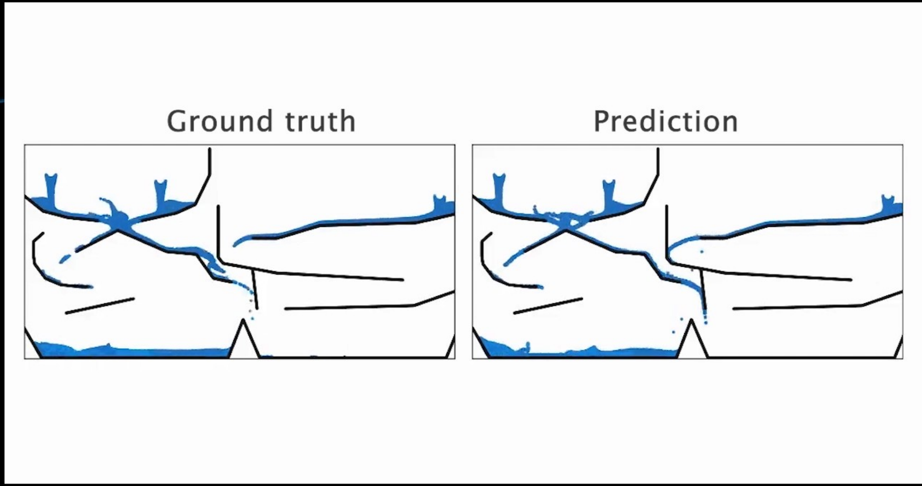
Graph Neural Networks





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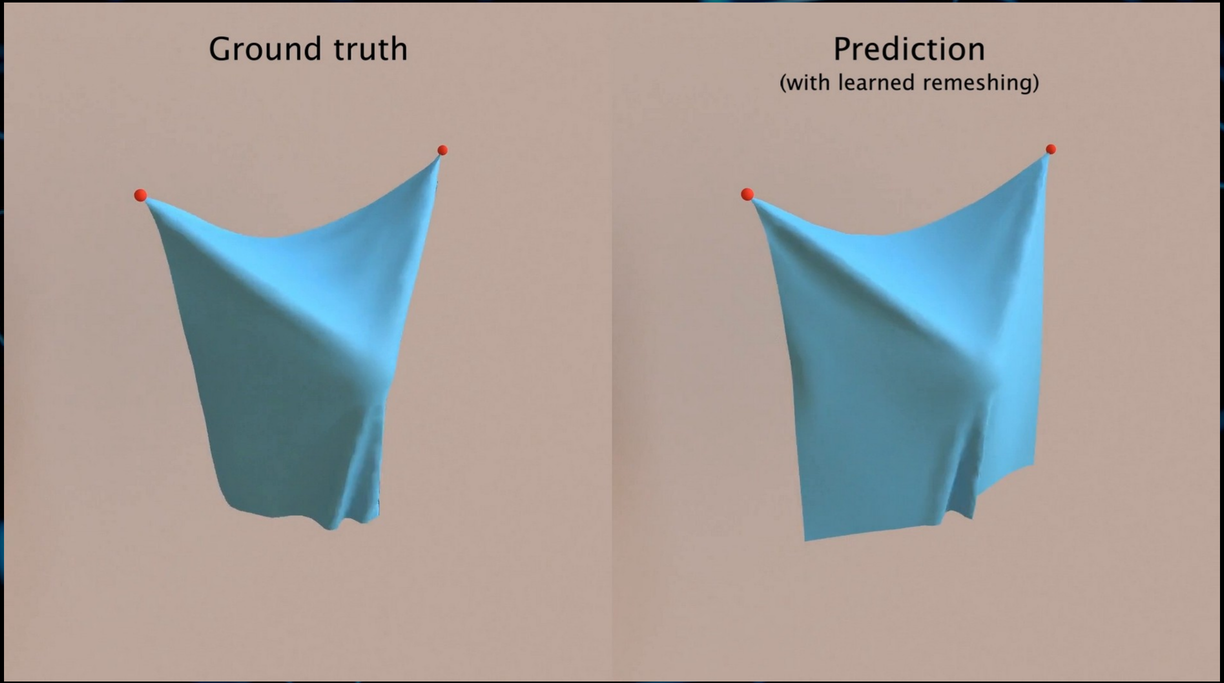

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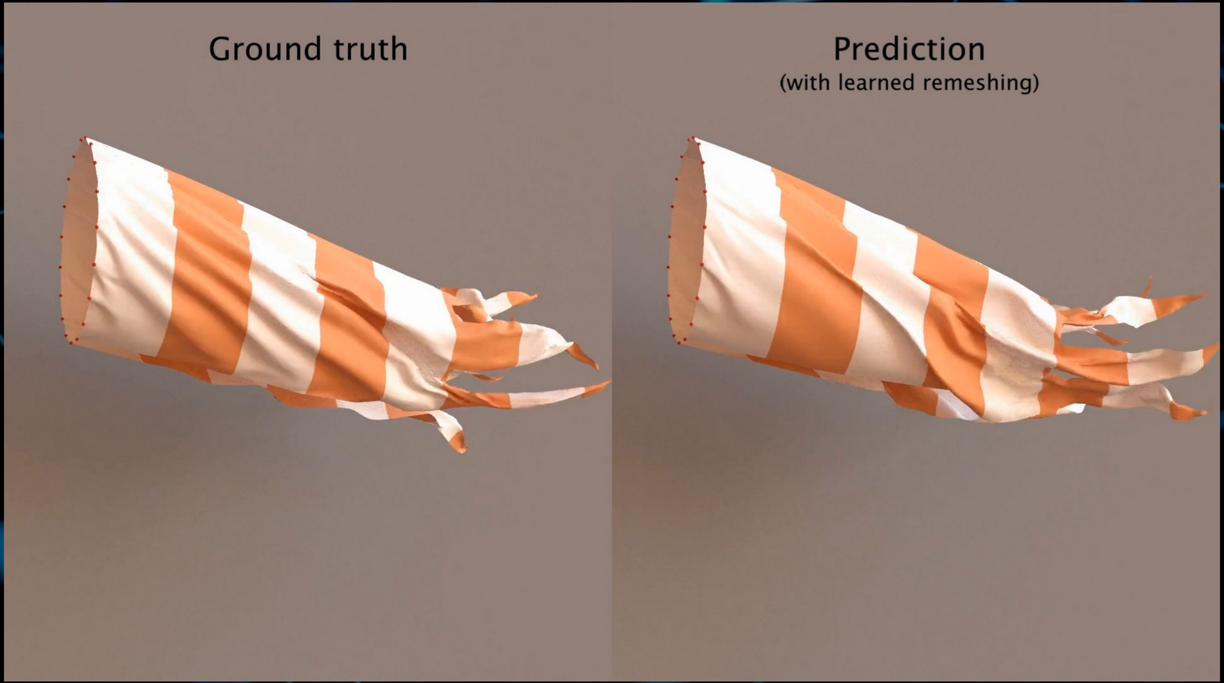
Graph Neural Networks



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Current Research

- Domain Decomposition
- Importance sampling
- Optimization method in PINN training (e.g. stoch. Versions of trust region methods and L-BFGS)
- Conditional PINNs in Micromagnetism
- Time-dependent PDEs

Acknowledgements

- Austrian Science Fund (FWF) via project P 31140 ”Reduced Order Approaches for Micromagnetics (ROAM)”
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