Physics-aligned Field Reconstruction with Diffusion Bridge

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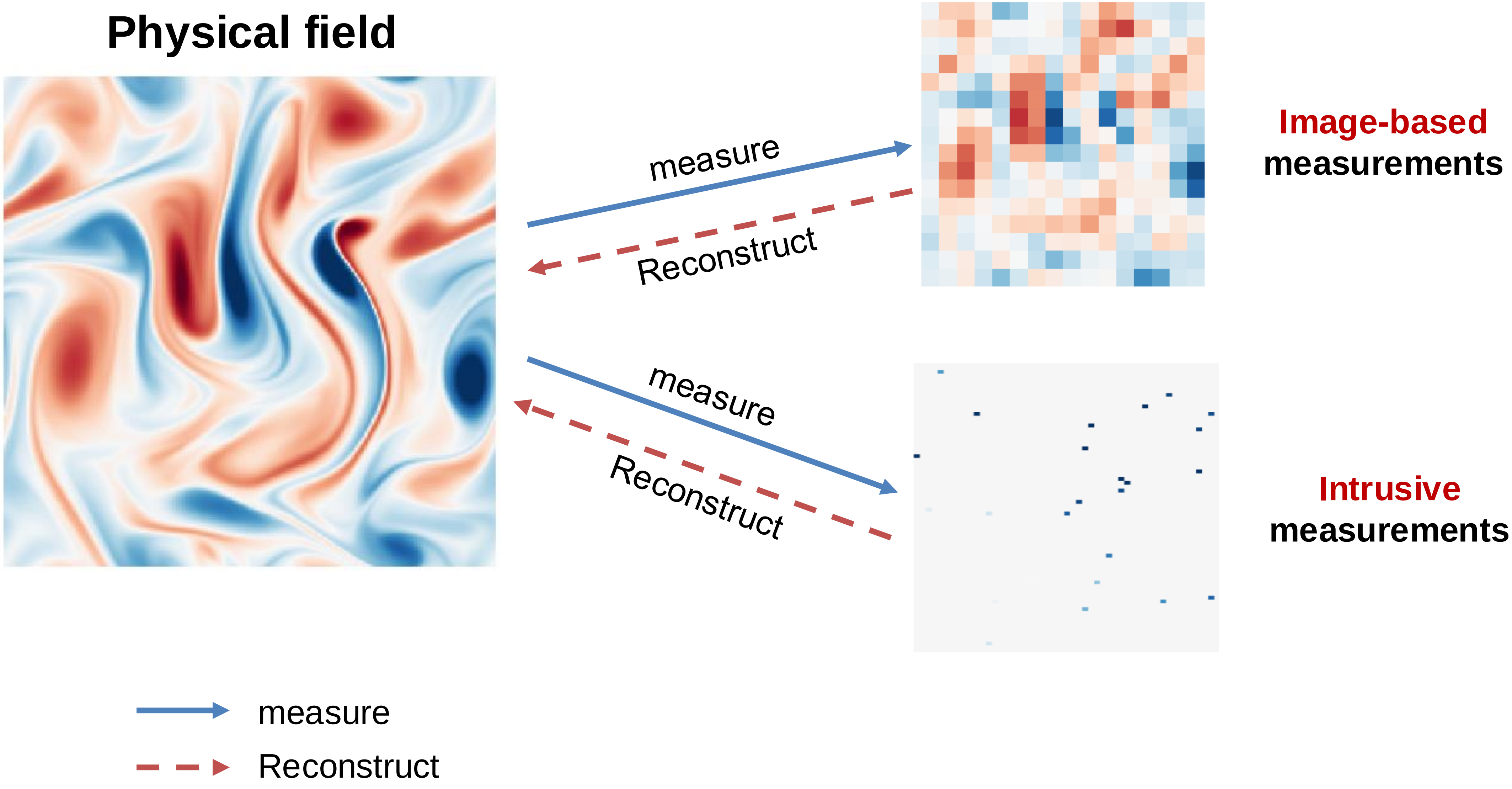
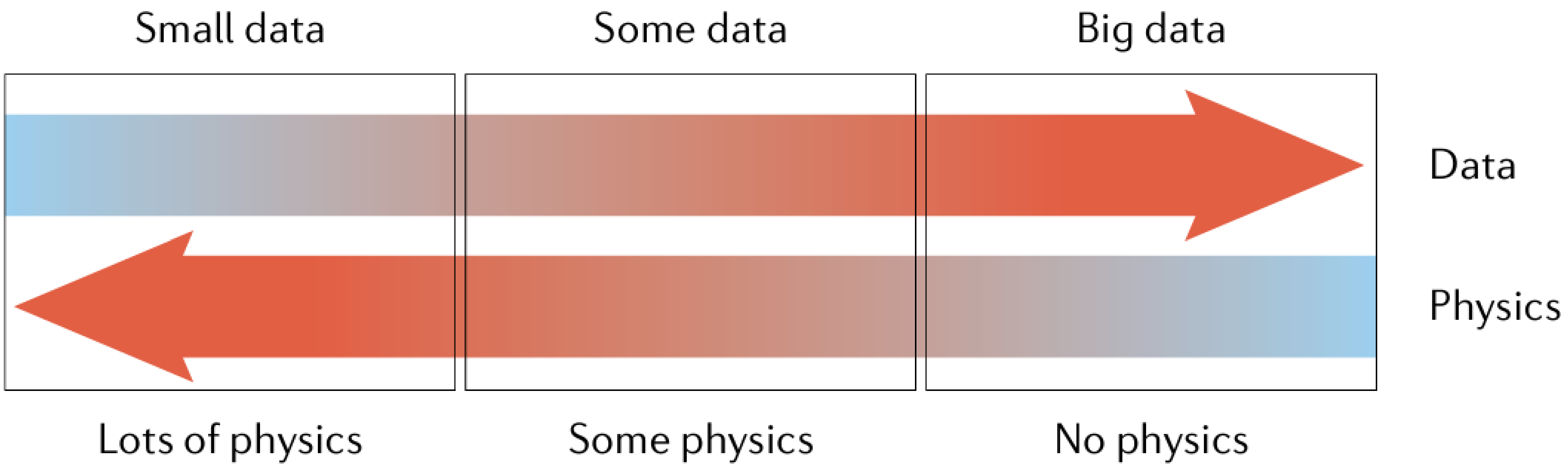
The Thirteenth International Conference of Learning Representation (ICLR2025)

What is field reconstruction?



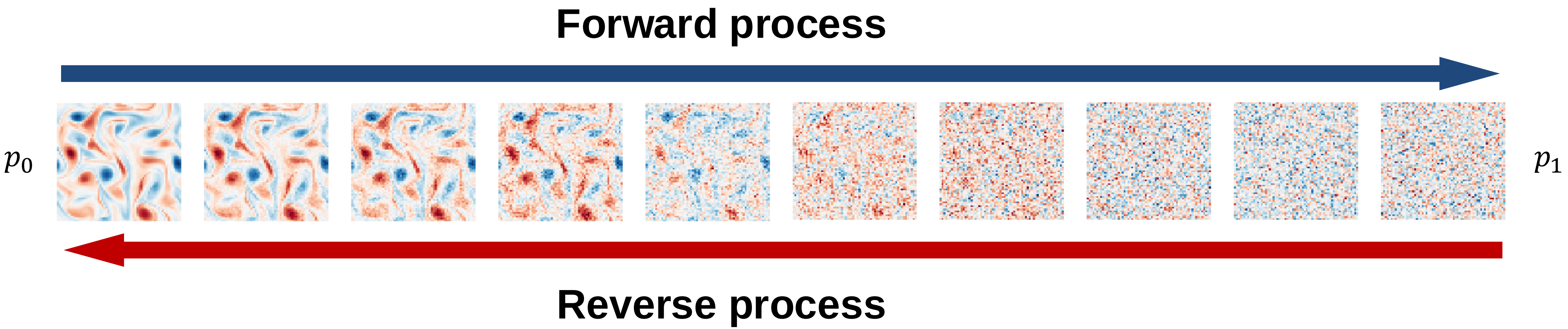
How to reconstruct physical field?



- **physics-based**
  - **PINN**
  - **Variational data assimilation**
- **data-driven**
  - **ROM-based**
  - **End2End (CNN, NO)**
  - **Generative models (VAE, GAN, Diffusion)**

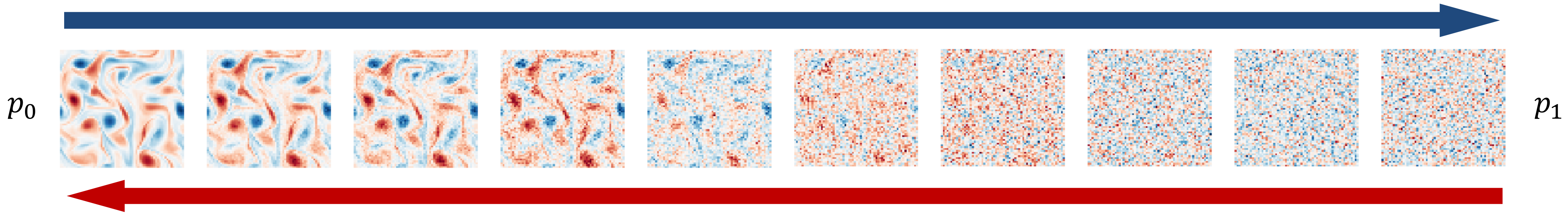
Karniadakis et. al, 2021 *Nat. Rev. Phys.*

Quick introduction of diffusion models



Diffusion models for field reconstruction

Forward process

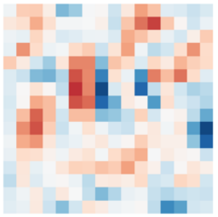


Reverse process

Guidance

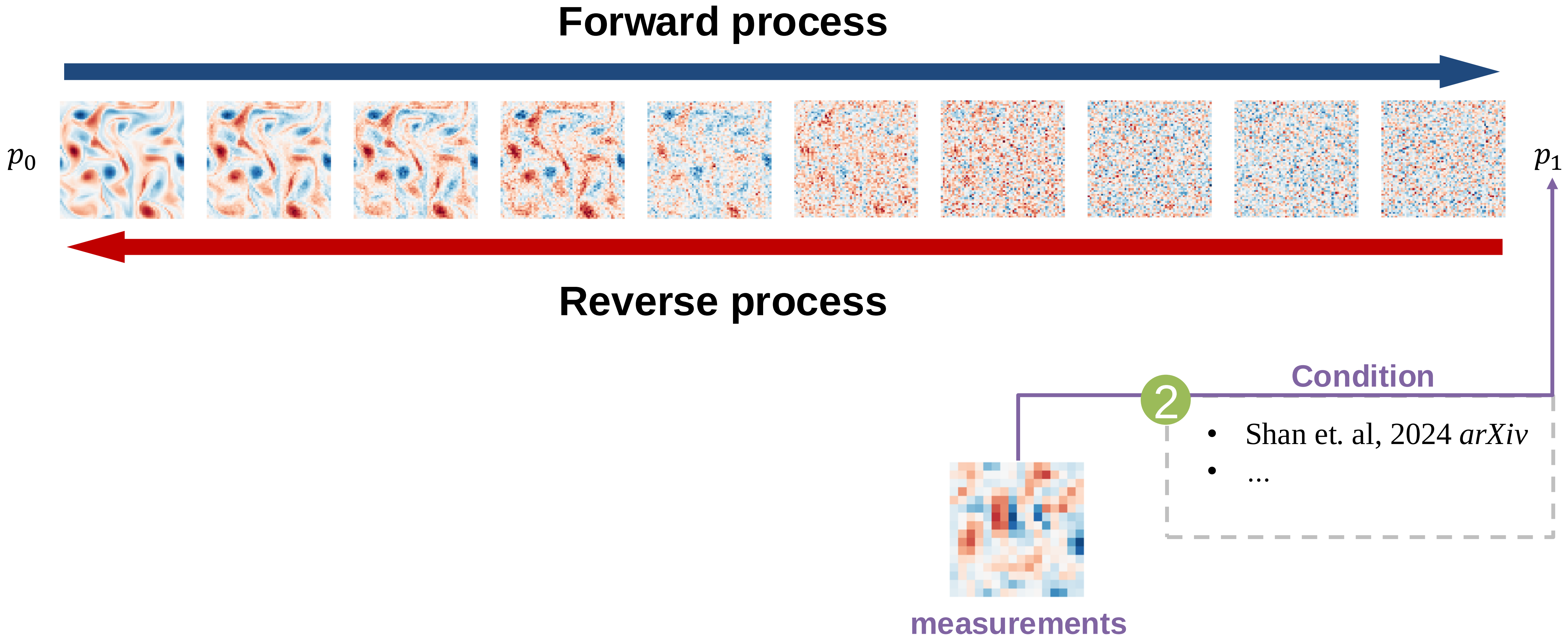
1

- Shu et. al, 2023 *JCP*
- Li et. al, 2024 *NMI*
- …

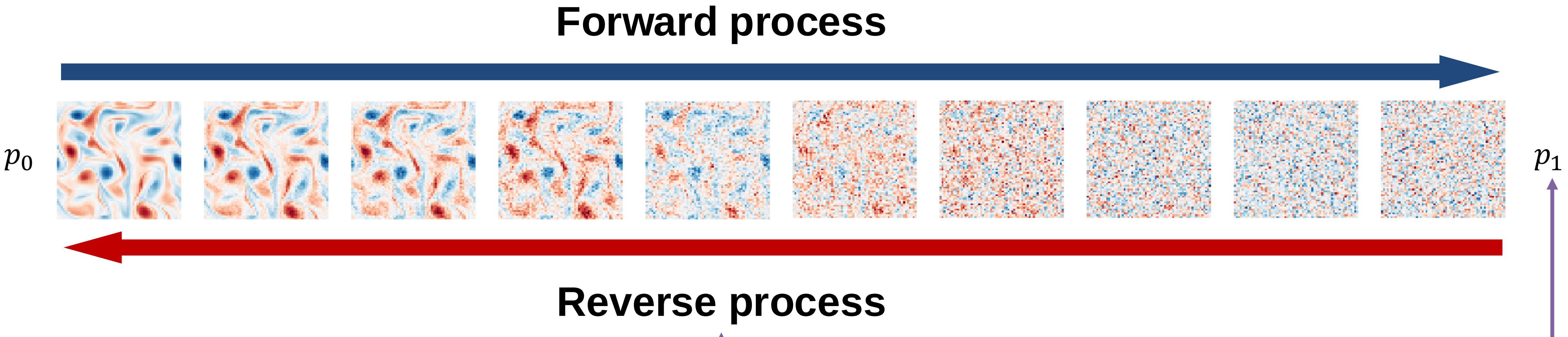


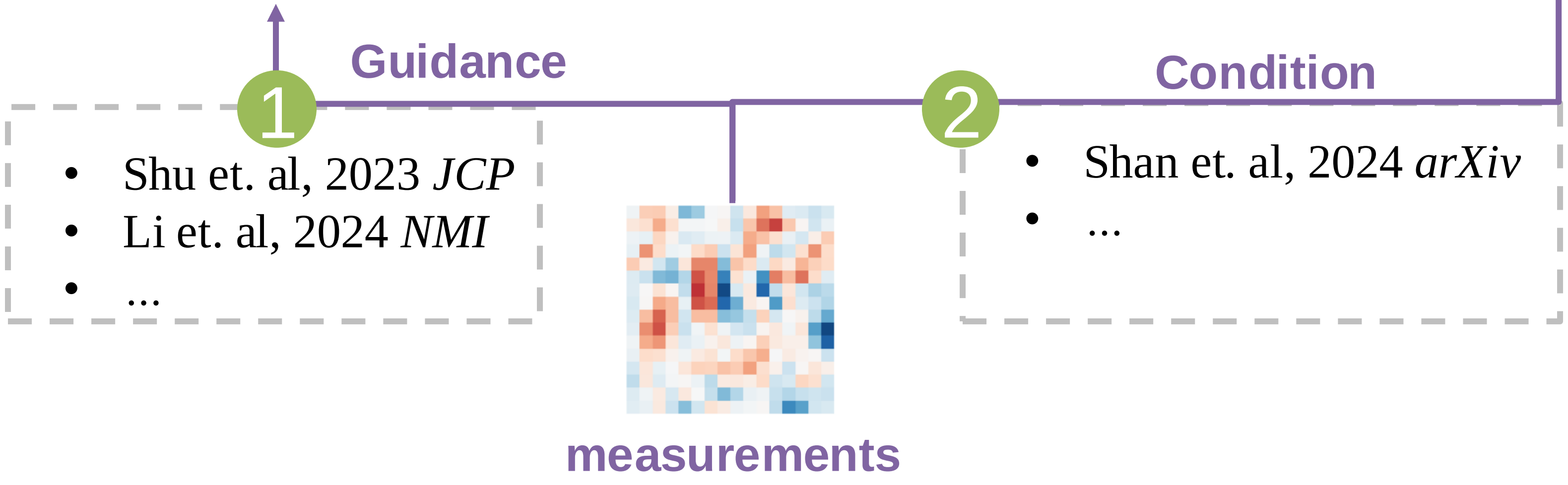
measurements

Diffusion models for field reconstruction



Diffusion models for field reconstruction



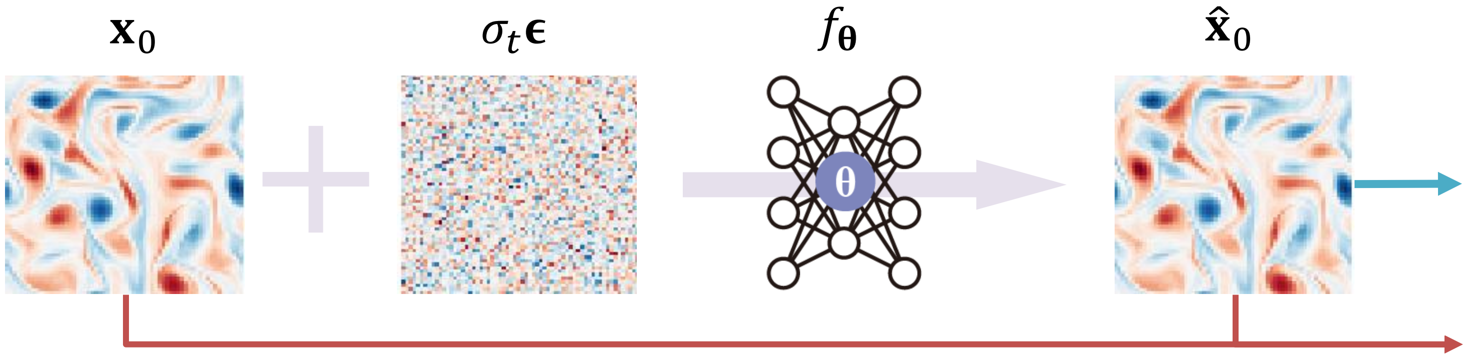


- Data fidelity ✓
- Training speed ✗
- sampling speed ✗

Does the generated field comply with the physics?

- **PINN loss in training**

- Shan et. al, 2024 *arXiv*

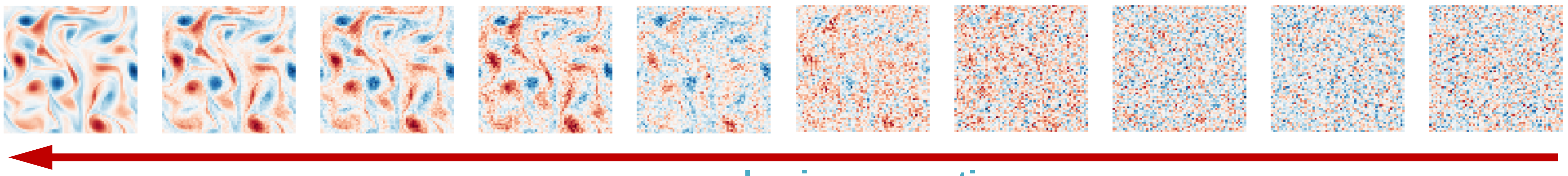


physics loss $\|\mathcal{F}(\hat{\mathbf{x}}_0)\|_2^2$

Diffusion loss $\|\hat{\mathbf{x}}_0 - \mathbf{x}_0\|_2^2$

- **PINN loss in sampling**

- Jacobsen et. al, 2024 *arXiv*
- Gao et. al, 2024 *Nat. Commun.*



physics correction

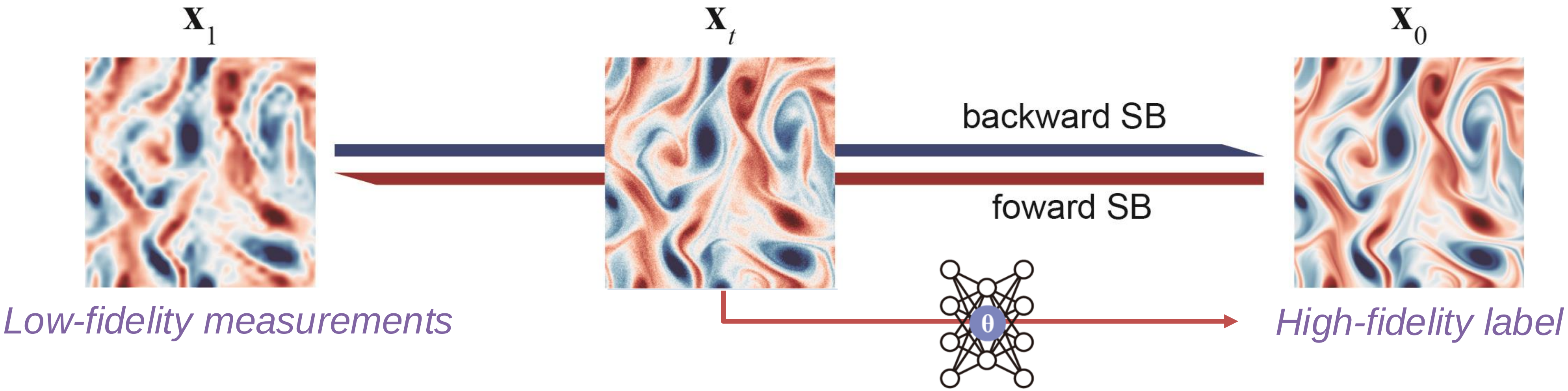
$$\mathbf{x}_{t-1} \leftarrow \text{Diffusion update}(\mathbf{x}_t) - \nabla_{\mathbf{x}_t} \|\mathcal{F}(\hat{\mathbf{x}}_0)\|_2^2, \text{where } \hat{\mathbf{x}}_0 = f_{\boldsymbol{\theta}}(\mathbf{x}_t)$$

- **The one-step prediction $\hat{\mathbf{x}}_0$ is rough!**

Physics-aligned Schrödinger Bridge (PalSB)

- High data fidelity
- Fast training & sampling
- physically plausible

Efficient training & sampling through diffusion bridge

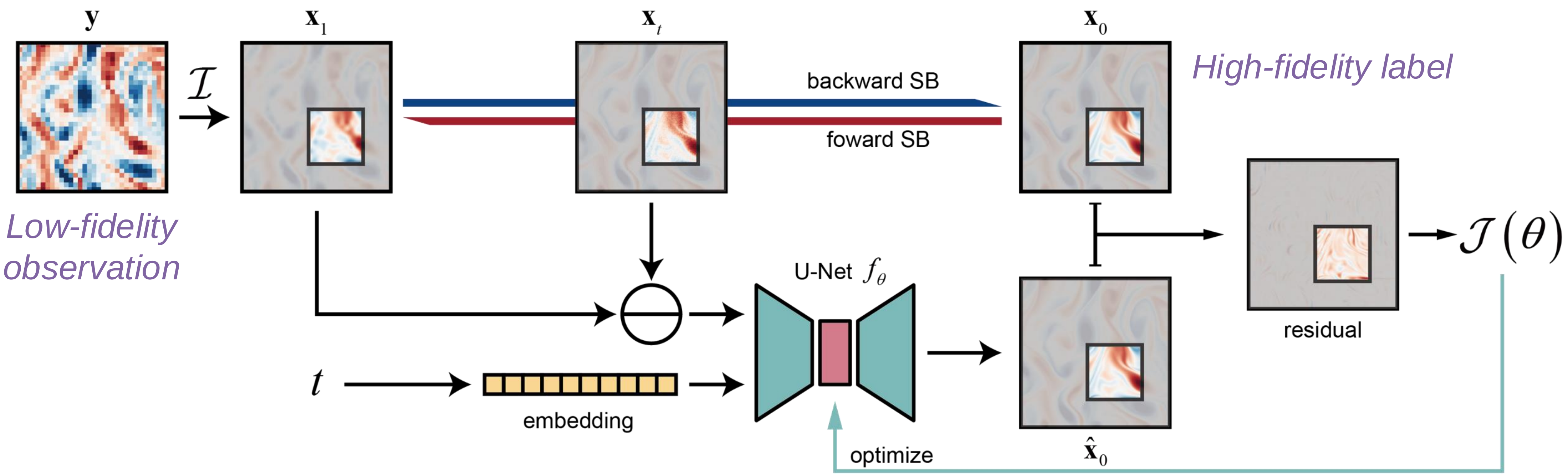


- **Forward SB:** $d\mathbf{x}_t = \mathbf{f}(t)dt + \sqrt{\beta(t)}dW_t, \mathbf{x}_0 \sim \hat{\Psi}(\cdot, 0)$
- **Backward SB:** $d\mathbf{x}_t = \mathbf{f}(t)dt + \sqrt{\beta(t)}d\overline{W}_t, \mathbf{x}_1 \sim \Psi(\cdot, 1)$
- **Posterior distribution:** $p_t(\mathbf{x}_t, t|\mathbf{x}_0, \mathbf{x}_1) = \mathcal{N}\left(\mathbf{x}_t; \frac{\bar{\sigma}_t^2}{\bar{\sigma}_t^2 + \sigma_t^2}\mathbf{x}_0 + (1 - \frac{\bar{\sigma}_t^2}{\bar{\sigma}_t^2 + \sigma_t^2})\mathbf{x}_1, \frac{\bar{\sigma}_t^2 \sigma_t^2}{\bar{\sigma}_t^2 + \sigma_t^2}\mathbf{I}\right)$

[Liu et. al, 2023 *ICML*]

Dual-stage training

1. Pretraining stage (~5 hours with 64×64 patch size)

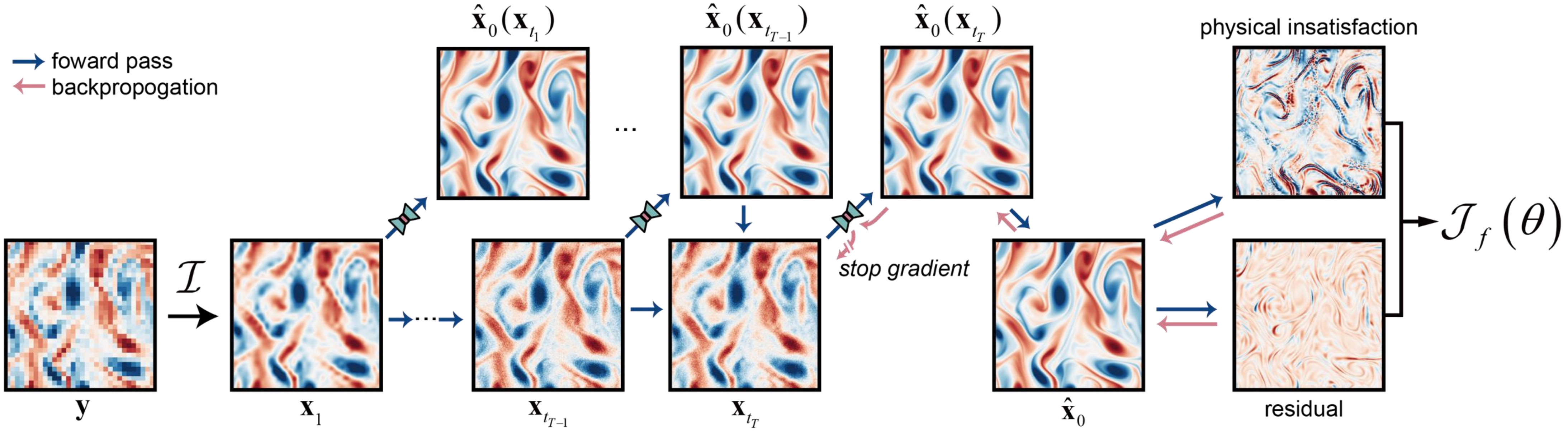


- **Patch-based training:** $\mathcal{J}(\theta) = \mathbb{E}_t \mathbb{E}_{\tilde{\mathbf{x}}_0, \tilde{\mathbf{x}}_1 \sim \mathrm{crop}(\mathbf{x}_0, \mathbf{x}_1)} \mathbb{E}_{\mathbf{x}_0, \mathbf{x}_1 \sim p_0, p_1} \left[\| f_\theta(\tilde{\mathbf{x}}_t, \tilde{\mathbf{x}}_1, t) - \tilde{\mathbf{x}}_0 \|^2 \right]$

where $\mathbf{x}_1 = \mathcal{I}(\mathbf{y}) = \mathcal{I}(\mathcal{H}(\mathbf{x}_0) + \epsilon), \quad \mathbf{x}_0 \sim p_0, \quad \epsilon \sim \mathcal{N}(\mathbf{0}, \sigma_\epsilon^2 \mathbf{I}_m)$

Dual-stage training

2. Aligning physics in finetuning stage (~0.25 hours on 256×256 field)



Regularized loss: $$\mathcal{J}_f(\theta) = \mathbb{E}_{\mathbf{y}}\mathbb{E}_{\hat{\mathbf{x}}_0 \sim p_\theta(\mathbf{x}_0|\mathbf{y})}\left[\underbrace{\gamma_{phys}\|\mathcal{F}(\hat{\mathbf{x}}_0)\|}_{\text{Physics loss}} + \underbrace{\gamma_{reg}\|\hat{\mathbf{x}}_0 - \mathbf{x}_0\|}_{\text{Regularizer}}\right]$$

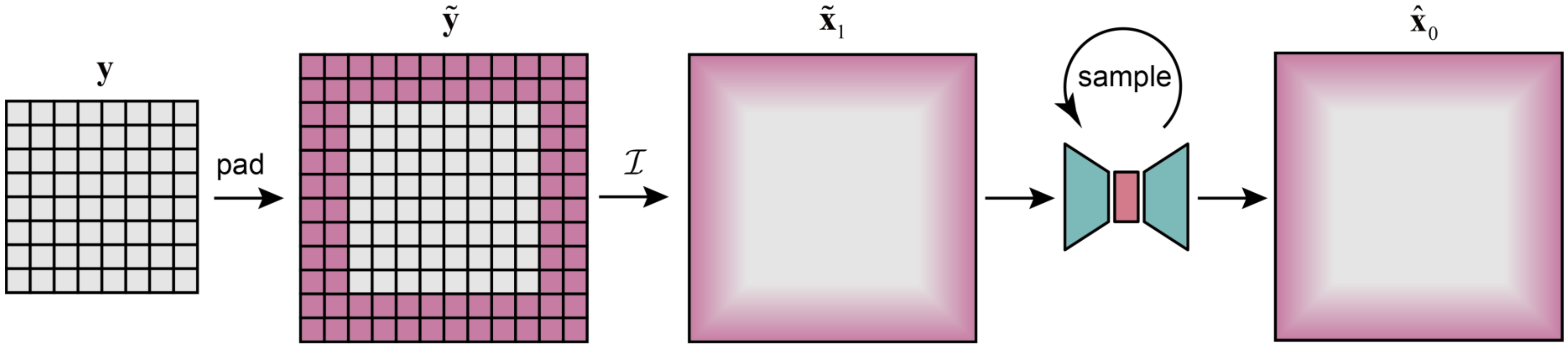
- **Better initialization achieved by pretraining**
- **Backpropagate through the sampling path:** $$\nabla_\theta \mathcal{J}_f(\theta) = \frac{\partial \mathcal{J}_f}{\partial \theta} + \sum_{i=1}^{T}\left(\frac{\partial \mathbf{x}_{t_i}}{\partial \theta}\right)^\top \frac{\partial \mathcal{J}_f}{\partial \mathbf{x}_{t_i}}$$

  (Truncated for all $i < T$, [Clark et. al, 2024 *ICLR*])

Efficient sampling process

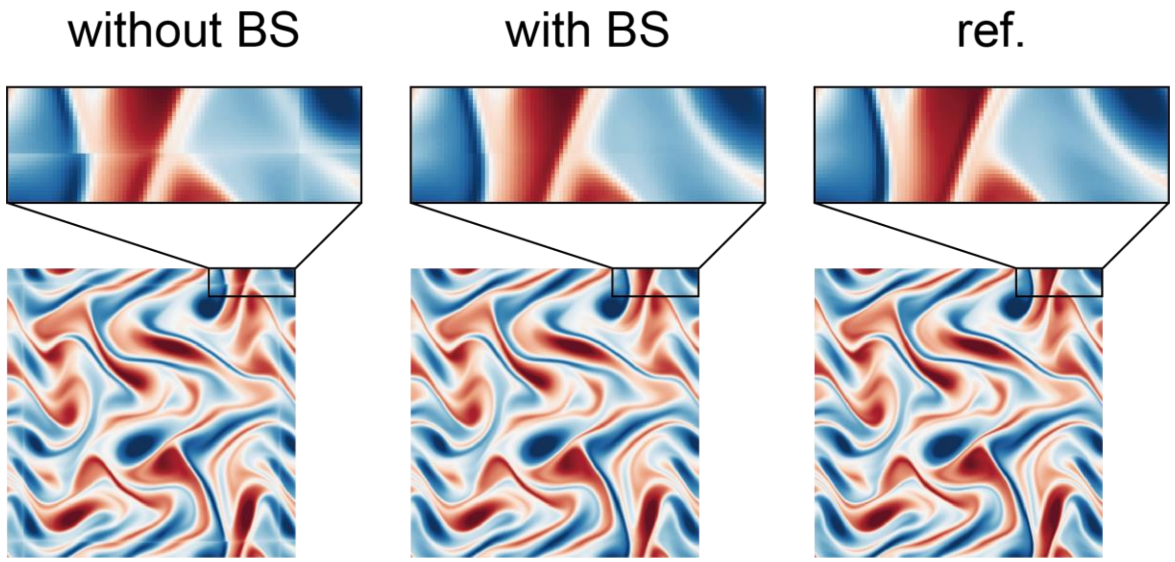
1. Take boundary condition into consideration

Low-fidelity observation



High-fidelity result

Reconstruction example:

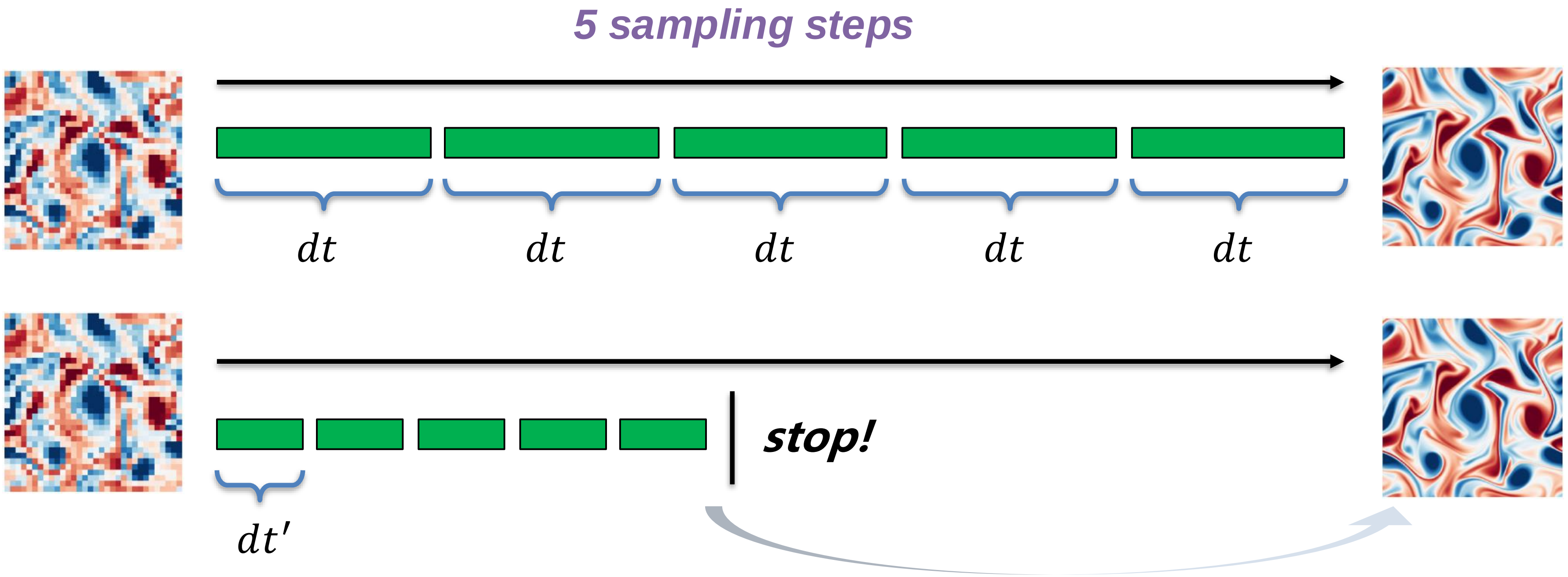


Efficient sampling process

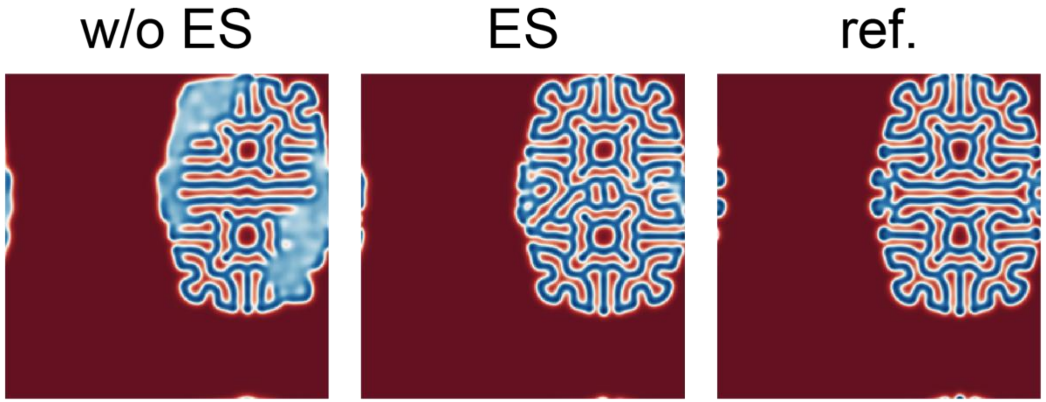
2. Early stop strategy

Conventional:

Early stop (ES):

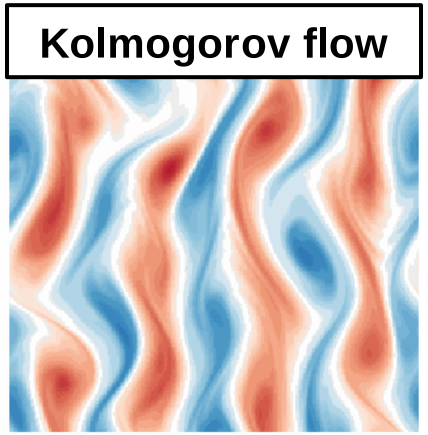


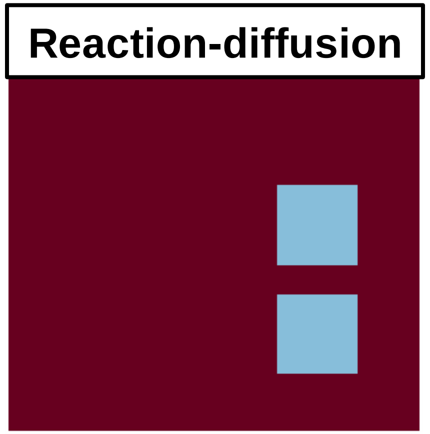
Reconstruction example:

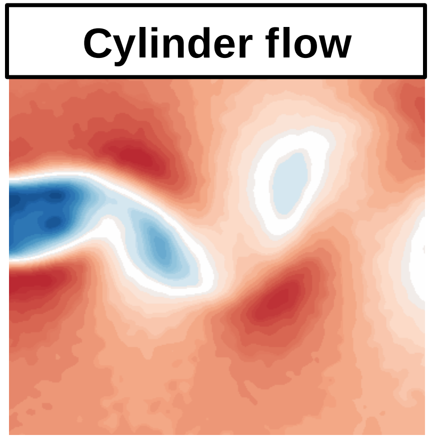


Experimental setups

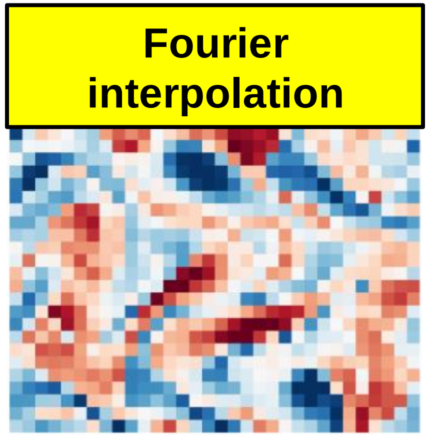
- **Three physical systems**

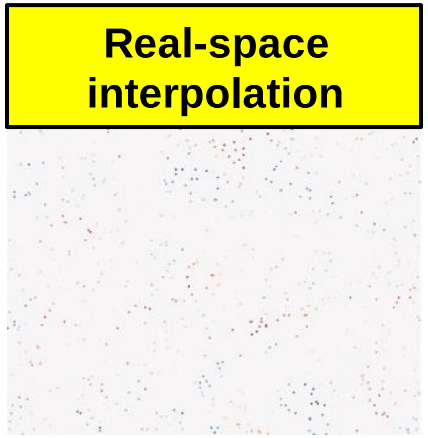






- **Two tasks**



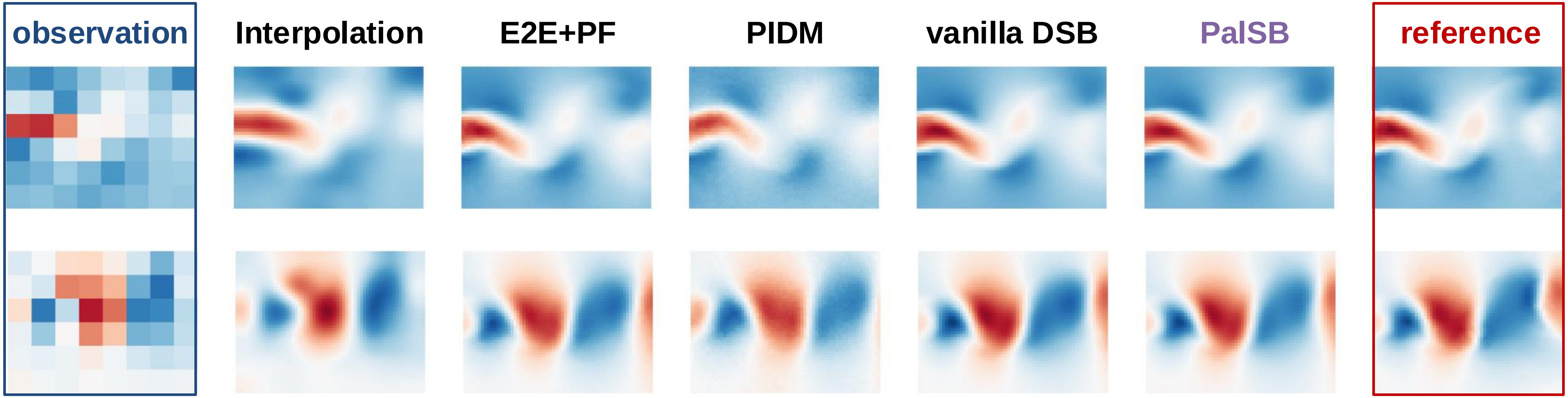


- **Baselines:** trivial methods (interpolation), End-to-End with physics loss [1], PIDM [2], vanilla DSB [3]
- **Evaluation metrics:** nRMSE, MSE, MAE, Correlation, nER (normalized equation residual)
- **Ablations:** early stop sampling (ES), boundary-aware sampling (BS), physics-aligned finetuning

[1] Li et. al, 2021, *ICLR*; [2] Shu et. al, 2023, *JCP*; [3] Liu et. al, 2023, *ICML*

Results on cylinder flow

Fourier interpolation (8x super-resolution)

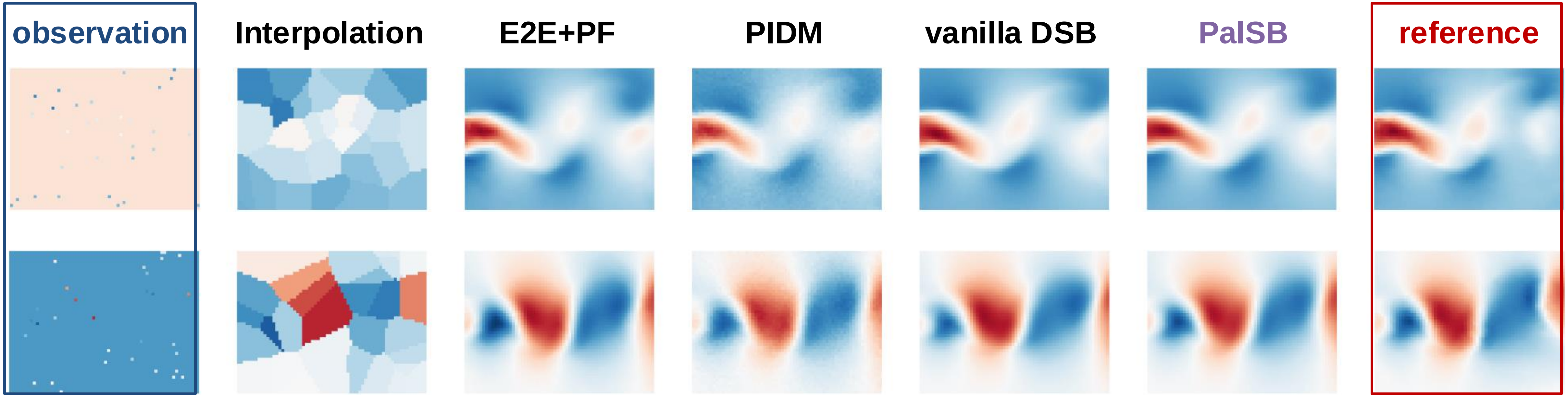


	Interpolation	E2E+PF	PIDM	vanilla DSB	PalSB
nRMSE ↓	0.274	0.094	0.261	0.063	**0.062**
MSE ↓	2.29e-5	3.42e-6	2.14e-5	**1.36e-6**	1.42e-6
MAE ↓	3.06e-3	1.08e-3	3.05e-3	7.18e-4	**7.04e-4**
Correlation ↑	0.843	0.972	0.766	**0.994**	0.974
nER ↓	5.90e-2	8.32e-3	1.60e-2	1.50e-2	**1.22e-3**

Poor physical compliance for vanilla DSB!

Results on cylinder flow

Real-space interpolation (1% observable points)

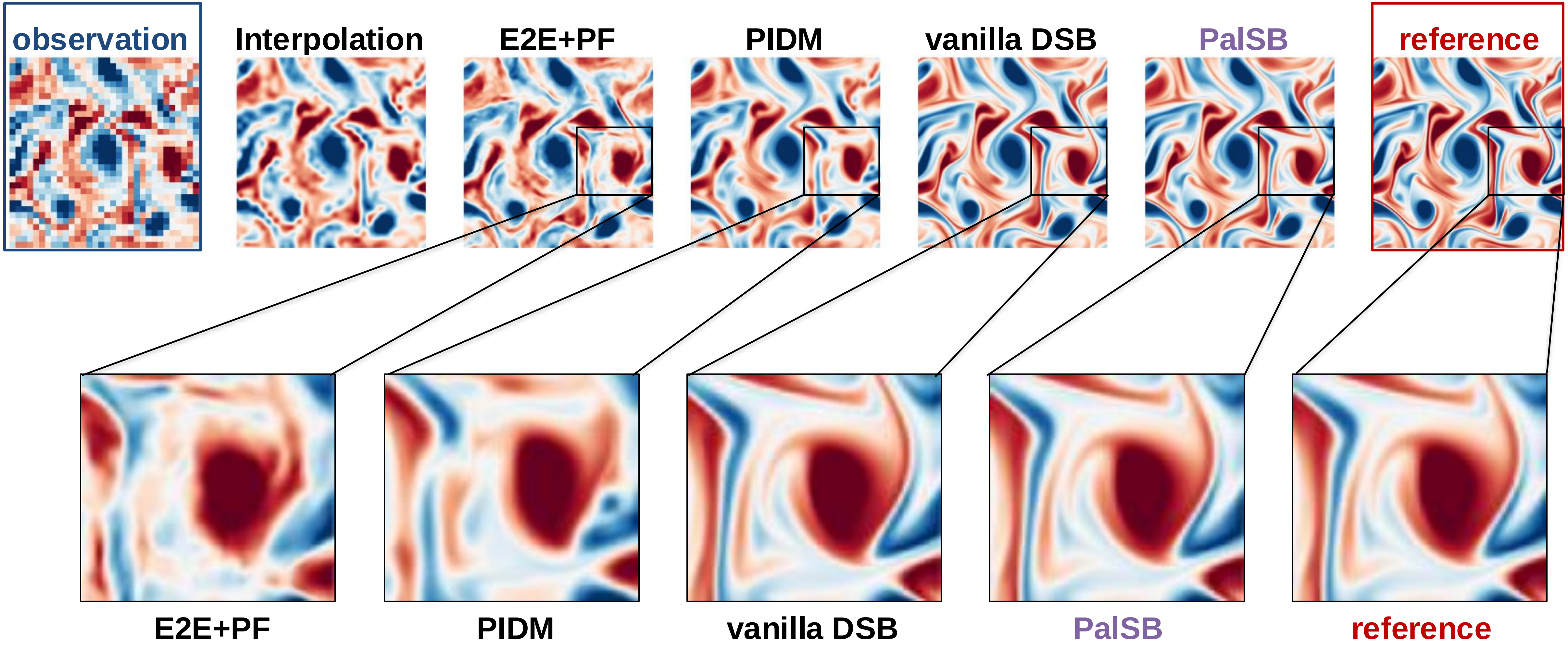


nRMSE ↓	0.301	0.100	0.121	0.092	**0.090**
MSE ↓	2.80e-5	3.81e-6	4.97e-5	2.92e-6	**2.75e-6**
MAE ↓	3.10e-3	1.17e-3	1.45e-3	1.04e-4	**1.02e-4**
Correlation ↑	0.898	0.906	0.894	**0.972**	0.955
nER ↓	1.70	9.48e-3	4.50e-2	2.10e-2	**8.74e-4**

Poor physical compliance for vanilla DSB!

Results on Kolmogorov flow

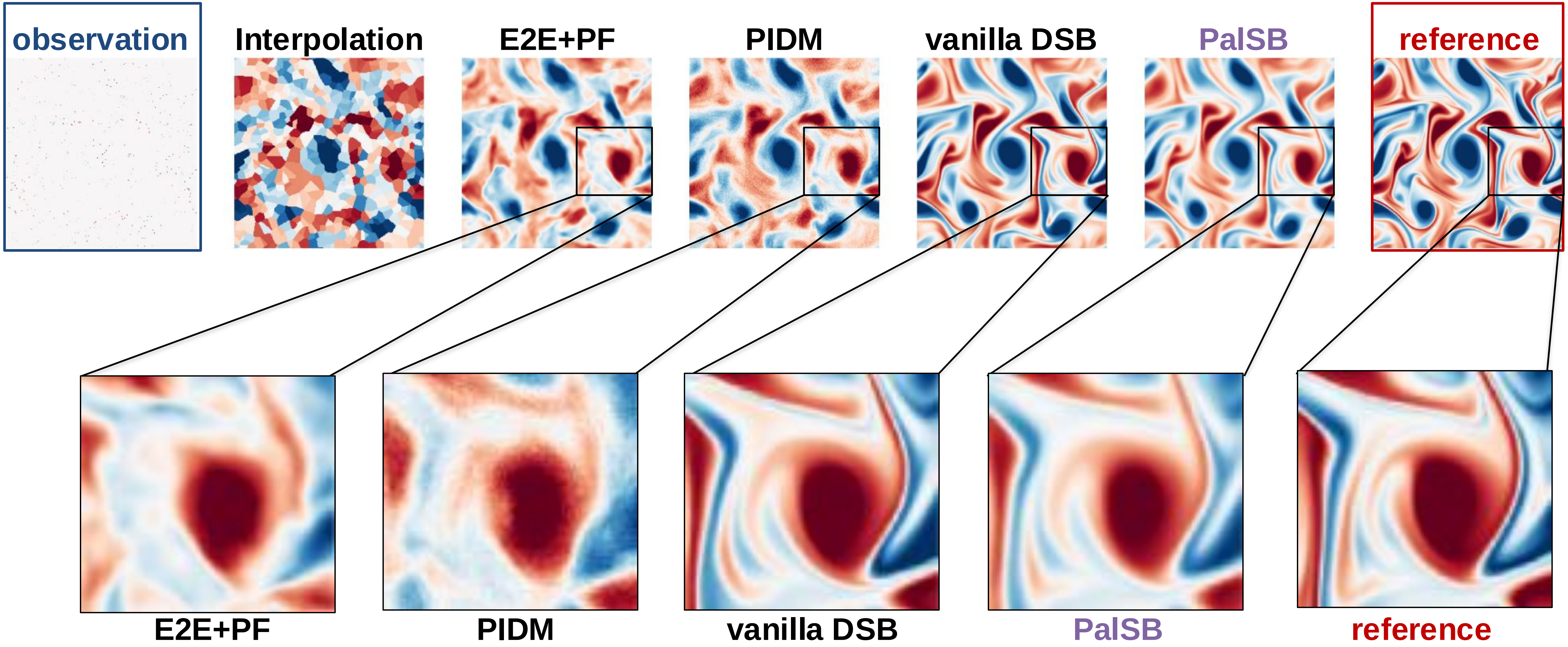
Fourier interpolation (8x super-resolution)



nER ↓	0.391	0.345	0.080	**0.024**

Results on Kolmogorov flow

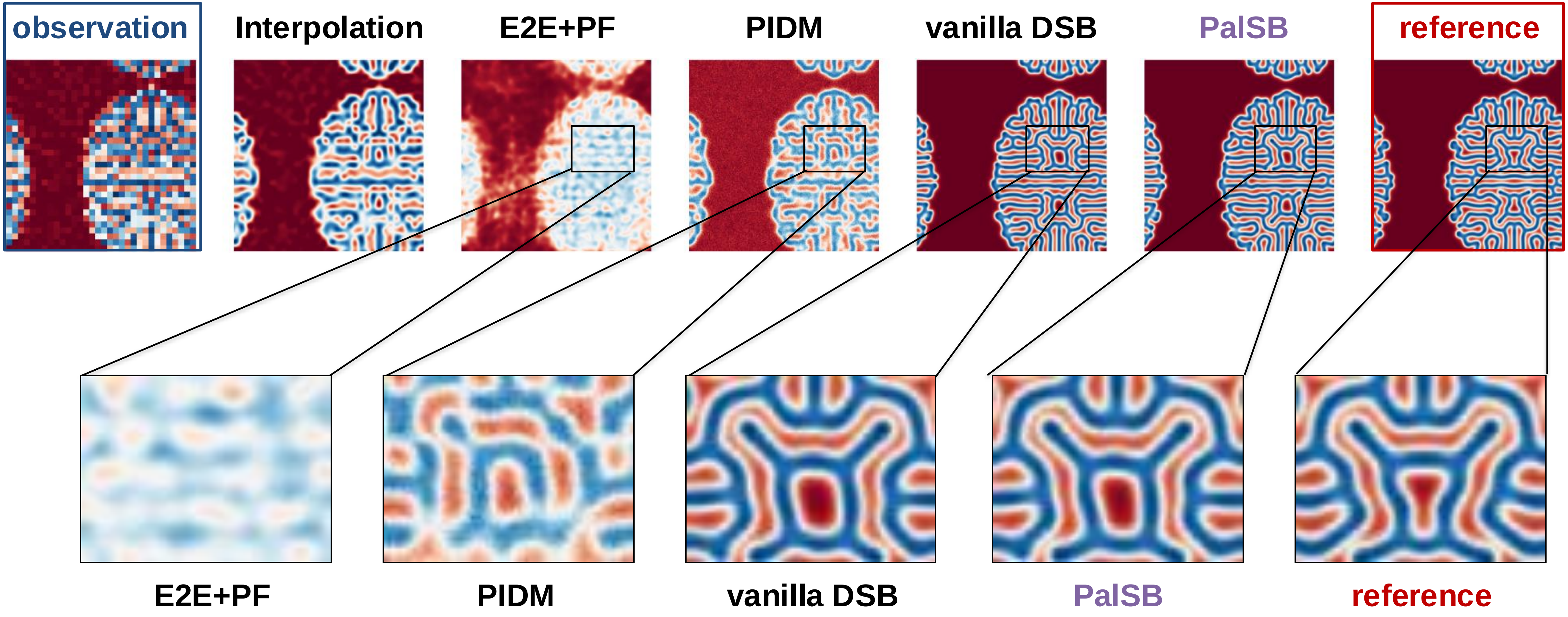
Real-space interpolation (1% observable points)



	E2E+PF	PIDM	vanilla DSB	PalSB
nER ↓	2.68	27.3	1.95	**0.565**

Results on Reaction-diffusion system

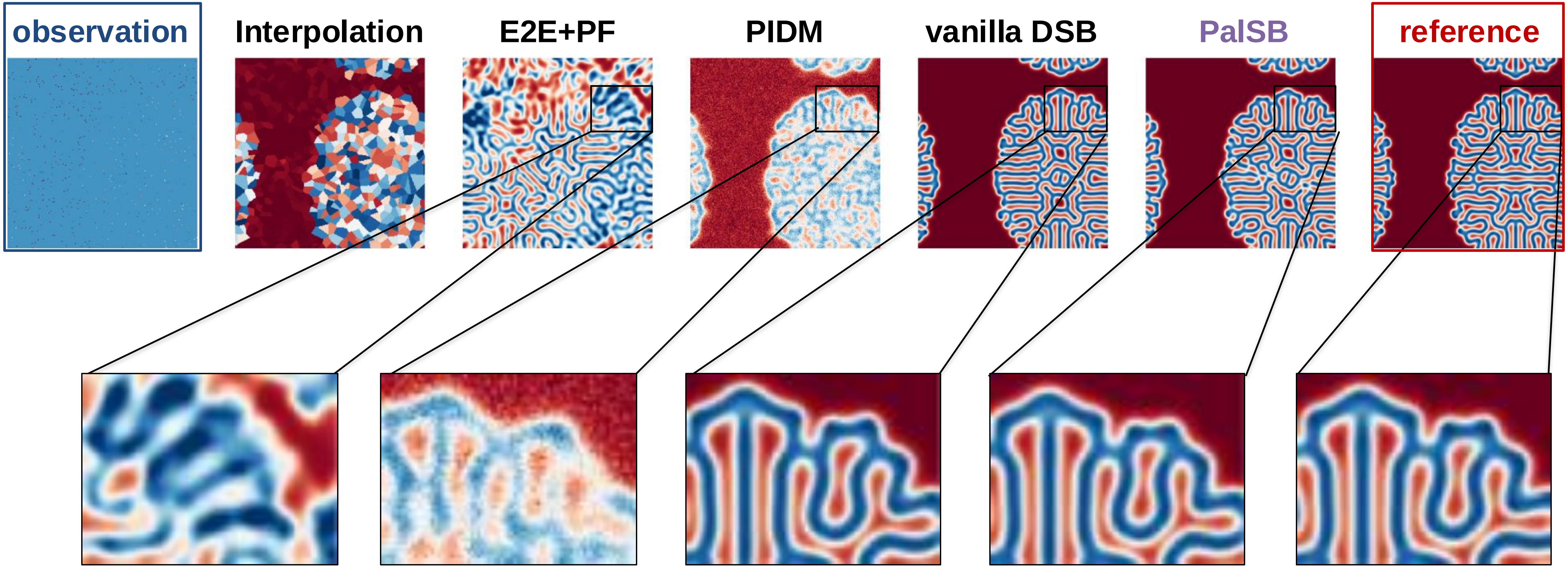
Fourier interpolation (8x super-resolution)



	E2E+PF	PIDM	vanilla DSB	PaISB	reference
nER ↓	8.17e-5	1.23e-3	1.58e-6	**8.91e-8**	

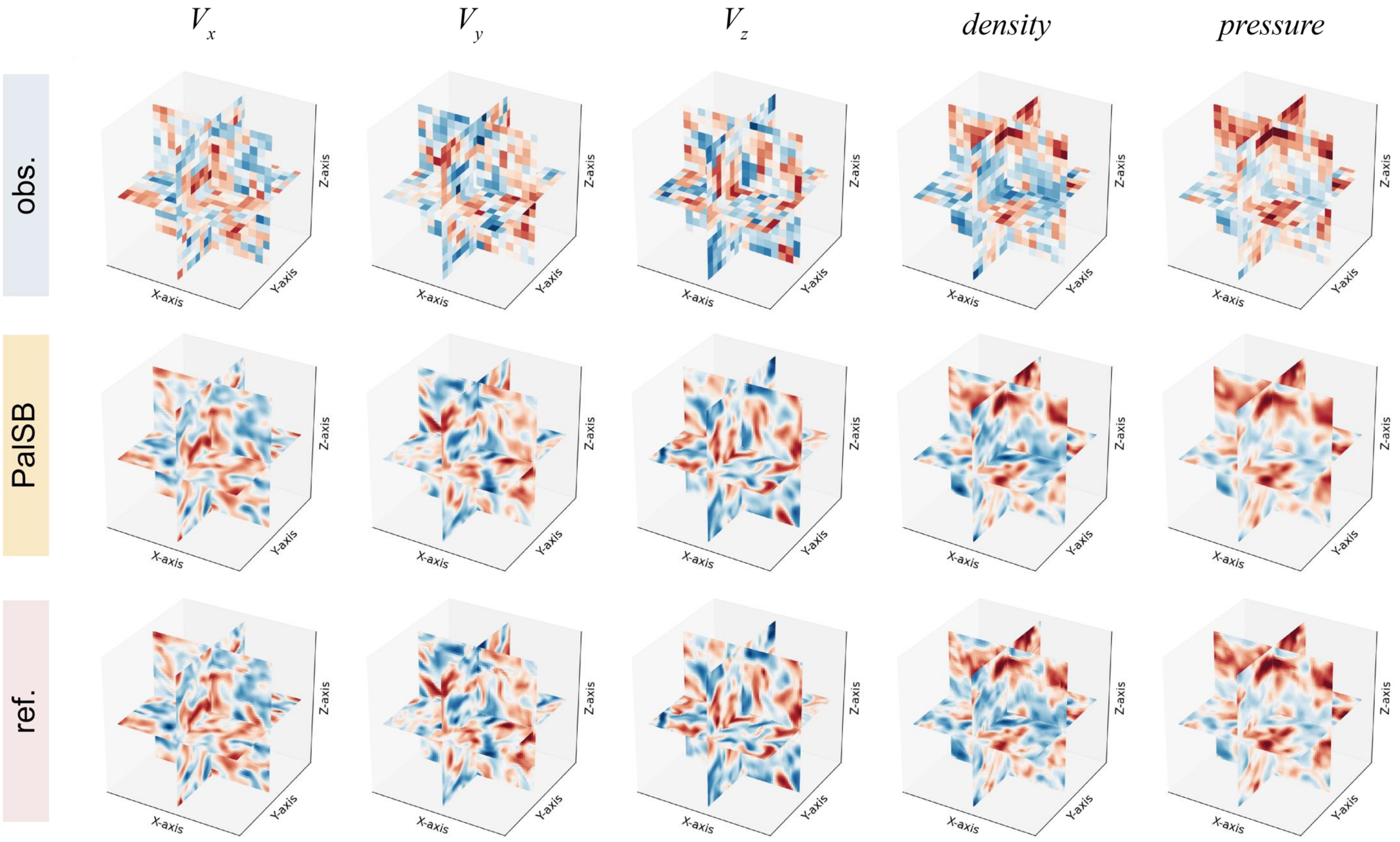
Results on Reaction-diffusion system

Real-space interpolation (1% observable points)



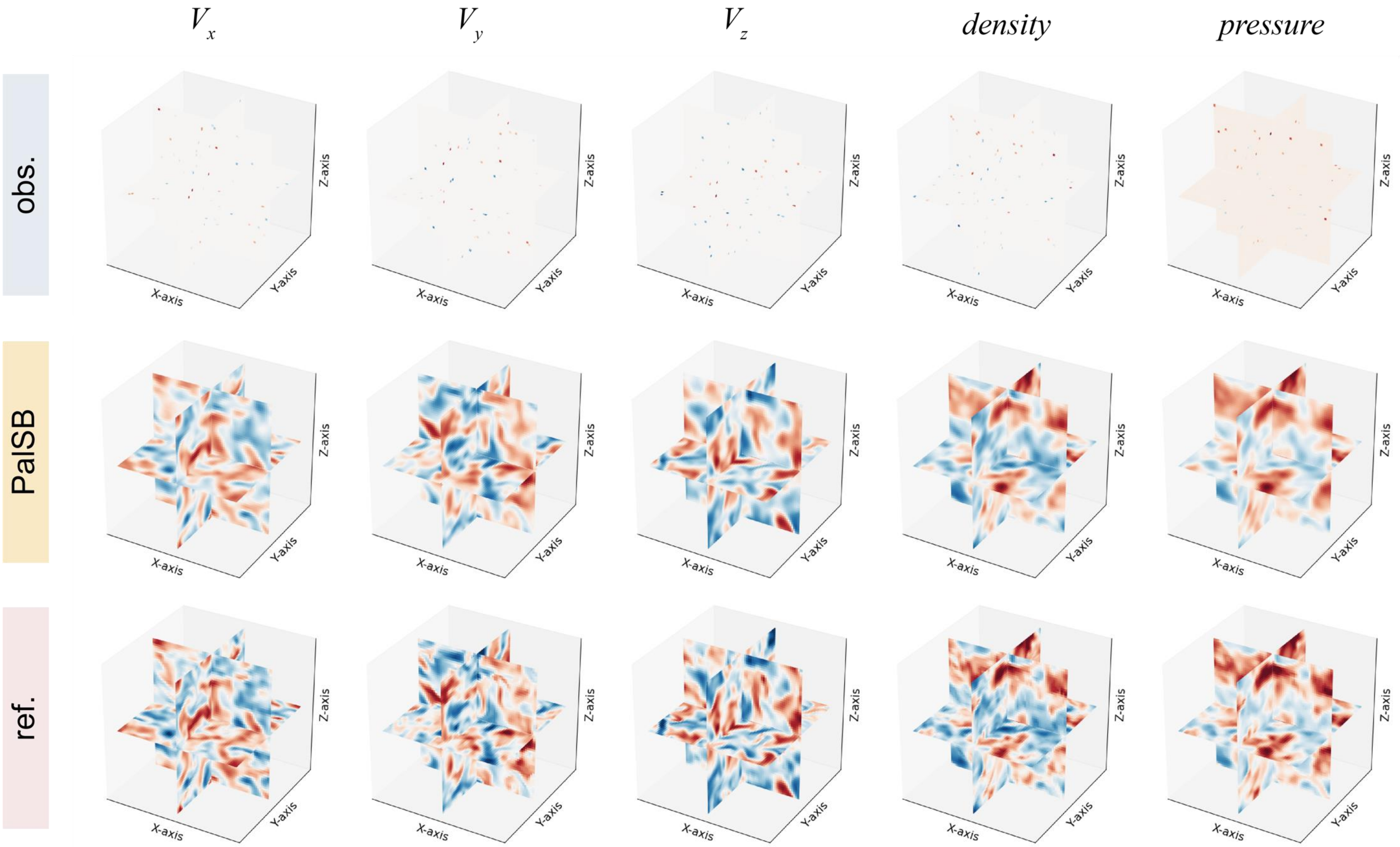
	E2E+PF	PIDM	vanilla DSB	PaISB	reference
nER ↓	5.37e-5	3.83e-3	1.86e-6	**1.69e-7**	

Fourier interpolation (4x super-resolution)



Results on 3D turbulence

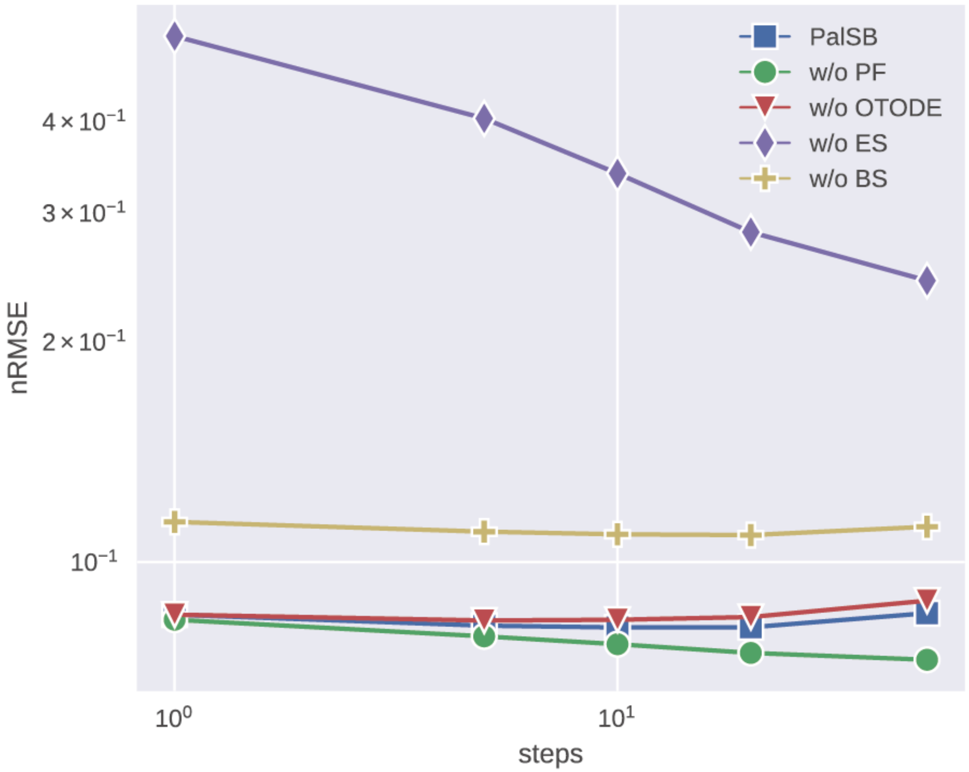
Real-space interpolation (1% observable points)



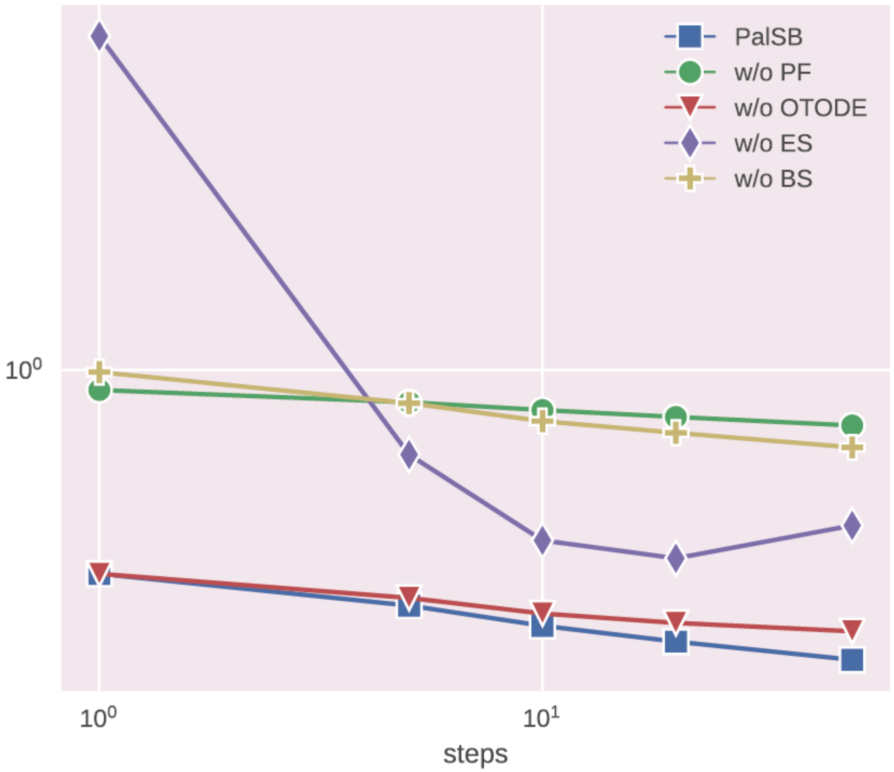
Ablation studies

An instance on Kolmogorov flow

Relative error



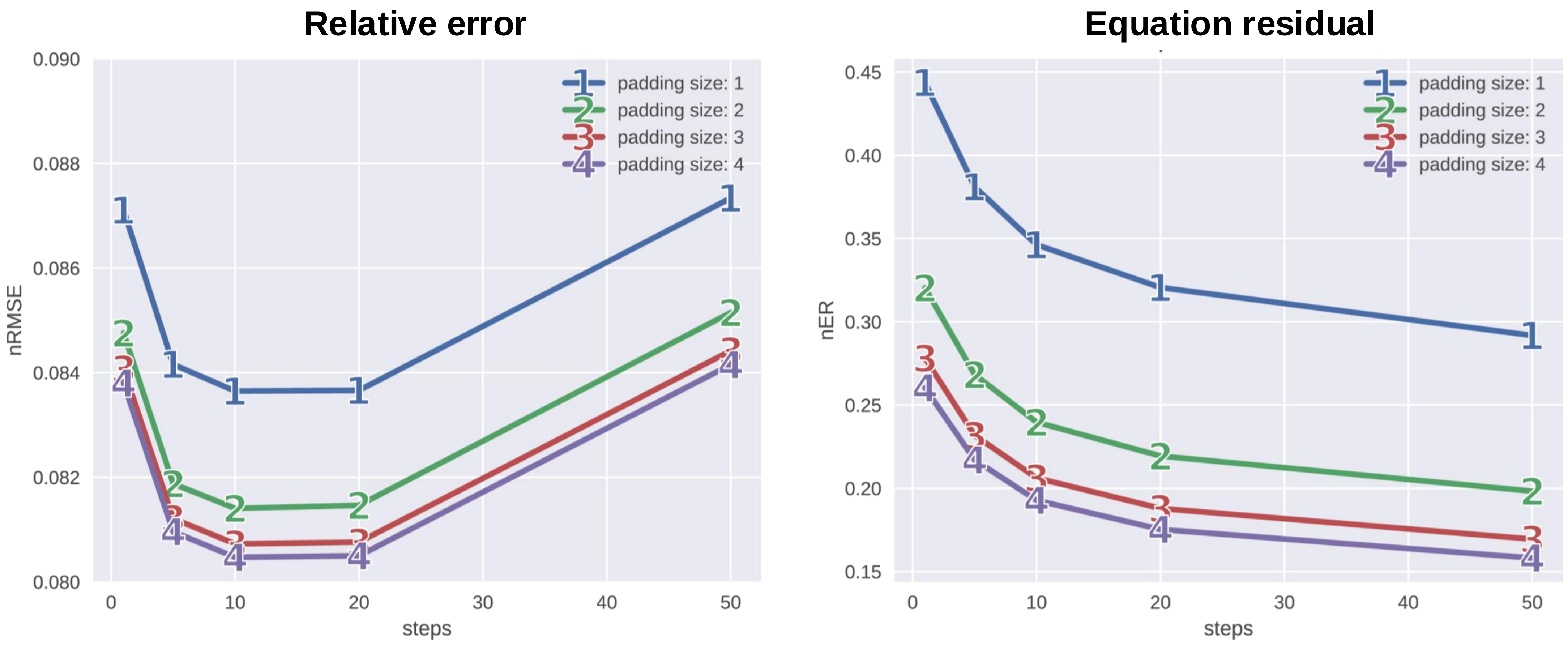
Equation residual



- **PF**: physics-aligned finetune
- **OTODE**: deterministic sampling
- **ES**: early stop sampling
- **BS**: boundary-aware sampling

Ablation studies

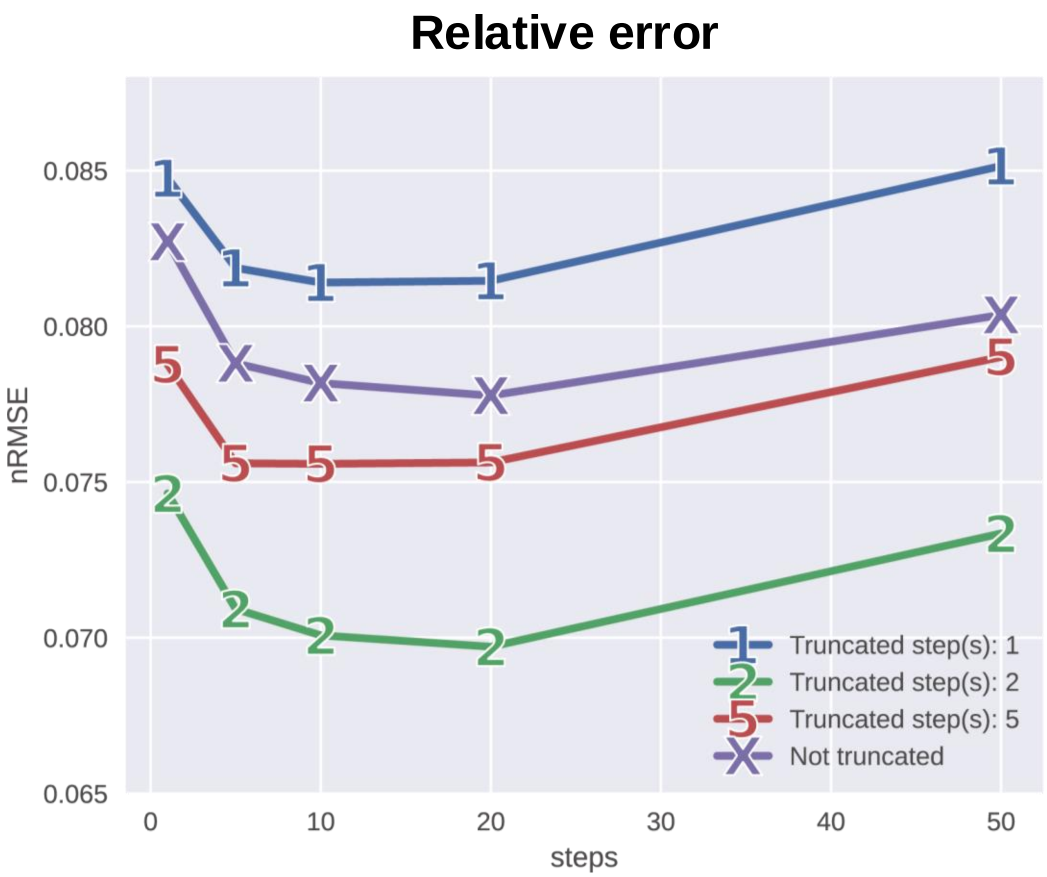
Padding size in boundary-aware sampling

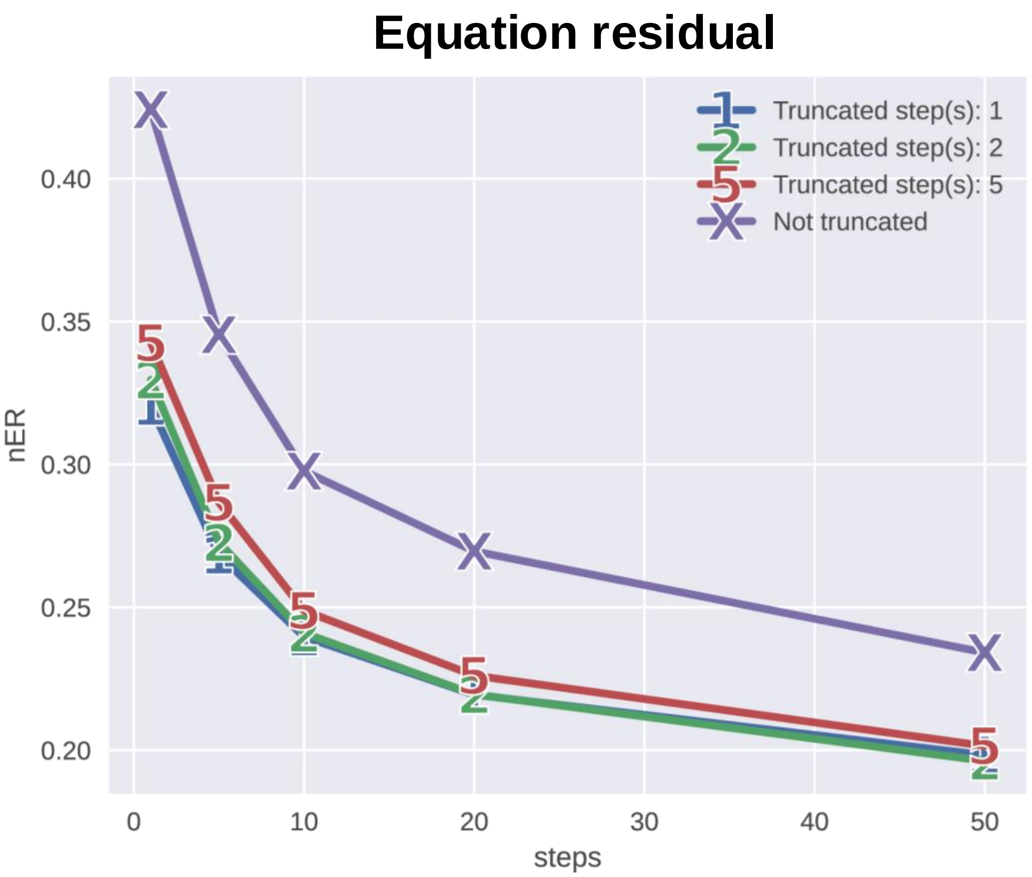


- **Larger padding size leads to better performance**
- **Larger padding size leads to higher computational demand**

Ablation studies

Number of truncated steps in finetuning stage





- **More truncated steps leads to worse physical compliance**
- **More truncated steps do not necessarily reduce prediction error**

Conclusion

- **We explore the application of DSB in physical field reconstruction from sparse measurements.**
- **We develop a physics-aligned fine-tuning approach for generative models to address optimization challenges associated with physics-informed loss functions.**
- **We introduce an innovative sampling technique that effectively incorporates boundary conditions into the generative process.**

Thanks!

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Github: https://github.com/lzy12301/PaISB