DeepLag: Discovering Deep Lagrangian Dynamics for Intuitive Fluid Prediction

Qilong Ma[*], **Haixu Wu**[*], **Lanxiang Xing**, **Shangchen Miao**, **Mingsheng Long**[✉]
School of Software, BNRist, Tsinghua University, China
{mql22,wuhx23,xlx22,msc21}@mails.tsinghua.edu.cn, mingsheng@tsinghua.edu.cn


Qilong Ma

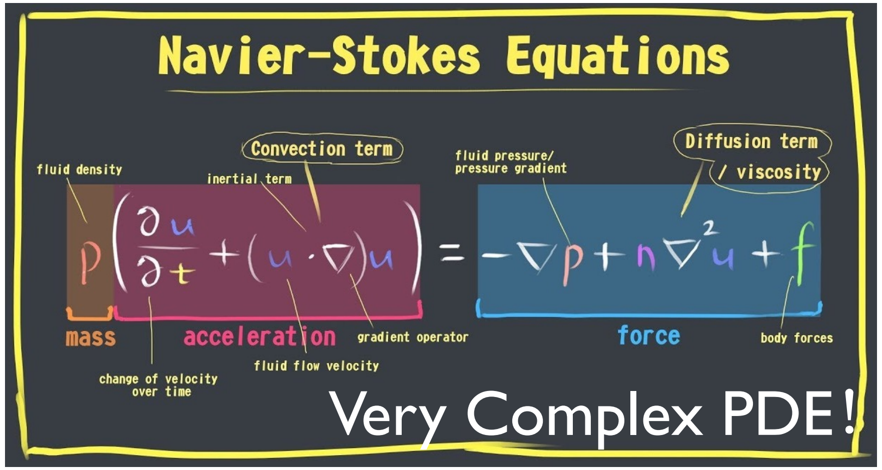

Haixu Wu


Lanxiang Xing

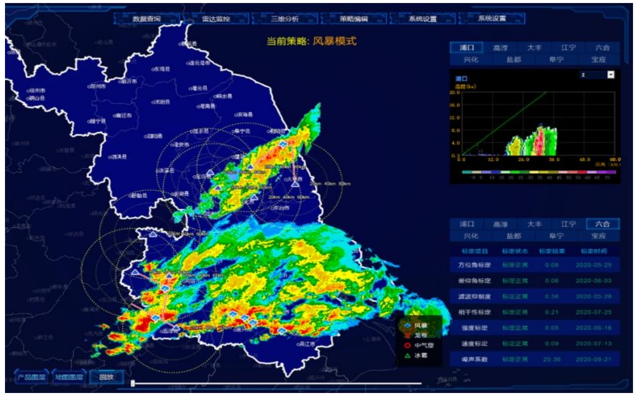

Shangchen Miao


Mingsheng Long

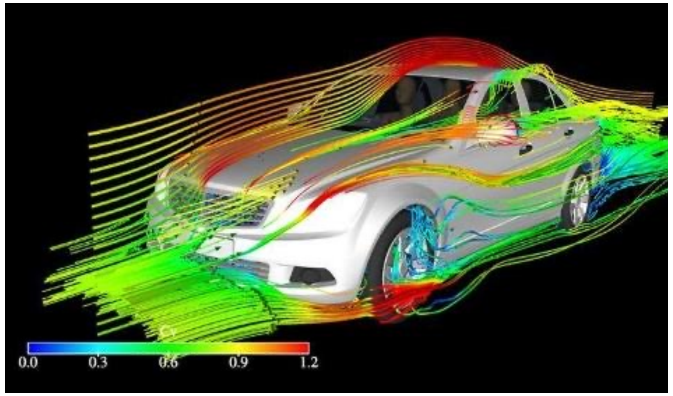
1.1 FLUID & ITS CHARACTERISTICS



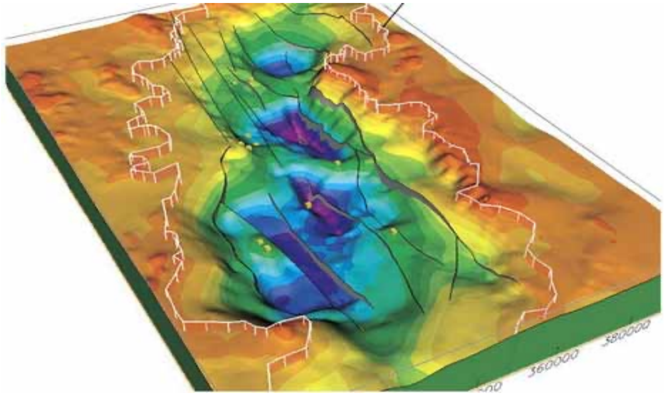
- **Fluids**: easily deform, with complex dynamics
- **Highly related to production and life**: Accurate prediction of future fluid evolution is of great significance in various fields



Weather forecasting and disaster warning



Aerodynamic design optimization



Prediction of underground oil and gas reservoir

1.2 SIGNIFICANCE: THE DIFFICULTIES OF CFD — PART 1

- **Empirical Models** that Simplify Equations
  - *Empirical parameters and assumptions* are used to *decompose and approximate* turbulent characteristics and viscous behaviour of fluids.

Reynolds-averaged Navier Stokes (RANS) equation[1]

$$\frac{\partial(\rho U_i)}{\partial t} + \frac{\partial(\rho U_i U_j)}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right)\boxed{-\rho\overline{u_i' u_j'}}\right] \Rightarrow$$

information loss ☹

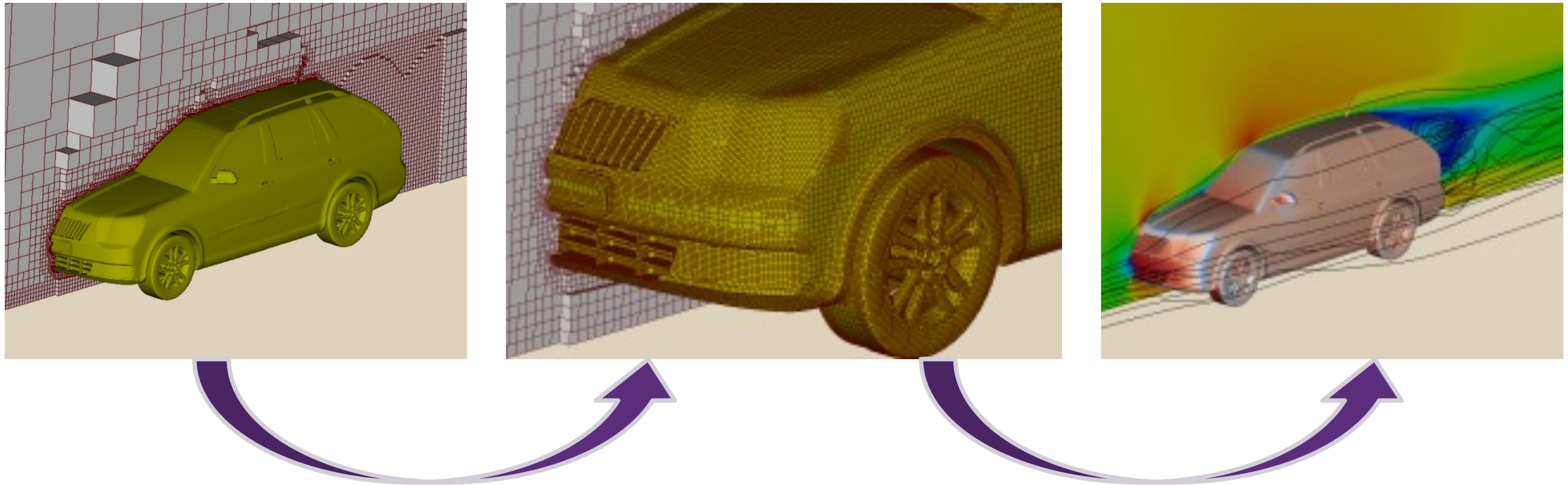
$$-\rho\overline{u_i' u_j'} = \underline{\mu_t\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3}\frac{\partial U_k}{\partial x_k}\delta_{ij}\right) - \frac{2}{3}\rho k \delta_{ij}} \Rightarrow$$

depends on the hypothesis ☹

[1] https://www.simscale.com/docs/simulation-setup/global-settings/k-omega-sst/

1.2 SIGNIFICANCE: THE DIFFICULTIES OF CFD — PART 2

- **Numerical Methods** that Simplify Computation
  - Define geometry and bounds, *discretize into mesh by different methods*, model physics, *iteratively solve numerical equations*, and analyse results.



partial observation ☹

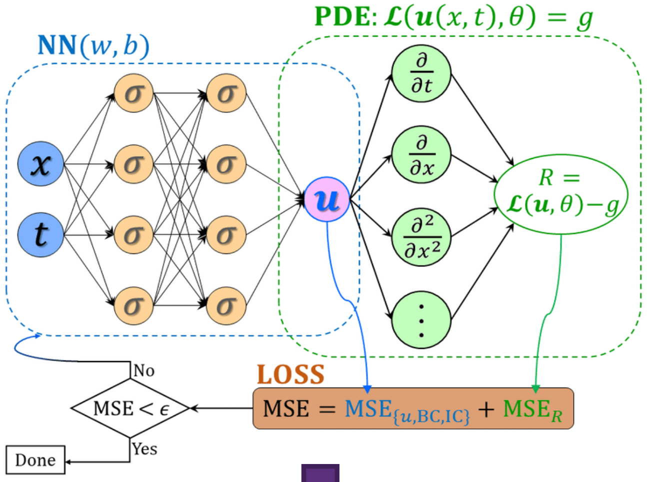
substantial computational cost ☹

Neural Fluid Prediction (NFP) with <u>Data-driven Deep Models</u> ☺

[figs] https://cfd.direct/openfoam/computational-fluid-dynamics/

1.3.1 NFP: PHYSICS-INFORMED NEURAL NETWORKS

- Learning the mapping between variables (inputs) and solutions (outputs) of PDEs
- Encoding physical (PDE residuals) and data (prediction error) constraints into the loss function



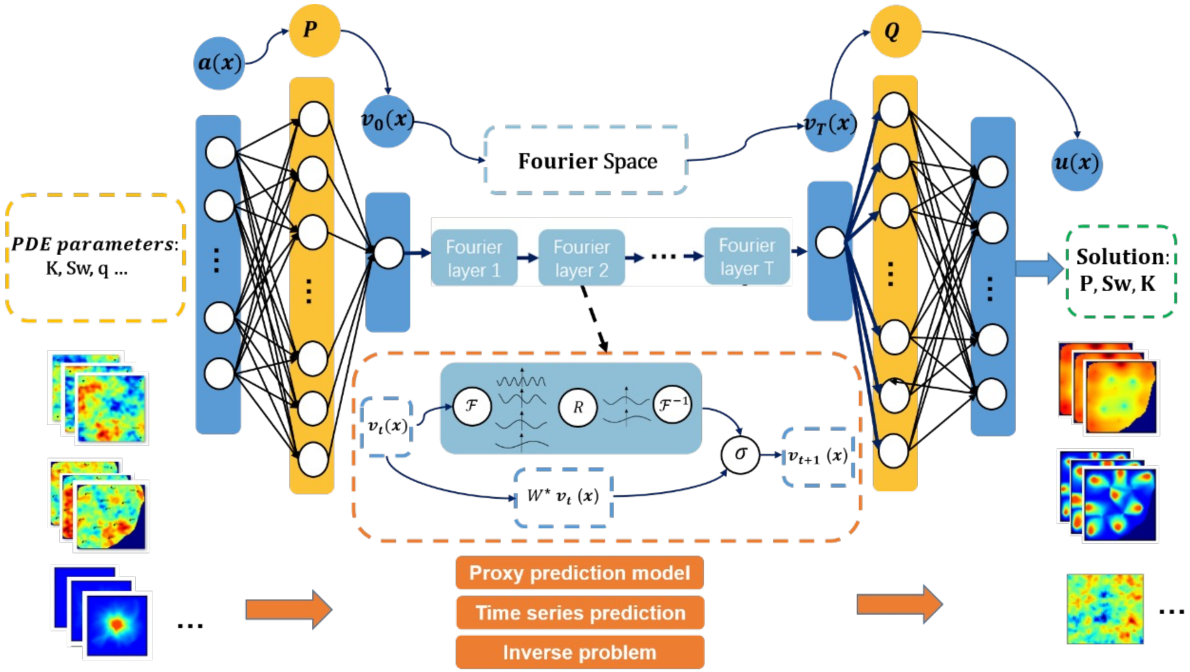
$$\mathcal{L} = \overbrace{\frac{\lambda_r}{N_r}\sum_{i=1}^{N_r}\|\mathcal{F}(u_w;\theta)(\boldsymbol{x}_i)\|^2}^{R} + \overbrace{\frac{\lambda_i}{N_i}\sum_{i=1}^{N_i}\|\mathcal{I}(u_w;\theta)(\boldsymbol{x}_i)\|^2}^{\mathrm{IC}}$$
$$+ \underbrace{\frac{\lambda_b}{N_b}\sum_{i=1}^{N_b}\|\mathcal{B}(u_w;\theta)(\boldsymbol{x}_i)\|^2}_{\mathrm{BC}} + \underbrace{\frac{\lambda_d}{N_d}\sum_{i=1}^{N}\|u_w(\boldsymbol{x}_i) - u(\boldsymbol{x}_i)\|^2}_{u}.$$

training difficulties ☹ poor generalization ☹

Raiss, et al. *Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations.* JCP 2019.

1.3.2 NFP: NEURAL OPERATORS

- Learn the mapping between two Banach spaces including function of input field and output field
- Encoding PDE parameters into the latent space then evolve with a theoretical method



high computational efficiency

easy to train

strong generalization

lacks interpretability

Li, et al. *Fourier neural operator for parametric partial differential equation.* ICLR 2021.

2.1 RECAP: TWO PERSPECTIVES & MULTI SCALES

- Physical priors ➡ Research focus
  - Insight 1: Two perspectives[1] of fluid motion

Eulerian Grid	Observe at fixed locations	Change rate of local fluid w.r.t. time
Lagrangian Particle	Track specific fluid elements	Change rate of moving element w.r.t speed

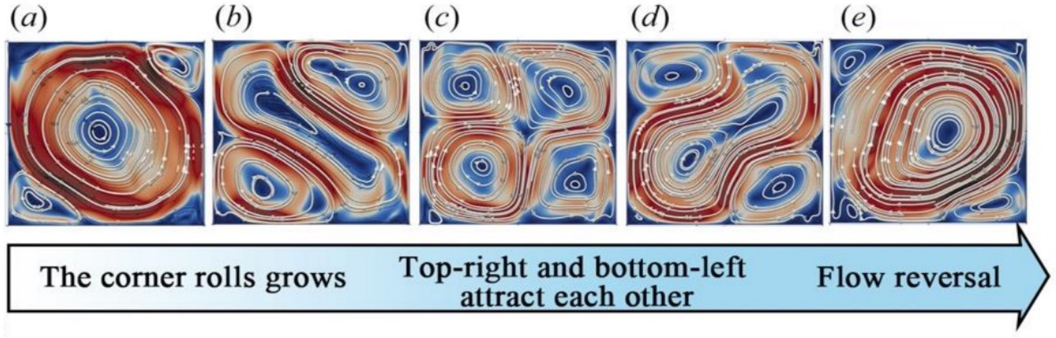
Focus 1: **Combining them for spatiotemporal evolution modelling**

temporal

$$\underbrace{\frac{D\mathbf{q}}{Dt}}_{\text{Material deri.}} \equiv \underbrace{\frac{\partial \mathbf{q}}{\partial t}}_{\text{Domain deri.}} + \underbrace{\mathbf{u} \cdot \nabla \mathbf{q}}_{\text{Convective deri.}} .$$

spatial

  - Insight 2: Different motion patterns at different scales



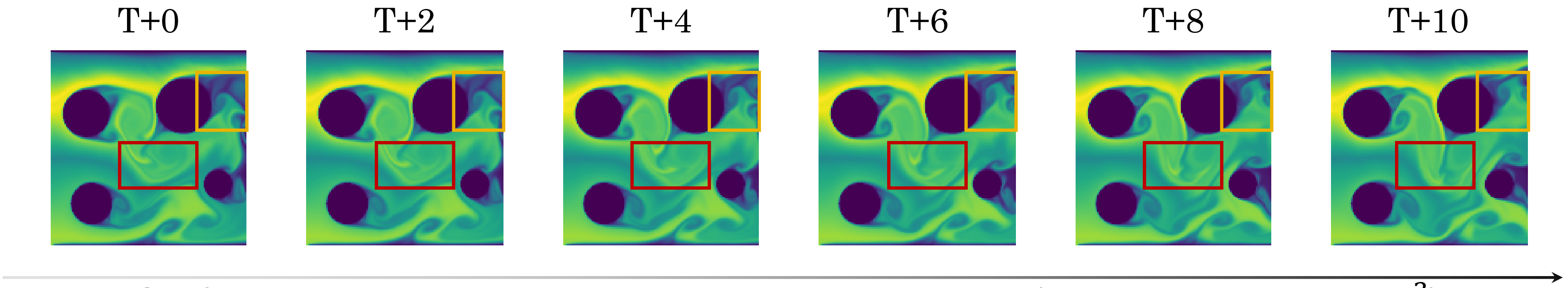
Focus 2:

Using multiscale model to perceive regional features

[1] White, F.M. *Fluid Mechanics*. McGraw-Hill, 2011.

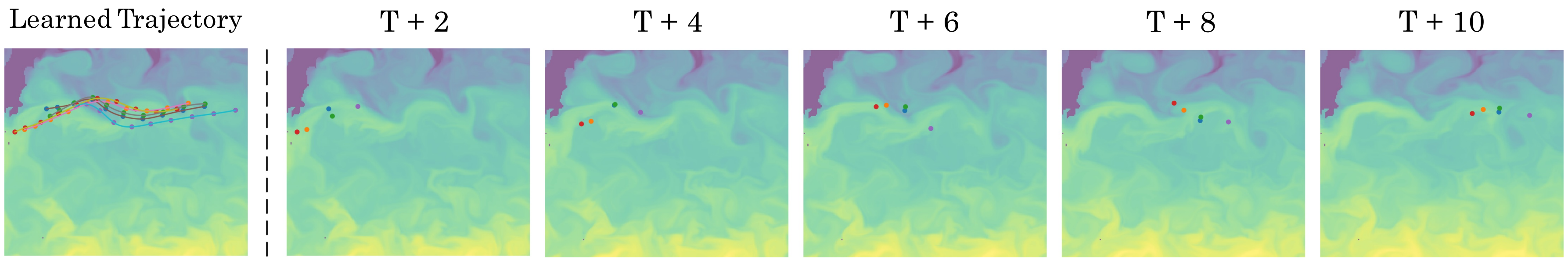
2.2 TARGET: COMPLEX SCENARIO & HARD PROBLEM

- High Reynold number with intricate Boundary conditions



Gas flow around multiple cylinders at high Reynolds number (Reynolds number: $1{\times}10^3$)

- Large-scale and Long-term



Ocean salinity variation[1] in the Northwest Pacific (375 km × 625 km, daily)

[1] CMEMS and MDS. *Global Ocean Physics Reanalysis.* DOI: 10.48670/moi-00021, 2023.

3.1 DEEPLAG: SETUP

- Learn the mapping of functions at adjacent time within the function space on the field
  - Given a bounded open subset $\mathcal{D} \subset \mathbb{R}^d$ in d-dimensional Euclidean space, the o variables observed at time t, $\boldsymbol{u}_t(\boldsymbol{x})$: $\mathbb{R}^d \to \mathbb{R}^o$, can be viewed as a vector-valued function defined on $\mathcal{D}$, forming the Banach space $\mathcal{U}(\mathcal{D}; \mathbb{R}^o)$.
  - The model $\mathcal{F}_\theta$ with parameter θ is expected to fit the mapping within $\mathcal{U}$:

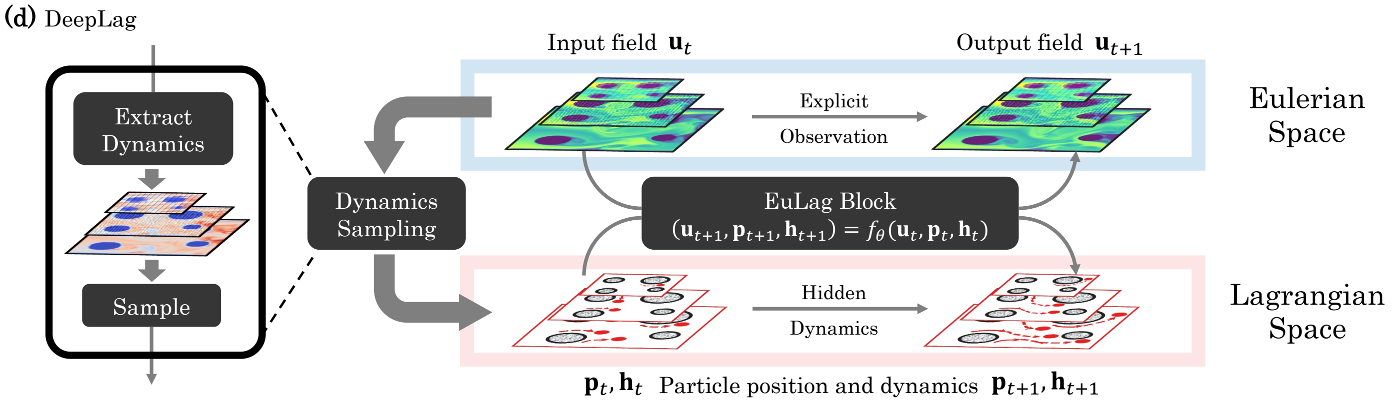
$$\Phi:\ \boldsymbol{u}_t(\boldsymbol{x}) \to \boldsymbol{u}_{t+1}(\boldsymbol{x})$$

- Multi-step autoregressive joint optimization paradigm
  - Input recent p steps of observation, predict the next step. Replace old obs. with new pred.

$$\mathrm{U}_t = \{\boldsymbol{u}_{t-p+1}, \boldsymbol{u}_{t-p+2}, \dots, \boldsymbol{u}_t\} \to \boldsymbol{u}_{t+1}, t = p, p+1, \dots$$

  - Uncertainty Loss are used to balance each step, enabling joint gradient backpropagation

3.2.1 DEEPLAG: MULTI-SCALE ARCHITECTURE



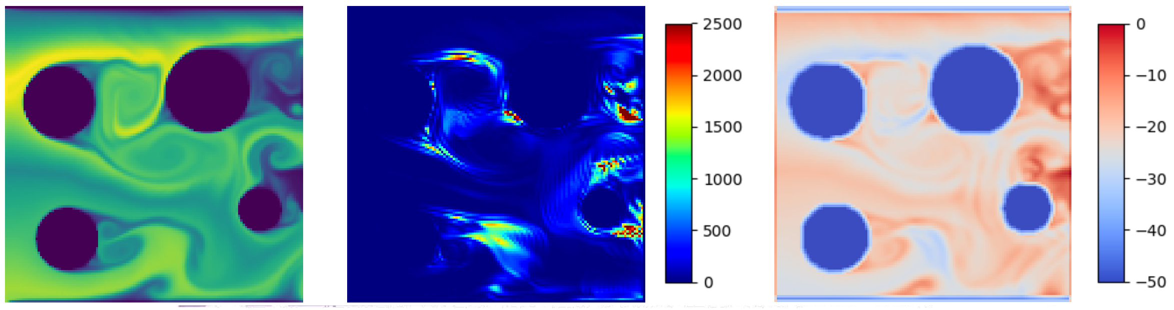
- Inter-scale information exchange
  - Up-sampling and down-sampling to create new fuse neighboring scales
- Feature mapping within scale l
  - The Lagrangian quantity $\boldsymbol{h}_t^l$ and particle position $\boldsymbol{p}_t^l$ aid Eulerian field $\boldsymbol{u}_t^l$ to evolve

$$\boldsymbol{u}_{t+1}^l, \boldsymbol{h}_{t+1}^l | \boldsymbol{p}_{t+1}^l = f_\theta^l(\boldsymbol{u}_t^l, \boldsymbol{h}_t^l | \boldsymbol{p}_t^l)$$

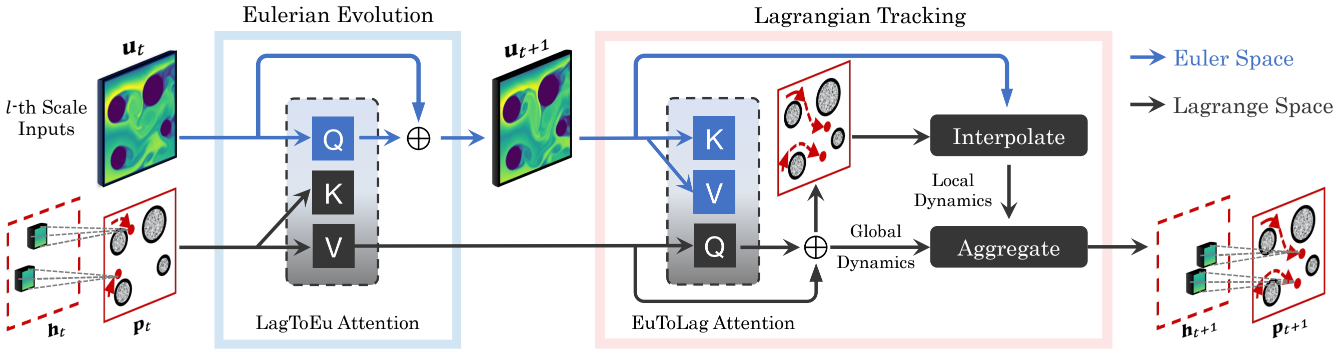
EuLag Block

  - Key particles are sampled based on the complexity of local dynamics
    - Input multi-frame vorticity: $\zeta = \frac{\partial v_y}{\partial x} - \frac{\partial v_x}{\partial y}$
    - Sampled particles via its pointwise variance:

$$\boldsymbol{p}_t \sim std(\zeta)$$



3.2.2 DEEPLAG: EULAG BLOCK



- Lagrangian (L) → Eulerian (E)
  - Distance-weighted cross-attention

$$\boldsymbol{u}_{t+1} = \boldsymbol{u}_t + \mathrm{softmax}\left(\frac{\boldsymbol{W}_Q\boldsymbol{u}_t(\boldsymbol{W}_K\boldsymbol{h}_t)^T}{\sqrt{C}} \cdot \boldsymbol{M}\right)\boldsymbol{W}_V\boldsymbol{h}_t$$

- Eulerian (E) → Lagrangian (L)
  - Global: Distance-weighted cross-attention

$$\boldsymbol{h}_{t+1,\,\mathrm{global}} = \boldsymbol{h}_t + \mathrm{softmax}\left(\frac{\boldsymbol{W'}_Q\boldsymbol{h}_t(\boldsymbol{W'}_K\boldsymbol{u}_t)^T}{\sqrt{C}} \cdot \boldsymbol{M}\right)\boldsymbol{W'}_V\boldsymbol{u}_t$$

  - Local: Eulerian features are interpolated at tracked particle coordinates to obtain $\boldsymbol{h}_{t+1,\,\mathrm{local}}$
  - MLP is used to fuse global and local results

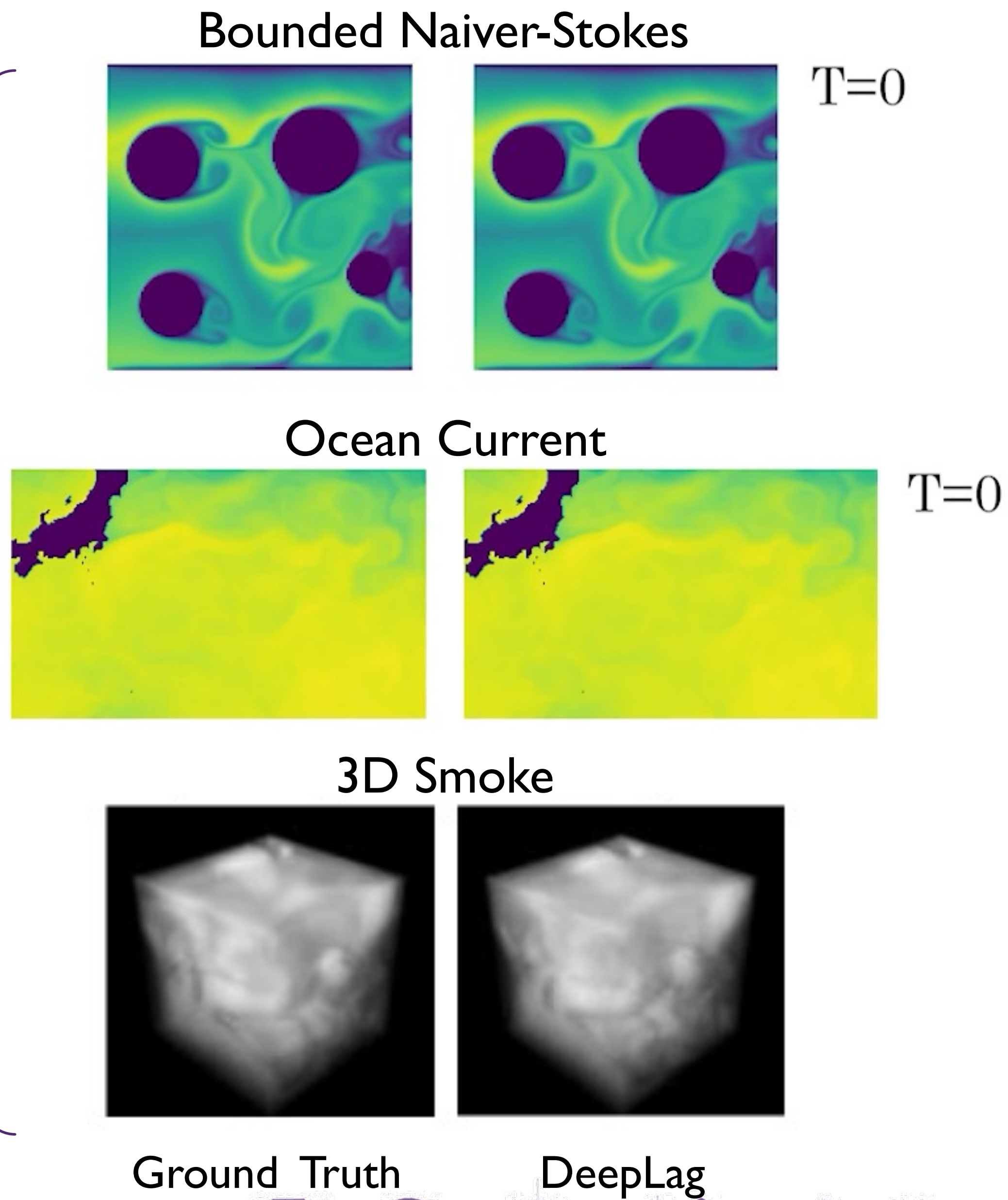
Self-Attn	O(n^2)
EuLag-Attn	O(n)

4 EXPERIMENTS

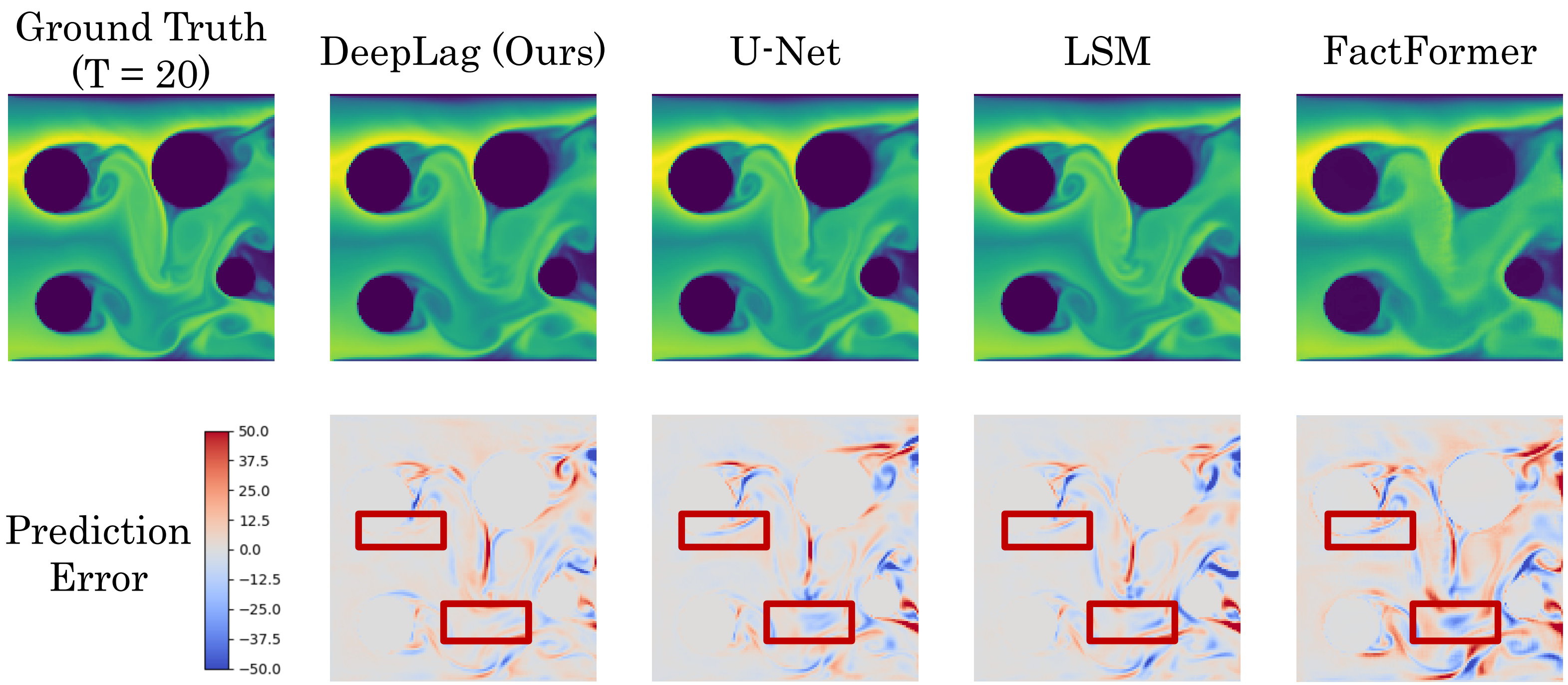
Strong performance on all tasks within the linear complexity

- Benchmarks
  - Bounded Naiver-Stokes
    - 13.8% relative promotion
  - Ocean Current
    - 30 days prediction, 12.8% relative promotion
  - 3D Smoke
    - 34.4% relative promotion

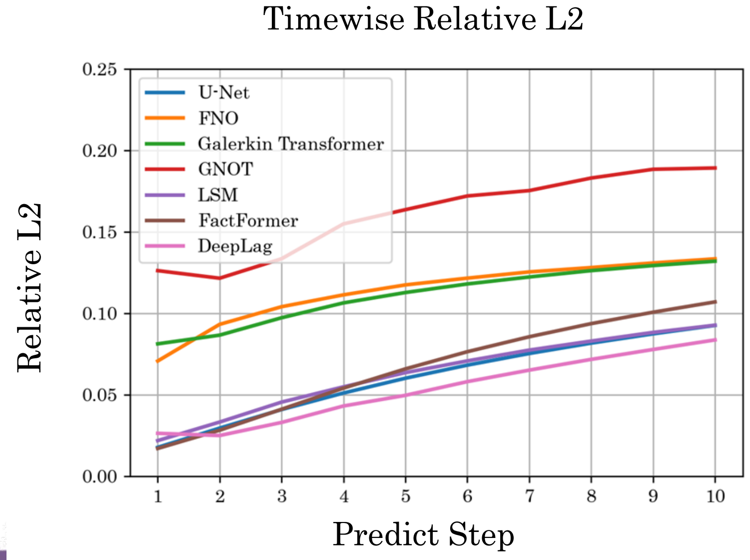
Datasets	Type	#Var	#Dim	#Space
Bounded N-S	Simulation	1	2D	128×128
Ocean Current	Real World	5	2D	180×300
3D Smoke	Simulation	4	3D	32^3



4.1 BOUNDED NAIVER-STOKES



Model	Relative L2 (↓)	
	10 Frames	30 Frames
U-Net [32]	<u>0.0618</u>	0.1038
FNO [21]	0.1041	0.1282
Galerkin Transformer [3]	0.1084	0.1369
Vortex [7]	0.1999	NaN
GNOT [14]	0.1388	0.1793
LSM [52]	0.0643	<u>0.1020</u>
FactFormer [20]	0.0733	0.1195
DeepLag (Ours)	**0.0543**	**0.0993**
Promotion	13.8%	2.7%

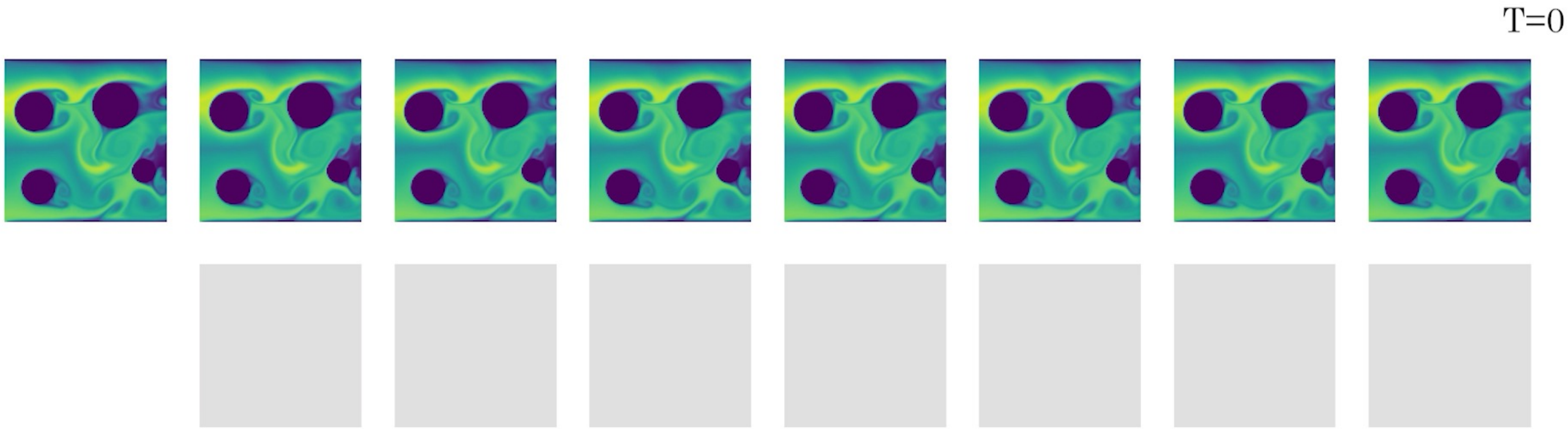


Precisely illustrate the vortex and give a reasonable motion mode of the Kármán vortex phenomenon[1]

[1] Wille, R. *Karman vortex streets.* Advances in Applied Mechanics, 1960.

4.1 BOUNDED NAIVER-STOKES

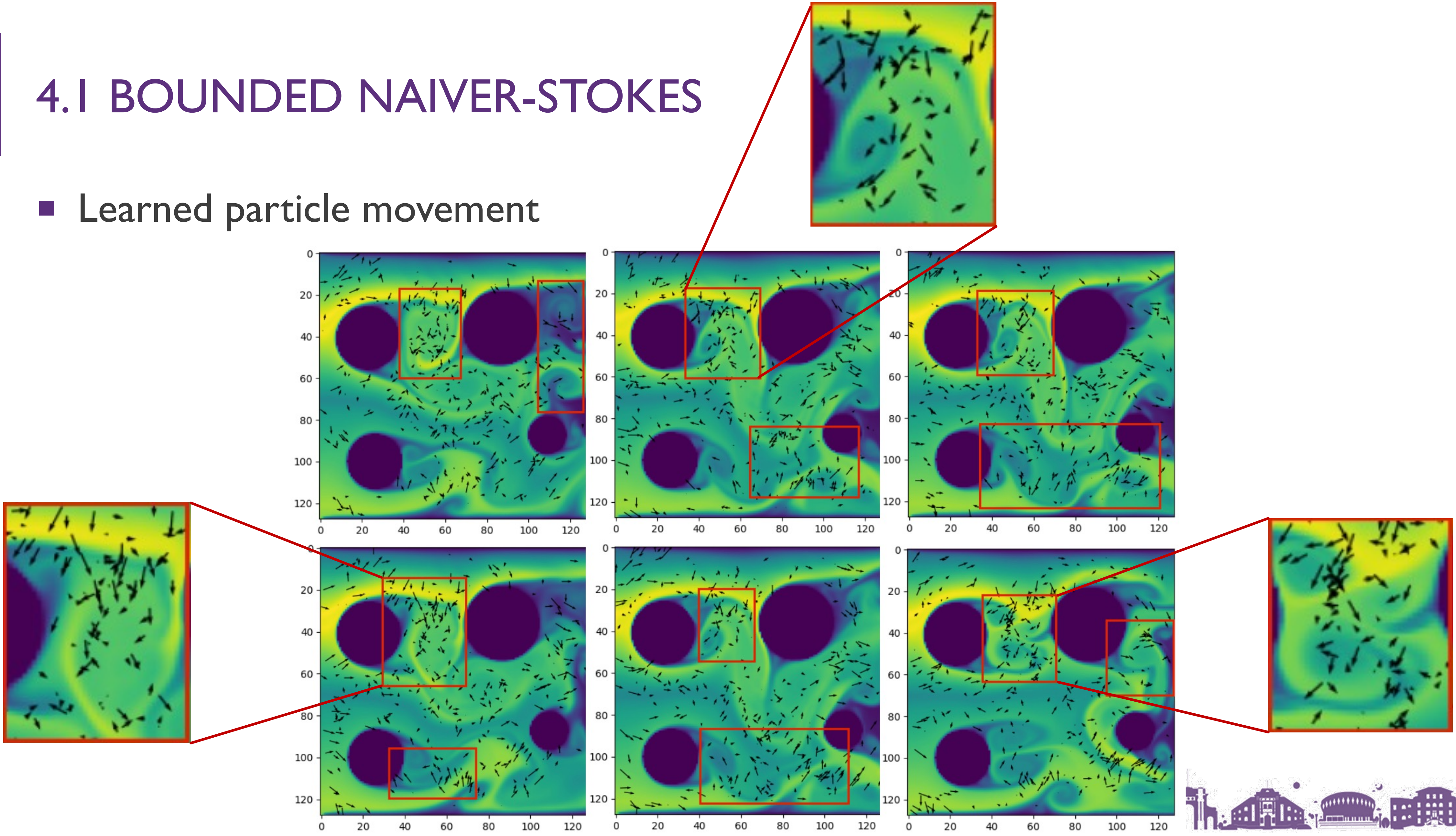
- Video of Long-term prediction (100 frames)



Ground Truth | **DeepLag (Ours)** | FactFormer | FNO | Galerkin Transformer | GNOT | LSM | U-Net

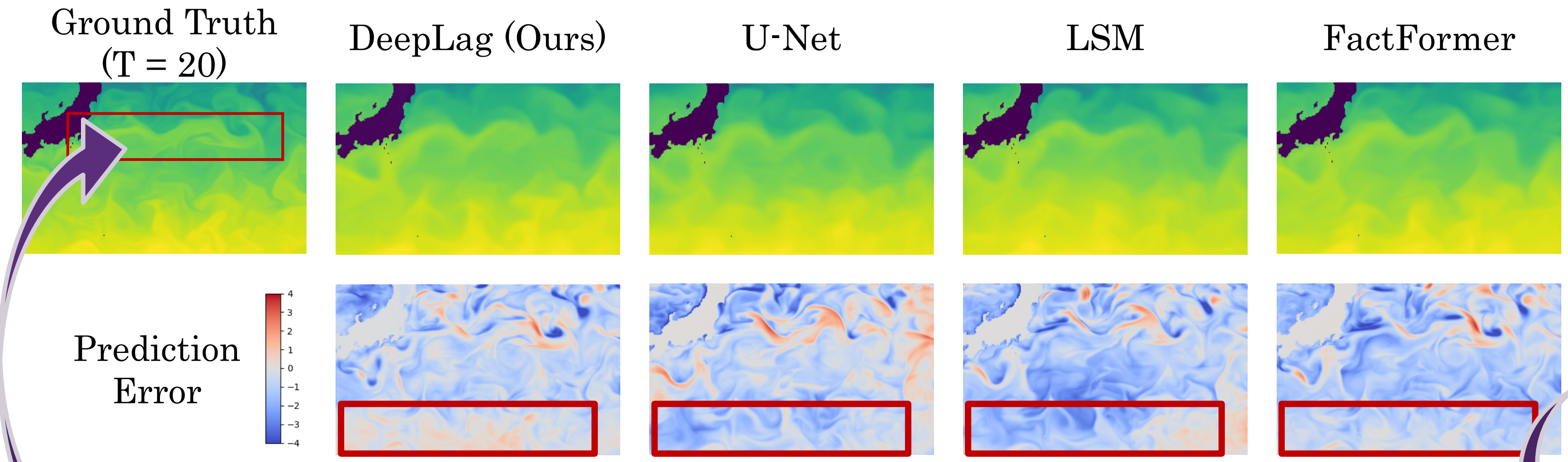
4.1 BOUNDED NAIVER-STOKES

- Learned particle movement



4.2 OCEAN CURRENT

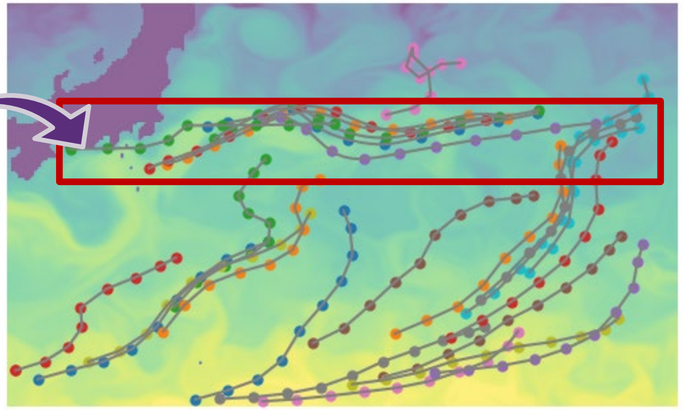
Performs well in real-world, large-scale fluids, which usually involve more inherent stochasticity



Provides a clear depiction of the Kuroshio pattern[1]

Model	Relative L2 (↓)	
	10 Days	30 Days
U-Net [32]	0.0185	0.0297
FNO [21]	0.0246	0.0420
Galerkin Transformer [3]	0.0323	0.0515
Vortex [7]	0.9548	NaN
GNOT [14]	0.0206	0.0336
LSM [52]	<u>0.0182</u>	<u>0.0290</u>
FactFormer [20]	0.0183	0.0296
DeepLag (Ours)	**0.0168**	**0.0257**
Promotion	8.3%	12.8%

Estimated Particle Trajectory
(T = 10 ~ 20)

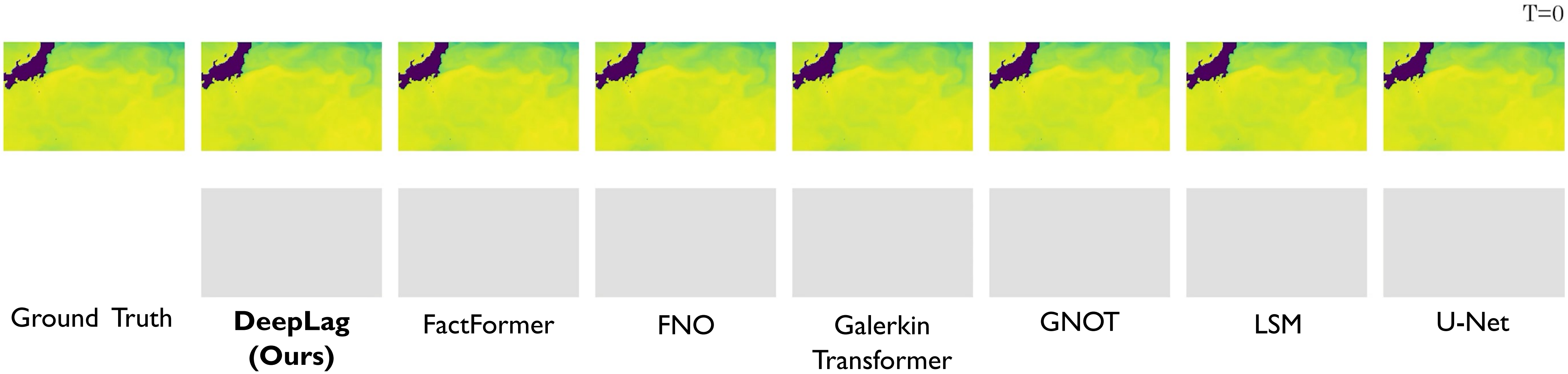


The movement of upper particles matches the sinuous trajectory of the Kuroshio current

[1] Tang, et al. *The flow pattern north of Taiwan and the migration of the Kuroshio.* Continental Shelf Research, 2021.

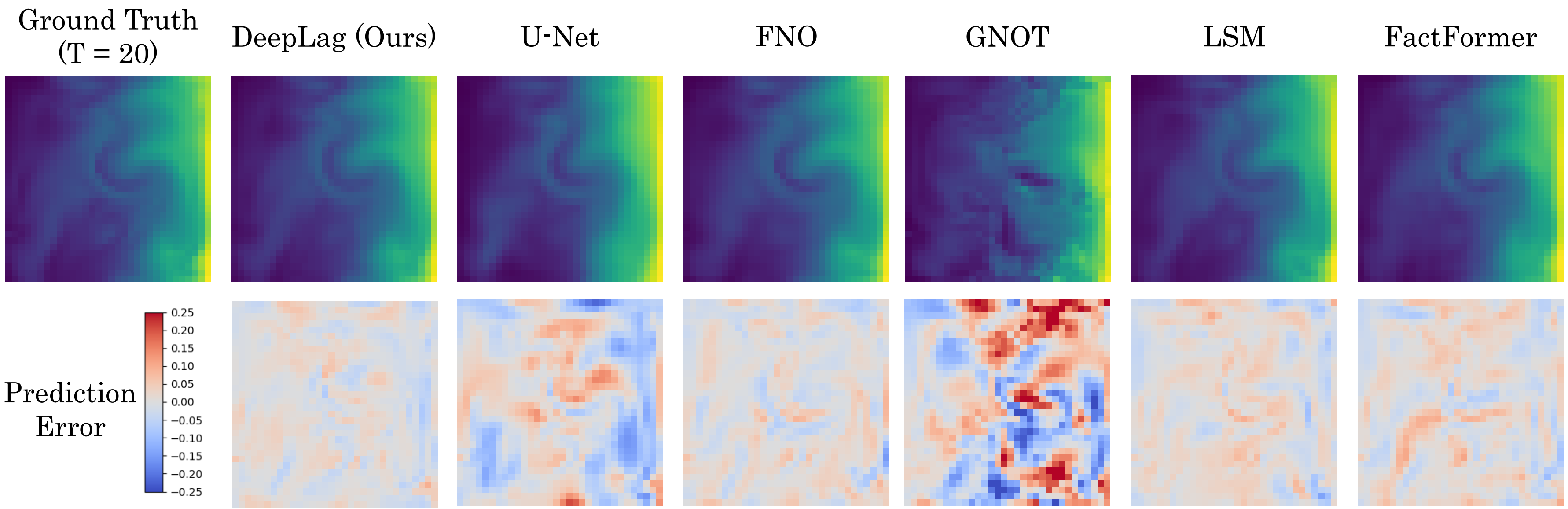
4.2 OCEAN CURRENT

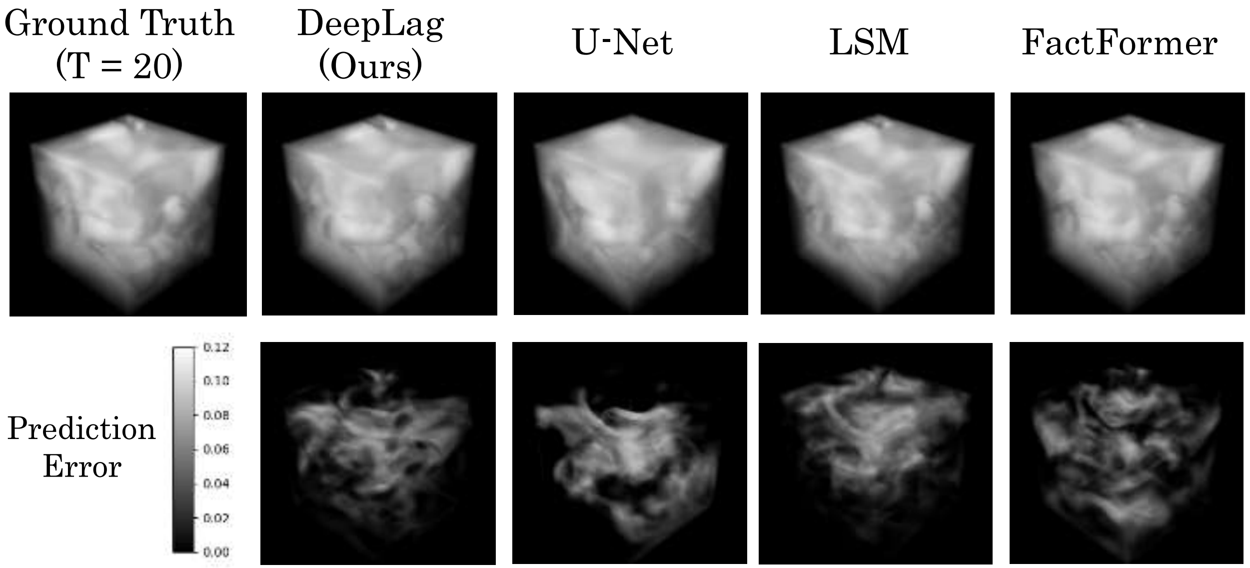
- Video of Long-term prediction (100 frames)



4.3 3D SMOKE

More gain on 3D scenario





Model	Relative L2 (↓)
U-Net [32]	0.0508
FNO [21]	0.0635
Galerkin Transformer [3]	0.1066
GNOT [14]	0.2100
LSM [52]	0.0527
FactFormer [20]	0.0793
DeepLag (Ours)	**0.0378**
Promotion	34.4%

4.4.1 ABLATIONS

- Module removing
  - w/o Lagrangian particle tracking, w/o Eularian feature evolving, w/o learnable sampling
- Hyperparameter sensitivity
  - Adjust number of {tracking particles, spatial scales, latent dimensions}
- Swap the order of EuToLag and LagToEu cross-attention

(a) Module Removing

Design	Relative L2 (↓)
DeepLag	**0.0543**
w/o LagToEu(·)	0.0556
w/o EuToLag(·)	0.0547
w/o Learnable Sampling	0.0552

(b) Hyperparameter Sensitivity

#Particle	Relative L2 (↓)	#Scale	Relative L2 (↓)	#Latent	Relative L2 (↓)
128	0.0559	1	0.0789	16	0.0656
256	0.0553	2	0.0658	32	0.0594
512(ori)	**0.0543**	4(ori)	**0.0543**	64(ori)	**0.0543**
768	0.0547	5	0.0554	128	0.0614

(c) Attention Swapping

Data	Original (↓)	Swapped (↓)
2D	**0.0543**	0.0545
3D	0.0378	0.0378

4.4.2 GENERALIZATION

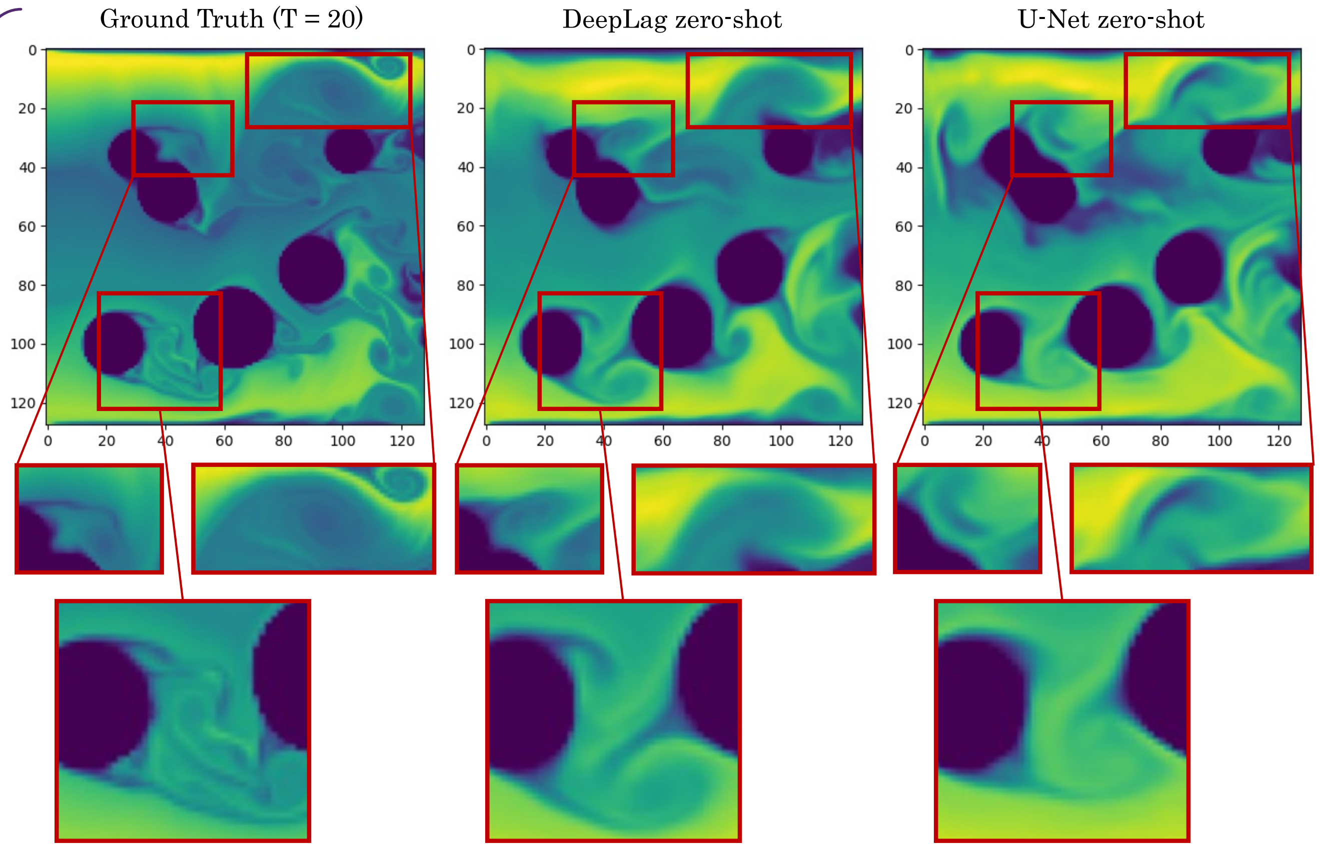
- On high-resolution data

Resolution	Mem	Time	Relative L2 (↓)
128×128	5420MB	1150s/ep	0.0543
256×256	13916MB	1300s/ep	**0.0514**

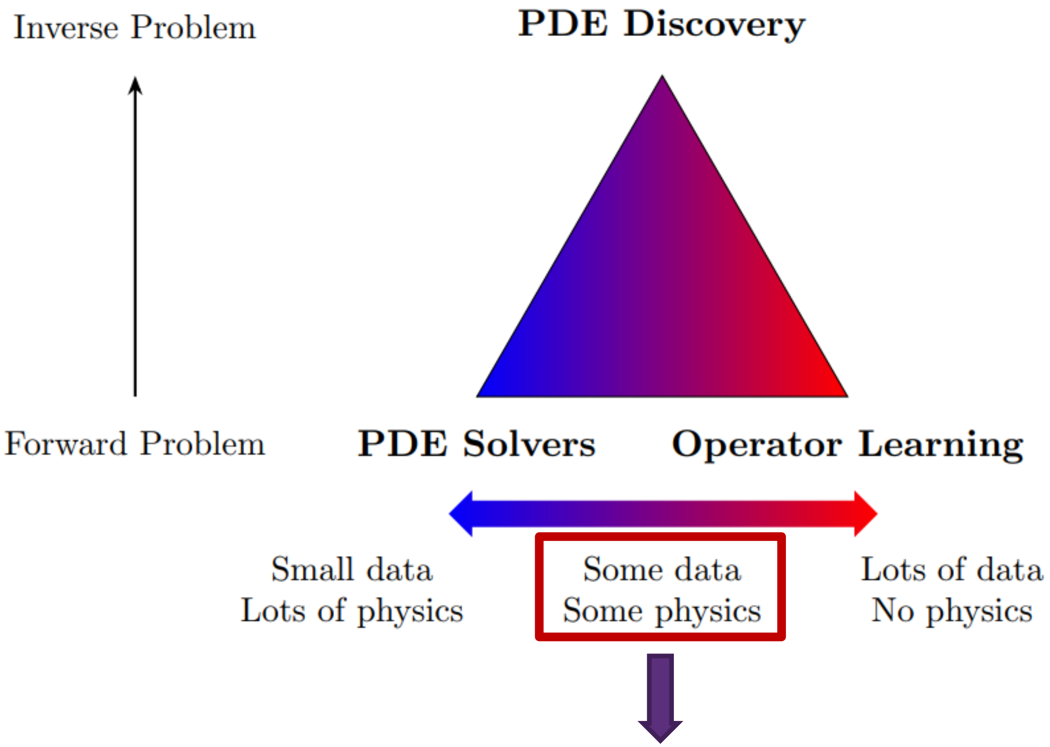
256×256, U-Net relative L2: 0.0600

- On unseen boundary conditions

Model	Relative L2
U-Net	0.217
DeepLag	**0.203**



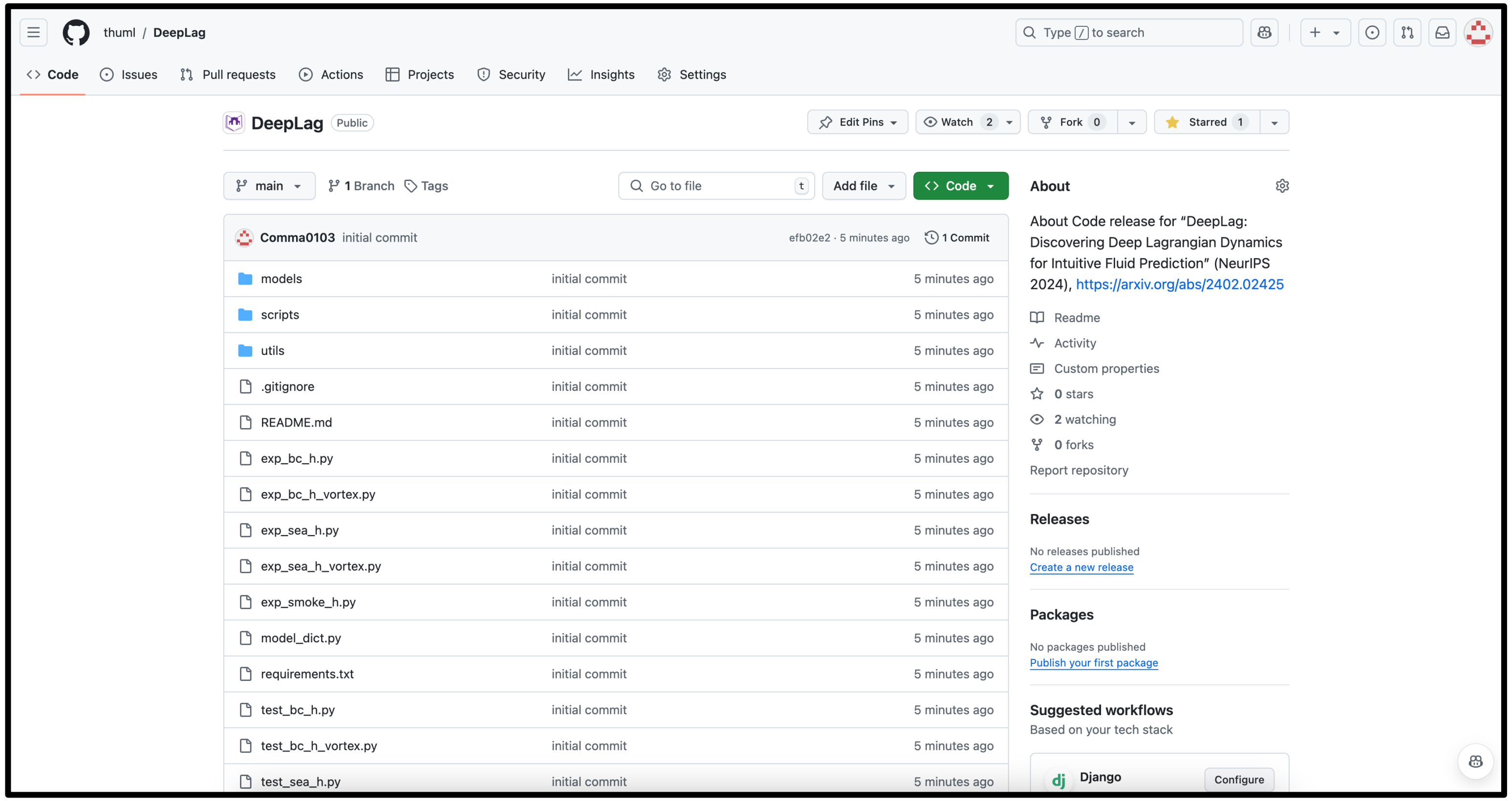
5 SUMMARY AND FUTURE WORK



Feature: A data-driven DL approach with physical interpretability through **Deep Lagrangian Dynamics**

- Addressing the interpretability of learned particle trajectories by aligning with Lagrangian numerical methods
- Introducing motion decomposition mechanisms and fluid-specific principles for specific scenarios to develop downstream specialized methods

OPEN SOURCE



https://github.com/thuml/DeepLag

Complete benchmarks & code & models

THANKS FOR LISTENING!

mql22@mails.tsinghua.edu.cn

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