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# Continuous PDE Dynamics Forecasting with Implicit Neural Representations

Yuan Yin,<sup>\*1</sup> Matthieu Kirchmeyer,<sup>\*1,2</sup> Jean-Yves Franceschi,<sup>\*2</sup> Alain Rakotomamonjy,<sup>2</sup> Patrick Gallinari<sup>1,2</sup> *\*Equal Contribution* <sup>1</sup>Sorbonne Université, CNRS, ISIR <sup>2</sup>Criteo AI Lab



## MOTIVATION

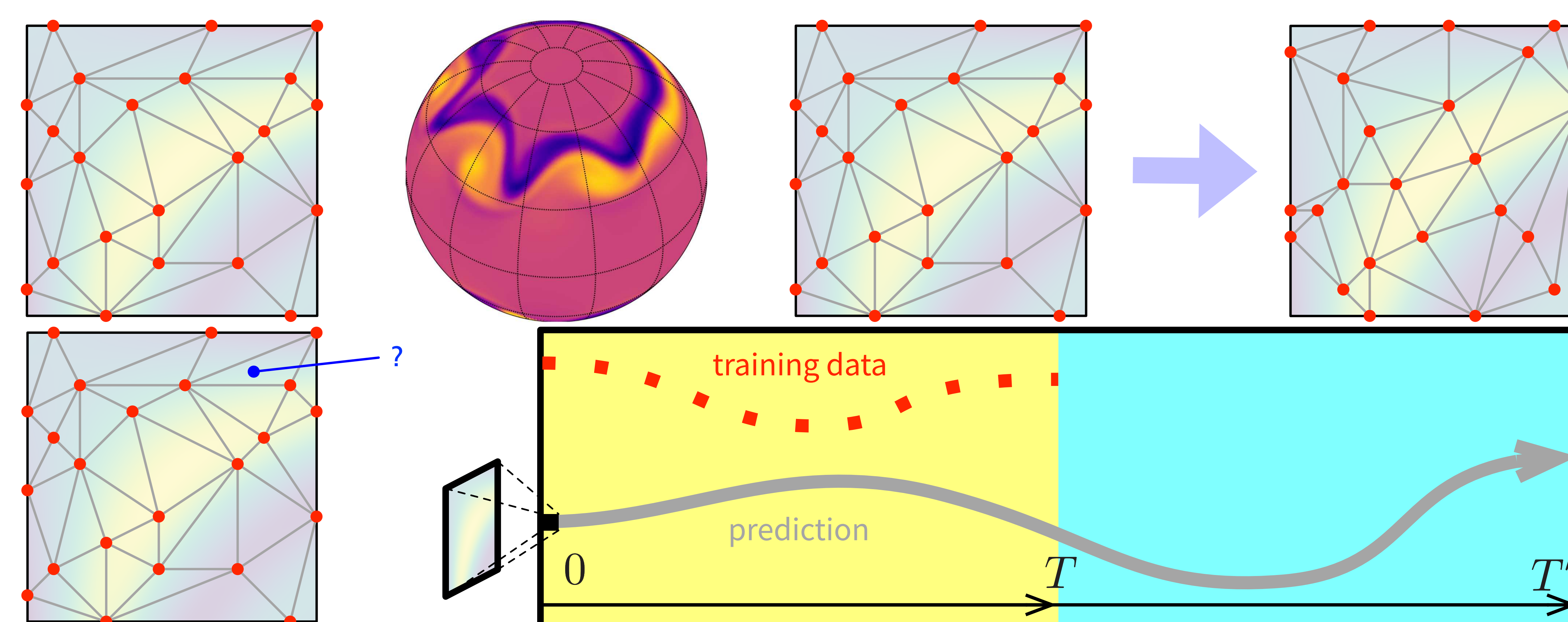
➤ Data-driven modeling of Partial Differential Equations (PDEs):

$$\frac{\partial v(x, t)}{\partial t} = F\left(x, v(x, t), \frac{\partial v(x, t)}{\partial x}, \frac{\partial^2 v(x, t)}{\partial x^2}, \dots\right)$$

➤ Variety of neural PDE forecasters... but with limitations.

➤ Spatial and temporal flexibility requirements.

- [1] Chen et al. Neural ordinary differential equations. *NeurIPS 2018*.
- [2] Brandstetter et al. Message passing neural PDE solvers. *ICLR 2022*.
- [3] Li et al. Markov neural operators for learning chaotic systems. *arXiv, 2021*.
- [4] Lu et al. Learning nonlinear operators via DeepONet based on the universal approximation theorem of operators. *Nature Machine Intelligence, 2021*.
- [5] Sitzmann et al. INRs with periodic activation functions. *NeurIPS 2020*.
- [6] Fathony et al. Multiplicative filter networks. *ICLR 2021*.



Model	Ref.	Space			Time		PDE agnostic, new initial conditions
		Train / test grid independence	Free-form grid and topology	Evaluation at un-observed locations	Time continuous	Time extrapolation	
Dis-crete	{ NODE [1] MP-PDE [2]	{ X X	{ X ✓	{ X X	{ ✓ X	{ ✓ ✓	{ ✓ ✓
NO	{ MNO [3] DeepONet [4]	{ ✓ X	{ X ✓	{ X ✓	{ X ✓	{ ✓ X	{ ✓ ✓
INR	{ SIREN, MFN [5, 6] Ours	{ ✓ ✓	{ ✓ ✓	{ ✓ ✓	{ ✓ ✓	{ X ✓	{ X ✓

➤ DINO solves prior limitations by combining INRs and ODEs.

## DINO: SPACE-TIME-CONTINUOUS FORECASTING

### INFERENCE

➤ INR-based decoder with hypernet:

$$(DEC) \forall t, \tilde{v}_t = I_{h_\phi}(\alpha_t)$$

➤ Encoding via auto-decoding, without explicit encoder NN:

$$(ENC) \alpha_0 = \text{auto-dec}(v_0)$$

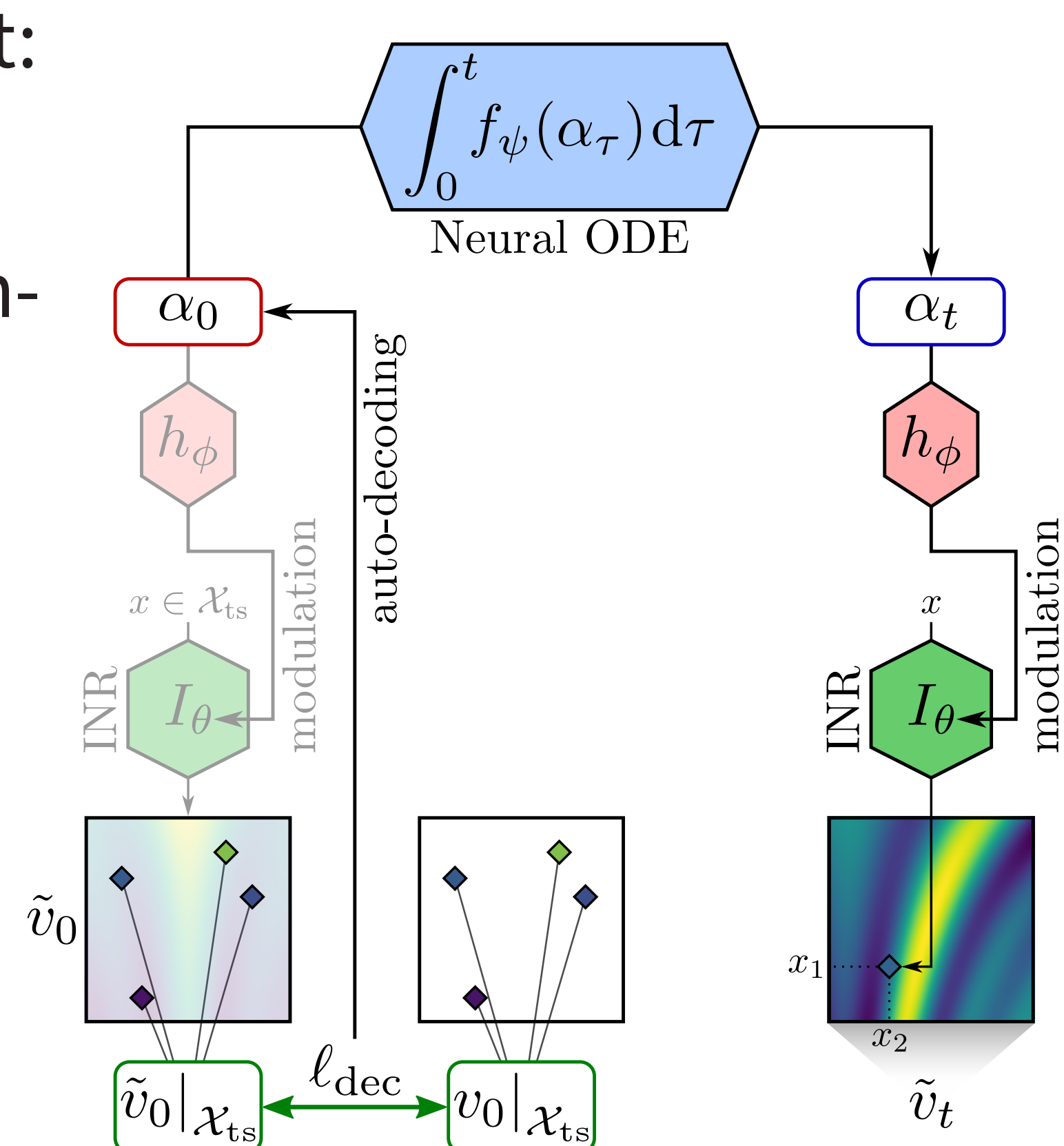
Inverse problem solved by gradient descent:

$$\alpha_0^k = \alpha_0^{k-1} - \eta \nabla_{\alpha_t} \ell_{\text{dec}}(\phi, \alpha_t^{k-1}; v_t),$$

$$\alpha_0 = \alpha_0^K$$

➤ Neural ODE as dynamics model:

$$(DYN) \frac{d\alpha_t}{dt} = f_\psi(\alpha_t)$$



### TWO-STAGE TRAINING PROCESS

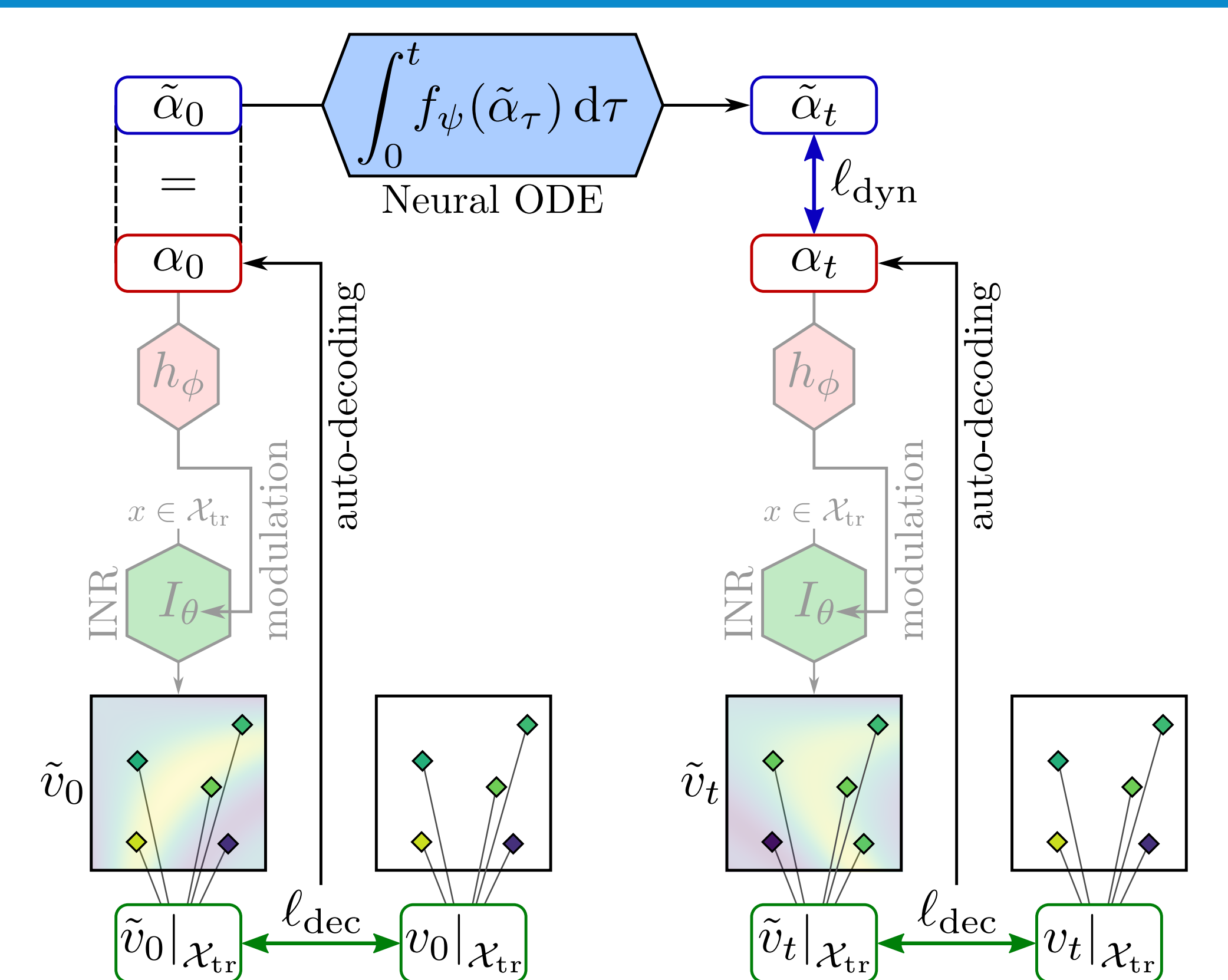
Separate training of model components:

1. Train (ENC)-(DEC):

- hypernetwork  $h_\phi$ ;
- latent state  $\{\alpha_t\}_t$ .

2. Train (DYN) on the learned  $\{\alpha_t\}_t$ :

- dynamics  $f_\psi$ .



➤ Stable training of model components.

## FOURIERNET AND AMPLITUDE MODULATION

➤ We modulated a Multiplicative Filter Network (Fathony et al., 2021) with a linear hypernet from the latent state  $\alpha_t$ .

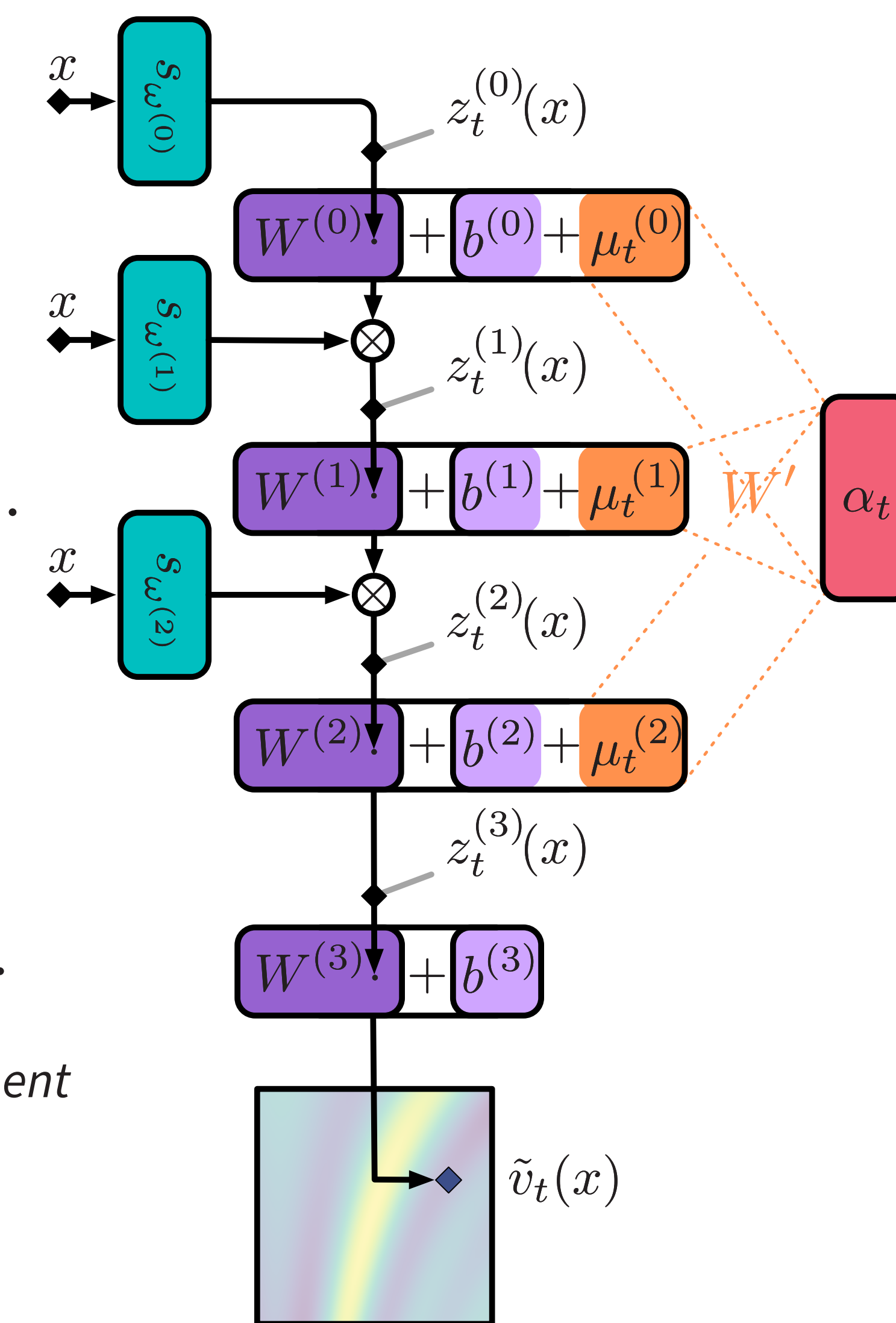
➤ We use a FourierNet:

$$s_{\omega(t)}(x) = [\cos(\omega(t)x), \sin(\omega(t)x)].$$

**Proposition 1** (Separation of time and space variables).

$$\tilde{v}_t(x) = \sum_m \underbrace{c^{(m)}(\alpha_t)}_{\text{time-dependent coefficient}} \times \underbrace{s_{\gamma^{(m)}}(x)}_{\text{spatial basis element}}$$

→ Inductive bias for better time extrapolation.



## MORE INFORMATION



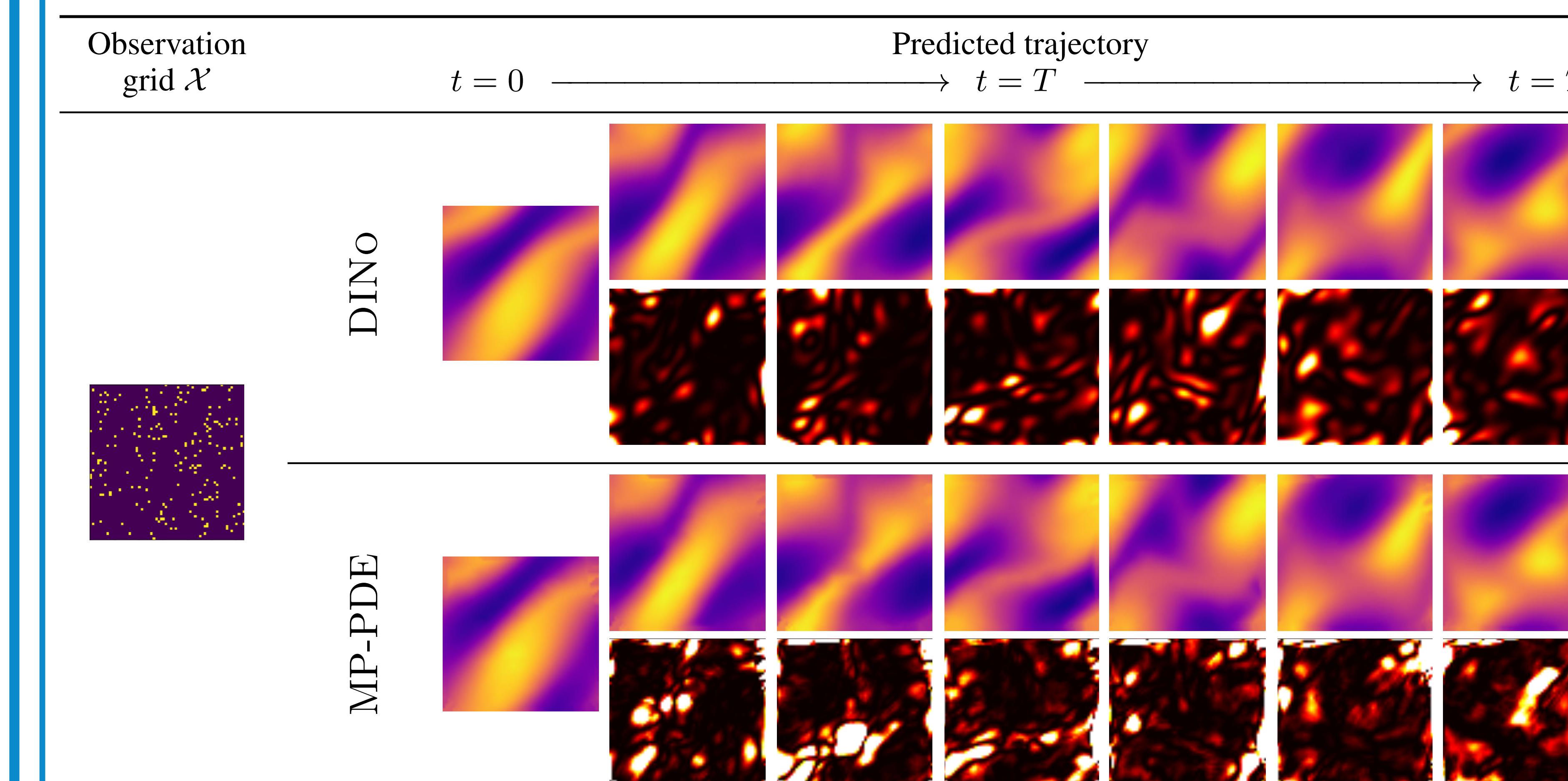
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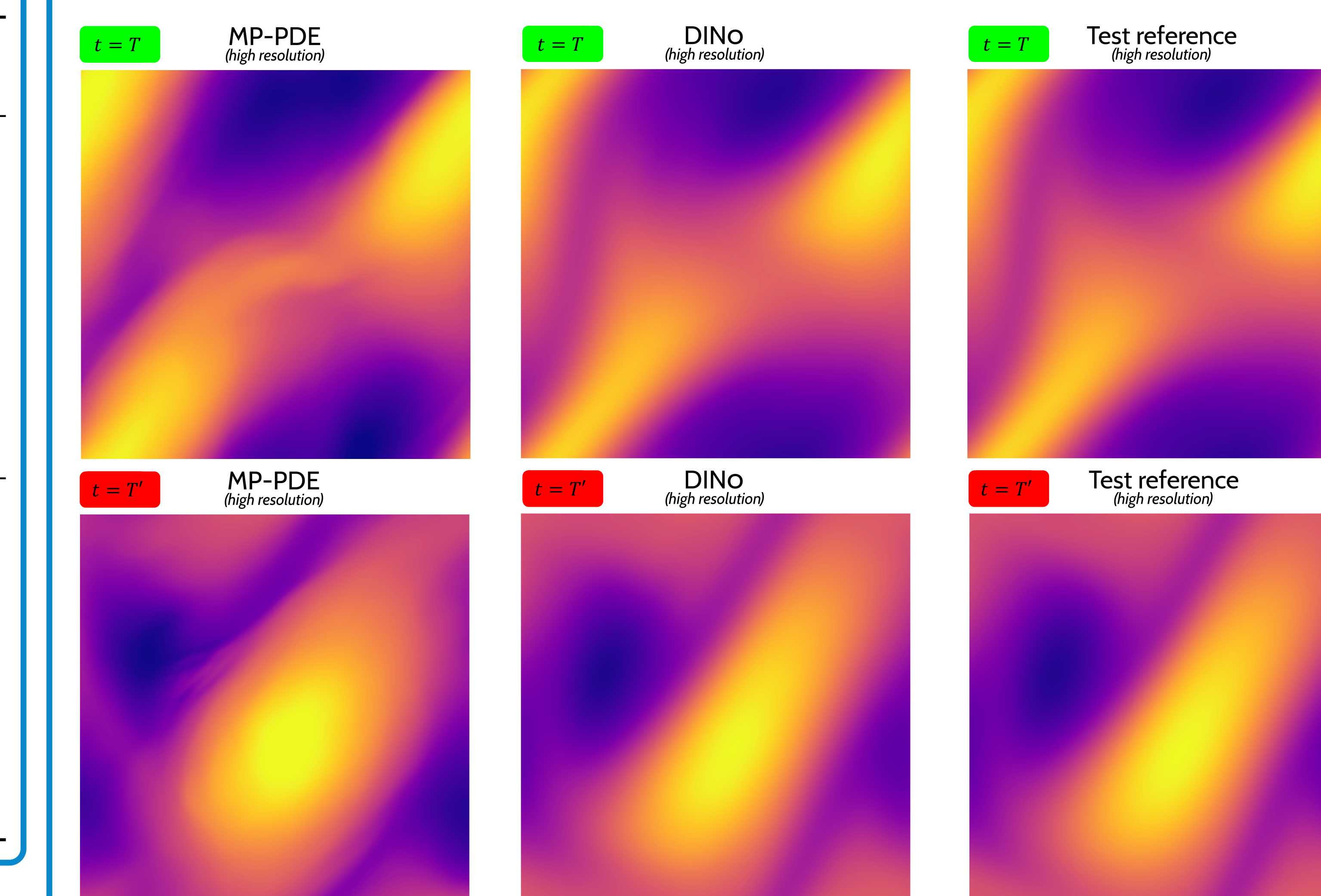
## DIVERSE EVALUATION SCENARIOS

➤ Comparison to recent neural PDE forecasters [1, 2, 3, 4, 5, 6] on planar (*Wave*, *Navier-Stokes*) and spherical (*Shallow-Water*) PDEs.

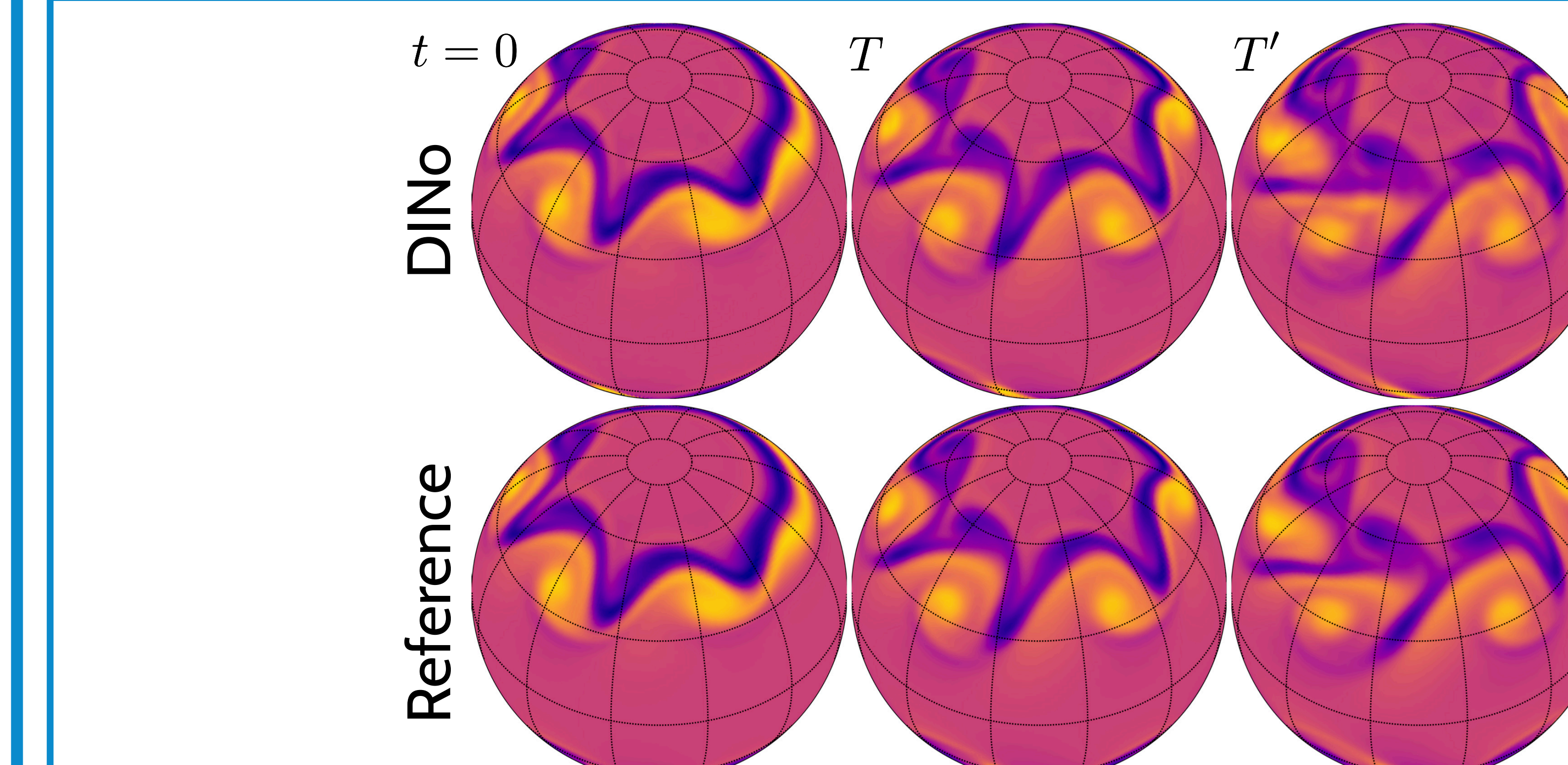
### COMPARISON TO STANDARD INTERPOLATION



### GENERALIZATION TO HIGHER RESOLUTION



### MODELING PDES ON MANIFOLDS



### FINER TIME RESOLUTION

Model	In-t	Out-t
I-DINO (linear)	$3.459 \times 10^{-4}$	$5.598 \times 10^{-4}$
I-DINO (quadratic)	$2.165 \times 10^{-4}$	$4.473 \times 10^{-4}$
DINO (ODE solve)	<b><math>2.151 \times 10^{-4}</math></b>	<b><math>4.388 \times 10^{-4}</math></b>

