NEURAL INFORMATION PROCESSING SYSTEMS

# DeepLag: Discovering Deep Lagrangian Dynamics for Intuitive Fluid Prediction

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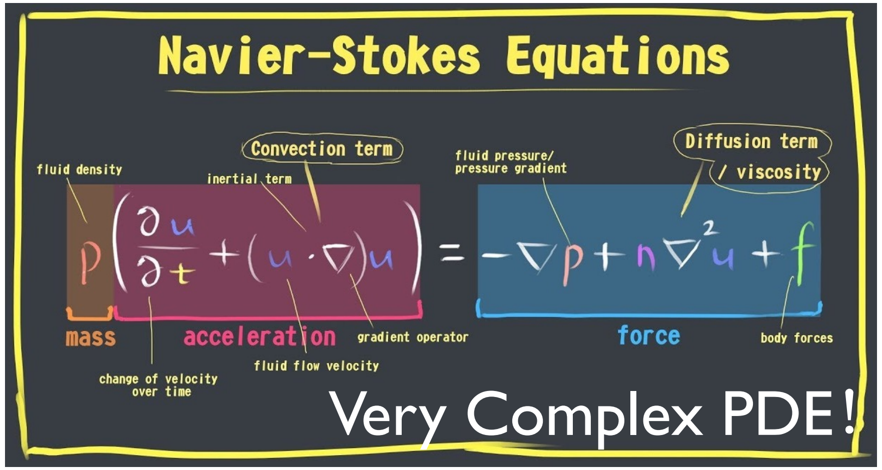
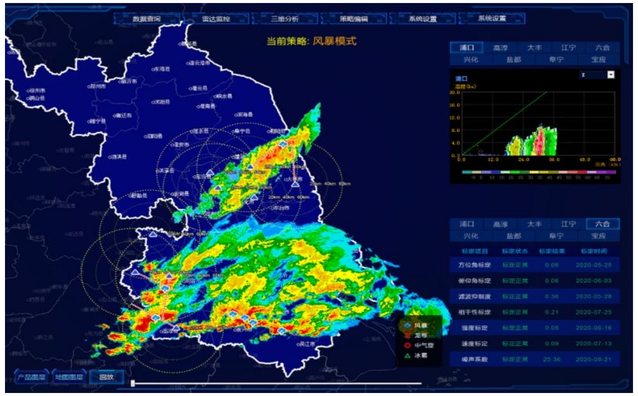
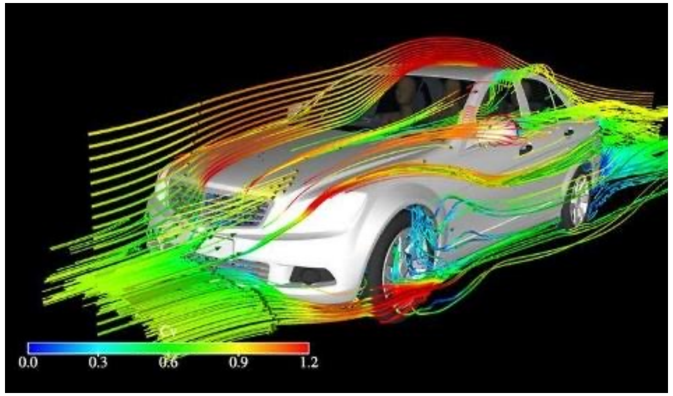
# 1.1 FLUID & ITS CHARACTERISTICS



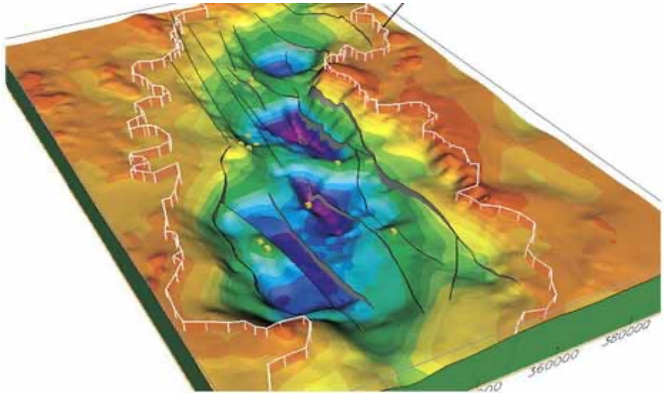

- **Fluids**: easily deform, with complex dynamics
- **Highly related to production and life**: Accurate prediction of future fluid evolution is of great significance in various fields



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]

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

→ information loss ☹

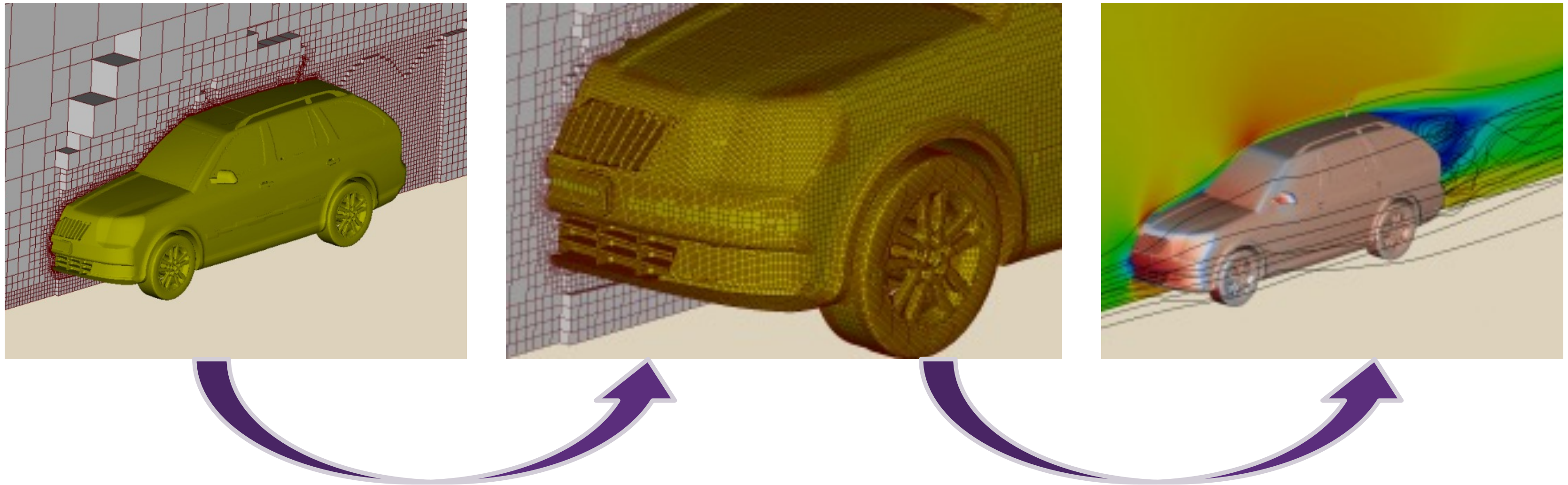
$$-\rho\overline{u_i' u_j'} = \mu_t\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3}\frac{\partial U_k}{\partial x_k}\delta_{ij}\right) - \frac{2}{3}\rho k \delta_{ij}$$

→ 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 ☹

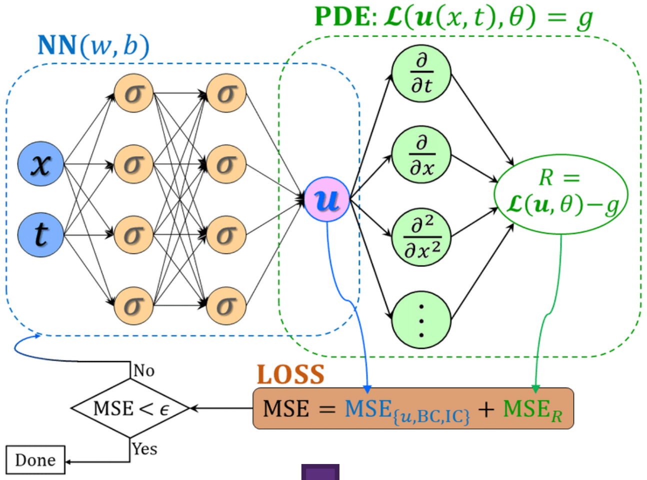
substantial computational cost ☹

Neural Fluid Prediction (NFP) with Data-driven Deep Models ☺

[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



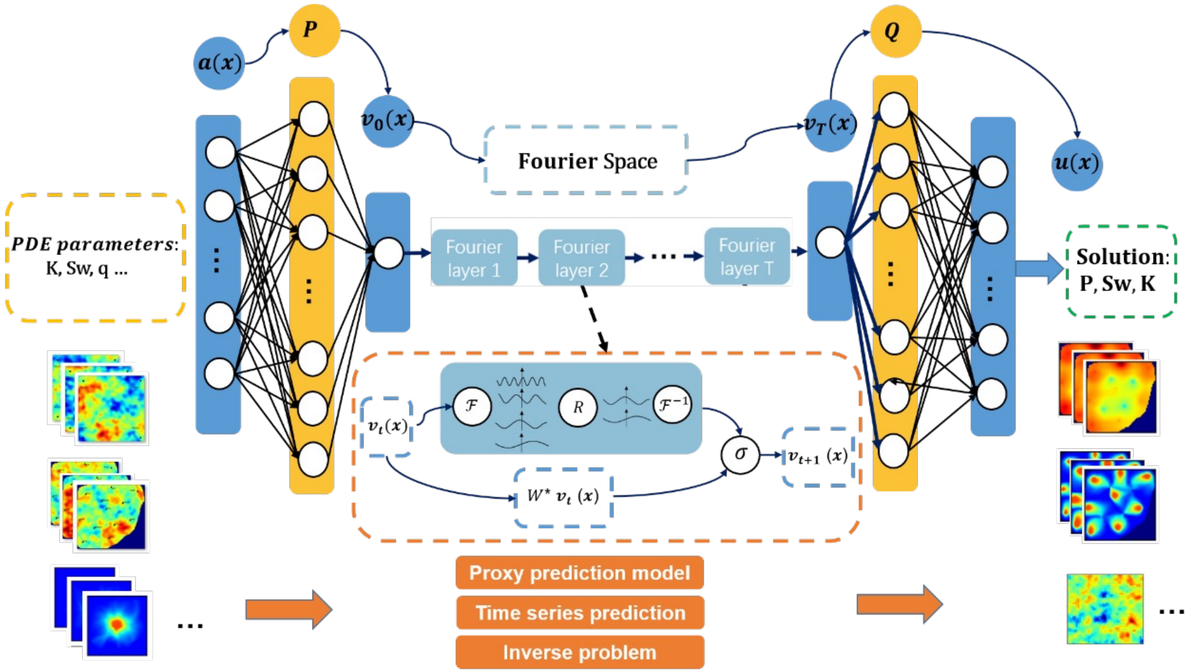

$$\mathcal{L} = \overbrace{\frac{\lambda_r}{N_r}\sum_{i=1}^{N_r}\|\mathcal{F}(u_w;\theta)(\boldsymbol{x}_i)\|^2}^{R} + \overbrace{\frac{\lambda_i}{N_i}\sum_{i=1}^{N_i}\|\mathcal{I}(u_w;\theta)(\boldsymbol{x}_i)\|^2}^{\mathrm{IC}}$$
$$+ \underbrace{\frac{\lambda_b}{N_b}\sum_{i=1}^{N_b}\|\mathcal{B}(u_w;\theta)(\boldsymbol{x}_i)\|^2}_{\mathrm{BC}}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

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 |

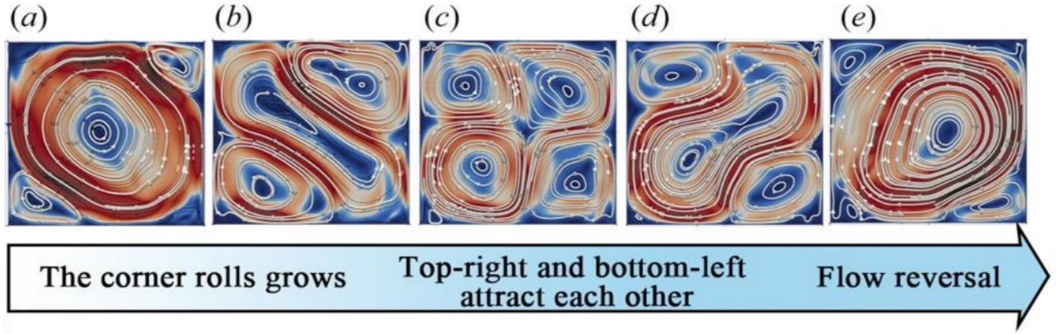
Focus 1: **Combining them for spatiotemporal evolution modelling**

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



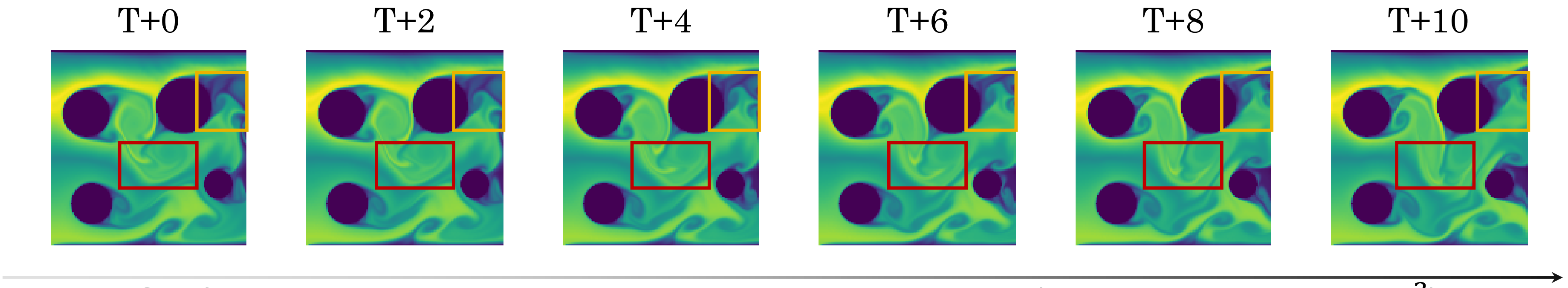

Focus 2:

**Using multiscale model to perceive regional features**

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

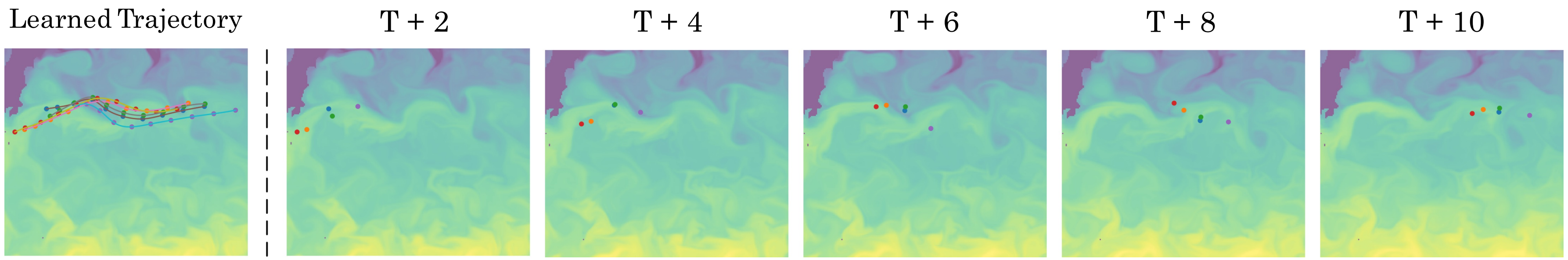
# 2.2 TARGET:  COMPLEX SCENARIO & HARD PROBLEM

- 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 $\times$ 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 $t$, $\boldsymbol{u}_t(\boldsymbol{x})$: $\mathbb{R}^d \rightarrow \mathbb{R}^o$, 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 $\theta$ is expected to fit the mapping within $\mathcal{U}$:

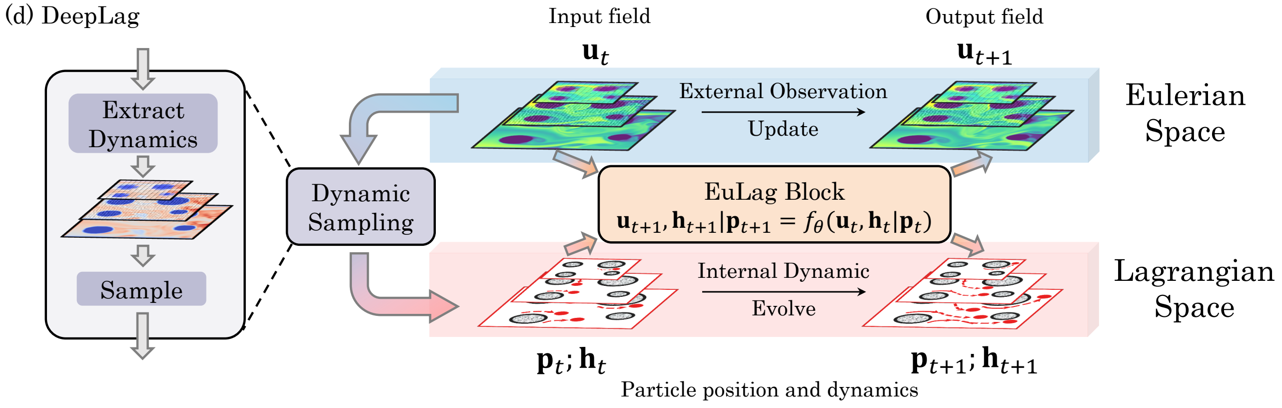
$$\Phi:\ \boldsymbol{u}_t(\boldsymbol{x}) \rightarrow \boldsymbol{u}_{t+1}(\boldsymbol{x})$$

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

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

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

# 3.2.1 DEEPLAG: MULTI-SCALE ARCHITECTURE

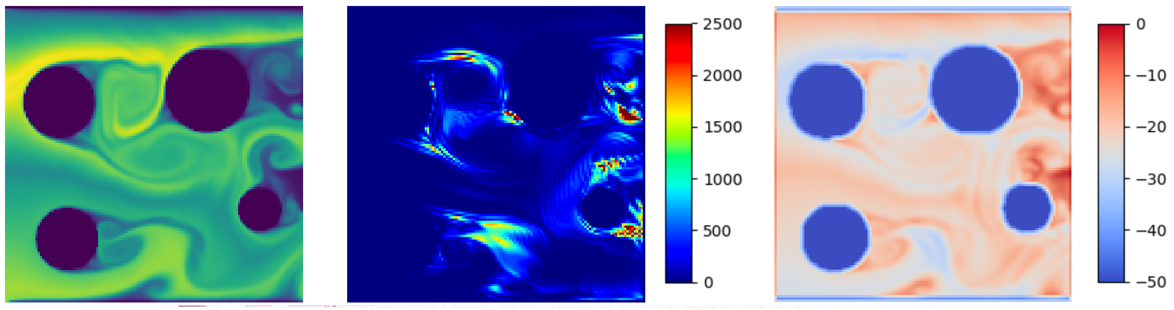



- Inter-scale information exchange
  - Up-sampling and down-sampling to create new fuse neighboring scales
- Feature mapping within scale $l$
  - The Lagrangian quantity $\boldsymbol{h}_t^l$ and particle position $\boldsymbol{p}_t^l$ aid Eulerian field $\boldsymbol{u}_t^l$ to evolve

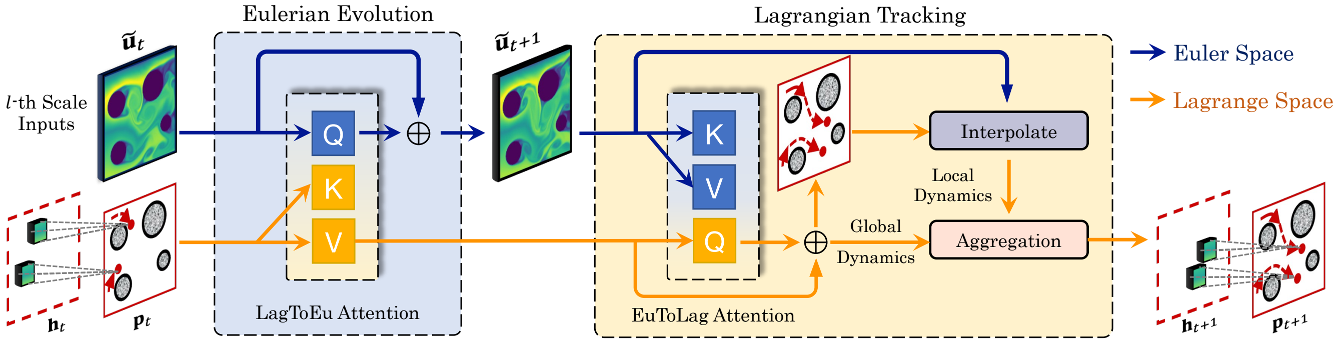
$$\boldsymbol{u}_{t+1}^l, \boldsymbol{h}_{t+1}^l | \boldsymbol{p}_{t+1}^l = f_\theta^l(\boldsymbol{u}_t^l, \boldsymbol{h}_t^l | \boldsymbol{p}_t^l)$$ ➡ EuLag Block

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

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



# 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

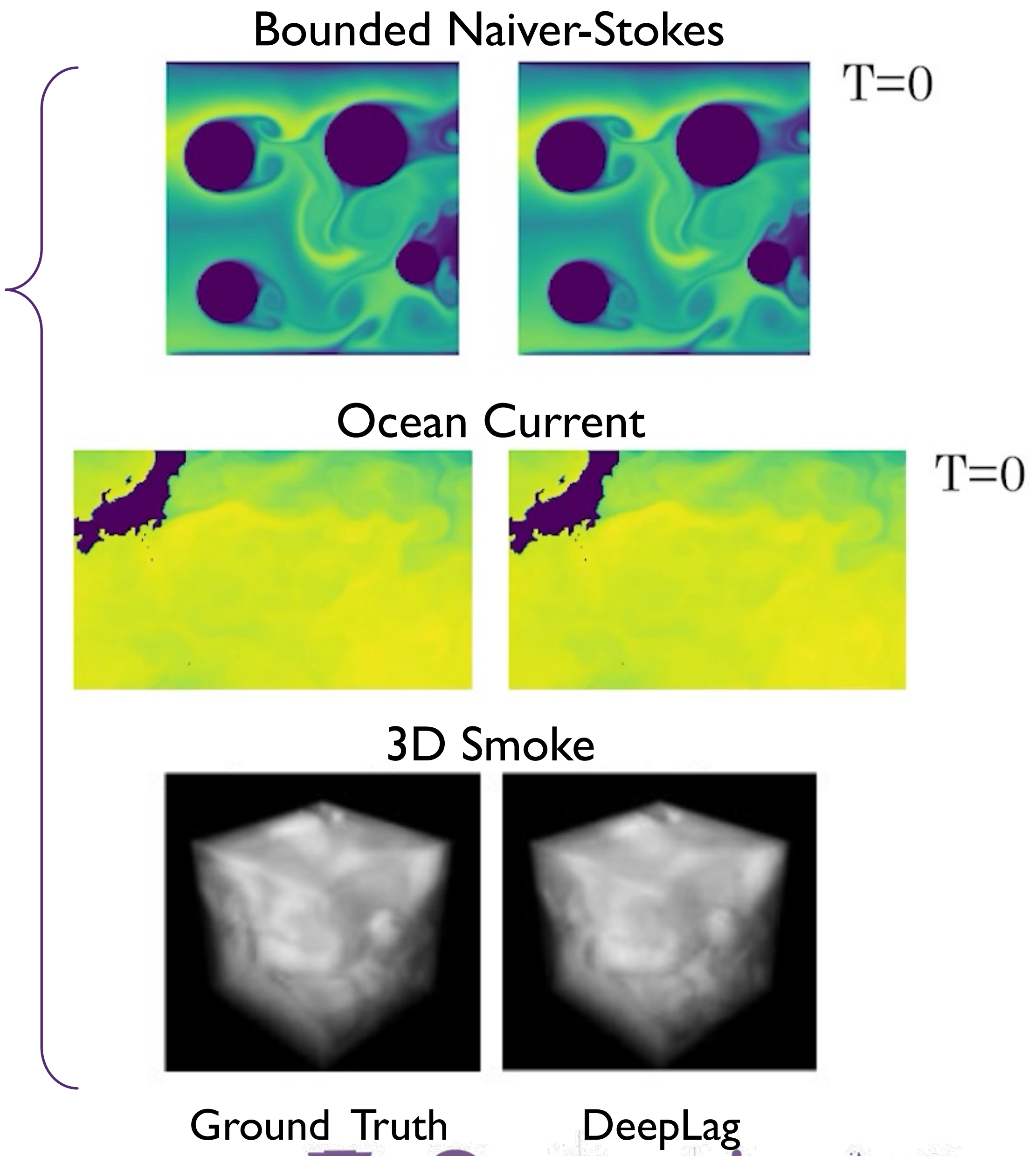
| Self-Attn | O(n^2) |
| --- | --- |
| EuLag-Attn | O(n) |

## 4 EXPERIMENTS

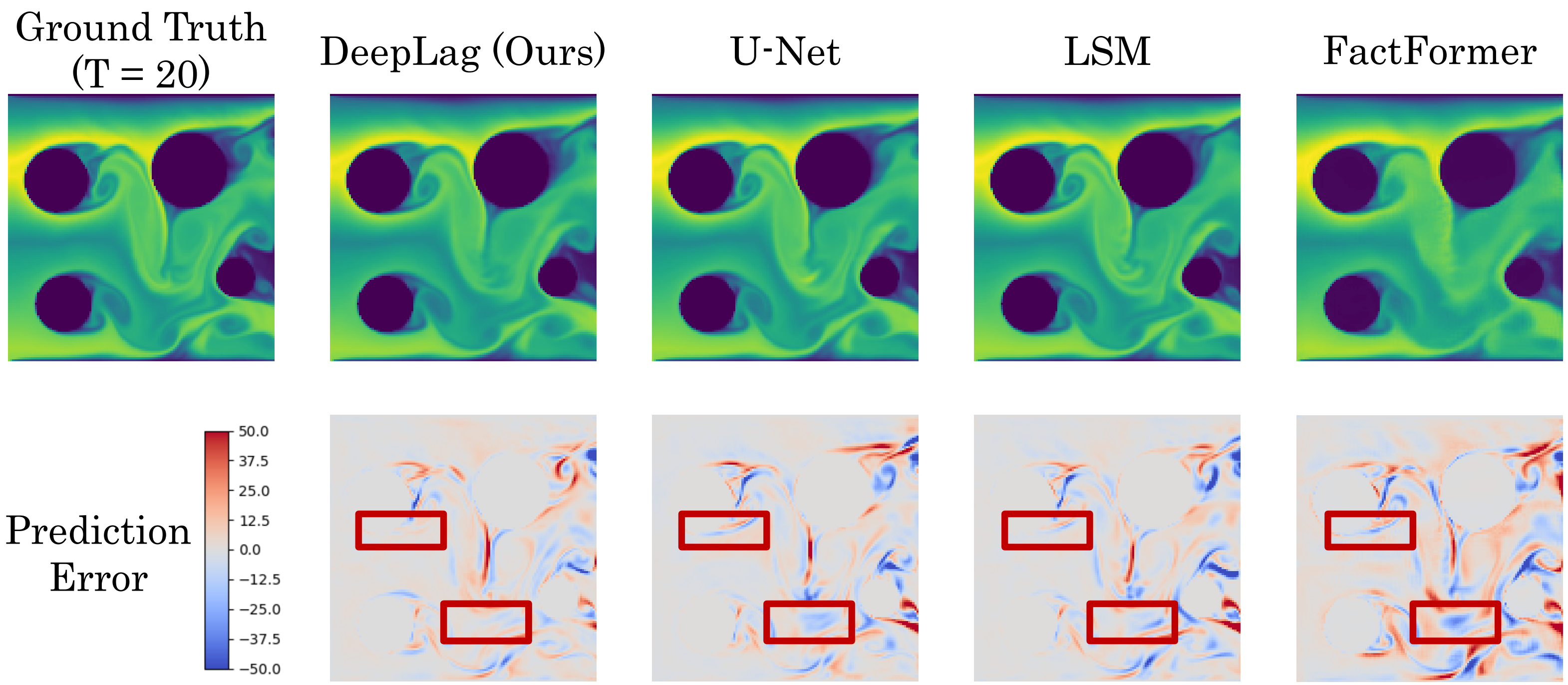
**Strong performance on all tasks within the linear complexity**

- 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 | $128 \times 128$ |
| Ocean Current | Real World | 5 | 2D | $180 \times 300$ |
| 3D Smoke | Simulation | 4 | 3D | $32^3$ |

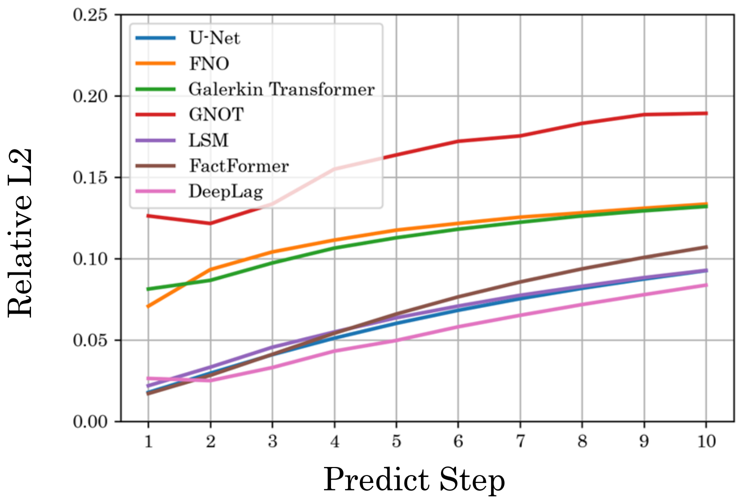


# 4.1 BOUNDED NAIVER-STOKES




| Model | Relative L2 (↓) 10 Frames | Relative L2 (↓) 30 Frames |
|---|---|---|
| U-Net [32] | 0.0618 | 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 | 0.1020 |
| FactFormer [20] | 0.0733 | 0.1195 |
| DeepLag (Ours) | **0.0543** | **0.0993** |
| Promotion | 13.8% | 2.7% |

Timewise Relative L2



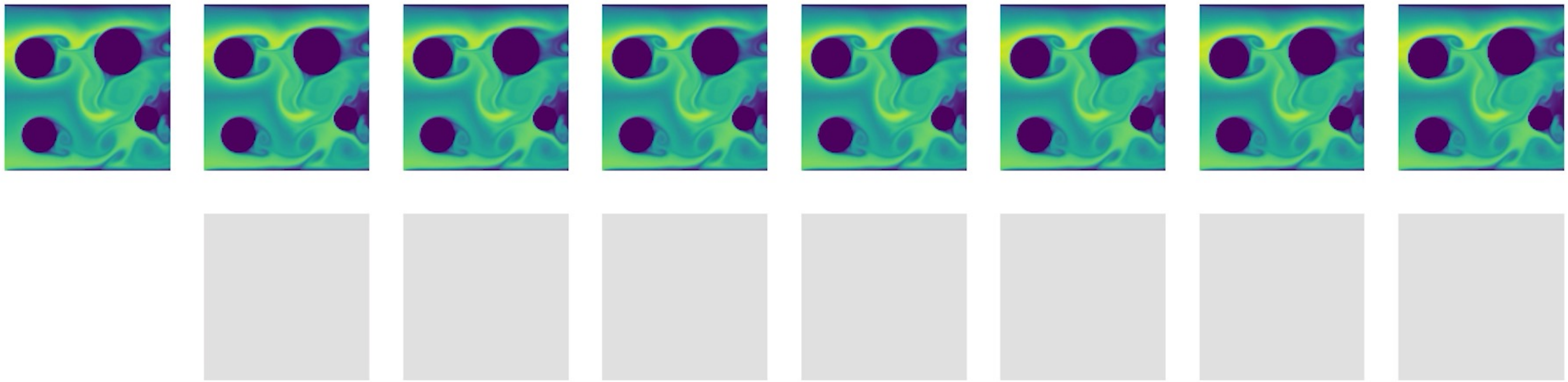

Precisely illustrate the vortex and give a reasonable motion mode of the Kármán vortex phenomenon[1]

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

## 4.1 BOUNDED NAIVER-STOKES

- Video of Long-term prediction (100 frames)

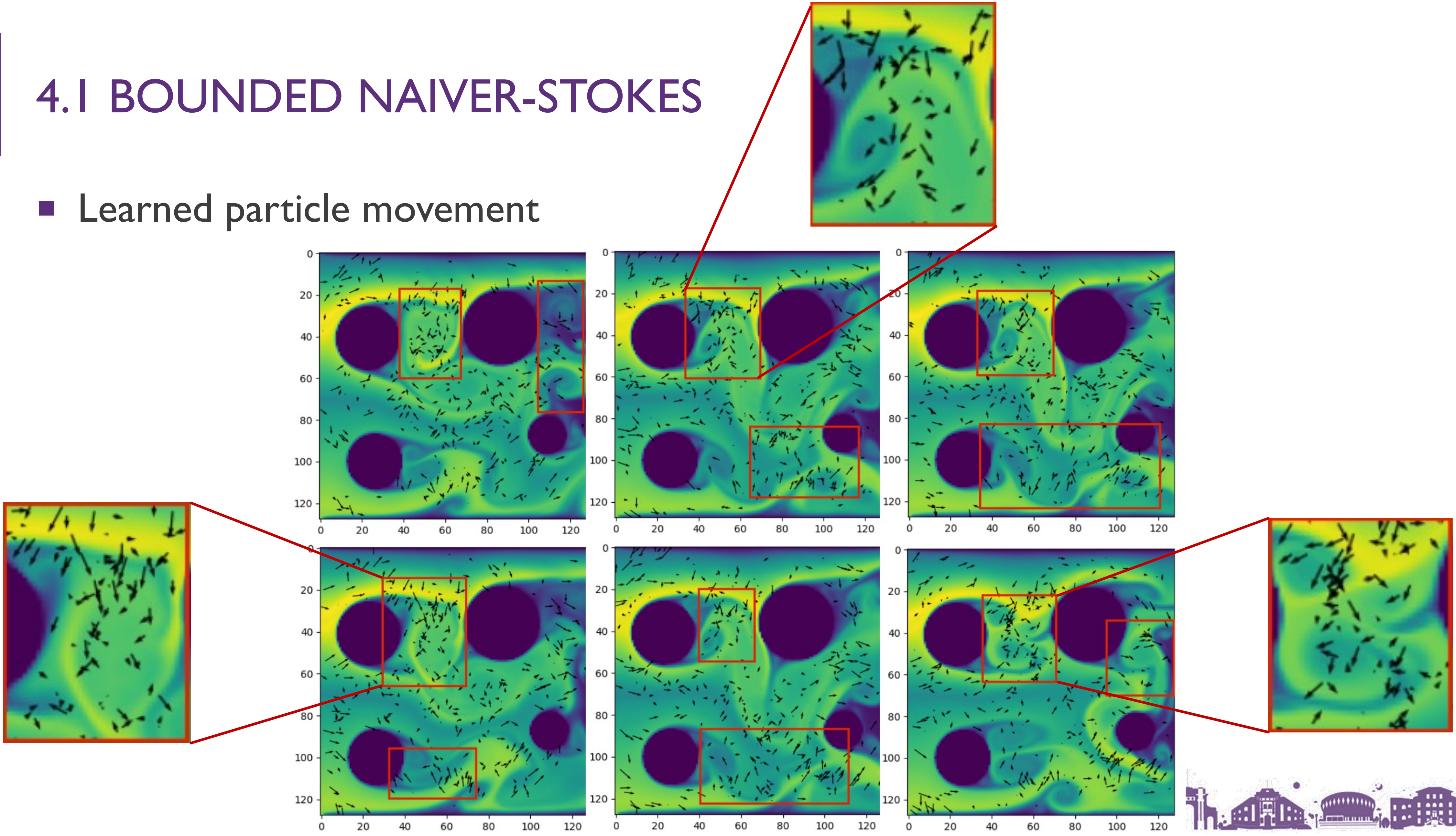
T=0



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

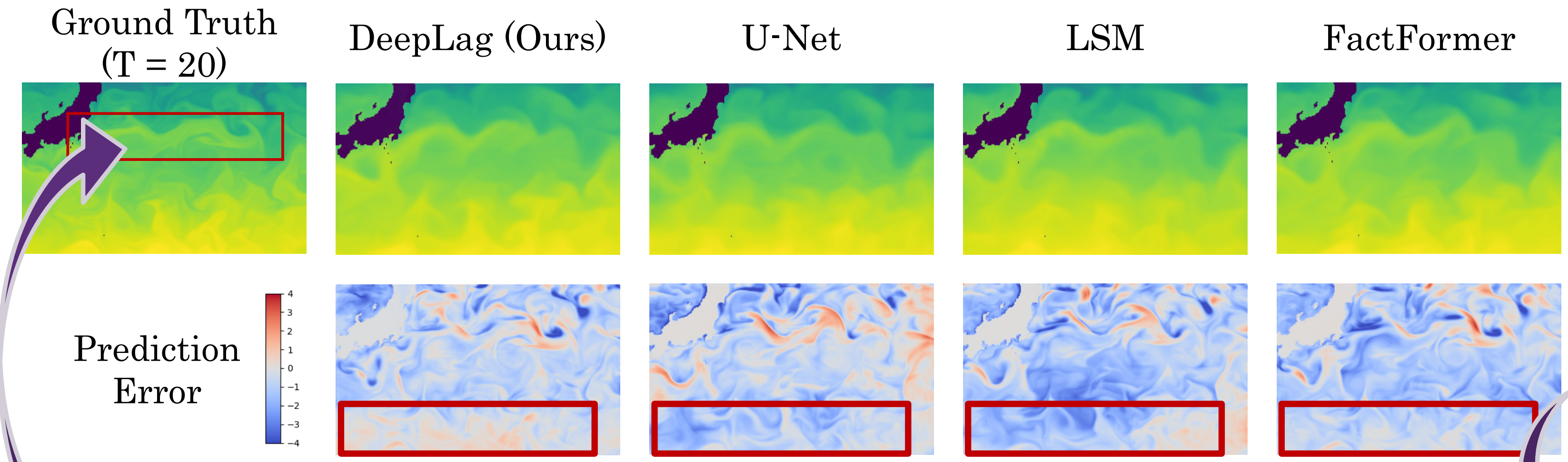
# 4.1 BOUNDED NAIVER-STOKES

- Learned particle movement



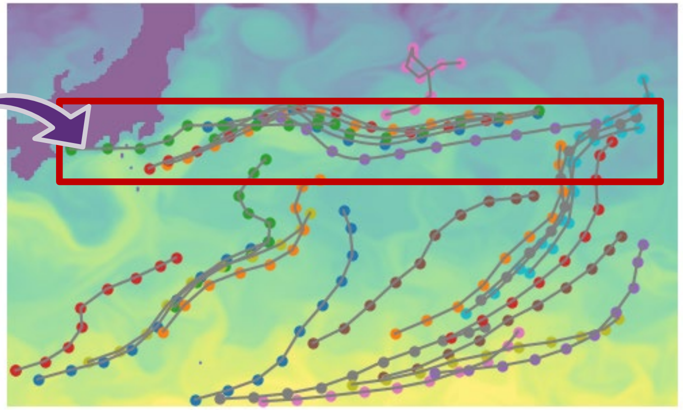
# 4.2 OCEAN CURRENT

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




| 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)



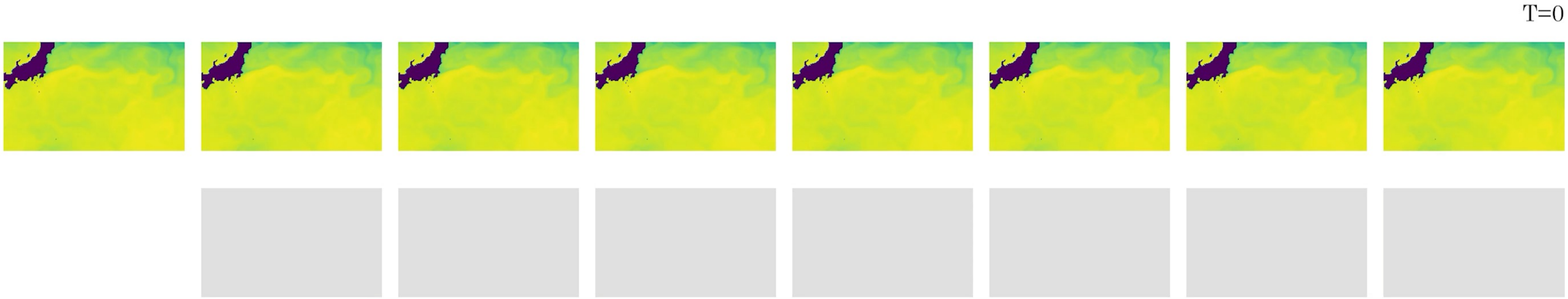
Provides a clear depiction of the Kuroshio pattern[1]

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

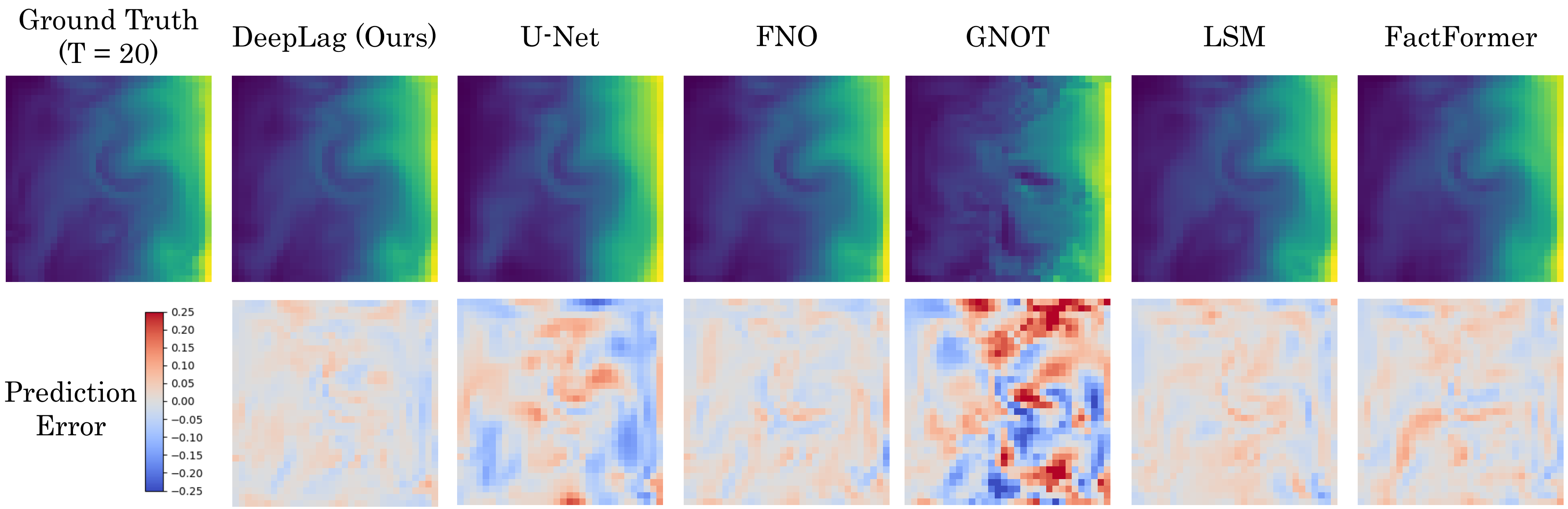
- Video of Long-term prediction (100 frames)

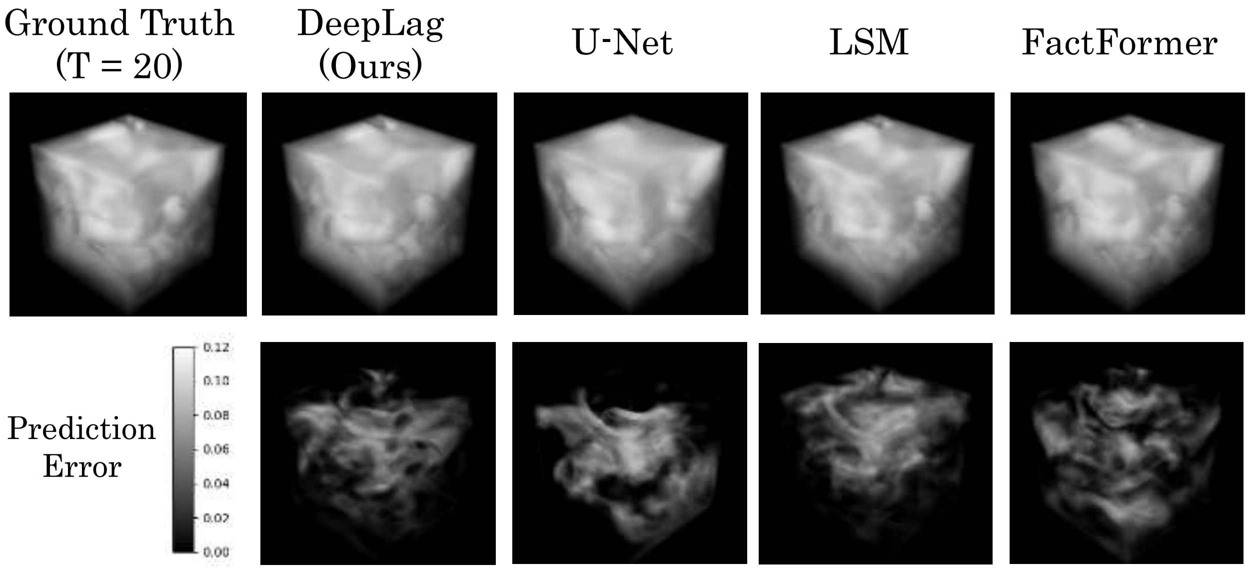



Ground Truth | **DeepLag (Ours)** | FactFormer | FNO | Galerkin Transformer | GNOT | LSM | U-Net

## 4.3 3D SMOKE

**More gain on 3D scenario**




| Model | Relative L2 (↓) |
|---|---|
| U-Net [32] | <u>0.0508</u> |
| 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

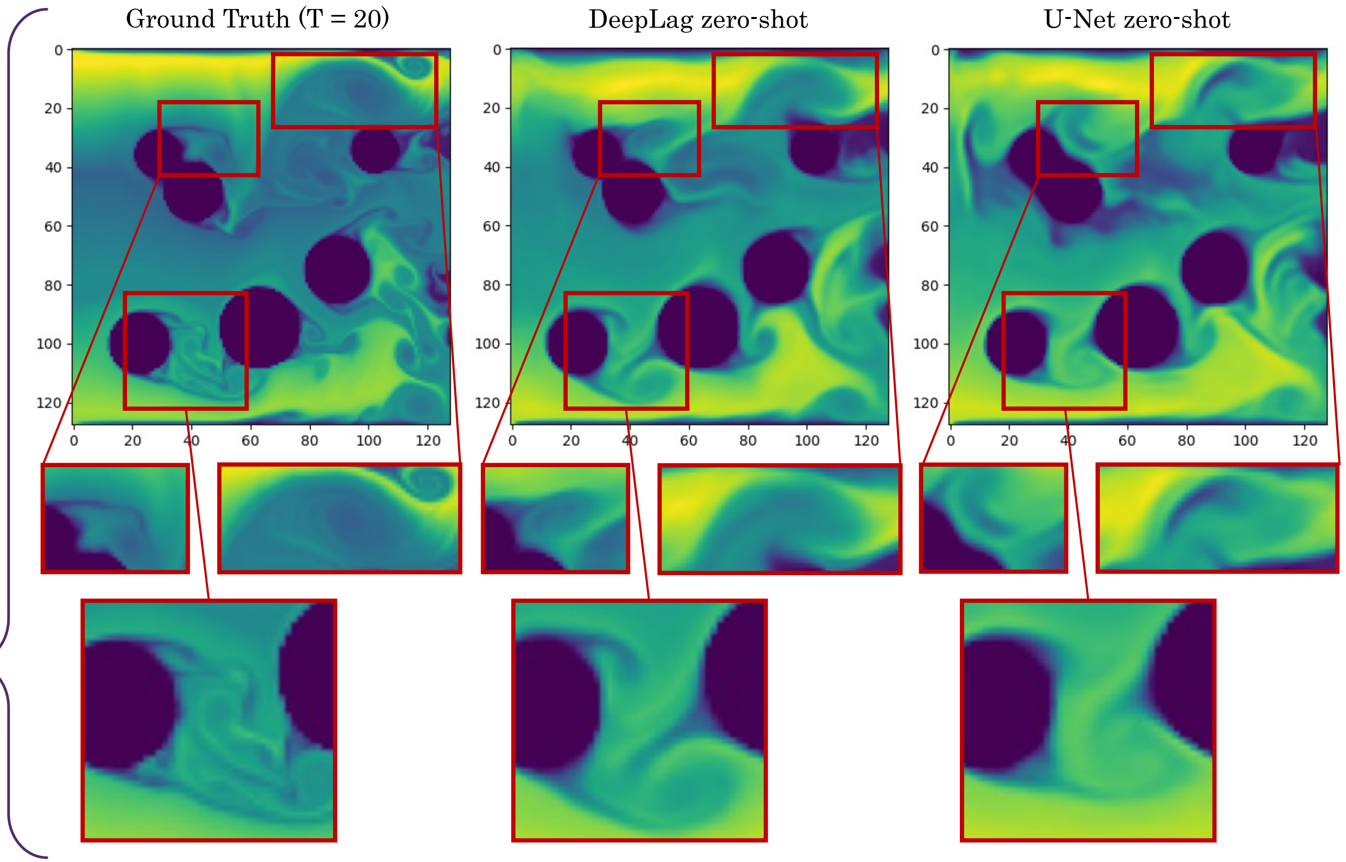
- On high-resolution data

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

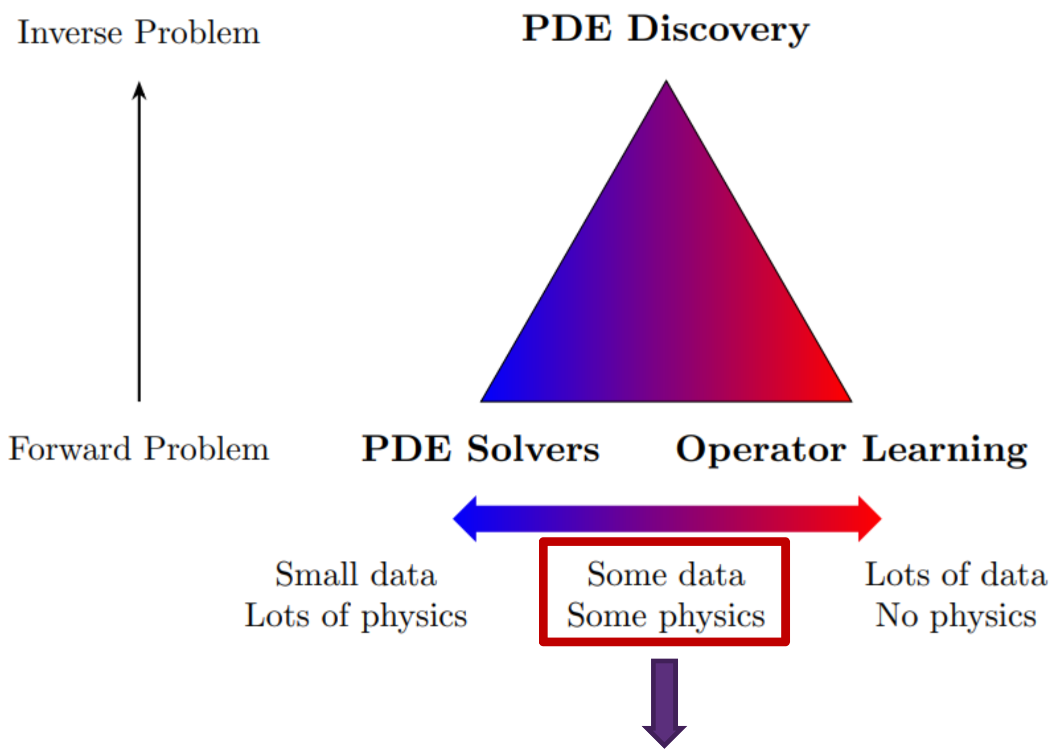
256×256, U-Net relative L2: 0.0600

- On unseen boundary conditions

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



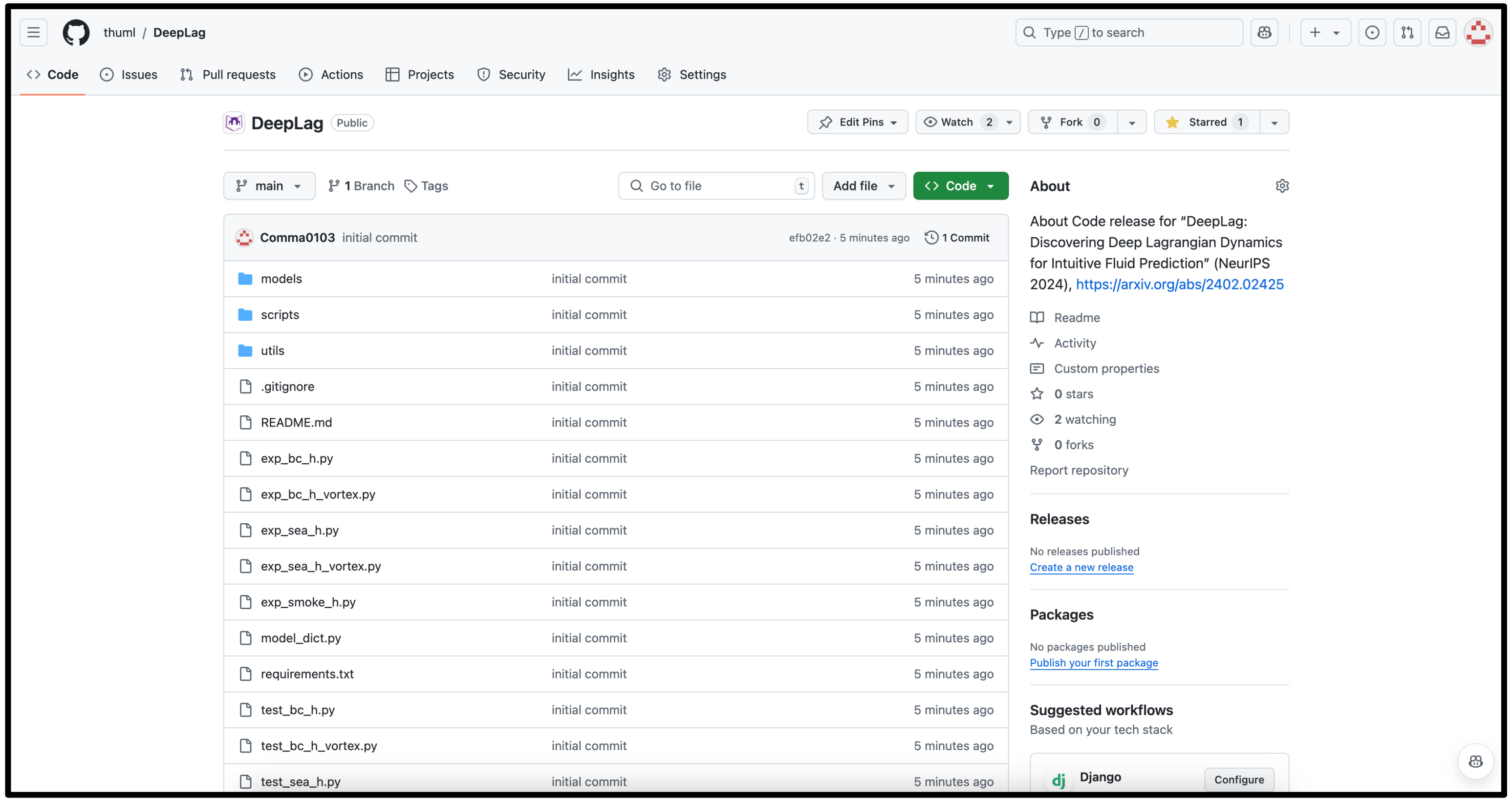
# 5 SUMMARY AND FUTURE WORK




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 & datasets & scripts

# THANKS FOR LISTENING!

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