Infinite-Fidelity Coregionalization for Physical Simulation

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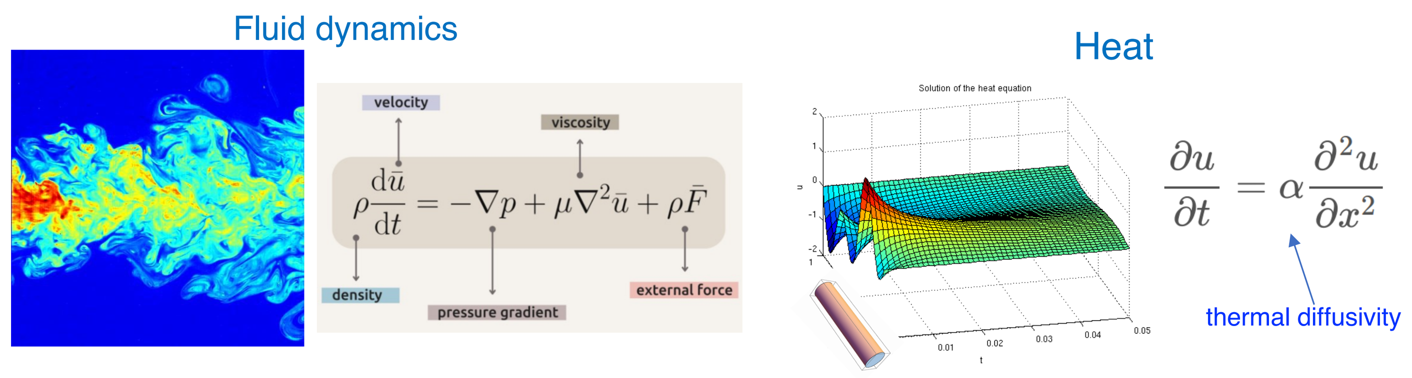
Abstract

Multi-fidelity modeling and learning is important in physical simulation related applications. It can leverage both low-fidelity and high-fidelity examples for training so as to reduce the cost of data generation yet still achieving good performance. While existing approaches only model finite, discrete fidelities, in practice, the feasible fidelity choice is often infinite, which can correspond to a continuous mesh spacing or finite element length. In this paper, we propose Infinite Fidelity Coregionalization (IFC). Given the data, our method can extract and exploit rich information within infinite, continuous fidelities to bolster the prediction accuracy. Our model can interpolate and/or extrapolate the predictions to novel fidelities that are not covered by the training data. Specifically, we introduce a low-dimensional latent output as a continuous function of the fidelity and input, and multiple it with a basis matrix to predict high-dimensional solution outputs. We model the latent output as a neural Ordinary Differential Equation (ODE) to capture the complex relationships within and integrate information throughout the continuous fidelities. We then use Gaussian processes or another ODE to estimate the fidelity-varying bases. For efficient inference, we reorganize the bases as a tensor, and use a tensor-Gaussian variational posterior approximation to develop a scalable inference algorithm for massive outputs. We show the advantage of our method in several benchmark tasks in computational physics.

Motivation

Physical Simulations by Solving PDEs:
- Daily phenomena are dominated by fundamental *physical laws*
- Fundamental physical laws are written as *Partial differential equations (PDEs) systems*

Key challenges of scientific computing:
- *Identify* the governing model for complex systems
- Efficiently *solving* large-scale non-linear systems of equations



Numerical Solvers:
- (Exact) accurate yet solutions
- Slow
- Do not generalize over the same domain

Data-drive Solvers(Surrogate Learning, Operator Learning):
- Fast inference with new PDE
- Generalize over domain problems
- Prepare large amount of data from numerical solvers

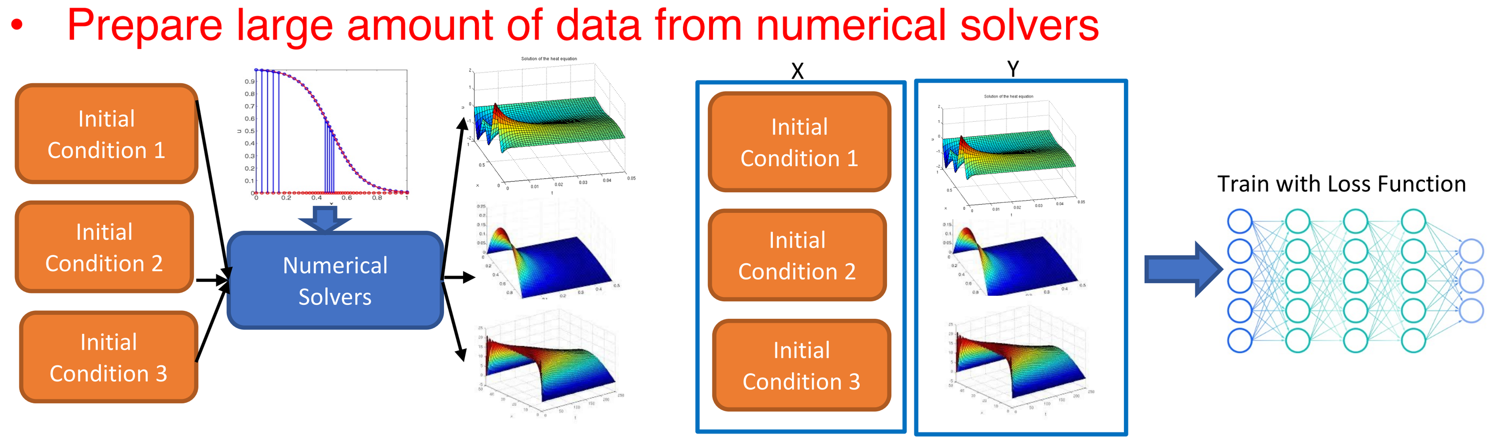
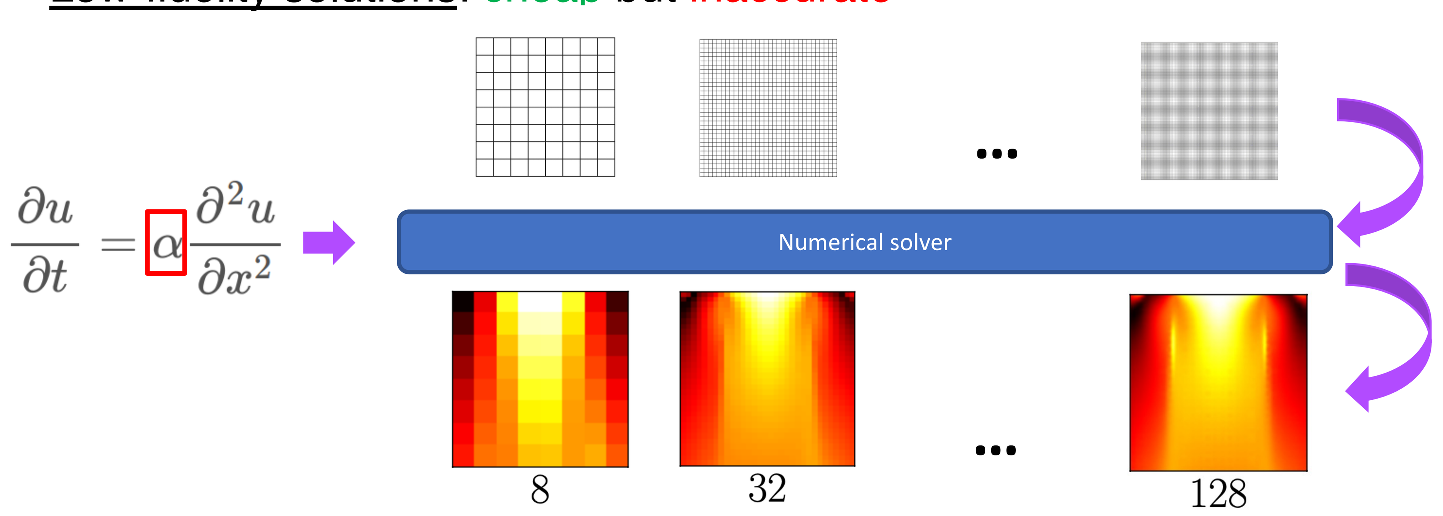


Figure 1. Conventional PDEs solvers

Figure 2. Data-driven PDEs solvers

Multi-fidelity Modeling:
- Conventional solvers usually have multi-fidelity evaluations natively
- High-fidelity solutions: expensive but accurate
- Low-fidelity solutions: cheap but inaccurate

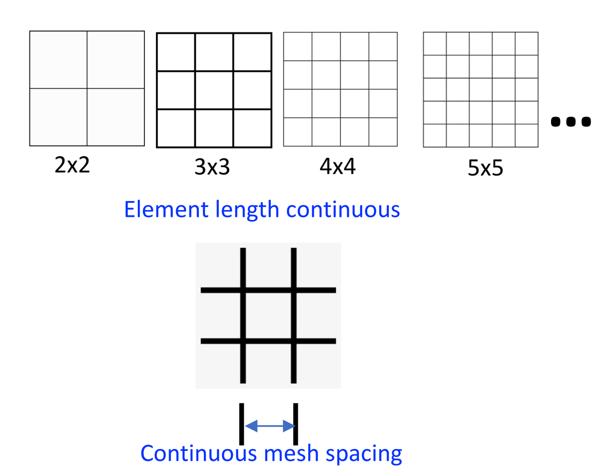


Linear Model of Coregionalization (LMC):
- *Low-dimensional inputs,*
- *very-high dimensional outputs*

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

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 Params

Our Contribution:
- *IFC*: A novel multi-fidelity modeling for very high-dimensional outputs
- Flexibly handles infinity/continuous fidelities while captures all fidelities' nonlinear, non-stationary correlations.
- Predicts on unseen fidelities.



	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 **all** fidelities?	✗	✗	✗	✓
Predict on **unseen** fidelities?	✗	✗	✗	✓
Extrapolate to **higher than target** fidelities?	✗	✗	✗	✓

Methods

Modeling:

Latent output of m-th fidelity — Actual output of m-th fidelity

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

NN that generate m-th fidelity latent outputs — Shared basis of m-th fidelity

Step 1: extending the latent outputs to the infinite fidelity case

$$\mathbf{h}(m,\mathbf{x}) = \mathbf{h}(m-\Delta,\mathbf{x}) + \boldsymbol{\psi}$$

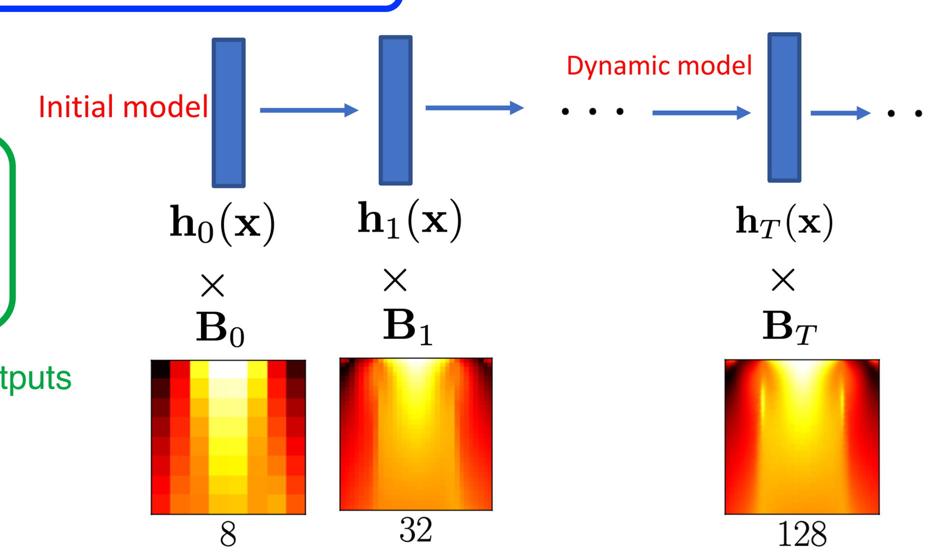
Infinitesimal fidelity — Adjustment term $\quad \lim_{\Delta\to 0} \boldsymbol{\psi} = \mathbf{0}$

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

Rearrange the terms

$$\frac{\partial \mathbf{h}(m,\mathbf{x})}{\partial m} = \boldsymbol{\phi}\left(m, \mathbf{h}(m,\mathbf{x}), \mathbf{x}\right)$$
$$\mathbf{h}(0,\mathbf{x}) = \boldsymbol{\beta}(\mathbf{x})$$

A parametric ODE model for latent outputs



Step 2: project the latent outputs through shared basis

- 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-ODE² (*ODE* treatment of basis matrix)

$$\frac{\partial b_{ij}(m)}{\partial m} = \gamma(b_{ij}, m), \quad b_{ij}(0) = \nu_{ij}$$
$$p(\mathcal{Y}|\mathbf{X}) = \prod_{n=1}^{N}\mathcal{N}(\mathbf{y}_n|\mathbf{B}_n\mathbf{h}(m_n,\mathbf{x}_n),\sigma^2\mathbf{I})$$

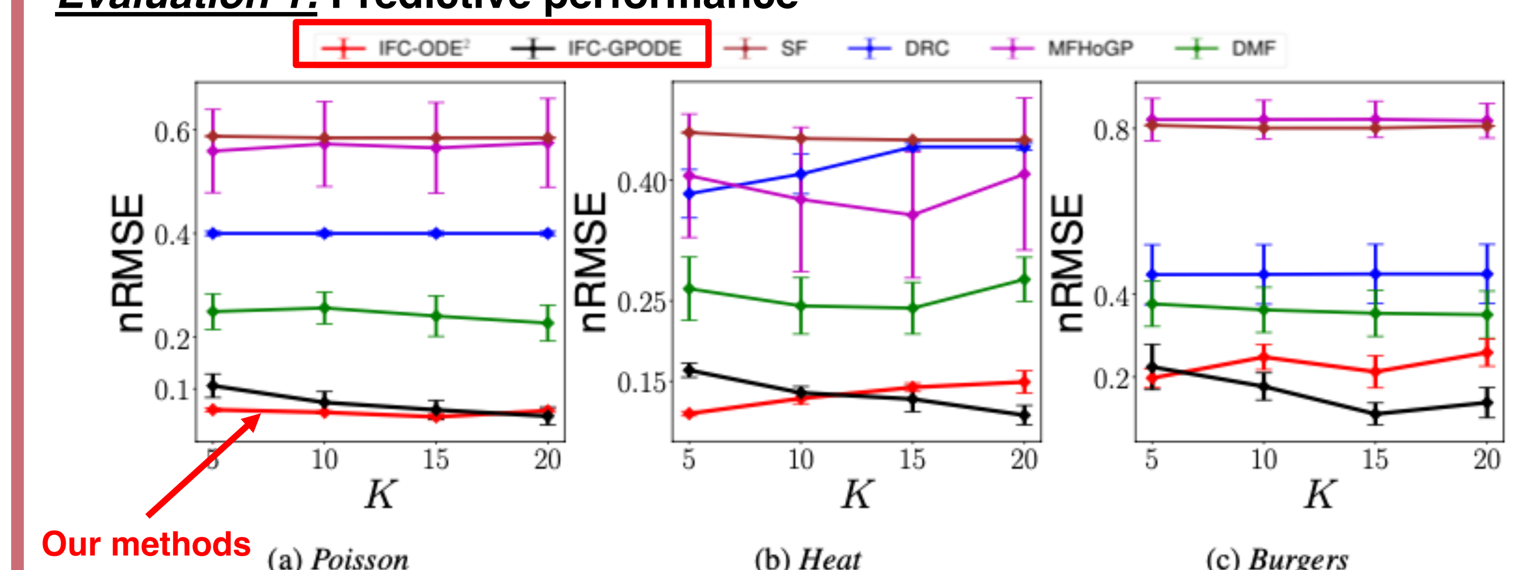
Learning / Inference:
- IFC-GPODE: SVI with Kronecker tensor normal

$$q(\mathcal{B}) = \mathcal{TN}(\mathcal{B}|\mathcal{U}, \boldsymbol{\Sigma}_1, \ldots, \boldsymbol{\Sigma}_R, \boldsymbol{\Sigma}_{R+1}, \boldsymbol{\Sigma}_{R+2}) = \mathcal{N}(\mathrm{vec}(\mathcal{B})|\mathrm{vec}(\mathcal{U}), \boldsymbol{\Sigma}_1\otimes\ldots\otimes\boldsymbol{\Sigma}_{R+2})$$

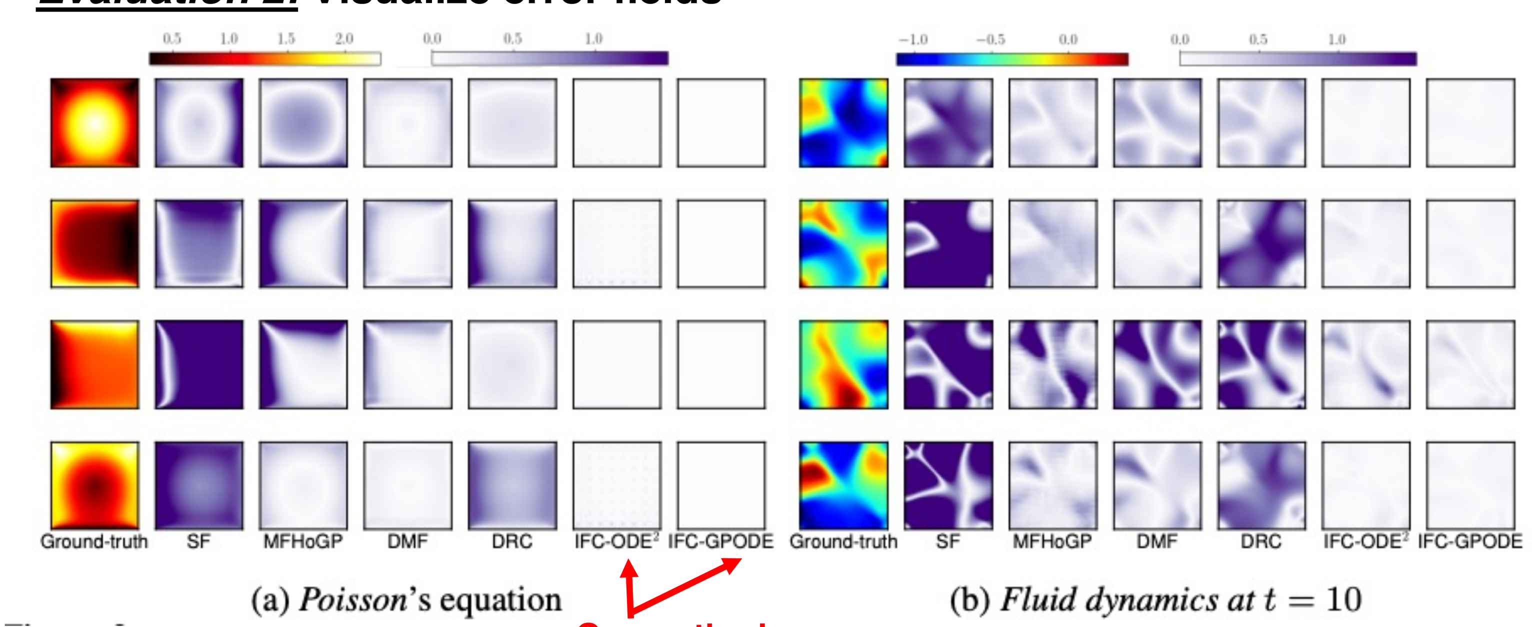
- IFC-ODE²: end-to-end parametric ODE learning

Experiment

Evaluation 1: **Predictive performance**



Evaluation 2: **Visualize error fields**



Evaluation 3: **Predict on unseen fidelities**