Wavelet Diffusion Neural Operator

Peiyan Hu[2#*], Rui Wang[3#*], Xiang Zheng[4#], Tao Zhang[1], Haodong Feng[1], Ruiqi Feng[1], Long Wei[1],

Yue Wang[5], Zhi-Ming Ma[2], Tailin Wu[1†]

[1] Department of Artificial Intelligence, School of Engineering, Westlake University,

[2] Academy of Mathematics and Systems Science, Chinese Academy of Sciences,

[3] Fudan University, [4] South China University of Technology, [5] Microsoft AI4Science

(* equal contributions; # intern at Westlake University, † corresponding author)

Corresponding to: {hupeiyan,wutailin}@westlake.edu.cn, ruiwang18@fudan.edu.cn

Motivation

- **Motivation: abrupt changes & multi-resolution**

- **Generation in the wavelet domain.**
  - Wavelet transform is both space and frequency localized and excels at approximating functions with abrupt changes.
  - Due to the linearity and locality of the wavelet transform, it can integrate seamlessly with the multi-resolution training.
- **Multi-resolution training.**
  - Generalization to higher-resolution simulations.

Preliminary

- **Diffusion model:**
- Forward process: add noise

$$q(x_{k+1}|x_k) = \mathcal{N}(x_{k+1}; \sqrt{\alpha_k}x_k, (1-\alpha_k)\mathrm{I})$$

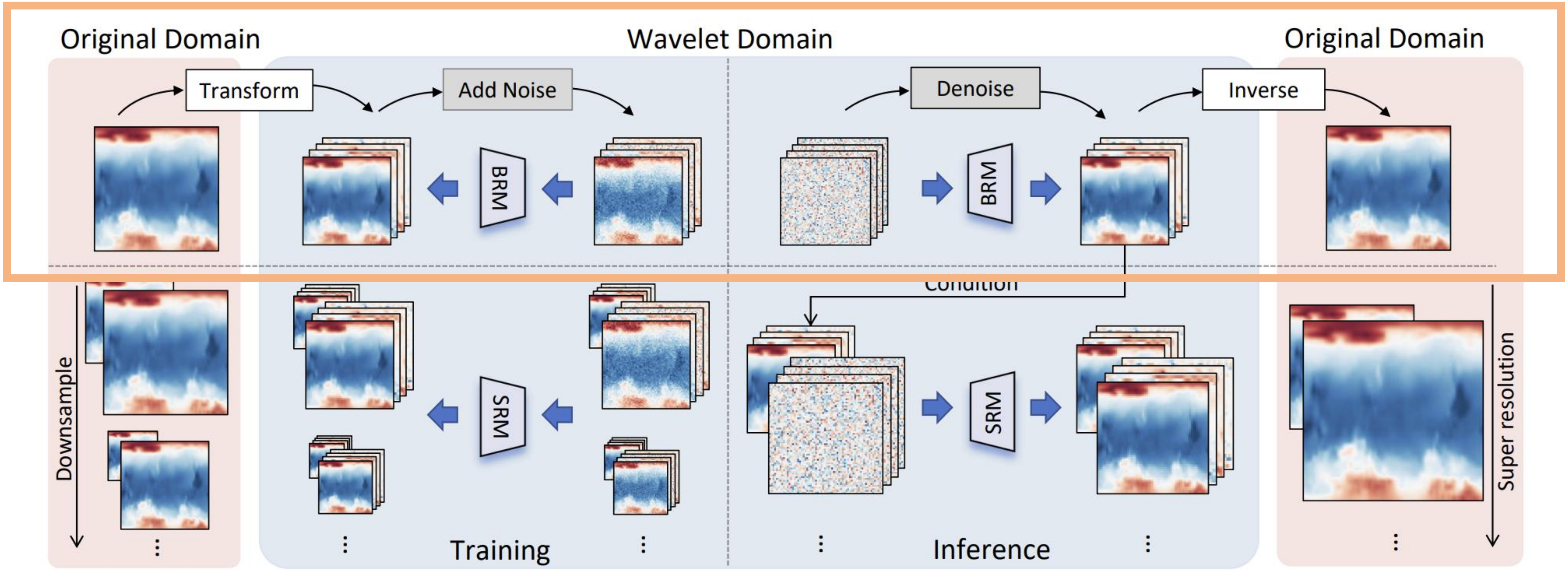
- Reverse process: denoise

$$p_\theta(x_{k-1}|x_k) = \mathcal{N}(x_{k-1}; \mu_\theta(x_k, \mathrm{k}), \sigma_k \mathrm{I})$$

- Train the denoising model ϵ_θ:

$$\mathcal{L} = \mathbb{E}_{k\sim U(1,K),\mathbf{x}_0\sim p(x),\boldsymbol{\epsilon}\sim\mathcal{N}(\mathbf{0},\mathbf{I})}[||\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_k}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_k}\boldsymbol{\epsilon}, k)||_2^2]$$

Method


Original Domain
Wavelet Domain
Original Domain
Transform
Add Noise
Denoise
Inverse
BRM
BRM
Condition
Downsample
SRM
SRM
Super resolution
Training
Inference

Method – Generation in the Wavelet Domain

- **Wavelet basis:** we use wavelet analysis to represent signals with basis functions localized in both space-time and frequency domains, taking values only within finite intervals.

$$u(x) = \sum_m c_L(m)\phi_{L,m}(x) + \sum_m d_L(m)\psi_{L,m}(x).$$

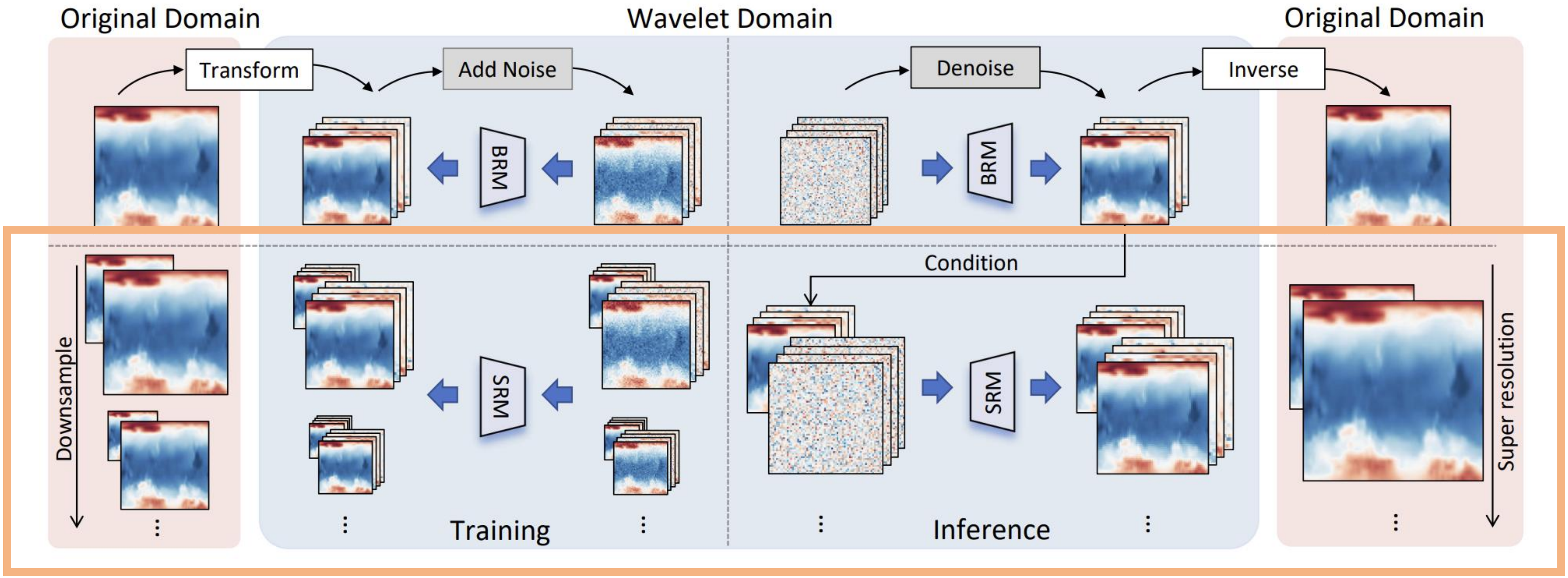
- **WDNO for simulation:**

$$W_{u_{[0,T]}}^{(k-1)} = W_{u_{[0,T]}}^{(k)} - \eta\boldsymbol{\epsilon}_\theta(W_{u_{[0,T]}}^{(k)}, W_a, k) + \xi, \quad \xi \sim \mathcal{N}(\mathbf{0}, \sigma_k^2\mathbf{I})$$

- **WDNO for control:**

$$W_{f_{[0,T]}}^{(k-1)} = W_{f_{[0,T]}}^{(k)} - \eta\left(\epsilon_\theta(W_{f_{[0,T]}}^{(k)}, W_a, k) + \lambda\nabla_{W_{f_{[0,T]}}}\mathcal{J}(\hat{W}_{f_{[0,T]}}^{(k)})\right) + \xi, \quad \xi \sim \mathcal{N}(\mathbf{0}, \sigma_k^2\mathbf{I})$$

Method – Multi-resolution Training



Results

- Our method tested in 5 different simulation tasks and 2 control tasks:

  Simulation:
  - 1D Burgers’ equation state control
  - 1D Advection equation
  - 1D compressible Navier–Stokes equation
  - 2D incompressible fluid
  - ERA5 dataset for weather forecasting

  Control:
  - 1D Burgers’ equation state control
  - 2D incompressible fluid control

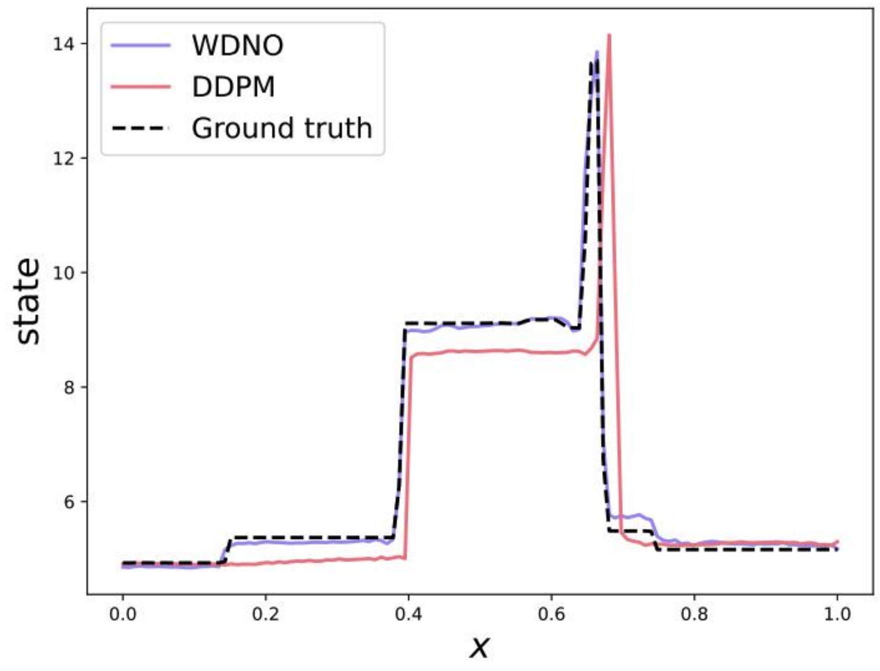
- WDNO demonstrates superior simulation and control performance
  - Significant improvements in long-term and detail prediction accuracy.
  - WDNO reduces the smoke leakage by 33.2% compared to the second-best baseline in indirect control task.

Simulation Results

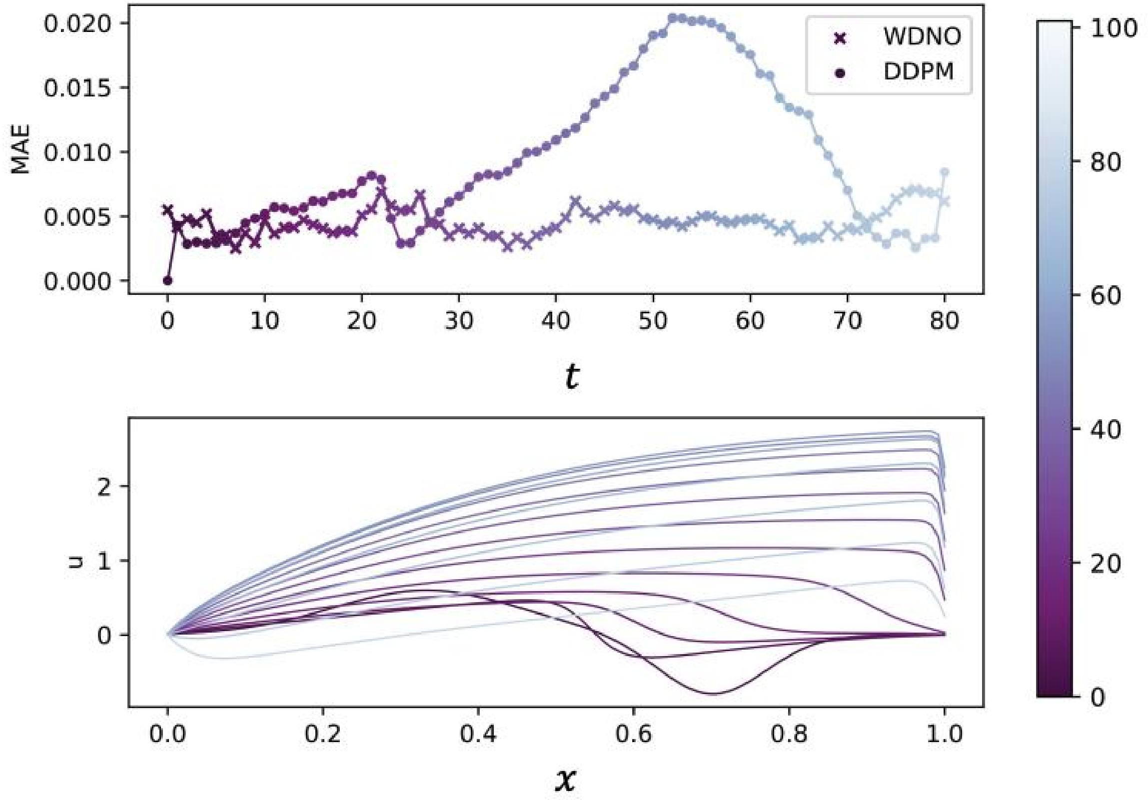
Methods	1D			2D	
	Burgers'	Advection	Navier-Stokes	Fluid	ERA5
WNO	0.00572	4.216e-02	6.5428	0.07975	–
MWT	0.00052	3.468e-04	1.3830	0.01556	21.85750
OFormer	0.00023	1.858e-04	0.6227	0.04303	18.26230
FNO	0.00015	9.712e-04	<u>0.2575</u>	<u>0.00684</u>	<u>14.38638</u>
CNN (1D) / U-Net (2D)	0.00198	5.033e-04	12.4966	0.00737	15.51342
DDPM	**0.00013**	<u>4.209e-05</u>	5.5228	0.01578	15.21103
WDNO (ours)	<u>0.00014</u>	**2.898e-05**	**0.2195**	**0.00231**	**12.83291**

WDNO achieves the best Performance

Simulation Results – abrupt changes



1D Burgers' equation



1D Compressible Navier-Stokes

Control Results – 1D Burgers' equation

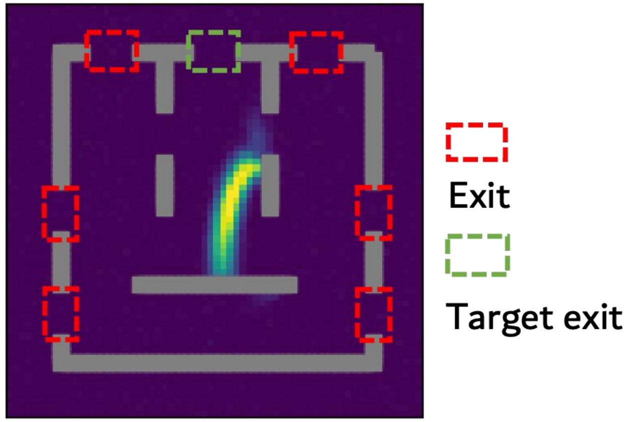
Control objective: ($u^*(x)$ is target state)

$$\mathcal{J} = \int_D |u(T,x) - u_d(x)|^2 \, dx + \alpha \int_{[0,T]\times D} |f(t,x)|^2 \, dt dx$$

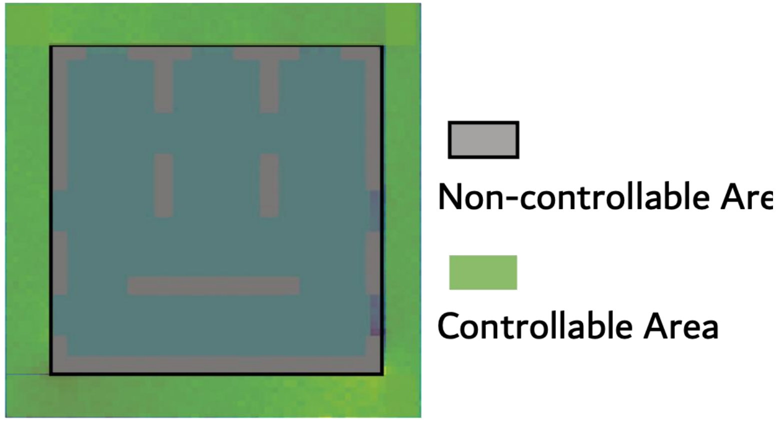
$$\begin{cases} \dfrac{\partial u(t,x)}{\partial t} = -u(t,x) \cdot \dfrac{\partial u(t,x)}{\partial x} + \nu \dfrac{\partial^2 u(t,x)}{\partial x^2} + f(t,x) & \text{in } [0,T] \times D \\ u(t,x) = 0 & \text{on } [0,T] \times \partial D \\ u(0,x) = u_0(x) & \text{at } \{t = 0\} \end{cases}$$

Methods	$\mathcal{J}$
PID (surrogate-solver)	0.6645
SAC (pseudo-online)	0.1376
SAC (offline)	0.3210
BC (surrogate-solver)	0.2998
BC (solver)	0.1879
BPPO (surrogate-solver)	0.3075
BPPO (solver)	0.1867
SL	0.0235
DDPM	0.0272
WDNO (ours)	**0.0205**

Control Results – 2D incompressible fluid

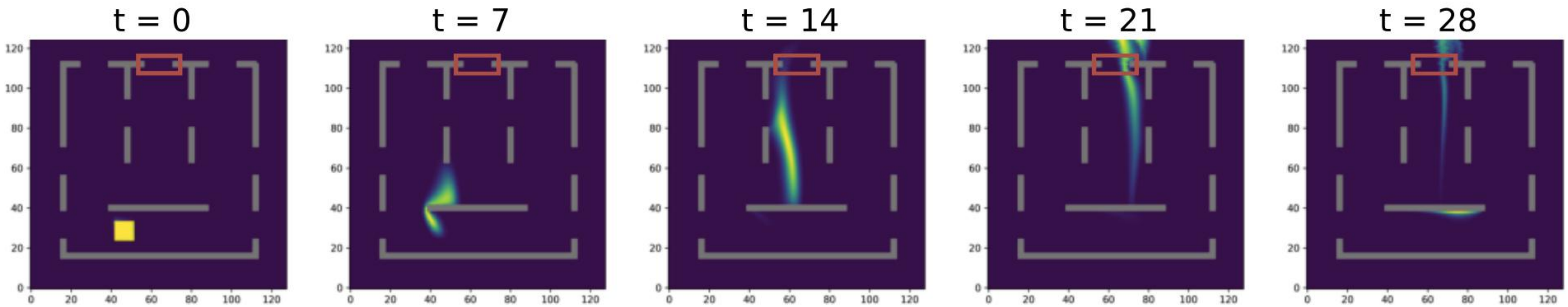


(a) Locations of exits and obstacles



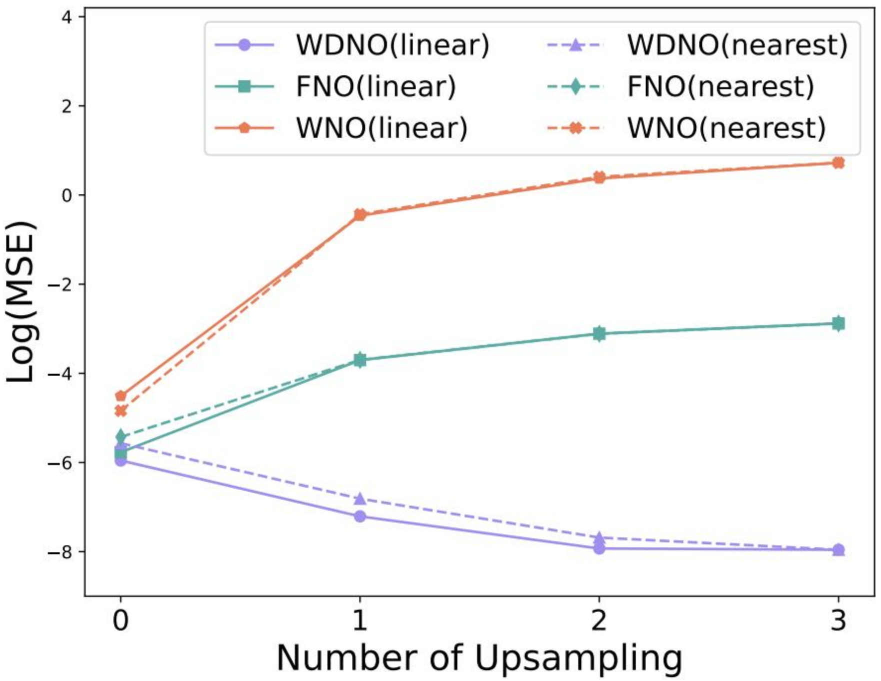
(b) Locations of controllable area

Methods	$\mathcal{J}$
BC	0.3085
BPPO	0.3066
SAC (pseudo-online)	0.3212
SAC (offline)	0.6503
DDPM	0.3124
WDNO (ours)	**0.2047**

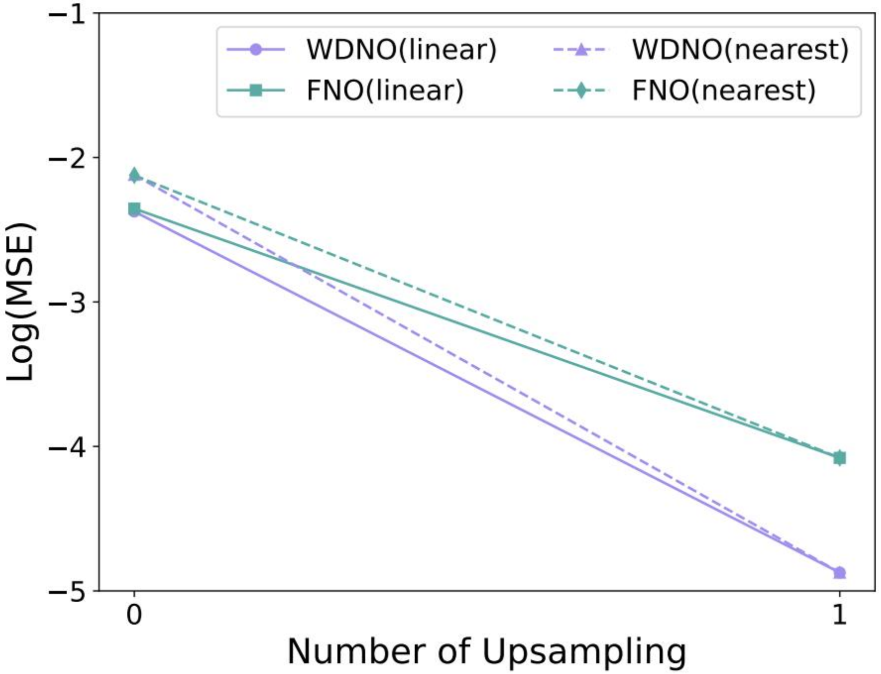


Results – zero-shot super-resolution

1D Burgers' equation

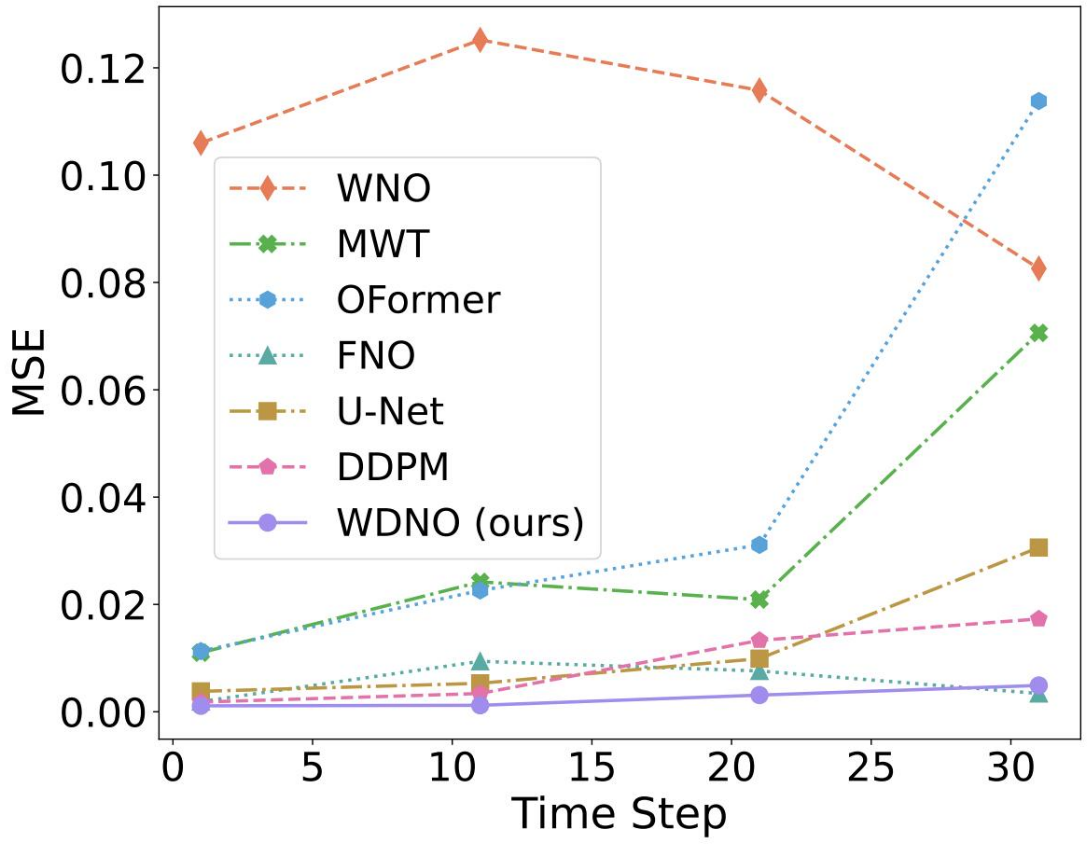


2D incompressible fluid



WDNO outperforms the mesh-invariant FNO and WNO

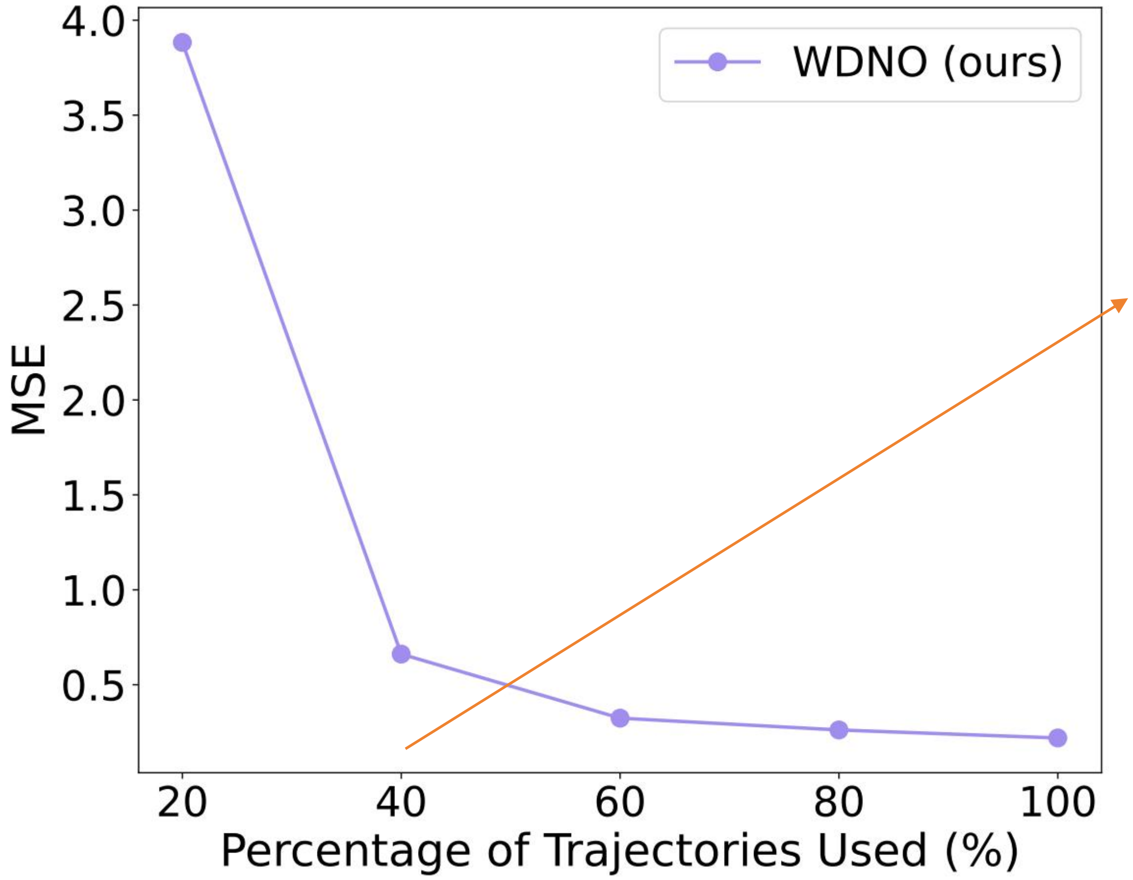
Results – Ablation studies



Long-term dependencies.

WDNO exhibits the slowest error growth.

Results – Ablation studies

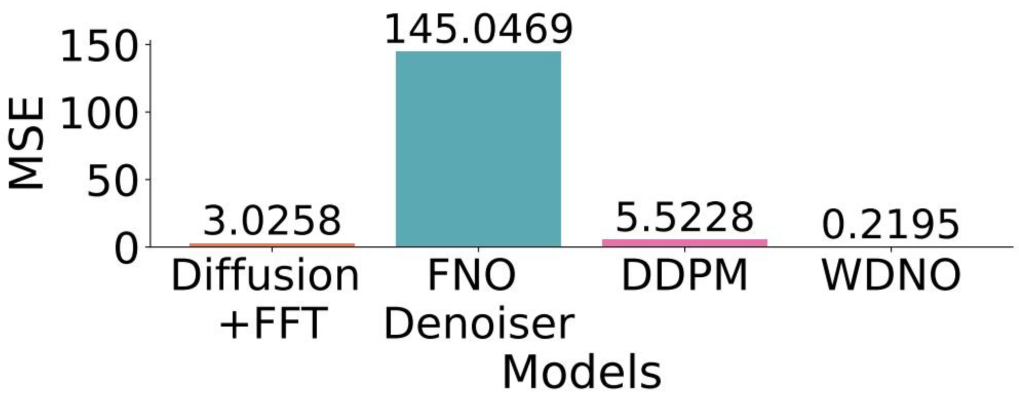


Number of training samples.

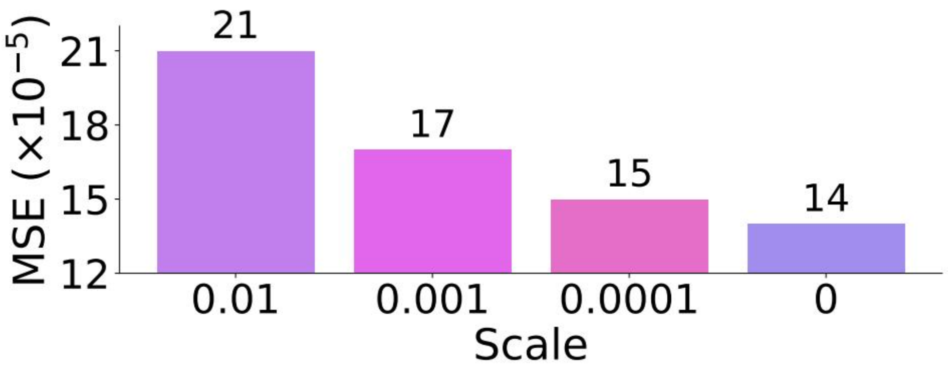
0.4 times：WDNO ’s error remains within a relatively small range.

Results – Ablation studies

1D compressible Navier-Stokes equation



Comparison with Fourier transform:
Wavelet transforms is more effective for learning complex system dynamics.



Measurement noise:
WDNO 's results exhibit minimal variation with changes in scale, demonstrating its robustness to noise.

Limitation and Future Work

- Real-World Application
  - WDNO is not limited to specific environments.
  - Potential real-world applications: turbulence, structural materials, plasma.

- Applicability to Irregular Data
  - WDNO (Wavelet transform& denoising model U-Net): only applicable to static, uniform grid data.
  - Future improvements:

    Geometric wavelets for irregular data;

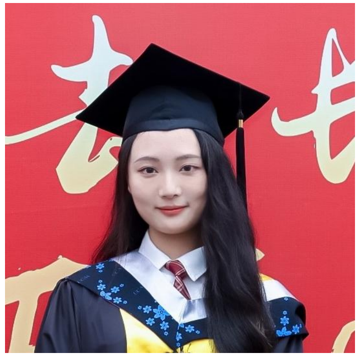
    Diffusion models for graph structures;

    Projecting irregular grids onto regular uniform grids

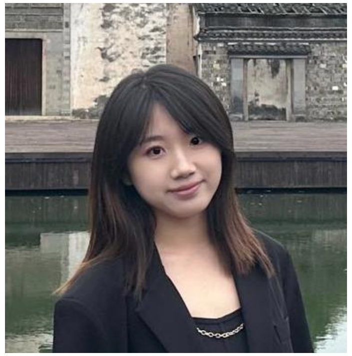
- Incorporating Physical Information
  - Current: not incorporate equation-based information
  - Add physics-informed loss based on the PDEs --> enhance the model’s accuracy, robustness, and generalizability.

Our group: AI for Scientific Simulation & Discovery Lab @ Westlake University

Group Website:



Peiyan Hu



Rui Wang

Xiang Zheng

Tao Zhang

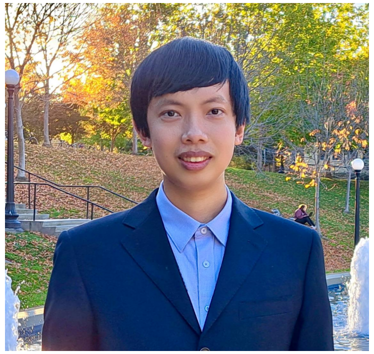
Haodong Feng

Ruiqi Feng

Long Wei

Yue Wang

Zhi-Ming Ma



Tailin Wu

Thank you!

If you have any questions, please feel free to contact us at:

hupeiyan18@mails.ucas.ac.cn

ruiwang18@fudan.edu.cn

wutailin@westlake.edu.cn

Group Website: