Infinite-Fidelity Coregionalization for Physical Simulation

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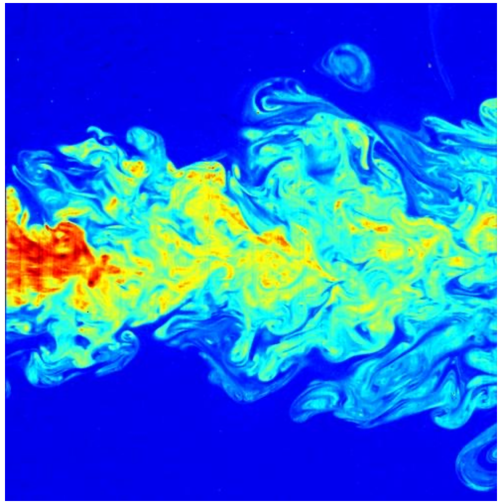
Physical Simulations by Solving PDEs

Fluid dynamics



velocity

viscosity

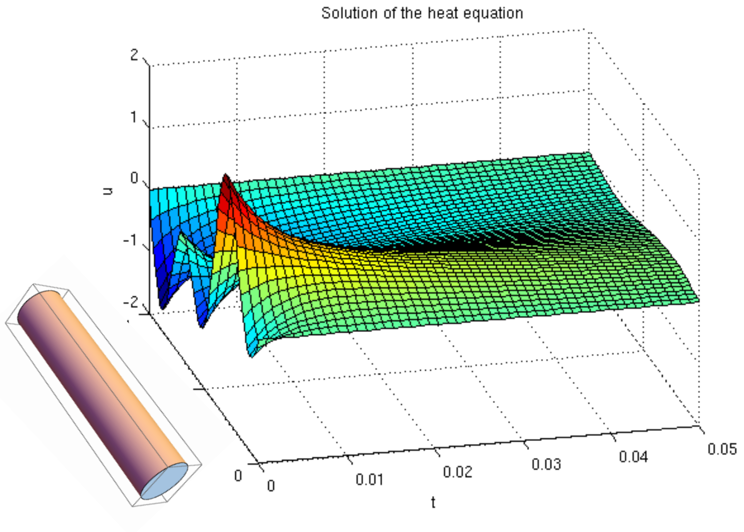
$$\rho\frac{\mathrm{d}\bar{u}}{\mathrm{d}t} = -\nabla p + \mu\nabla^2\bar{u} + \rho\bar{F}$$

density

pressure gradient

external force

Heat

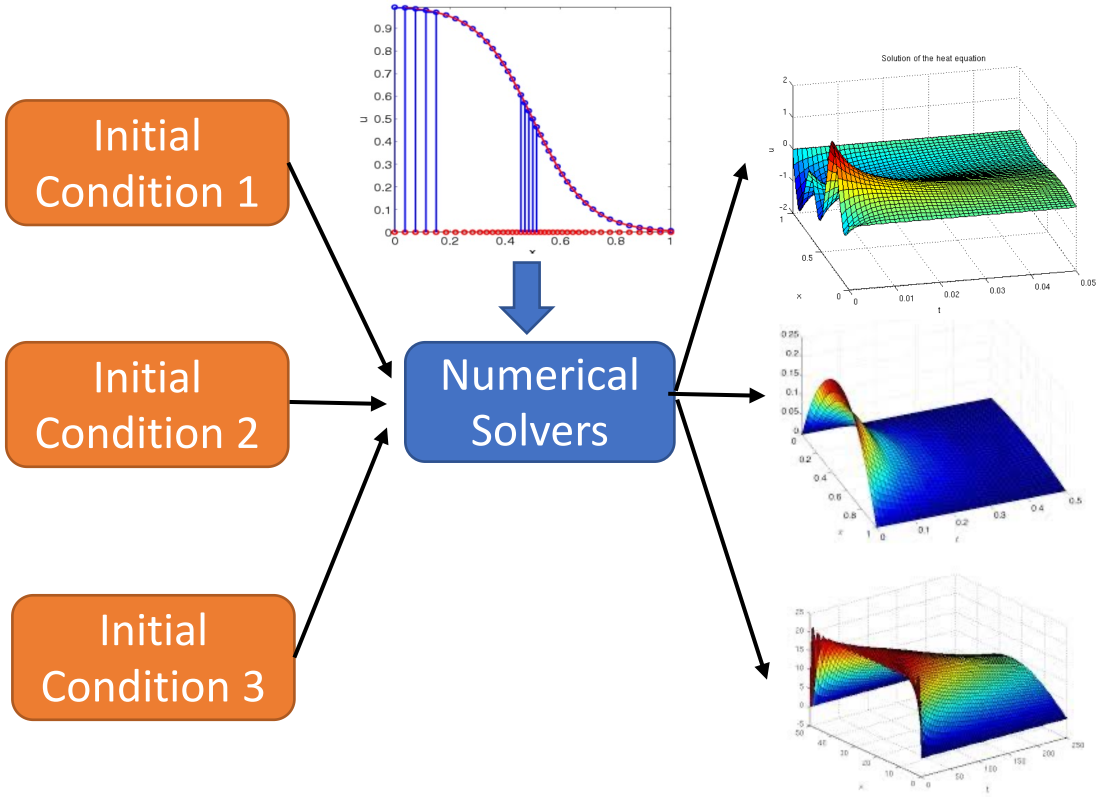


$$\frac{\partial u}{\partial t} = \alpha\frac{\partial^2 u}{\partial x^2}$$

thermal diffusivity

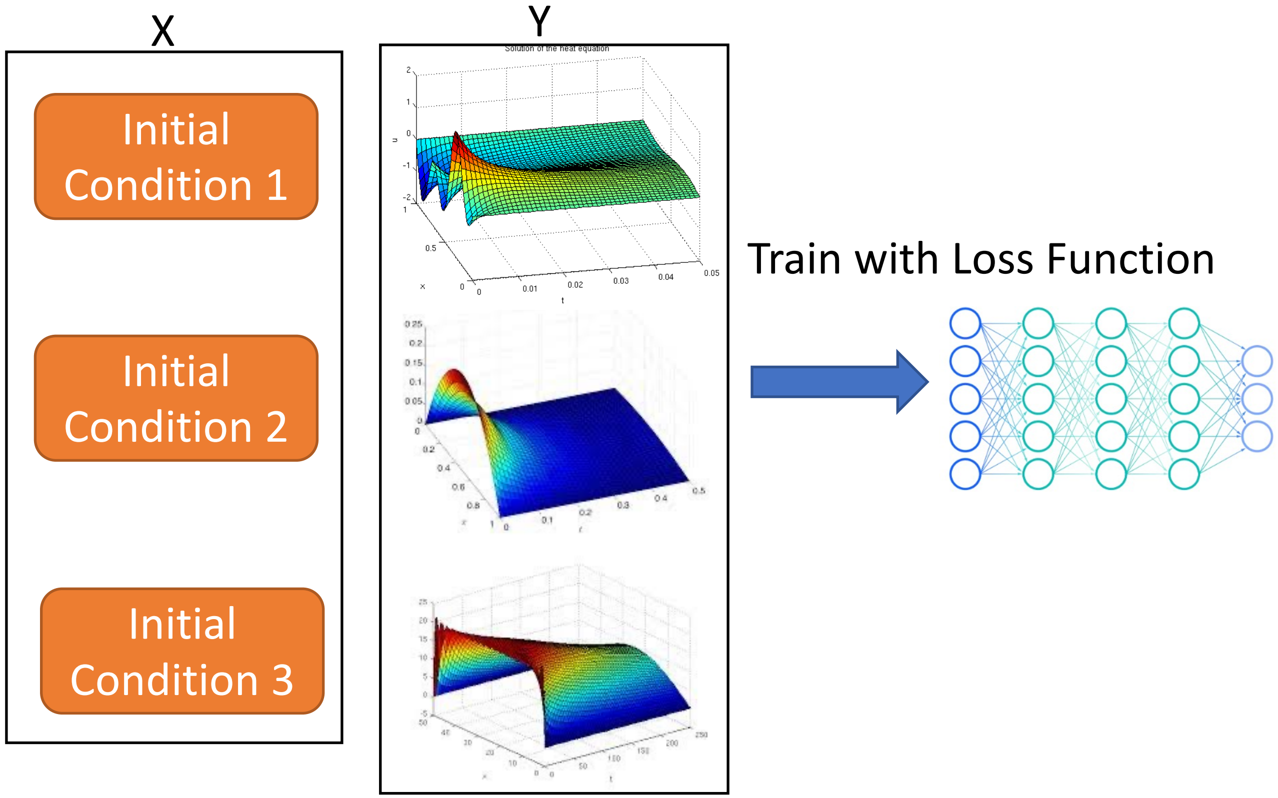
Physical Simulations by Solving PDEs

- Numerical methods



- (Exactly) Accurate Solution
- Slow
- Do not generalize over the same domain

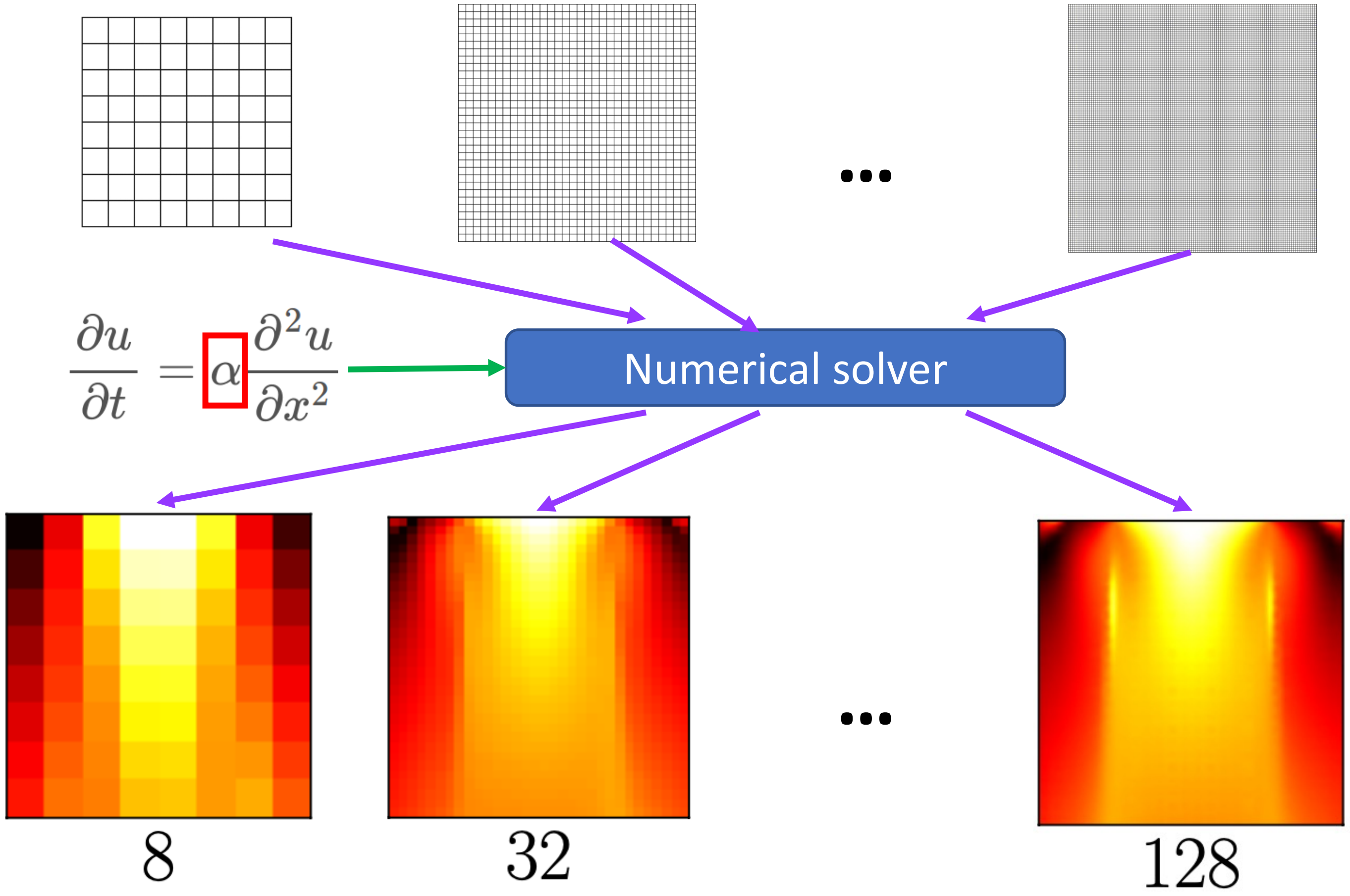
- Data-driven methods



- Fast inference with new PDE
- Generalize over domain
- Prepare large amount of data from numerical solvers

Multi-Fidelity Modeling

- High-dimensional outputs for physical simulations



Linear Model of Coregionalization (LMC)

$$\mathbf{f}(\mathbf{x}) = \sum_{k=1}^{K} h_k(\mathbf{x})\mathbf{b}_k = \mathbf{B} \cdot \mathbf{h}(\mathbf{x})$$

Low-dimensional output

$$\mathbf{h}(x) = [h_1(\mathbf{x}), \ldots, h_K(\mathbf{x})]^\top$$

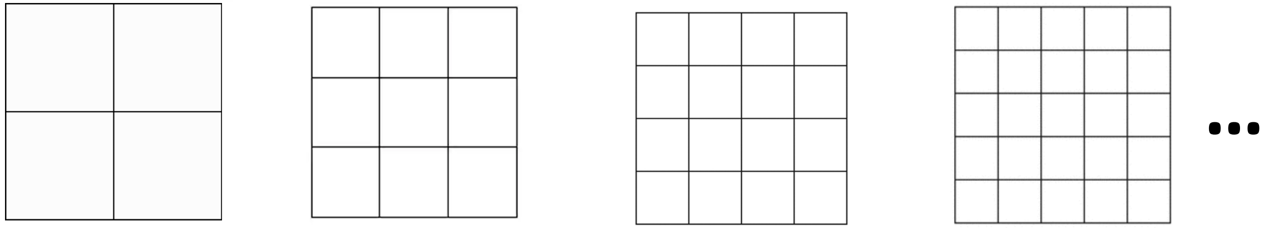
Basis Matrix

$$\mathbf{B} = [\mathbf{b}_1, \ldots, \mathbf{b}_K]$$

Learnable

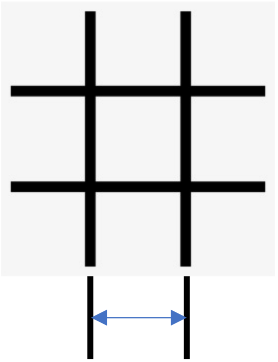
Multi-Fidelity Modeling

- Motivation: infinitely “continuous” fidelity



2x2 3x3 4x4 5x5 …

Element length continuous



Continuous mesh spacing

- ***Existing methods:*** fixed set of fidelities, do not generalize over the fidelities
- ***<u>Our methods:</u>*** model all fidelities simultaneously, capture rich information

	DRC (Xing et al 2021)	MFHoGP (Wang et al. 2021)	DMF (Li et al. 2022)	IFC (Ours)
Multi-Fidelity Modeling ?	✓	✓	✓	✓
Capture Complex Fidelities Correlations?	✓	✓	✓	✓
Models **<u>all</u>** fidelities?	✗	✗	✗	✓
Predict on **<u>unseen</u>** fidelities?	✗	✗	✗	✓
Extrapolate to **<u>higher than target</u>** fidelities?	✗	✗	✗	✓

Infinite-Fidelity Modeling

Recall LMC $\mathbf{h}_m(\mathbf{x}) = \boldsymbol{\alpha}\left(\mathbf{h}_{m-1}(\mathbf{x}), \mathbf{x}\right), \quad \mathbf{f}_m(\mathbf{x}) = \mathbf{B}_m \mathbf{h}_m(\mathbf{x})$

infinitesimal

correction term $\lim_{\Delta \to 0} \boldsymbol{\psi} = \mathbf{0}$

$$\mathbf{h}(m, \mathbf{x}) = \mathbf{h}(m - \Delta, \mathbf{x}) + \Delta \cdot \boldsymbol{\phi}\left(m, \mathbf{h}(m - \Delta, \mathbf{x}), \mathbf{x}\right)$$

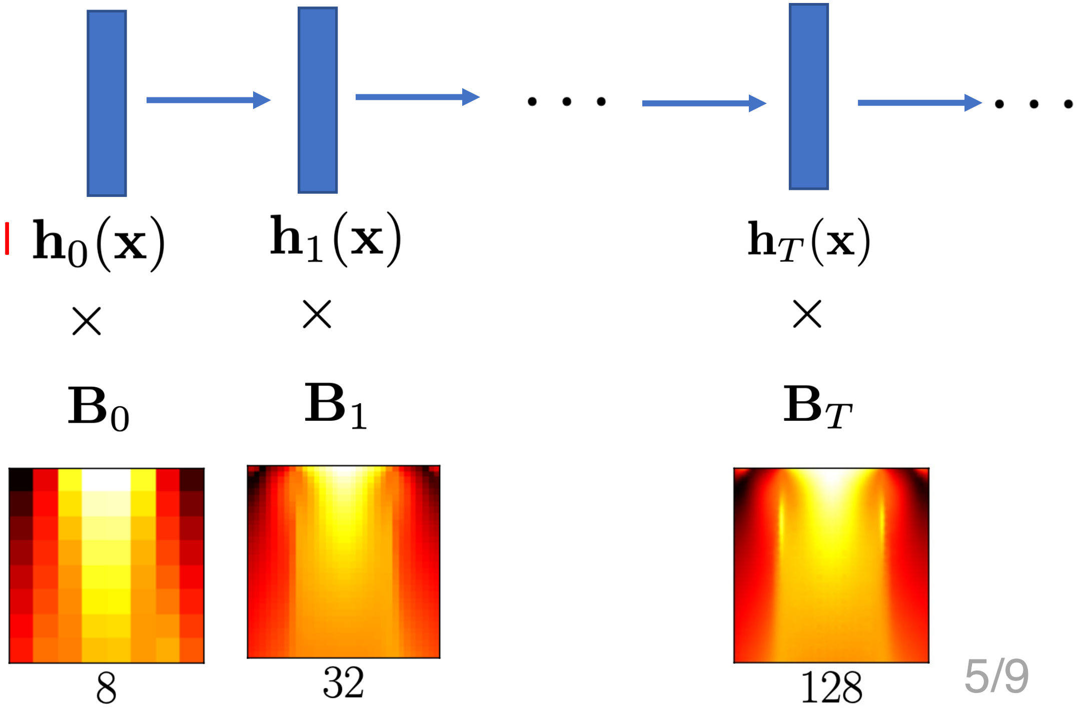
$$\frac{\partial \mathbf{h}(m, \mathbf{x})}{\partial m} = \boldsymbol{\phi}\left(m, \mathbf{h}(m, \mathbf{x}), \mathbf{x}\right)$$

$$\mathbf{h}(0, \mathbf{x}) = \boldsymbol{\beta}(\mathbf{x})$$

ODE model

ODE dynamic model

ODE initial model



Infinite-Fidelity Modeling

- IFC-GPODE (*GP* treatment of basis matrix)

$$b_{ij}(m) \sim \mathcal{GP}(0, \kappa(m, m'))$$

$$p(\mathcal{B}, \mathcal{Y}|\mathbf{X}) = \prod_{i=1}^{d} \prod_{k=1}^{K} \mathcal{N}(\mathbf{b}_{ij}|\mathbf{0}, \mathbf{K}) \prod_{n=1}^{N} \mathcal{N}(\mathbf{y}_n|\mathbf{B}_n\mathbf{h}(m_n, \mathbf{x}_n), \sigma^2\mathbf{I})$$

- IFC-ODE^2 (*ODE* treatment of basis matrix)

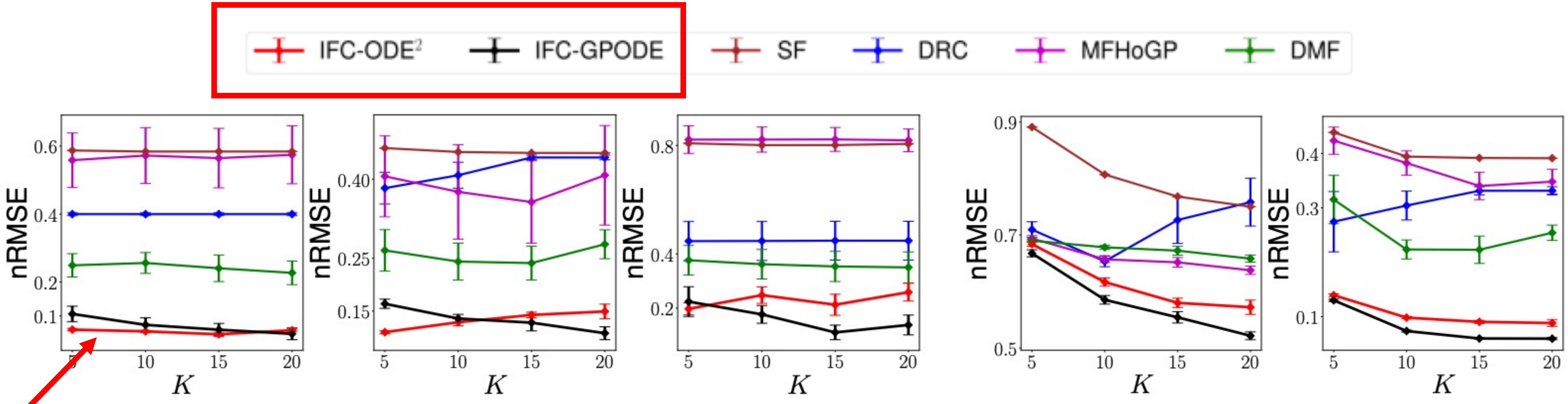
$$\frac{\partial b_{ij}(m)}{\partial m} = \gamma(b_{ij}, m), \quad b_{ij}(0) = \nu_{ij}$$

$$p(\mathcal{Y}|\mathbf{X}) = \prod_{n=1}^{N} \mathcal{N}(\mathbf{y}_n|\mathbf{B}_n\mathbf{h}(m_n, \mathbf{x}_n), \sigma^2\mathbf{I})$$

We have proposed ***efficient*** algorithms to train those two models. Refer our paper for more details.

Experiment

- Predictive performance

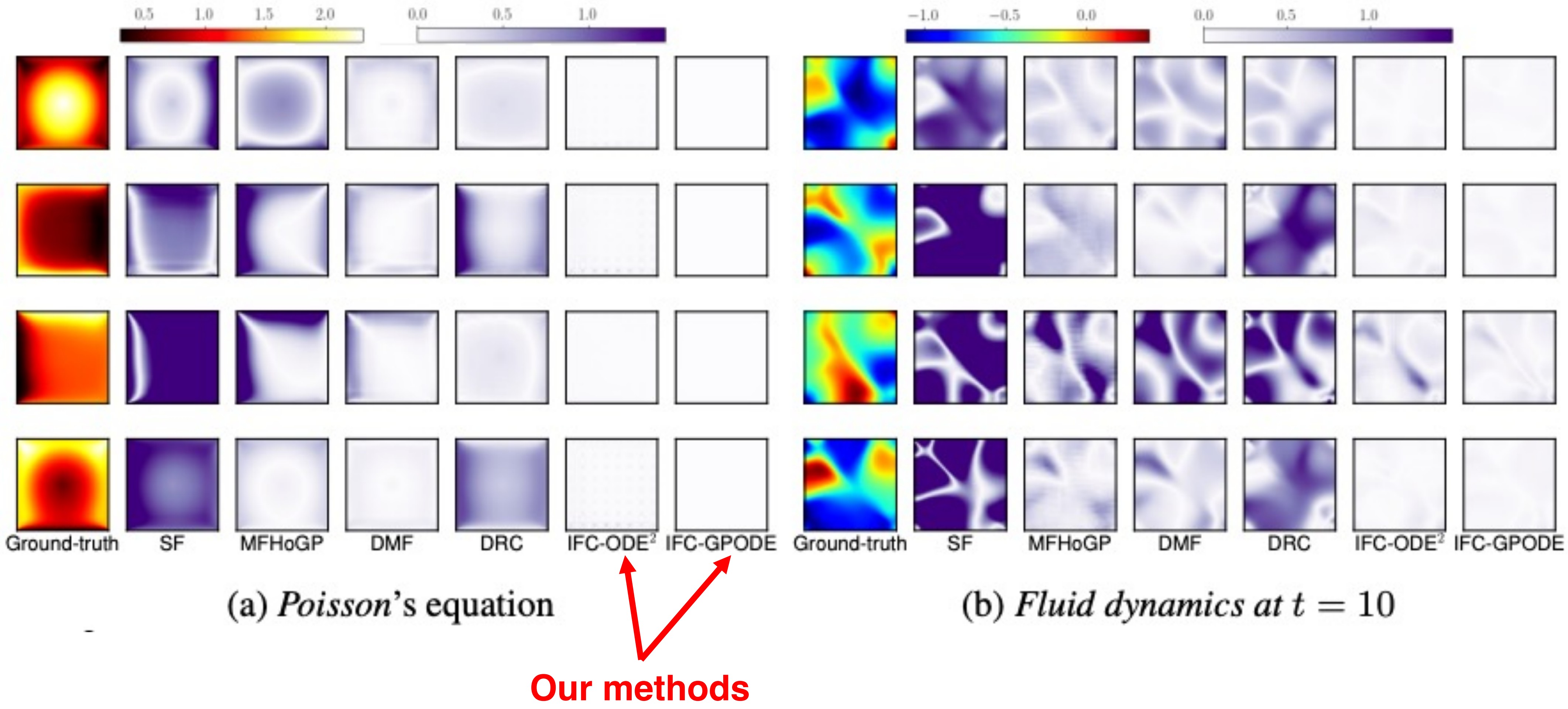


(a) *Poisson* (b) *Heat* (c) *Burgers* (a) *Topology Optimization* (b) *Fluid Dynamics*

Our methods

Experiment

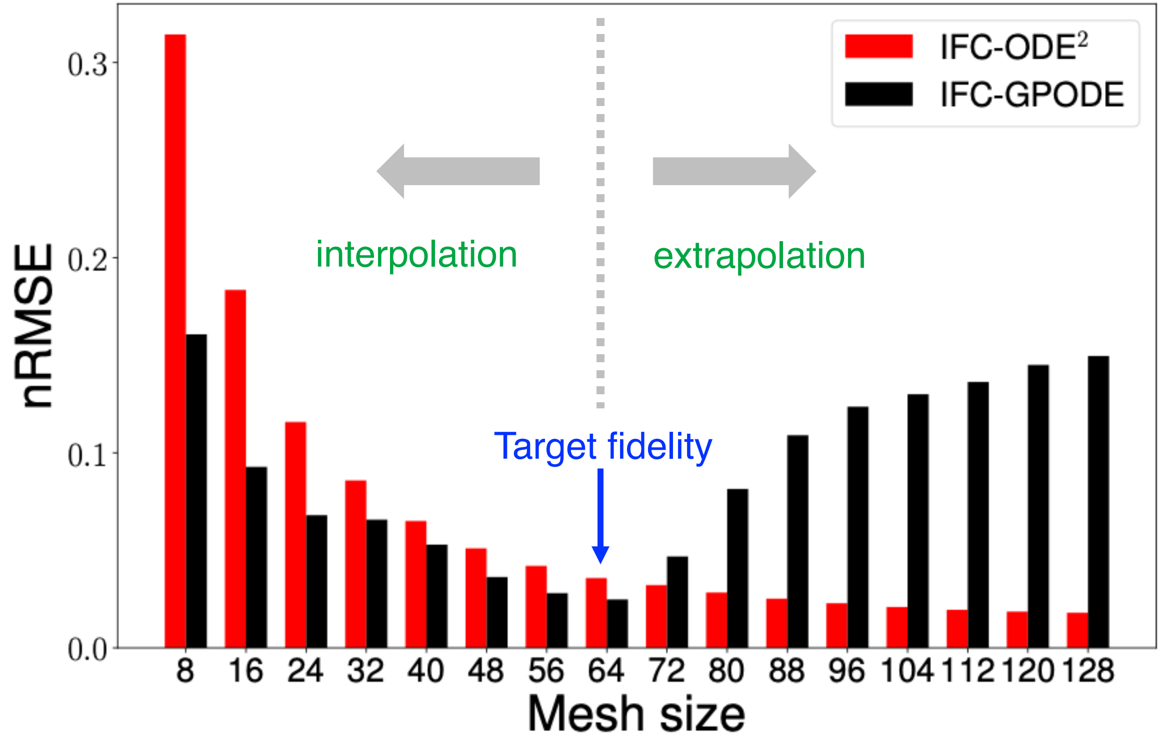
- Visualize error field



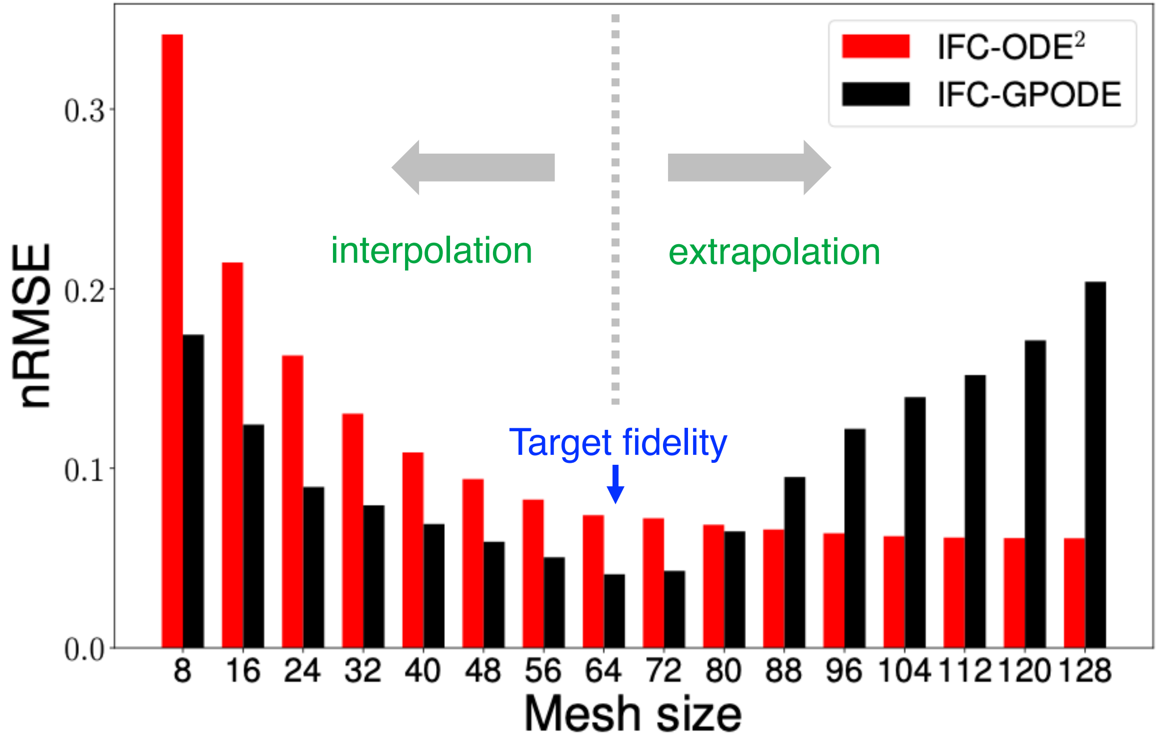
(a) *Poisson's equation* (b) *Fluid dynamics at* $t = 10$

Experiment

- Predict on ***unseen*** fidelities



(a) *Poisson*'s equation



(b) *Heat* equation

Welcome to our poster!

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