GridMix: Exploring Spatial Modulation for Neural Fields in PDE Modeling

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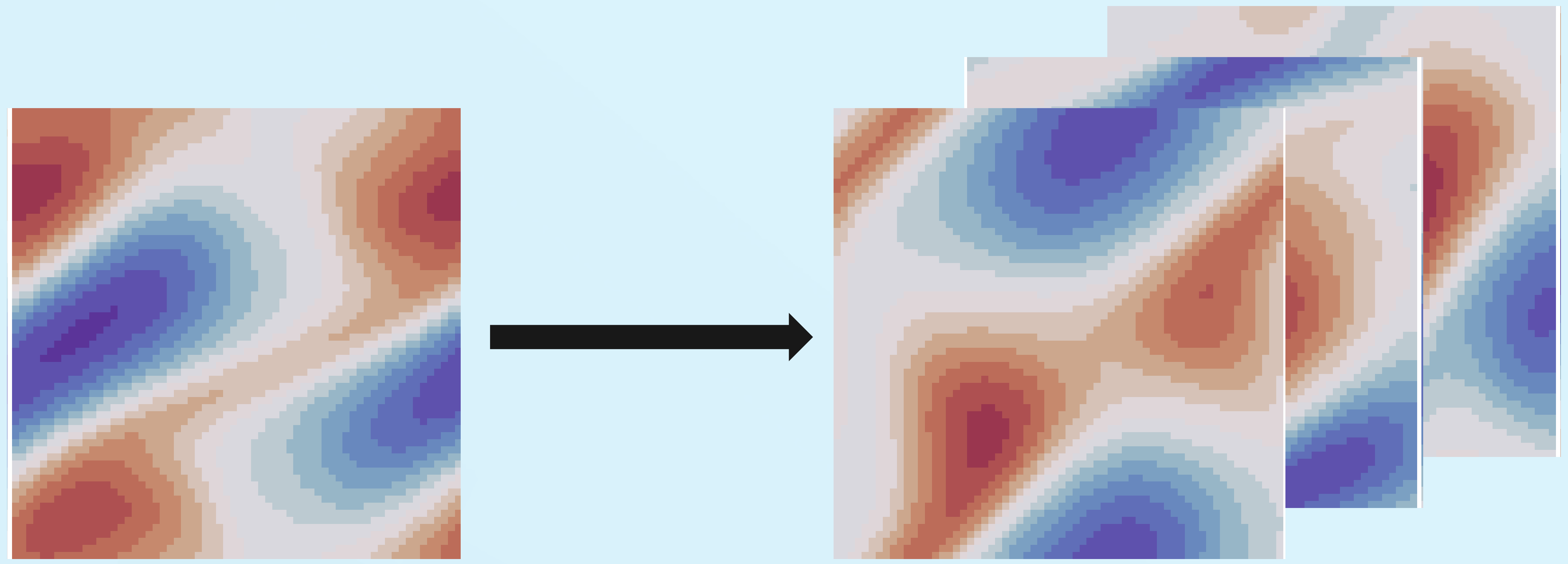
PDE Modeling

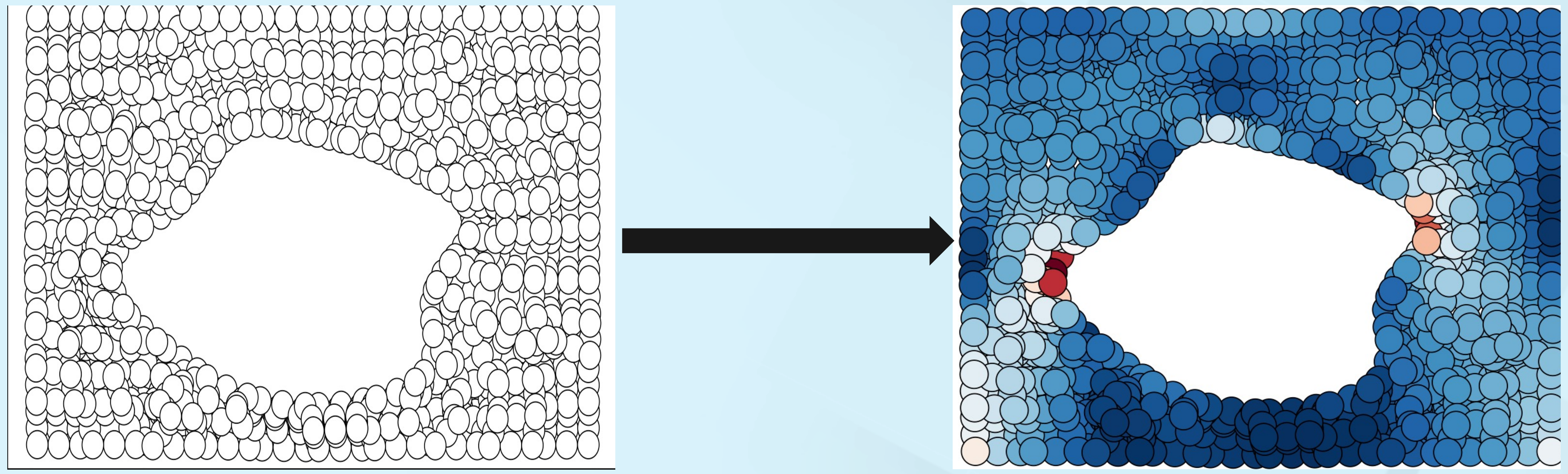
Input Space $\mathcal{A}$ $\xrightarrow[\textit{Governing by PDE}]{\text{Operator } \mathcal{G}}$ Output Space $\mathcal{U}$

Dynamics Modeling



$T = 0$ $\quad$ $T = 1:N$

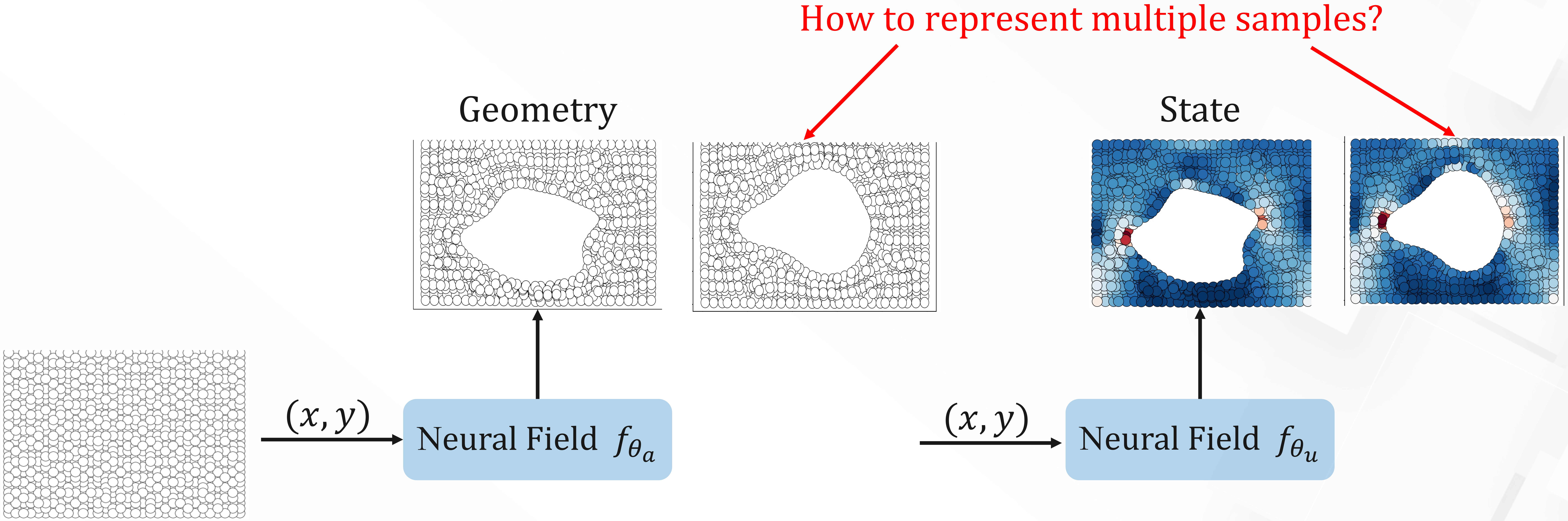
Geometric Prediction



Geometry $\quad$ State

Neural Fields

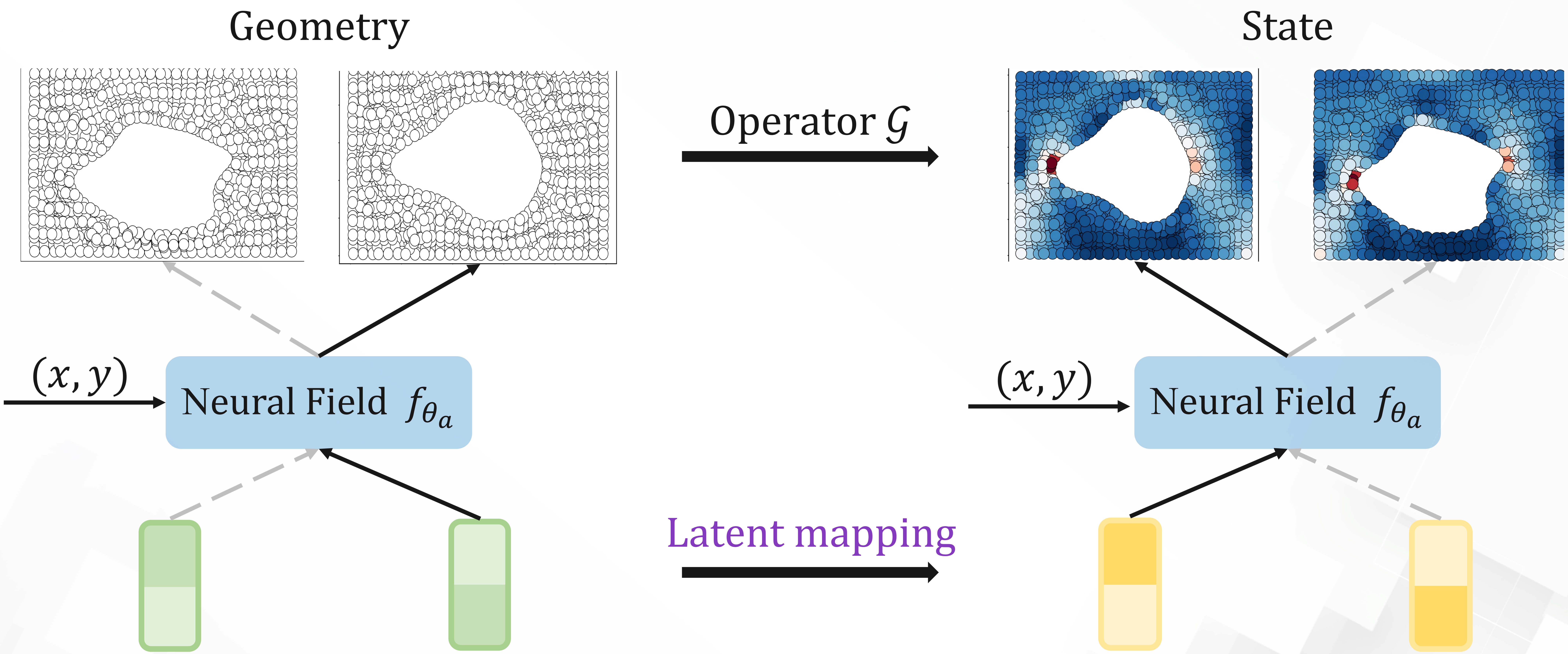
- *Continuous* data representation



[1] Serrano et al., NeurIPS 2023. Operator learning with neural fields.

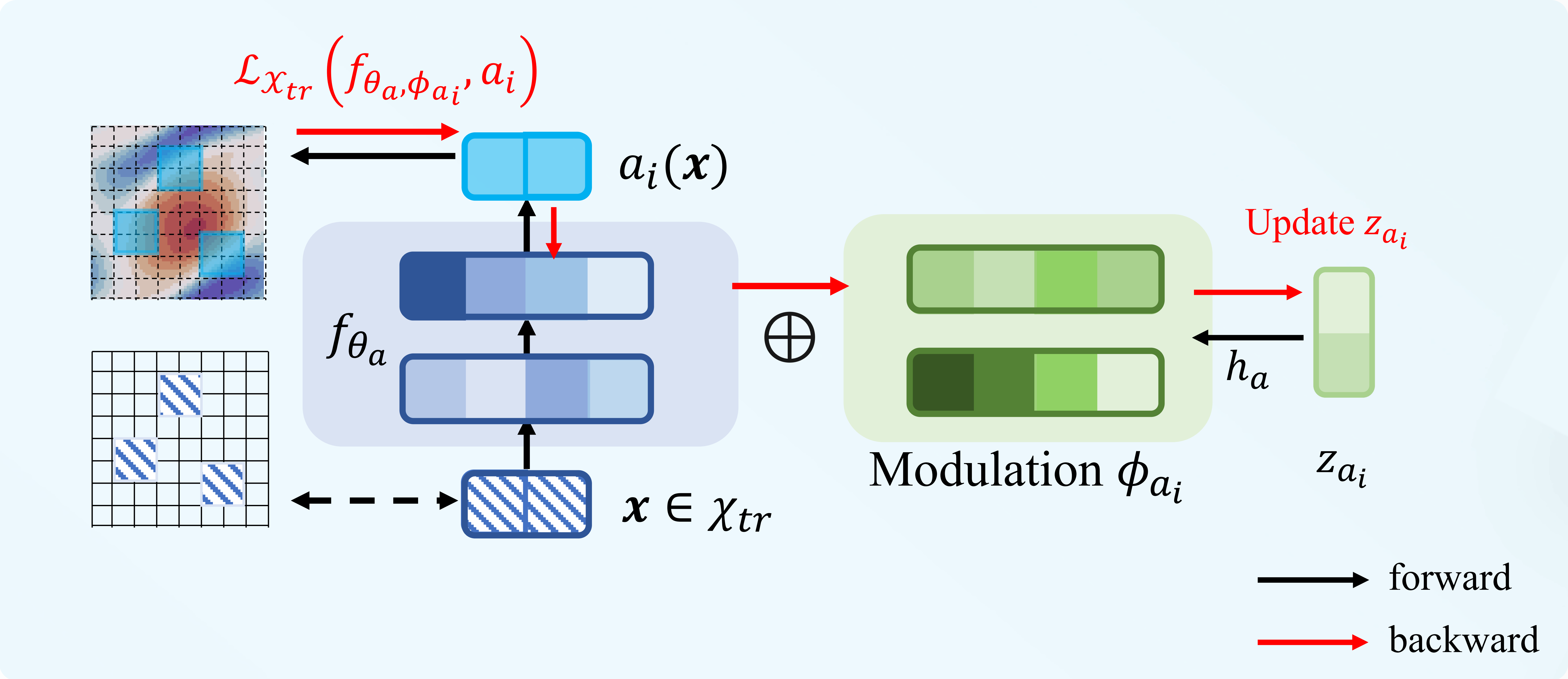
Neural Fields

- *Continuous* data representation
- Multi-sample representation via *modulation latent codes*



How to obtain modulations?

- Feature-wise Linear Modulation (FiLM)



- Auto-Decoding: optimize latent code to minimize the reconstruction loss

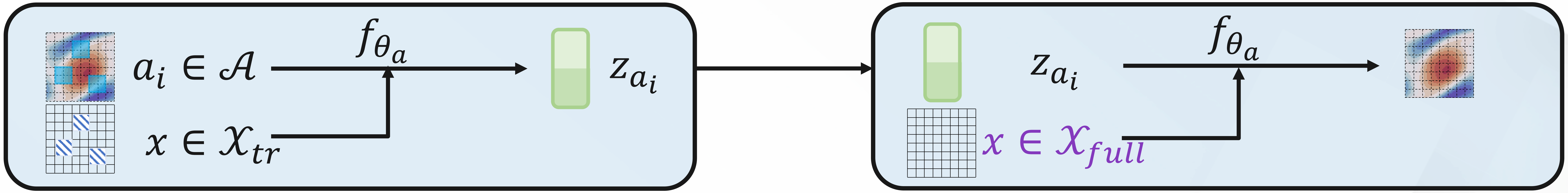
$$\mathcal{L}_{\chi_{tr}}\left(f_{\theta_a,\phi_{a_i}}, a_i\right) = \mathbb{E}_{x\sim\chi_{tr}} \left\| f_{\theta_a,\phi_{a_i}}(x) - a_i(x) \right\|^2$$

[2] Perez el al., AAAI 2018. Film: Visual reasoning with a general conditioning layer.
[3] Park et al., CVPR 2019. Deepsdf: Learning continuous signed distance functions for shape representation.

Advantages of Neural Fields

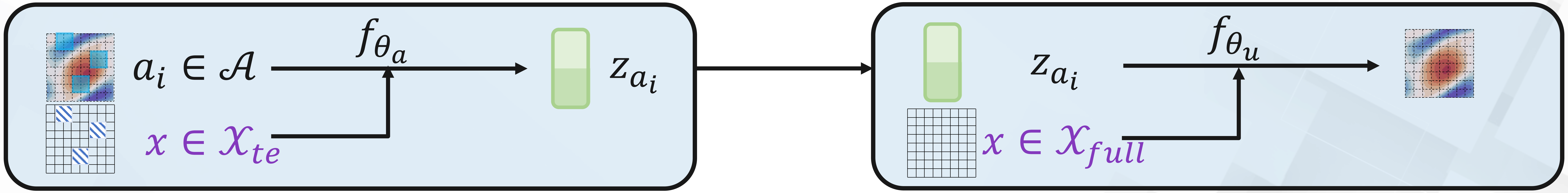
- ☐ Reconstruct data from *sparse* observation

Training: observe a_i on $\mathcal{X}_{tr}$ reconstruct a_i at $\mathcal{X}_{full}$



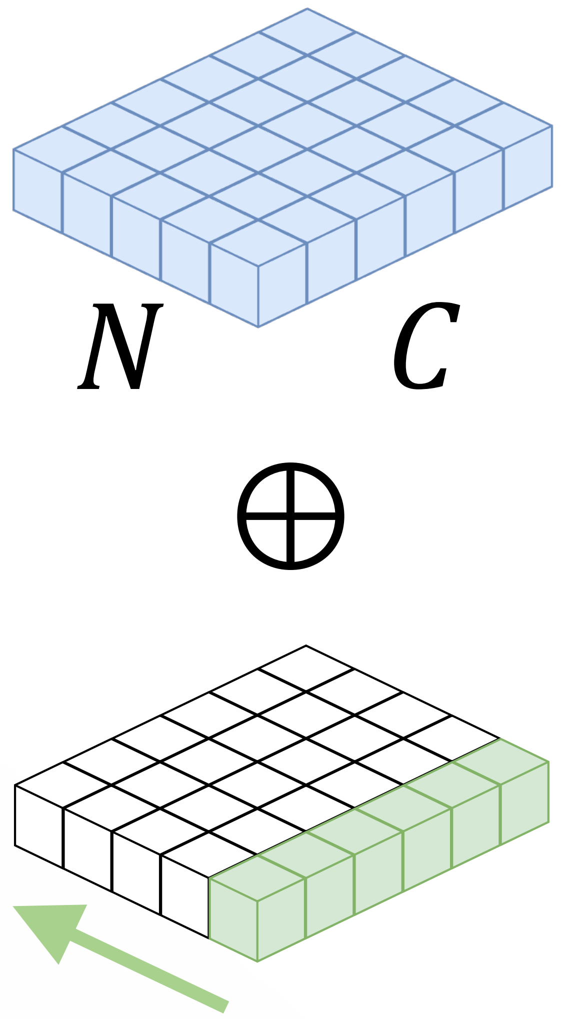
- ☐ Generalize to *unseen* spatial locations

Testing: observe a_i on unseen $\mathcal{X}_{te}$ reconstruct a_i at $\mathcal{X}_{full}$



Enhancing Neural Fields with Spatial Modulation

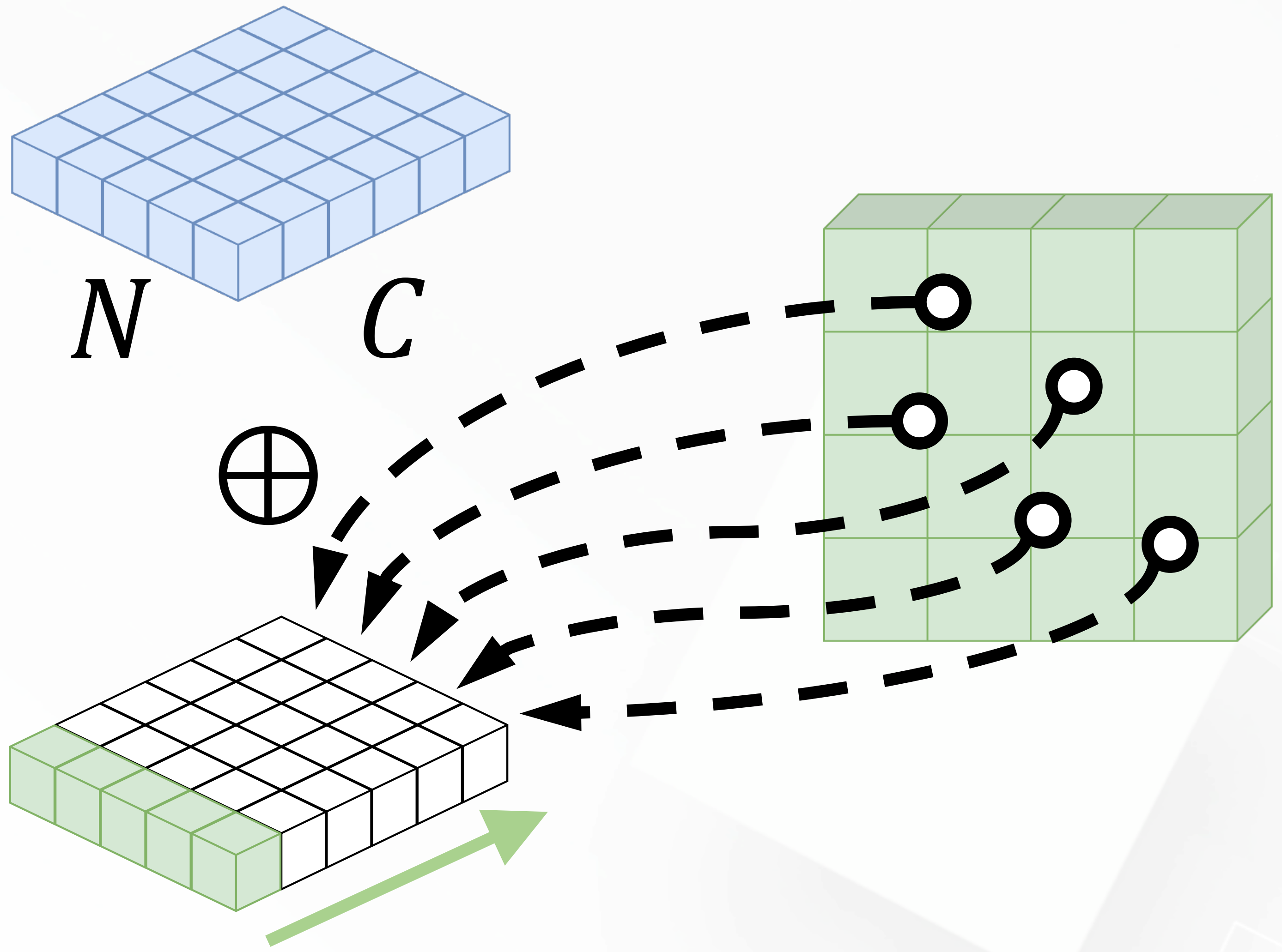
□ **Global** Modulation



$$\eta_{i+1}(x) = \sin(\omega_0(W_i\eta_i(x) + b_i + \varphi_i))$$

- All locations x share the same φ_i

□ **Spatial** Modulation



$$\eta_{i+1}(x) = \sin(\omega_0(W_i\eta_i(x) + b_i + \varphi_i(x)))$$

- Each location x learns an independent $\varphi_i(x)$

[4] Lee el al., ICLR 2024. Coordinate-aware modulation for neural fields.

Enhancing Neural Fields with Spatial Modulation

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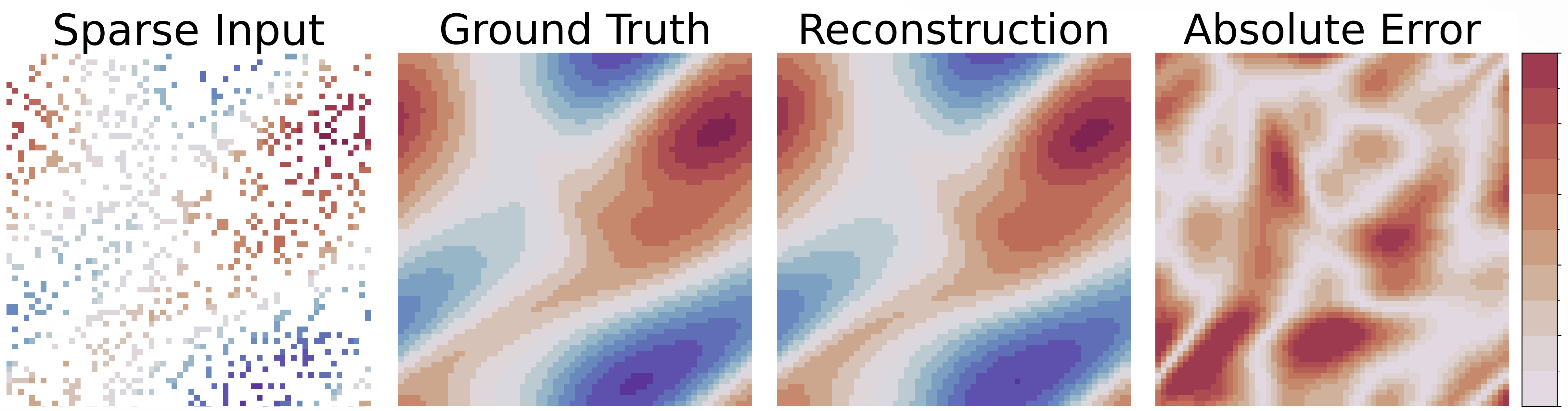
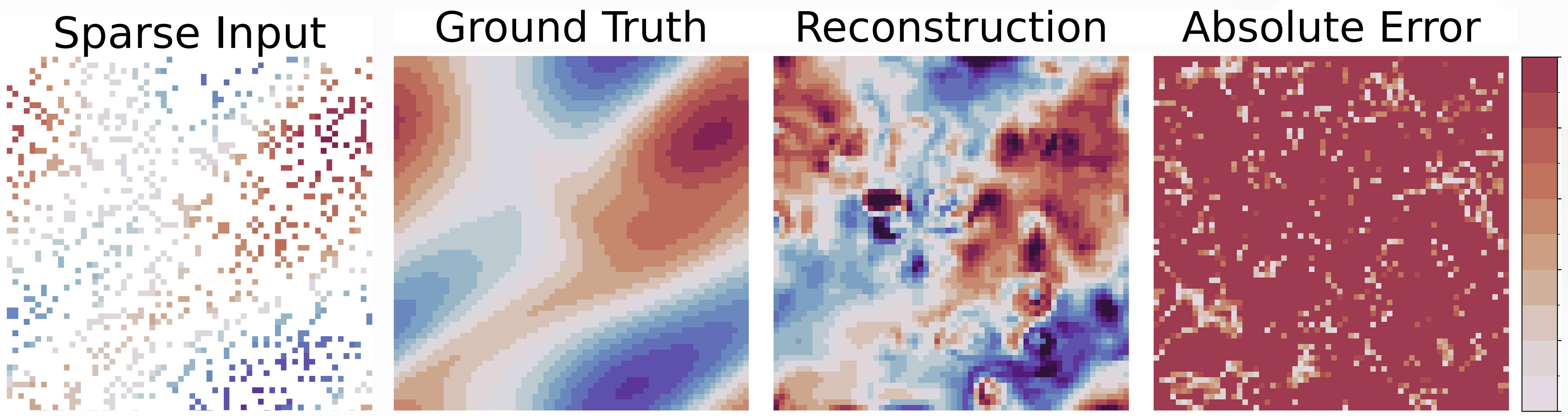
Global Modulation



- Limited in capturing fine local details

Spatial Modulation

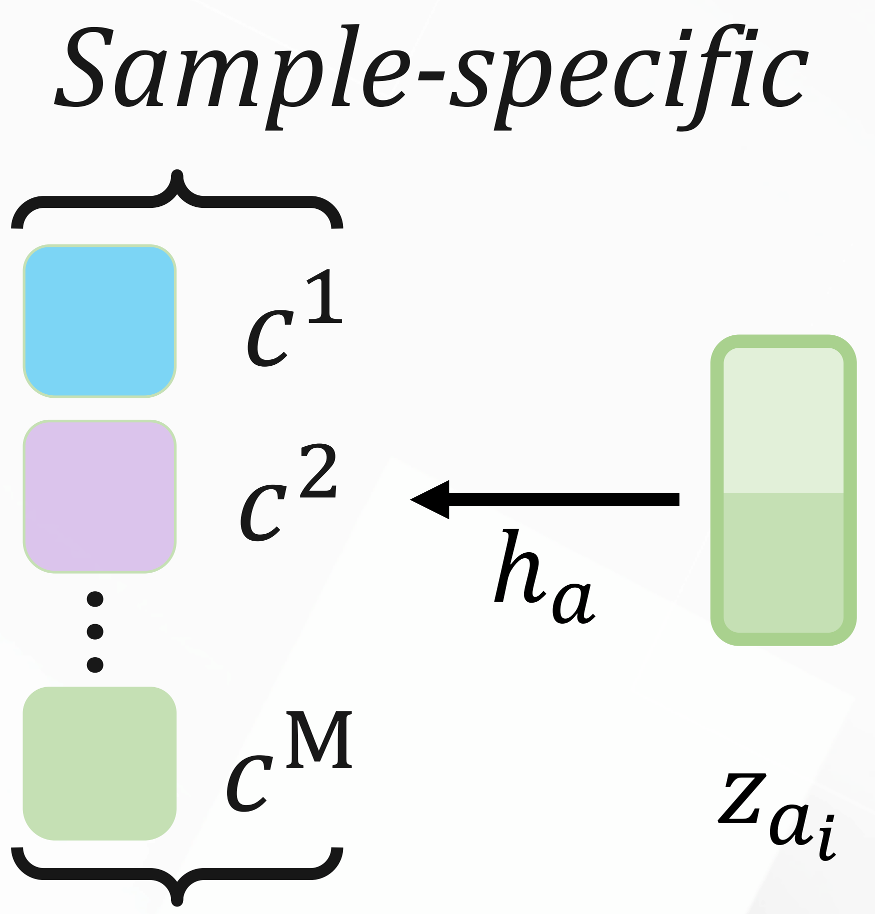


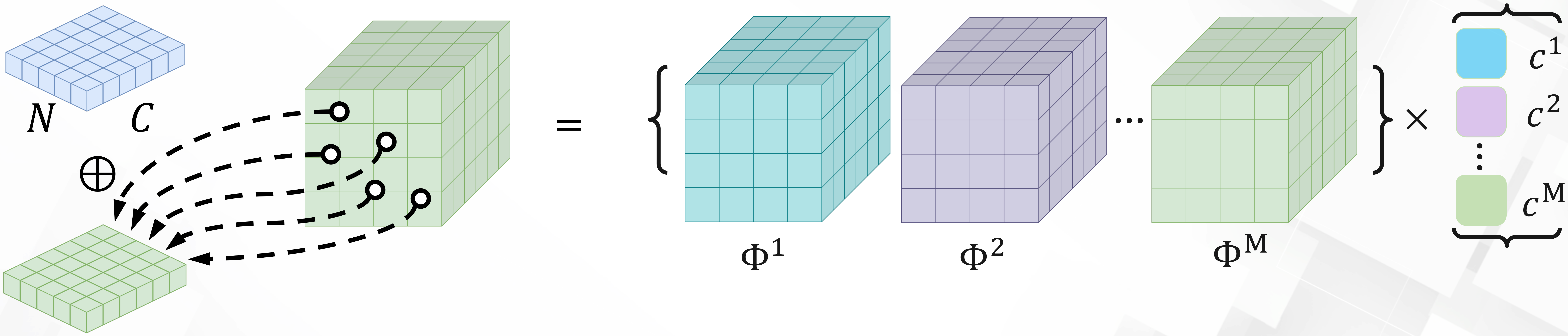
- Struggles to reconstruct global structure due to overfitting to the training grids

Represent Spatial Modulation as Mixtures of Grids

GridMix

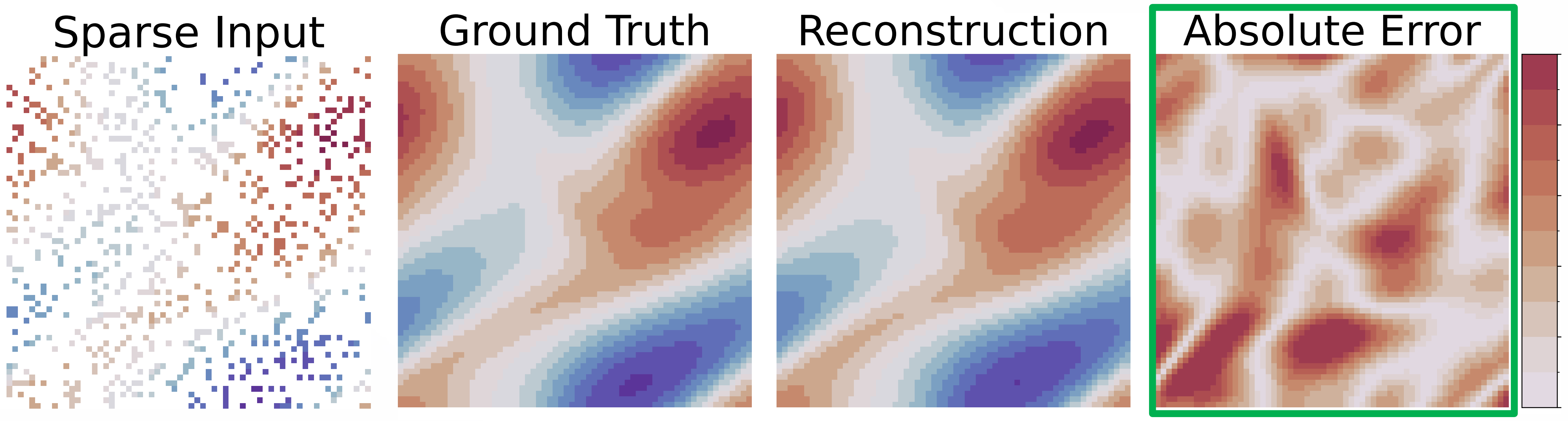
$$\varphi_i(x) = \sum_{m=1}^{M} c^m \Phi^m(x)$$



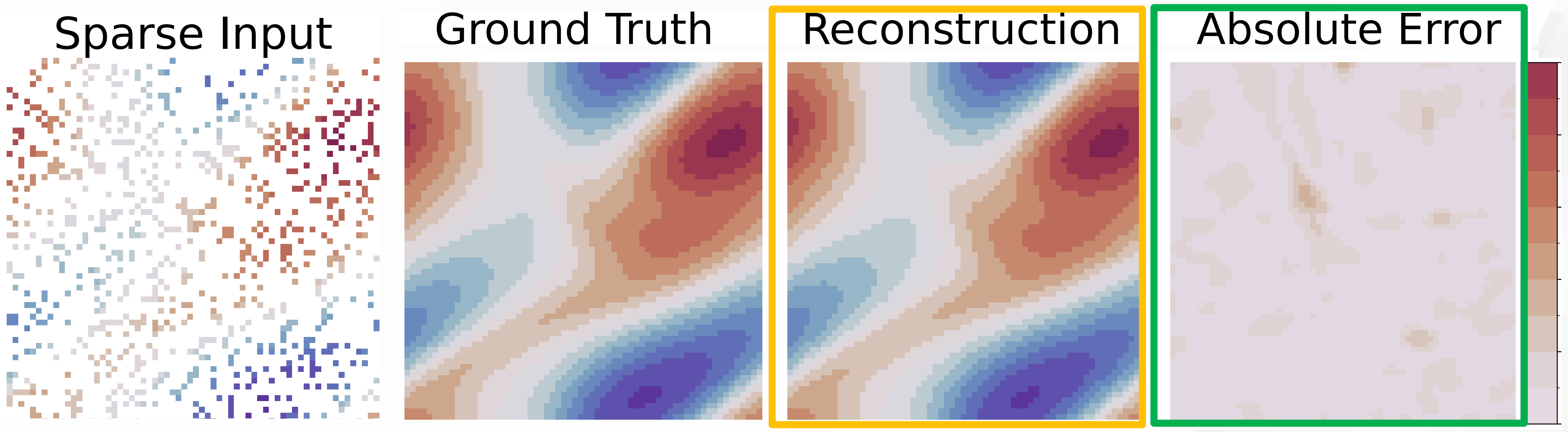


Represent Spatial Modulation as Mixtures of Grids

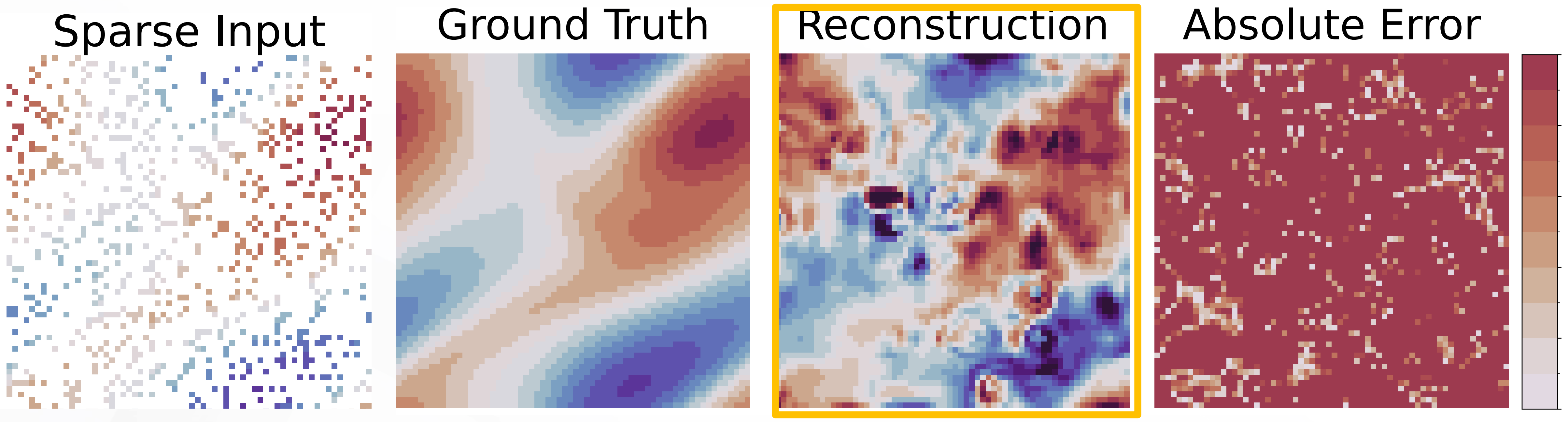
☐ Global Modulation



☐ GridMix



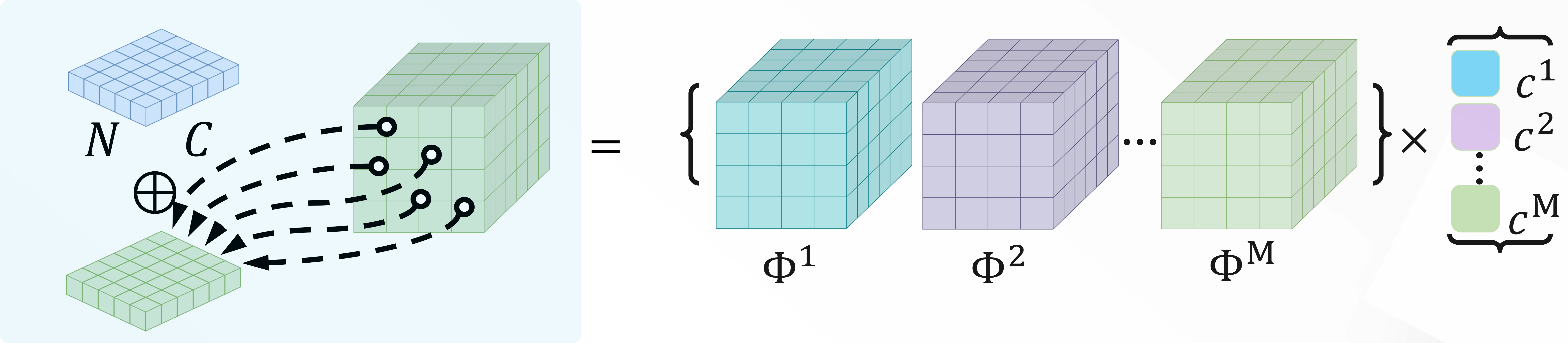
☐ Spatial Modulation



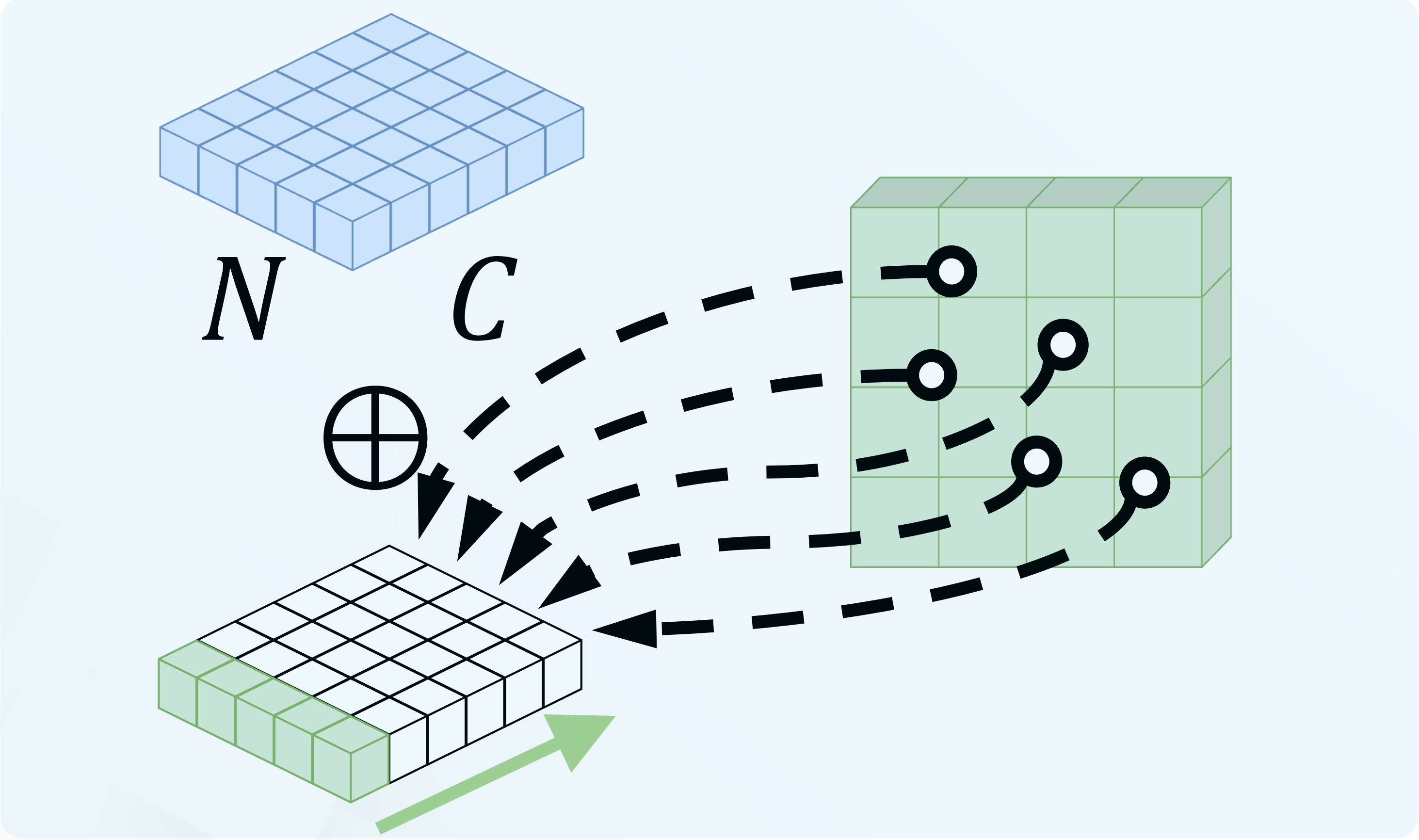
- Accurately captures fine-grained local features
- Effectively reconstructs global structure

Key Insights Behind GridMix

☐ GridMix



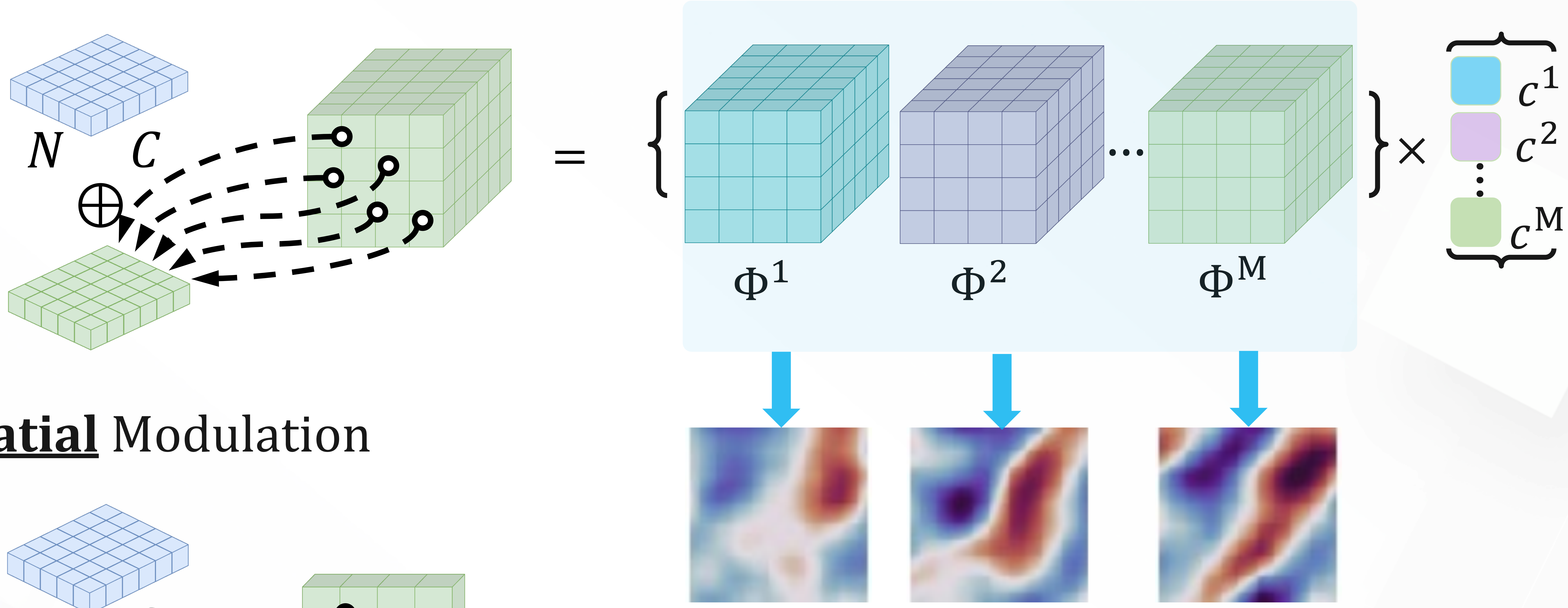
☐ **Spatial** Modulation



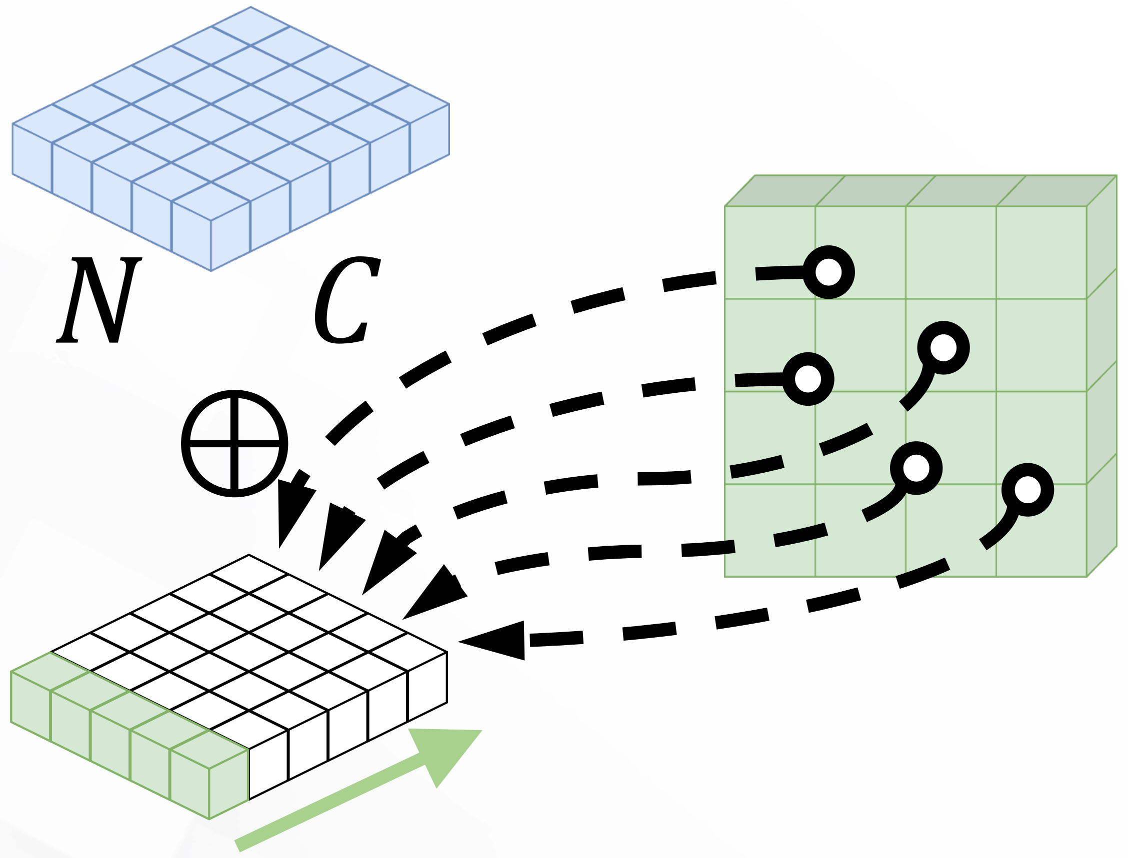
- Preserves fine-grained spatial locality

Key Insights Behind GridMix

GridMix



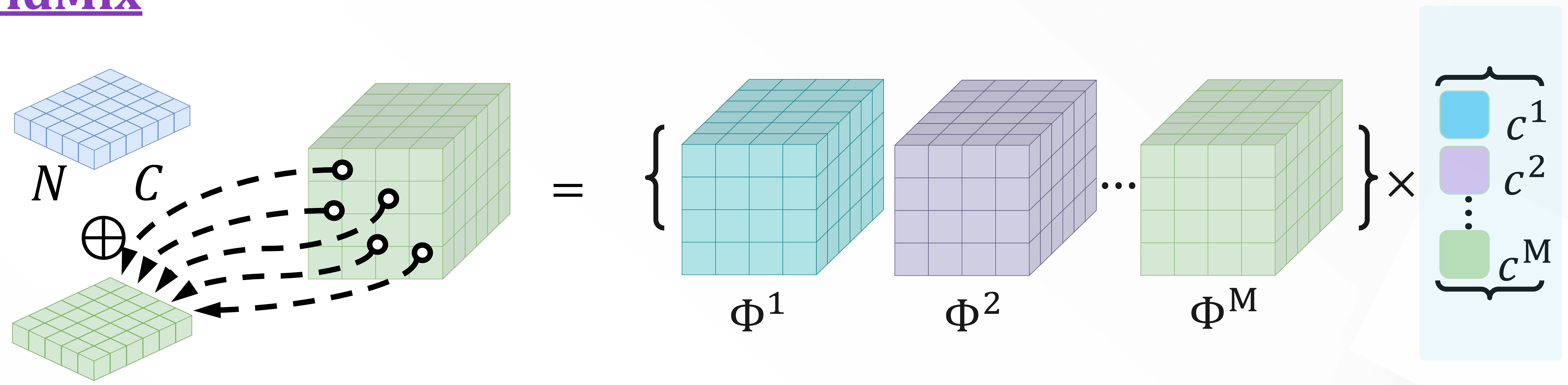
Spatial Modulation



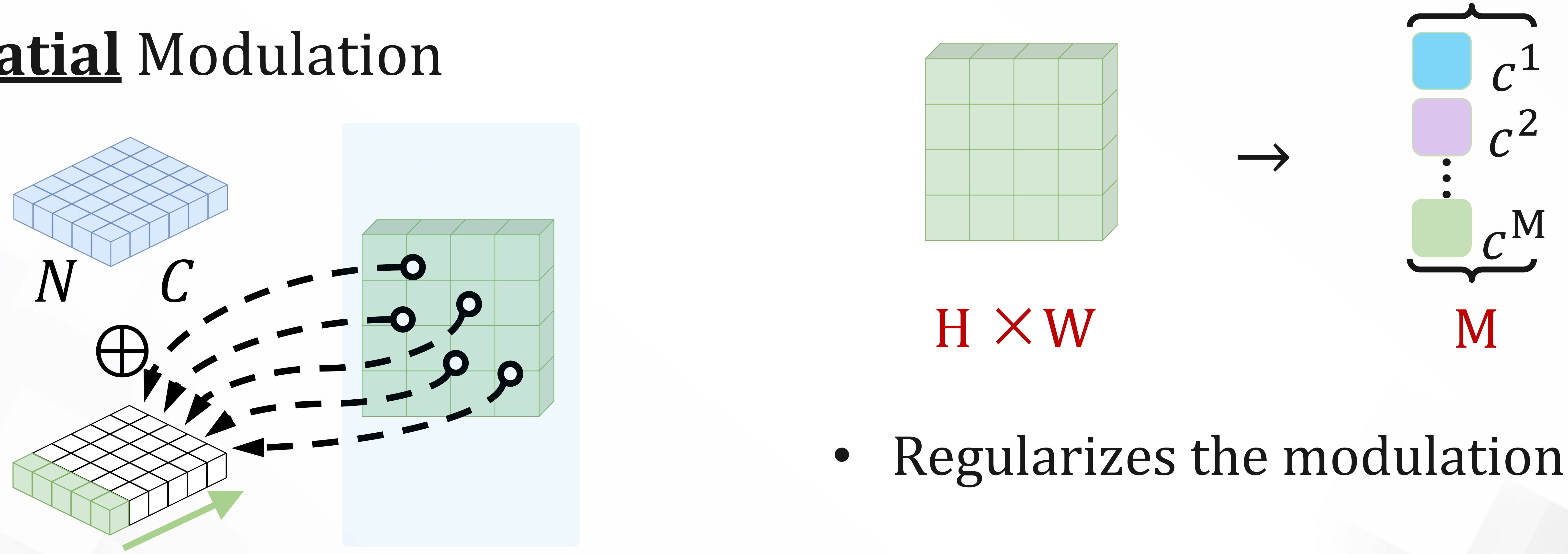
- Captures global structural patterns via shared basis functions

Key Insights Behind GridMix

GridMix



Spatial Modulation



- Regularizes the modulation space

Training

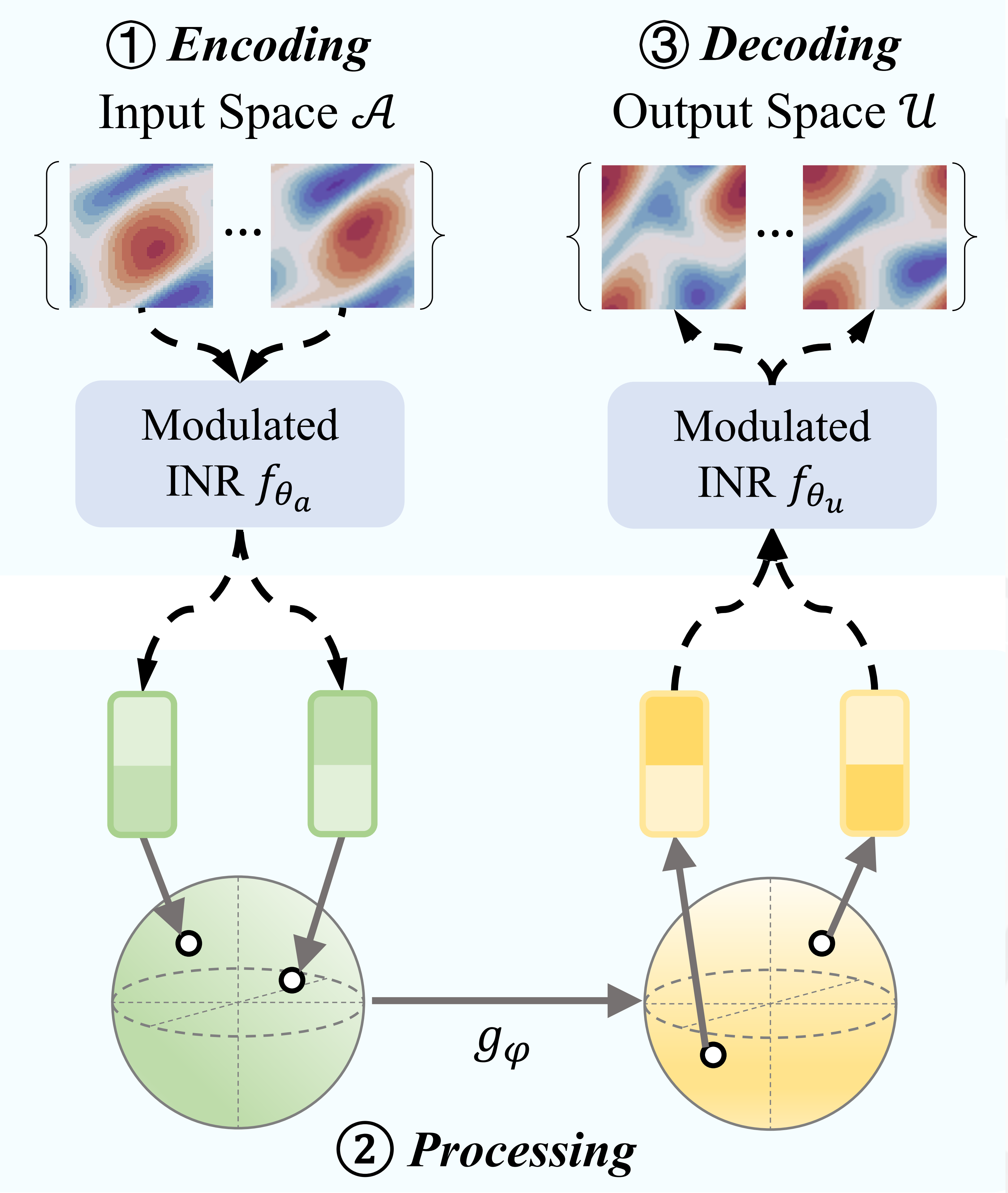
Two-stage training strategy

- **Representation**: Encode data as latent codes

$$a_i \in \mathcal{A} \xrightarrow{f_{\theta_a}} z_{a_i}$$
$$u_i \in \mathcal{U} \xrightarrow{f_{\theta_u}} z_{u_i}$$

- **Transformation**: Learn mapping in latent space

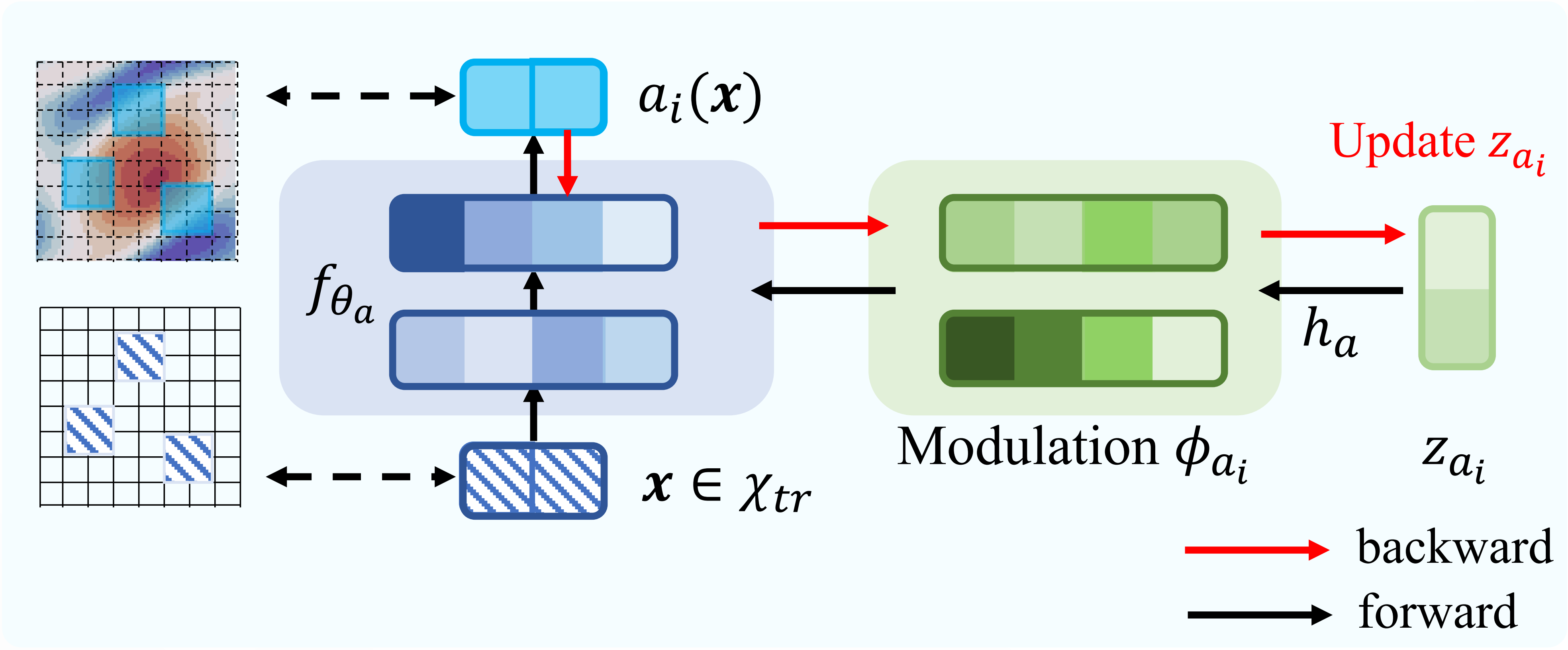
$$z_{a_i} \xrightarrow{g_\varphi} z_{u_i}$$



Meta-learning for Neural Fields and Modulations

☐ Alternatively update neural fields parameters θ_a and latent code a_i

- The encoding process (the inner loop) can be done in $K = 3$ steps



Input: $a_i \in \mathcal{A}, \theta_a$ *Outer loop*

Init: $z_{a_i}^{(0)} = 0$ *Inner loop*

for $k = \{1 \dots K\}$ do

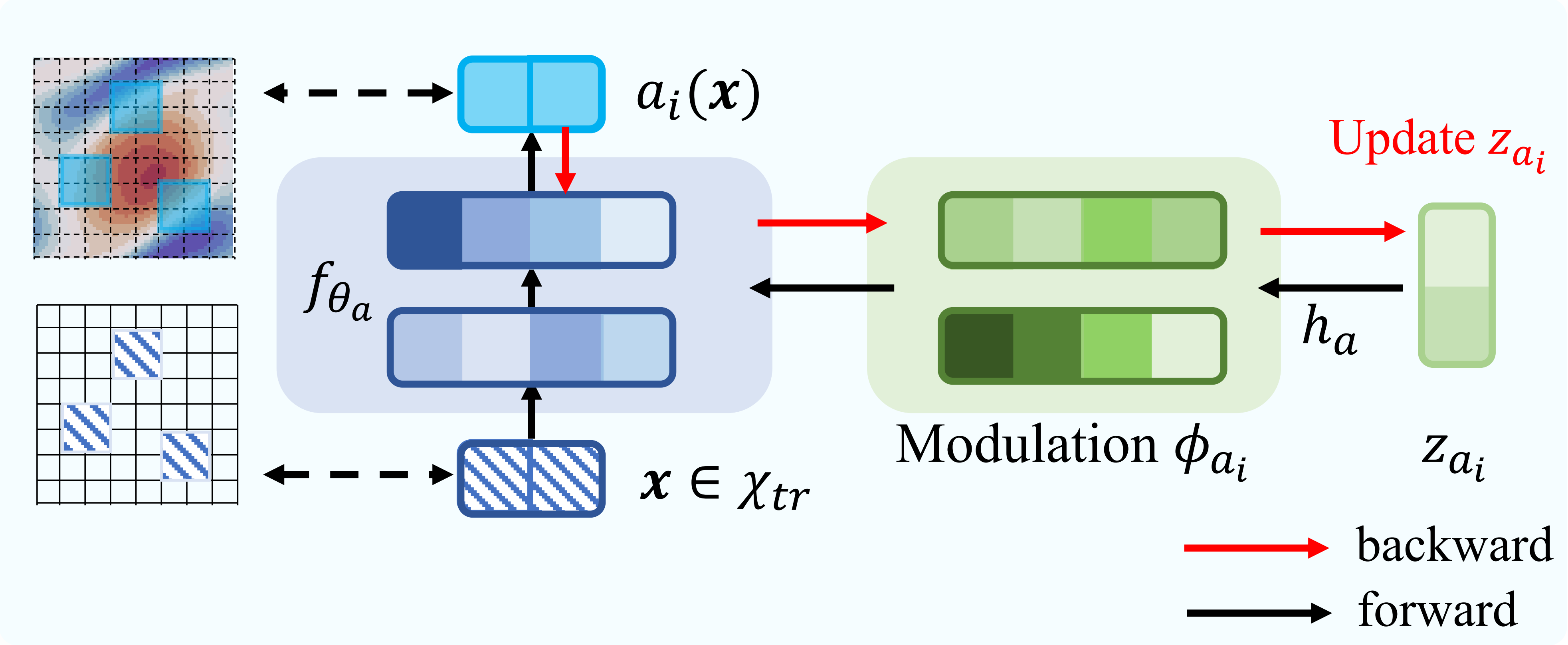
$$z_{a_i}^{(k)} = z_{a_i}^{(k-1)} - \alpha \nabla \mathcal{L}\left(f_{\theta_a}\left(\mathcal{X}_{tr}, z_{a_i}^{(k-1)}\right), a_i(x)\right)$$

end

$$\theta_a \leftarrow \theta_a - \beta \nabla \mathcal{L}\left(f_{\theta_a}\left(\mathcal{X}_{tr}, z_{a_i}^{(K)}\right), a_i(x)\right)$$

Spatial Domain Augmentation

- Simulate *__domain variations__* in training to improve generalization



Input: $a_i \in \mathcal{A}, \theta_a, \boldsymbol{\mathcal{X}_{out}} \supset \boldsymbol{\mathcal{X}_{tr}}$ *Outer loop*

Init: $z_{a_i}^{(0)} = 0, \boldsymbol{\mathcal{X}_{in}} \supset \boldsymbol{\mathcal{X}_{tr}}$ *Inner loop*

for $k = \{1 \dots K\}$ do

$$z_{a_i}^{(k)} = z_{a_i}^{(k-1)} - \alpha \nabla \mathcal{L}\left(f_{\theta_a}\left(\boldsymbol{\mathcal{X}_{out}}, z_{a_i}^{(k-1)}\right), a_i(x)\right)$$

end

$$\theta_a \leftarrow \theta_a - \beta \nabla \mathcal{L}\left(f_{\theta_a}\left(\boldsymbol{\mathcal{X}_{in}}, z_{a_i}^{(K)}\right), a_i(x)\right)$$

Experiments

Dynamics Modeling

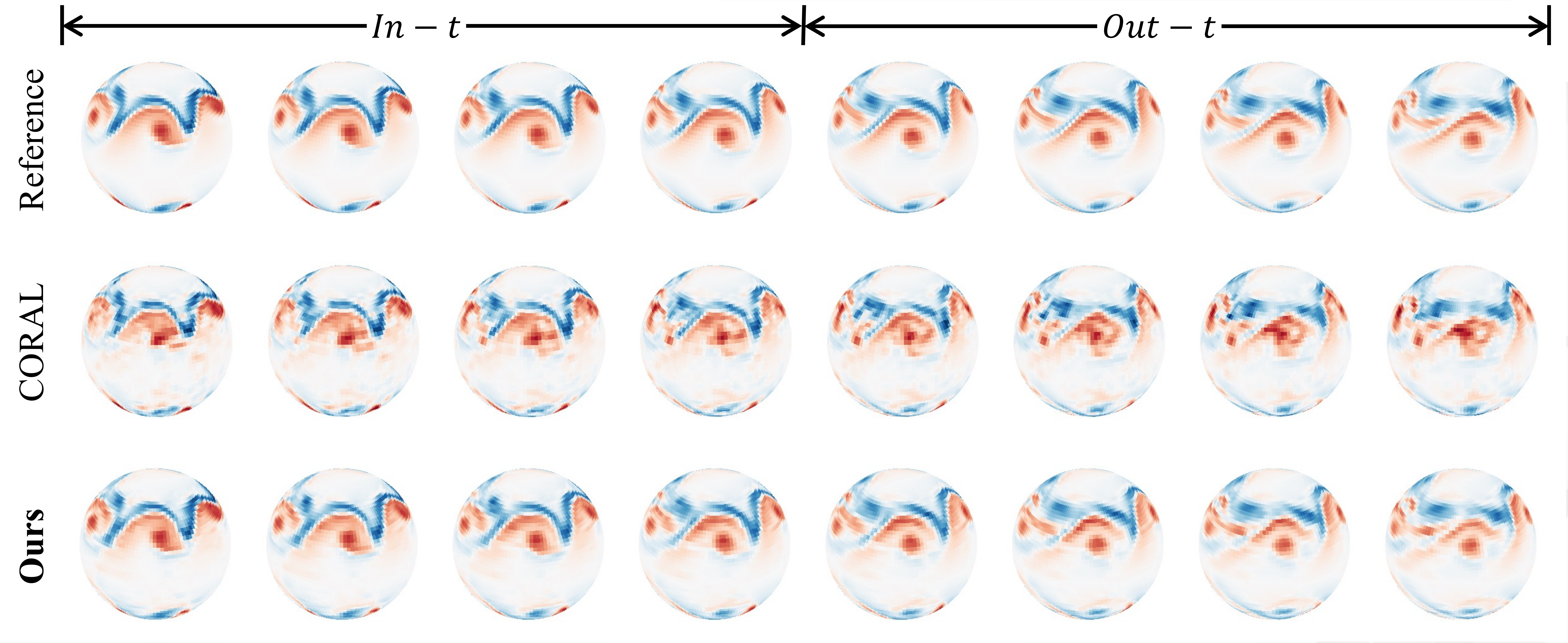
- *Sparse grid*
- *Temporal exploration*

$\mathcal{X}_{tr} \downarrow \mathcal{X}_{te}$	dataset →	*Navier-Stokes*		*Shallow-Water*	
		In-t	*Out-t*	*In-t*	*Out-t*
$\pi = 100\%$ regular grid	DeepONet	4.72e-2 ± 2.84e-2	9.58e-2 ± 1.83e-2	6.54e-3 ± 4.94e-4	8.93e-3 ± 9.42e-5
	FNO	5.68e-4 ± 7.62e-5	8.95e-3 ± 1.50e-3	3.20e-5 ± 2.51e-5	**1.17e-4 ± 3.01e-5**
	MP-PDE	4.39e-4 ± 8.78e-5	4.46e-3 ± 1.28e-3	9.37e-5 ± 5.56e-6	1.53e-3 ± 2.62e-4
	DINo	1.27e-3 ± 2.22e-5	1.11e-2 ± 2.28e-3	4.48e-5 ± 2.74e-6	2.63e-3 ± 1.36e-4
	CORAL	1.86e-4 ± 1.44e-5	1.02e-3 ± 8.62e-5	3.44e-6 ± 4.01e-7	4.82e-4 ± 5.16e-5
	MARBLE (Ours)	**3.52e-5 ± 5.31e-6**	**5.04e-4 ± 3.68e-5**	**8.21e-7 ± 1.13e-8**	1.42e-4 ± 7.07e-6
$\pi = 20\%$ irregular grid	DeepONet	8.37e-1 ± 2.07e-2	7.80e-1 ± 2.36e-2	1.05e-2 ± 5.01e-4	1.09e-2 ± 6.16e-4
	FNO + lin. int.	3.97e-3 ± 8.03e-4	9.92e-3 ± 2.36e-3	n.a.	n.a.
	MP-PDE	3,98e-2 ± 1,69e-2	1,31e-1 ± 5,34e-2	5.28e-3 ± 5.25e-4	2.56e-2 ± 8.23e-3
	DINo	9.99e-4 ± 6.71e-3	8.27e-3 ± 5.61e-3	2.20e-3 ± 1.06e-4	4.94e-3 ± 1.92e-4
	CORAL	2.18e-3 ± 6.88e-4	6.67e-3 ± 2.01e-3	1.41e-3 ± 1.39e-4	2.11e-3 ± 5.58e-5
13× lower	MARBLE (Ours)	**1.62e-4 ± 2.42e-5**	**9.27e-4 ± 1.44e-4**	**7.06e-4 ± 4.60e-5**	**8.45e-4 ± 3.01e-5**
$\pi = 5\%$ irregular grid	DeepONet	7.86e-1 ± 5.48e-2	7.48e-1 ± 2.76e-2	1.11e-2 ± 6.94e-4	1.12e-2 ± 7.79e-4
	FNO + lin. int.	3.87e-2 ± 1.44e-2	5.19e-2 ± 1.10e-2	n.a.	n.a.
	MP-PDE	1.92e-1 ± 9.27e-2	4.73e-1 ± 2.17e-1	1.10e-2 ± 4.23e-3	4.94e-2 ± 2.36e-2
	DINo	8.65e-2 ± 1.16e-2	9.36e-2 ± 9.34e-3	**1.22e-3 ± 2.05e-4**	1.52e-2 ± 3.74e-4
	CORAL	2.44e-2 ± 1.96e-2	4.57e-2 ± 1.78e-2	8.77e-3 ± 7.20e-4	1.29e-2 ± 1.92e-3
	MARBLE (Ours)	**1.43e-3 ± 5.66e-4**	**4.73e-3 ± 1.33e-3**	5.92e-3 ± 3.32e-4	**5.98e-3 ± 3.51e-4**

Experiments

Tsinghua University

□ Visualization results on *Shallow-Water* with $\pi = 20\%$ irregular grid

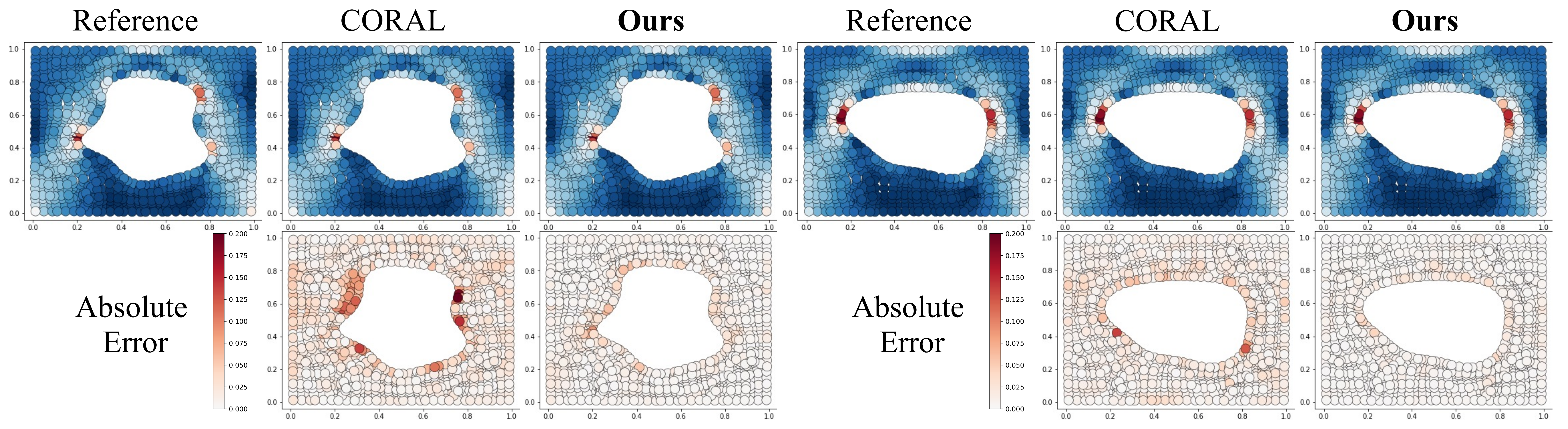


Experiments

Geometric Prediction

Model	*NACA-Euler*	*Elasticity*	*Pipe*
FNO	3.85e-2 ± 3.15e-3	4.95e-2 ± 1.21e-3	1.53e-2 ± 8.19e-3
UNet	5.05e-2 ± 1.25e-3	5.34e-2 ± 2.89e-4	2.98e-2 ± 1.08e-2
Geo-FNO	1.58e-2 ± 1.77e-3	3.41e-2 ± 1.93e-2	**6.59e-3** ± **4.67e-4**
Factorized-FNO	6.20e-3 ± 3.00e-4	1.96e-2 ± 2.00e-2	7.33e-3 ± 4.66e-4
CORAL	5.90e-3 ± 1.00e-4	1.67e-2 ± 4.18e-4	1.20e-2 ± 8.74e-4
MARBLE (Ours)	**5.79e-3** ± **9.67e-5**	**1.12e-2** ± **9.43e-5**	1.03e-2 ± 2.62e-4

Visualization results on *Elasticity*



Thank for your attention!

paper

code