Locally Subspace-Informed Neural Operators for Efficient Multiscale PDE Solving

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Problem Statement

- **The Core Method**: The **GMsFEM** (Generalized Multiscale Finite Element Method) provides high accuracy and robustness for PDEs with high-contrast coefficients by constructing local spectral basis functions.

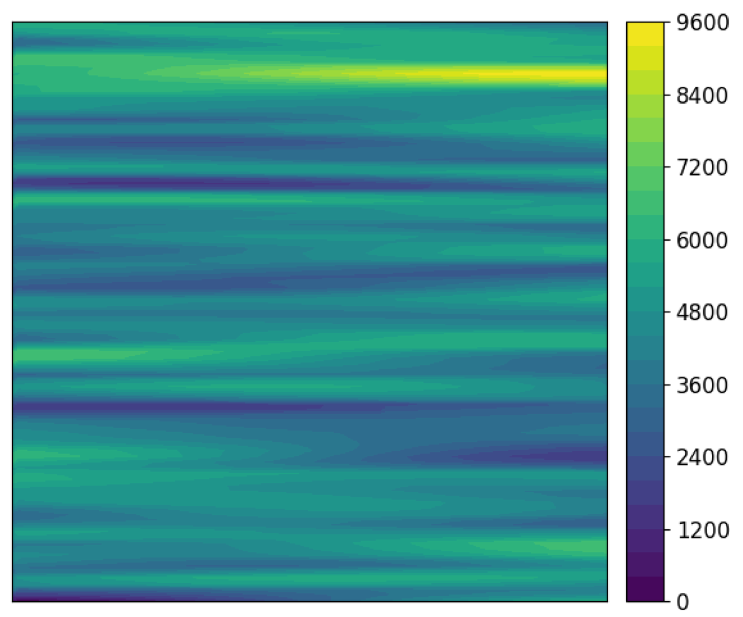

Fig. 1: Input high-contrast coefficient, $\kappa(x)$.

- **The Bottleneck**: Solving local eigenvalue problems during the offline stage of GMsFEM requires significant computational resources.
- **The Alternative**: Neural Operators (NO) are fast, but they lack robustness for highly heterogeneous media with high contrast and are heavily dependent on training data.

Objective

To develop a **hybrid framework** that combines the reliability of **GMsFEM** with the speed of **Neural Operators** by predicting the basis function subspace instead of performing costly classical computations.

Contributions

- **New Hybrid Approach (GMsFEM-NO)**: Utilizing NOs for the instantaneous generation of multiscale finite element method bases.
- **Subspace Alignment Loss (SAL)**: A novel loss function that optimizes the geometric distance between the ground-truth and predicted subspaces (Grassmannian distance) rather than attempting the point-wise reconstruction of individual functions.
- **Robustness and Efficiency**: Reducing basis construction time by over 60× while maintaining the accuracy of the original GMsFEM.
- **Grid and Source Invariance**: The method can be trained on a coarse grid and applied to a finer one; unlike pure NOs, the model remains independent of the source function $f(x)$.
- **Superiority over SOTA**: Higher accuracy and superior data efficiency compared to F-FNO, GNOT, and Transolver++ in high-contrast scenarios.

Proposed approach

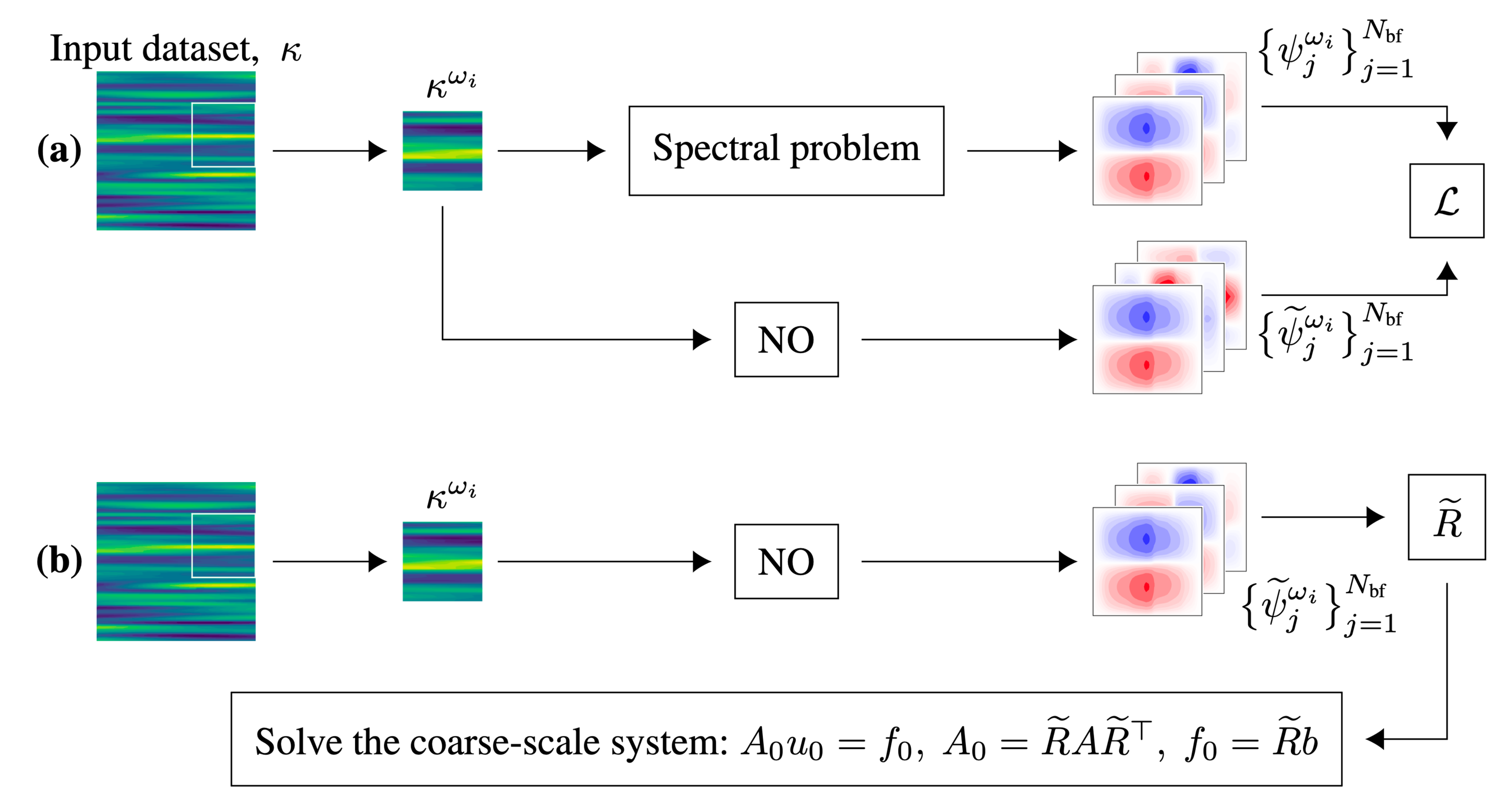

Fig. 2: Illustration of training **(a)** and inference **(b)** stages of the proposed GMsFEM-NO method. NO is trained on heterogeneous fields κ^{ω_i} that defined on subdomain ω_i to predict subspace of basis functions $\{\psi_j^{\omega_i}\}_{j=1}^{N_{\mathrm{bf}}}$, where N_{bf} is the number of basis functions. During training the subspace-informed loss $\mathcal{L}$ is applied to align predicted subspace $\{\widetilde{\psi}_j^{\omega_i}\}_{j=1}^{N_{\mathrm{bf}}}$ with $\{\psi_j^{\omega_i}\}_{j=1}^{N_{\mathrm{bf}}}$. During inference stage **(b)**, the predicted subspace forms the matrix $\widetilde{R}$ that projects matrix A and vectors to the coarse space.

Methodology:

- **Train**: The domain is partitioned into local subdomains ω_i of various types (**full**, **half**, and **corner**), for each of which a specialized NO is trained to predict $\{\psi_j^{\omega_i}\}_{j=1}^{N_{\mathrm{bf}}}$ basis functions ($N_{\mathrm{bf}} = 8$) using **SAL** loss.
- **Inference**: The trained NOs predict $\{\psi_j^{\omega_i}\}_{j=1}^{N_{\mathrm{bf}}}$ basis functions for each subdomain type; the projection matrix $\widetilde{R}$ is constructed from the predicted basis and used to solve the coarse-scale system:

$$\widetilde{R} A \widetilde{R}^\top u_0 = \widetilde{R} b, \qquad \widetilde{R} \in \mathbb{R}^{N_v \cdot N_{\mathrm{bf}} \times N_{\mathrm{fine}}},$$

where N_v is the number of local subdomains ω_i.

Subspace Alignment Loss (SAL)

Let $R^i = \left[\psi_1^{\omega_i}, \ldots, \psi_{N_{\mathrm{bf}}}^{\omega_i}\right]^\top$ represent the target subspace basis and $\widetilde{R}^i$ denote the predicted subspace. The **SAL** measures alignment between subspaces using their orthonormalized bases Q_{R^i} and $Q_{\widetilde{R}^i}$:

$$\mathcal{L}_{\mathrm{SAL}} = \mathbb{E}_i \left[N_{\mathrm{bf}} - \| Q_{R^i}^\top Q_{\widetilde{R}^i} \|_F^2 \right],$$

where the Frobenius norm term $\| Q_{R^i}^\top Q_{\widetilde{R}^i} \|_F^2$ quantifies the subspace overlap, achieving its maximum value N_{bf} when subspaces are perfectly aligned.

High-Contrast Problems

The **diffusion equation** with heterogeneous coefficient $\kappa(x)$:

$$-\nabla \cdot (\kappa(x) \nabla u(x)) = f(x), \quad x \in \Omega \equiv (0,\ 1)^D,\ u(x)\big|_{x \in \partial\Omega} = 0,$$

The steady-state version of **Richards' equation**:

$$-\nabla \cdot \big(\kappa(x, u(x)) \nabla u(x)\big) = f(x), \quad x \in \Omega \equiv (0,\ 1)^D,\ u(x)\big|_{x \in \partial\Omega} = 0,$$

where $\kappa\big(x, u(x)\big) = \kappa(x)\ (1 + |u|)^{-1}$ is unsaturated hydraulic conductivity.

Experiments

We consider two right-hand side configurations:

- Uniform unit forcing term

$$f(x) = 1. \tag{1}$$

- For 2D, spatially variable forcing defined by

$$f(x) \sim \gamma \cdot \mathcal{N}\Big(\alpha \cdot \big(I - \Delta\big)^{-\beta}\Big),\ \gamma = 2000,\ \alpha = 1,\ \beta = 0.5. \tag{2}$$

- For 3D, spatially variable forcing defined by

$$f(x) \sim \gamma \cdot \mathcal{N}\Big(\alpha \cdot \big(I - \Delta\big)^{-\beta}\Big),\ \gamma = 2000,\ \alpha = 2,\ \beta = 1. \tag{3}$$

GMsFEM vs. GMsFEM-NO for 2D

Performance comparison of GMsFEM and GMsFEM-NO for 2D (250×250, $N_v = 121$).

		GMsFEM		GMsFEM-NO, $\mathcal{L}_{\mathrm{SAL}}$	
N_{bf}	Dataset	L_2	H_1	L_2	H_1
8	Diffusion, 1	1.12%	14.01%	1.13%	13.92%
	Diffusion, 2	1.60%	21.49%	1.62%	22.50%
	Richards, 1	1.79%	14.57%	1.82%	14.27%
	Richards, 2	1.62%	21.76%	1.62%	22.62%

GMsFEM vs. GMsFEM-NO for 3D

Performance comparison of GMsFEM and GMsFEM-NO for 3D ($50 \times 50 \times 50$, $N_v = 216$).

		GMsFEM		GMsFEM-NO, $\mathcal{L}_{\mathrm{SAL}}$	
N_{bf}	Dataset	L_2	H_1	L_2	H_1
8	Diffusion, 1	3.07%	20.72%	3.10%	20.39%
	Diffusion, 3	5.08%	25.26%	5.01%	24.92%
	Richards, 1	4.04%	15.43%	4.12%	15.37%
	Richards, 3	5.02%	24.89%	5.02%	24.92%

GMsFEM vs. GMsFEM-NO for 3D

Performance comparison of GMsFEM and GMsFEM-NO for 3D ($100 \times 100 \times 100$, $N_v = 729$).

		GMsFEM		GMsFEM-NO, $\mathcal{L}_{\mathrm{SAL}}$	
N_{bf}	Dataset	L_2	H_1	L_2	H_1
8	Diffusion, 1	1.62%	14.76%	1.68%	14.98%
	Diffusion, 3	3.0%	12.55%	3.04%	12.84%
	Richards, 1	2.54%	17.83%	2.57%	17.91%
	Richards, 3	2.55%	17.85%	2.57%	17.91%

SOTA vs. GMsFEM-NO for 2D

Performance comparison of NOs and GMsFEM-NO (250×250 grid)

N_{bf}	Dataset	F-FNO	GNOT	Transolver++	GMsFEM-NO
8	Diffusion, 1	1.02%	1.26%	1.15%	1.05%
	Diffusion, 2	4.51%	14.29%	6.63%	1.60%
	Richards, 1	2.44%	2.34%	2.17%	1.72%
	Richards, 2	4.45%	14.69%	8.82%	1.60%

Comparison of F-FNO and GMsFEM-NO performance across different training dataset sizes for 250×250 grid.

$\mathcal{D}_{\mathrm{train}}$		Diffusion, 1	Diffusion, 2	Richards, 1	Richards, 2
200	GMsFEM-NO	**1.33**%	**1.77**%	**2.07**%	**1.77**%
	F-FNO	2.85%	11.56%	6.52%	11.49%
800	GMsFEM-NO	1.13%	**1.62**%	**1.82**%	**1.62**%
	F-FNO	**1.02**%	4.51%	2.44%	4.45%

Different grids for 2D

Evaluation of GMsFEM-NO trained on coarse grid and tested on finer grid, with comparison to standard GMsFEM.

		Diffusion, 1	Diffusion, 2	Richards, 1	Richards, 2
Train grid	Test grid	GMsFEM-NO			
100	500	2.42%	2.97%	4.70%	3.49%
250	500	1.45%	1.79%	2.25%	1.97%
		GMsFEM			
	500	1.17%	1.46%	1.93%	1.66%

Basis generation time

Basis generation time: GMsFEM-NO vs. GMsFEM offline stage.

Grid	N_v	GMsFEM, sec.	GMsFEM-NO, sec.
250×250	121	210.5	0.31
$50 \times 50 \times 50$	216	935.4	0.84
$100 \times 100 \times 100$	729	10547.2	1.33