

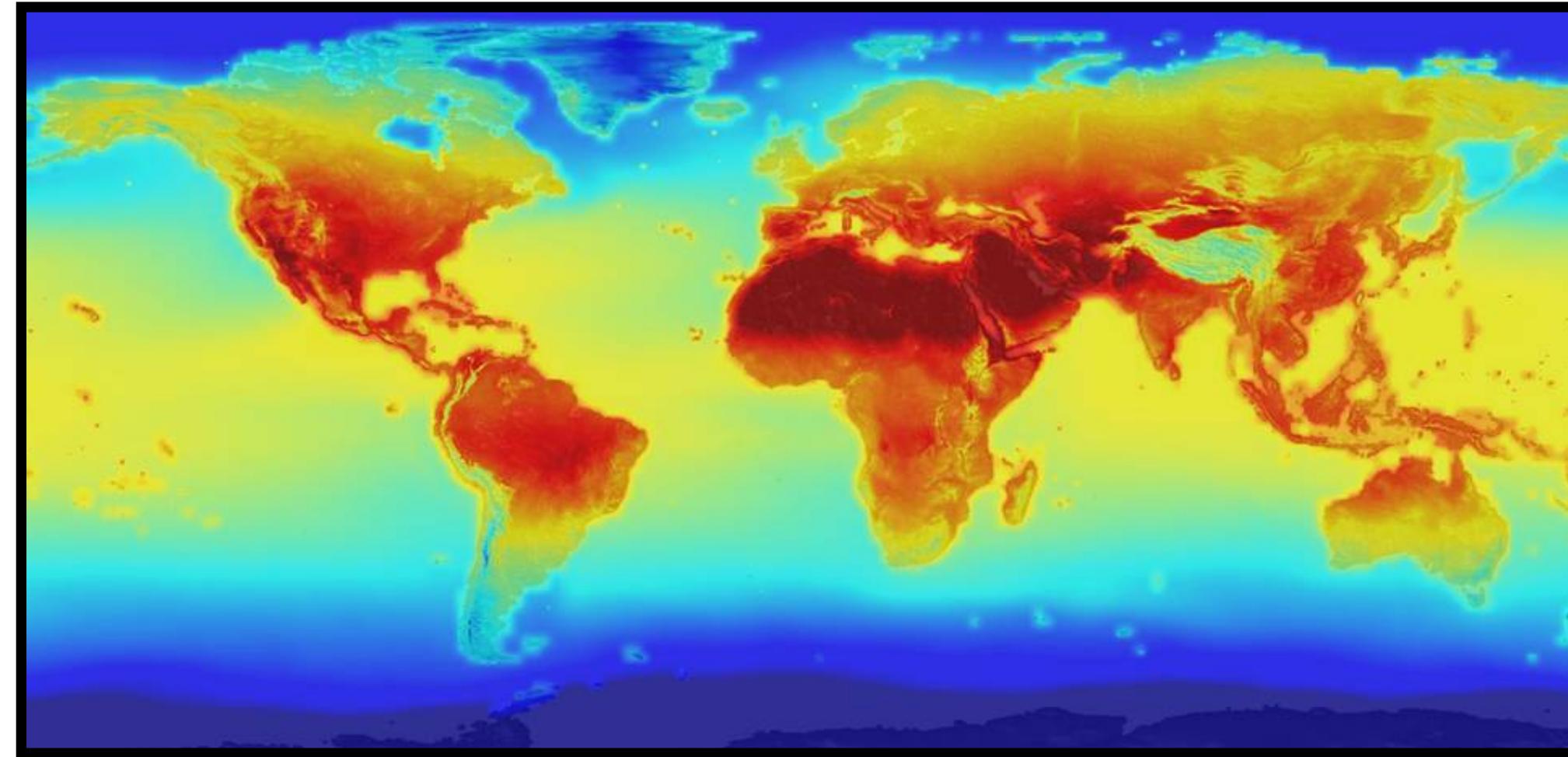
# **Learning and Forecasting the Effective Dynamics of Complex Systems across Scales**

Pantelis R. Vlachas  
Computational Science and Engineering Lab

# Motivation

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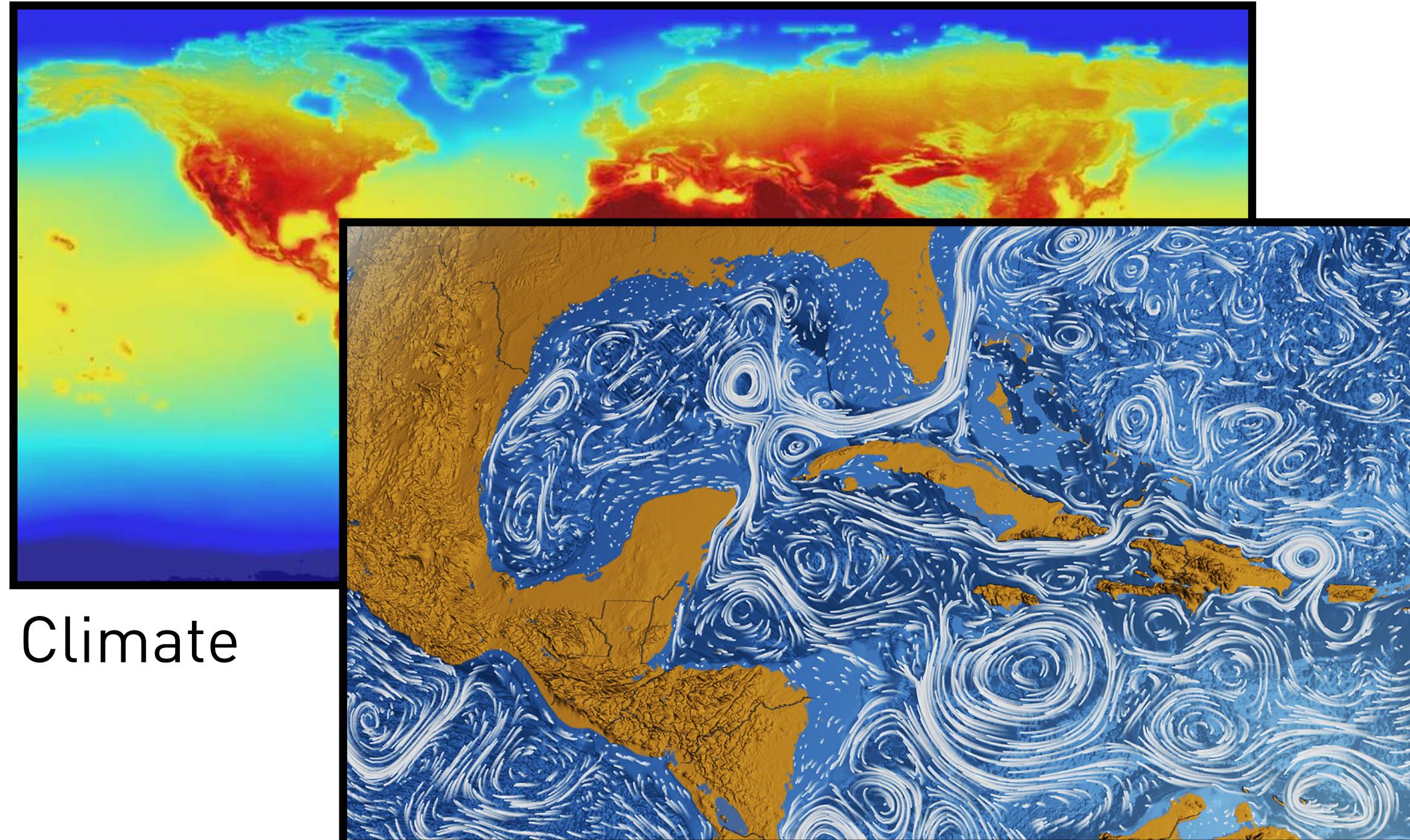
# Motivation



Climate

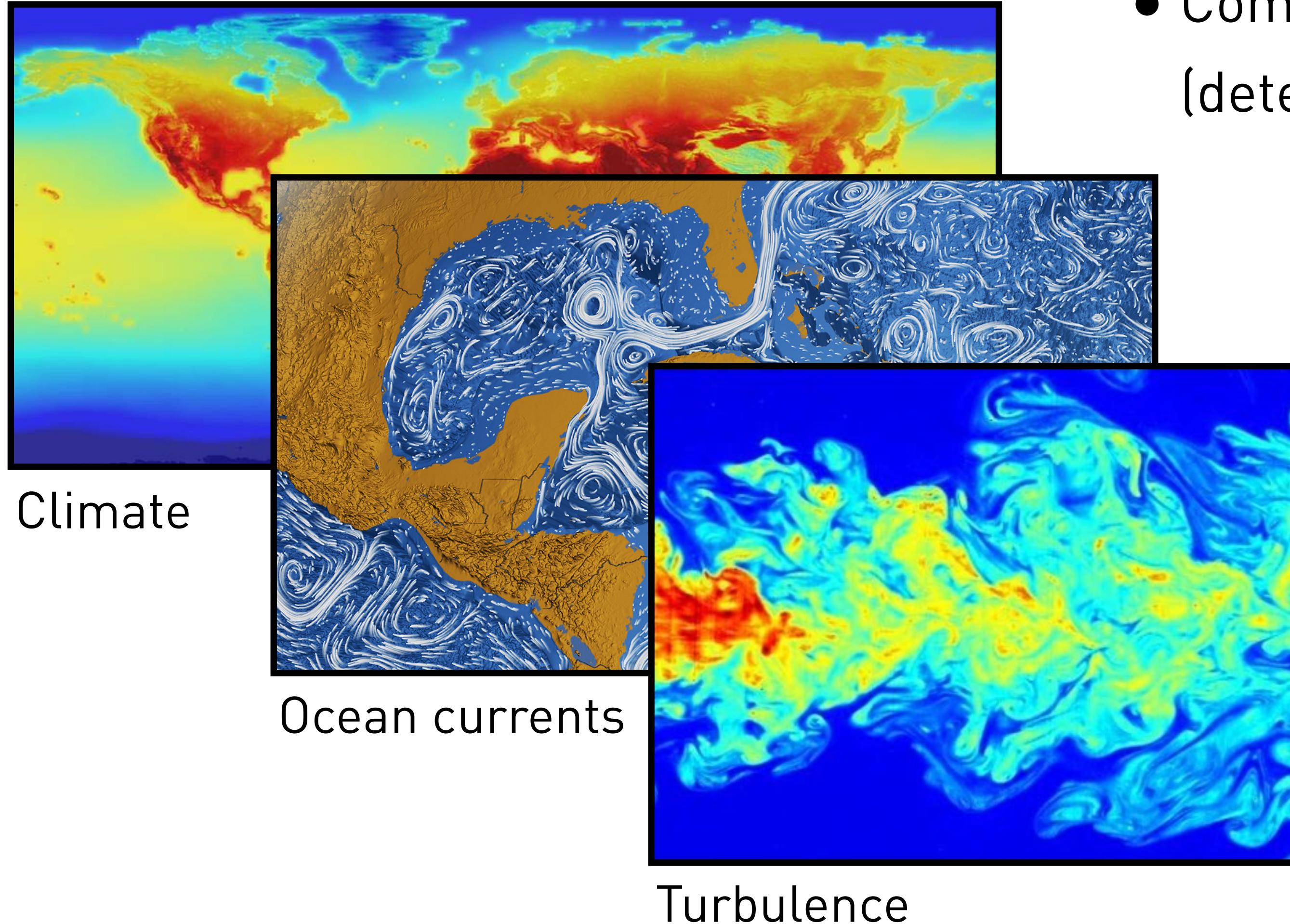
- Complex multiscale systems  
(deterministic, stochastic, chaotic)

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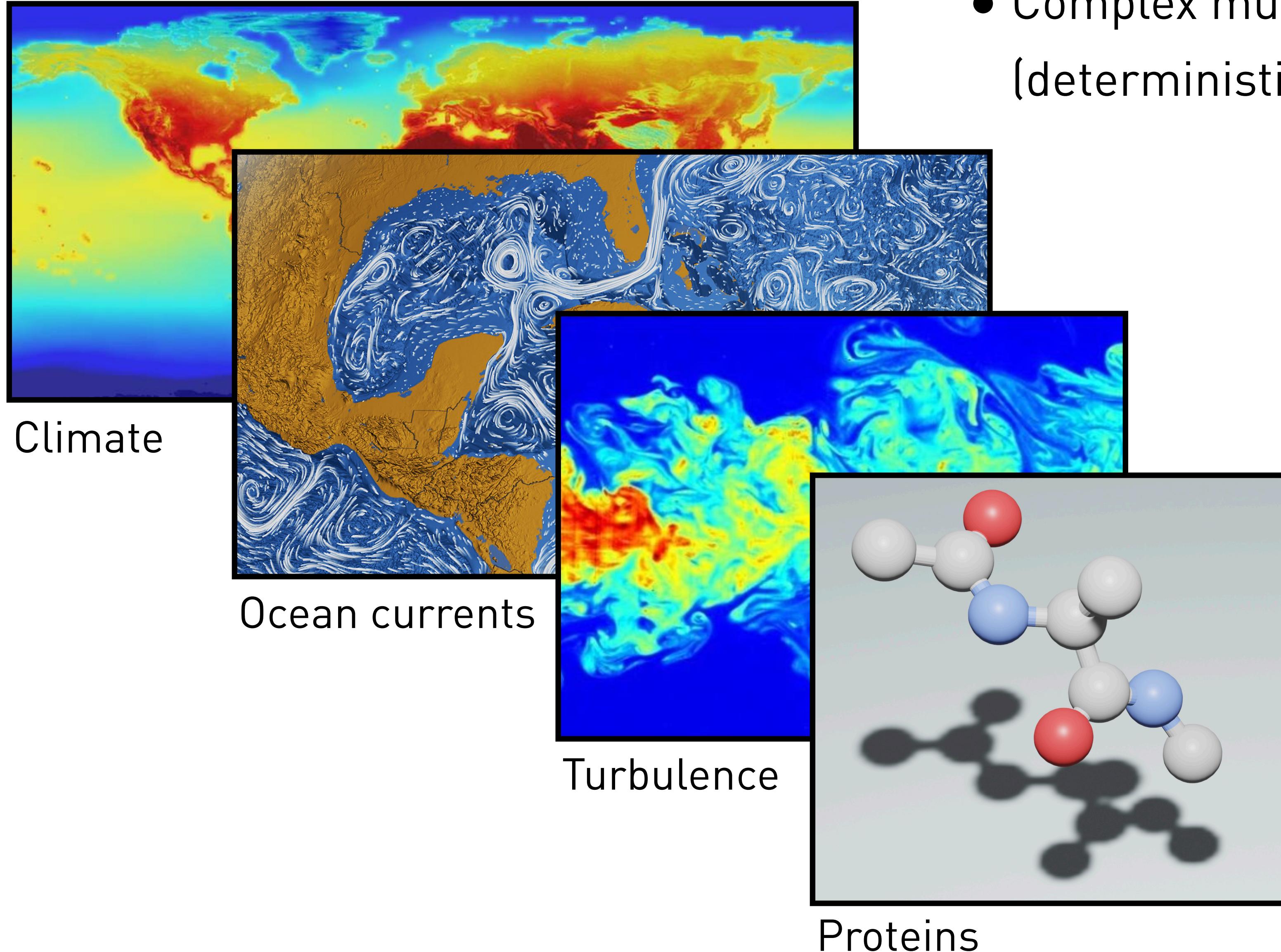
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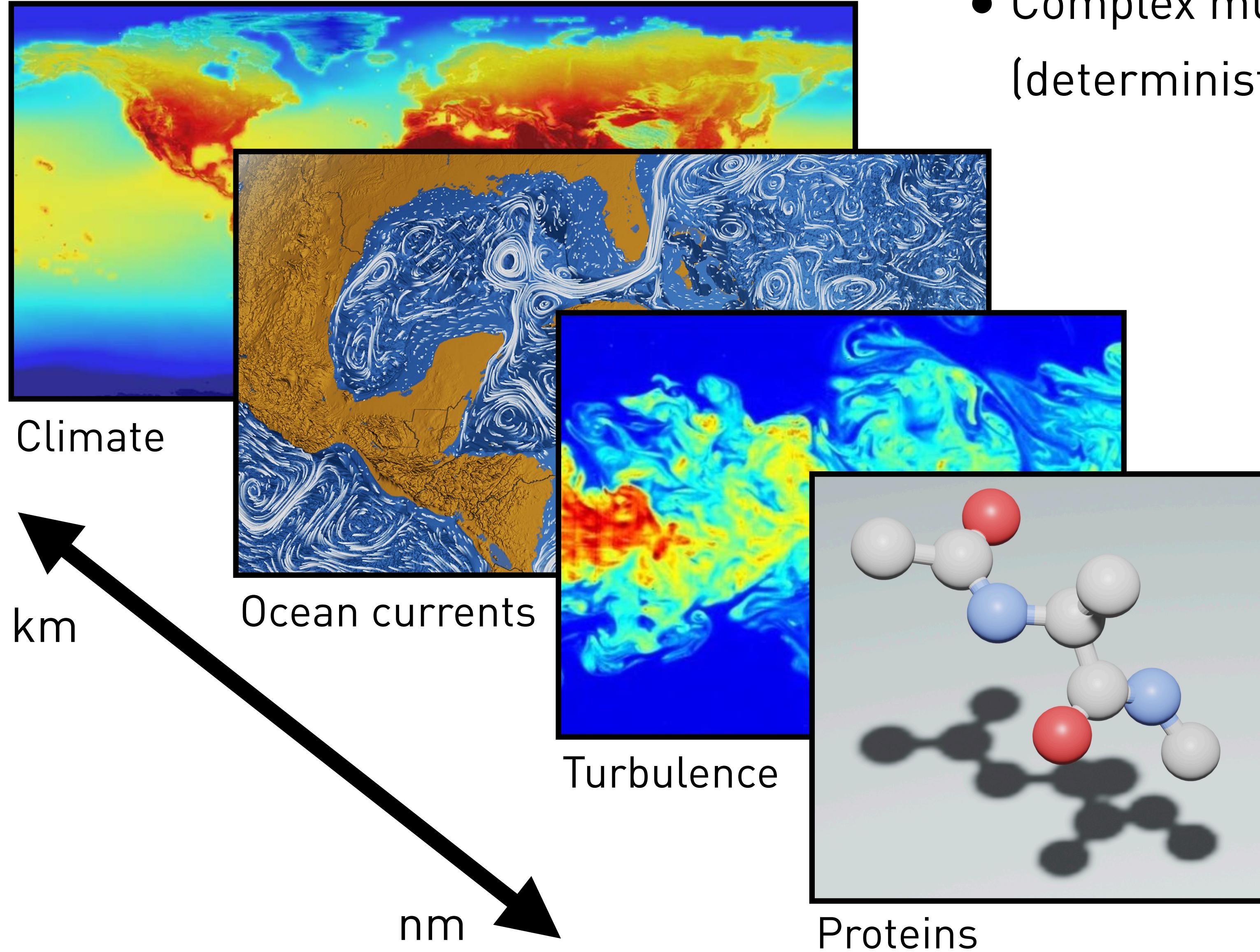
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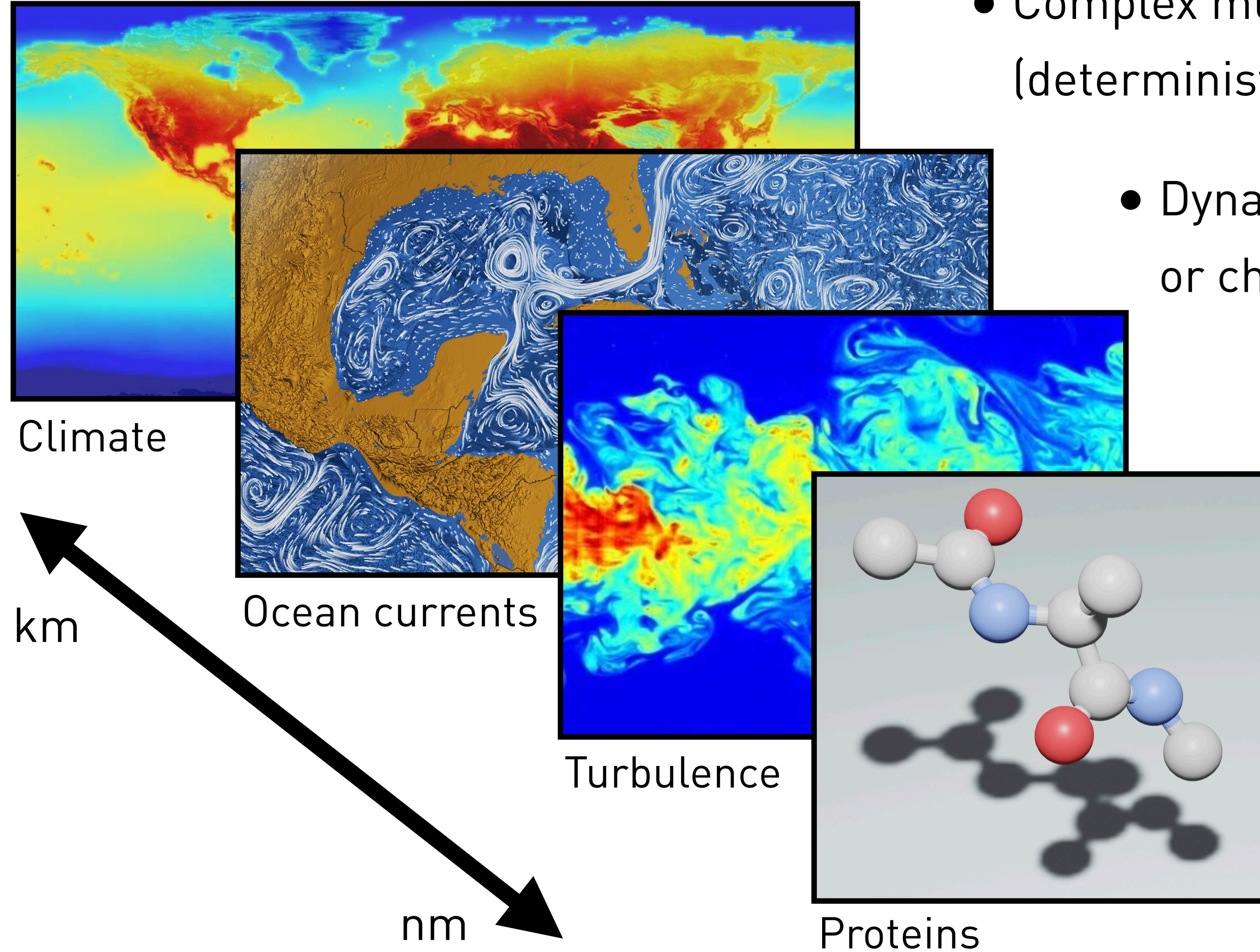
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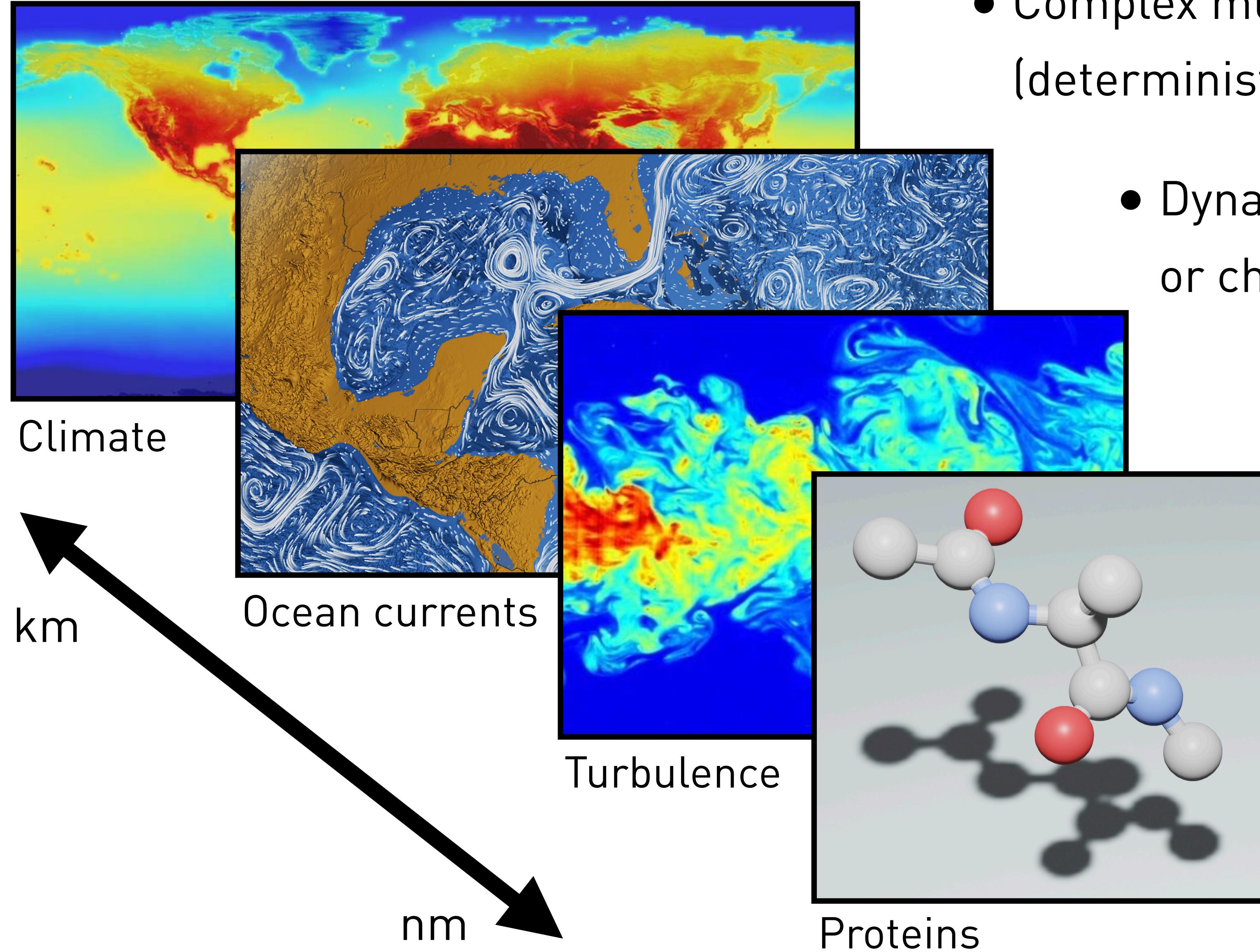
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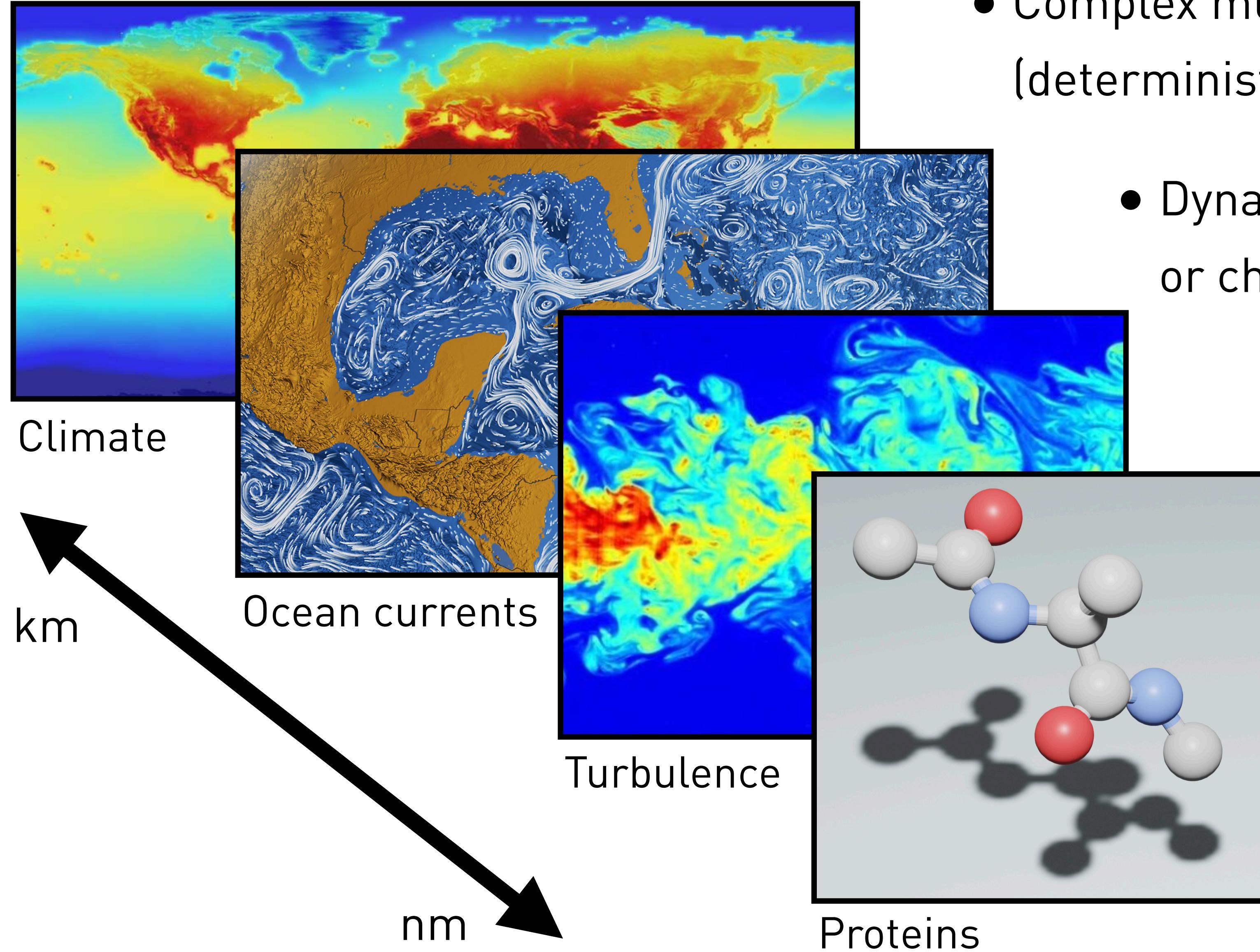
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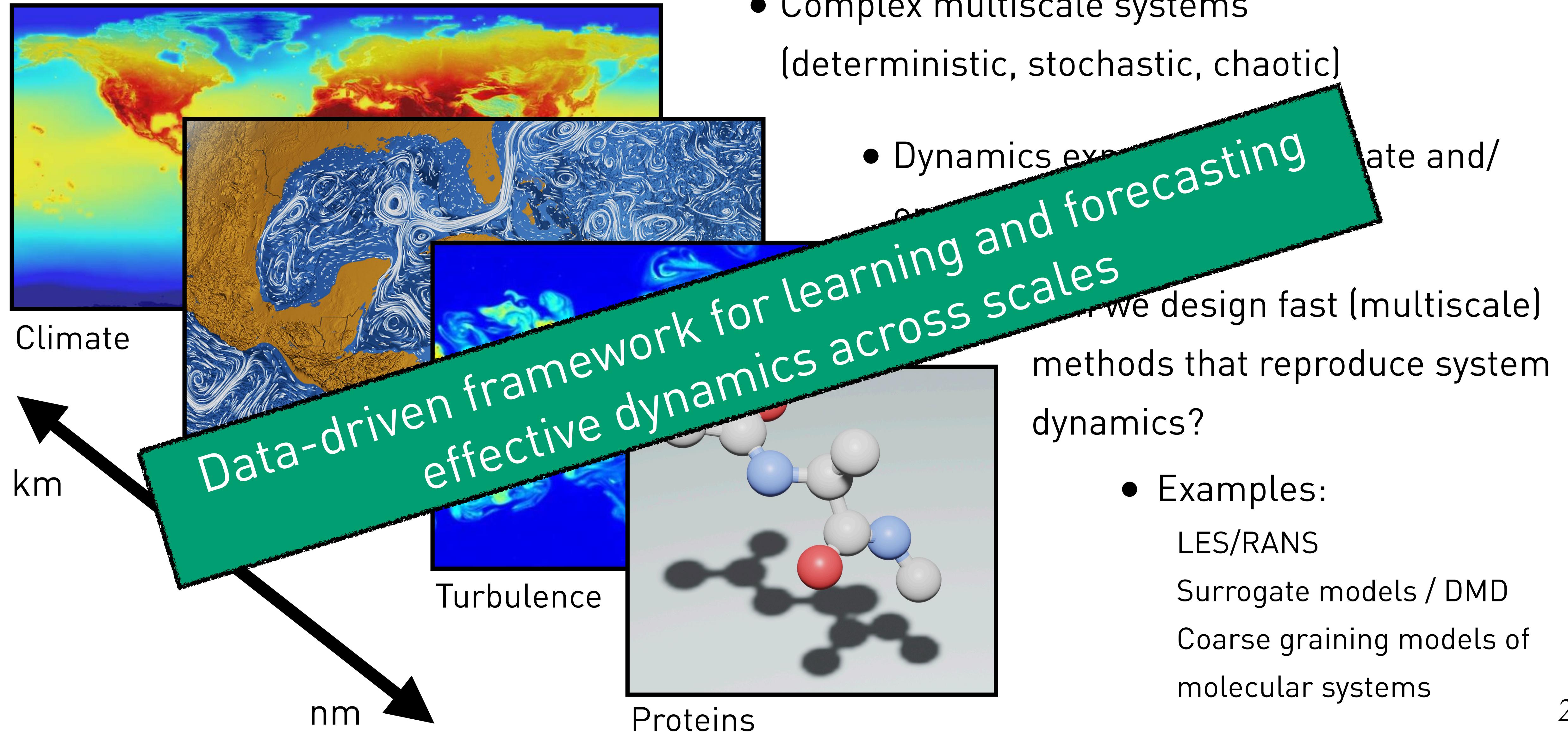
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- Can we design fast (multiscale)  
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dynamics?

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- Complex multiscale systems (deterministic, stochastic, chaotic)
- Dynamics expensive to simulate and/or challenging to forecast
- Can we design fast (multiscale) methods that reproduce system dynamics?
  - Examples:
    - LES/RANS
    - Surrogate models / DMD
    - Coarse graining models of molecular systems

# Motivation



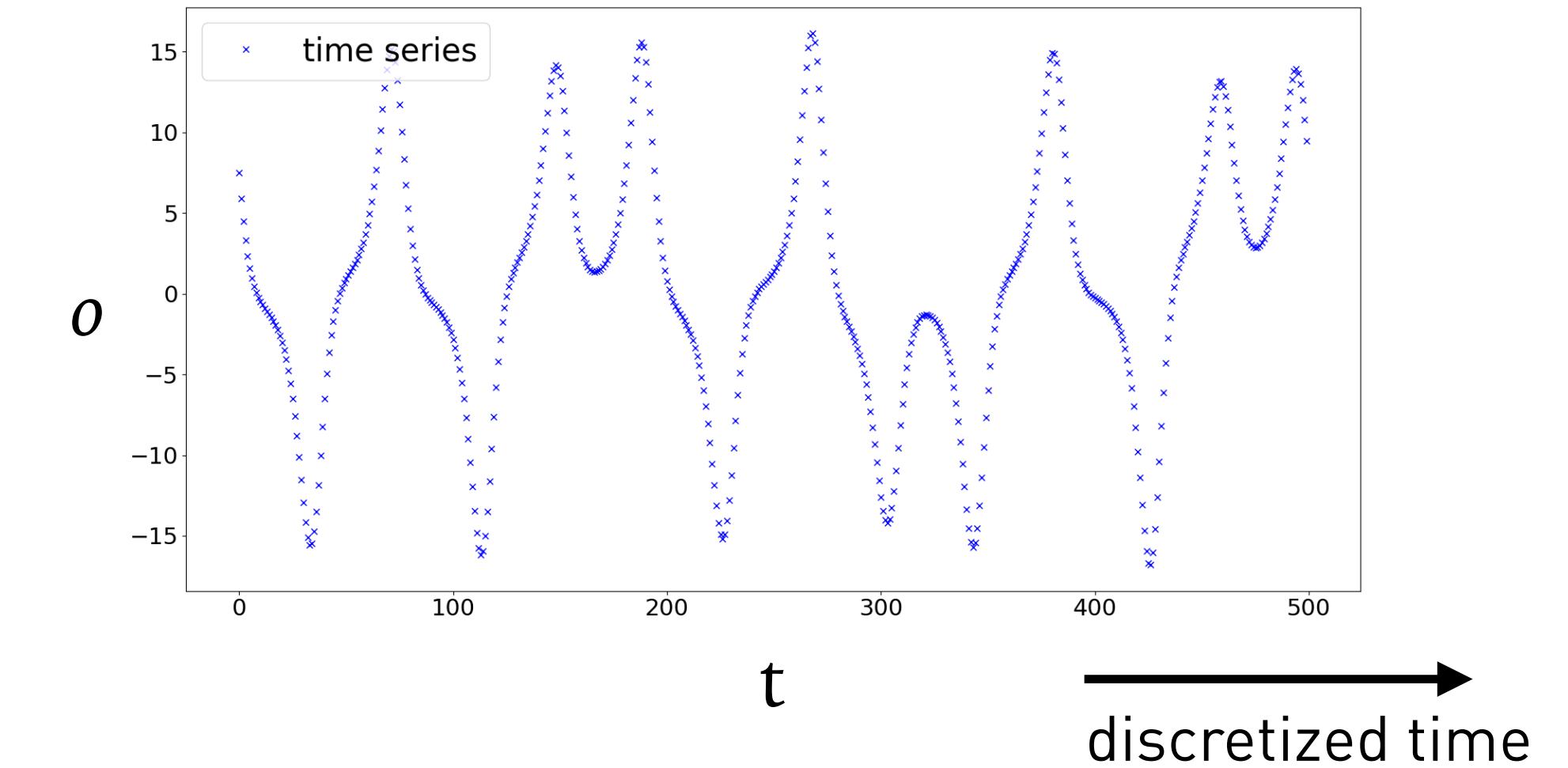
*I*

*Forecasting Complex Dynamics with  
Recurrent Neural Networks*

# Recurrent Neural Networks (RNNs)

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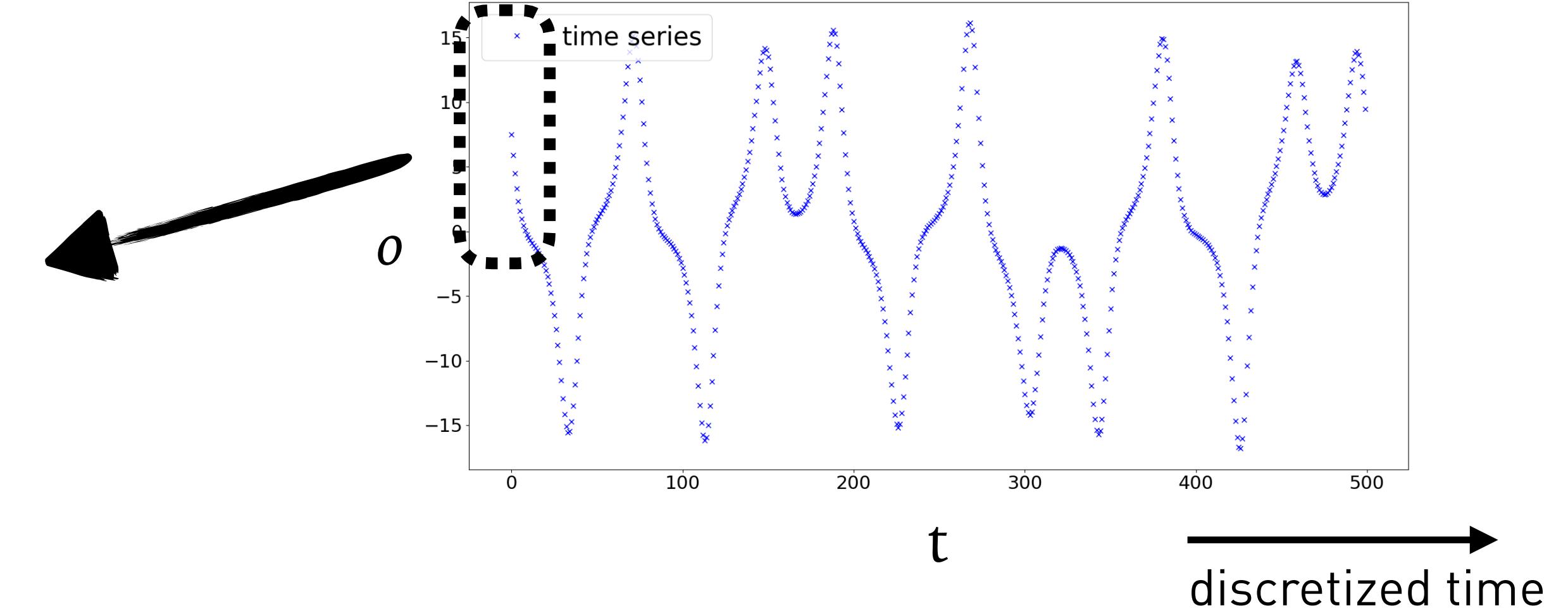
# Recurrent Neural Networks (RNNs)



Data from trajectories

- Sensory data / noisy
- Unknown underlying dynamics
- No equations based on first principles (physics)
- Does not describe full system state

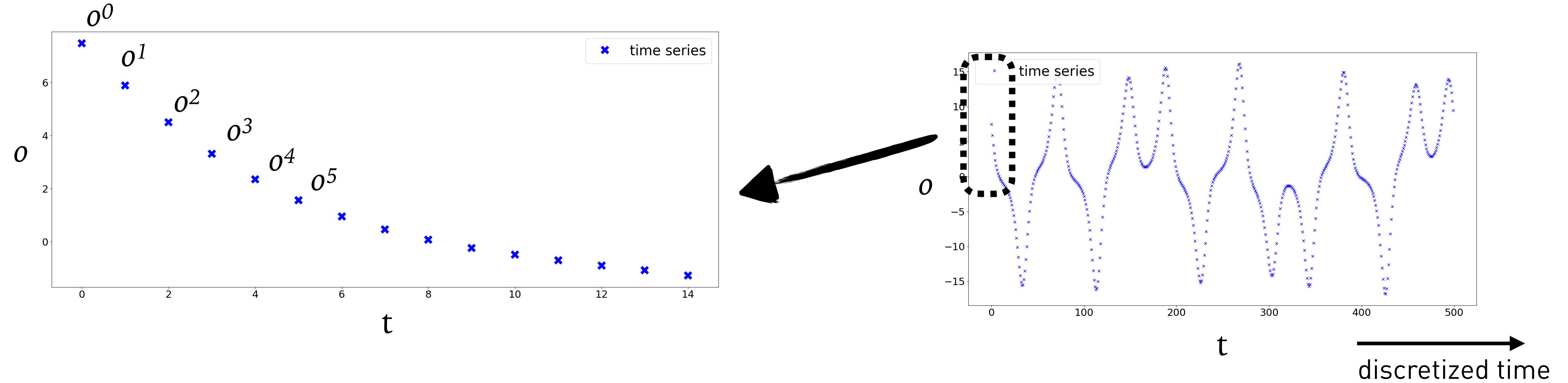
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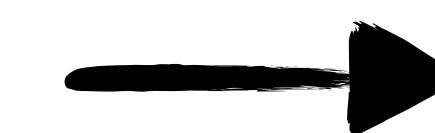
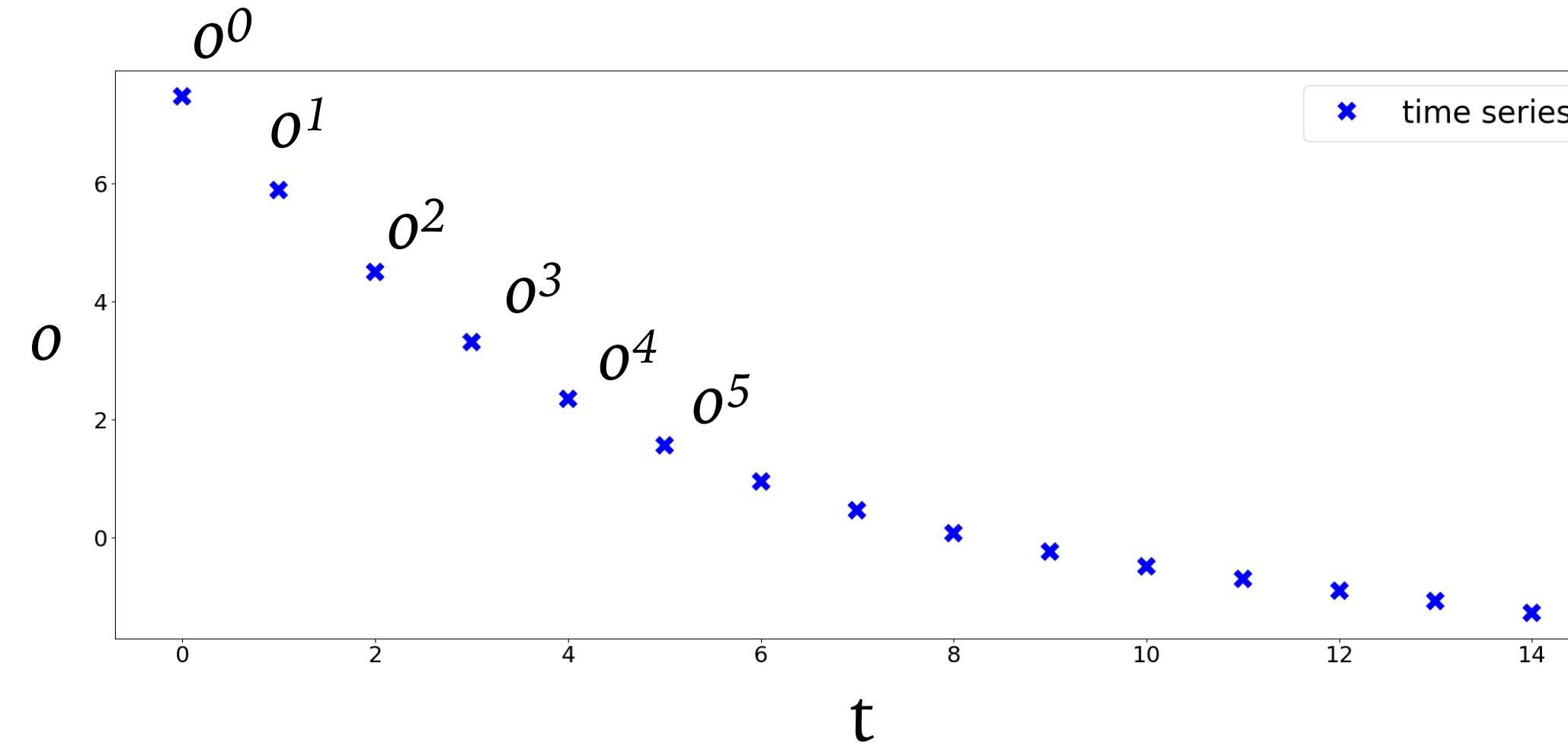
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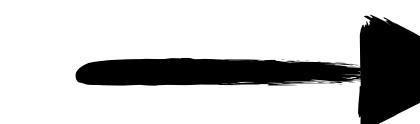
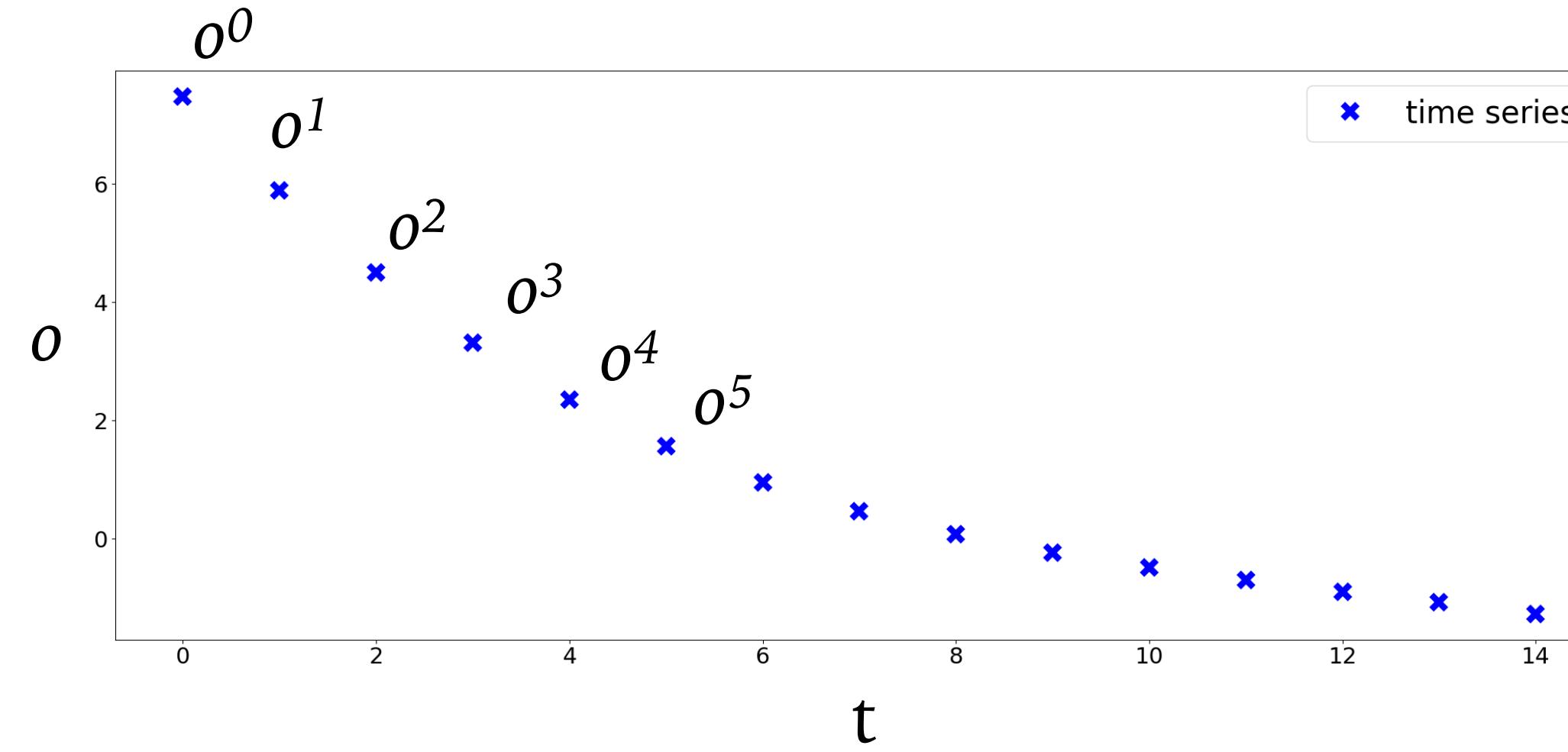
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with  $\dot{o}^t = f(o^t, o^{t-1}, o^{t-2}, \dots)$

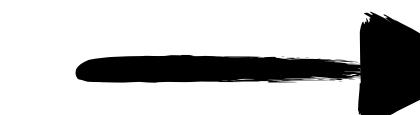
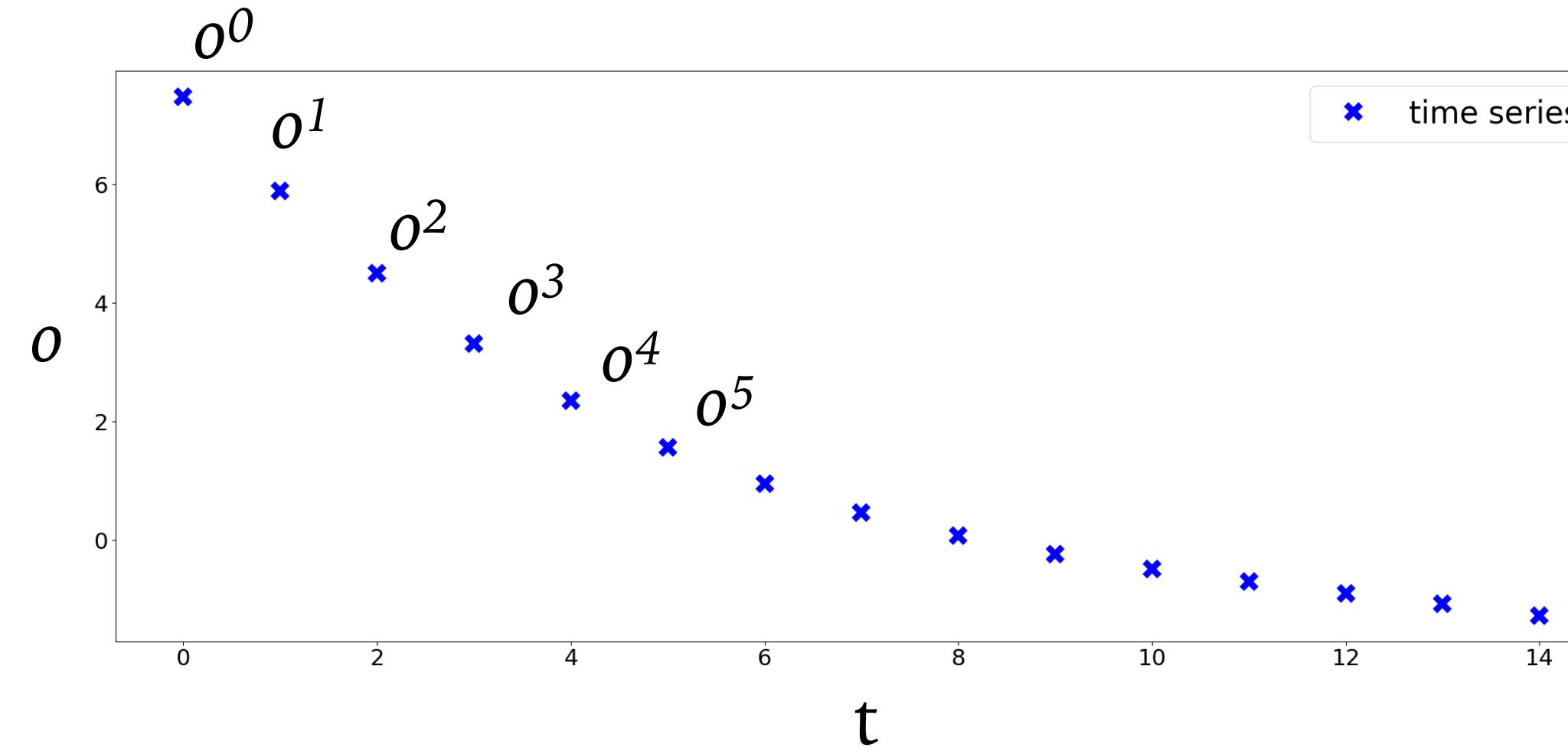
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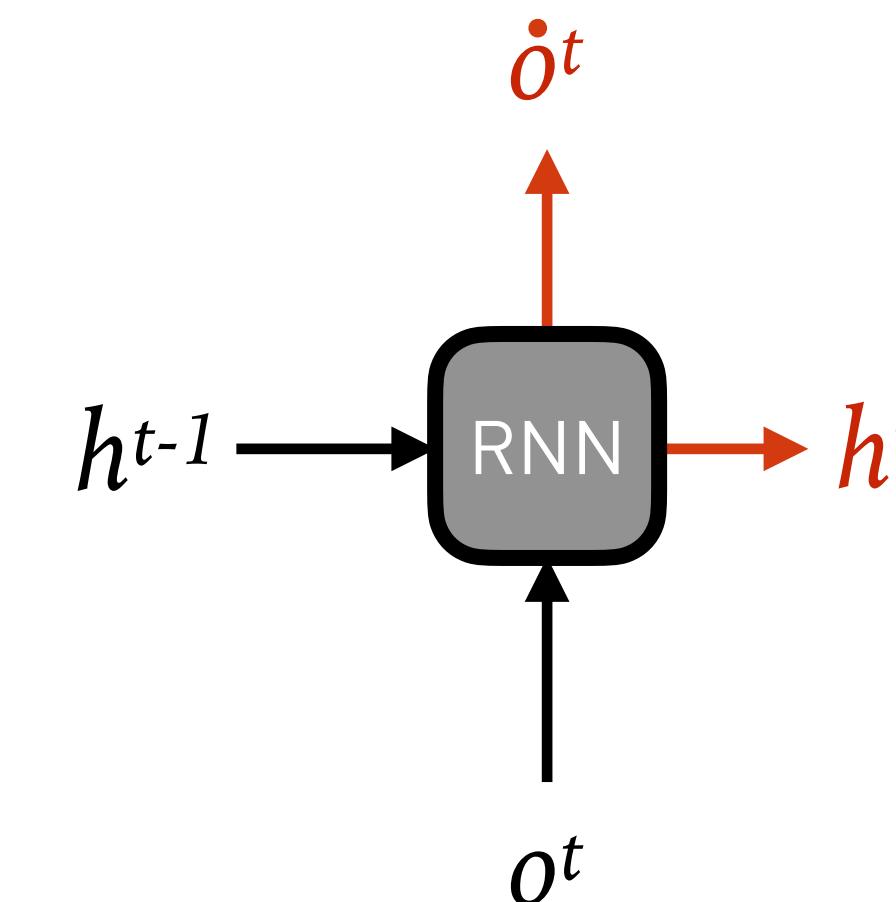
history  
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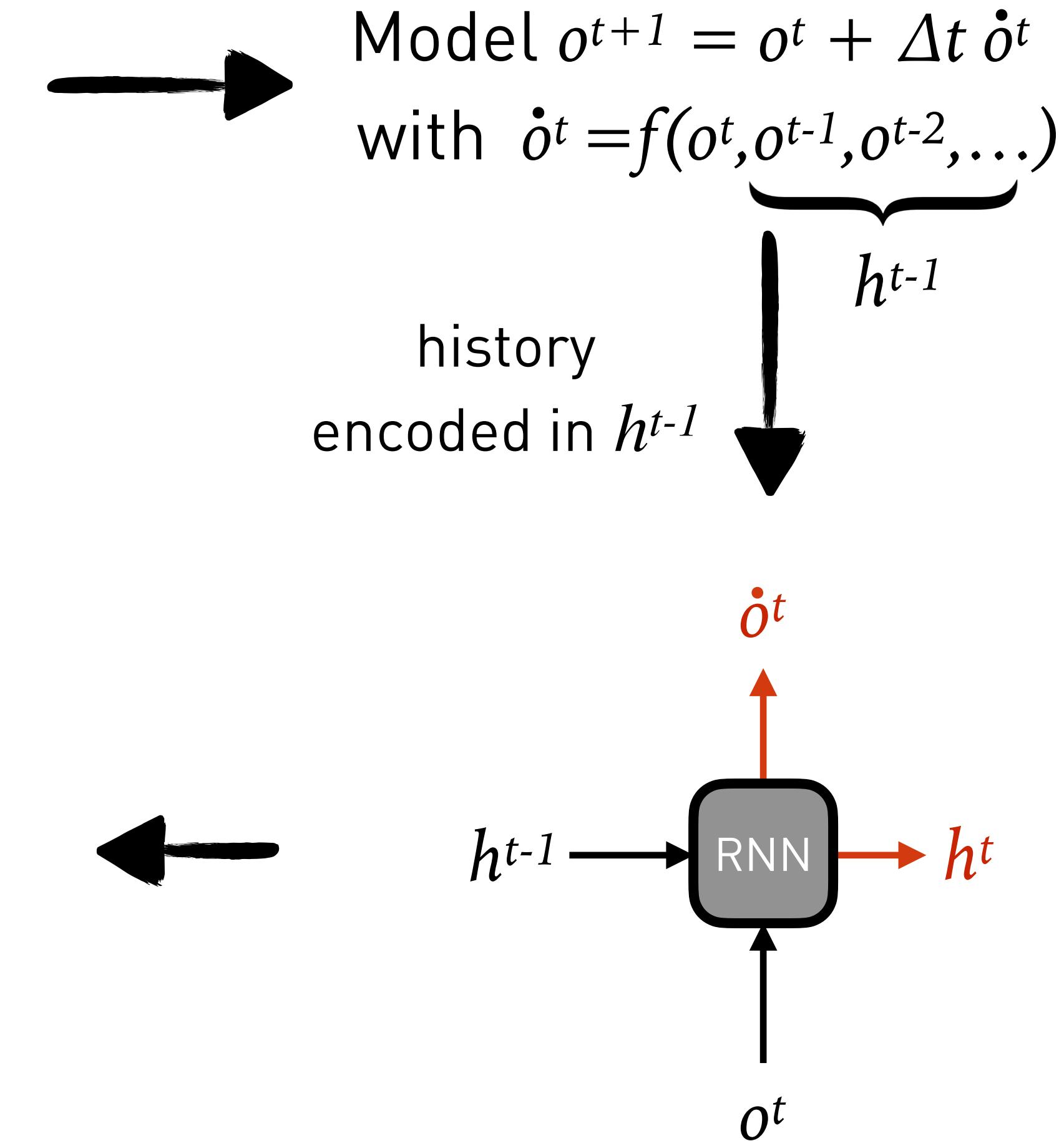
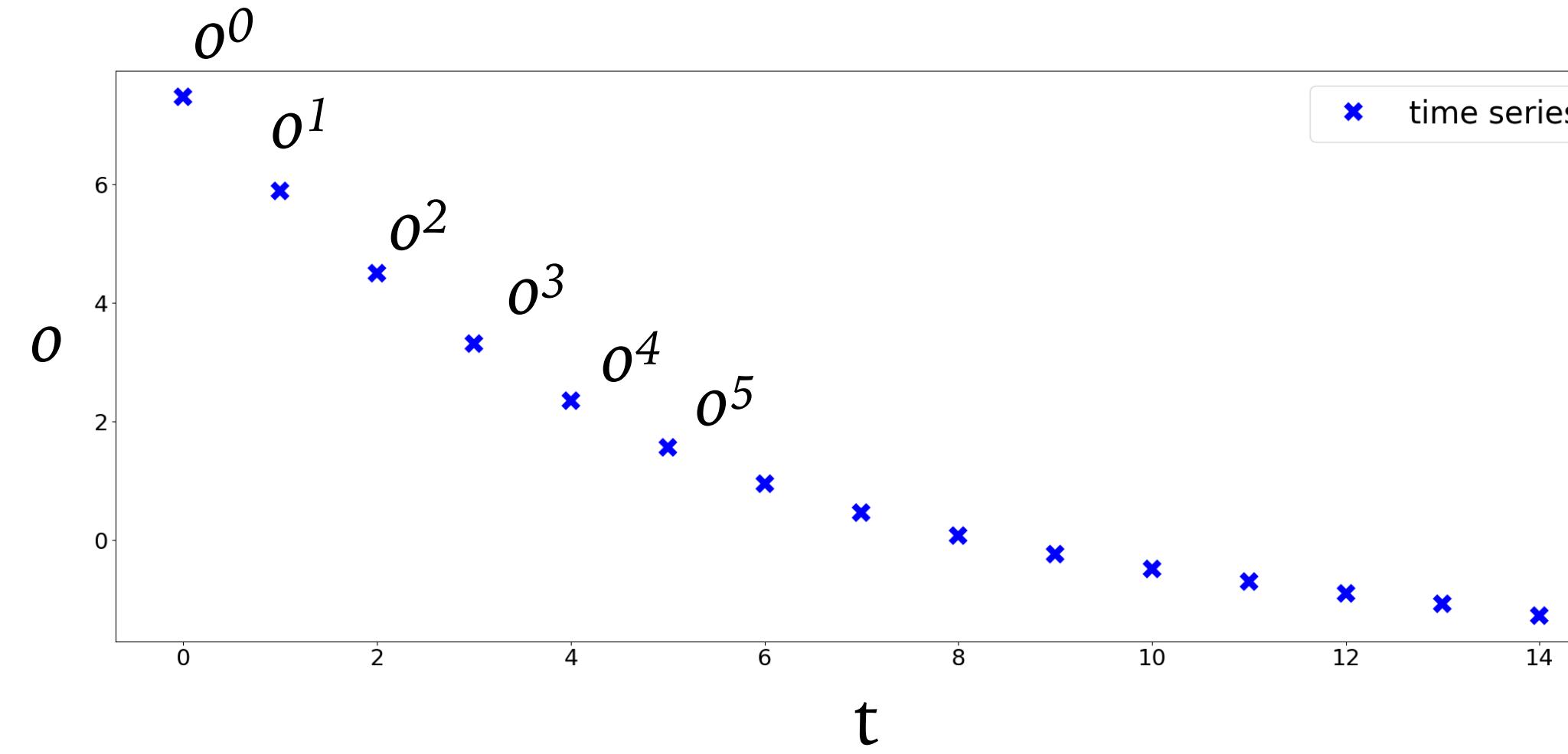


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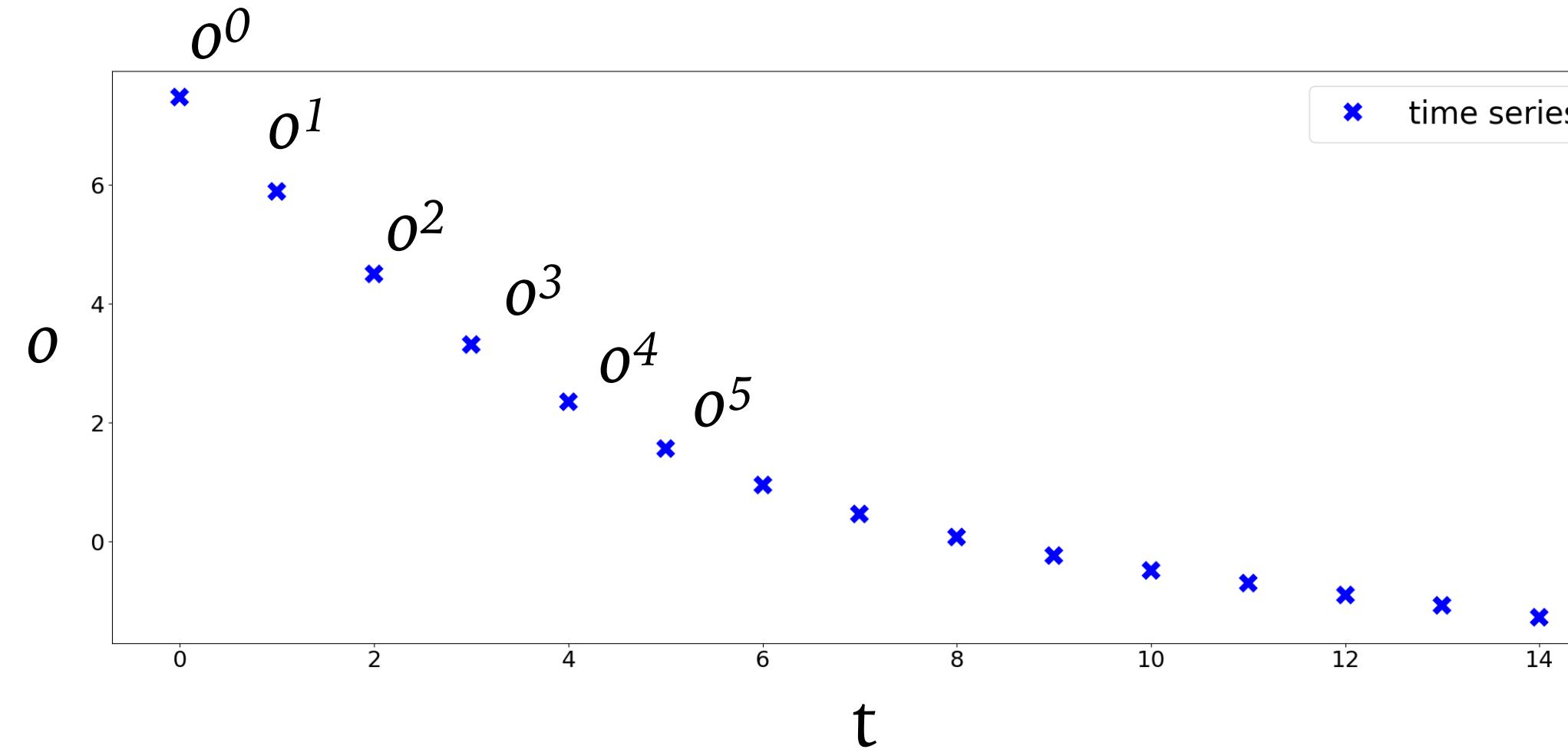
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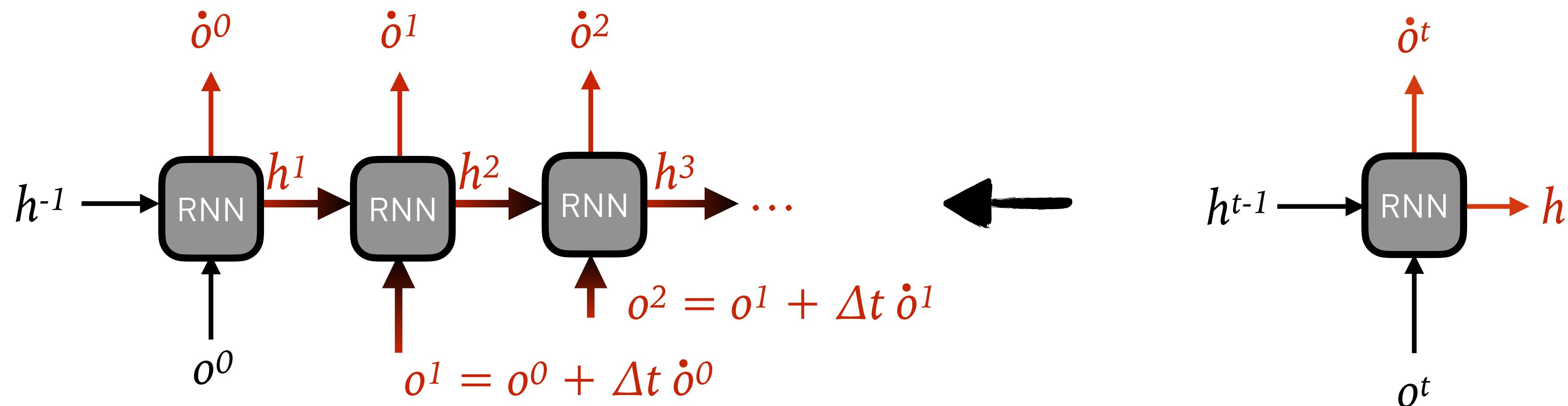


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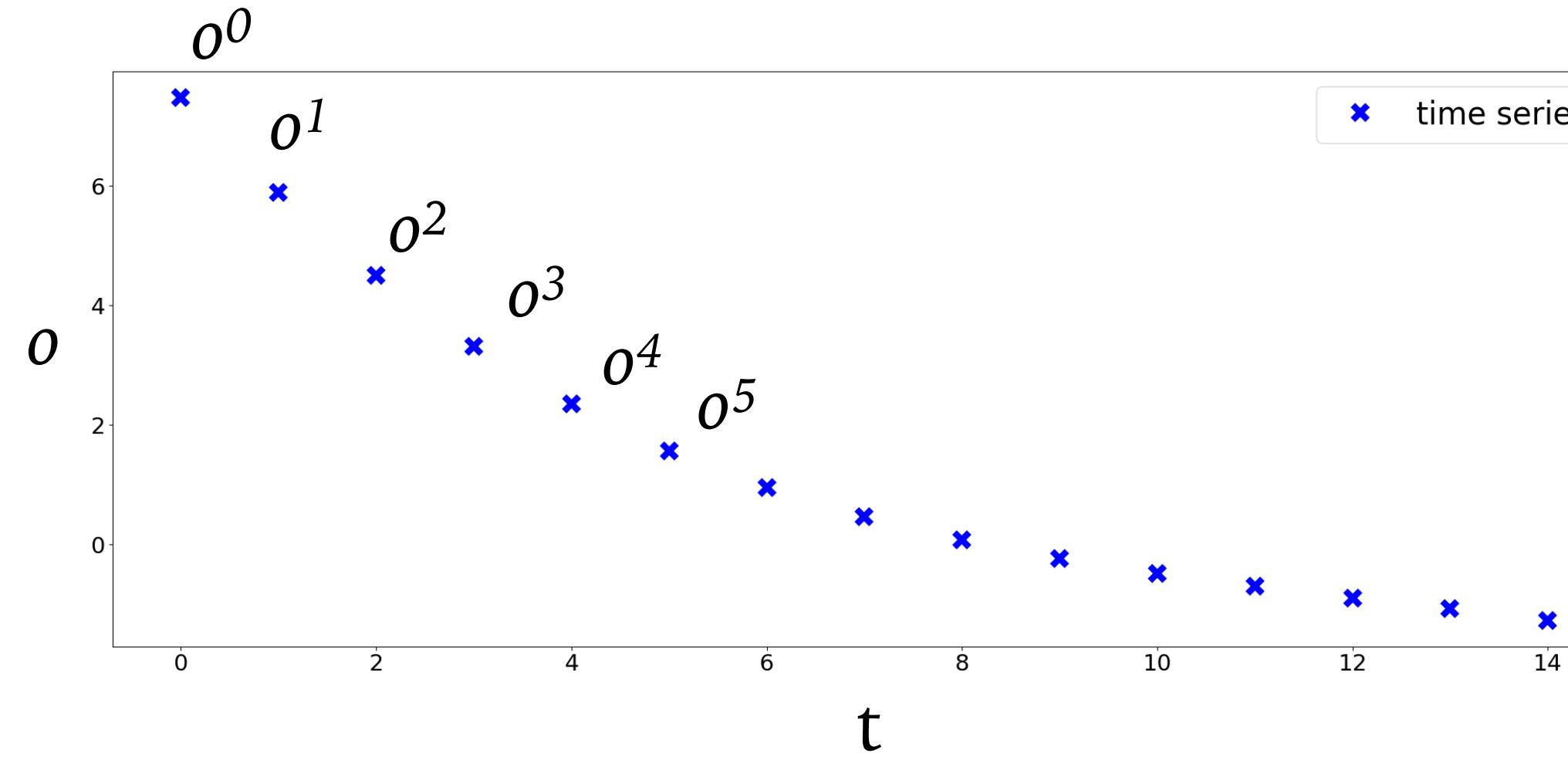


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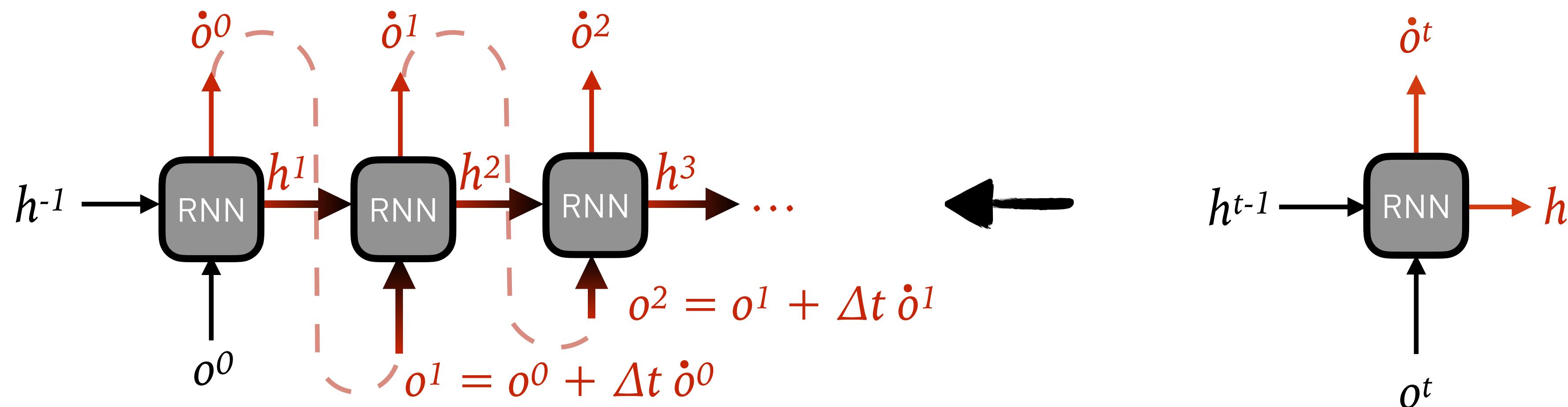


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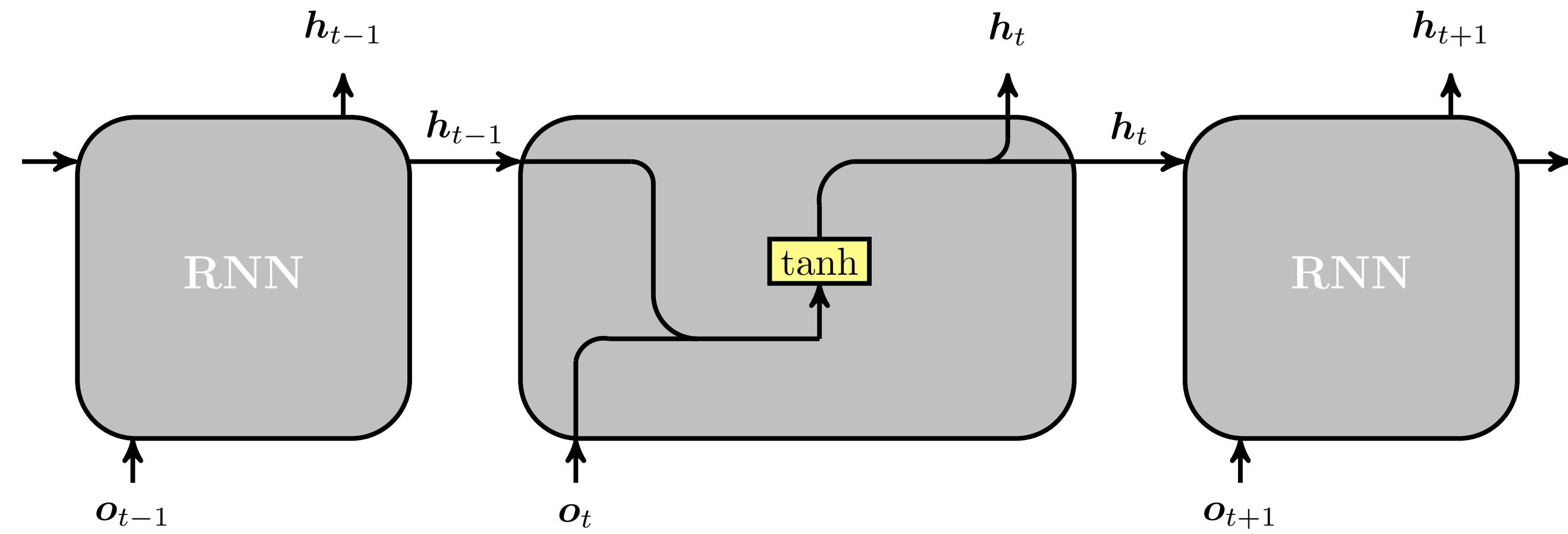


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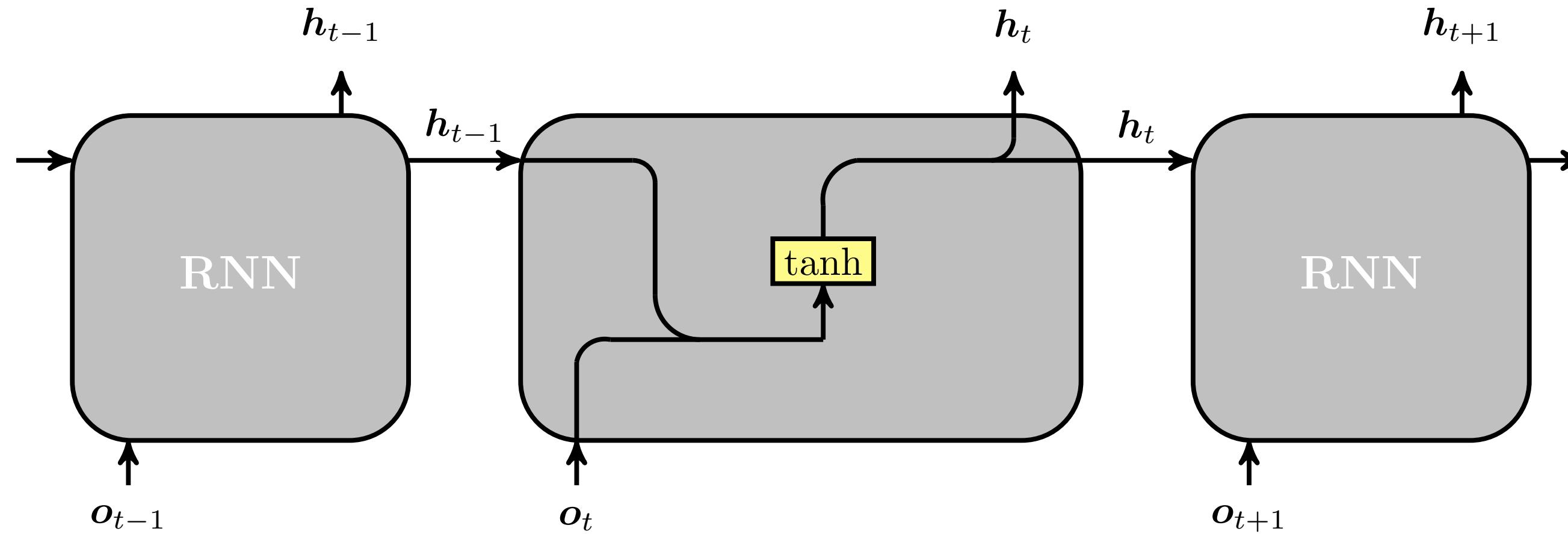
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# Elman RNN (1990)



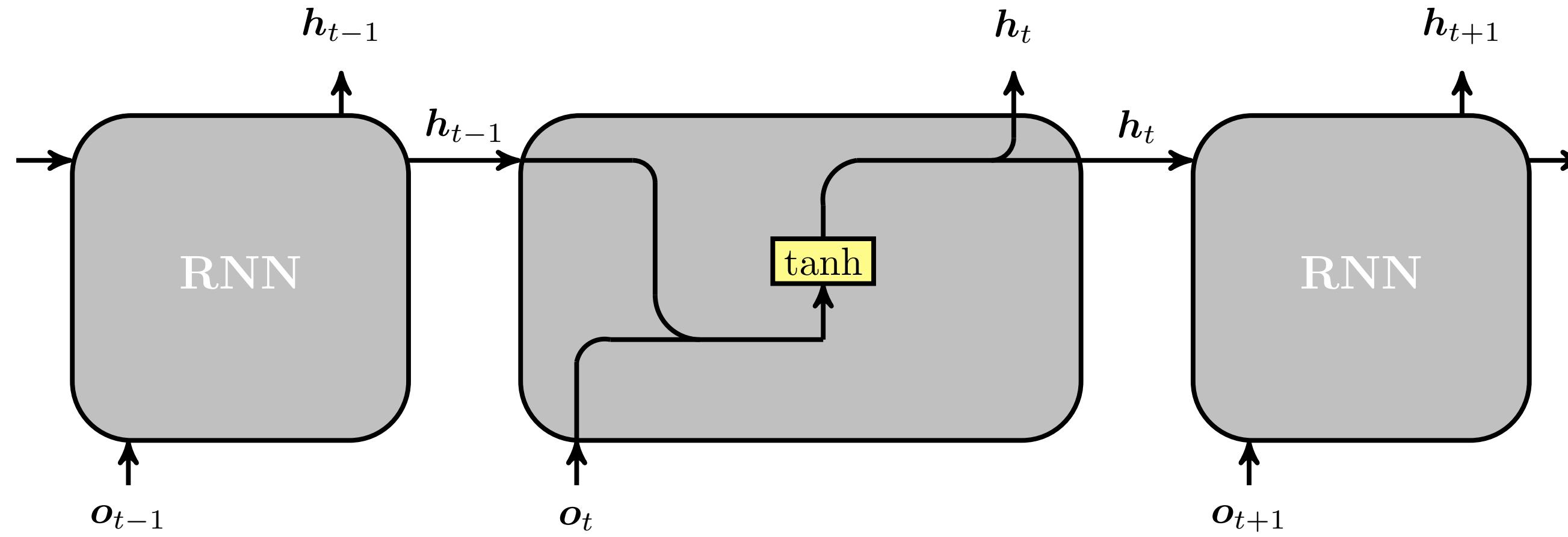
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Hidden-to-hidden mapping

$$h_t = \tanh(W_{ho} o_t + W_{hh} h_{t-1} + b_h)$$

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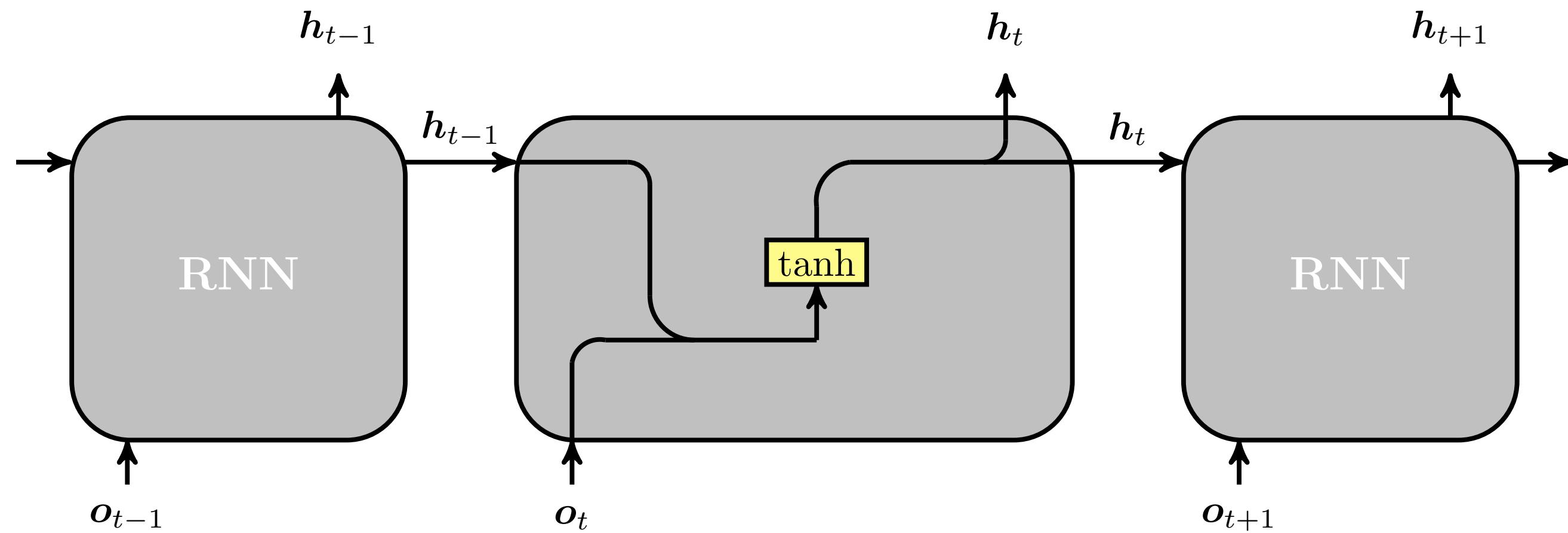
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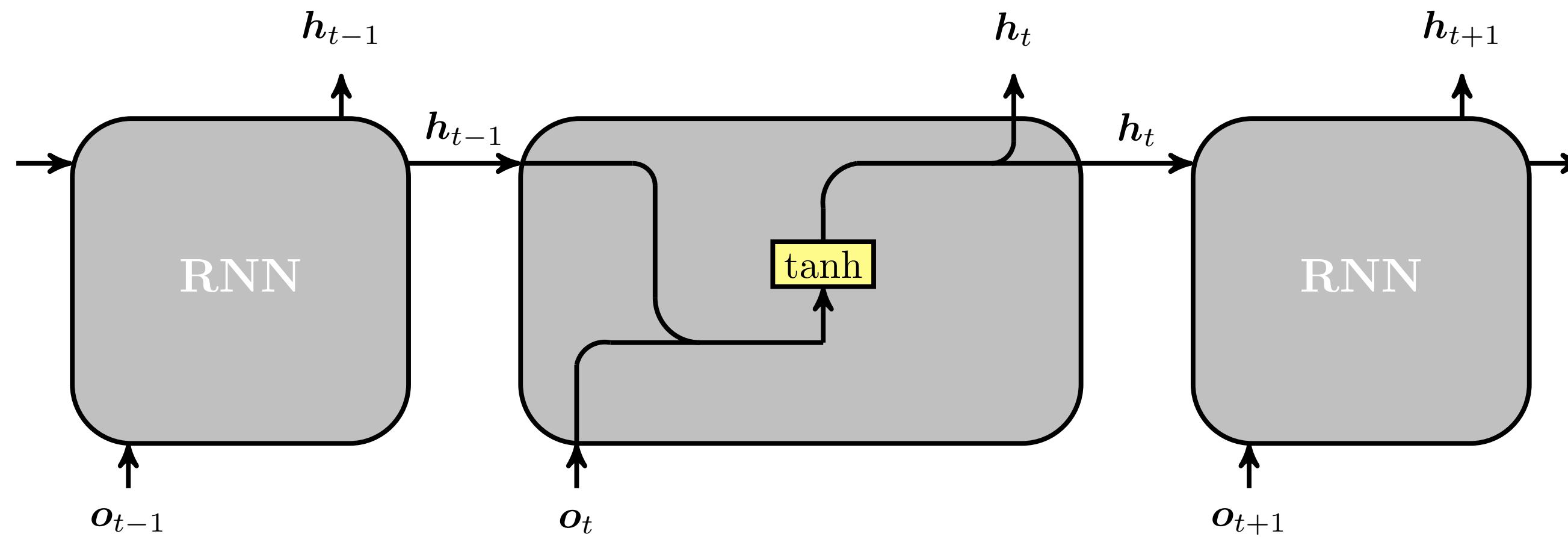
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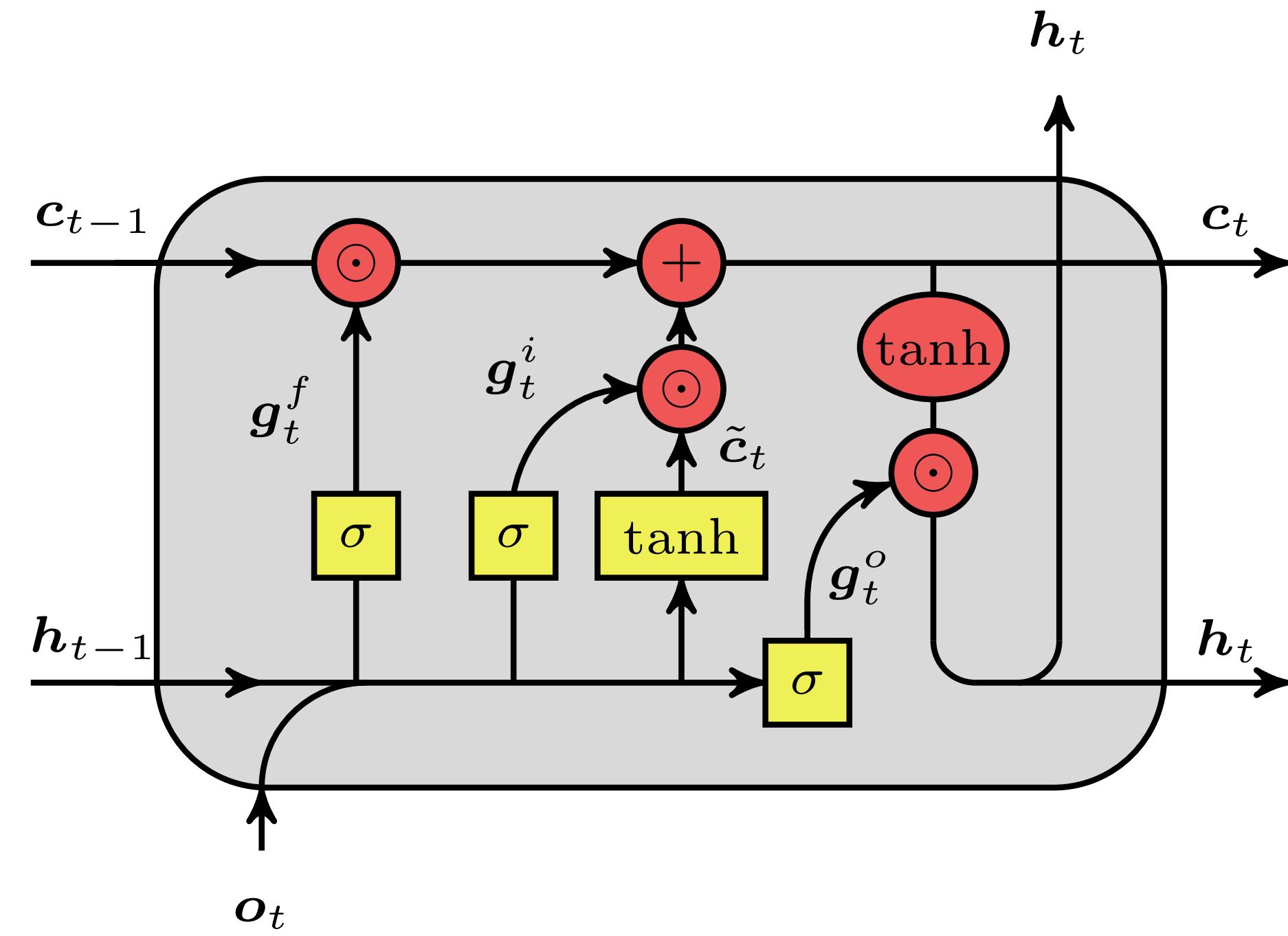
**Training** this network (fitting the WEIGHTS to data) is difficult.  
*(vanishing gradients problem)*

Parameters (WEIGHTS) to be learned:

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# Long Short-Term Memory (LSTM)

S. Hochreiter and J. Schmidhuber (1997)



Long Short-Term Memory Cell

# Kuramoto-Sivashinsky

---

$$\frac{\partial u}{\partial t} = -\nu \frac{\partial^4 u}{\partial x^4} - \frac{\partial^2 u}{\partial x^2} - u \frac{\partial u}{\partial x}$$

# Kuramoto-Sivashinsky

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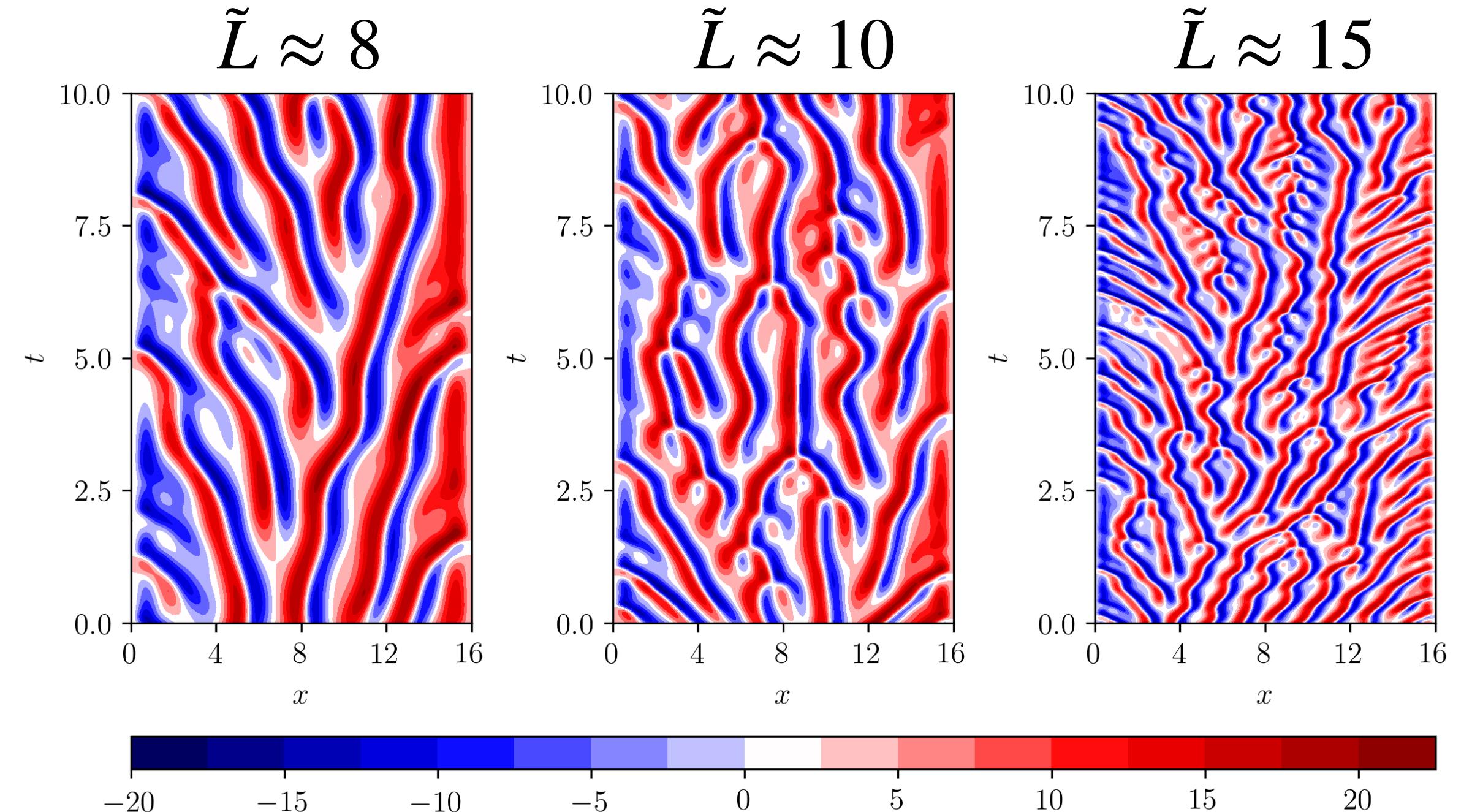
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- Fourth order PDE, negative viscosity  $\nu$
- Dirichlet & second order boundary conditions
- Domain  $x \in [0, L]$ ,  $L = 16$
- **Chaoticity scales with bifurcation parameter**

$$\tilde{L} = \frac{L}{2\pi\sqrt{\nu}}$$

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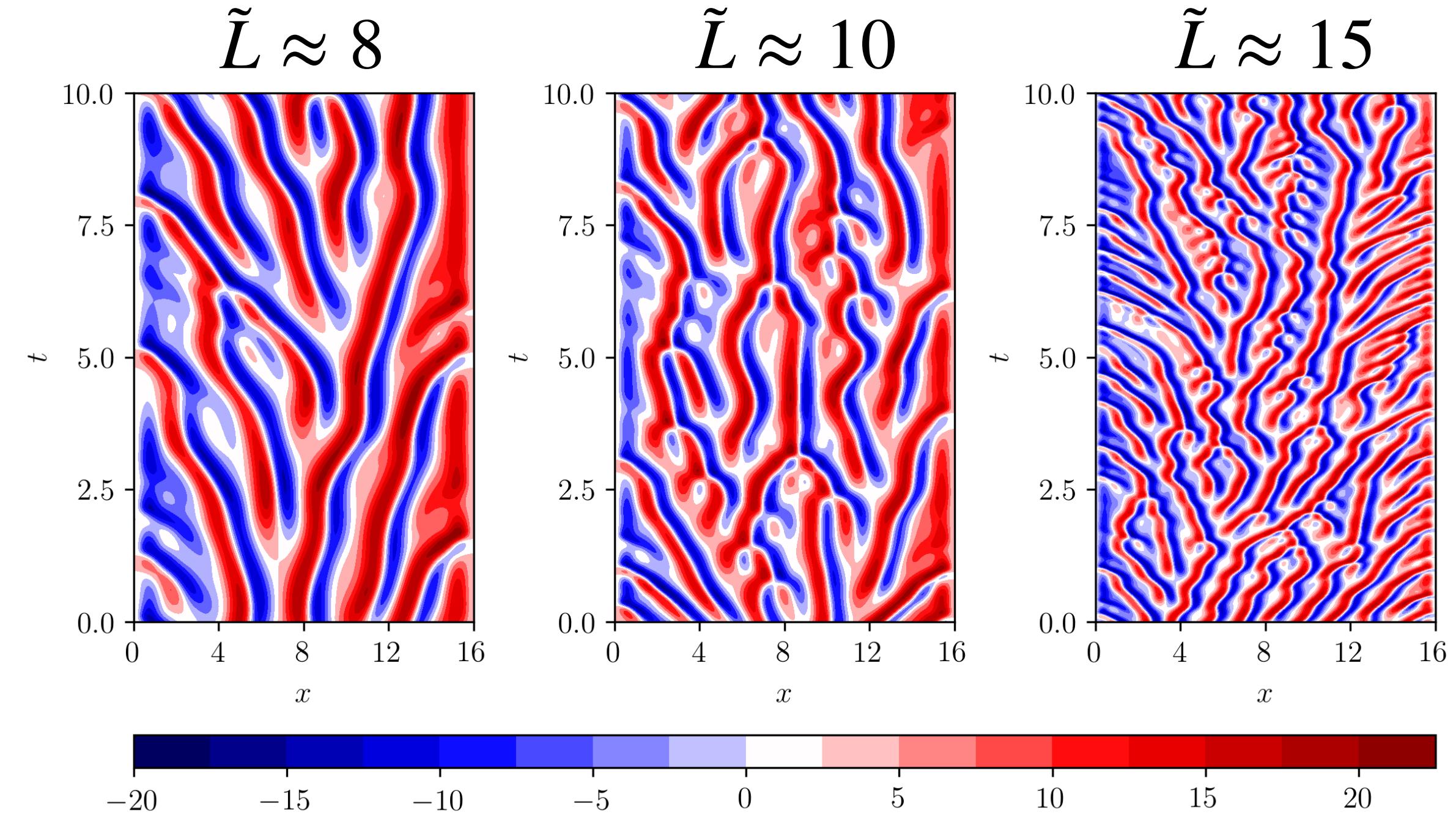


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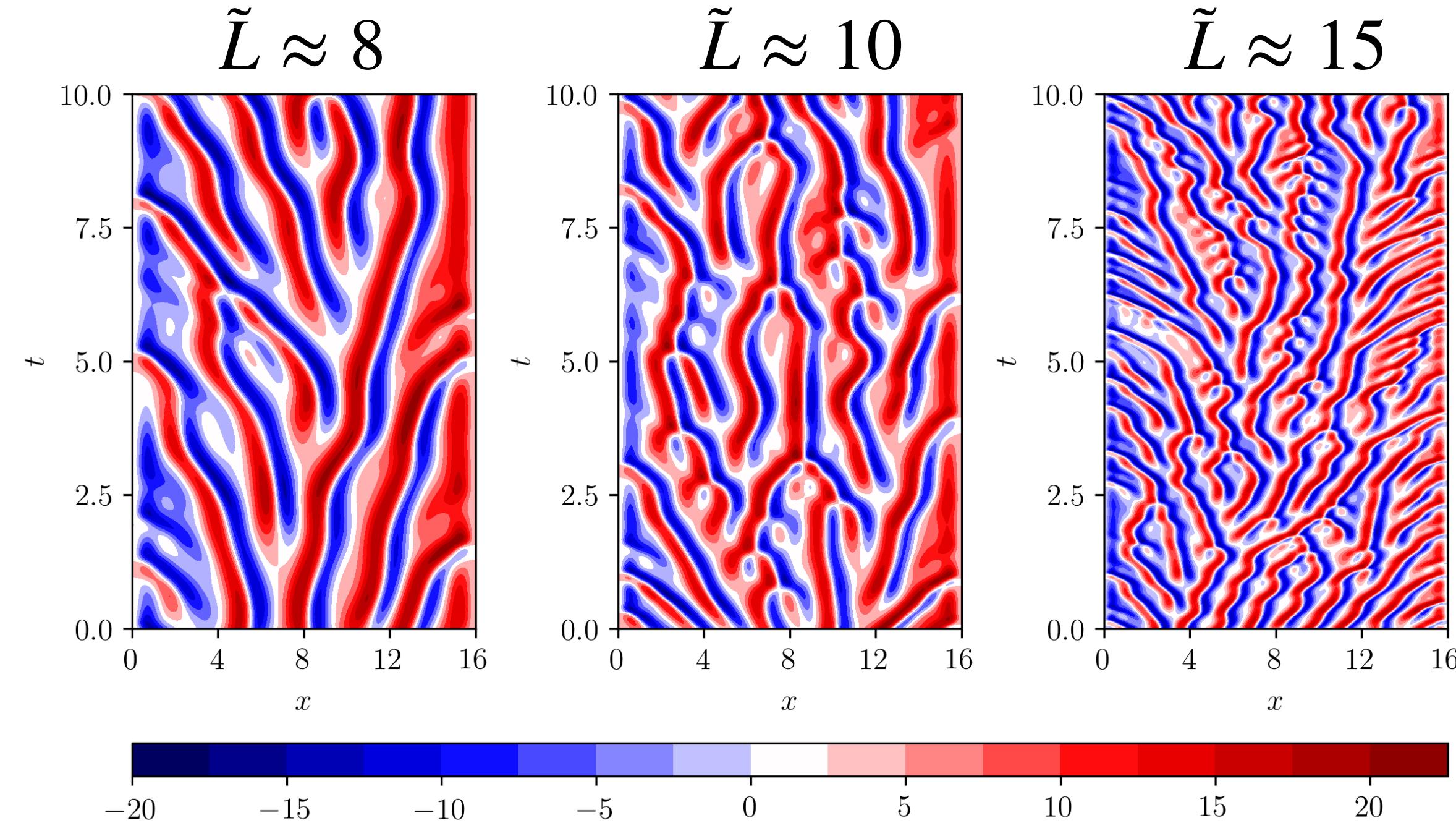
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Discretization with  
 $d_u = 512$  gridpoints

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$$\frac{du_i}{dt} = -\nu \frac{u_{i-2} - 4u_{i-1} + 6u_i - 4u_{i+1} + u_{i+2}}{\Delta x^4} - \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} - \frac{u_{i+1}^2 - u_{i-1}^2}{4\Delta x}$$

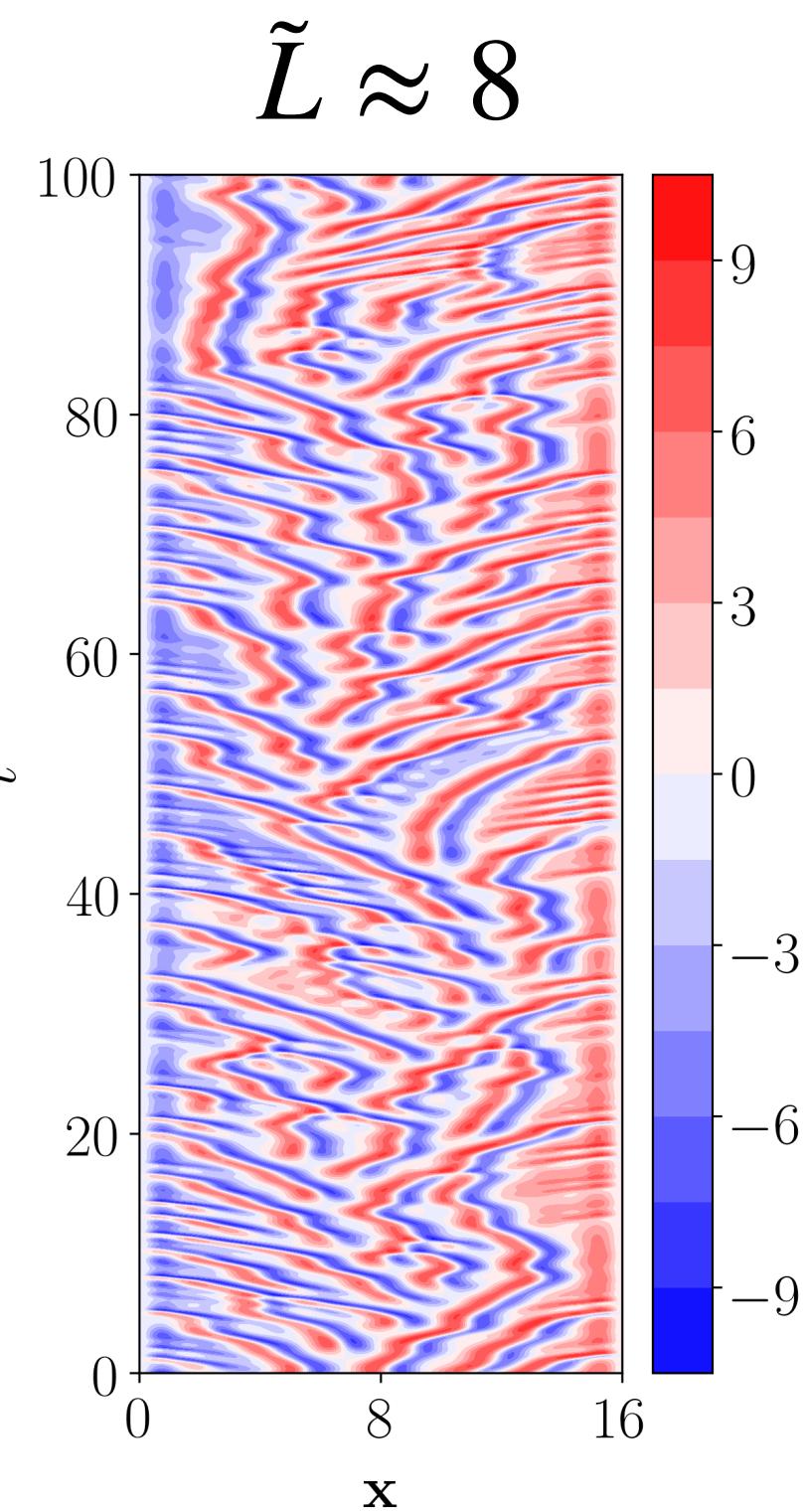
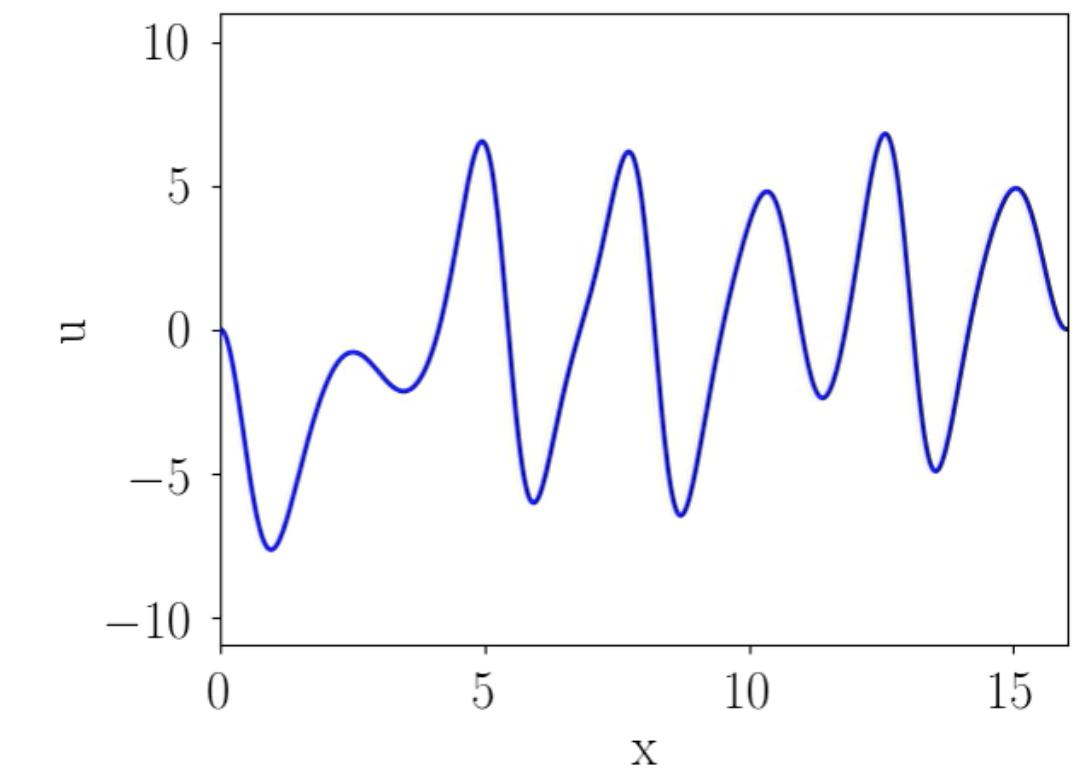
Integration with  $dt = 0.02$  up to  $T = 10^4$   
 (after discarding initial transients)  
**500.000 samples**

# Constructing the observable - training data

*High dimensional*

High dimensional  
simulation data

- $T = 10^4$
- half a million samples
- $u_t \in \mathbb{R}^{512}$

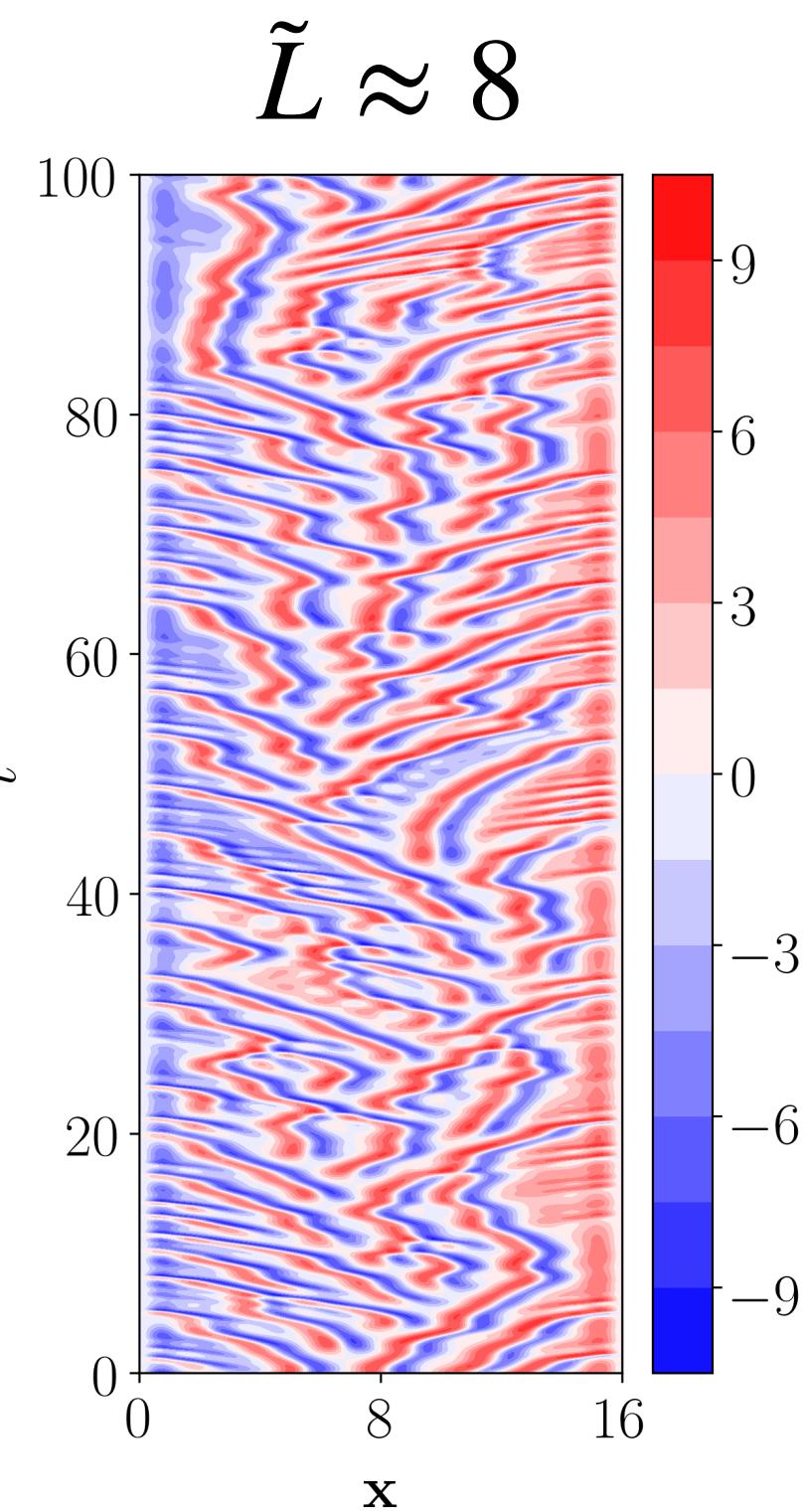
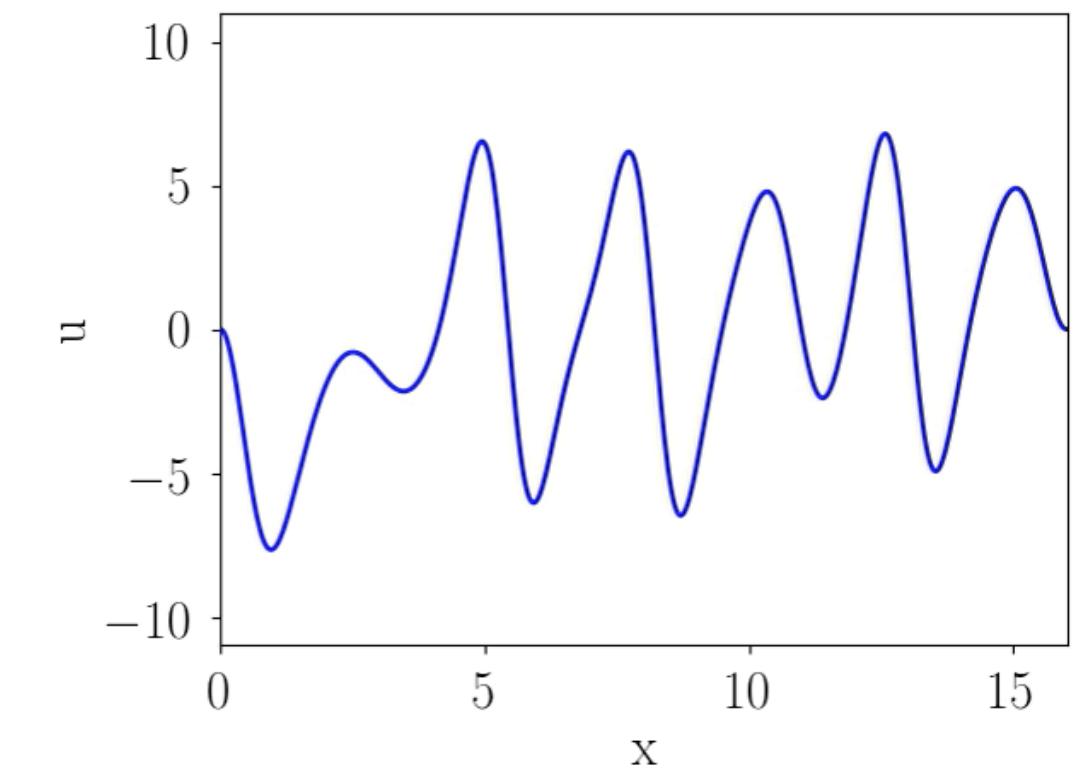


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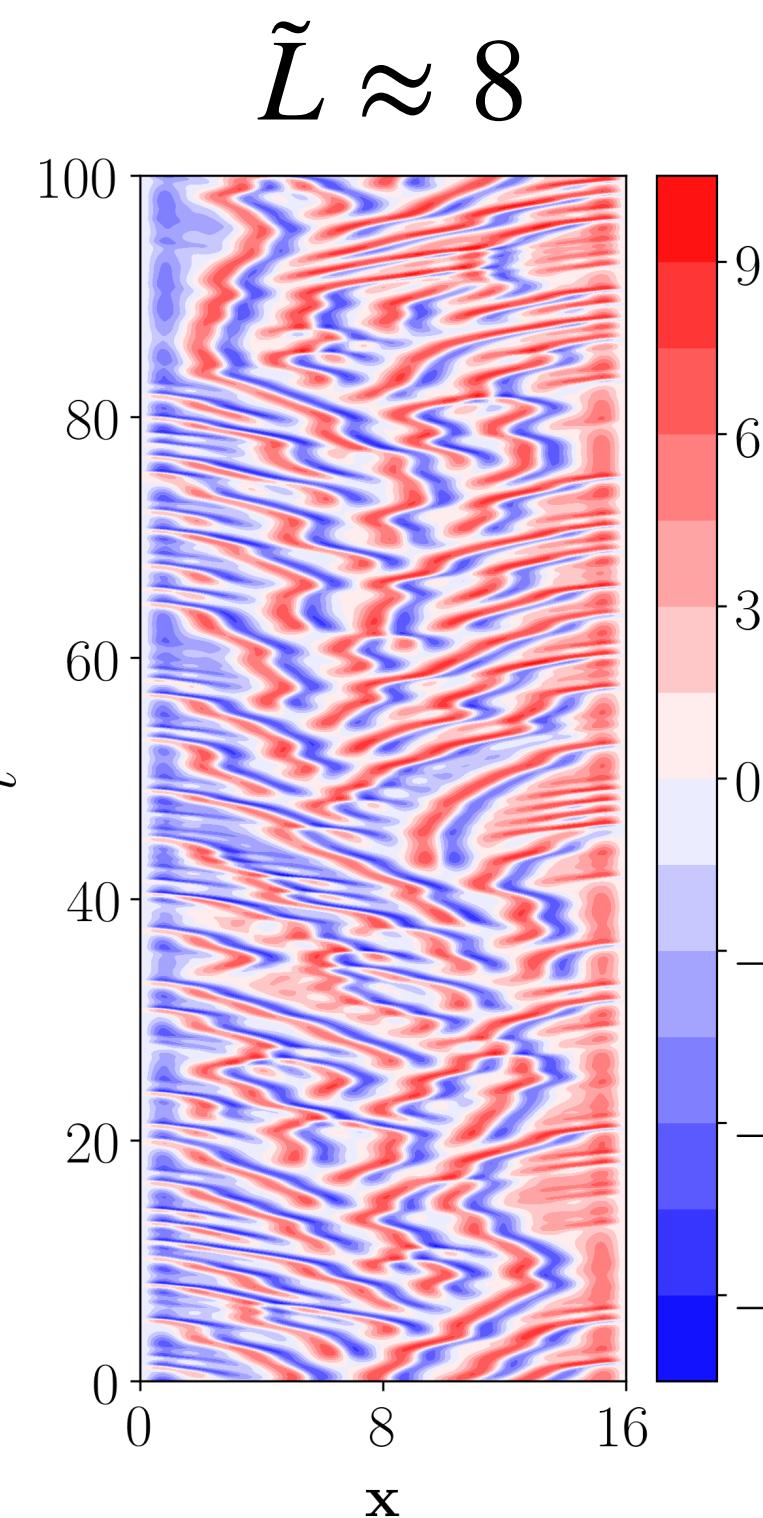
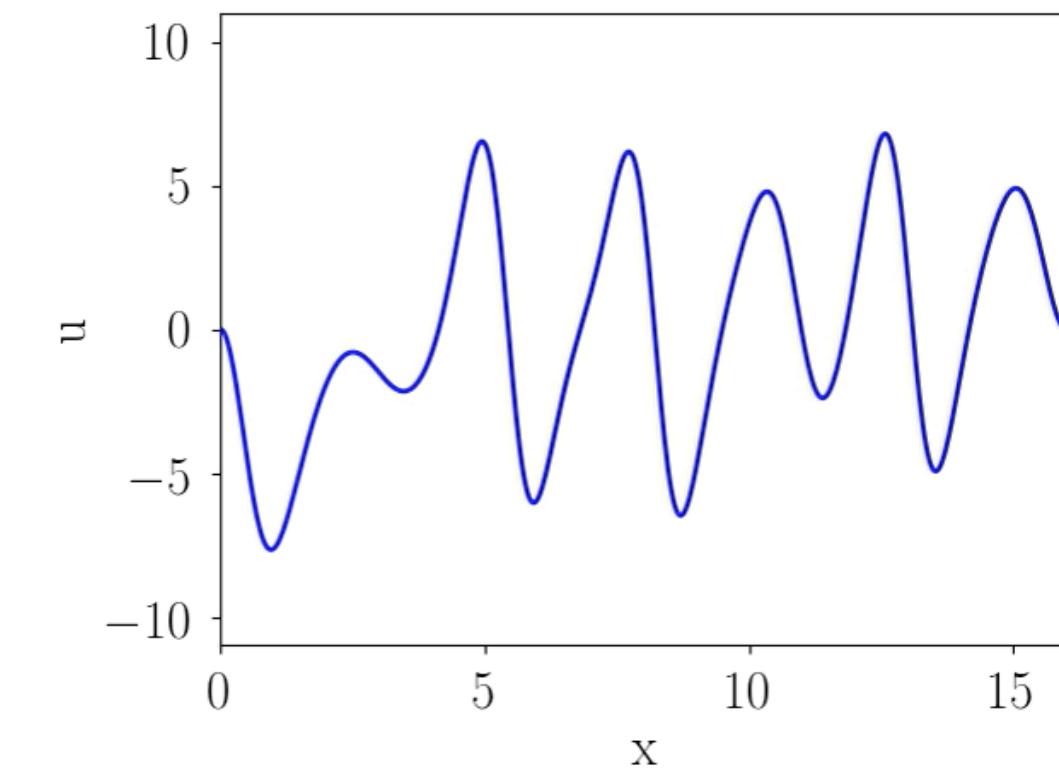


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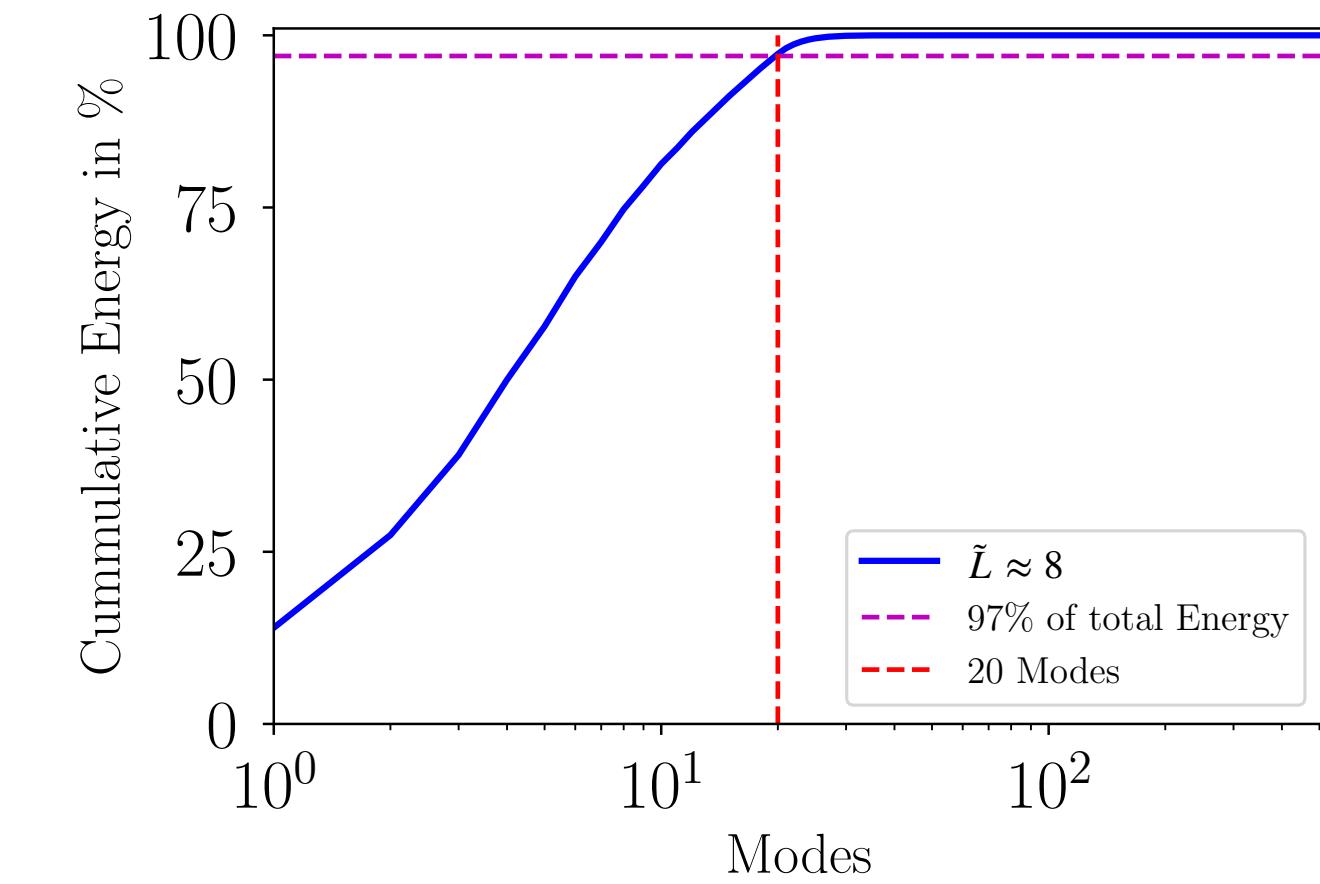
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**SVD / PCA**

Singular Value Decomposition

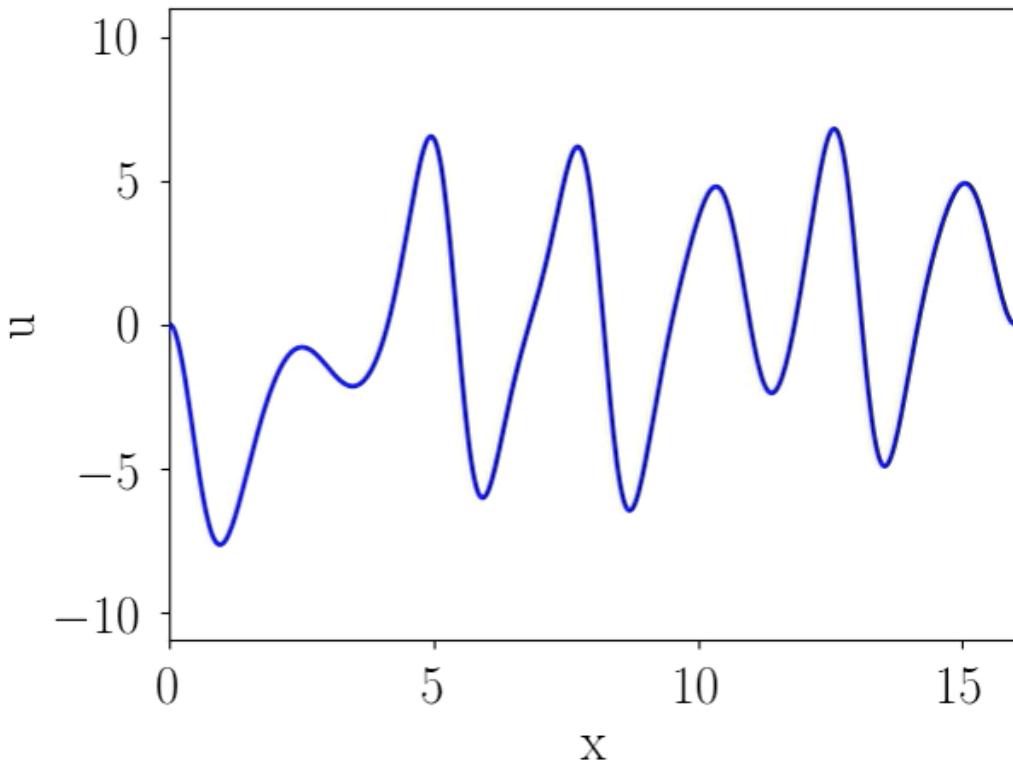


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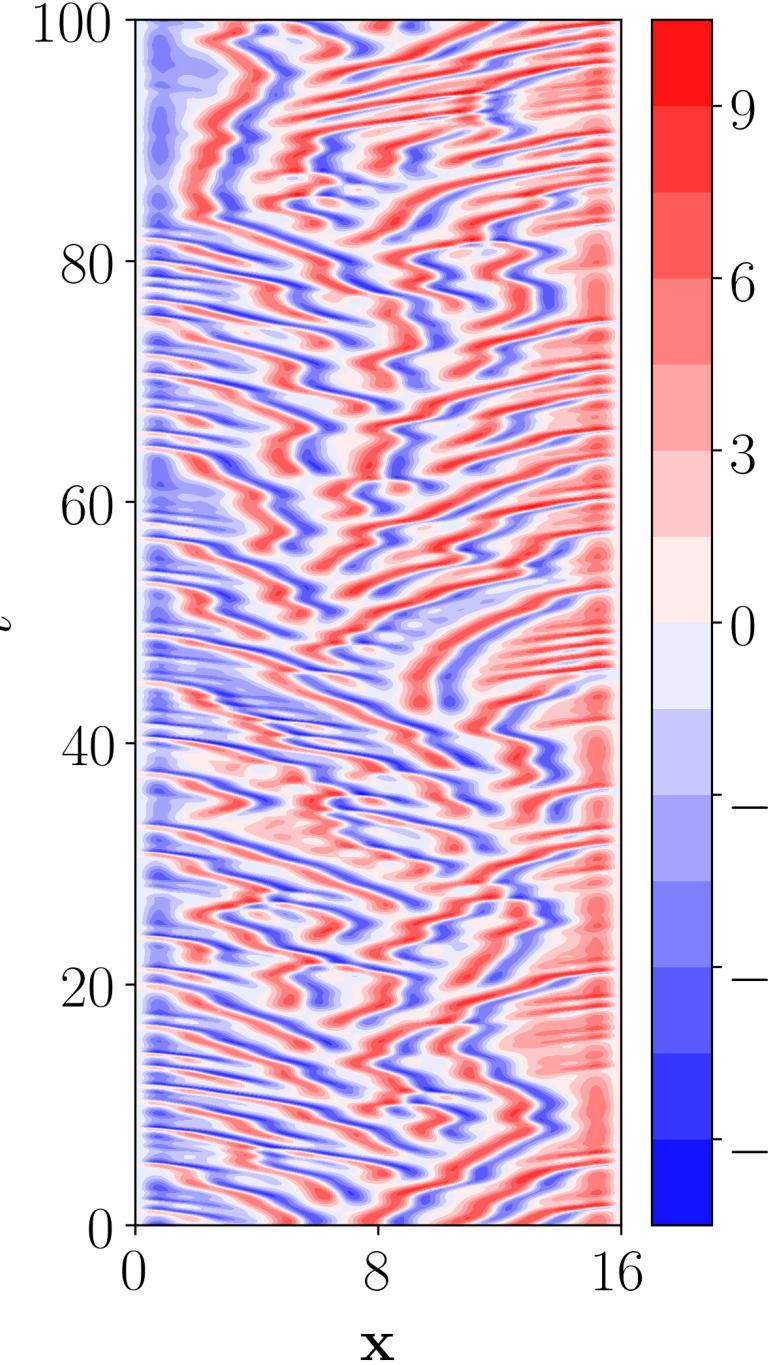
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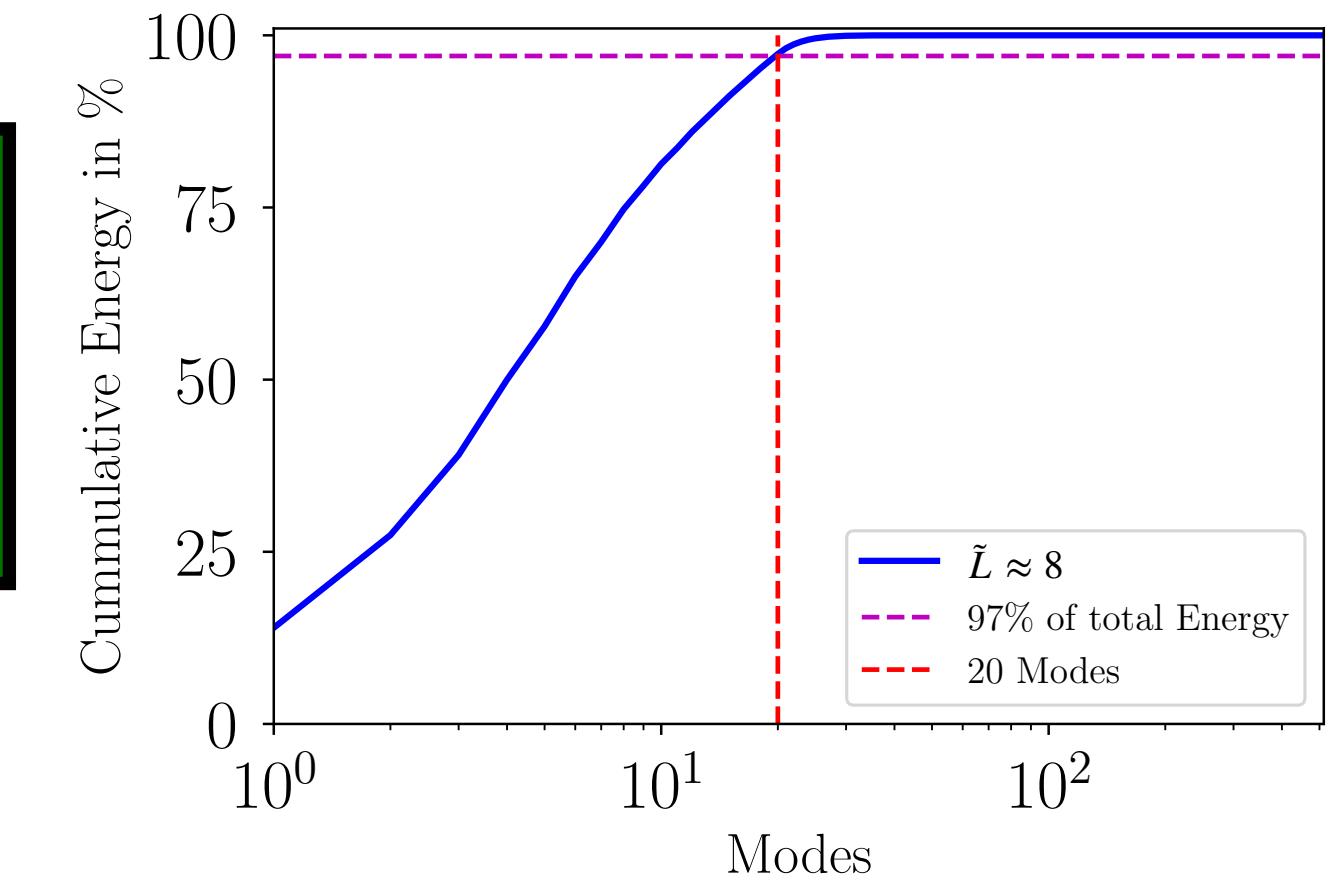
$\tilde{L} \approx 8$



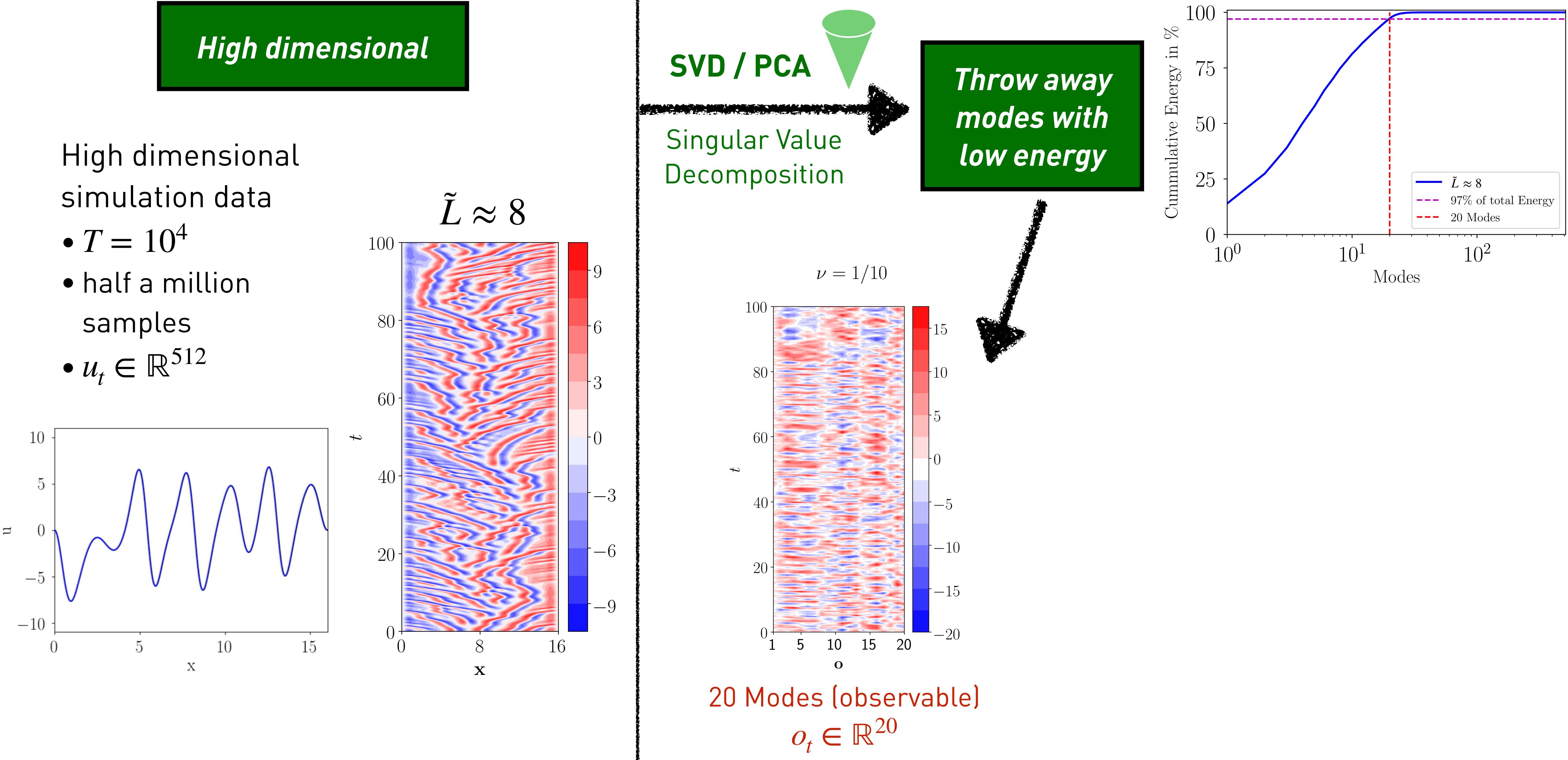
**SVD / PCA**

Singular Value Decomposition

***Throw away modes with low energy***



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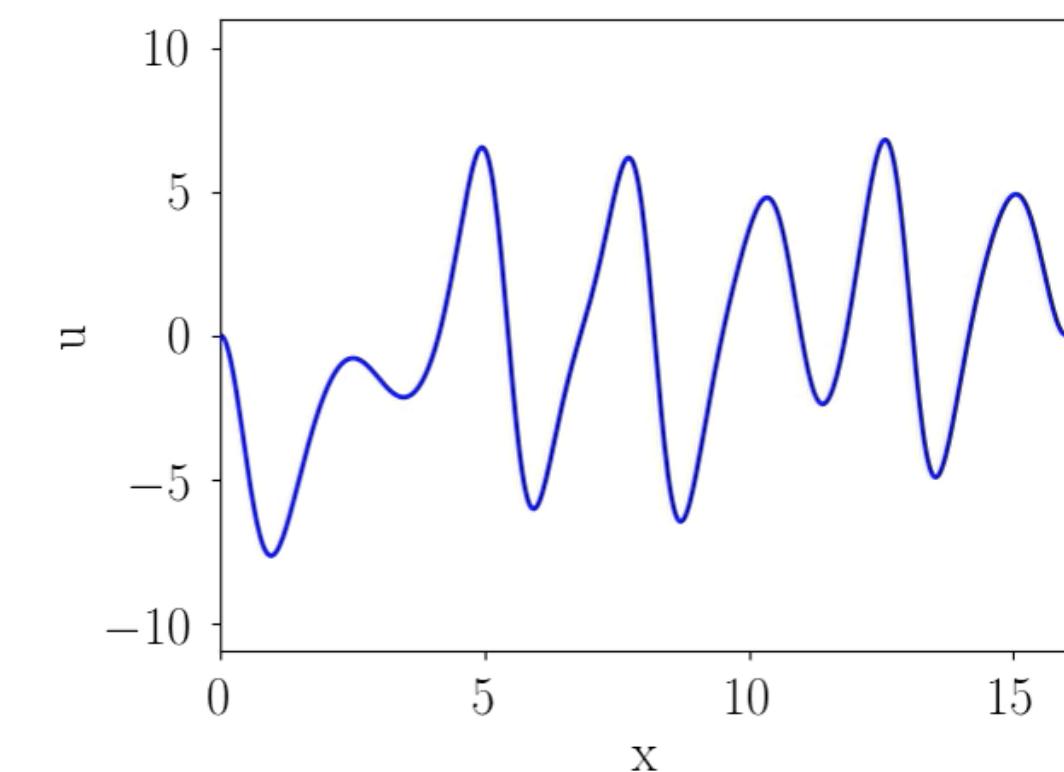


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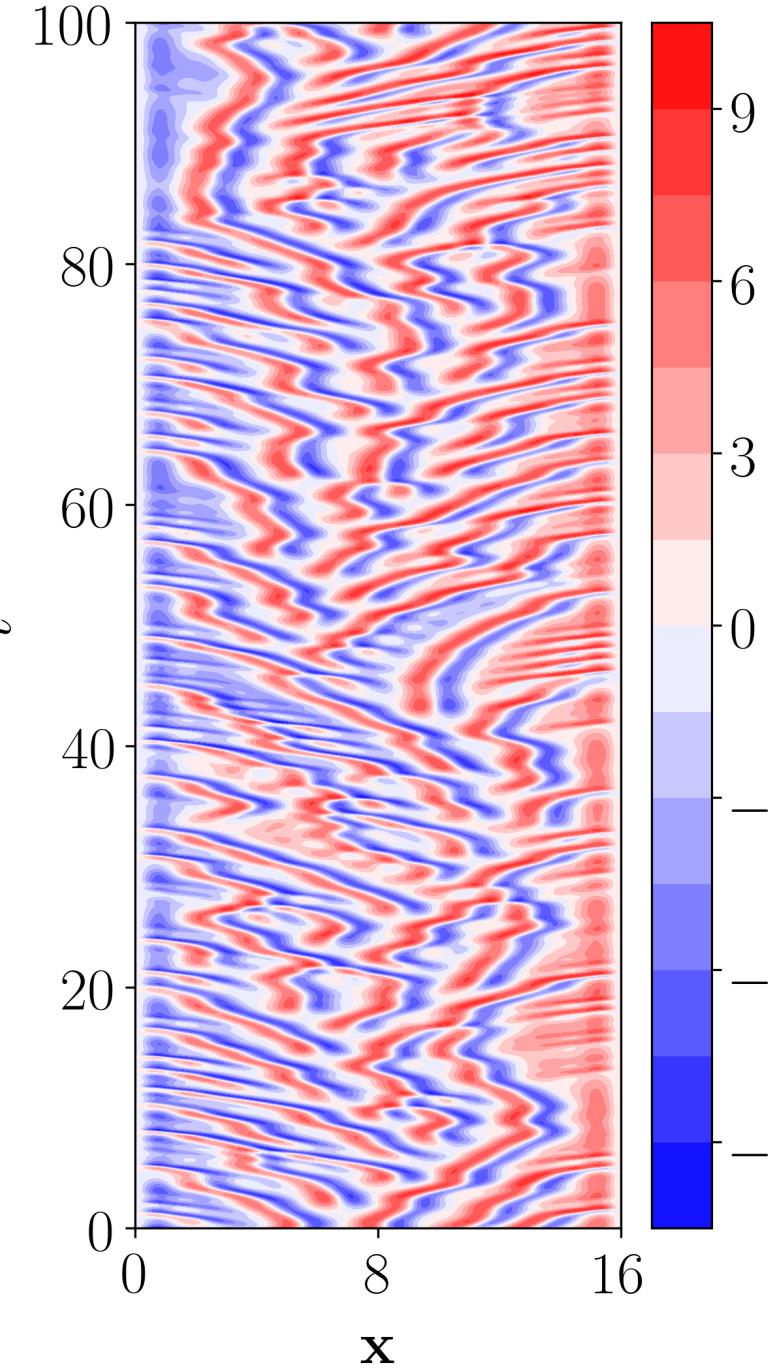
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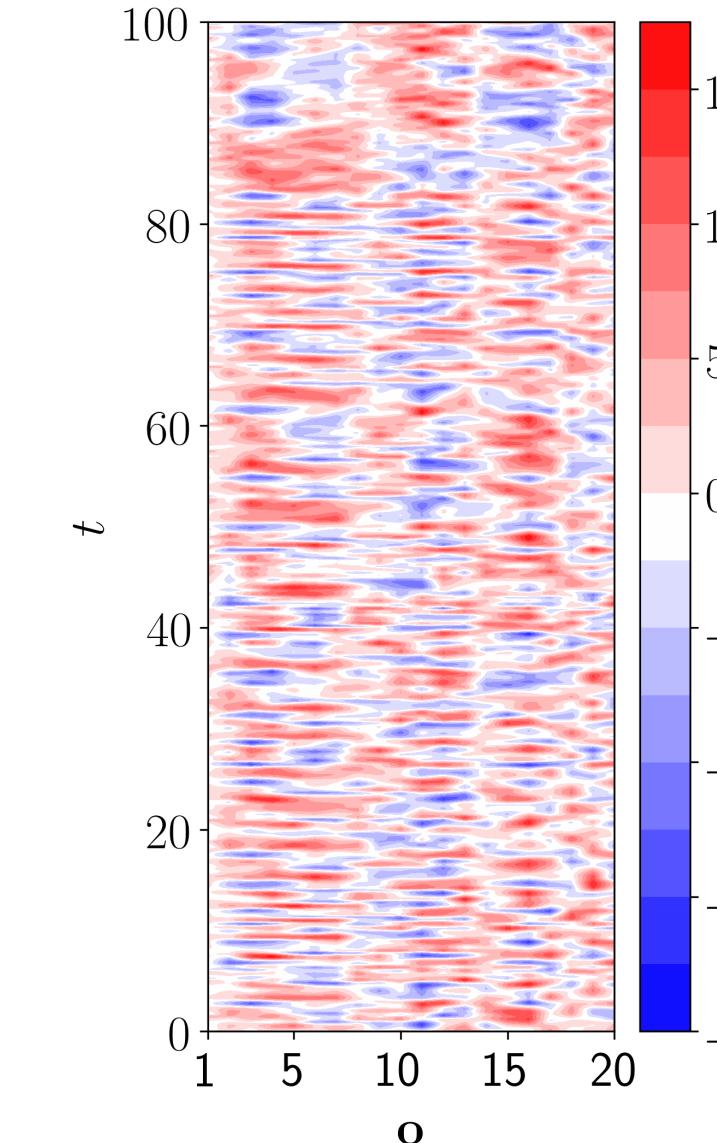


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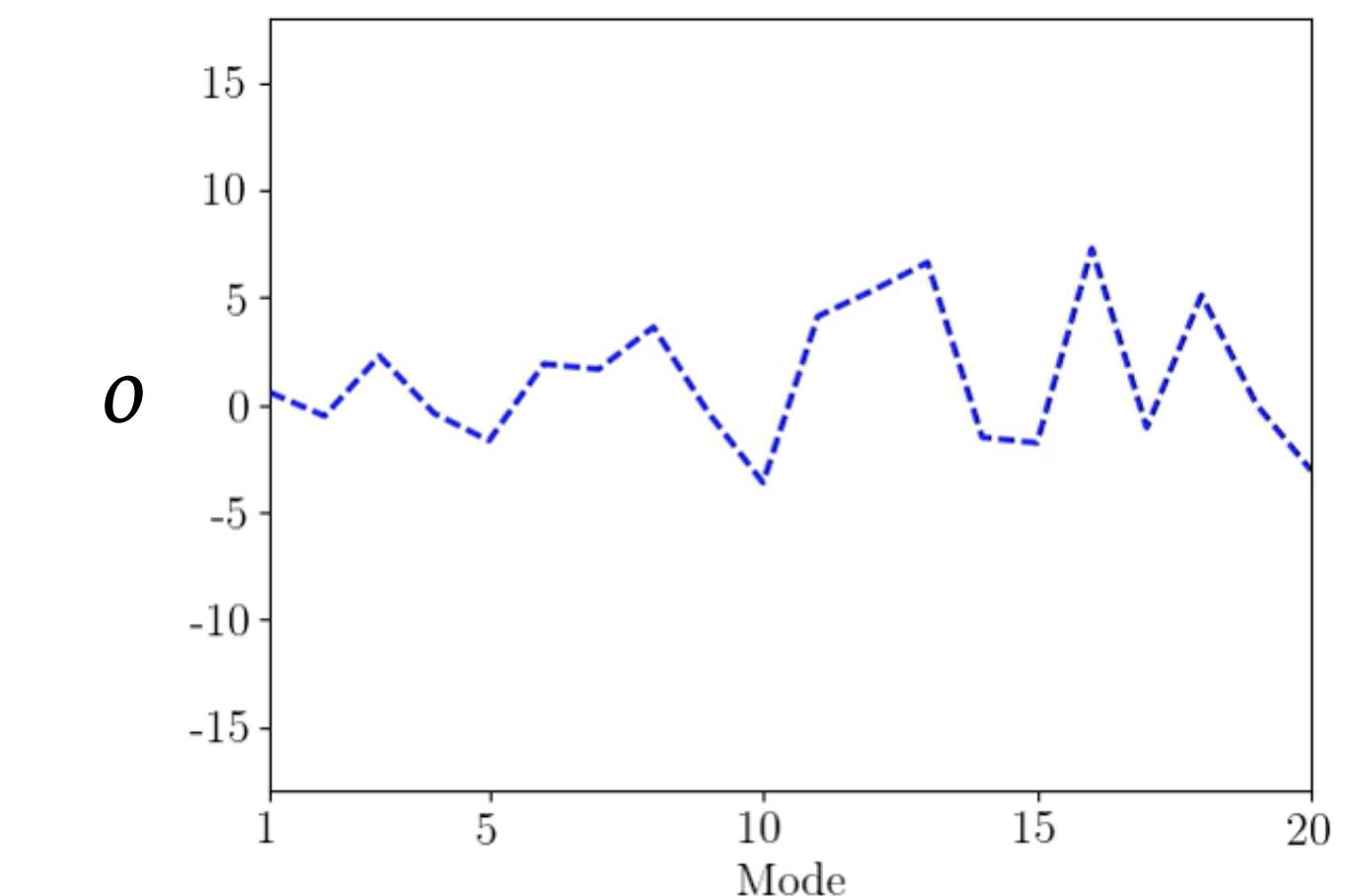
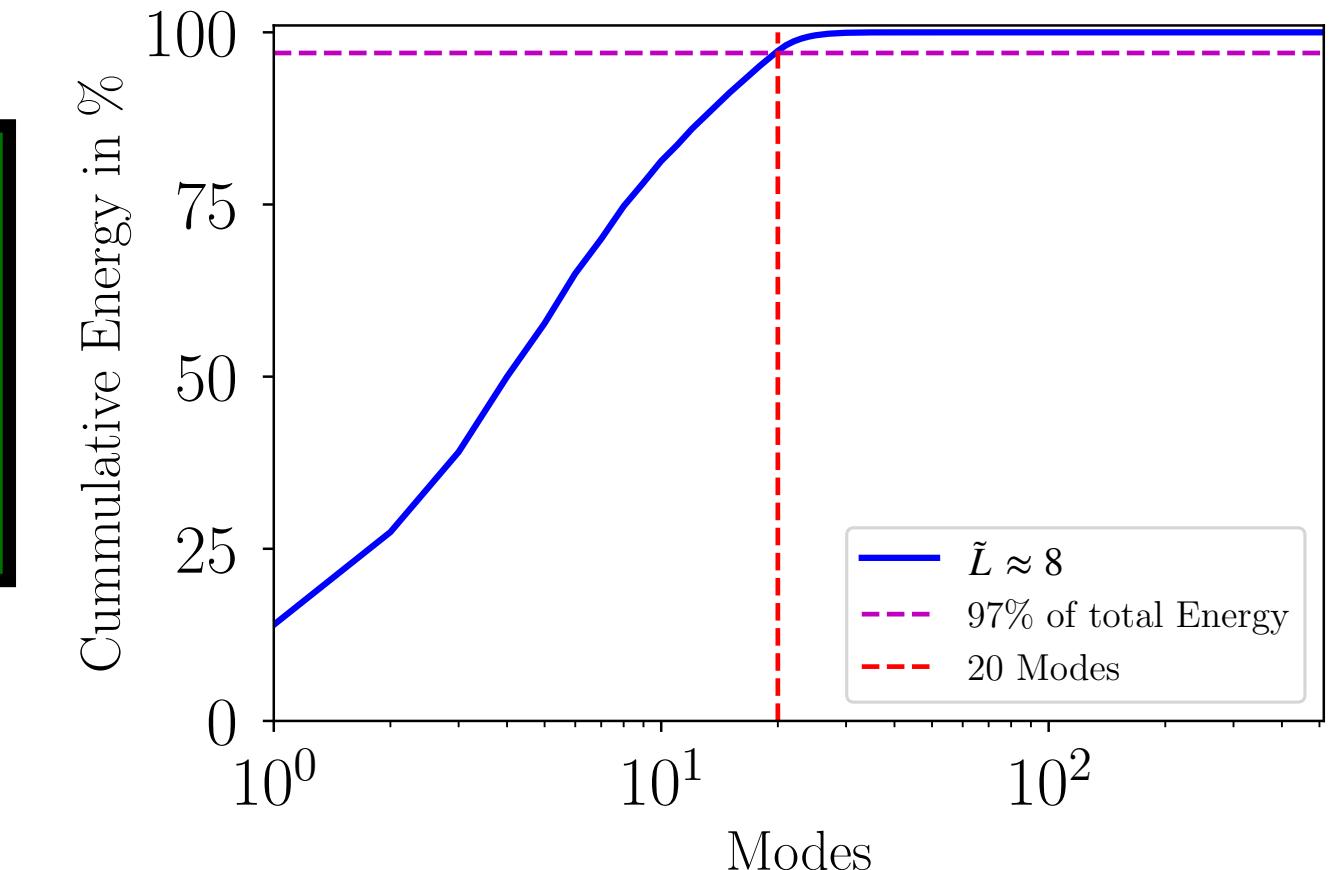
Singular Value  
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**Throw away  
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low energy**

$\nu = 1/10$



**20 Modes (observable)**  
 $o_t \in \mathbb{R}^{20}$



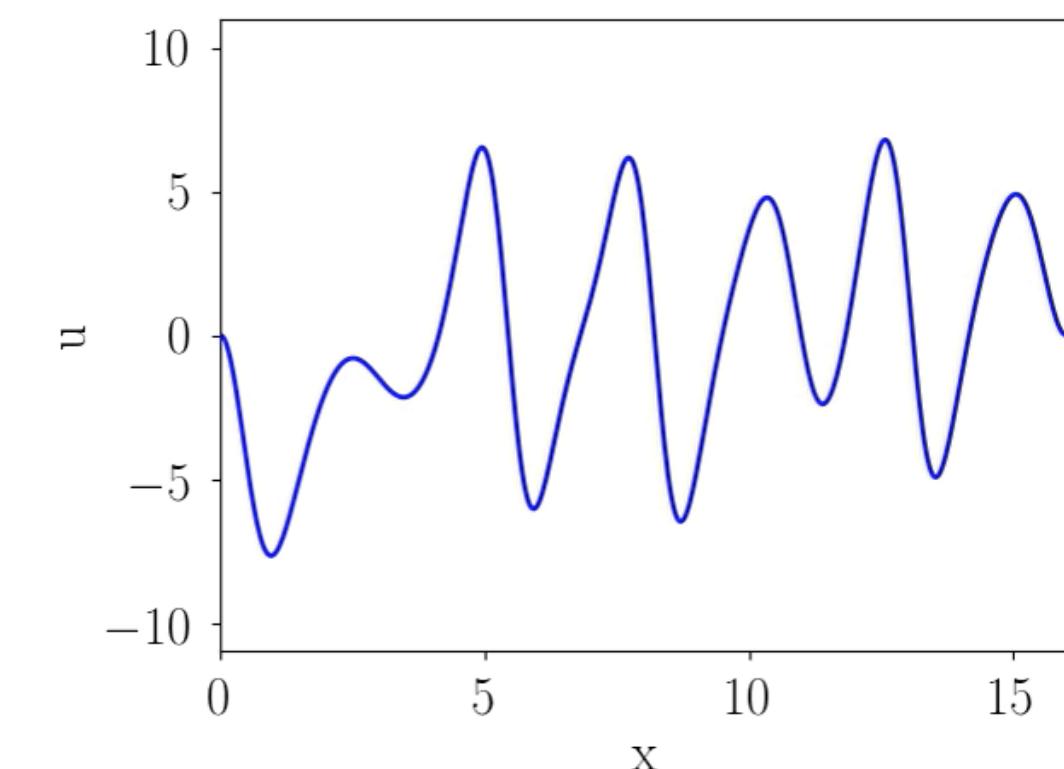
**Low dimensional  
reduced-order state  
(most energetic modes)**

# Constructing the observable - training data

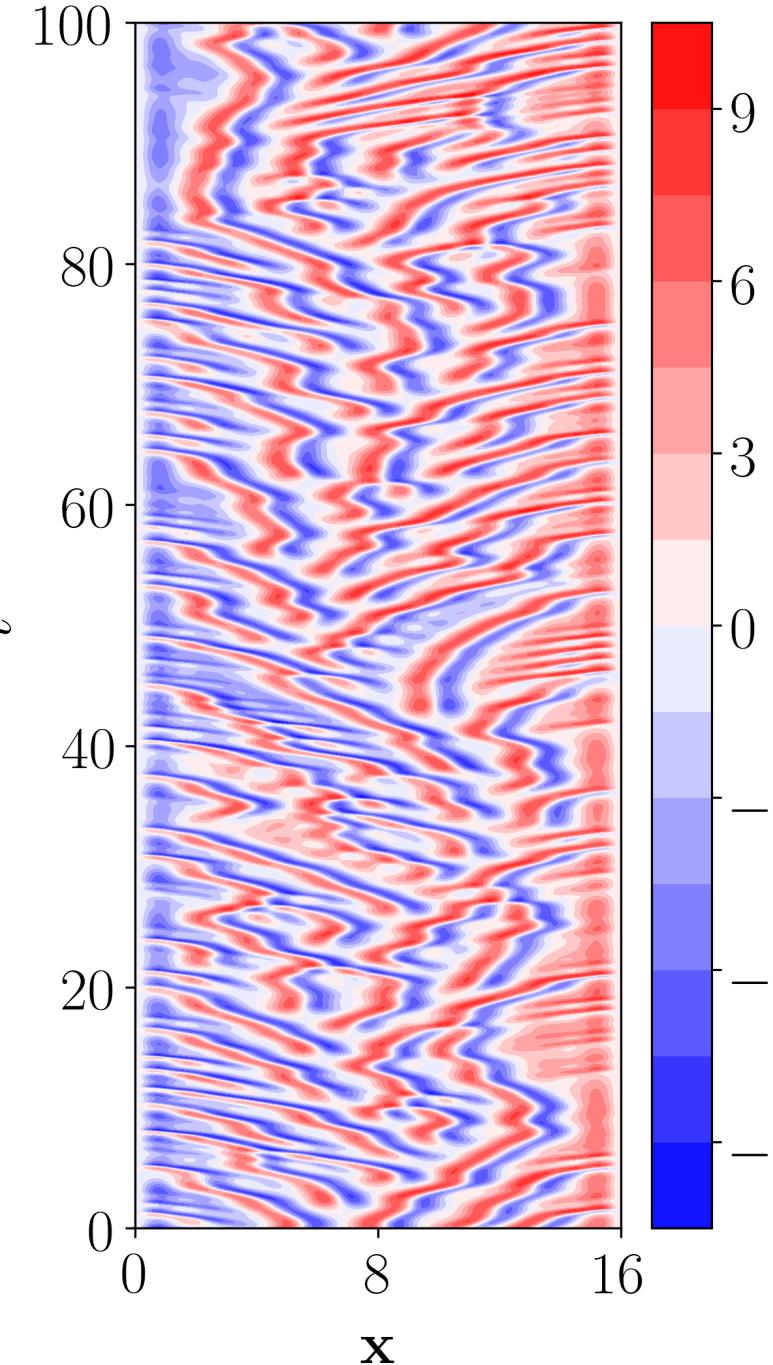
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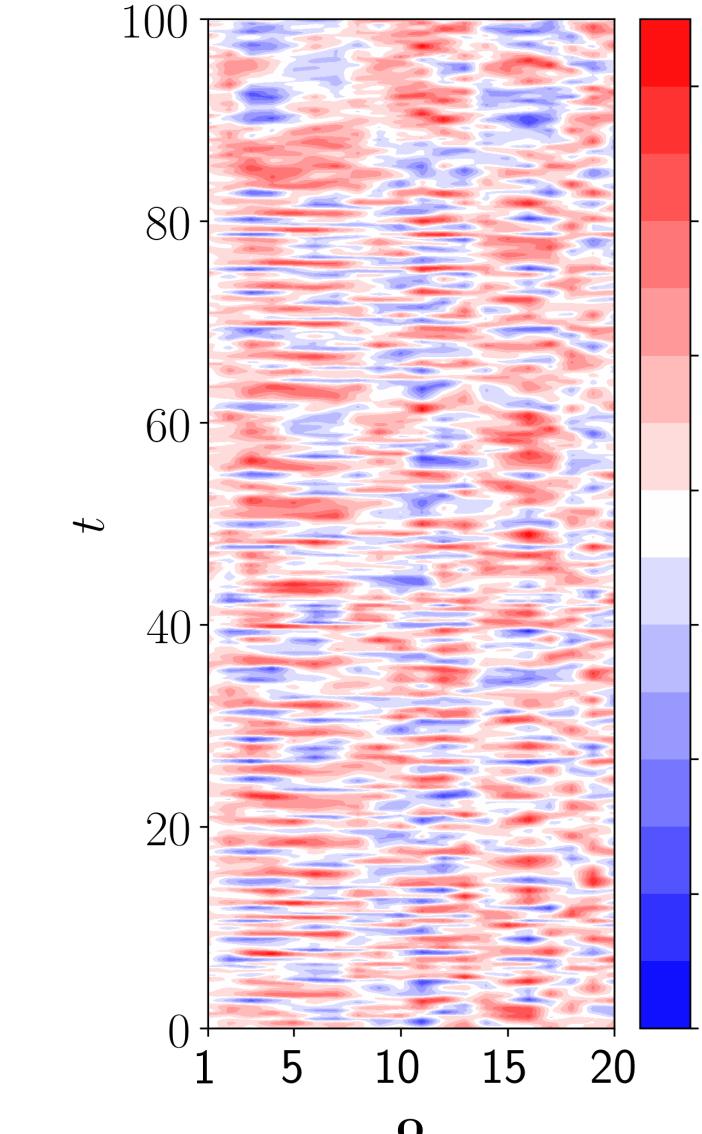


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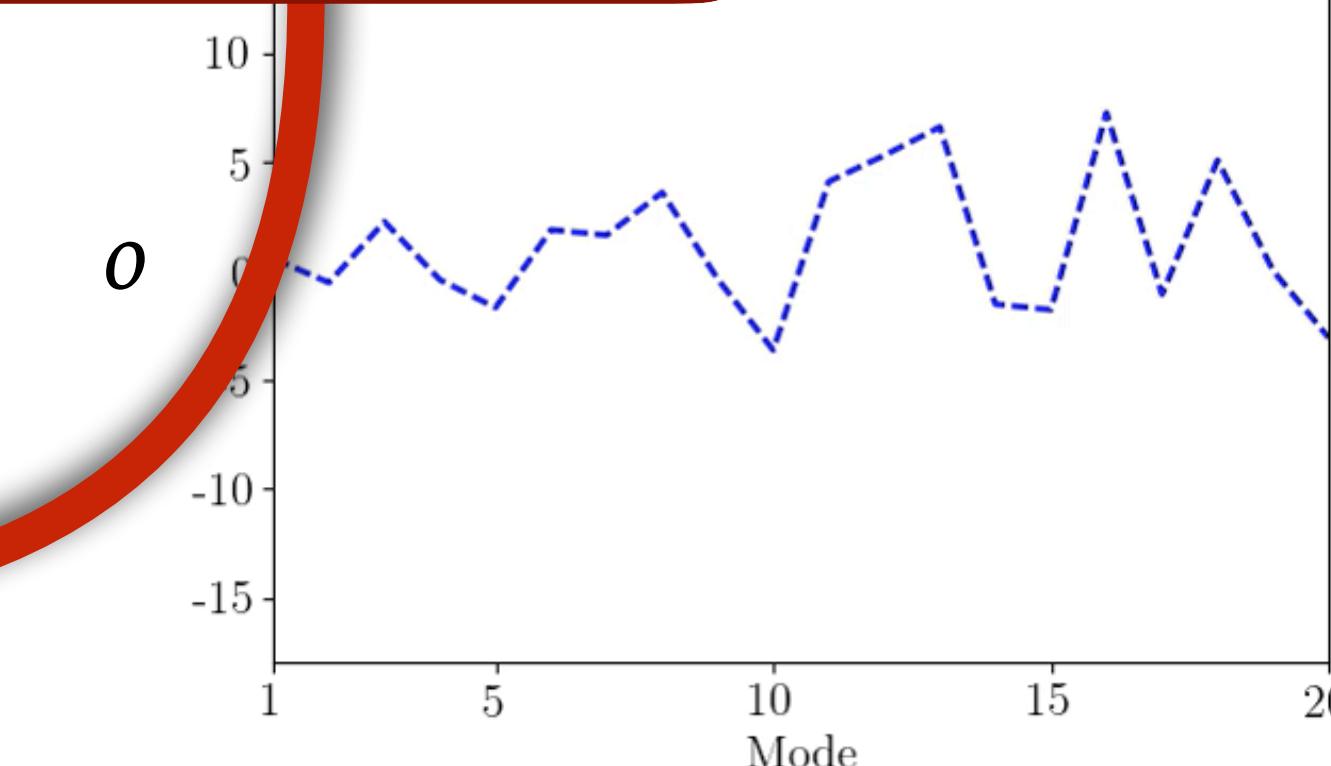
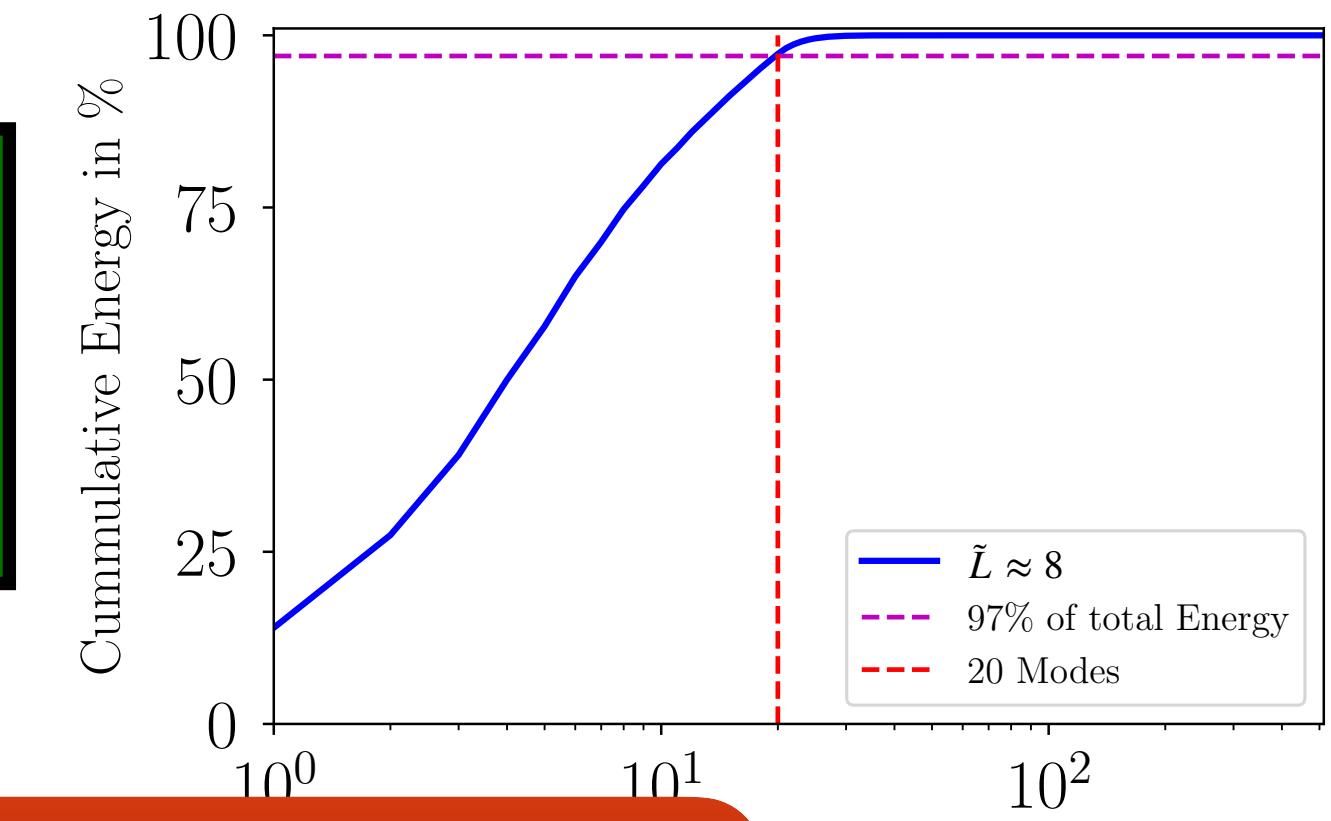
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**Training Data!**



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# Forecasting on UNSEEN data

- Iterative prediction in practice

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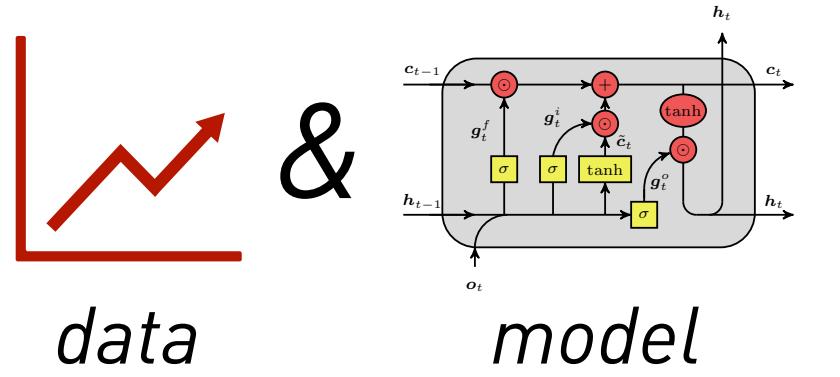
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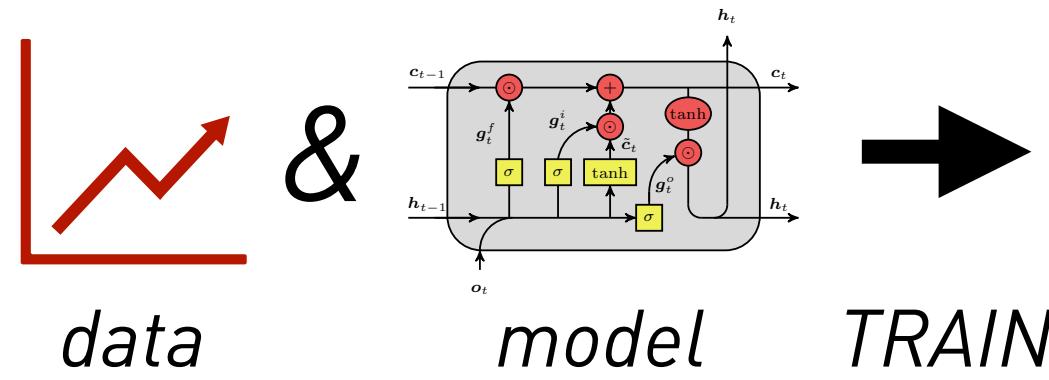
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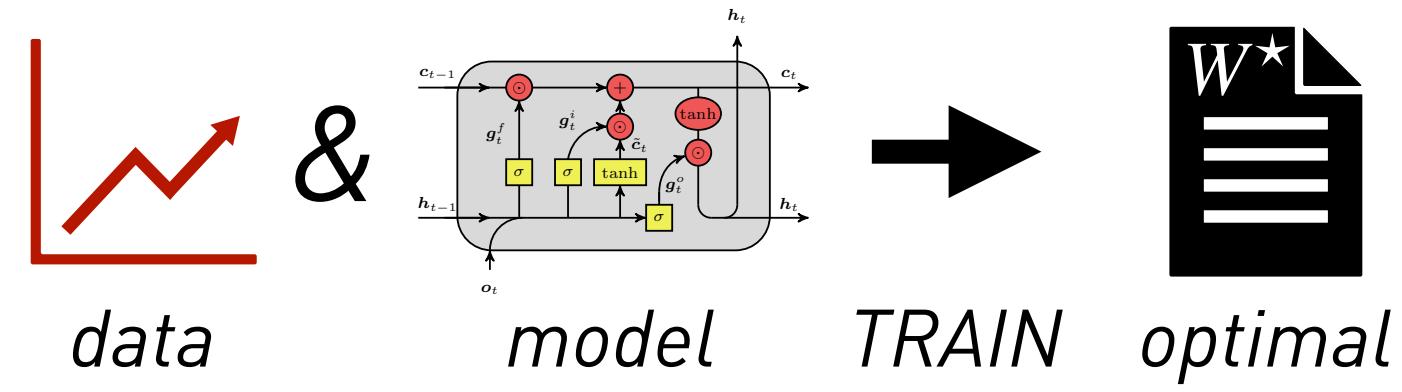
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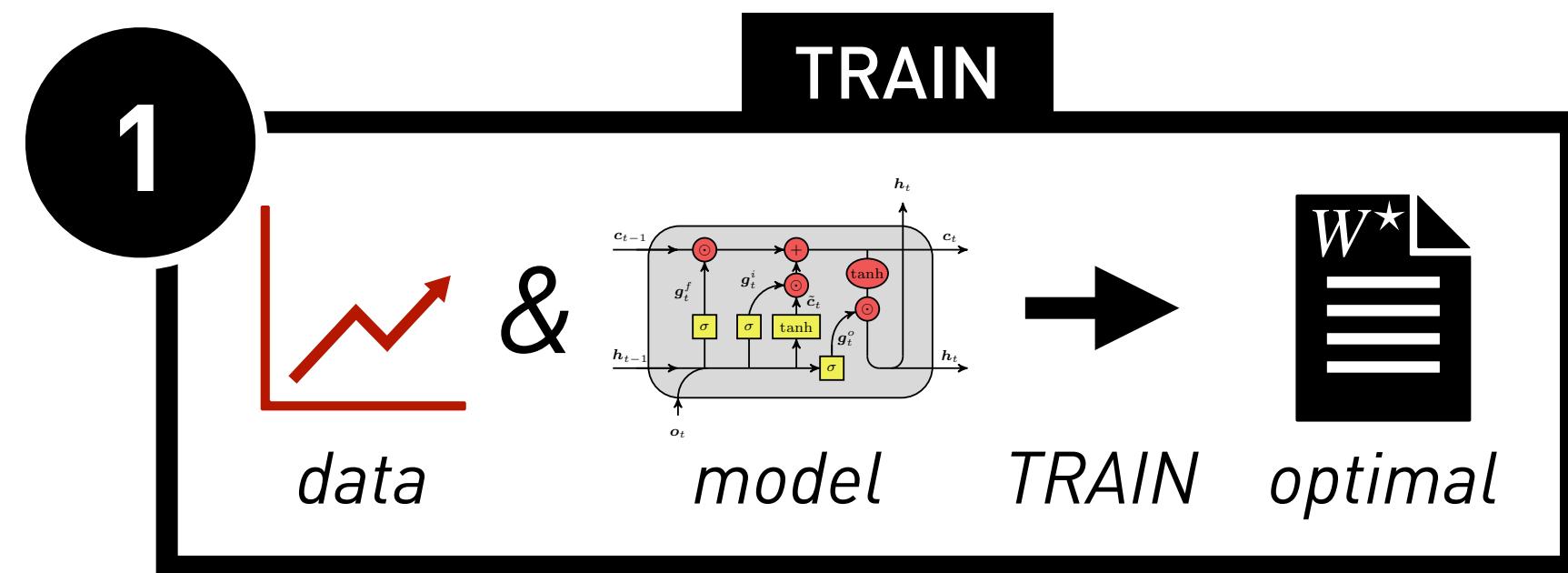


# Forecasting on UNSEEN data - Iterative prediction in practice



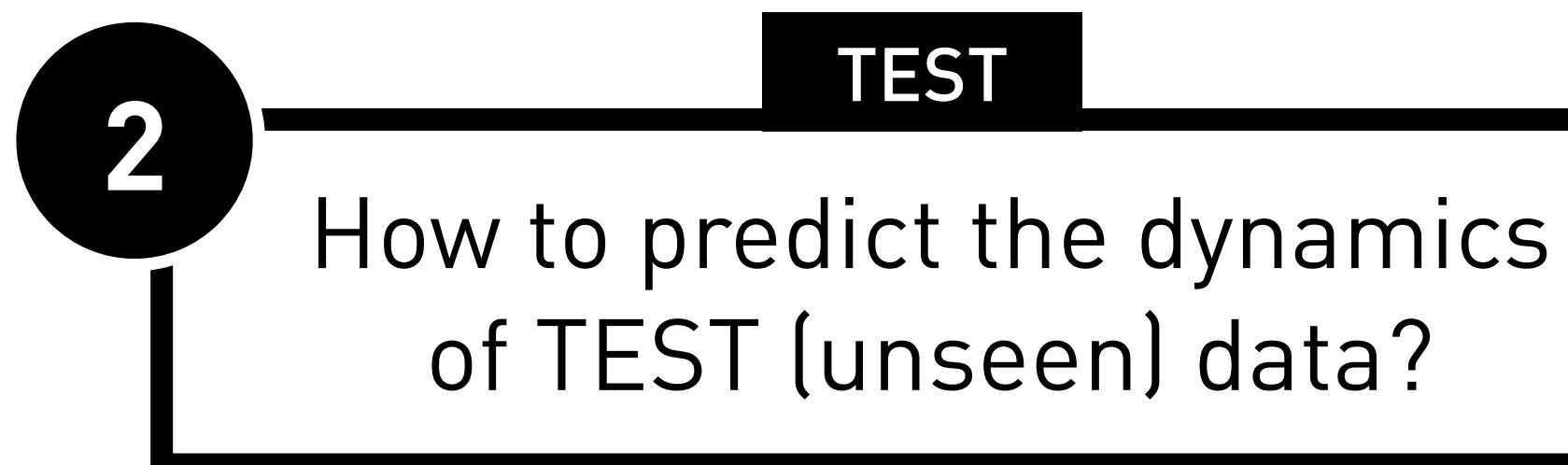
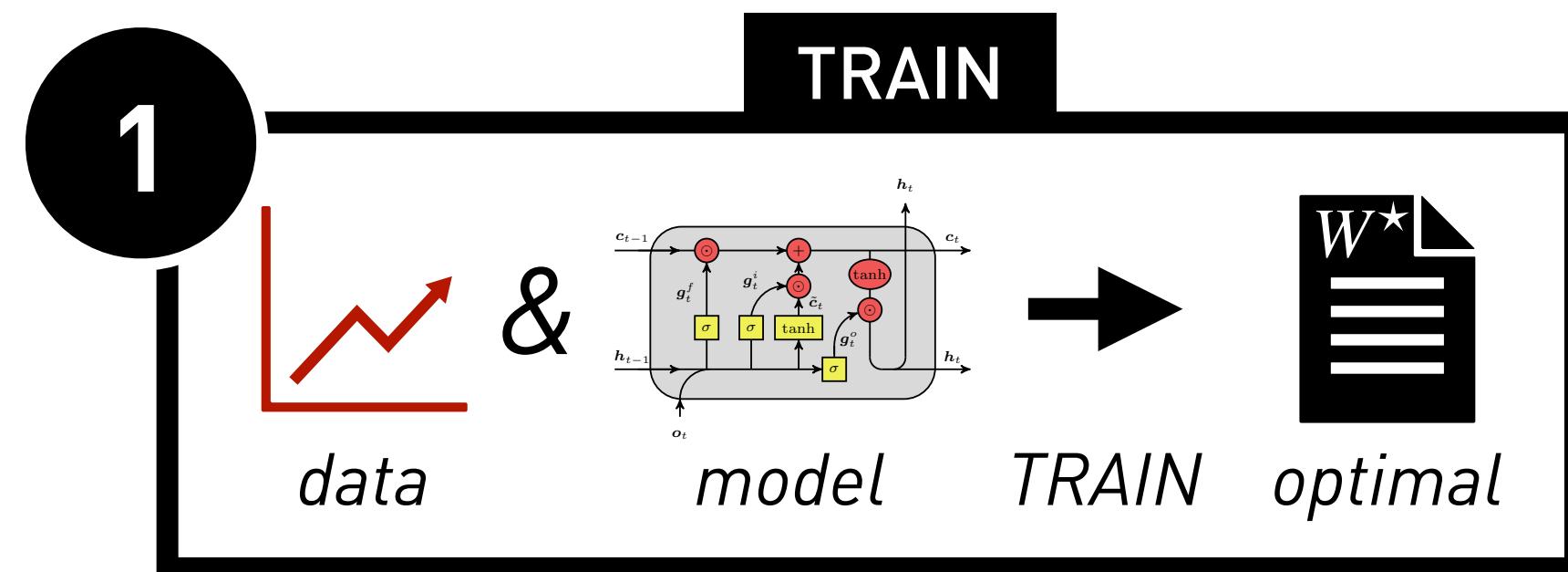
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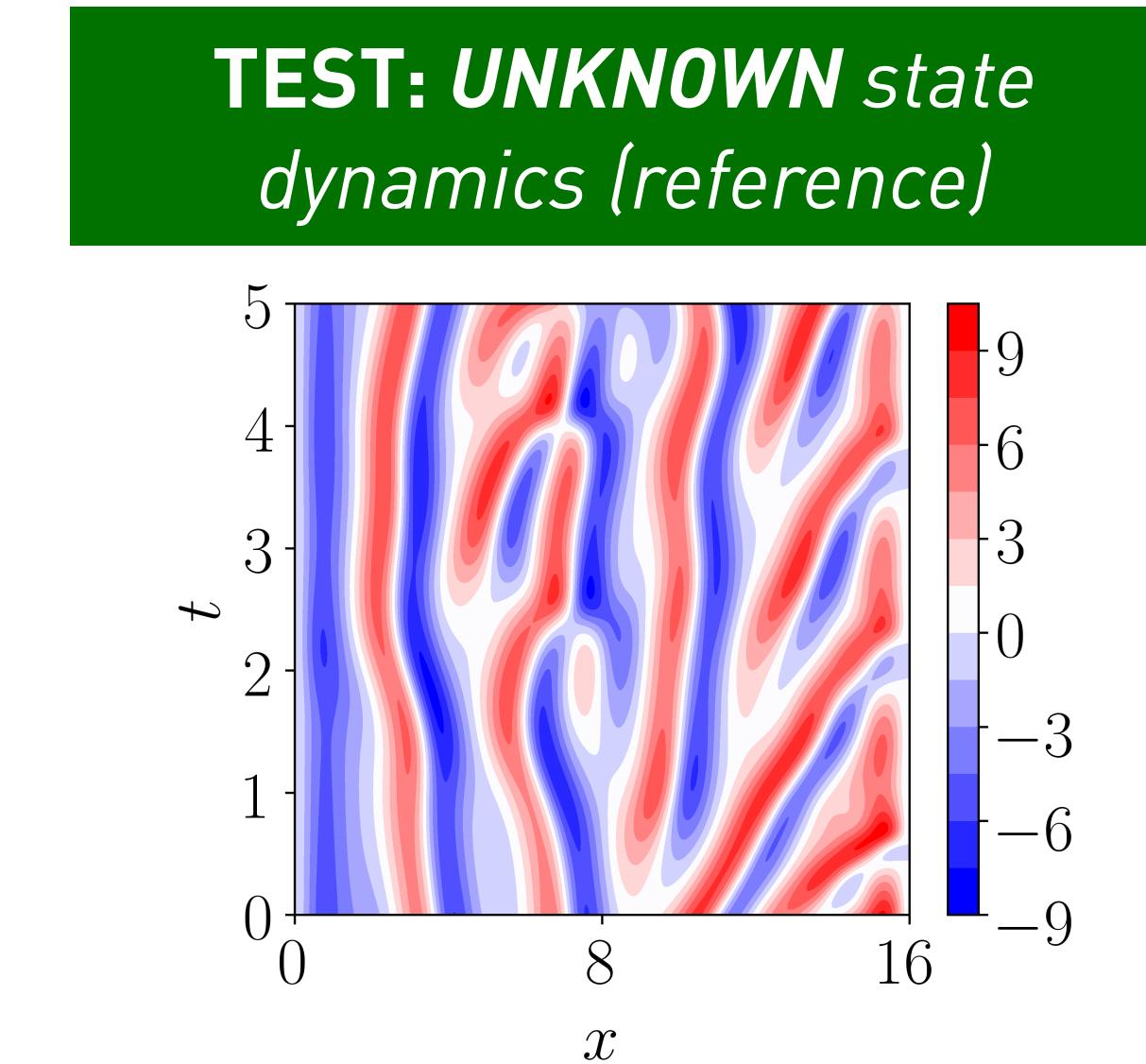
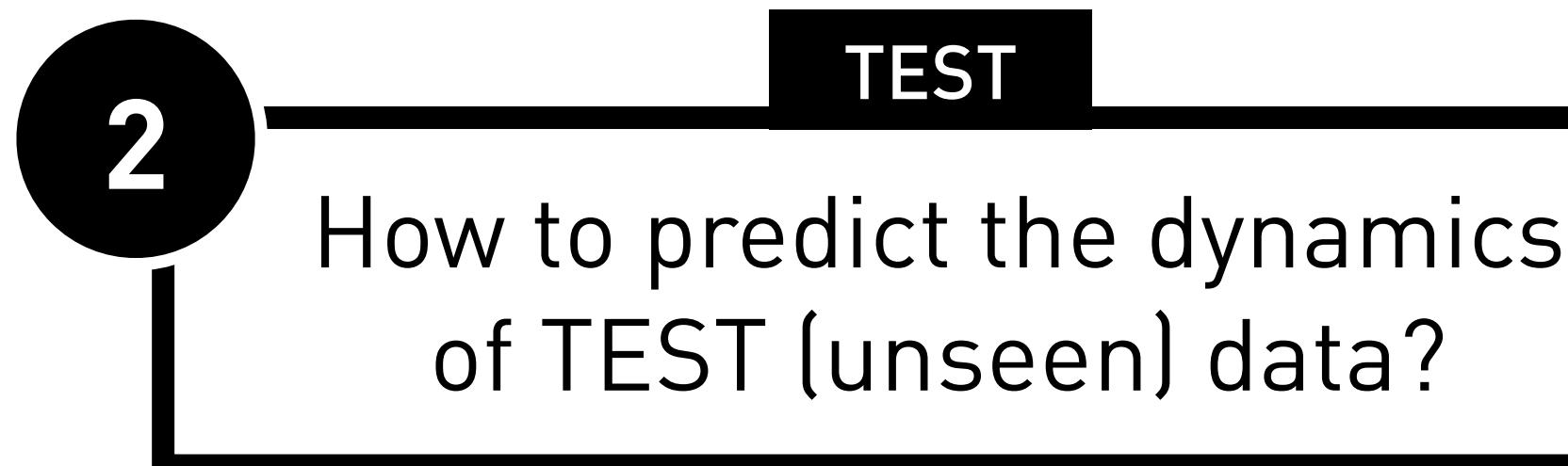
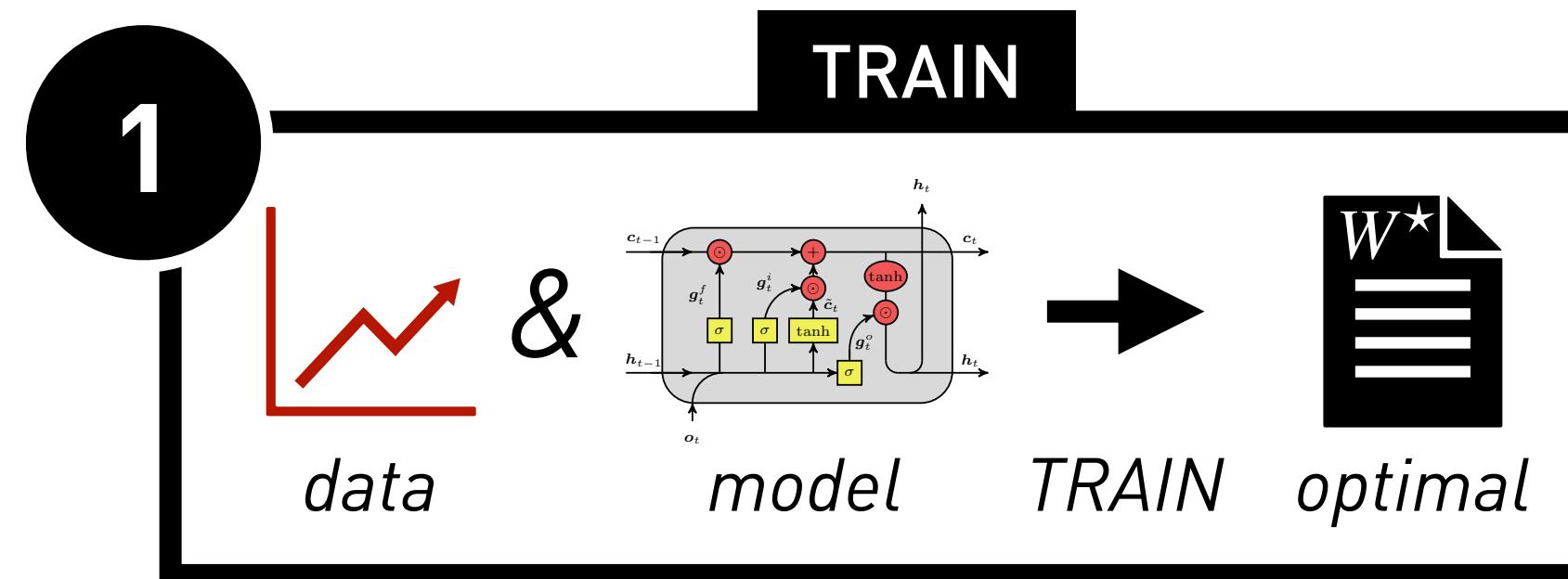
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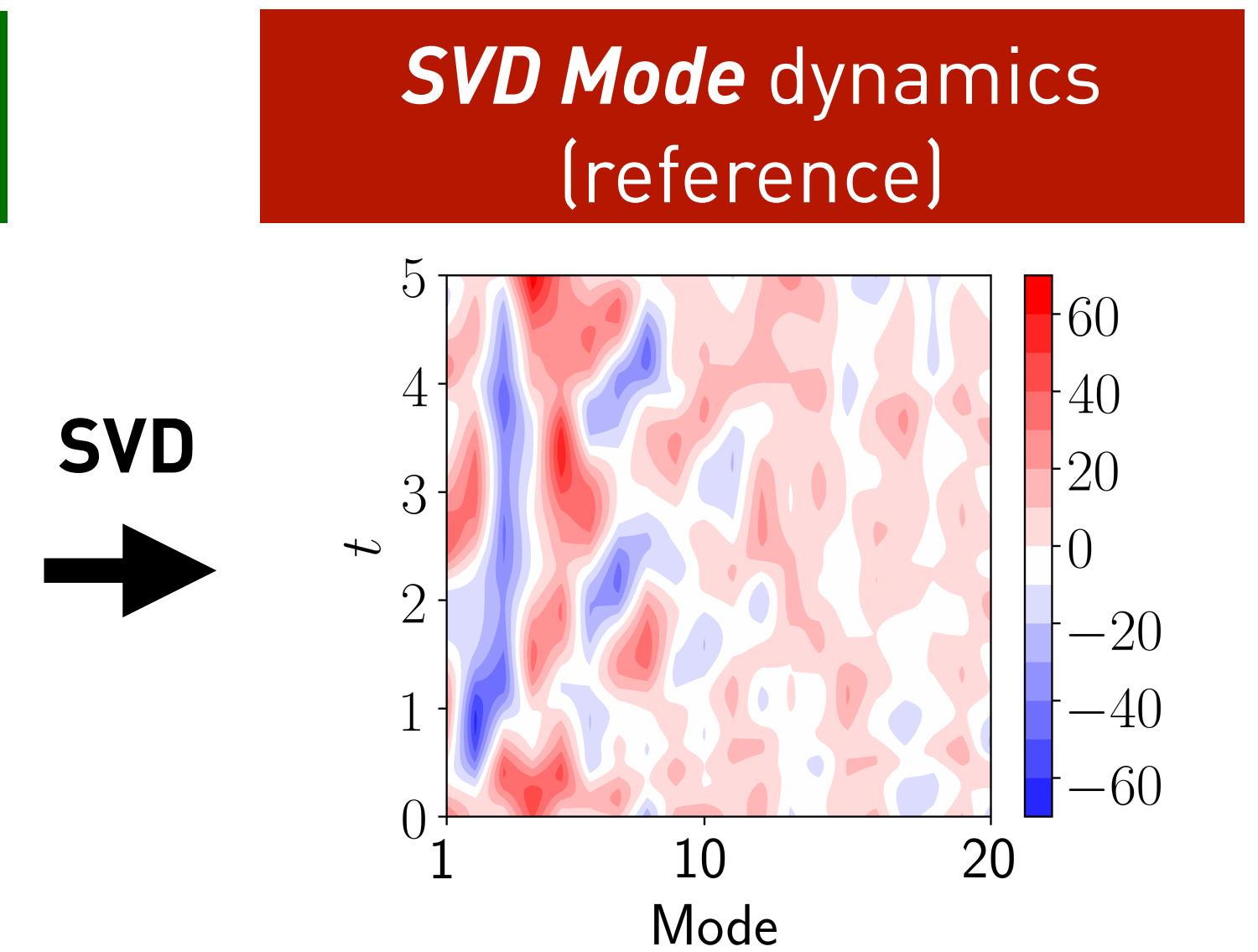
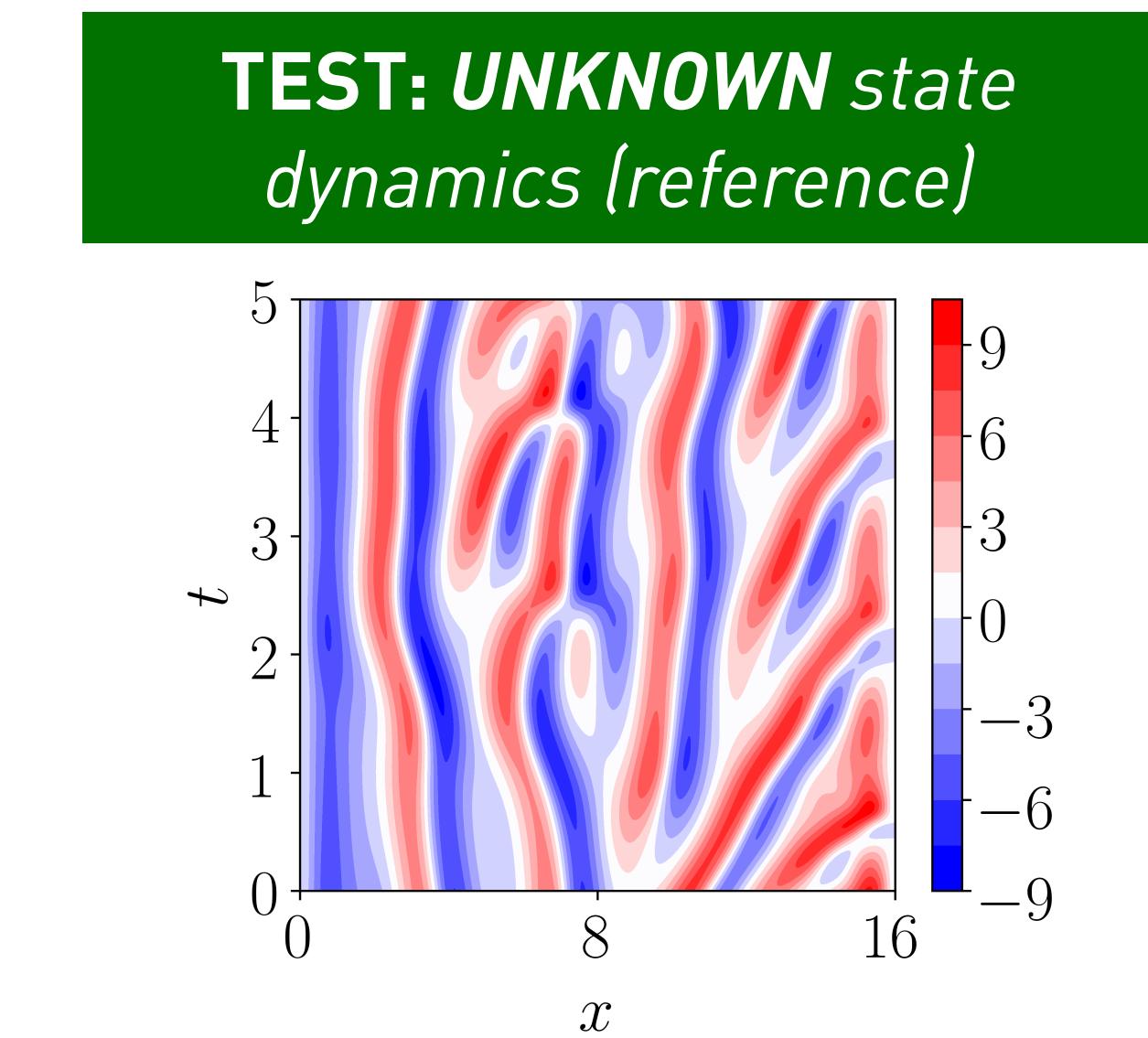
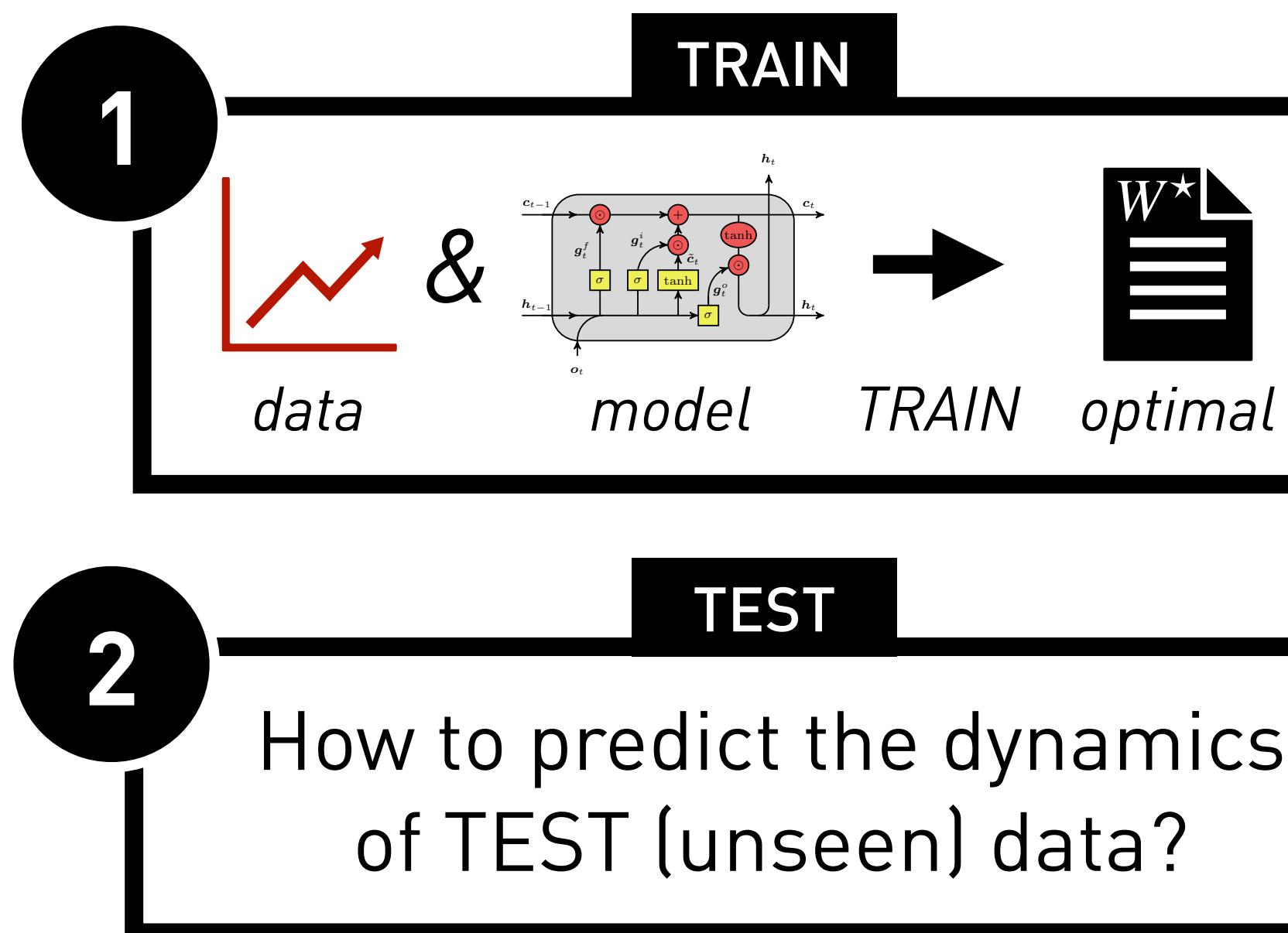
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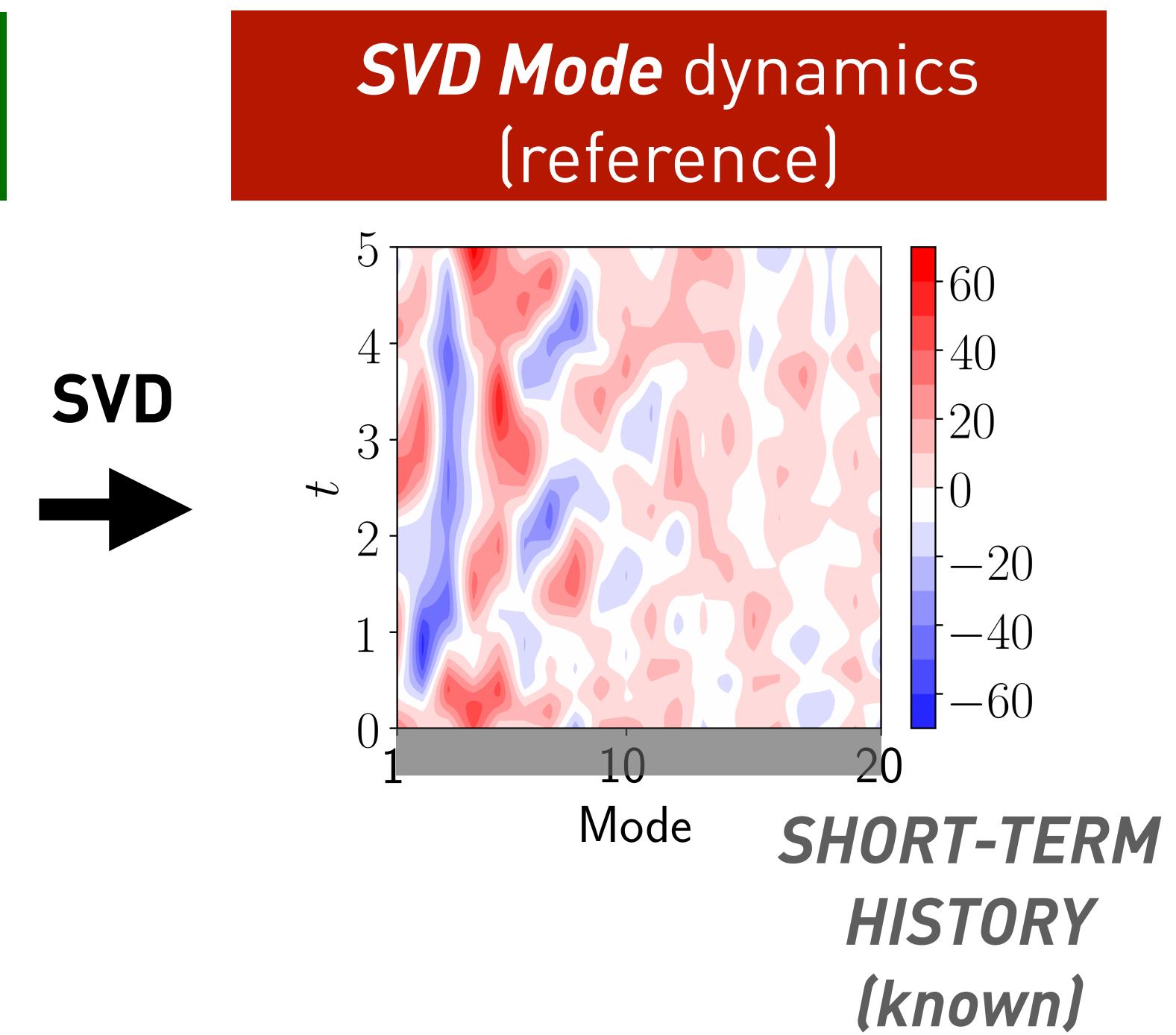
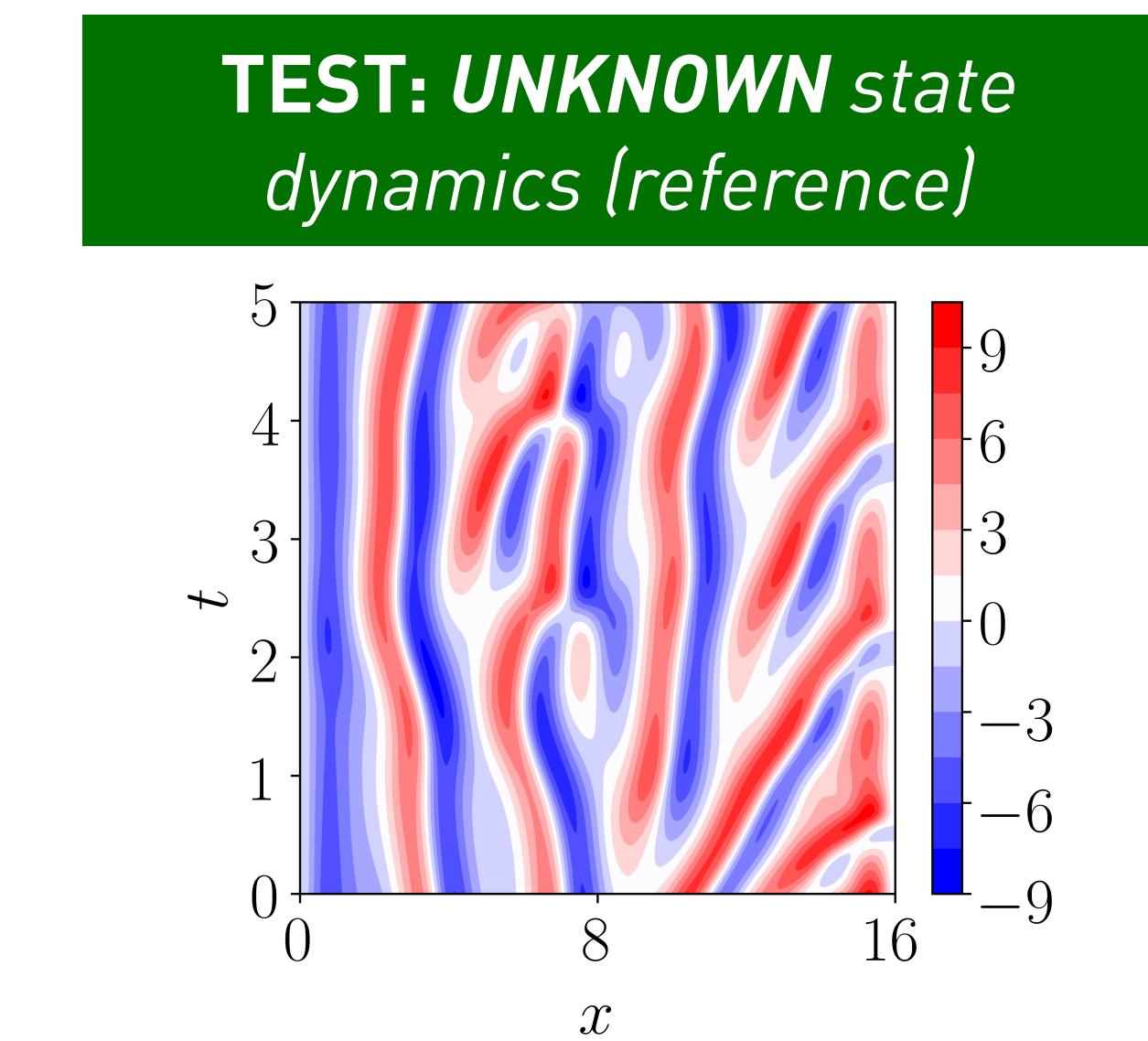
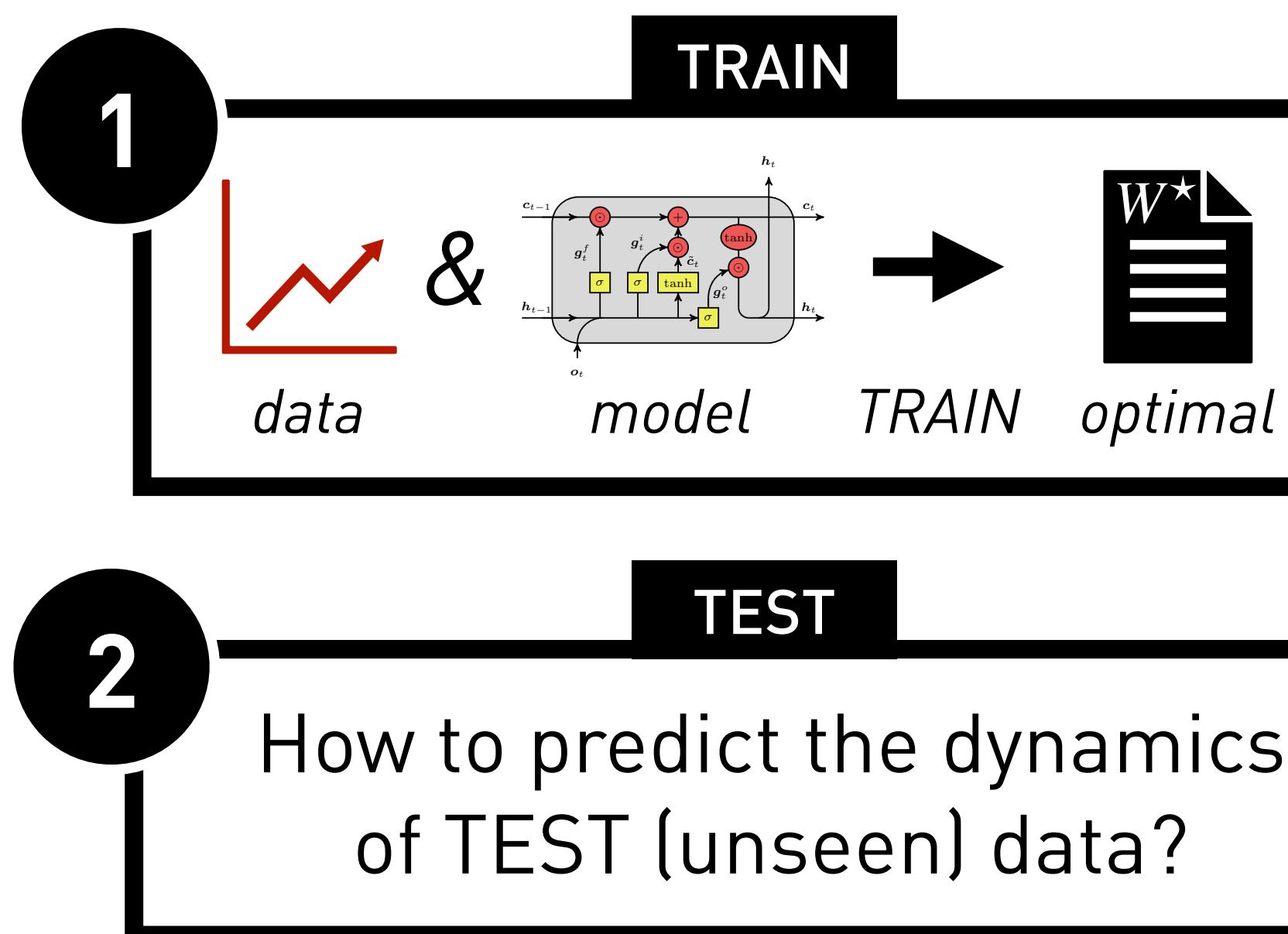
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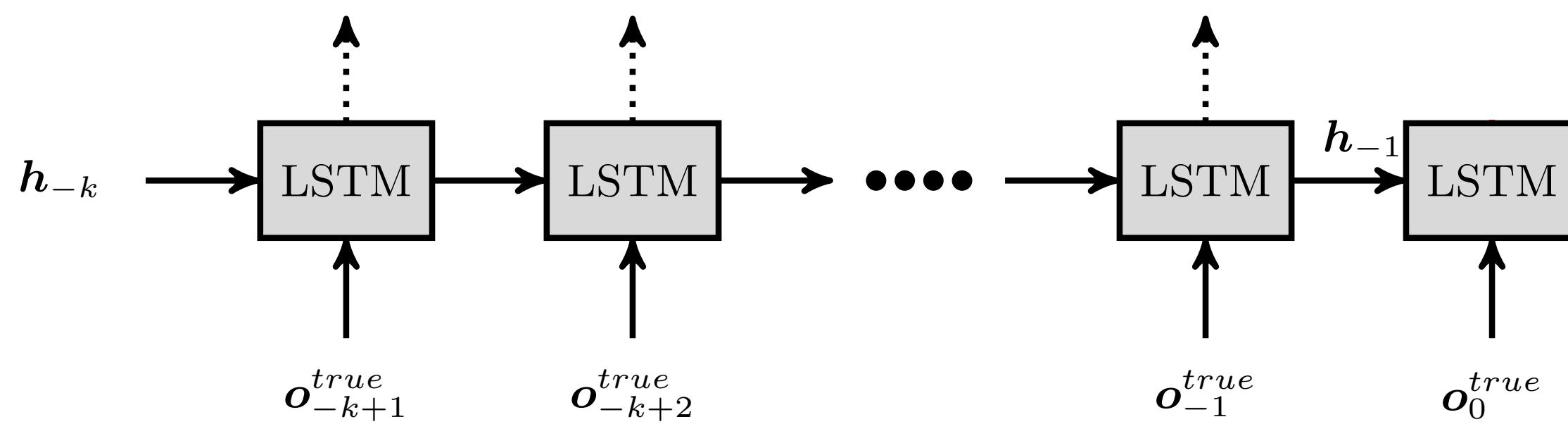
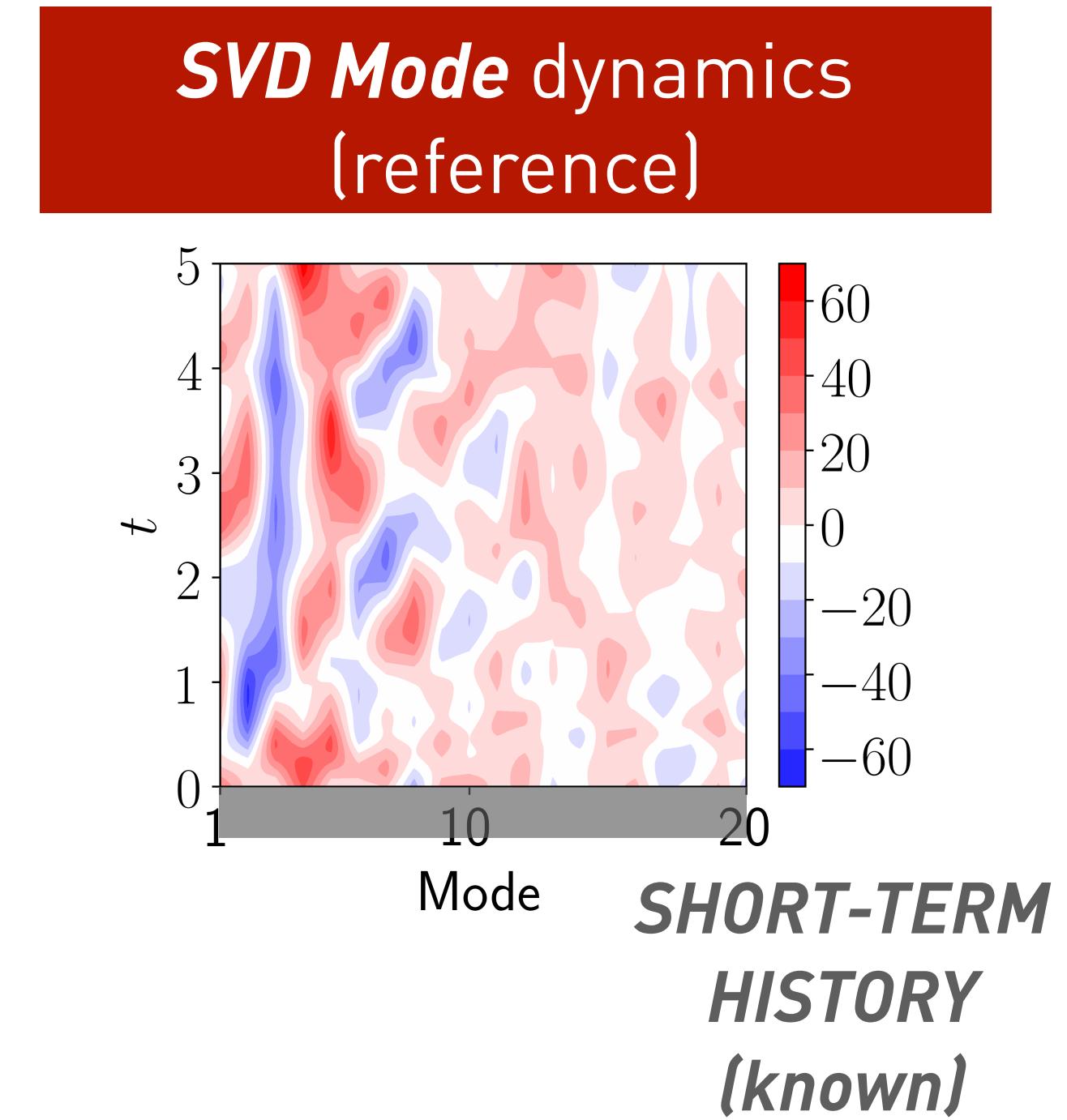
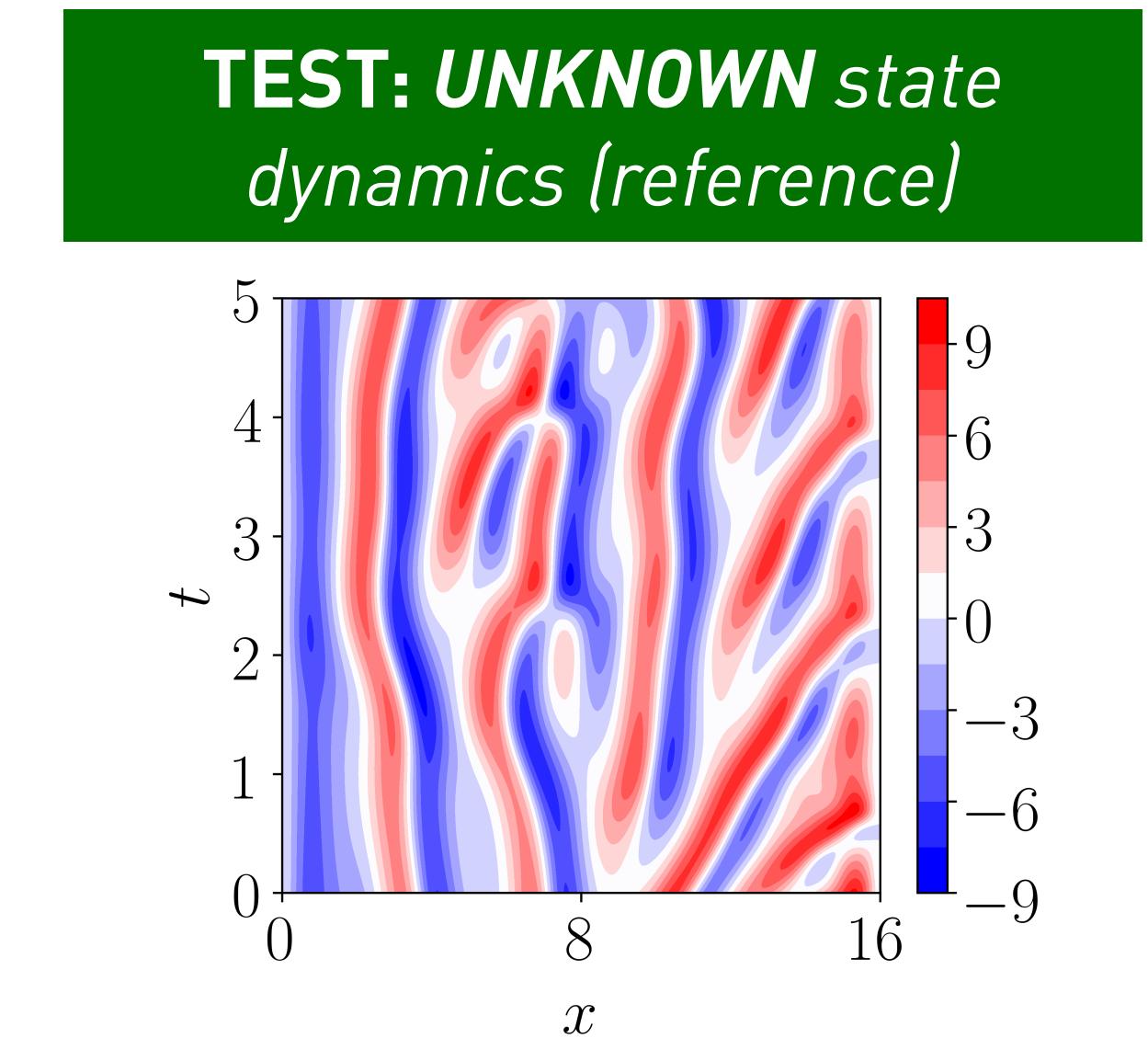
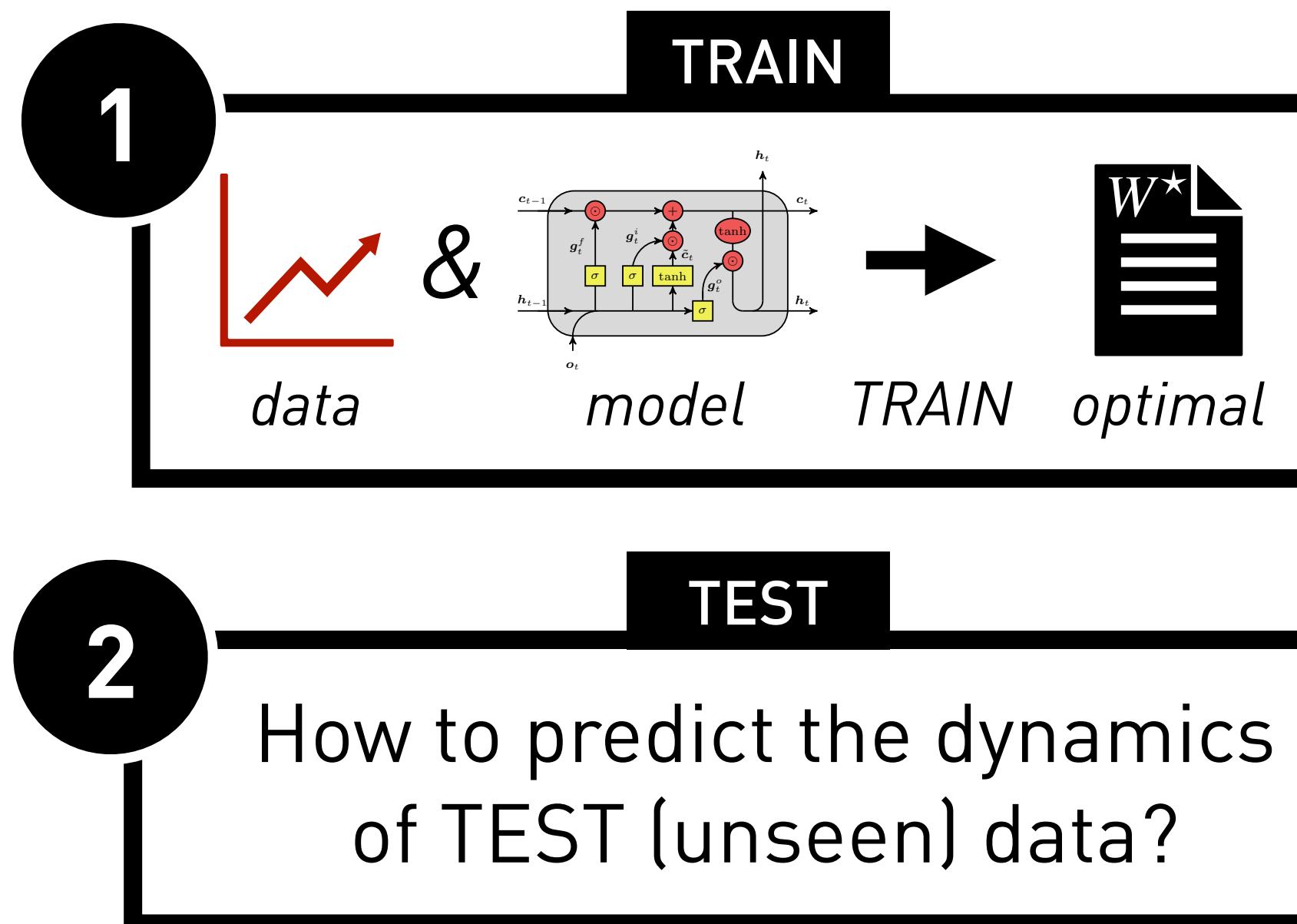
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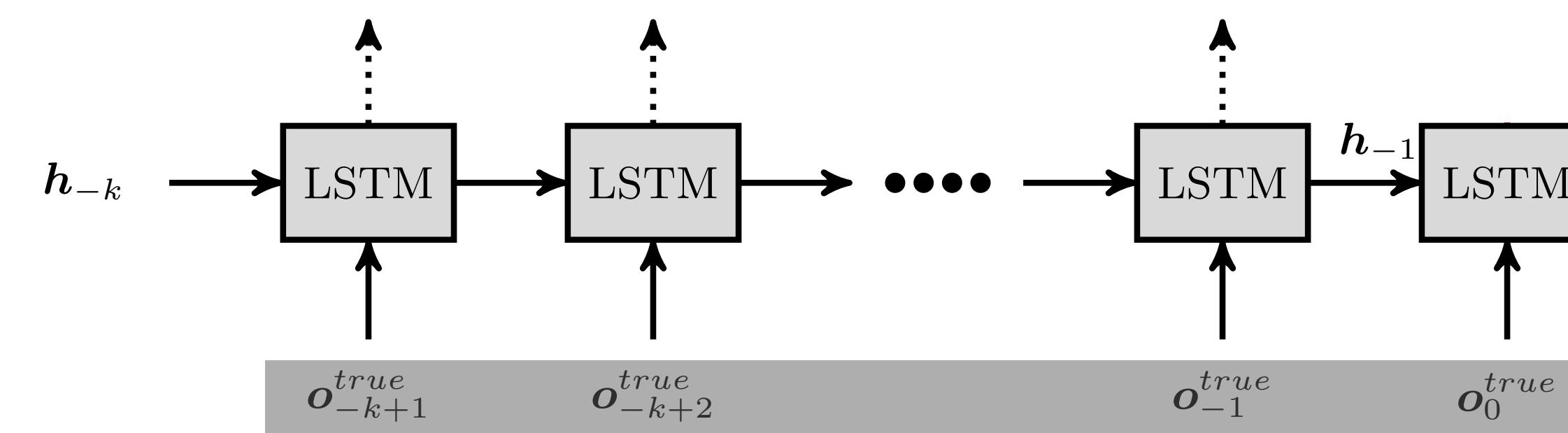
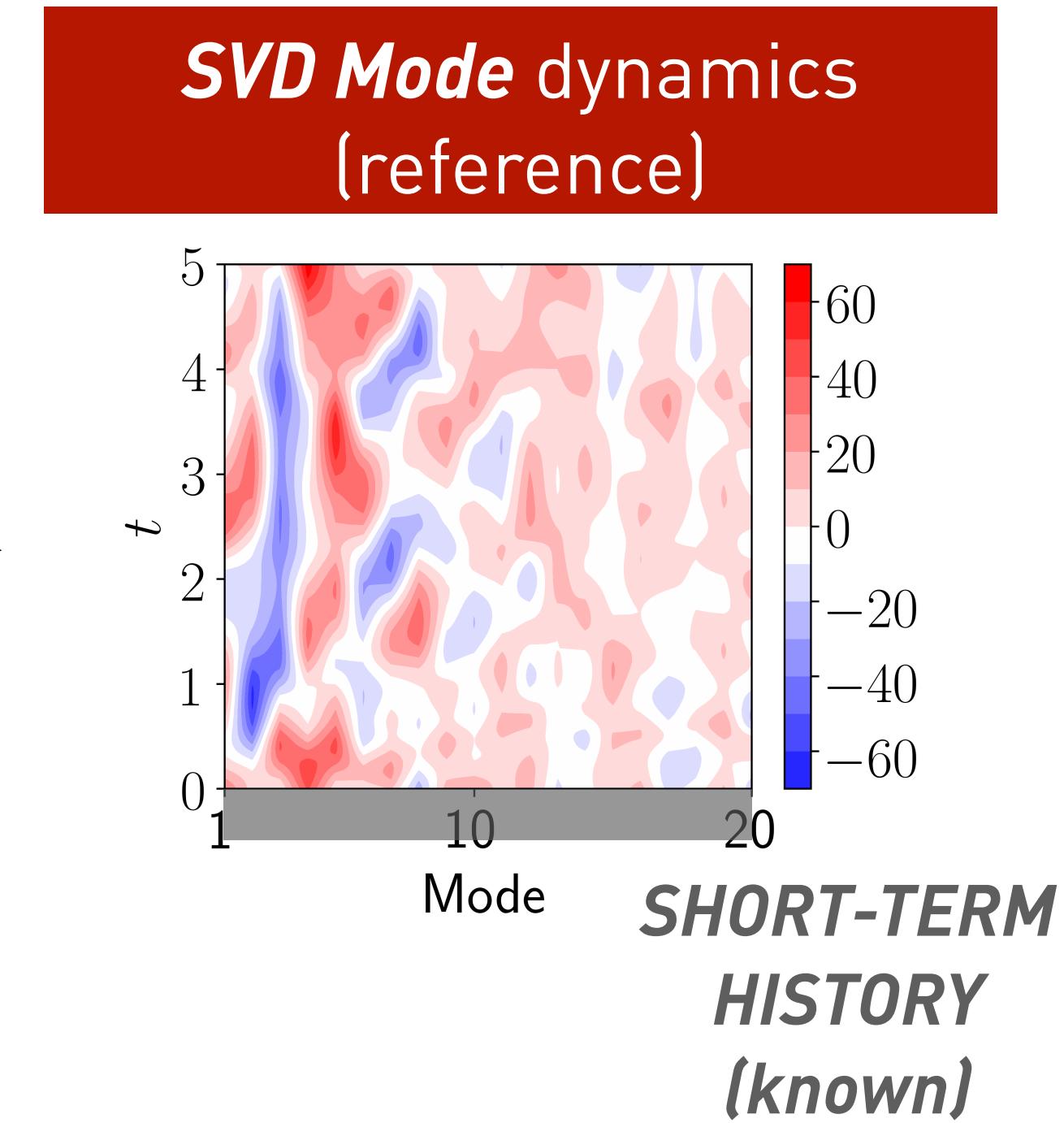
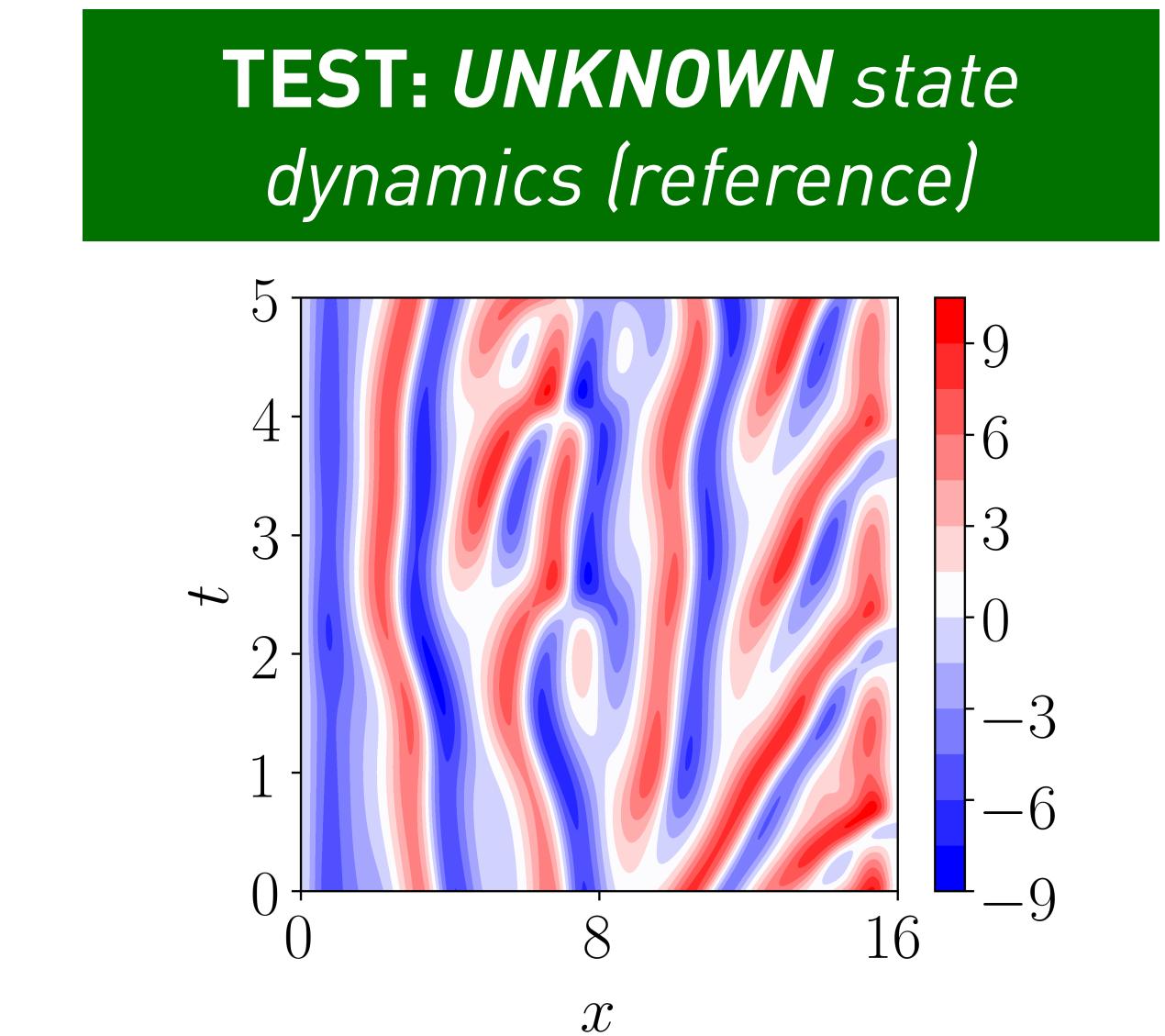
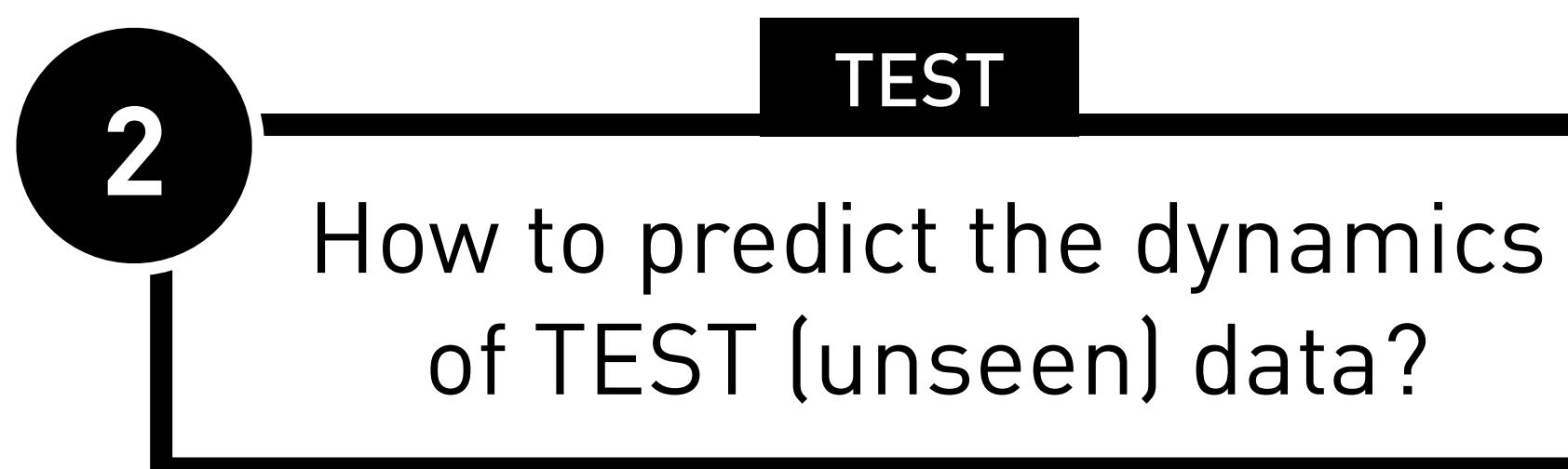
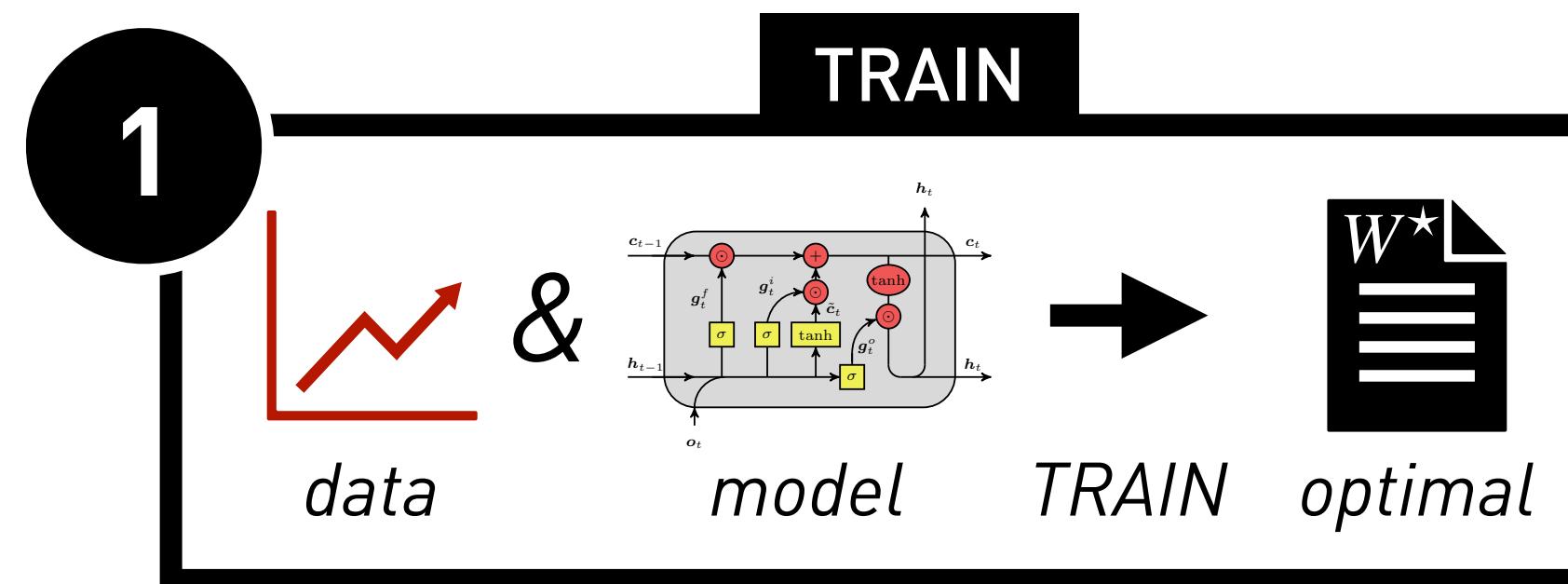
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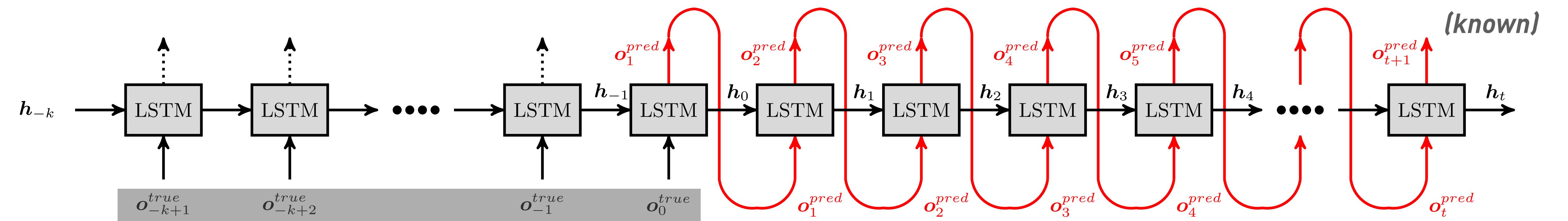
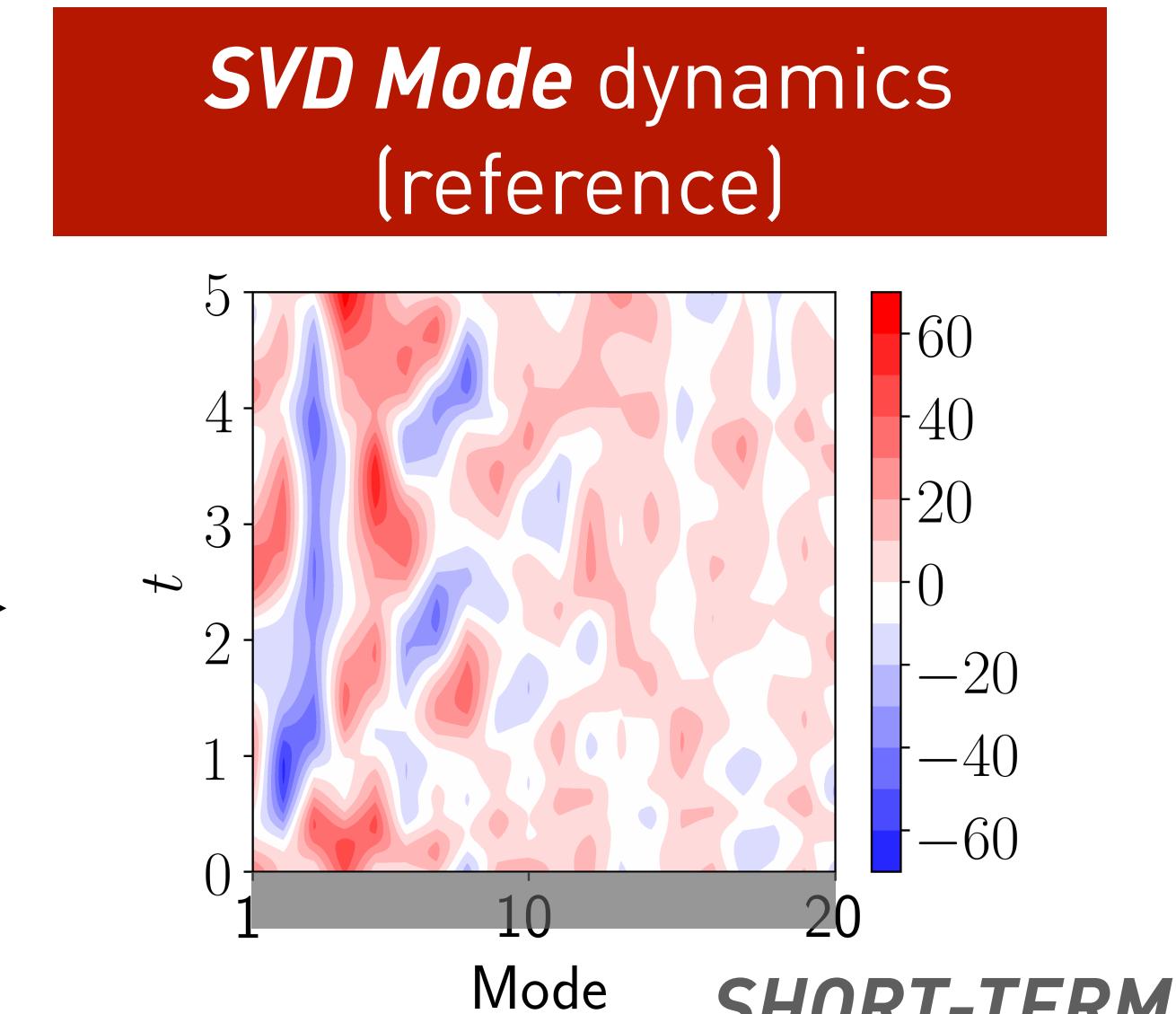
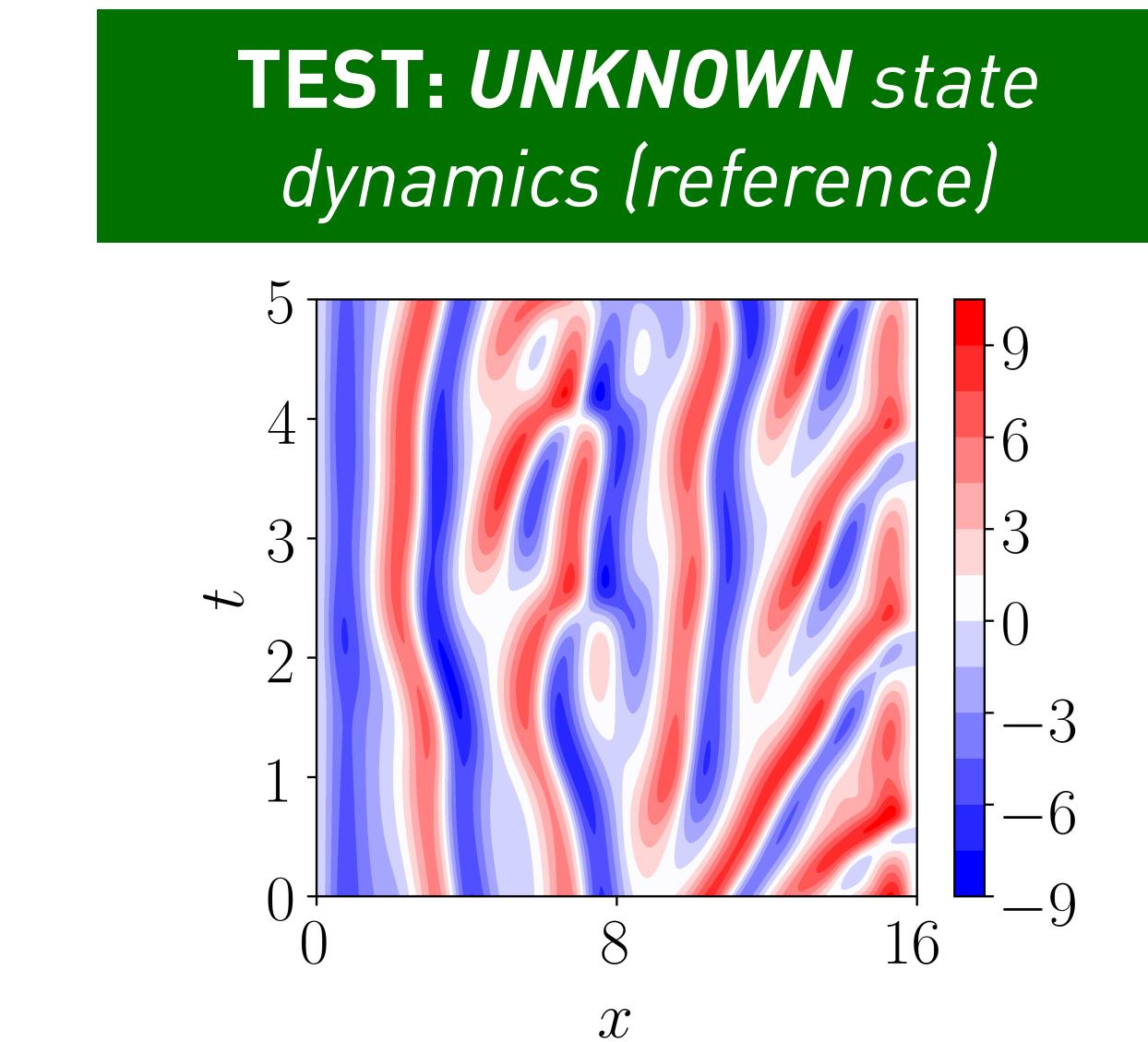
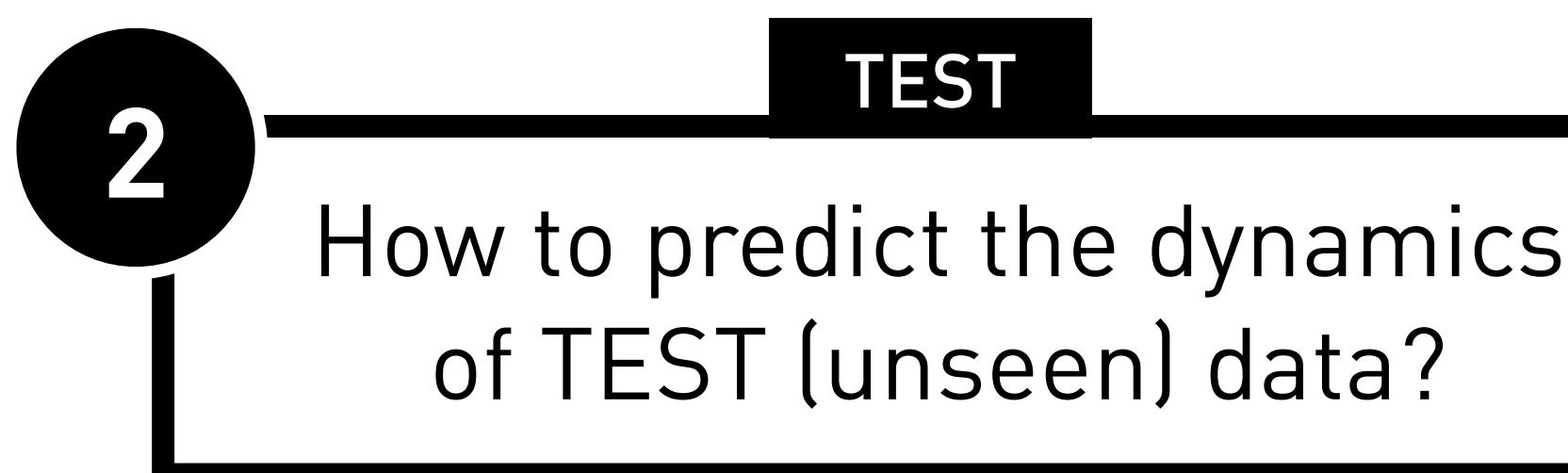
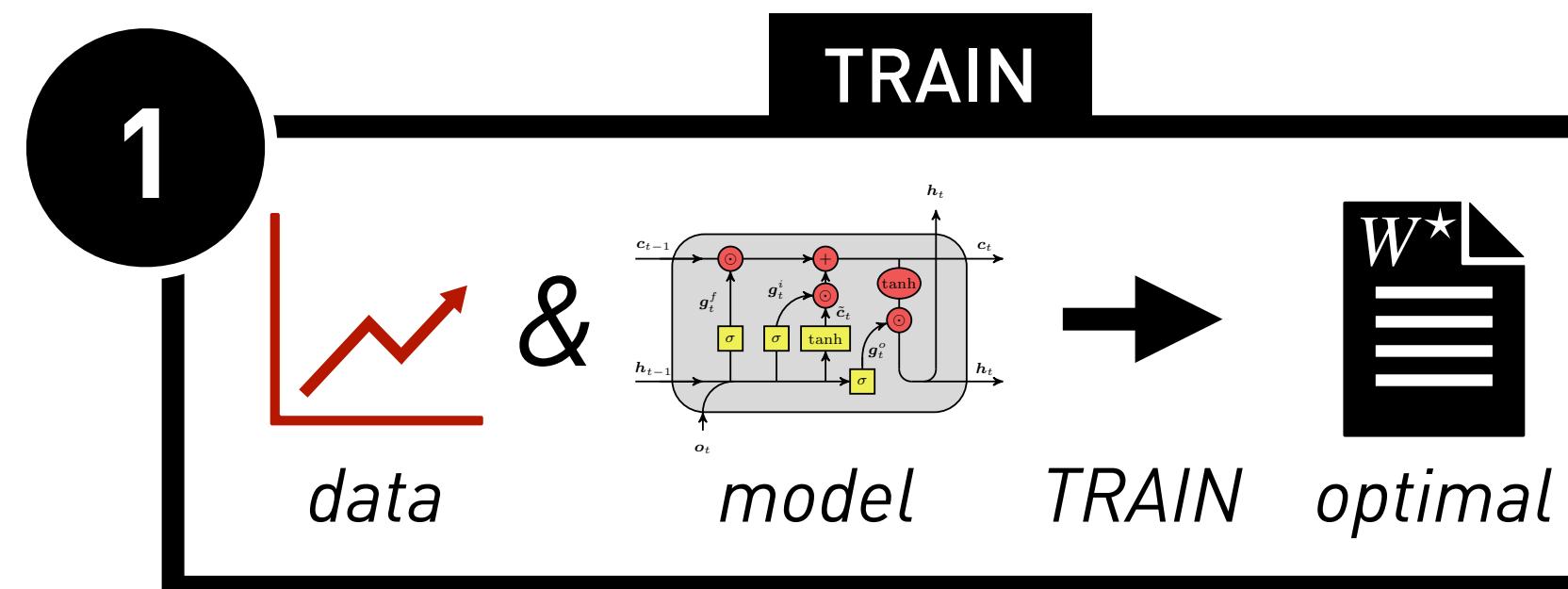
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**SHORT-TERM HISTORY (known)**

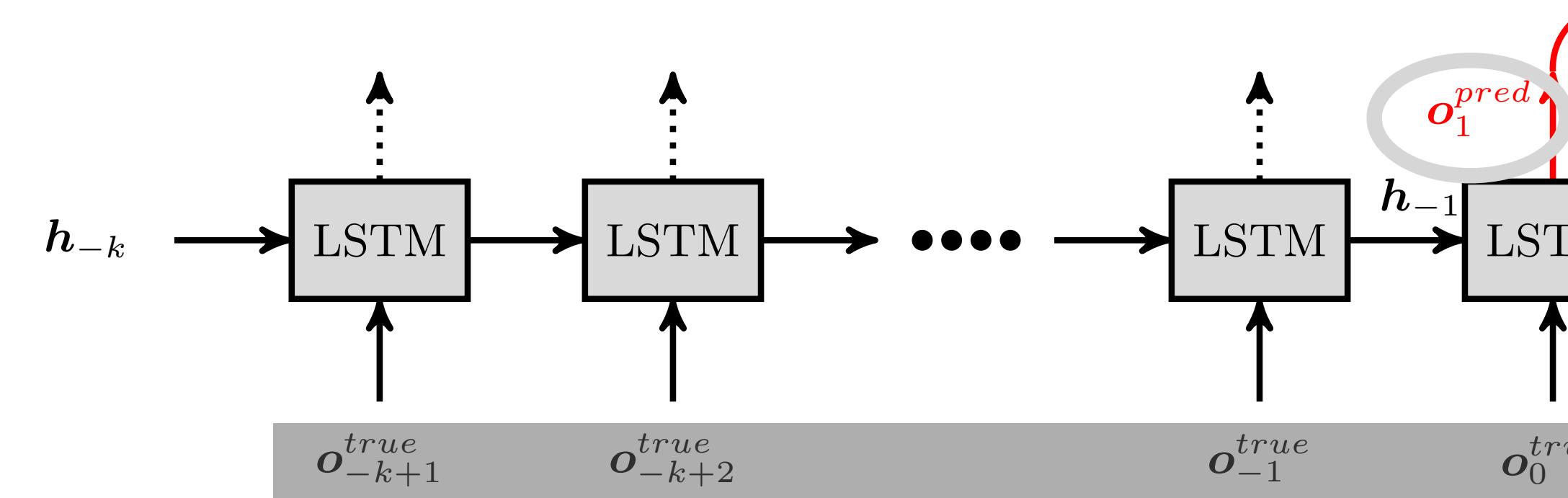
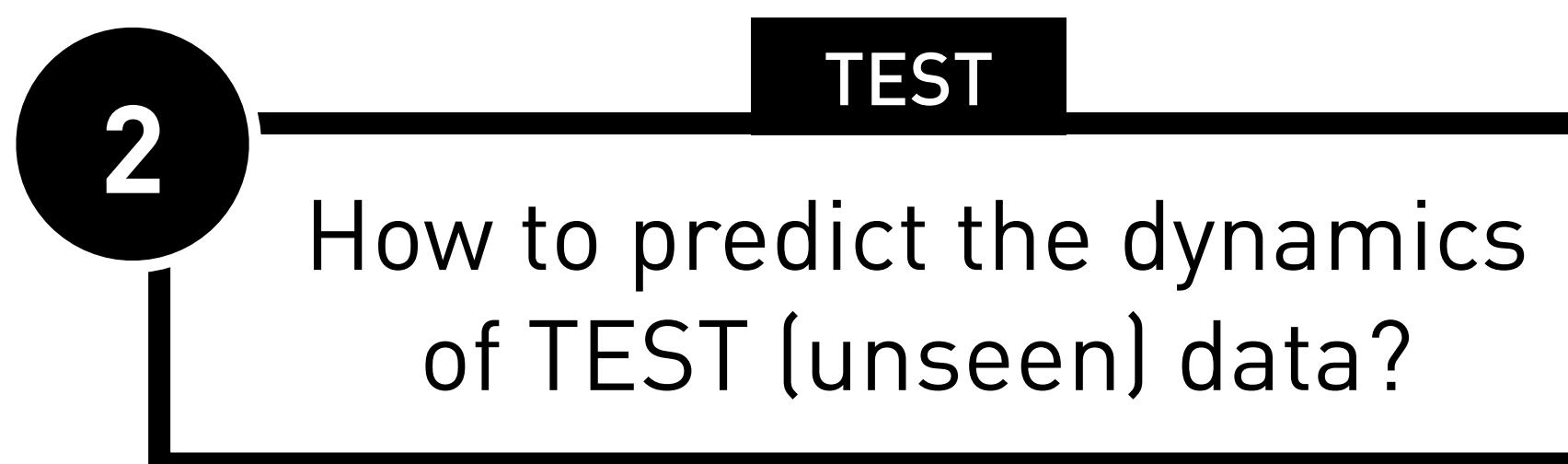
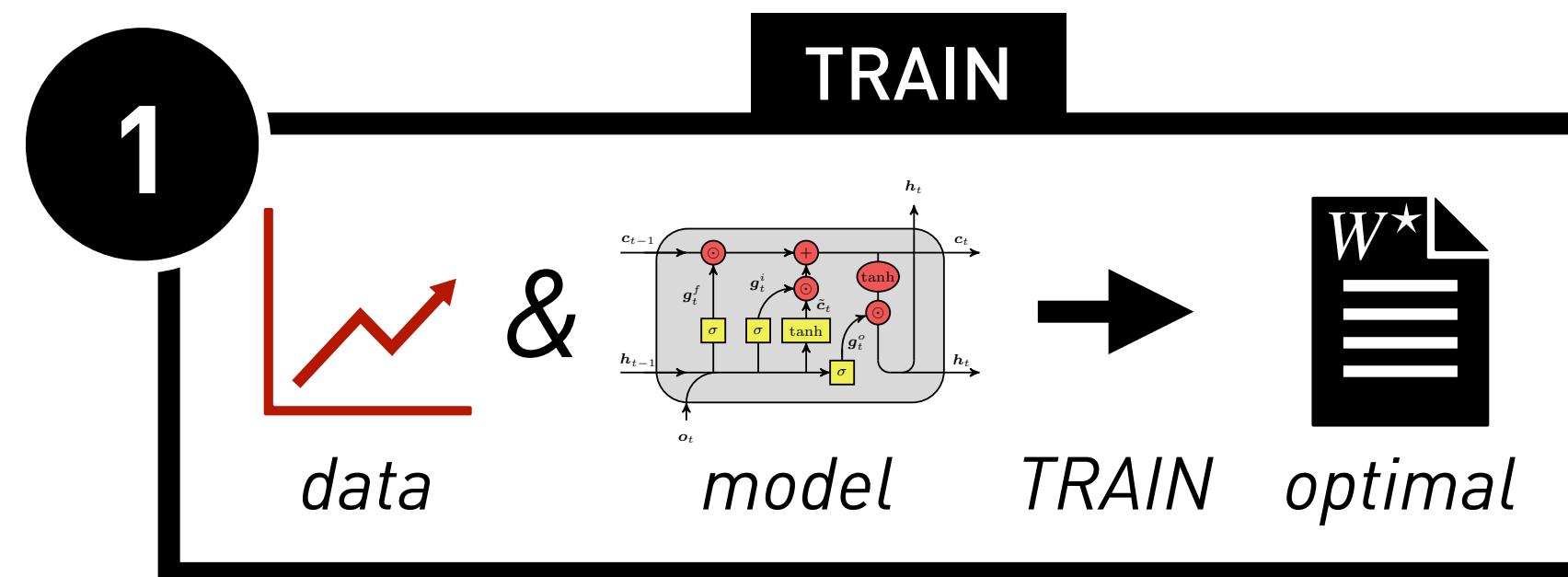
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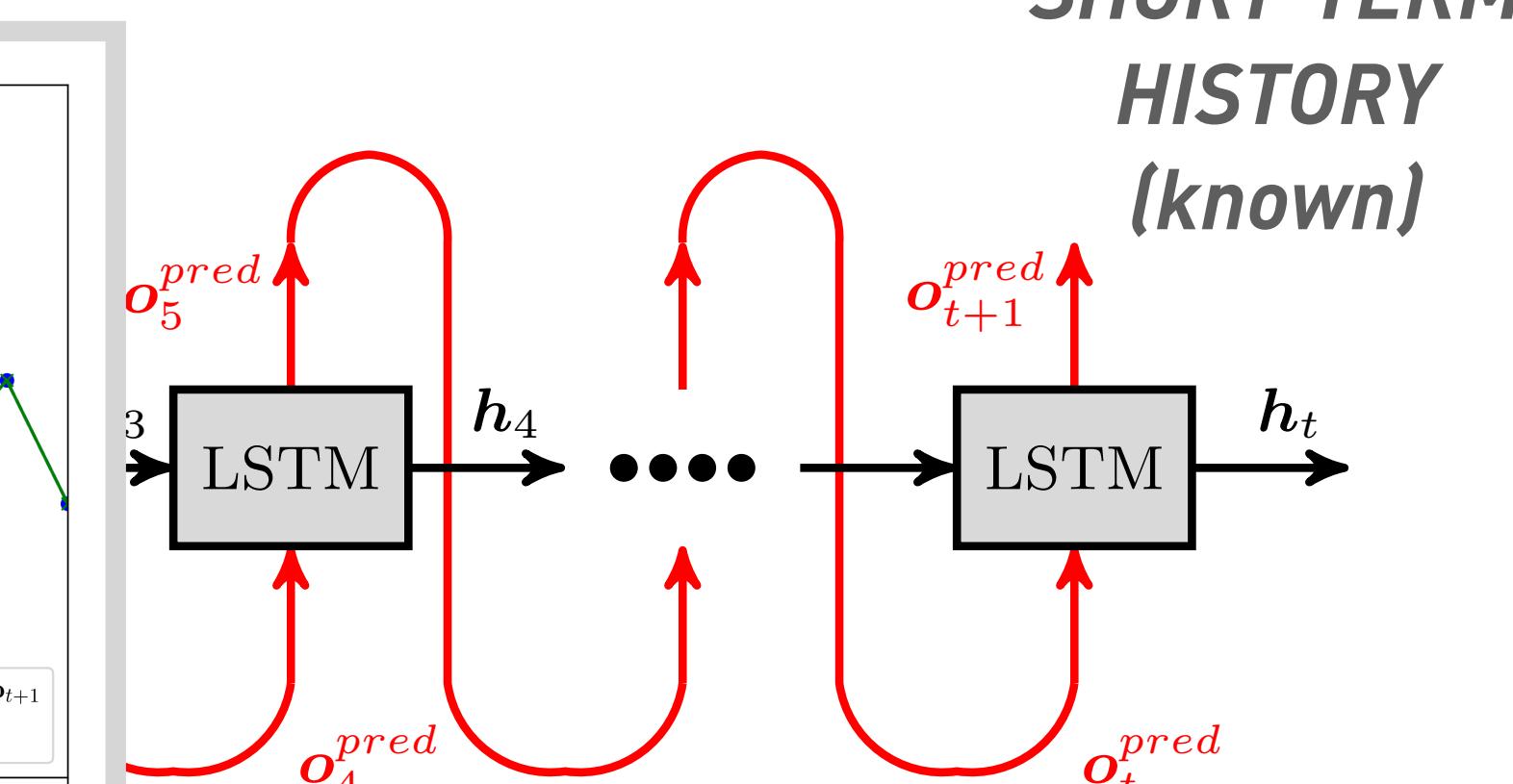
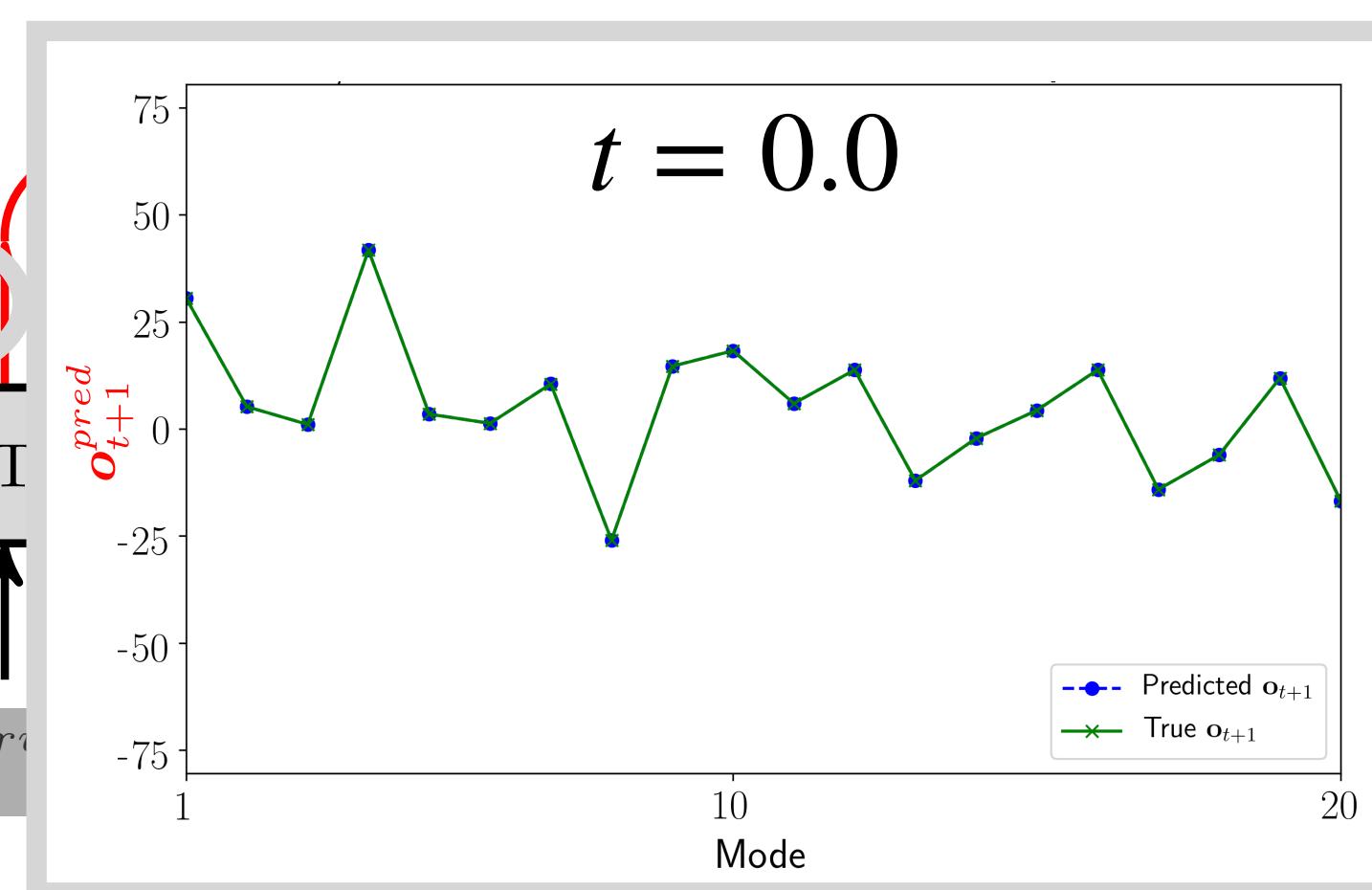
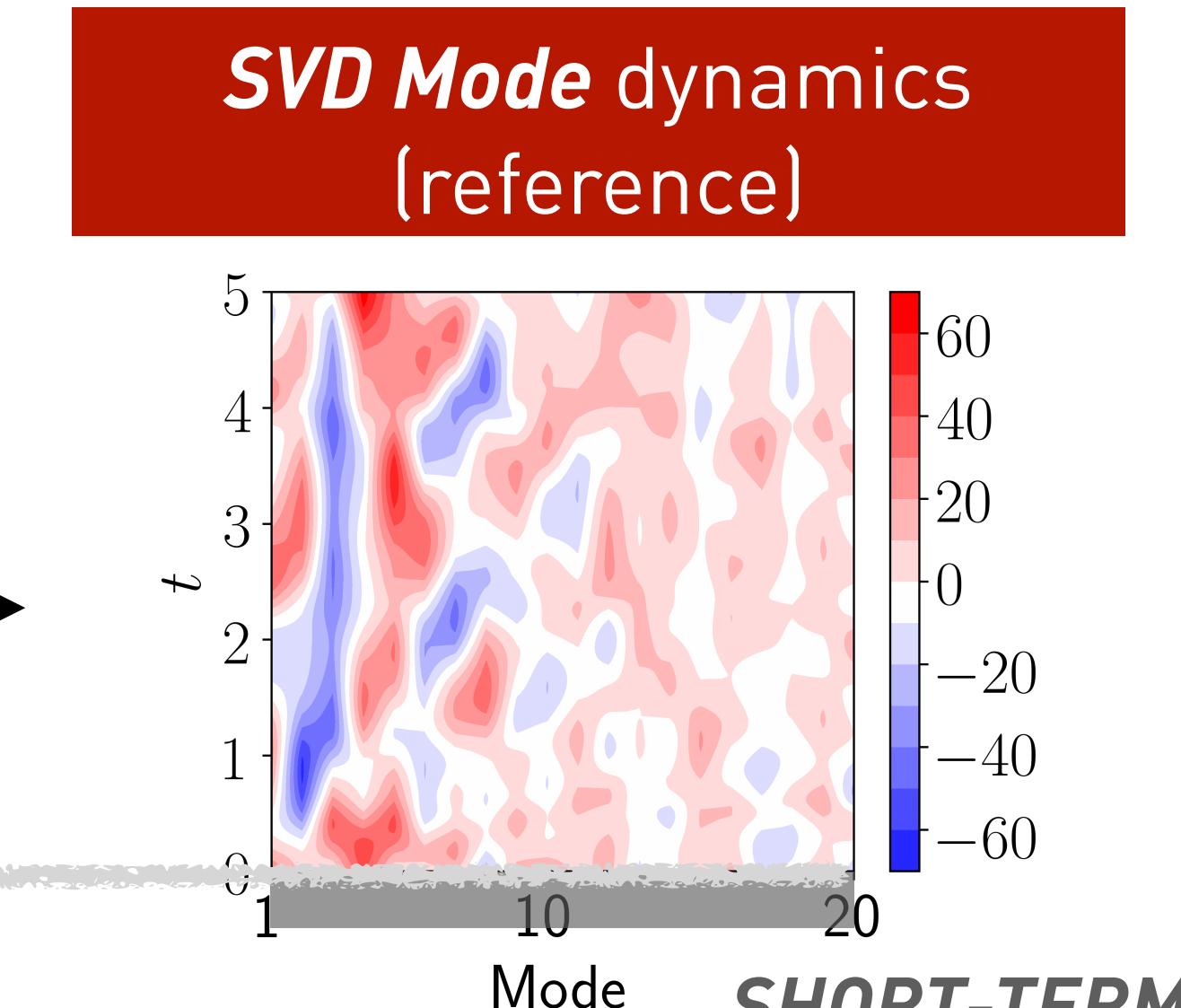
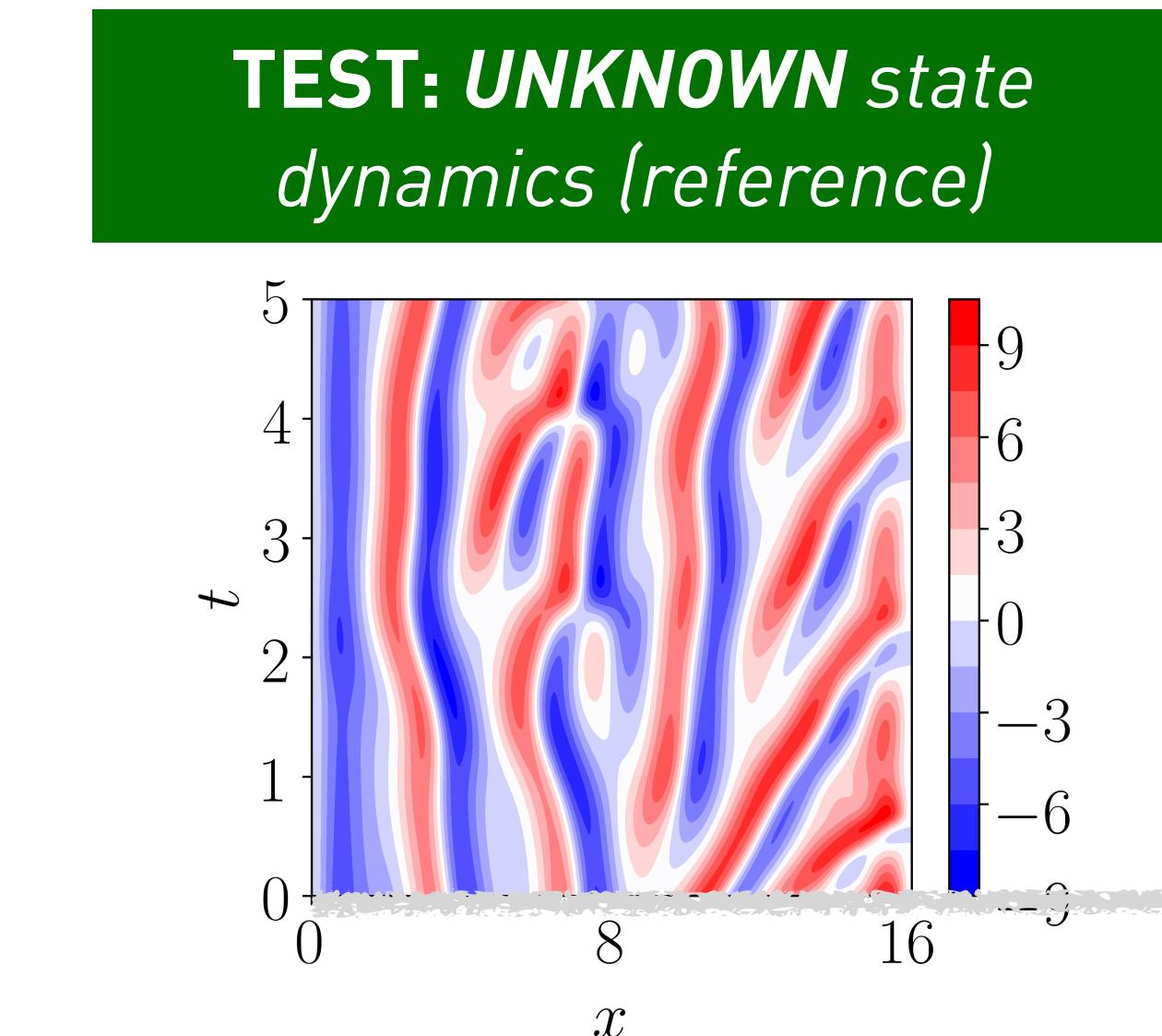


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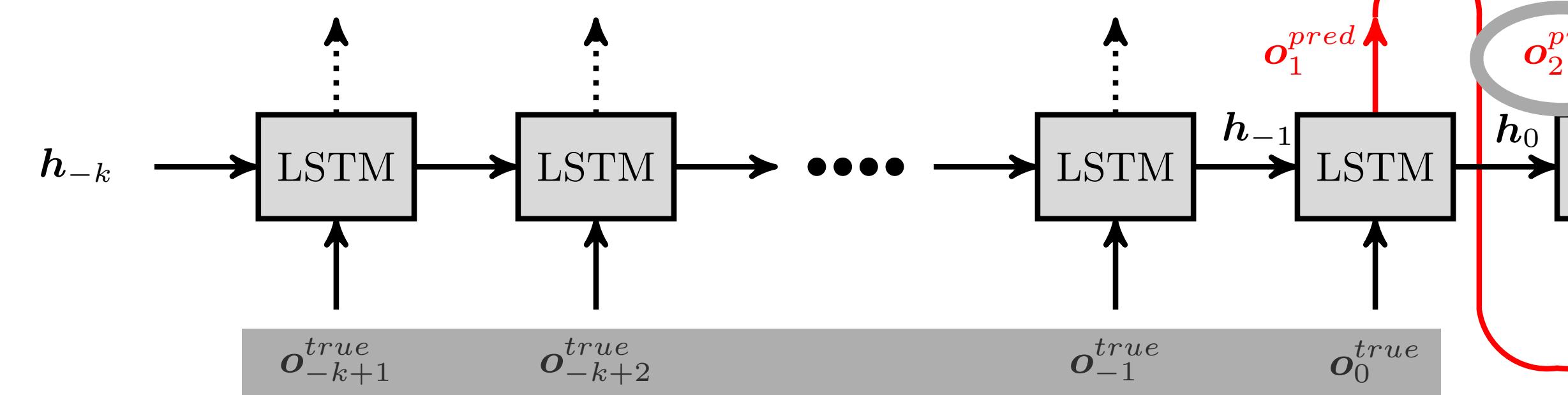
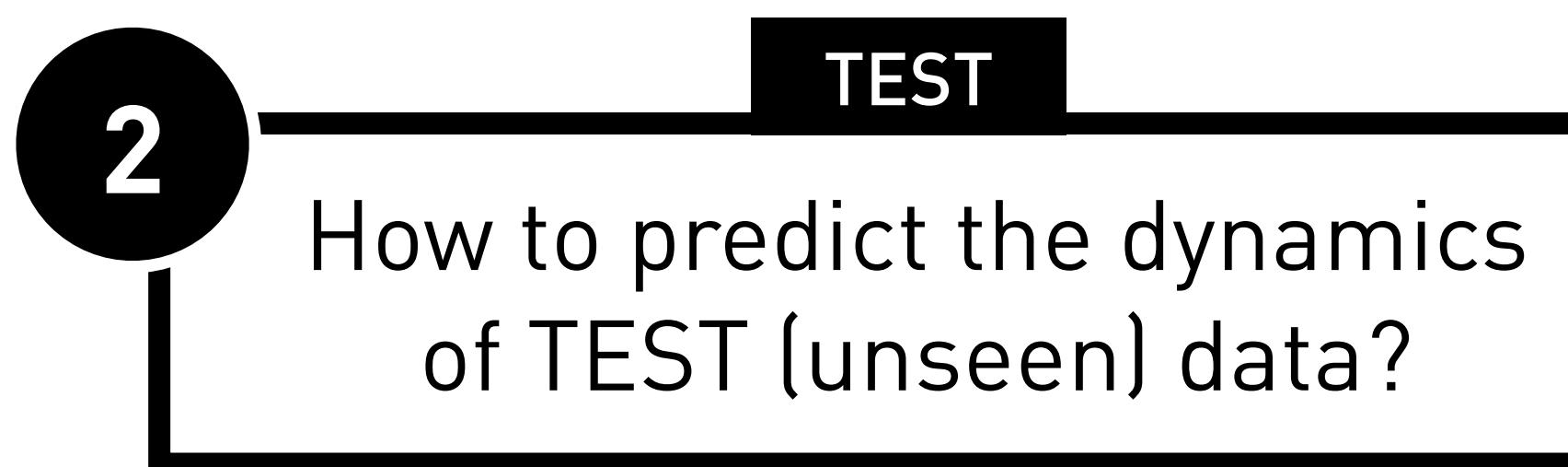
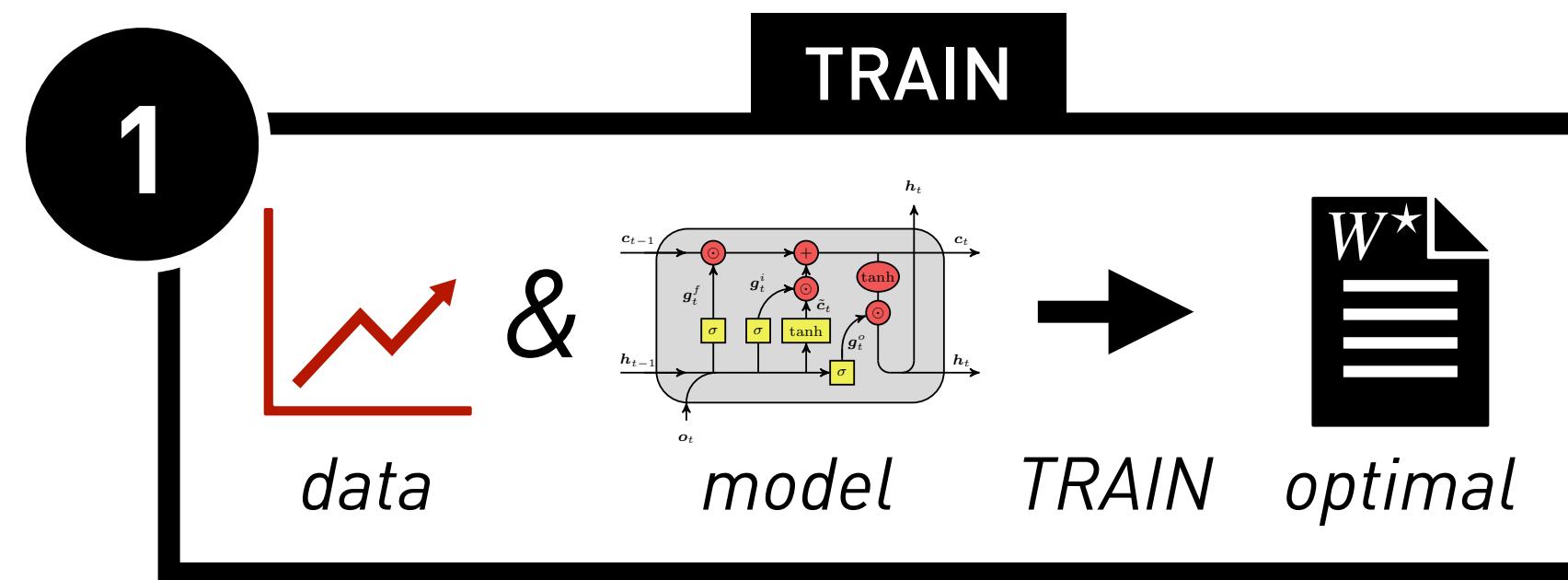


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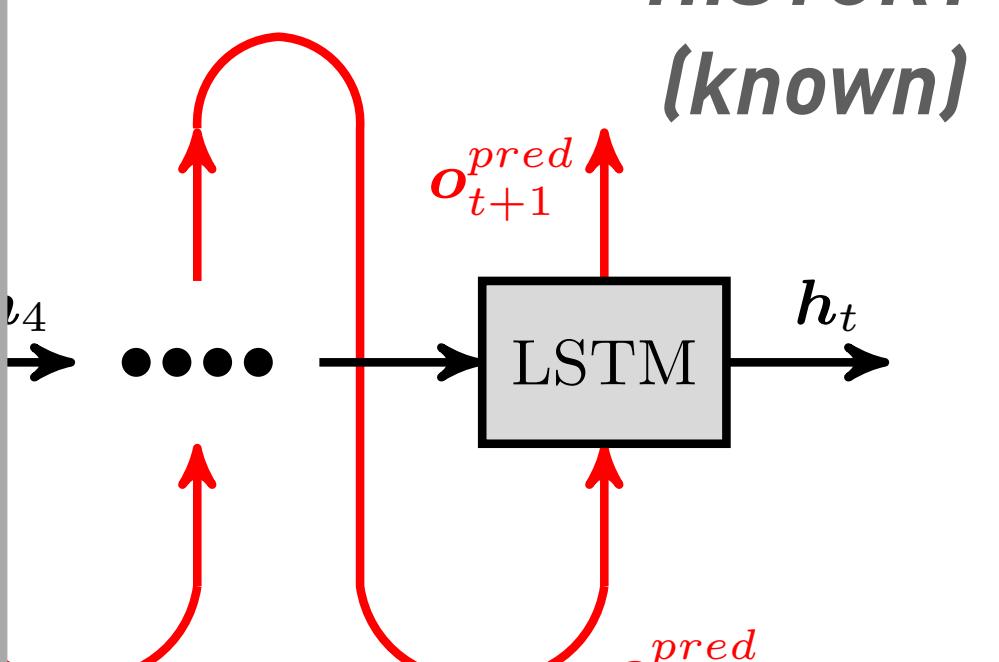
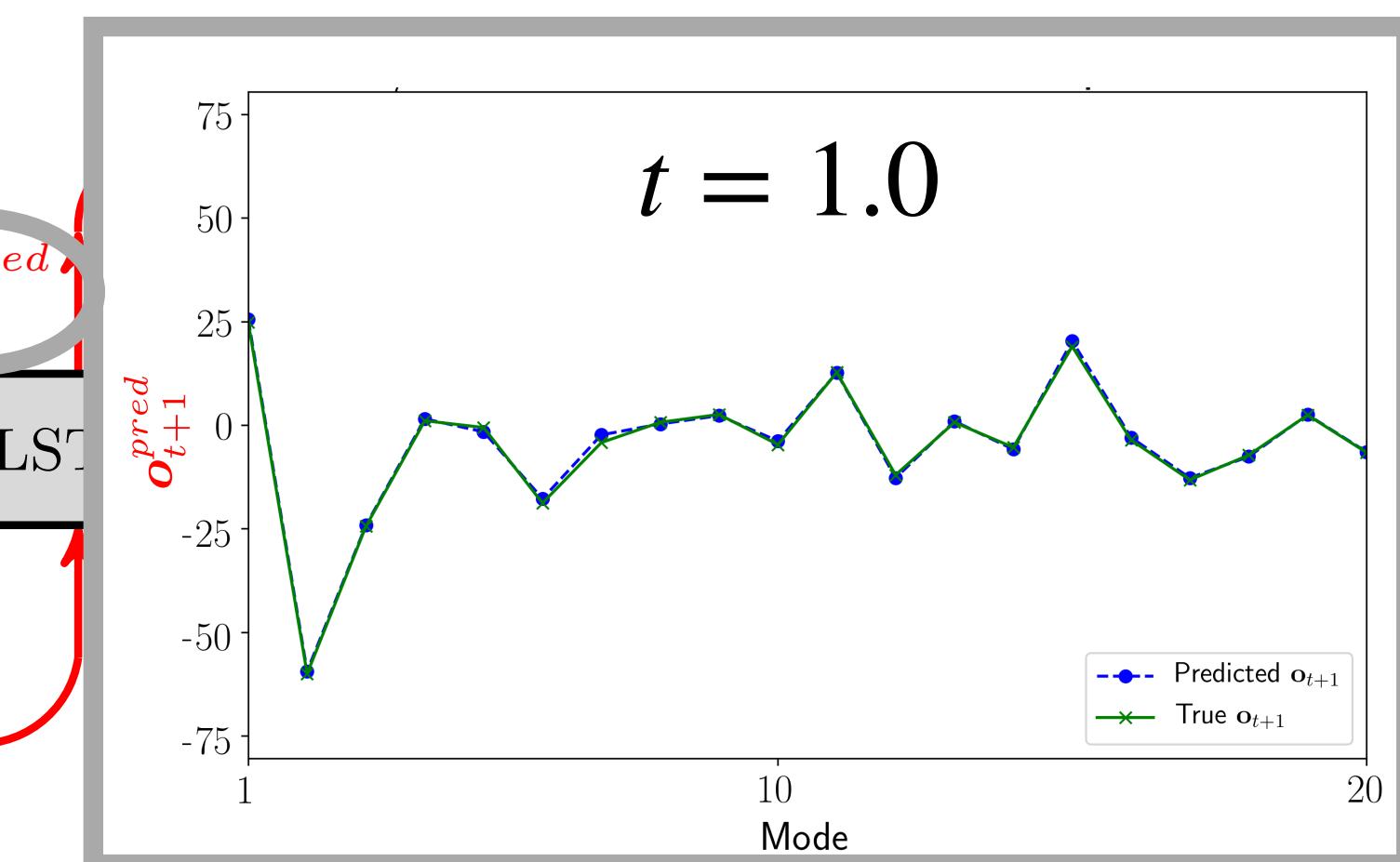
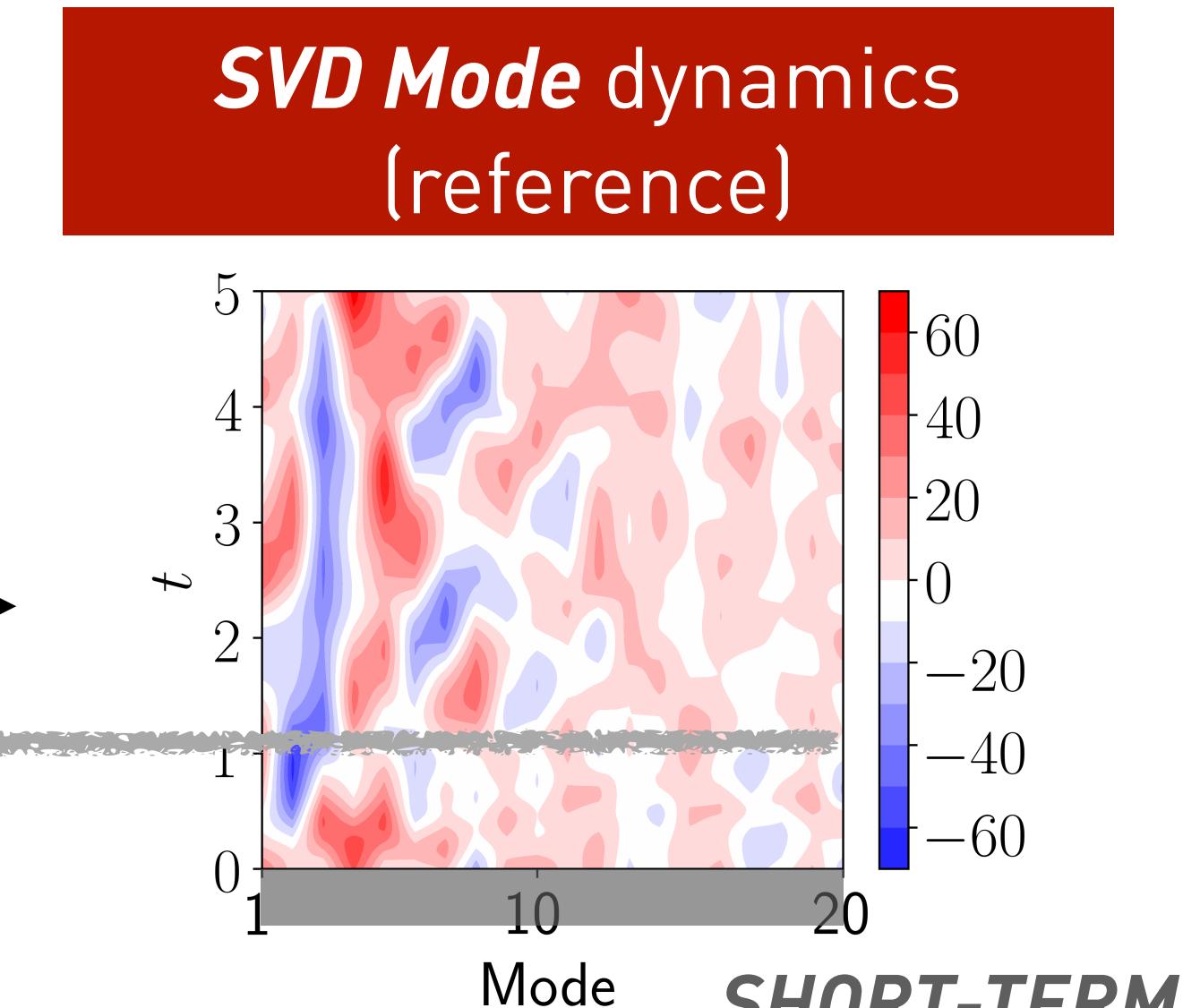
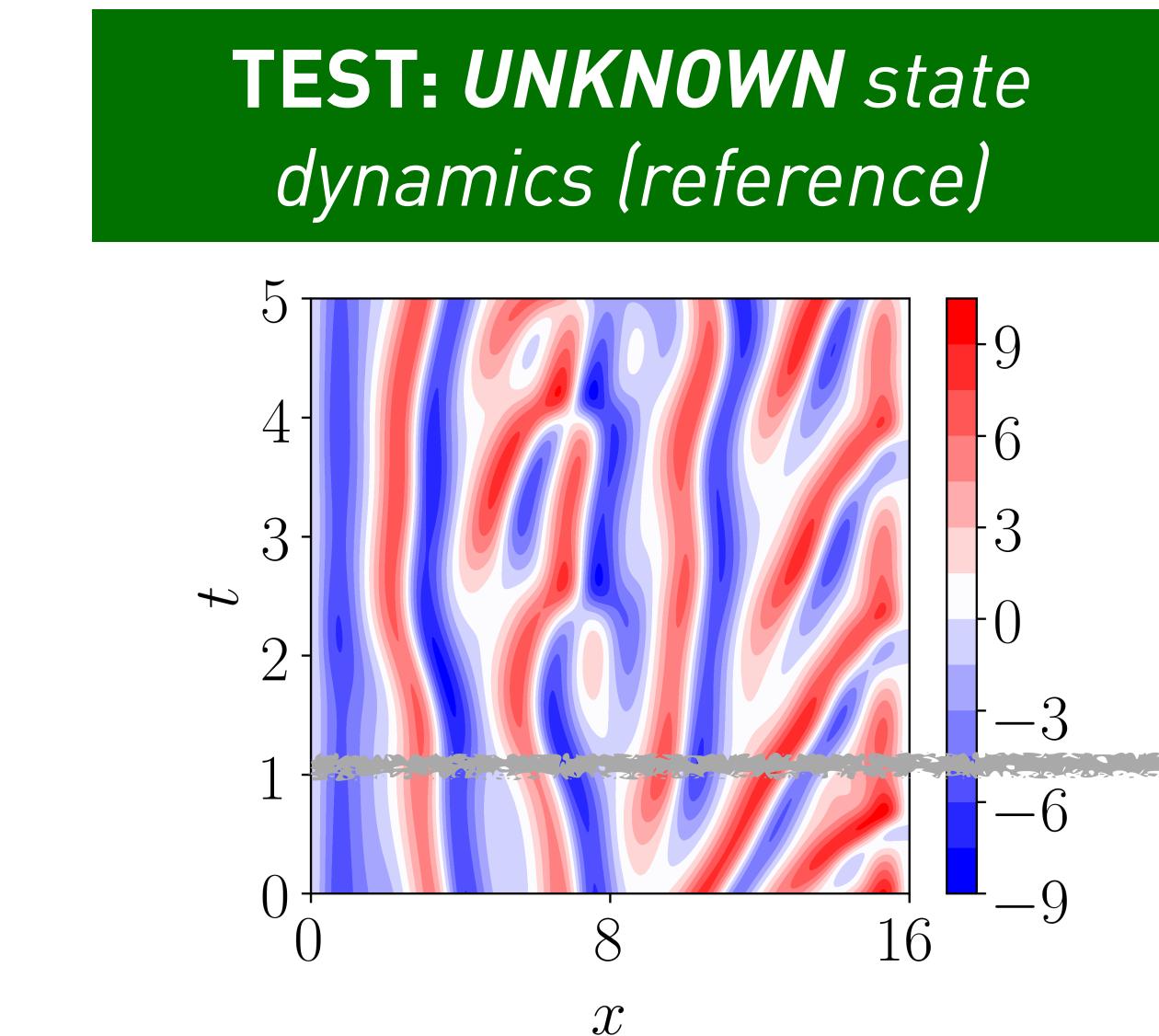


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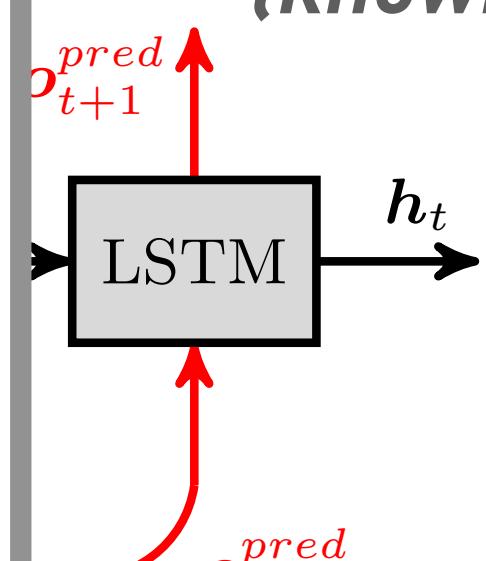
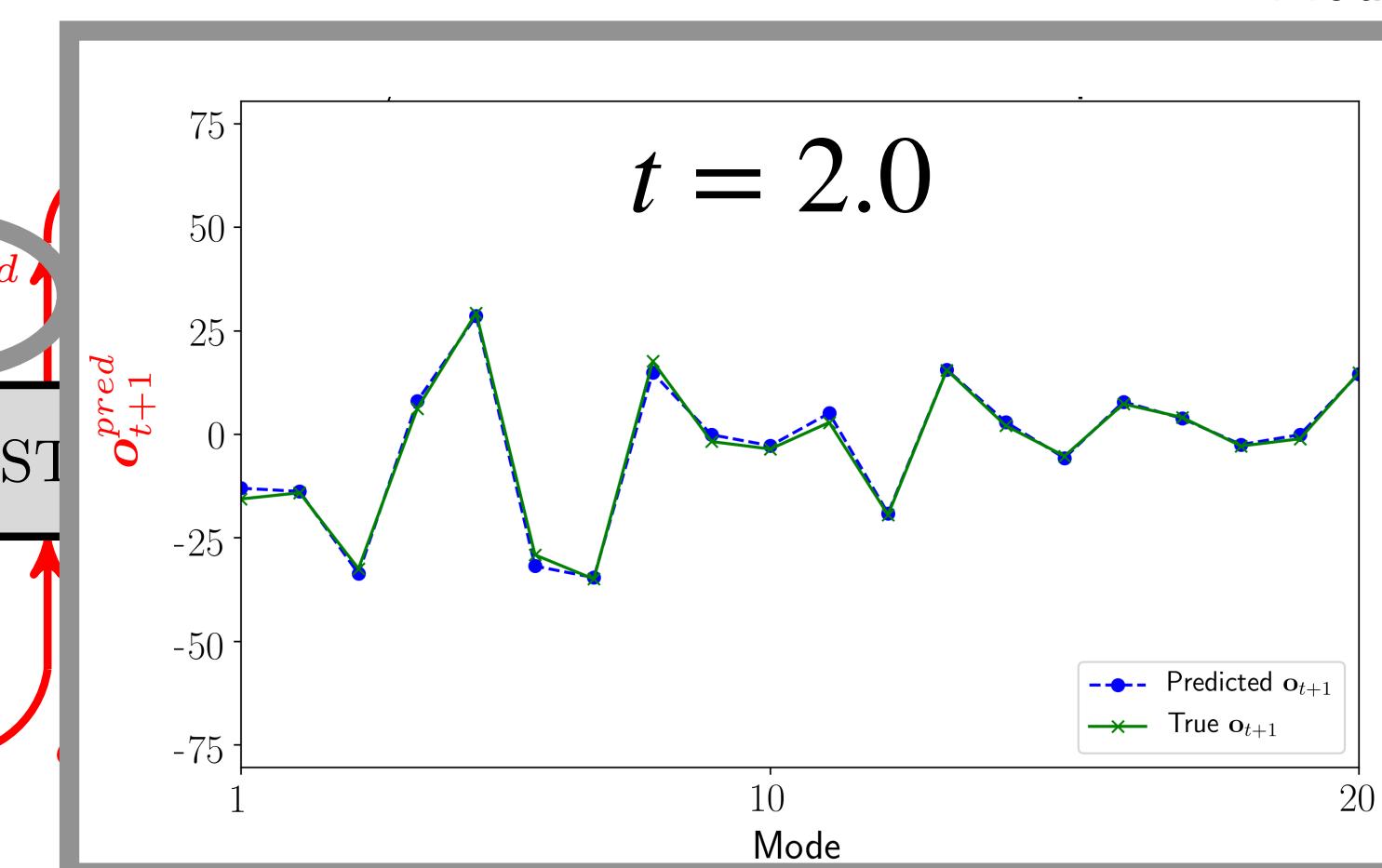
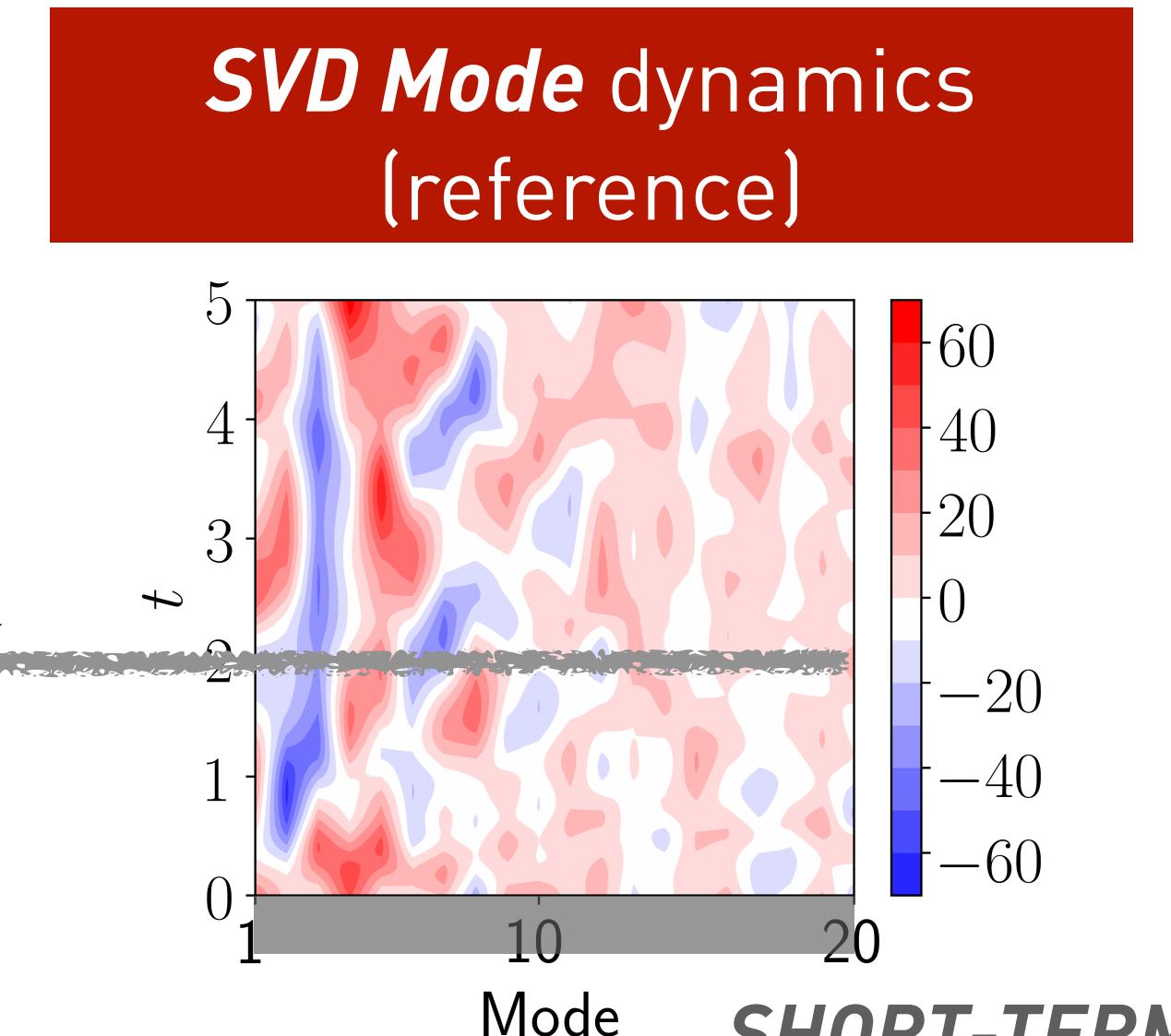
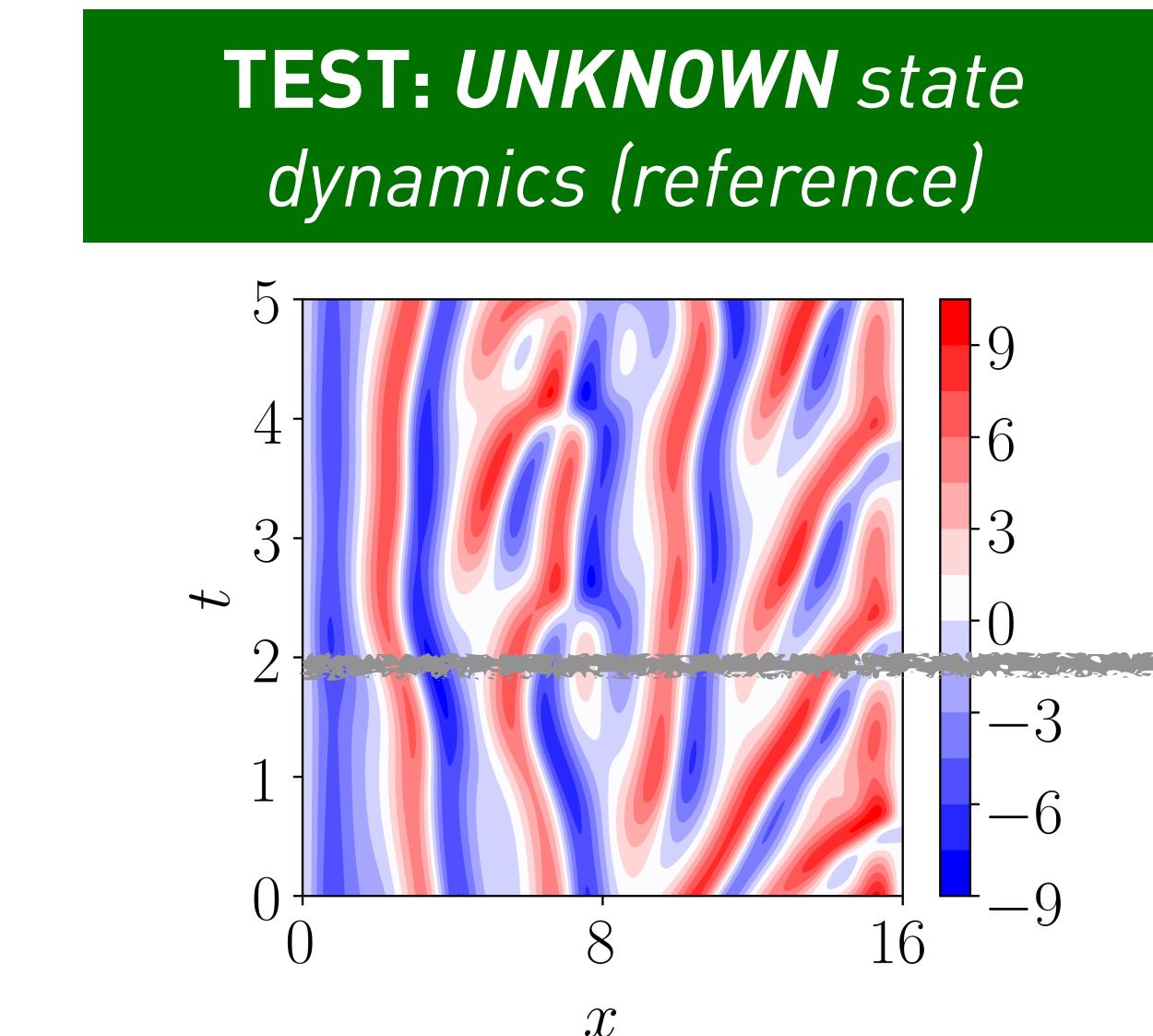
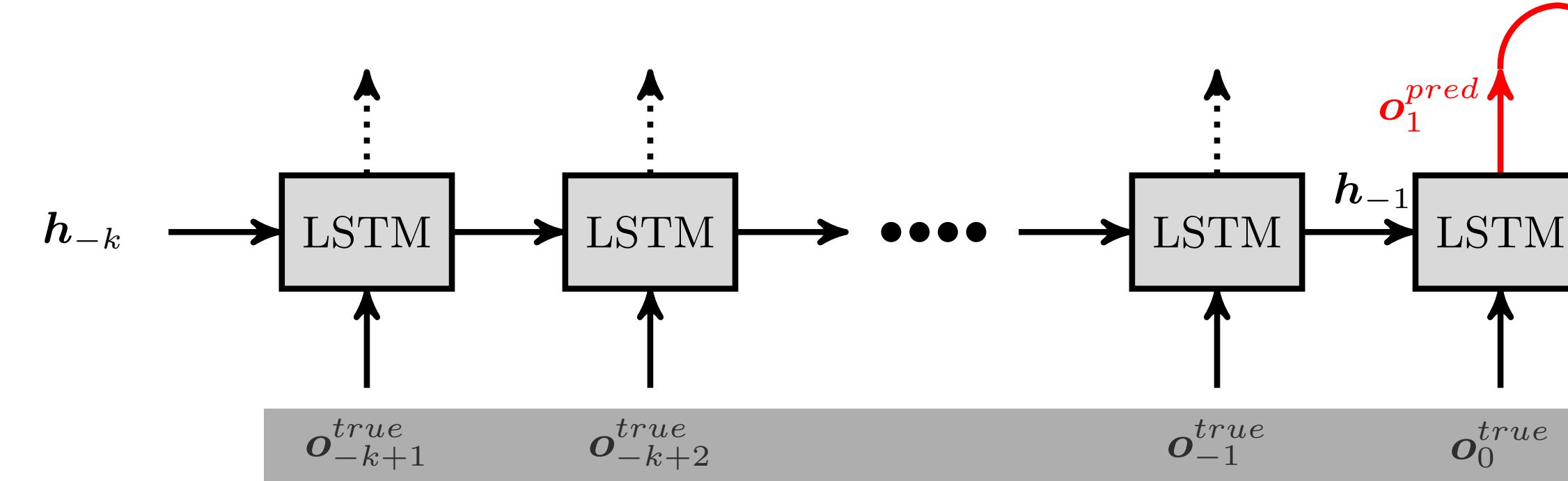
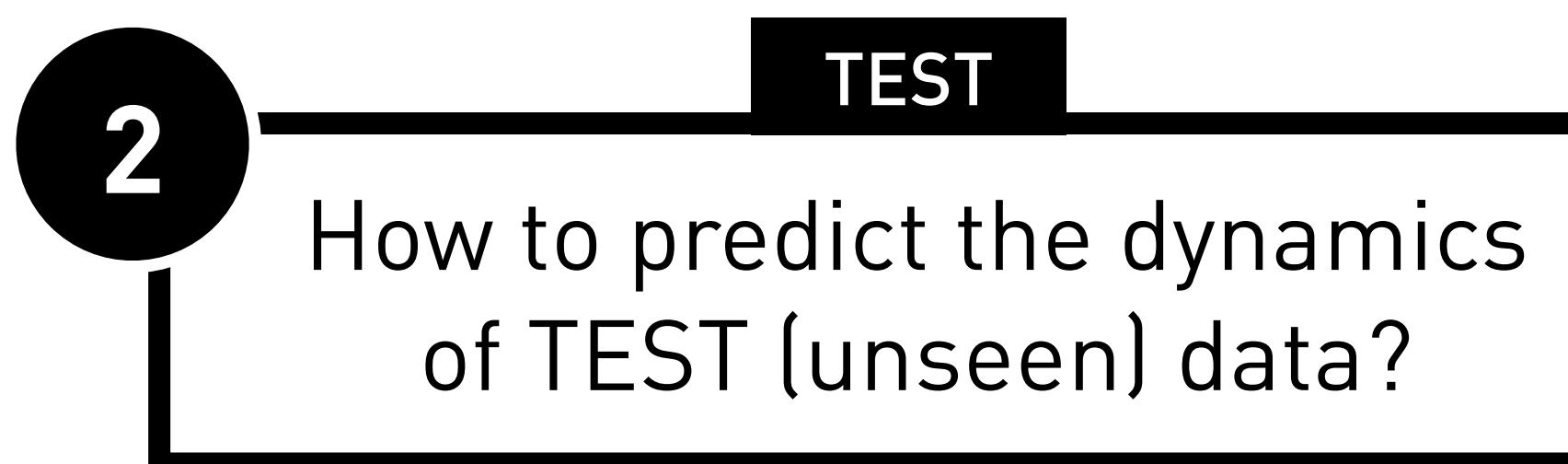
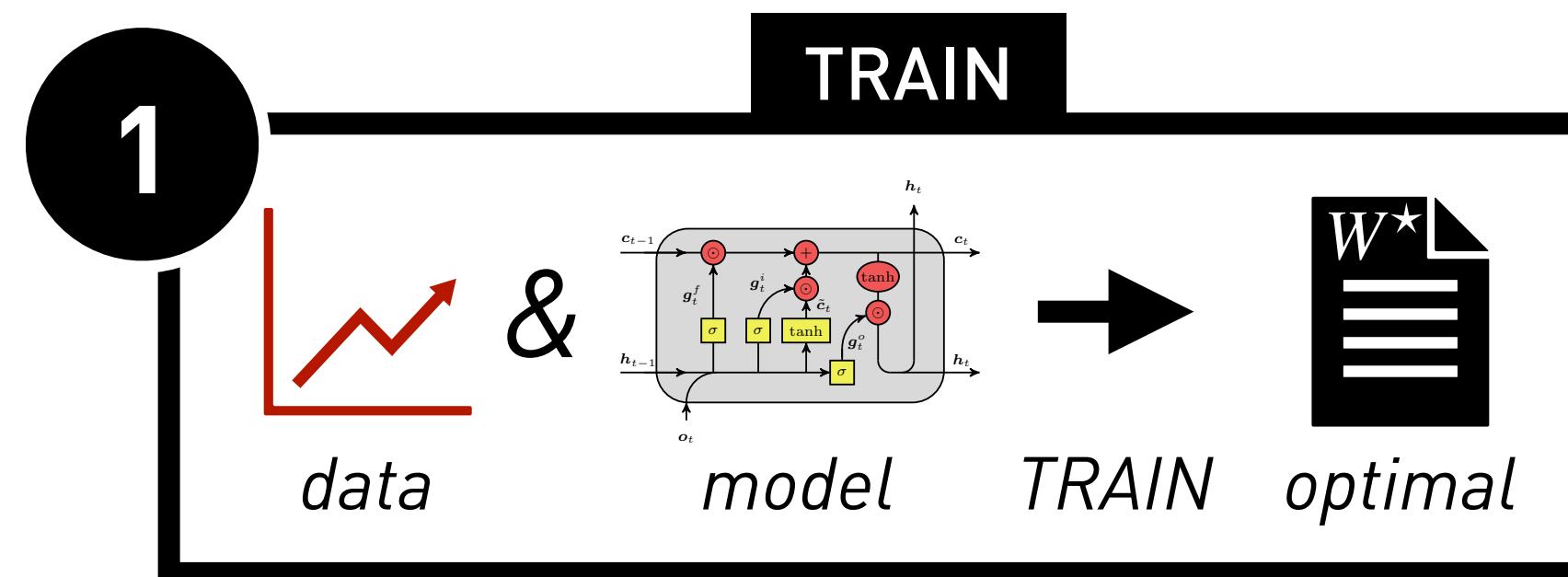


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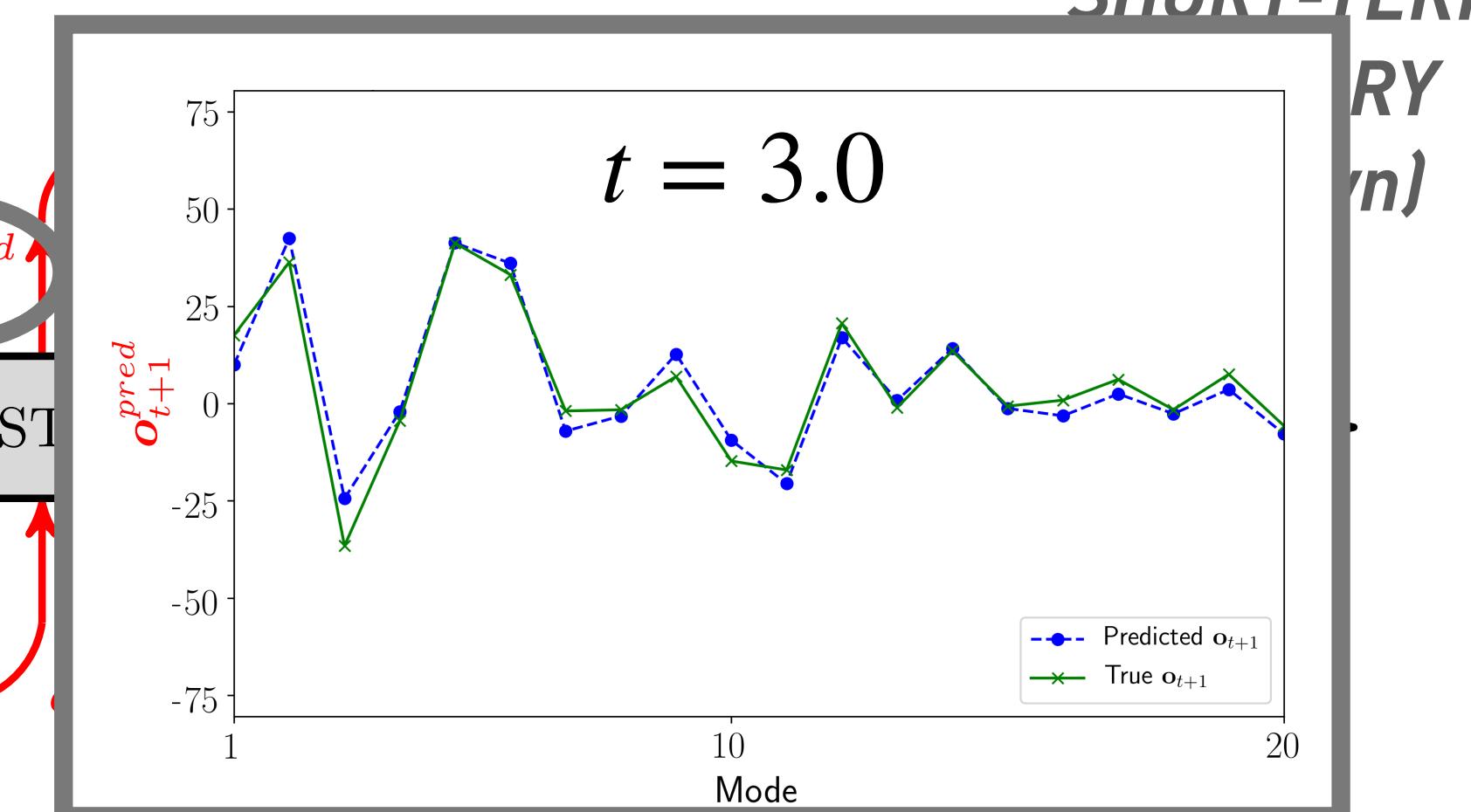
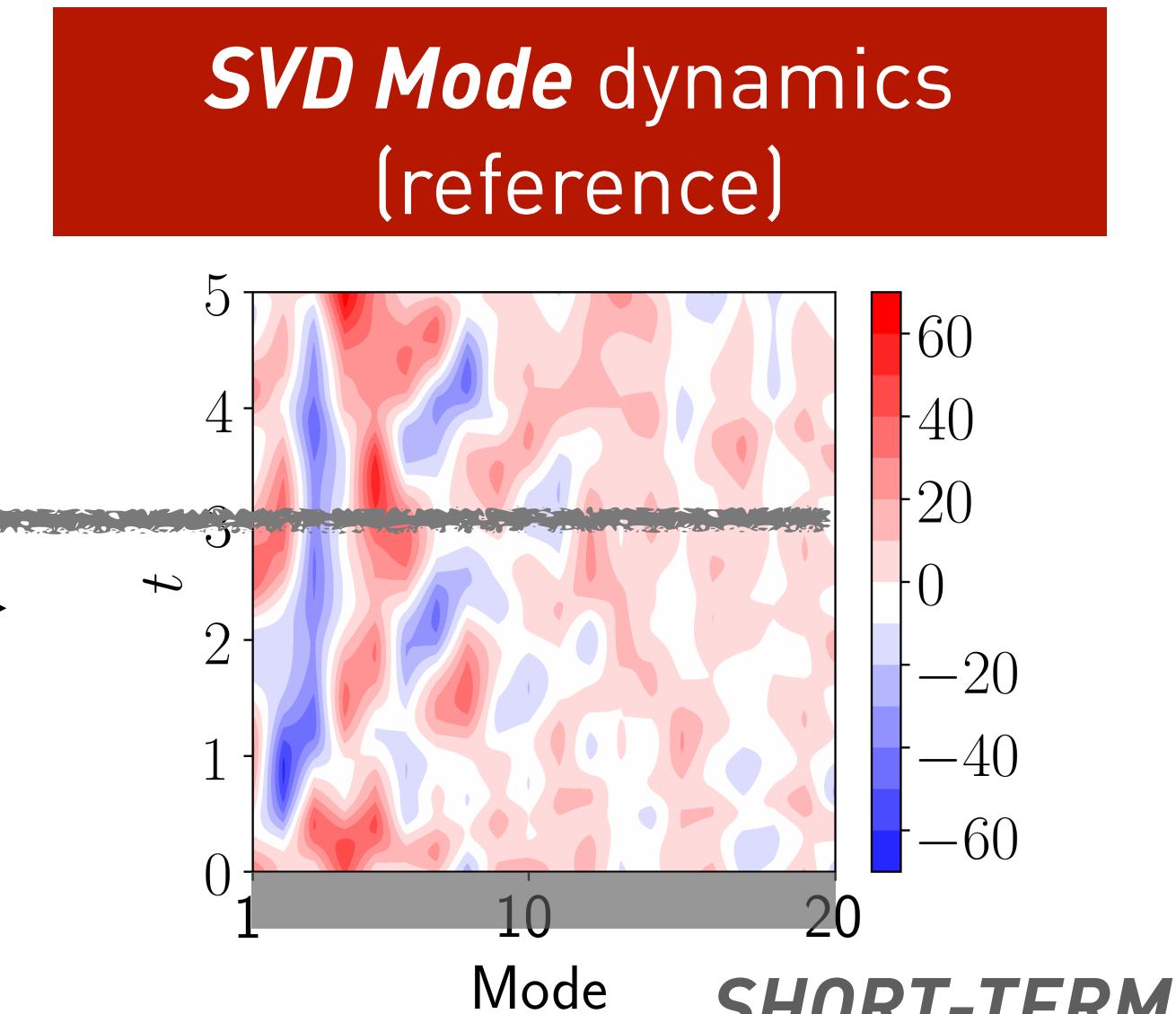
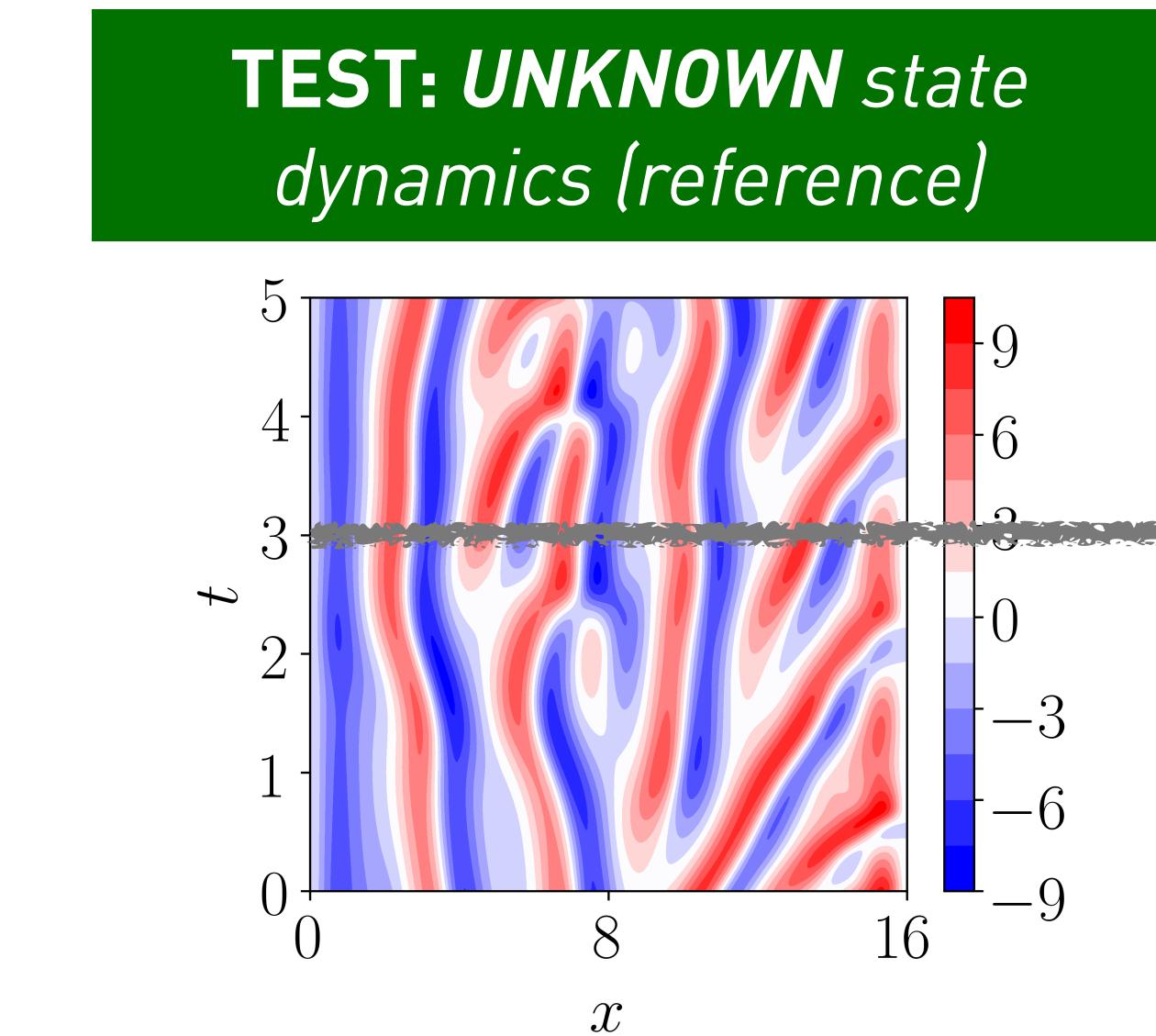
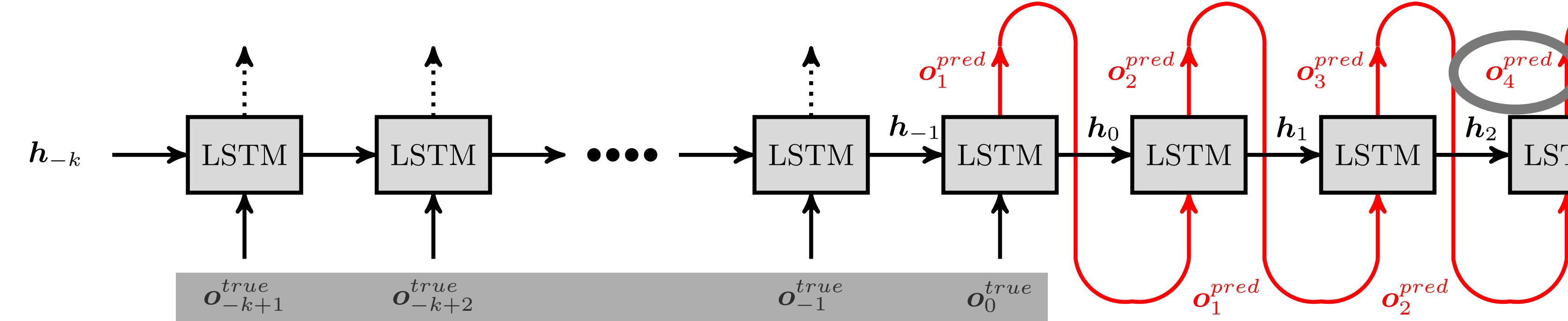
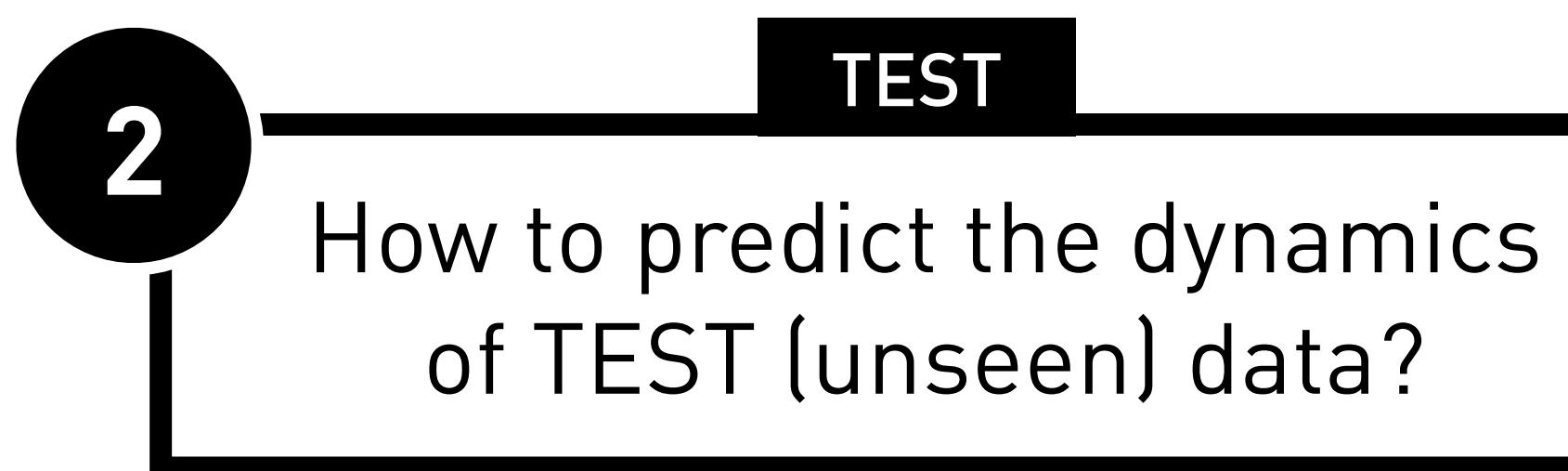
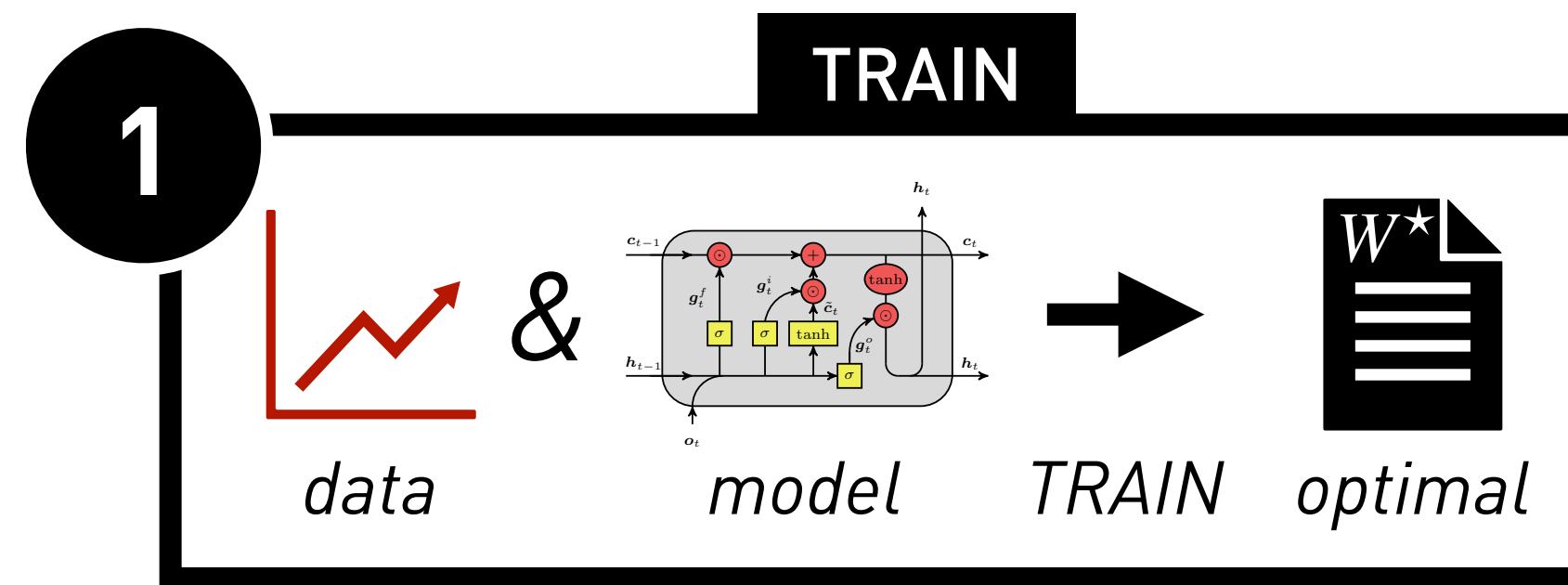
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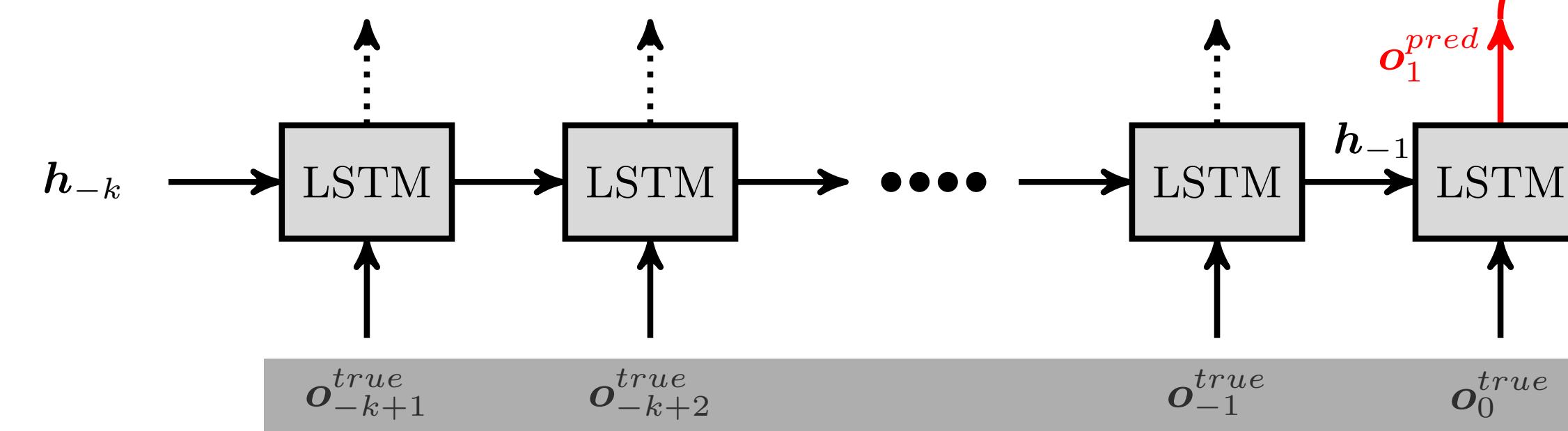
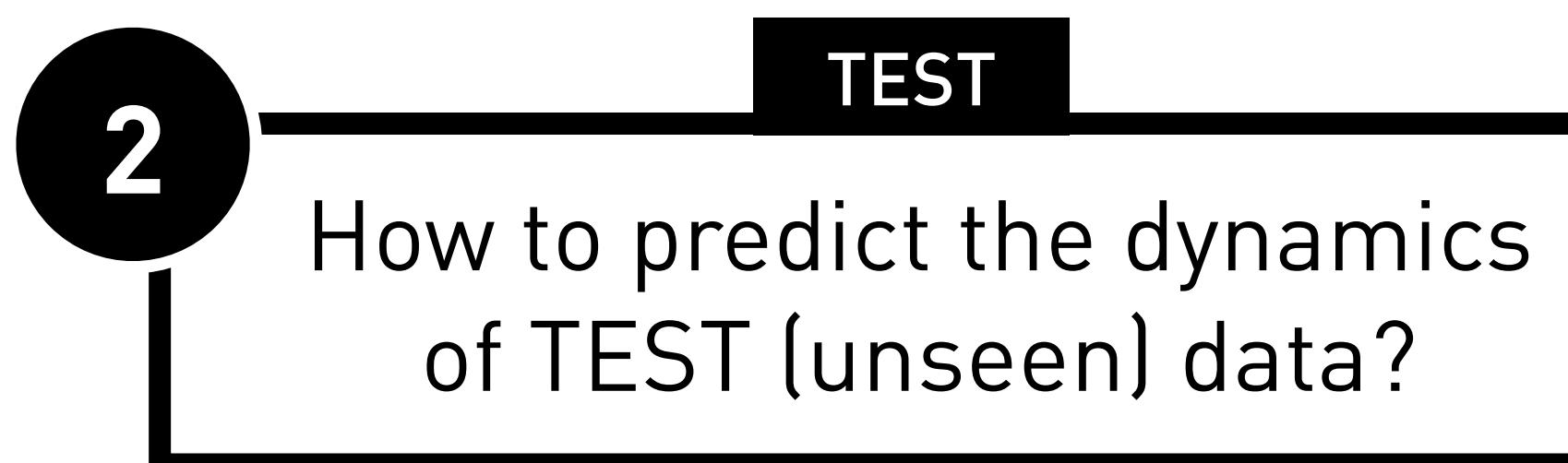
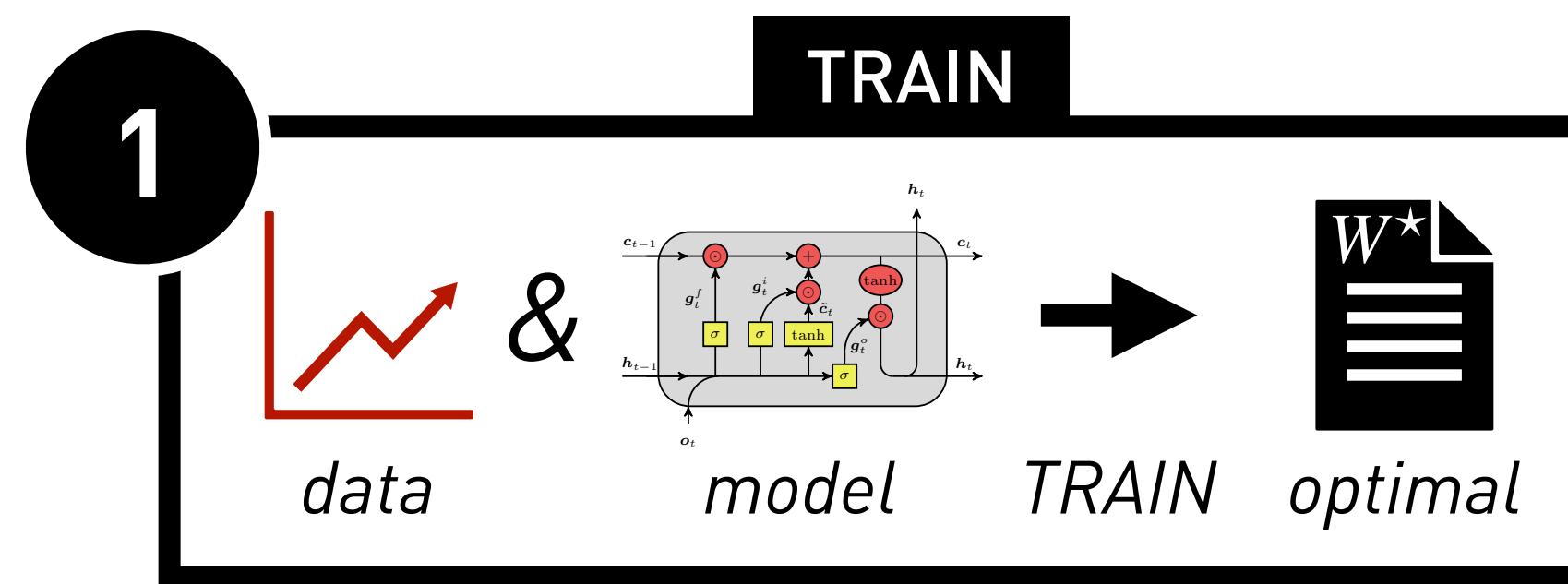
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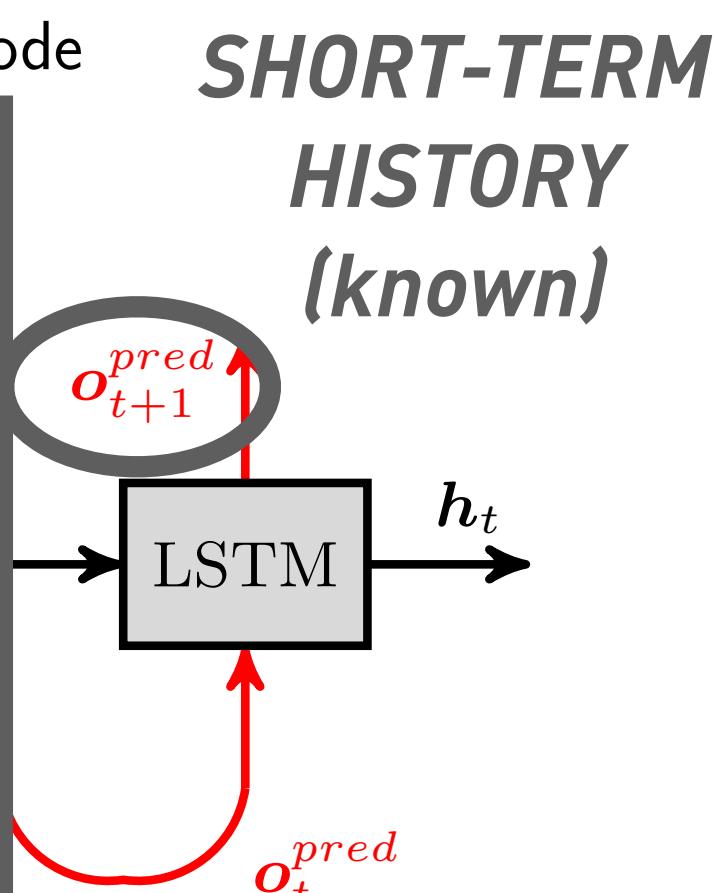
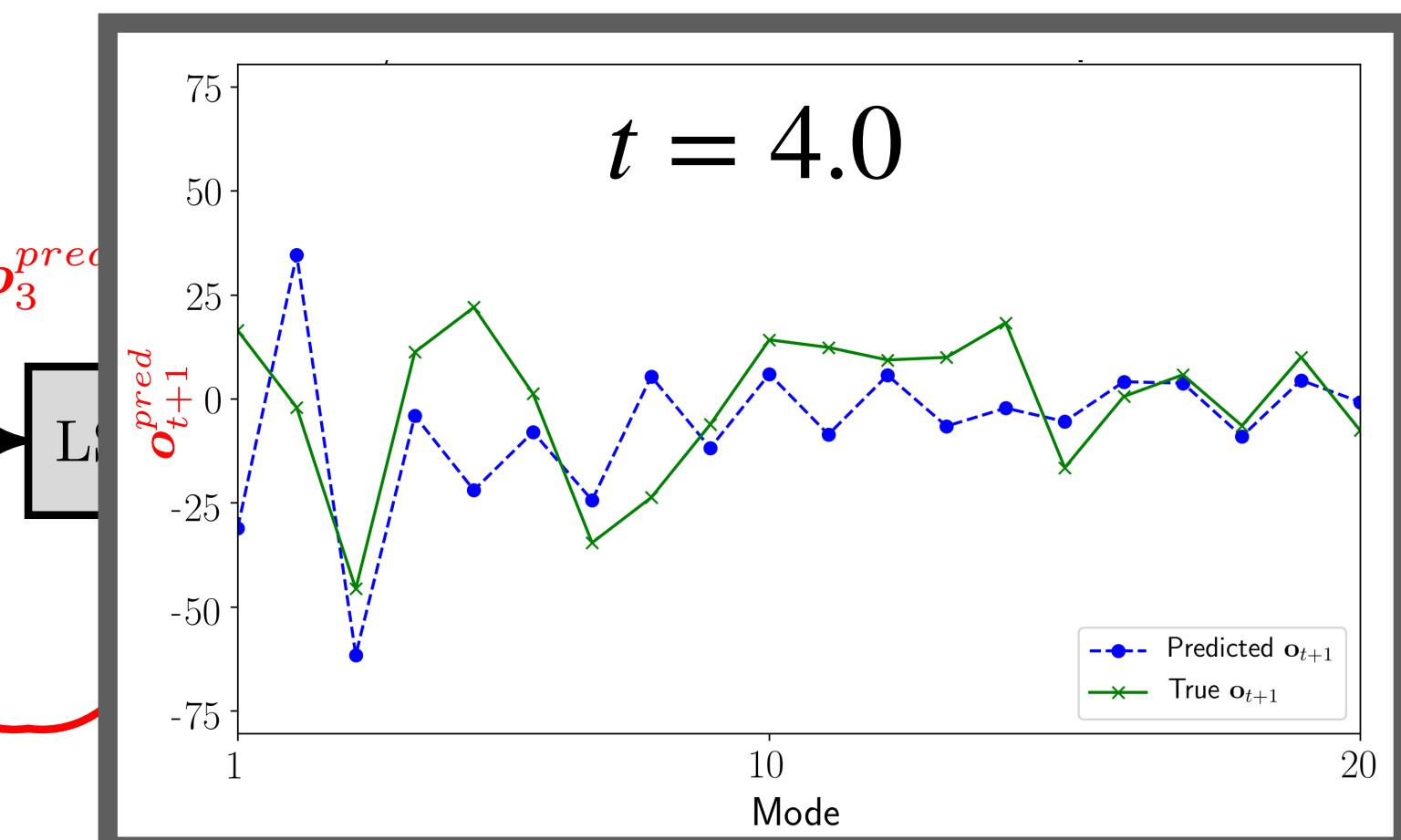
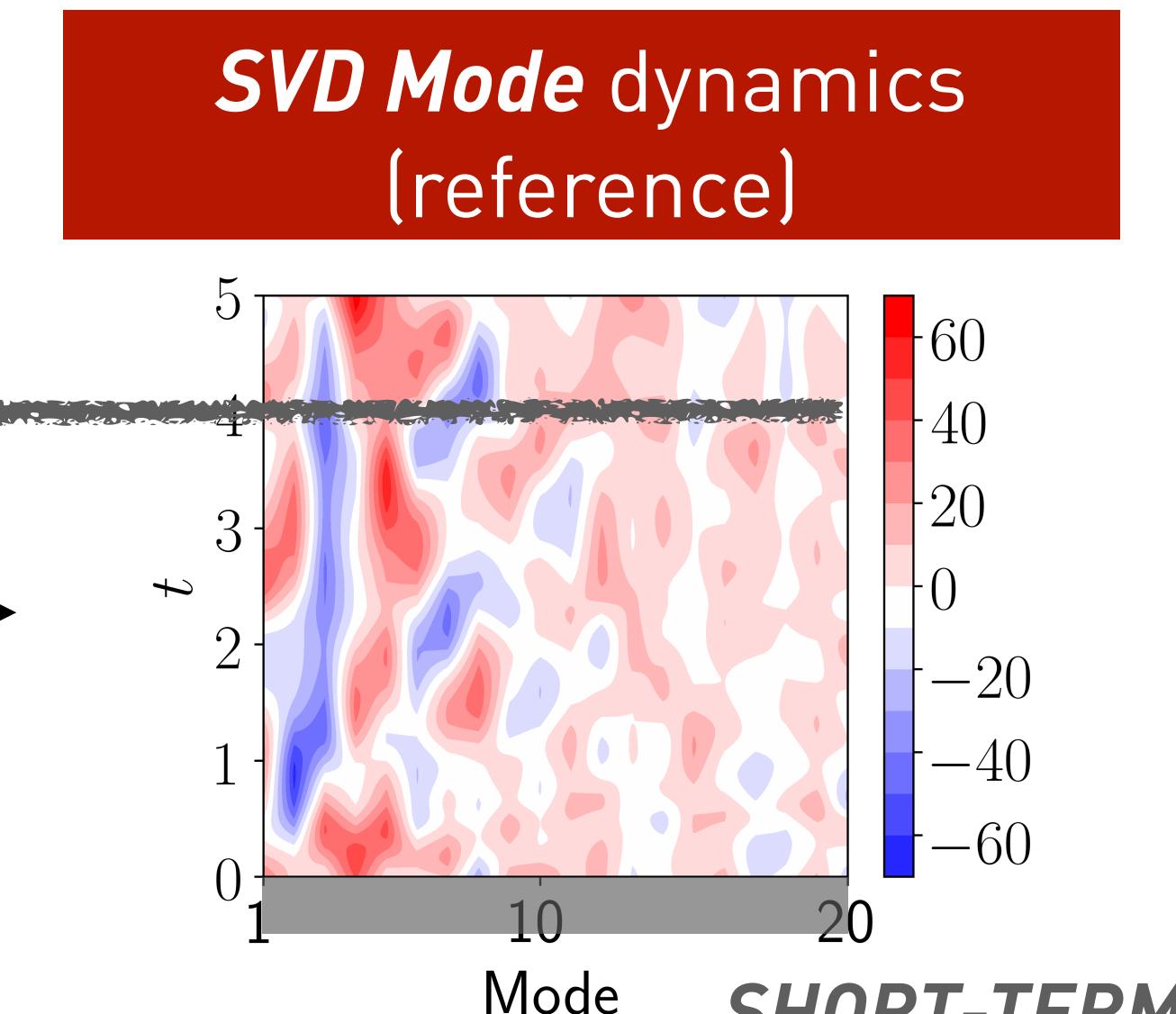
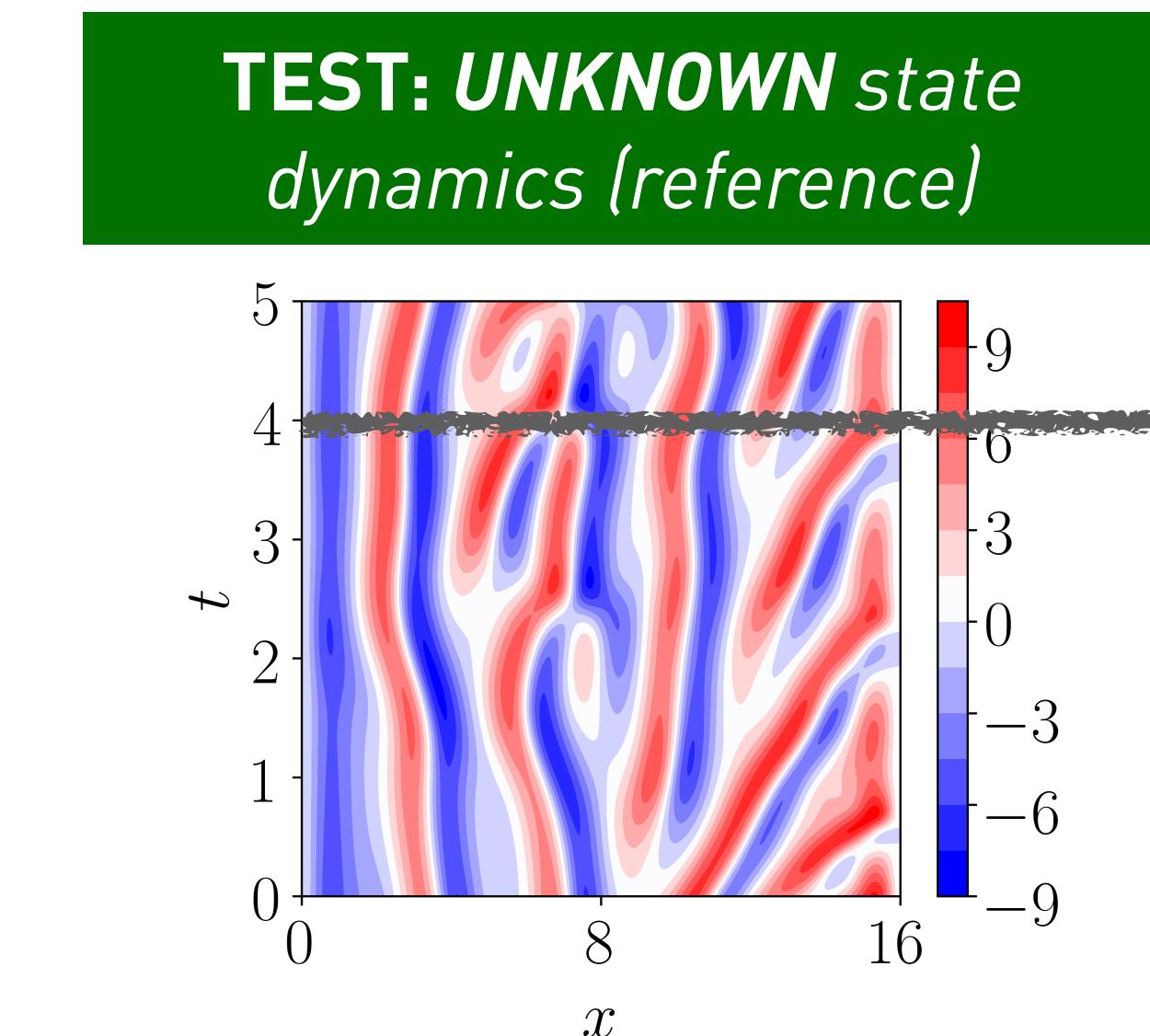


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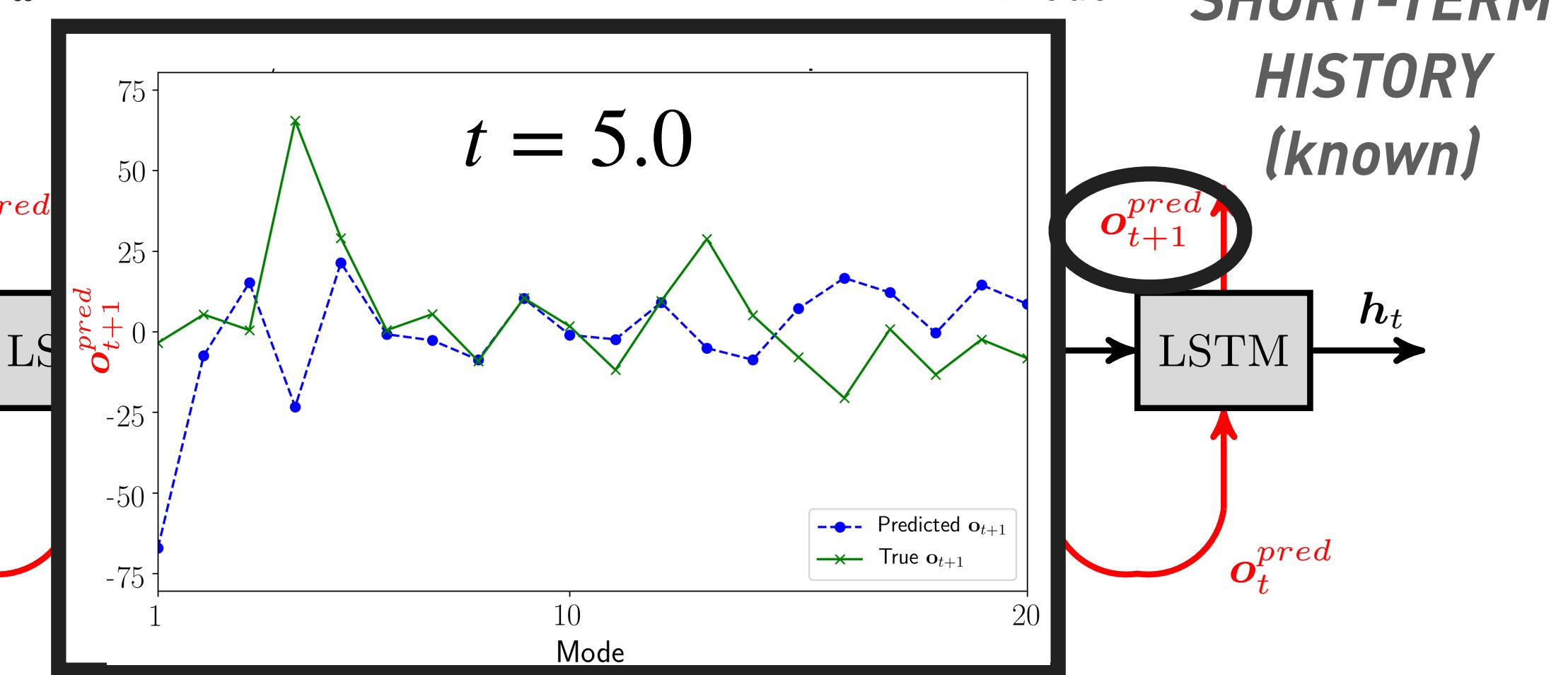
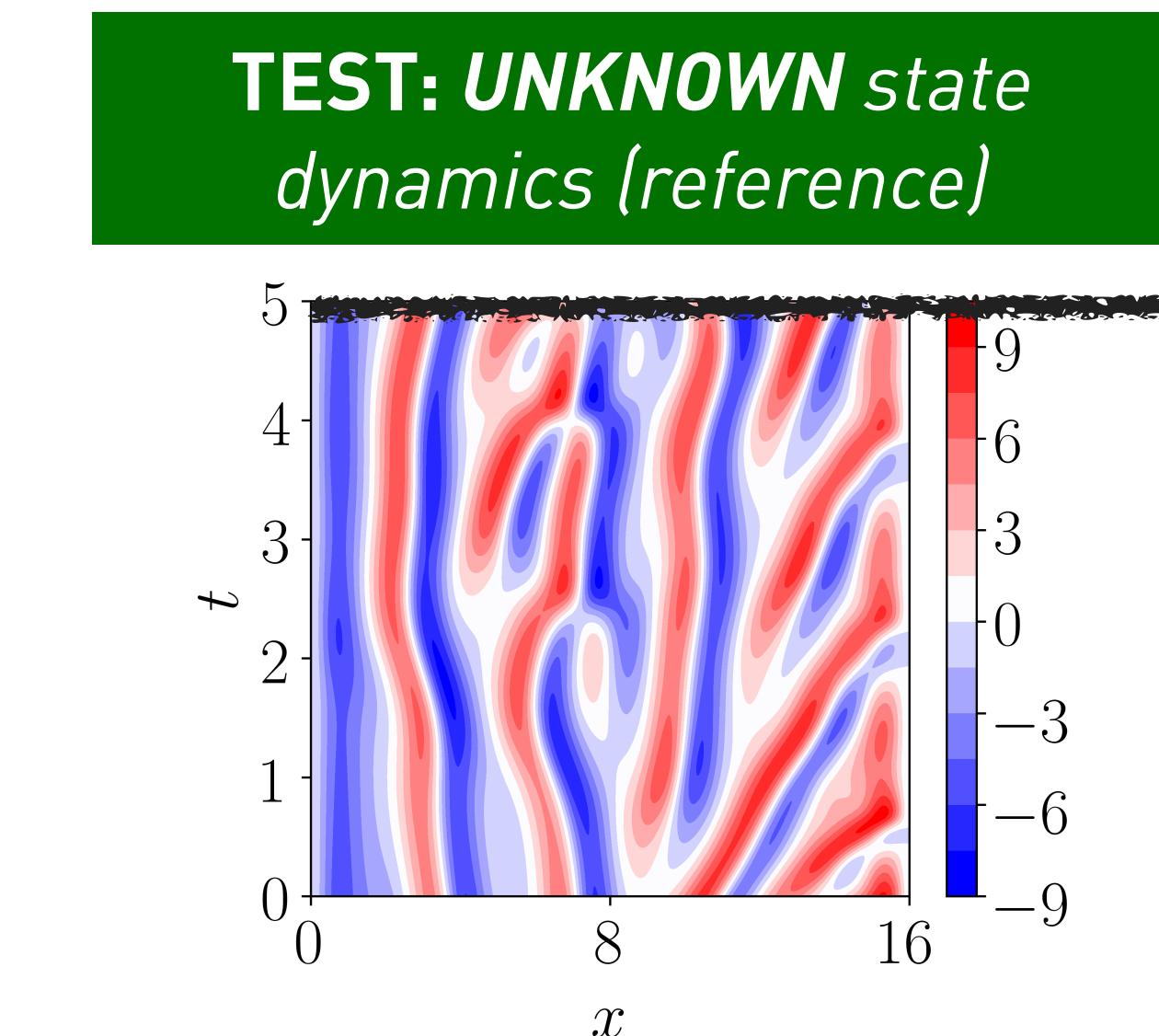
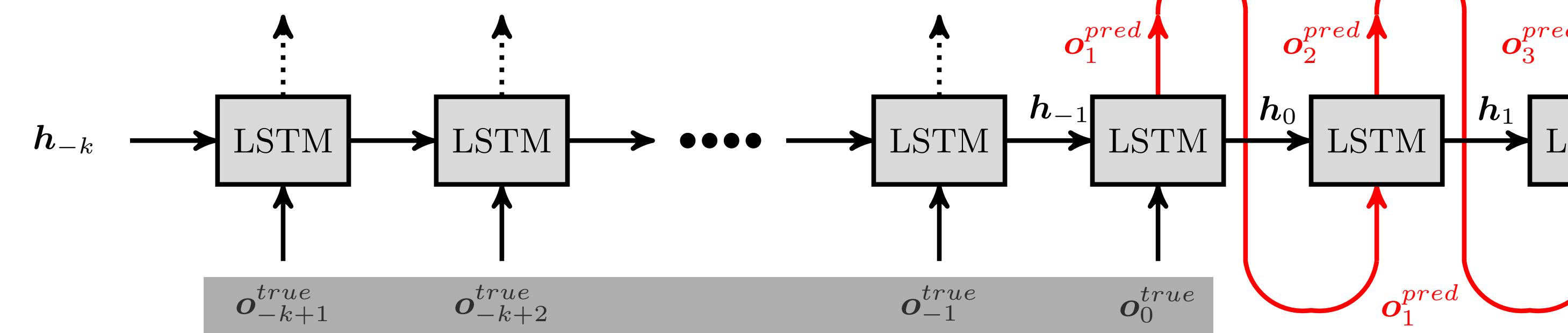
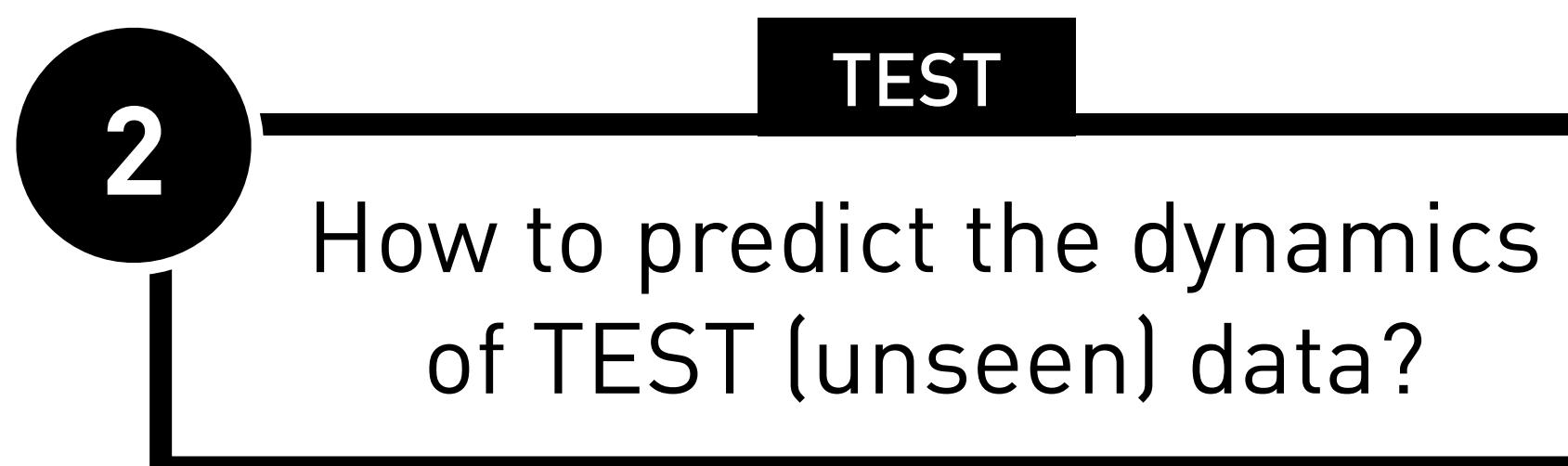
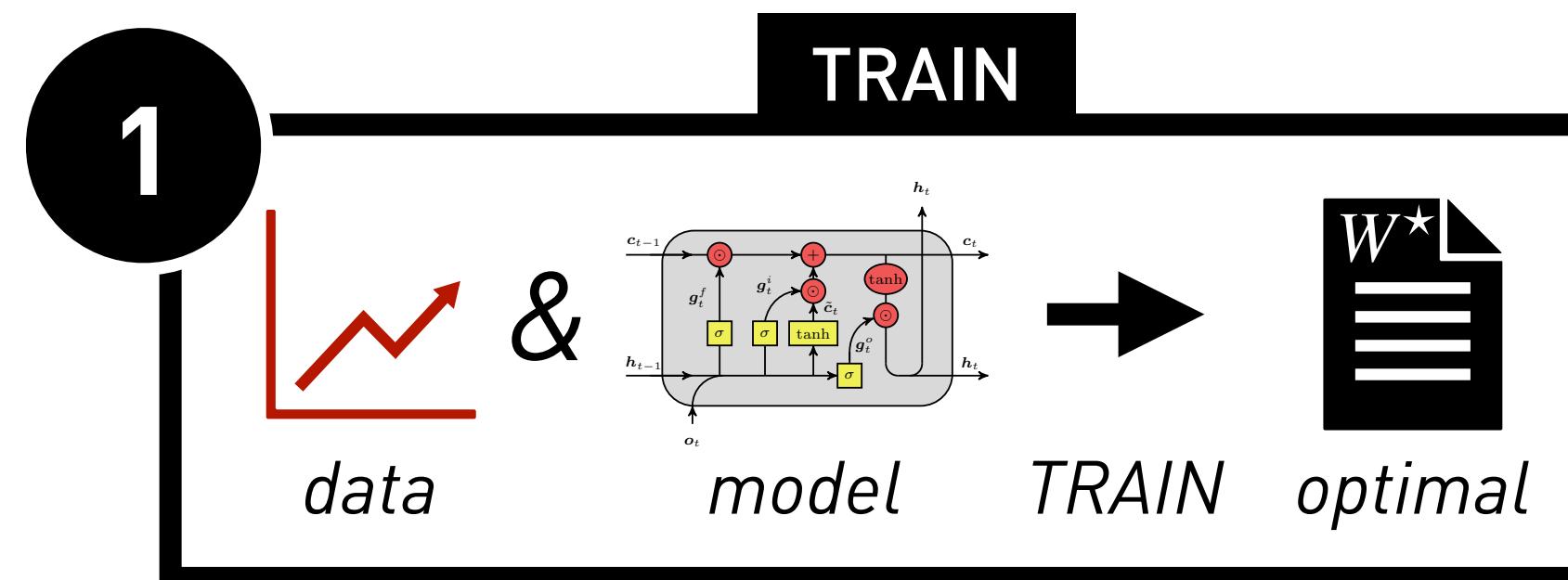


SHORT-TERM HISTORY  
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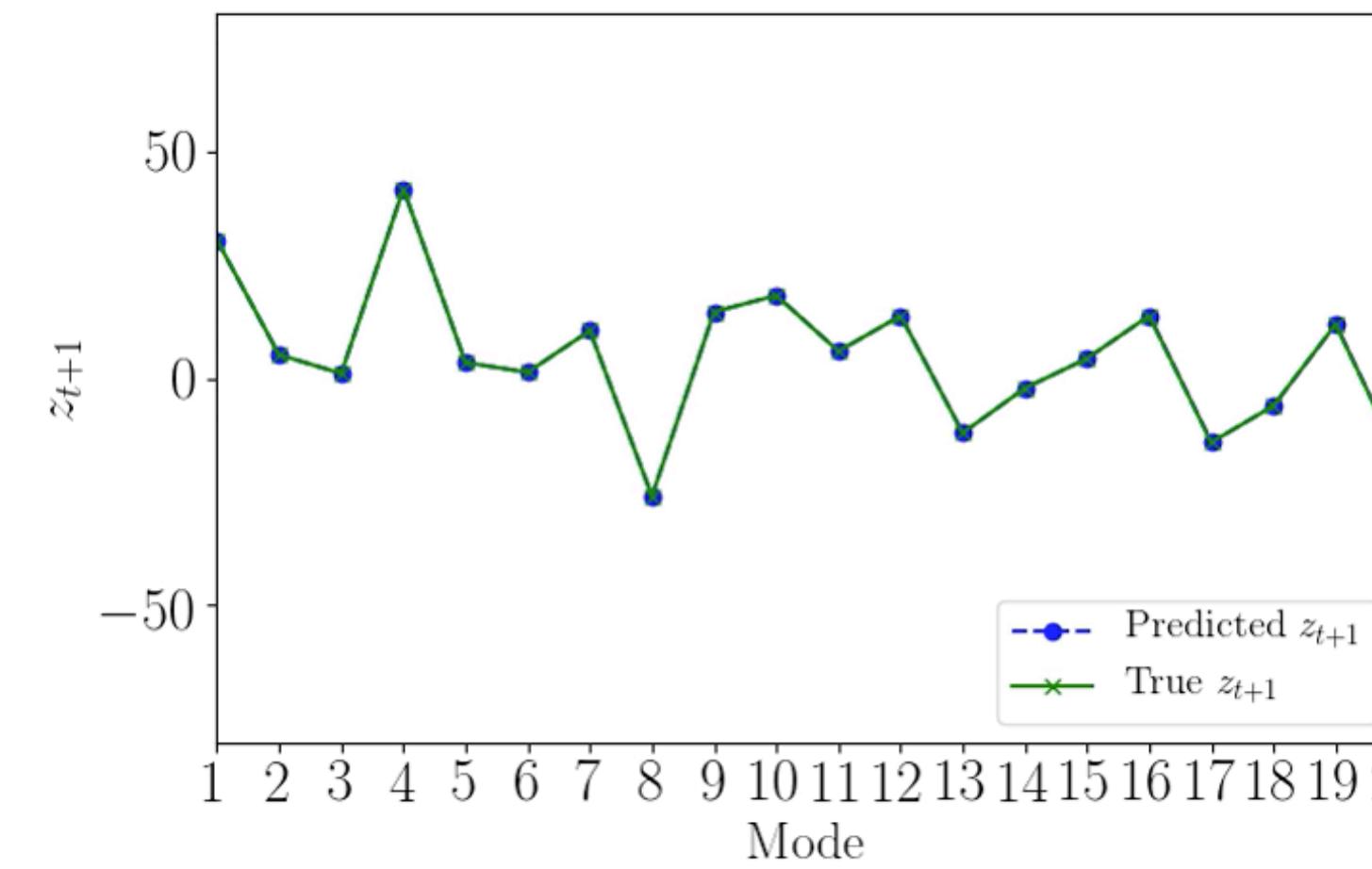


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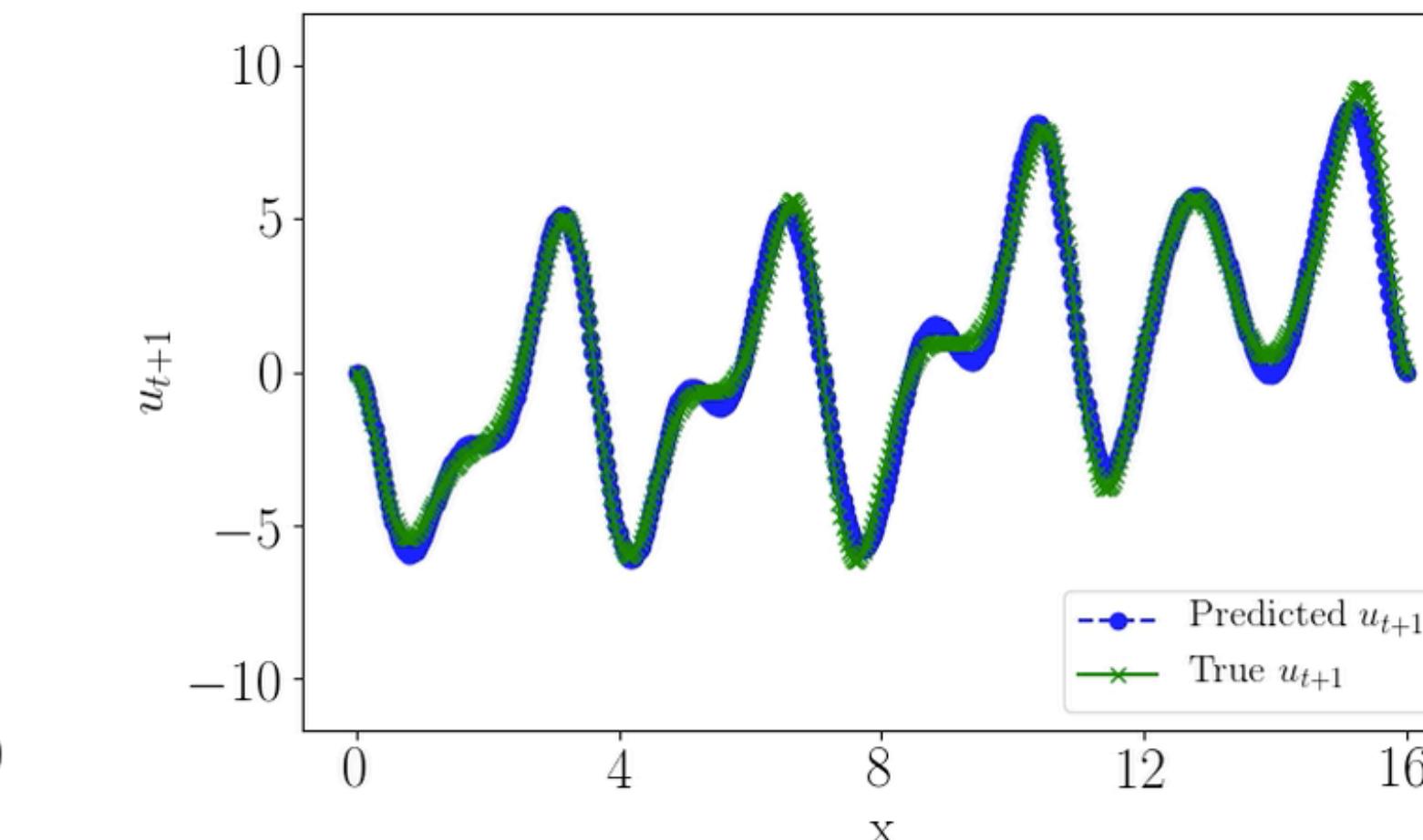
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prediction in **reduced space**

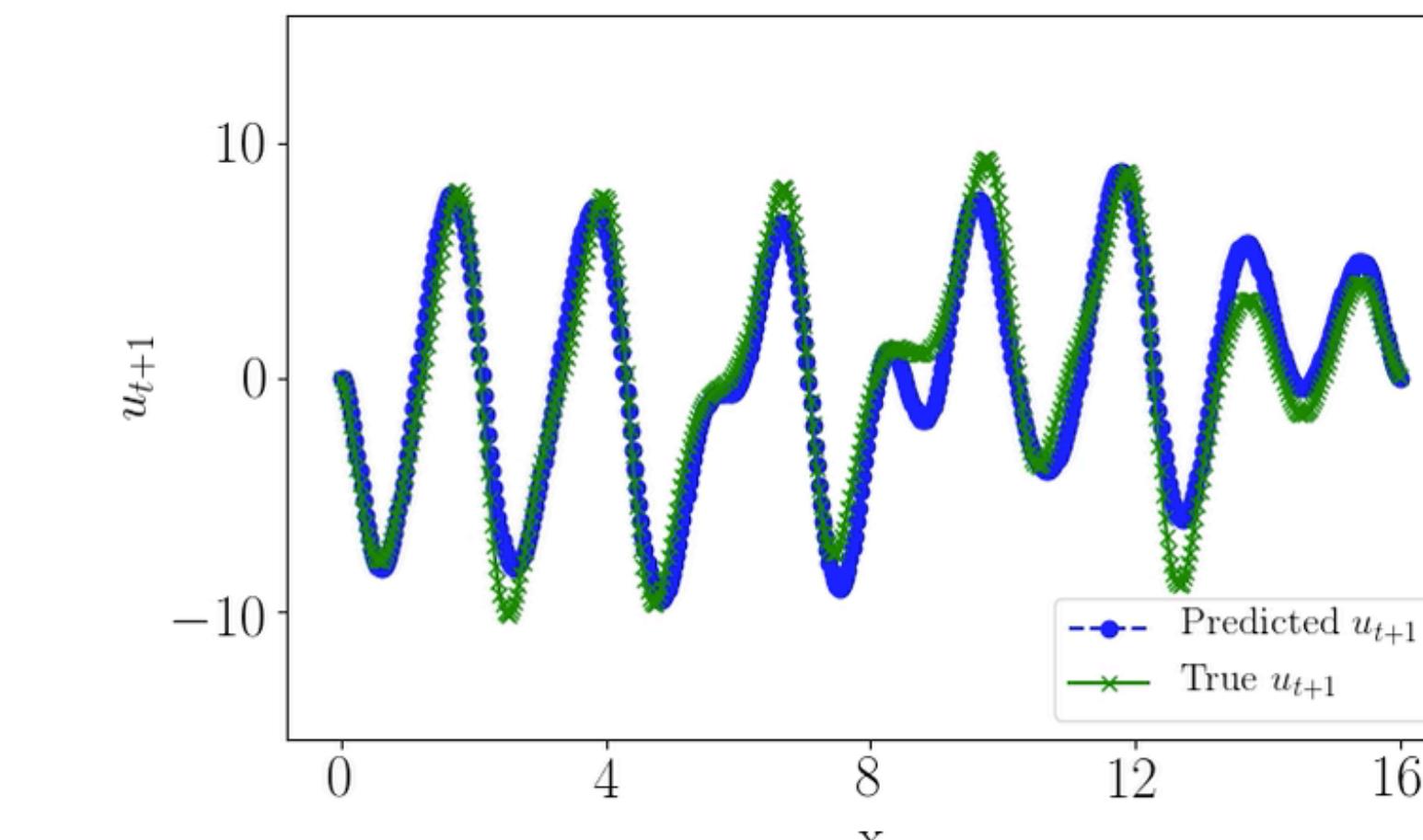
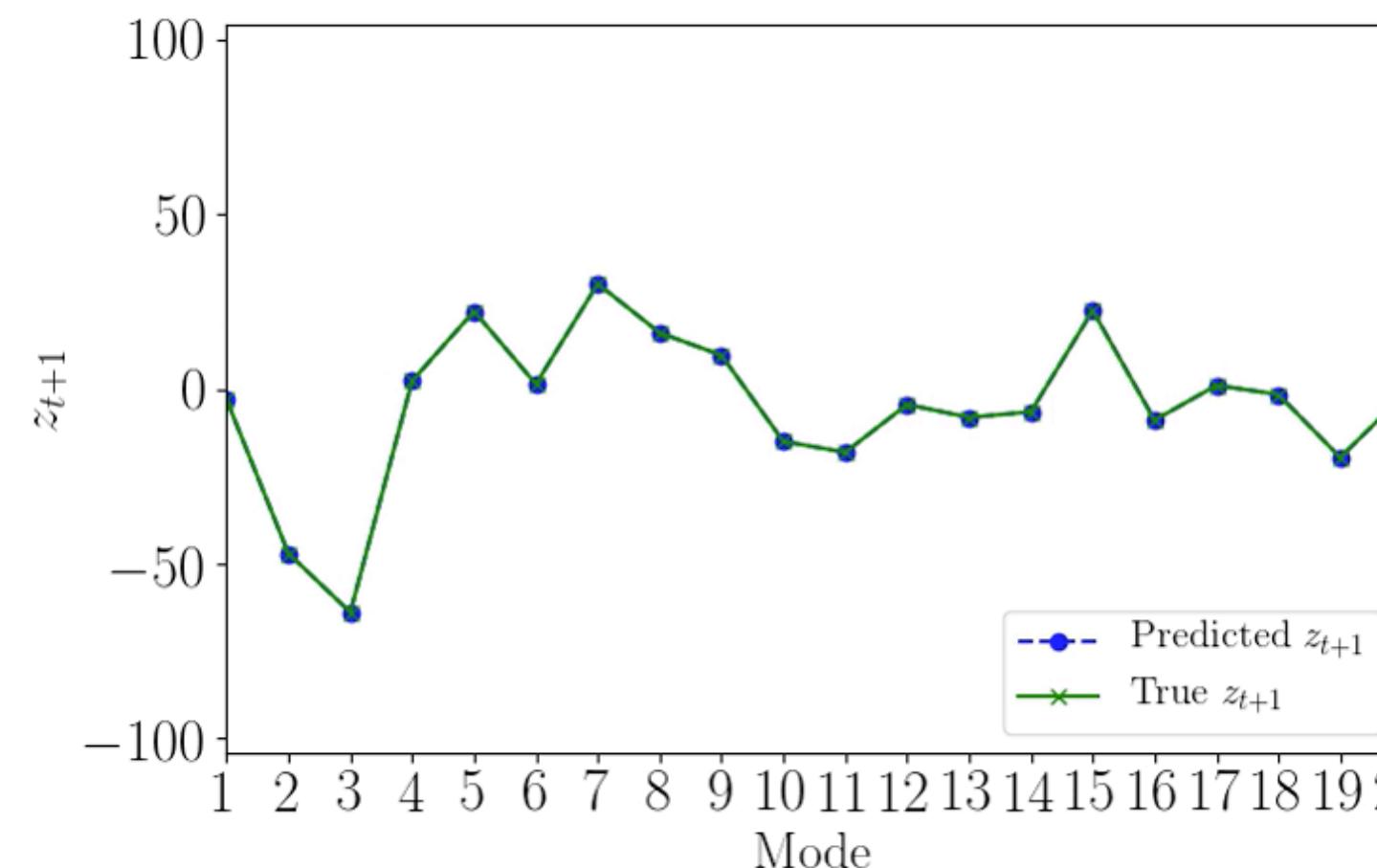
$$\tilde{L} \approx 8$$



expanded in **high-dimensional space**



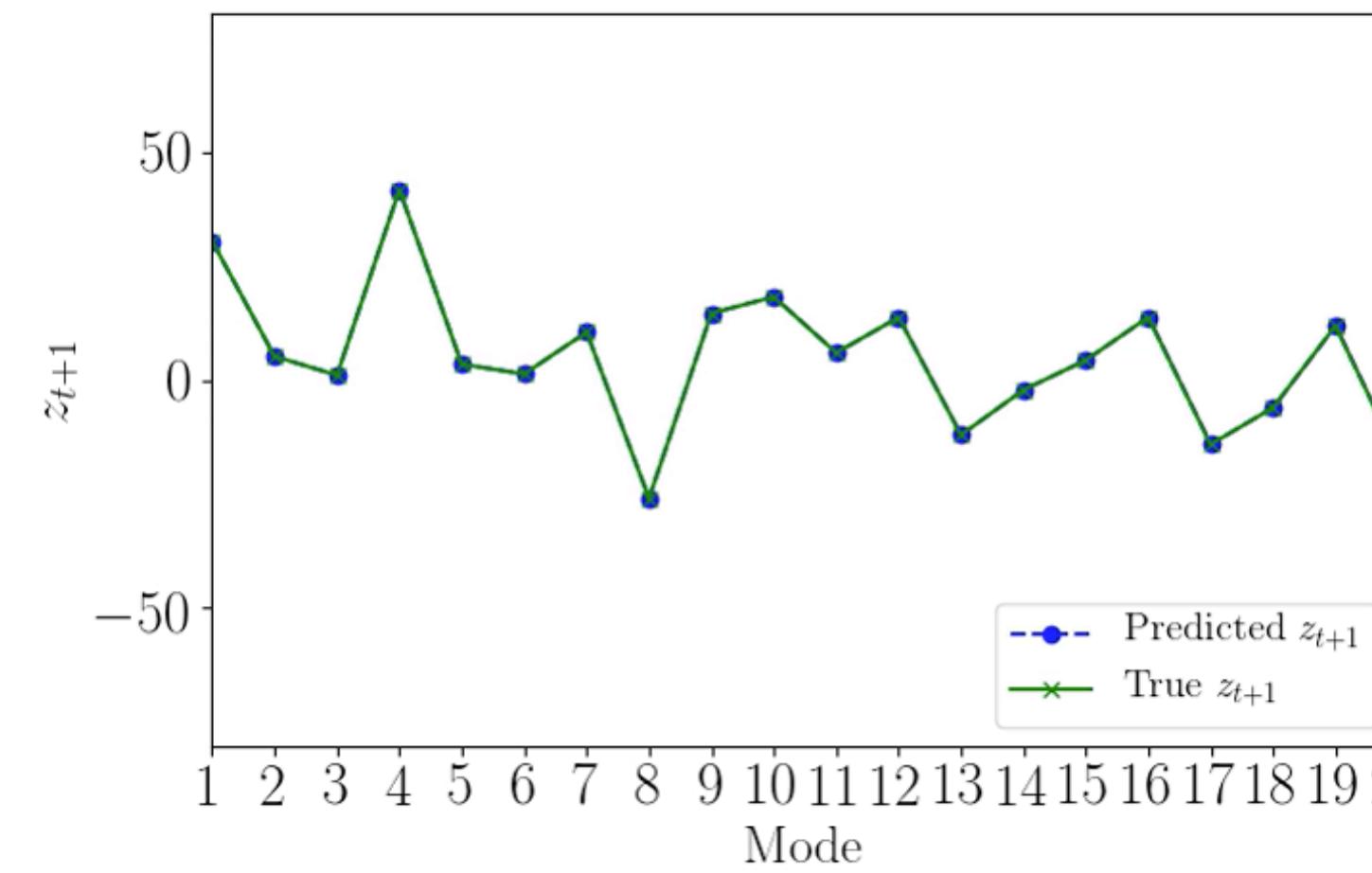
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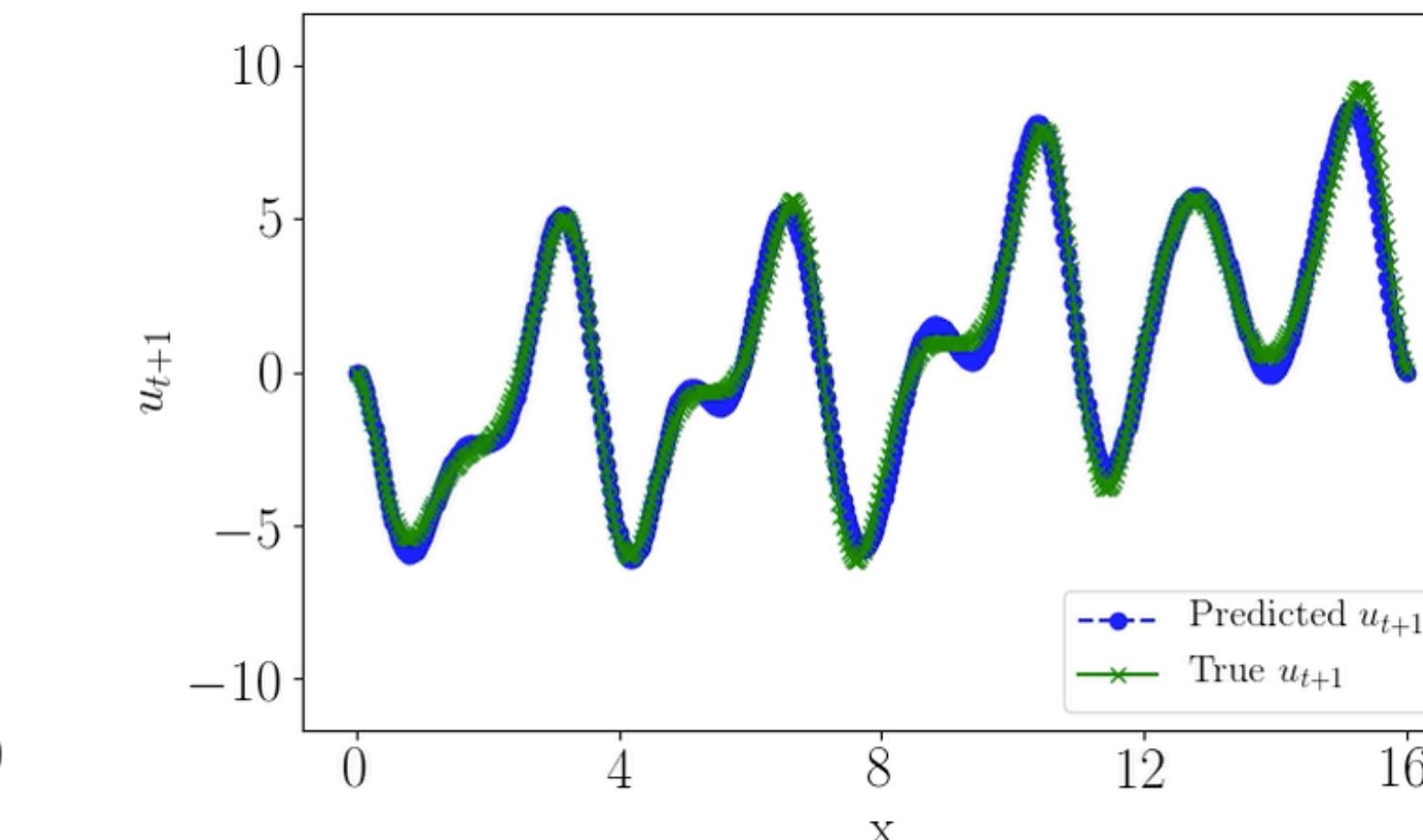
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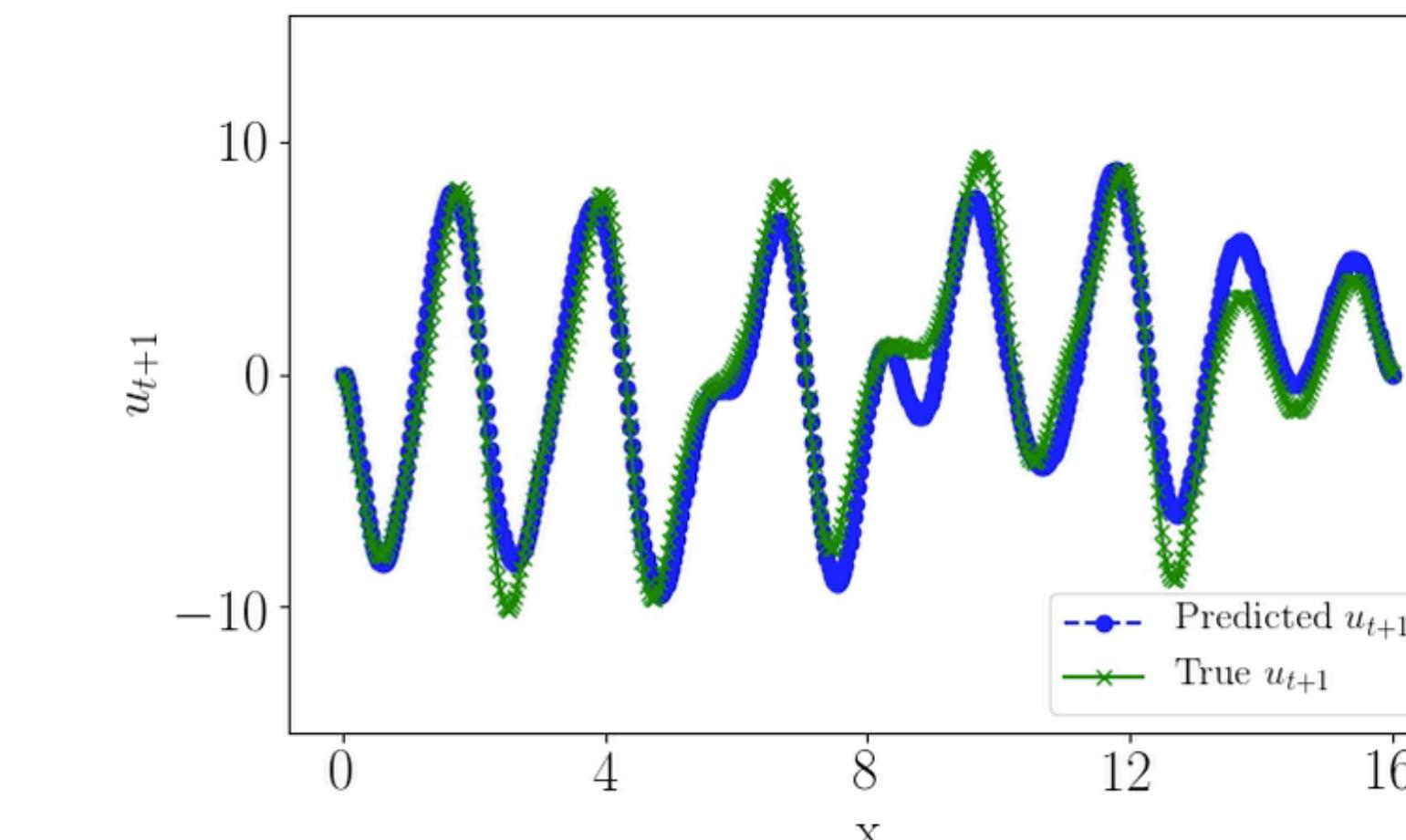
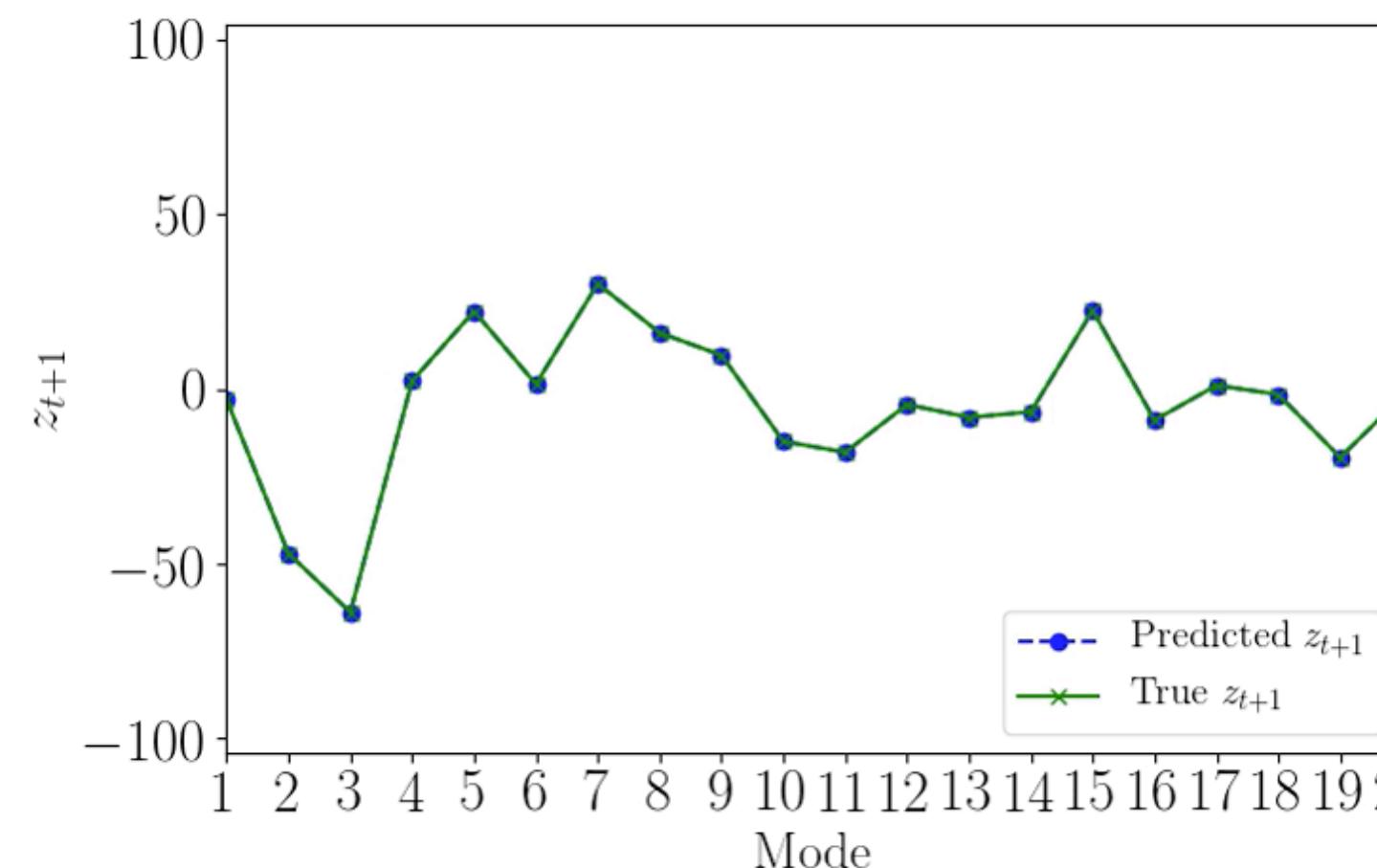
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[1] AJ Majda, J Harlim, *Filtering complex turbulent systems*, Cambridge University Press, 2012

[2] ZY Wan, TP Sapsis, *Reduced-space Gaussian Process Regression for data-driven probabilistic forecast of chaotic dynamical systems*, *Physica D: Nonlinear Phenomena*, 2017

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- Converges in the **long-term** in **mean statistical behavior**
- Efficient & effective in highly chaotic systems [1,2]

### Hybrid LSTM - MSM

$$\dot{z}_t = \begin{cases} \text{LSTM}^W(z_t, z_{t-1}, z_{t-2}, \dots) & \text{if } p_{train}(z_t) \geq \theta \\ \text{MSM}^{\zeta, c}(z_t) & \text{if } p_{train}(z_t) < \theta \end{cases}$$

Use MSM in attractor regions **underrepresented** in the training data or near attractor boundaries

### Mean Stochastic Model

$$dz_t = c z_t dt + \xi dW_t$$

parameters  
estimated from **data**

wiener  
process

$$\zeta = \sqrt{-2 c \sigma_z}$$

**data standard deviation**

$$c = \frac{1}{T}$$

**decorrelation time**

[1] AJ Majda, J Harlim, *Filtering complex turbulent systems*, Cambridge University Press, 2012

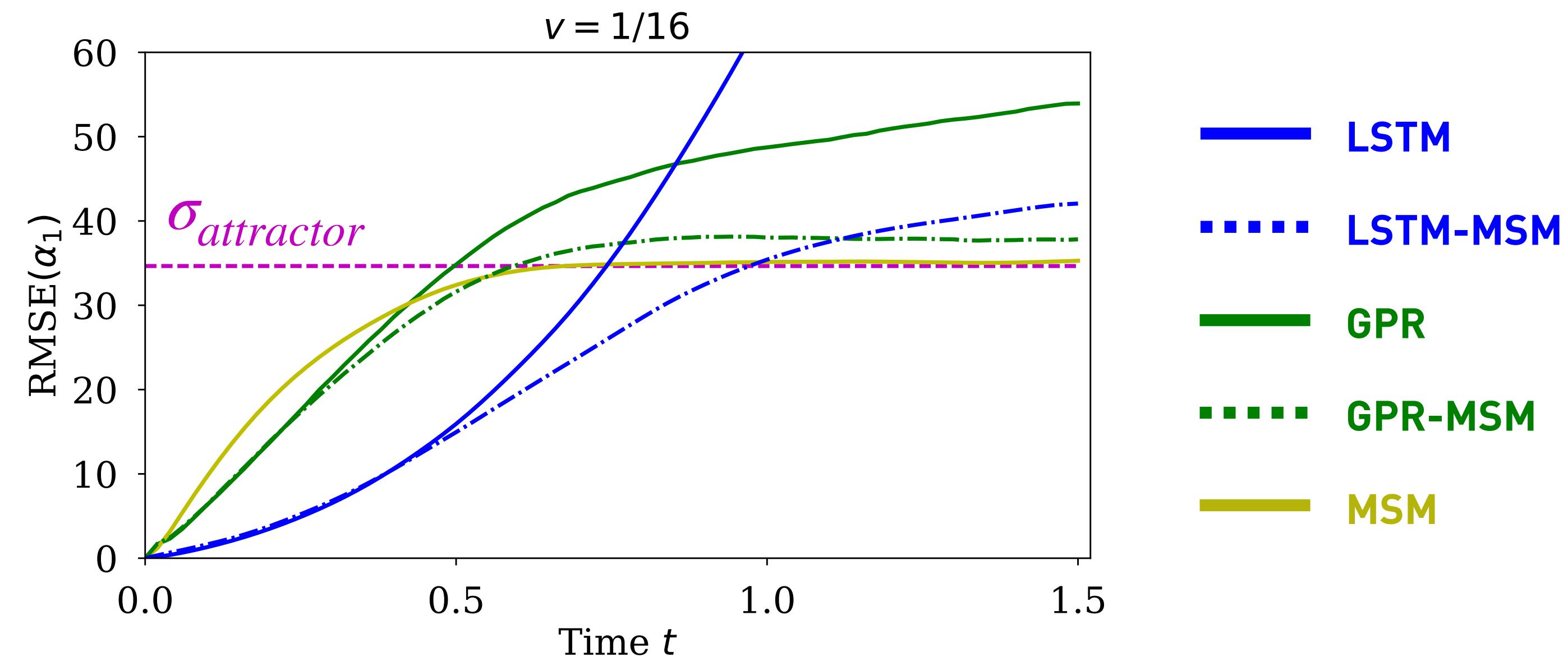
[2] ZY Wan, TP Sapsis, *Reduced-space Gaussian Process Regression for data-driven probabilistic forecast of chaotic dynamical systems*, *Physica D: Nonlinear Phenomena*, 2017

# Results on KS - Comparison with Gaussian Process Regression (GPR)

$V$	Total number of initial conditions ( <b>IC</b> )
$k$	Mode number
$i$	IC index
$z_k^i$	<b>True</b> state of mode $k$ starting from <b>IC</b> $i$
$\tilde{z}_k^i$	<b>Predicted</b> state of mode $k$ starting from <b>IC</b> $i$

Root mean square error:

$$\text{RMSE}(z_k) = \sqrt{\frac{1}{V} \sum_{i=1}^V (z_k^i - \tilde{z}_k^i)^2}$$



RMSE evolution in time of **the most energetic** mode  
(averaged over 1000 initial conditions)

# Challenges

1

Iterative prediction error **accumulates** leading to unphysical predictions  
*- divergence from attractor*

- Dynamics underrepresented in training data
- Scarce data in attractor boundaries
- Under-resolved high dimensional dynamics
- Models not generalising / distribution shift

**Mitigation? Hybrid LSTM - MSM approach**

# Challenges

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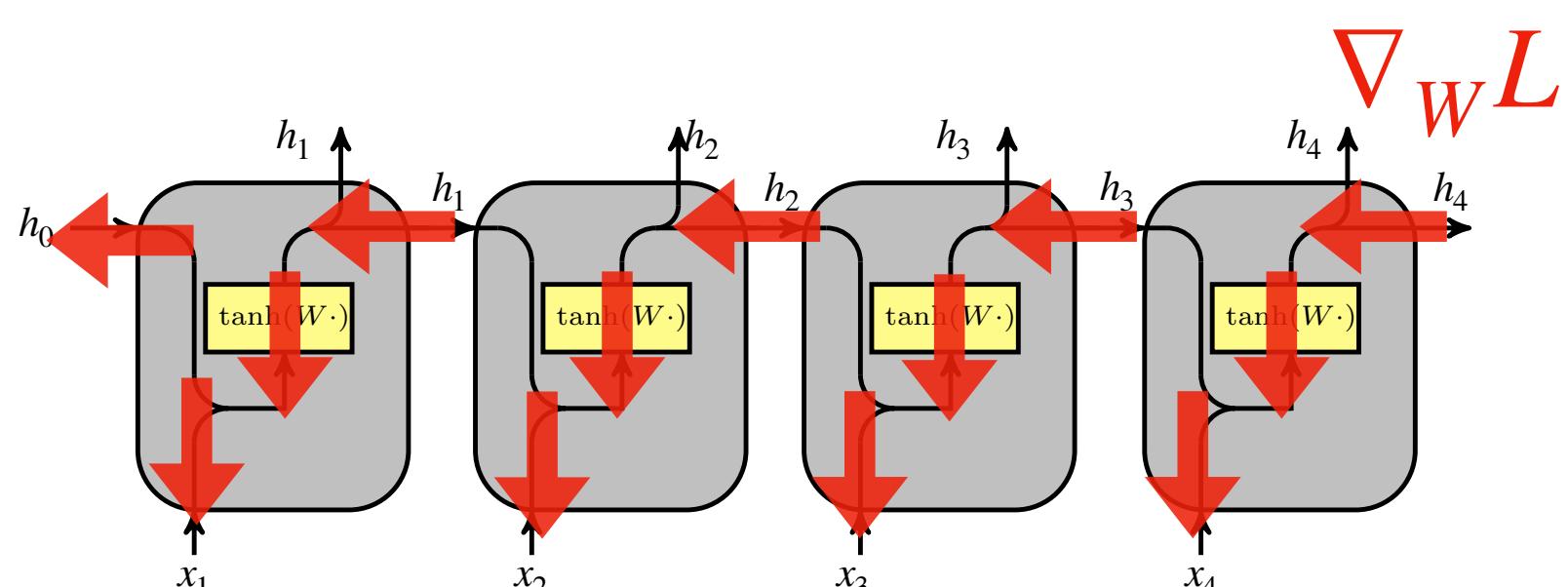
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**Vanishing gradients problem during training:** As the gradient is back-propagated during training of the networks it may **vanish to zero or explode.**



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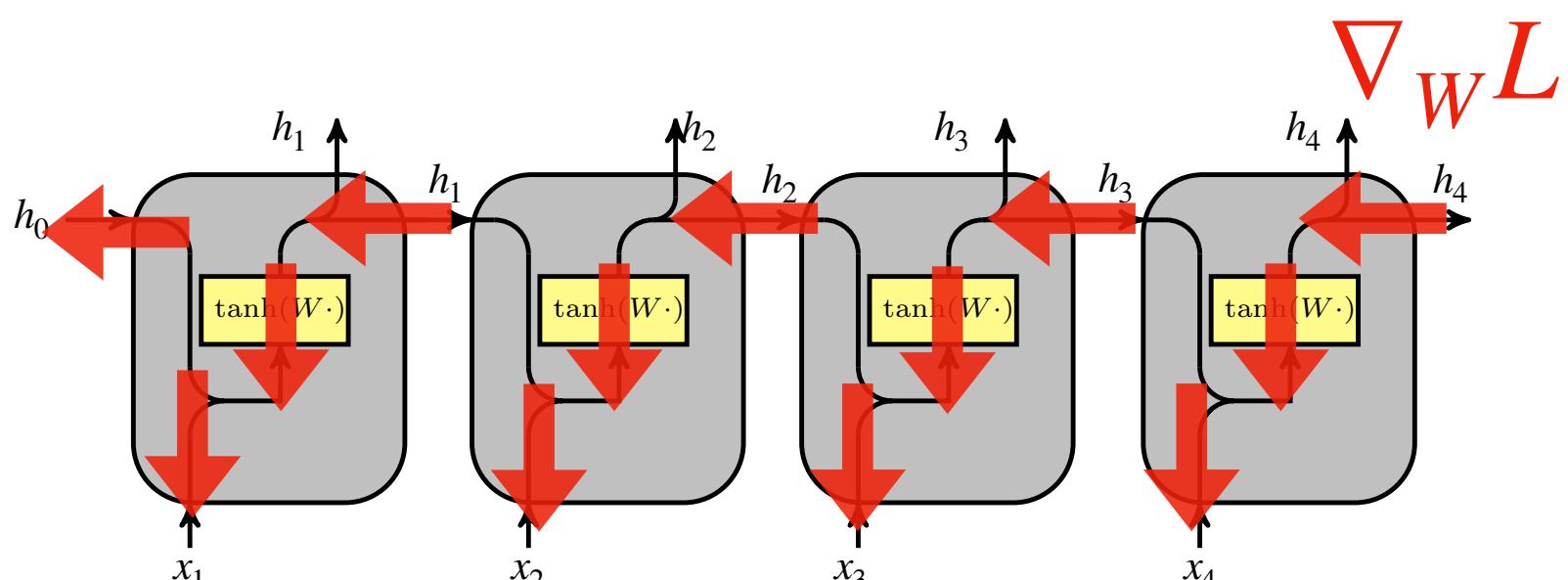
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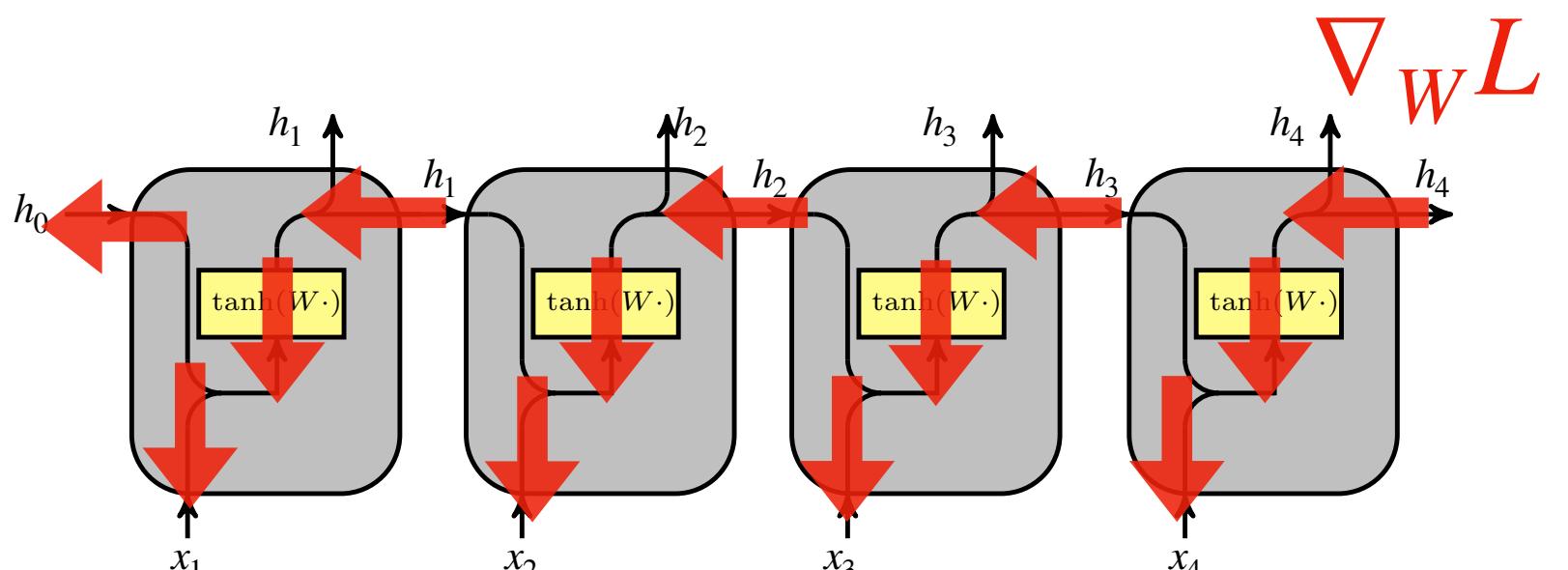
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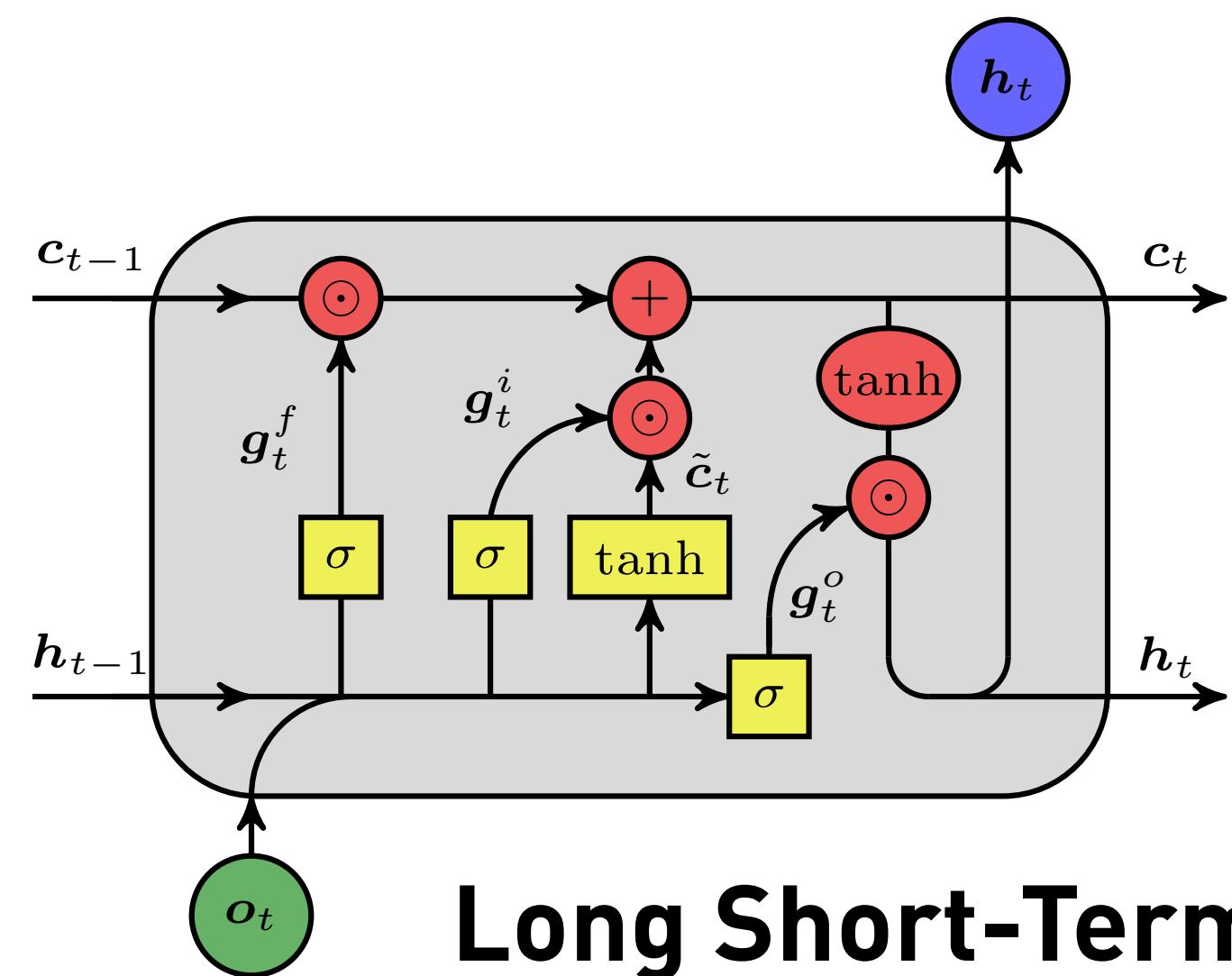
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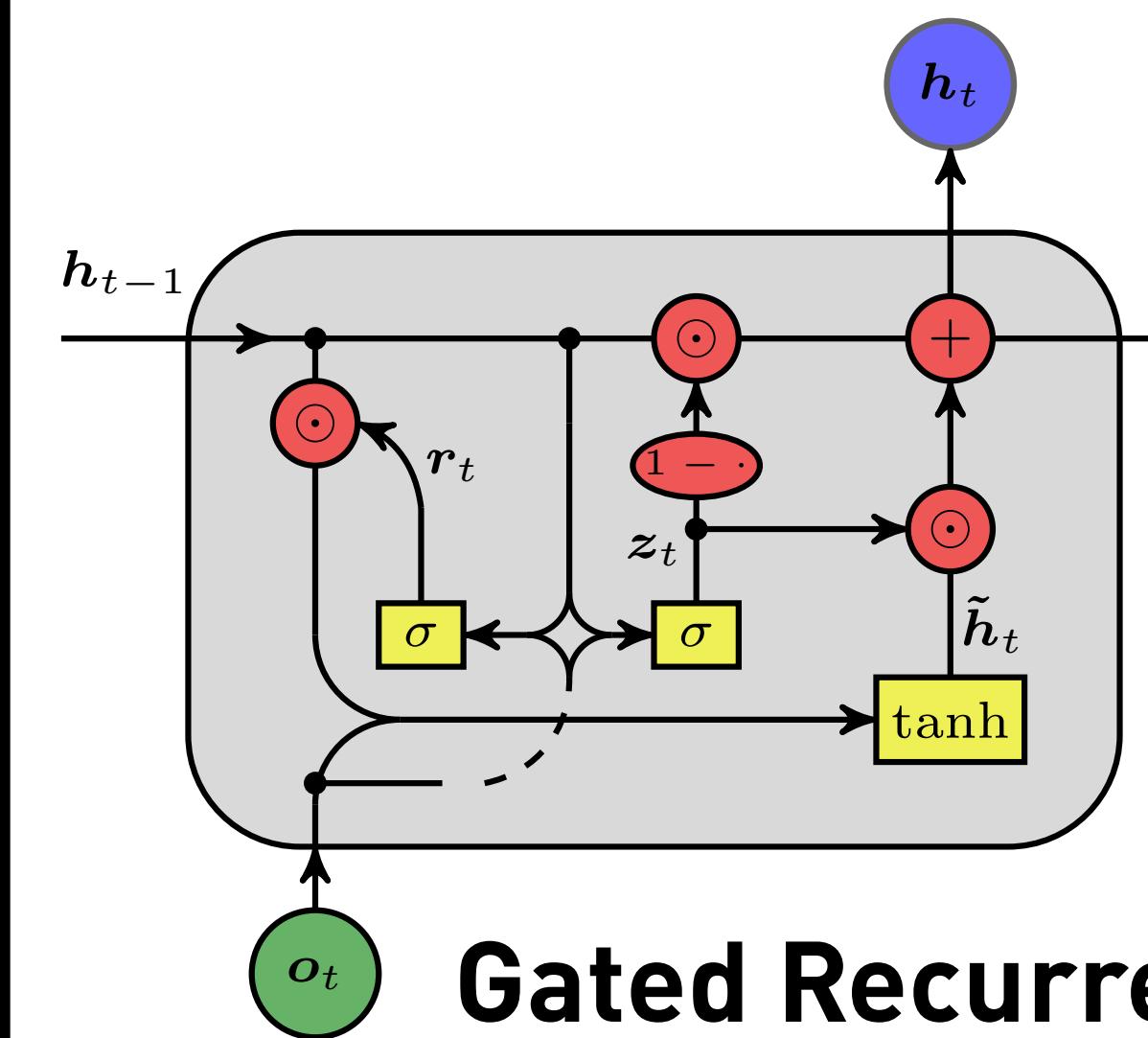


**Mitigation? Sophisticated architectures**



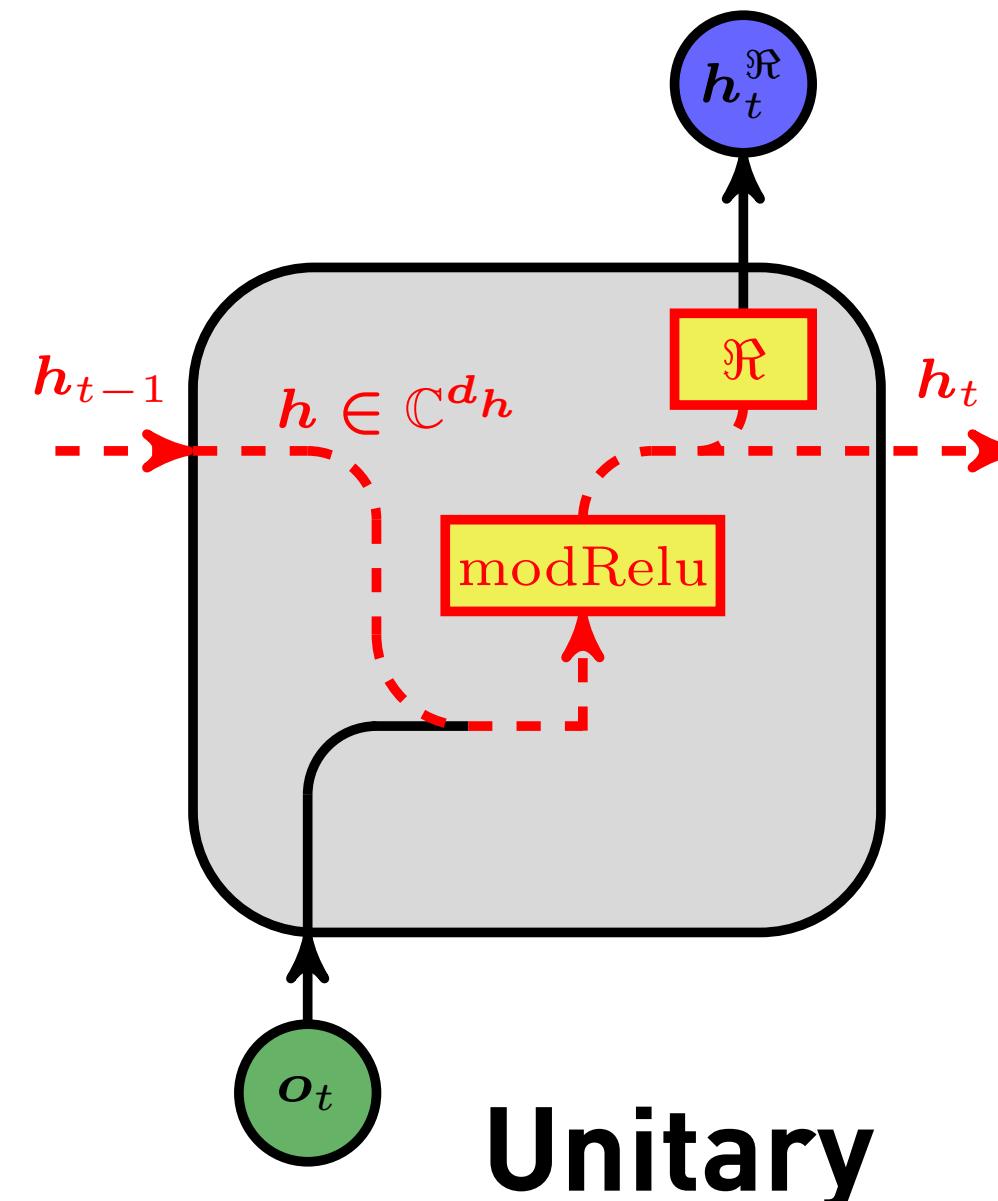
## Long Short-Term Memory (LSTM)

- Gating mechanisms
- Proposed by S. Hochreiter and J. Schmidhuber (1997)
- Trained with Backpropagation through time (BPTT)



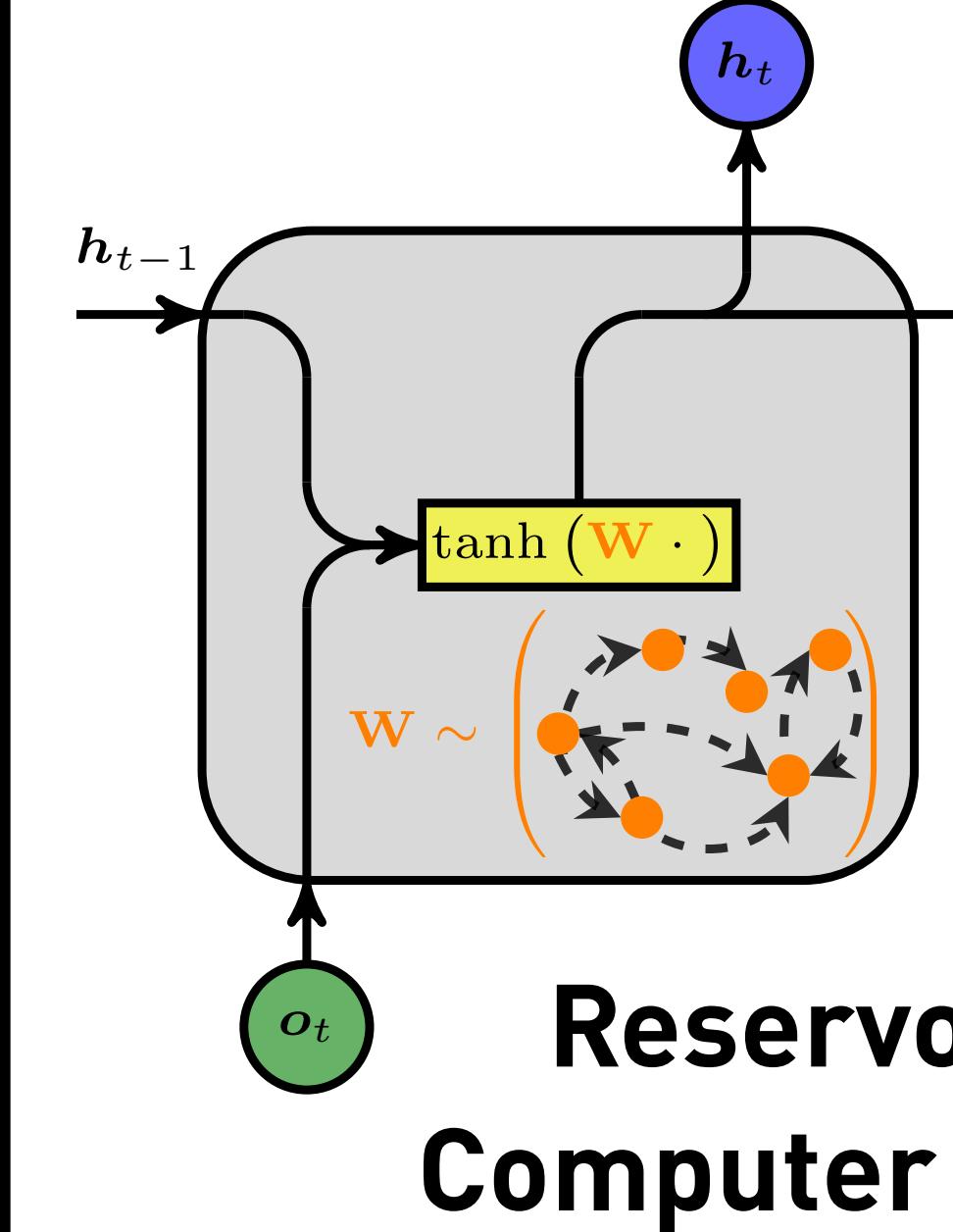
## Gated Recurrent Unit (GRU)

- Gating mechanisms
- Alternative to LSTM, less params., Cho et al. (2014)
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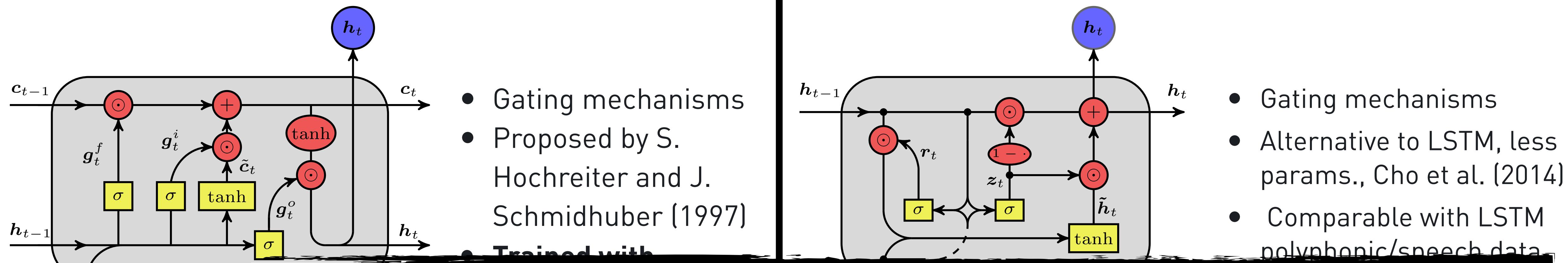
## Unitary

- Arjovsky et al. (2016); Jing et al. (2017)
- Recurrent weight matrix is complex unitary with spectral radius one
- Complex generalization of Elman RNNs
- modRelu as a activation
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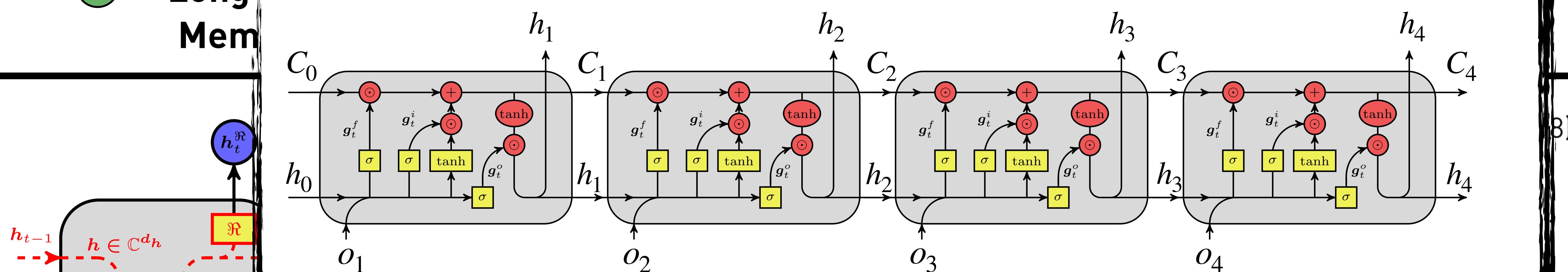


## Reservoir Computer (RC)

- Pathak, Ott, et. al. (2017, 2018)
- Echo state networks, Liquid state machines, Maass et. al. (2002), Jaeger et. al. (2007)
- Random sparse recurrent weight matrix with **spectral radius smaller than one**
- Train linear output layer with regularised least squares regression

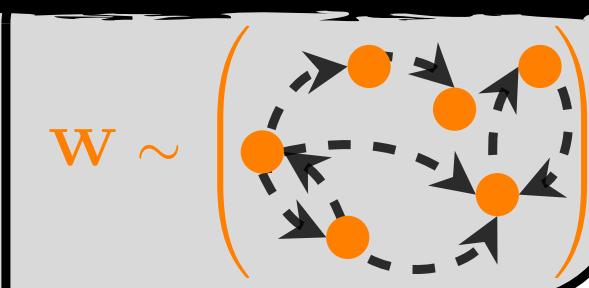


Gating architectures: *Uninterrupted gradient flow!*

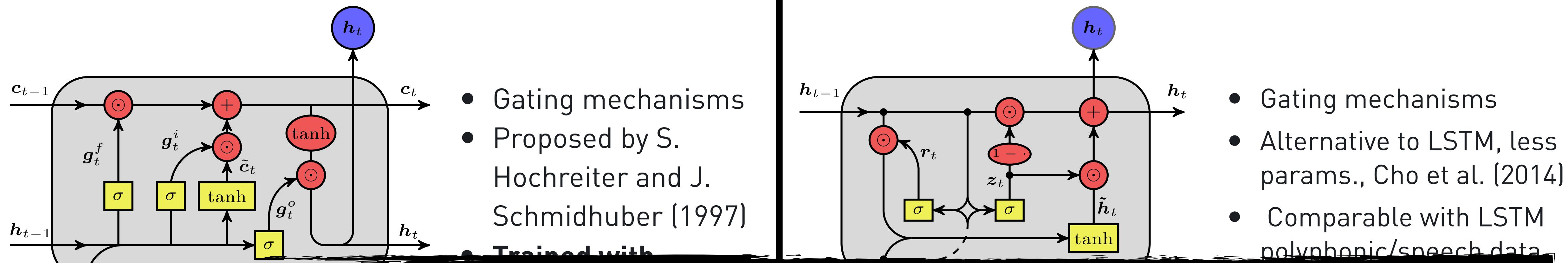


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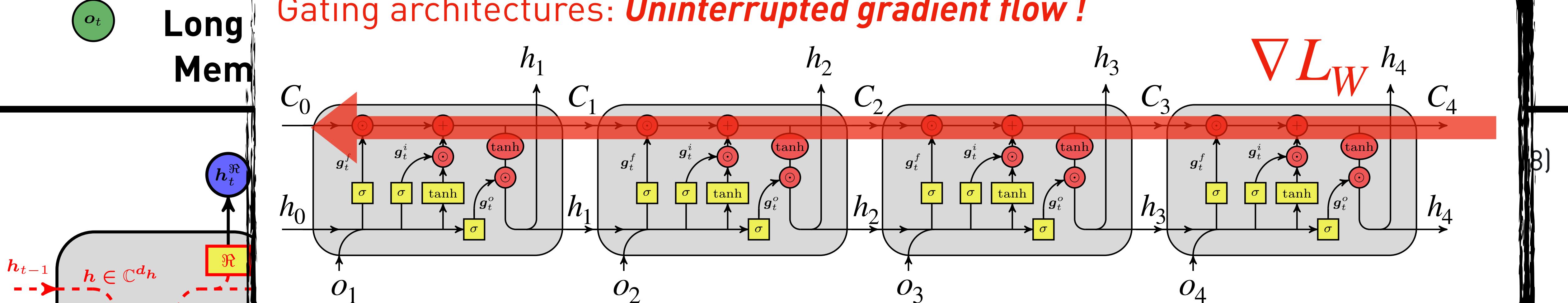
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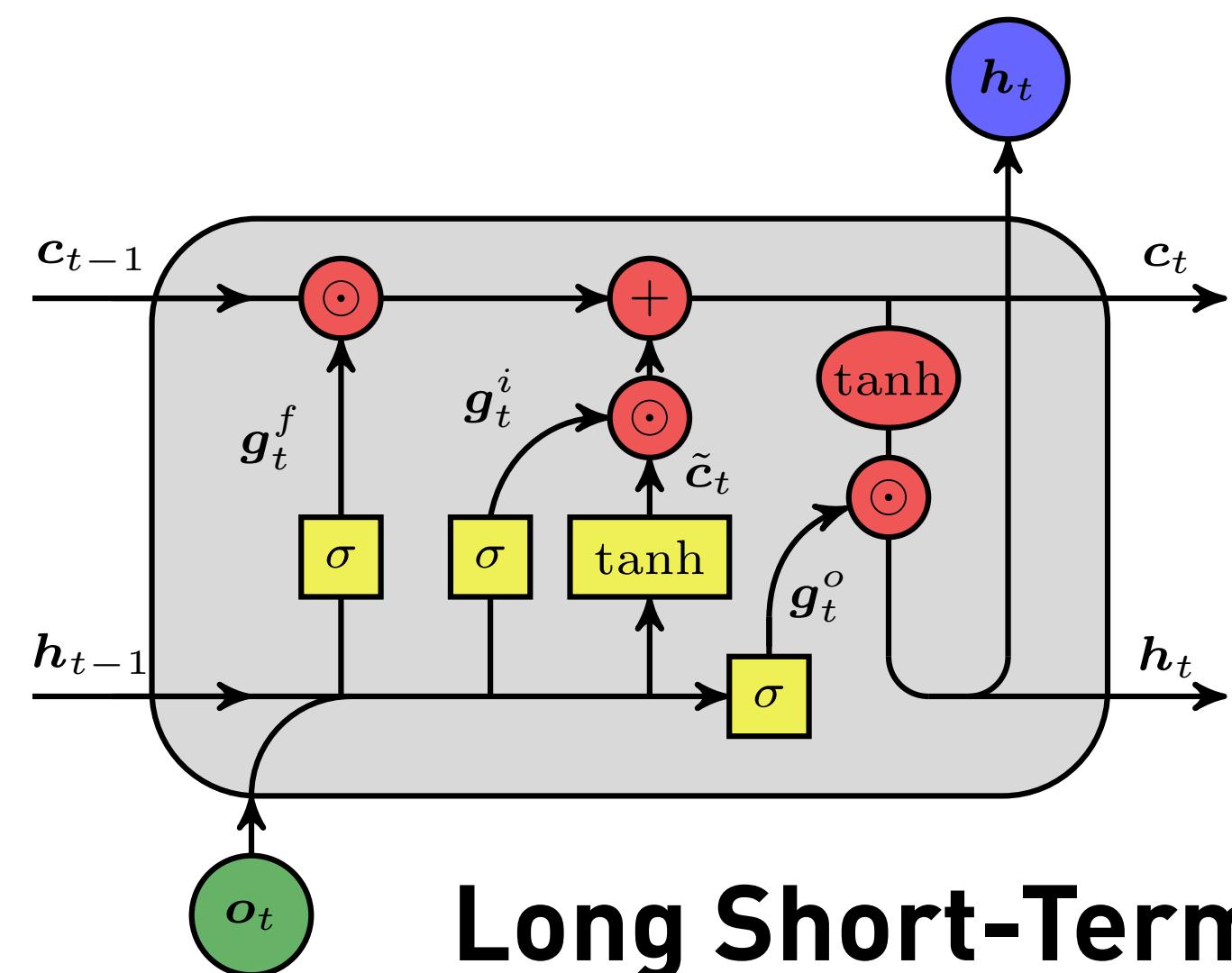
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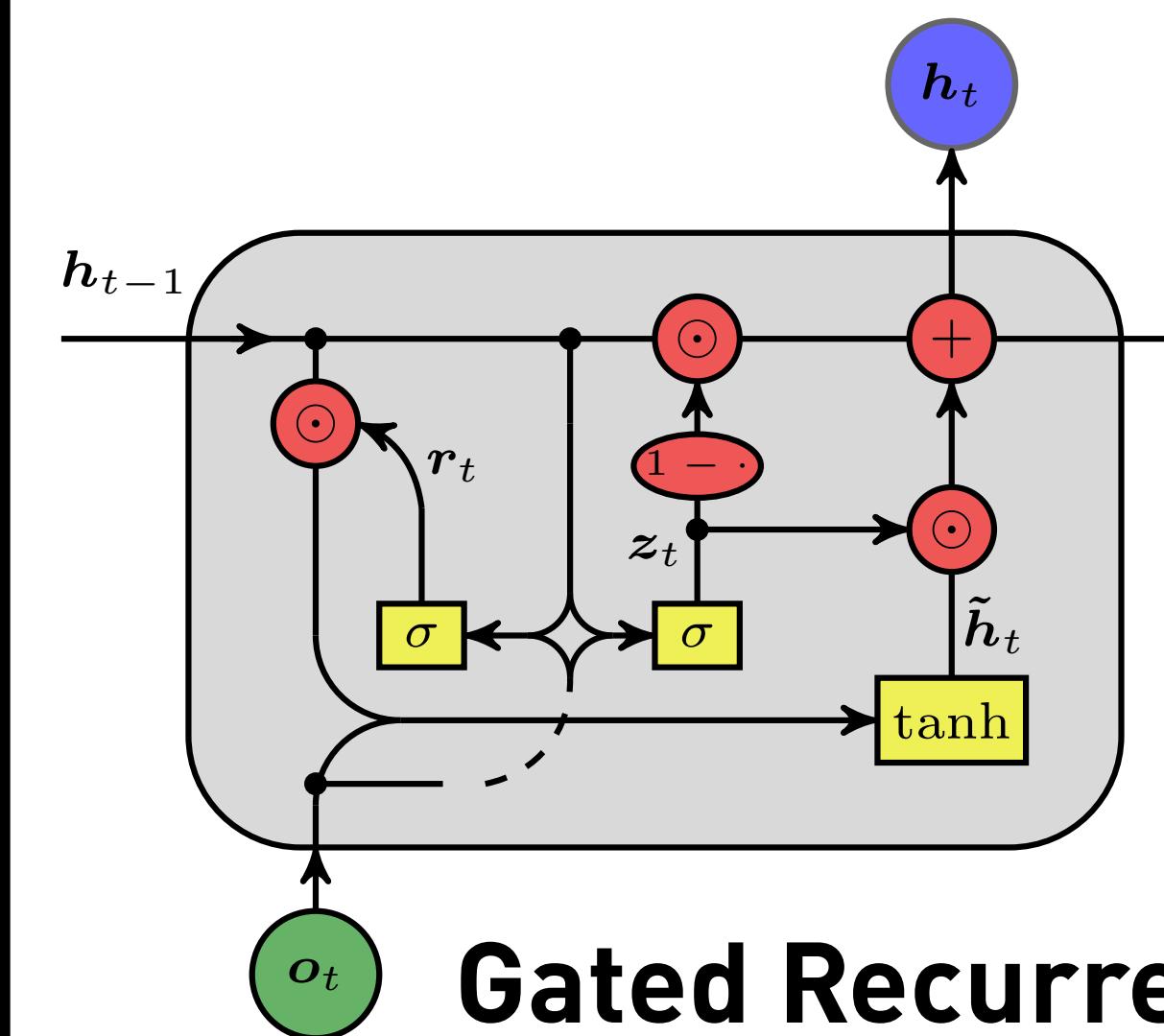
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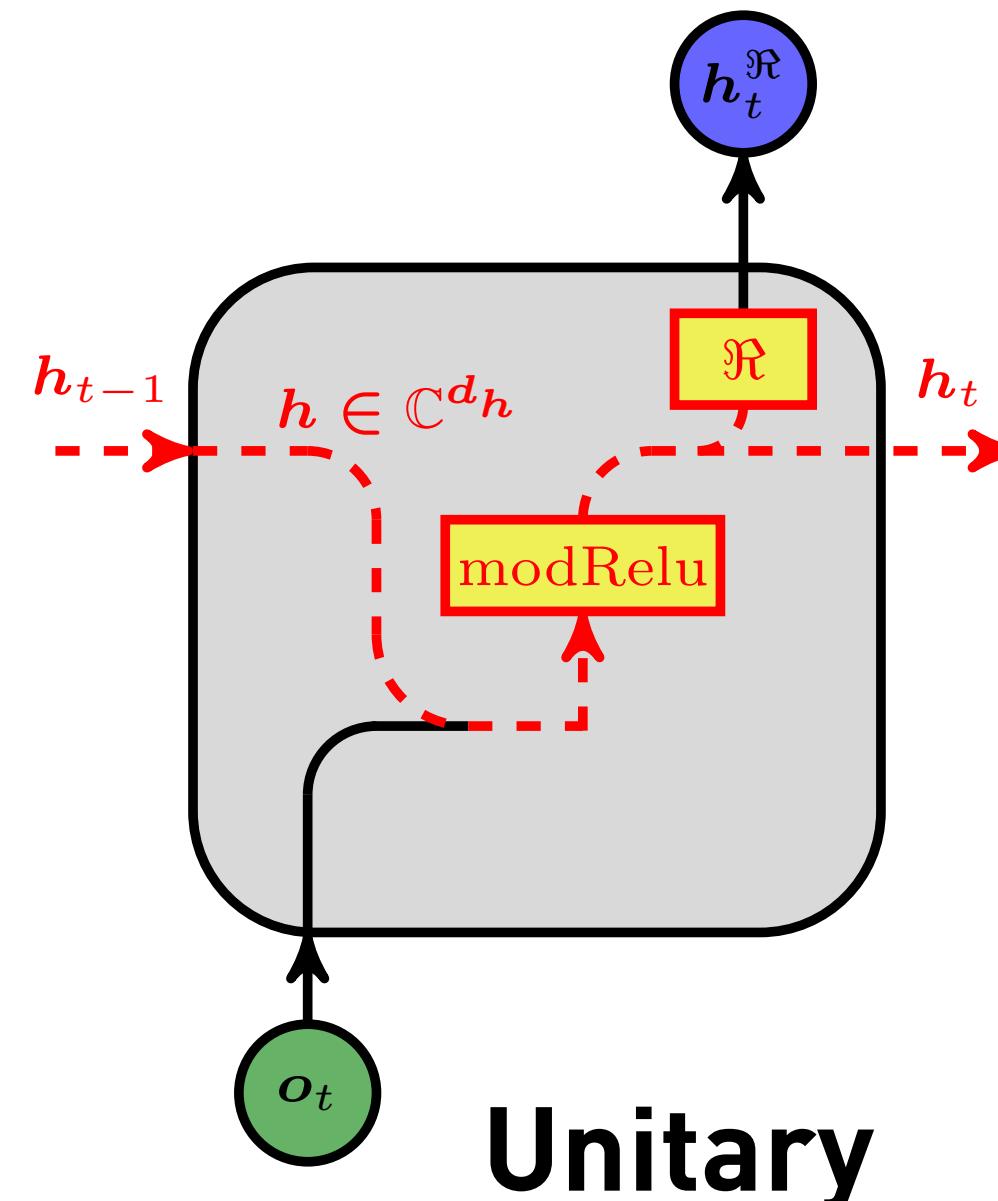
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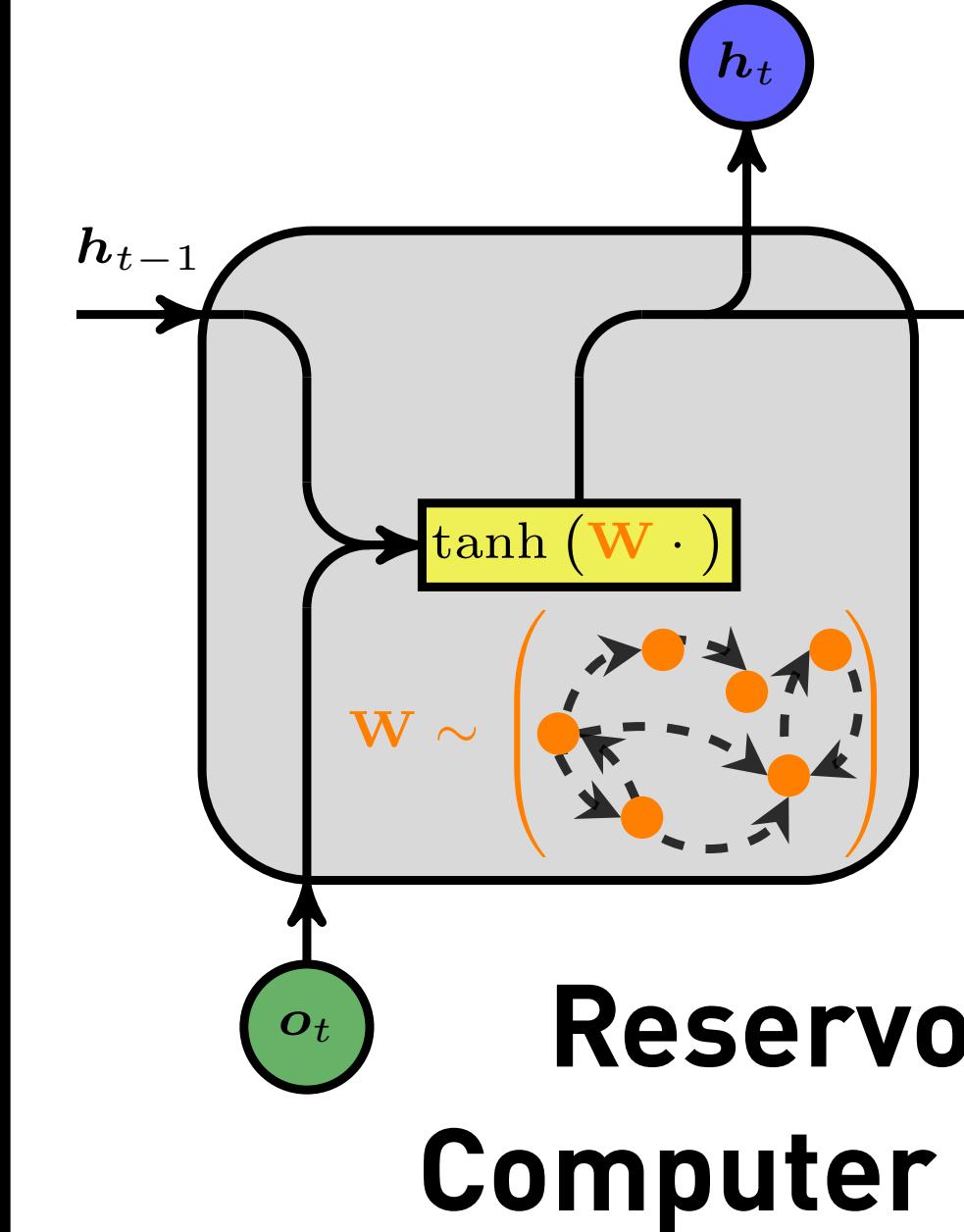
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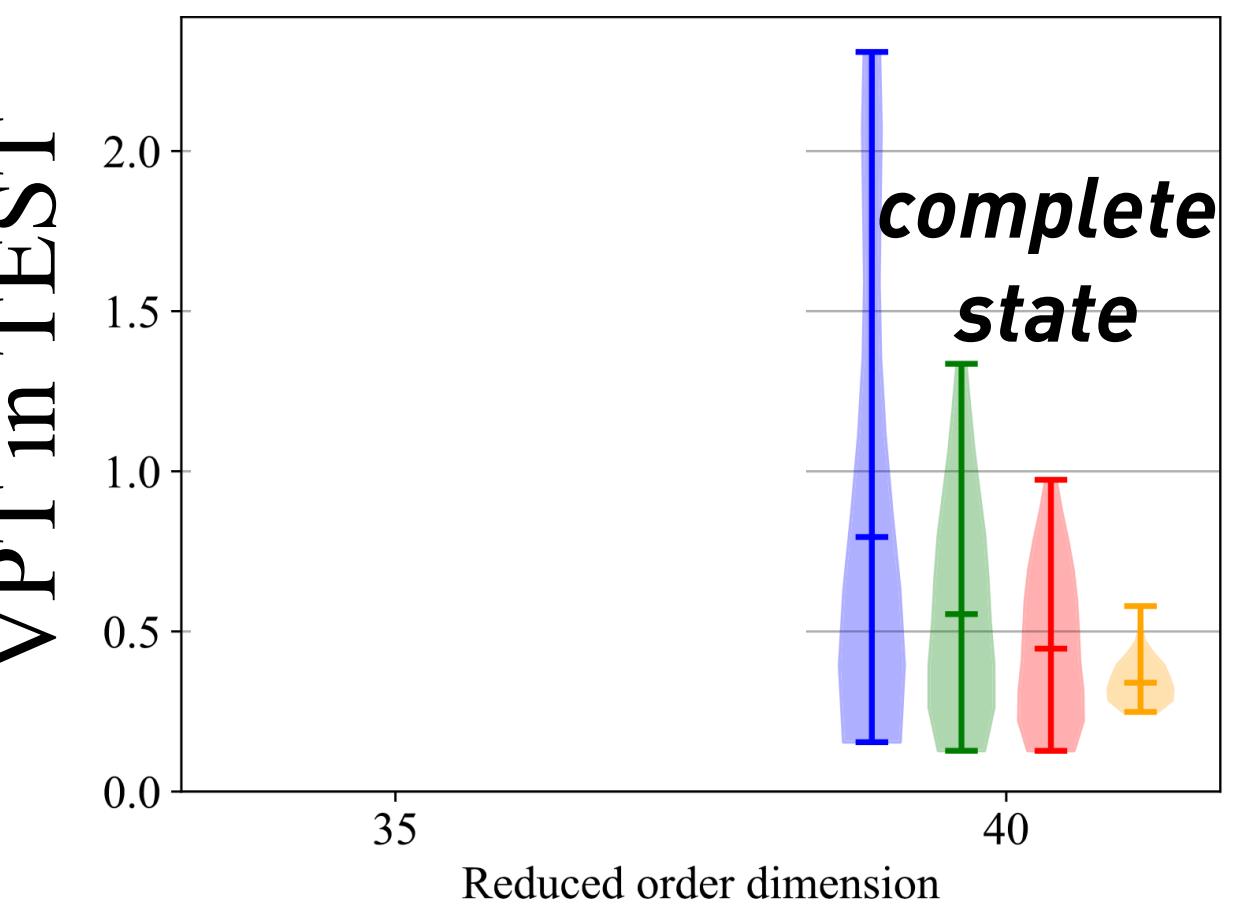
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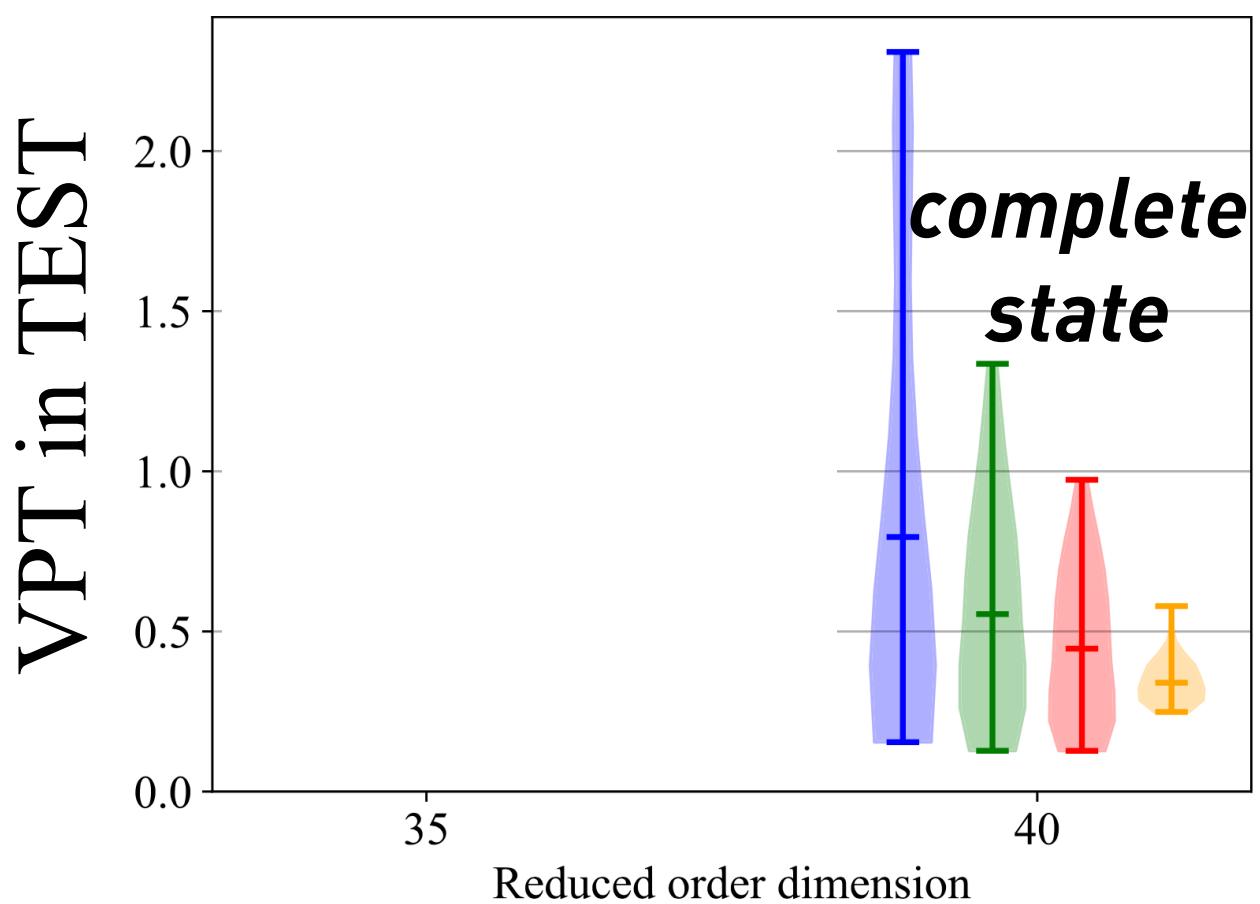


RC (or ) ; GRU (or ) ; LSTM (or ) ; Unit (or ) ; Ideal ;

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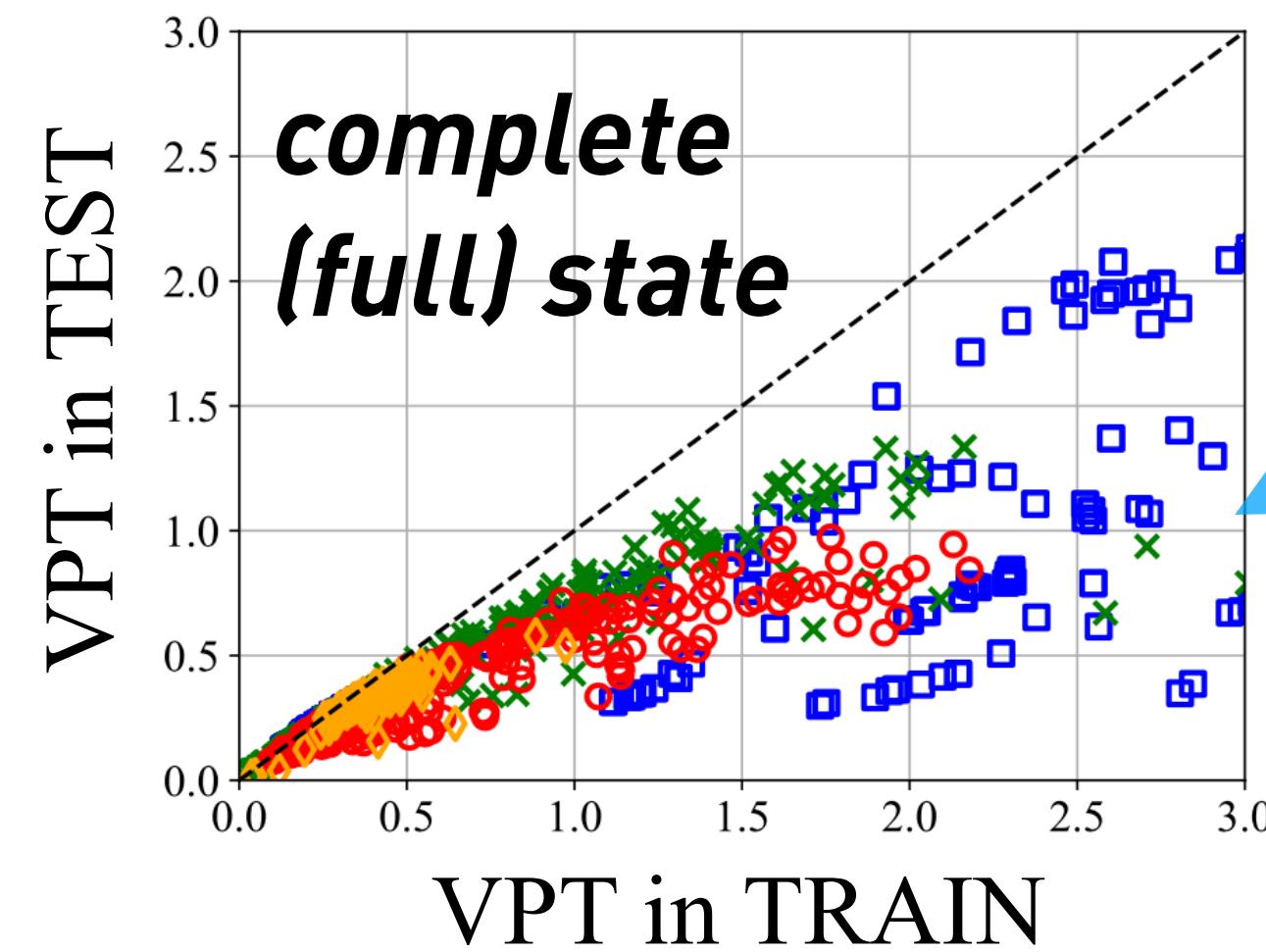
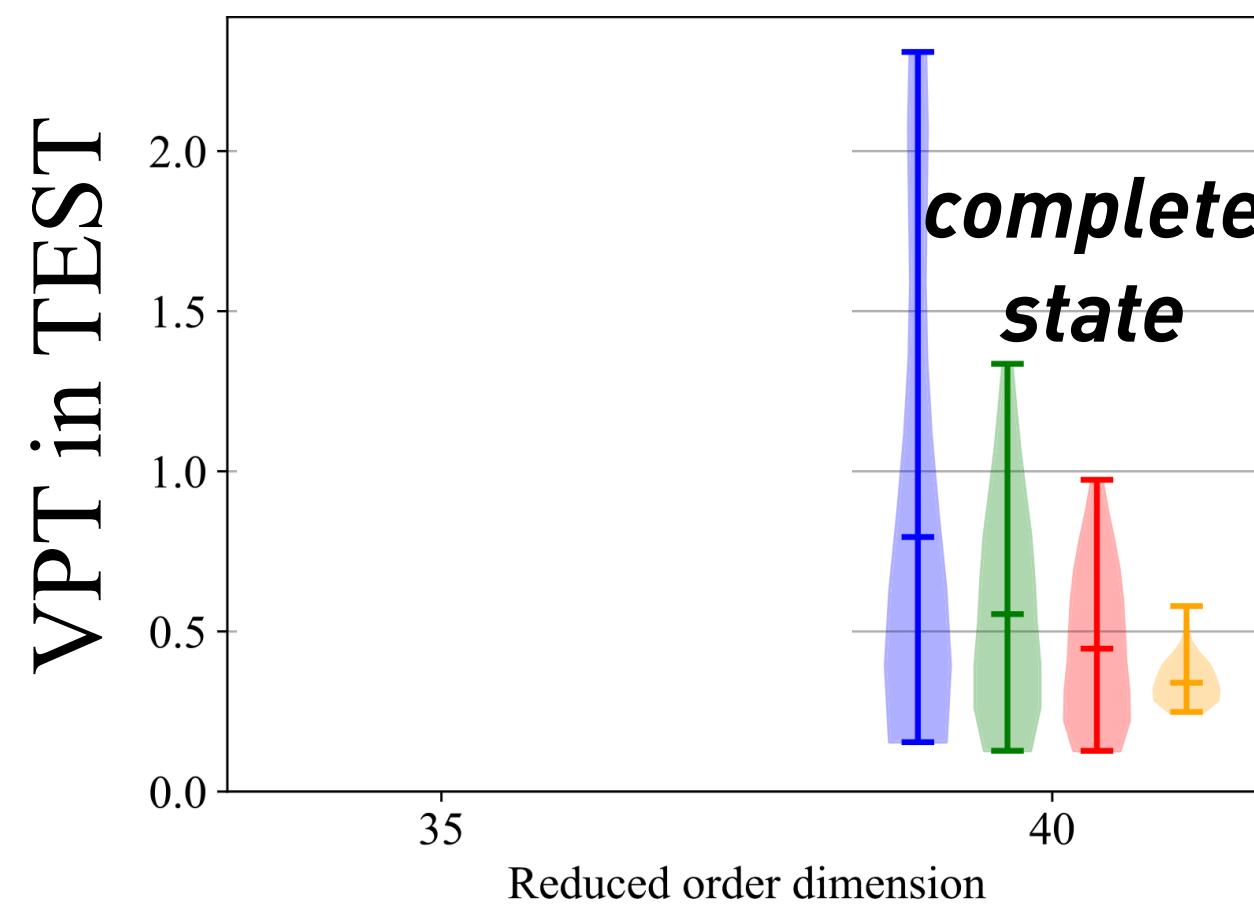


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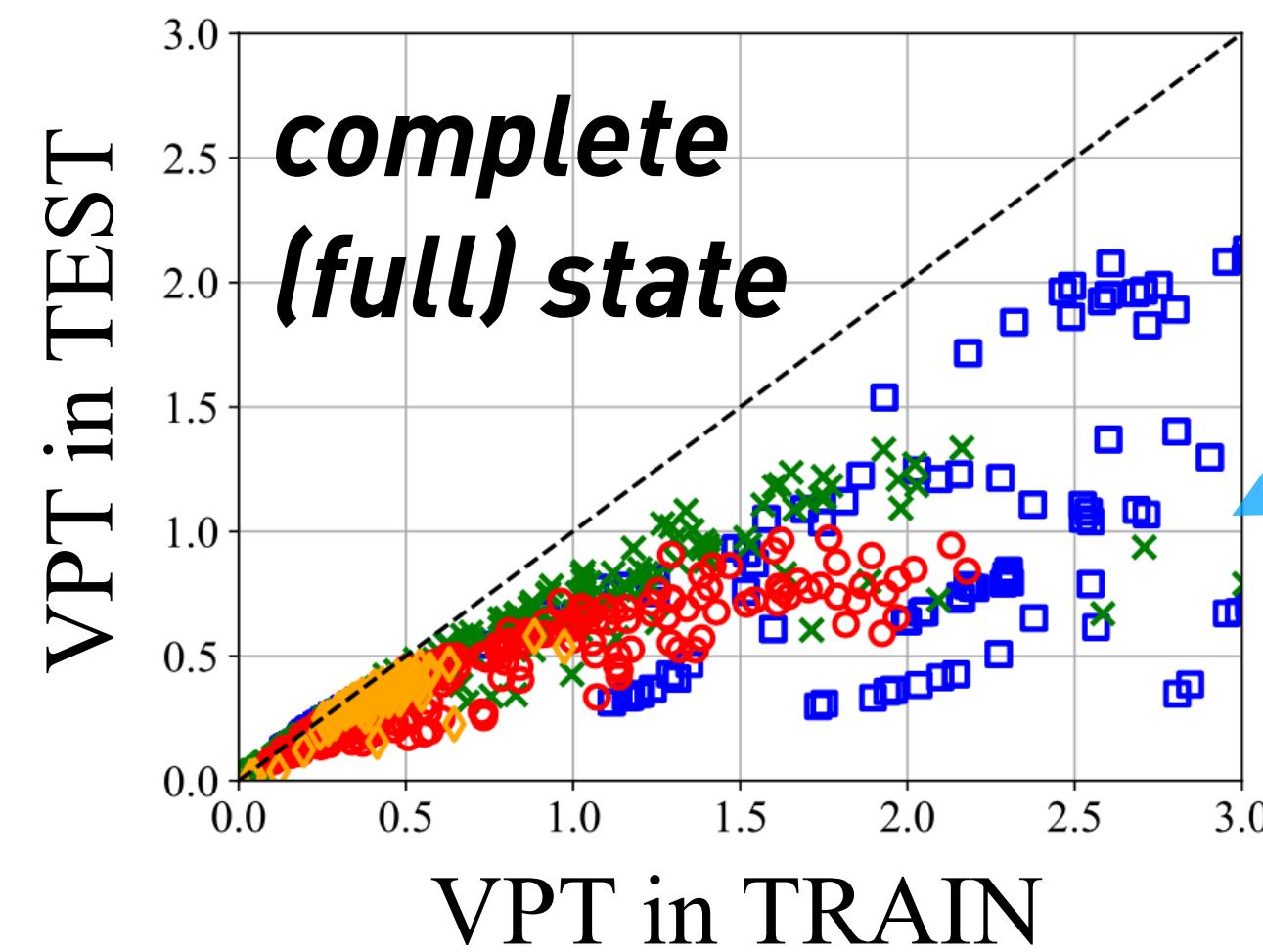
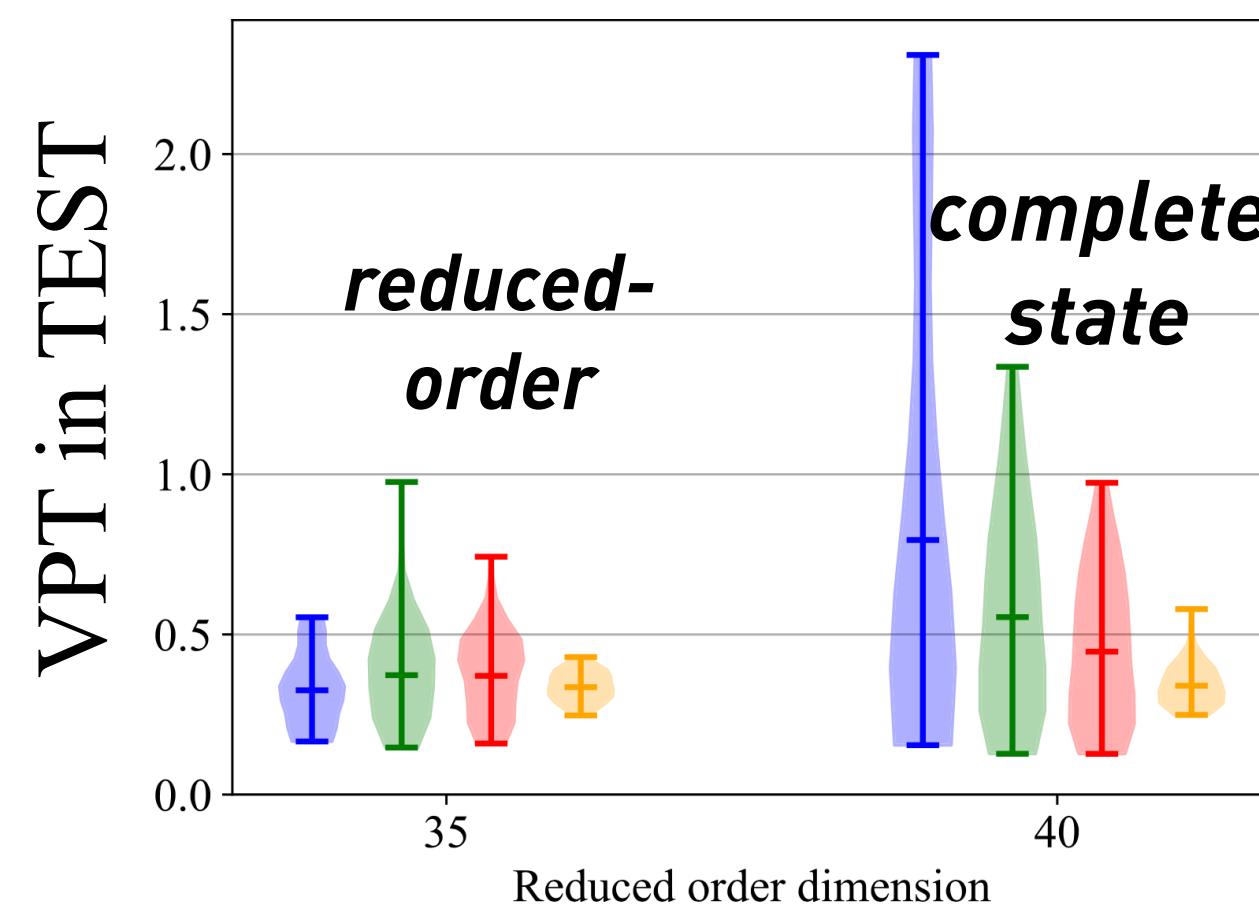


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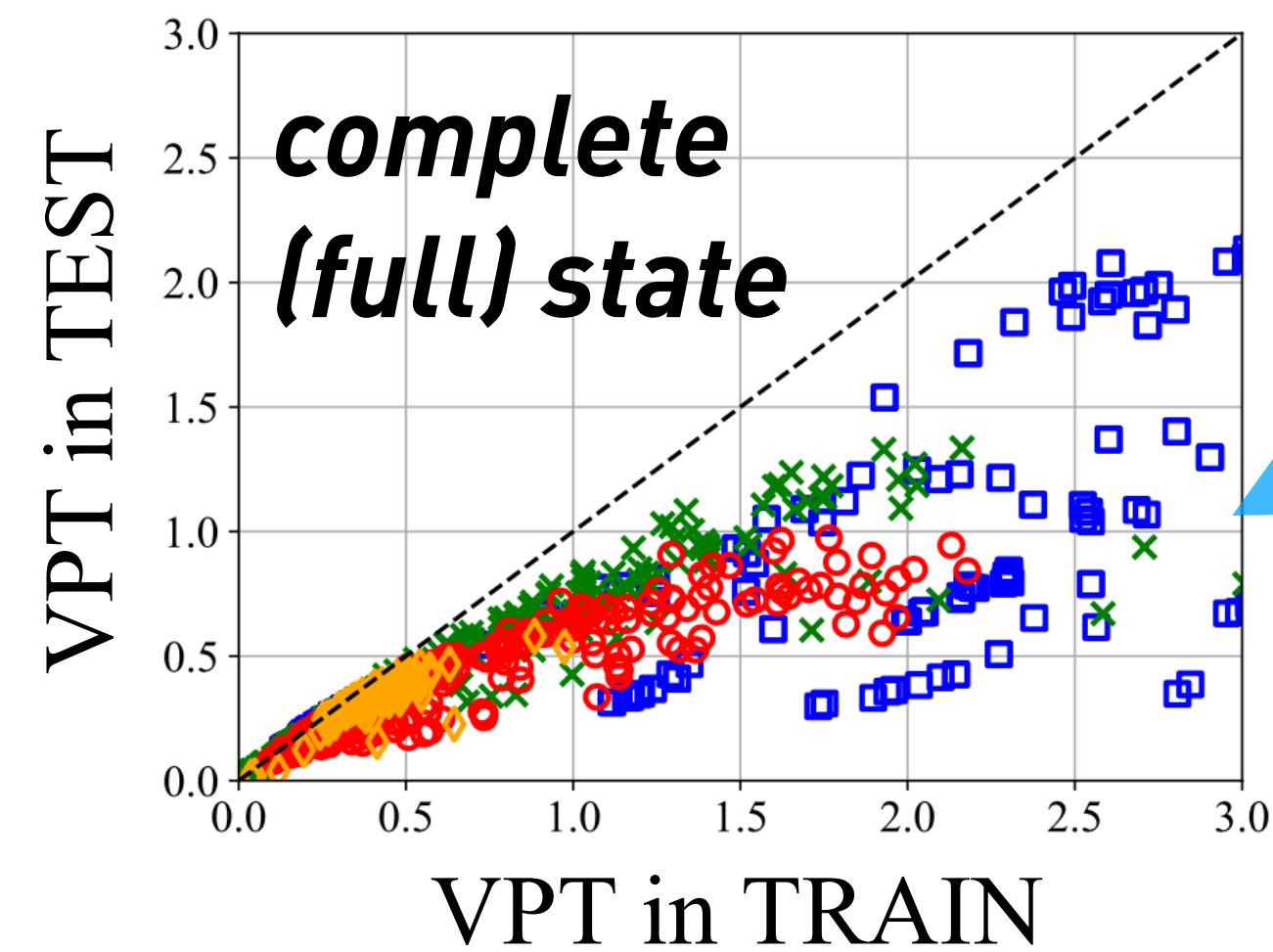
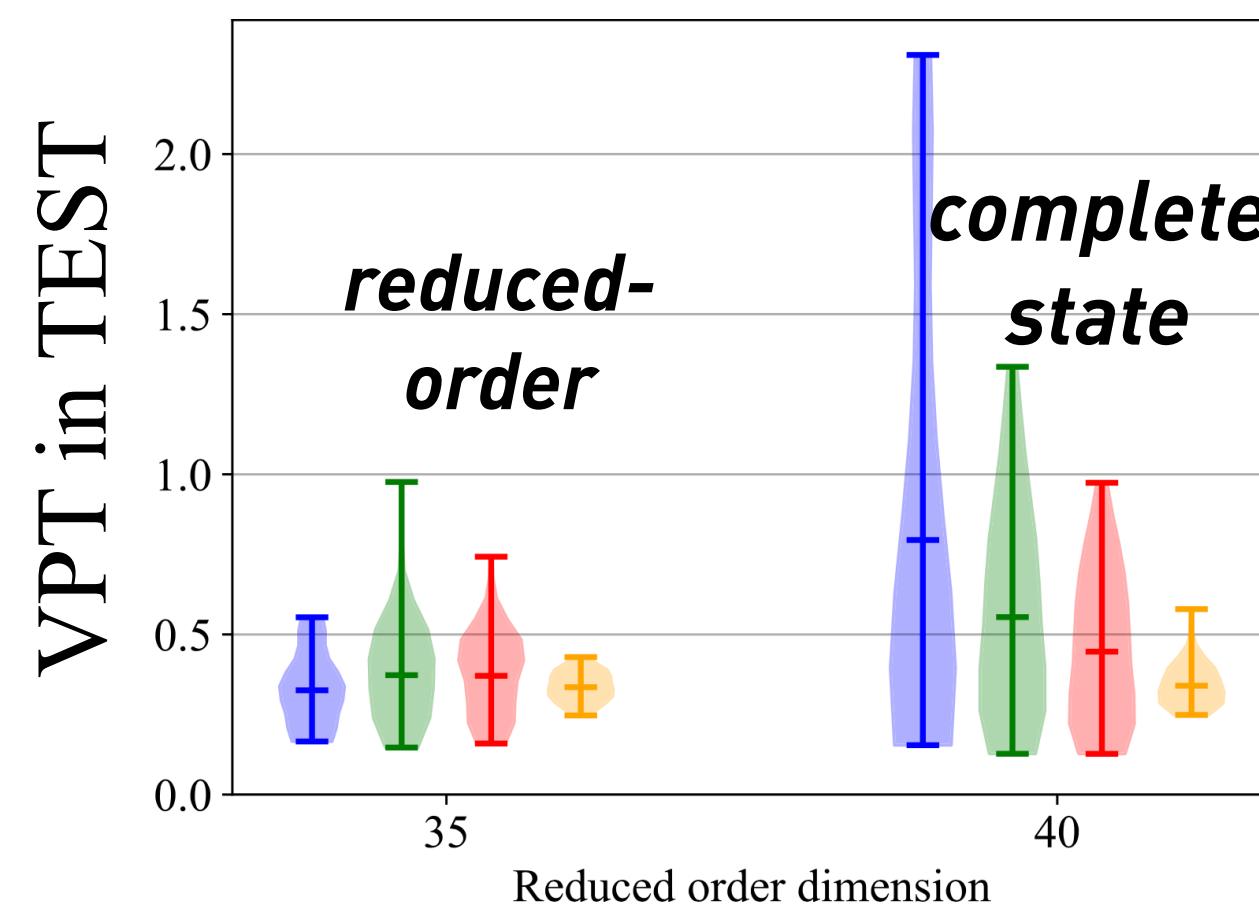


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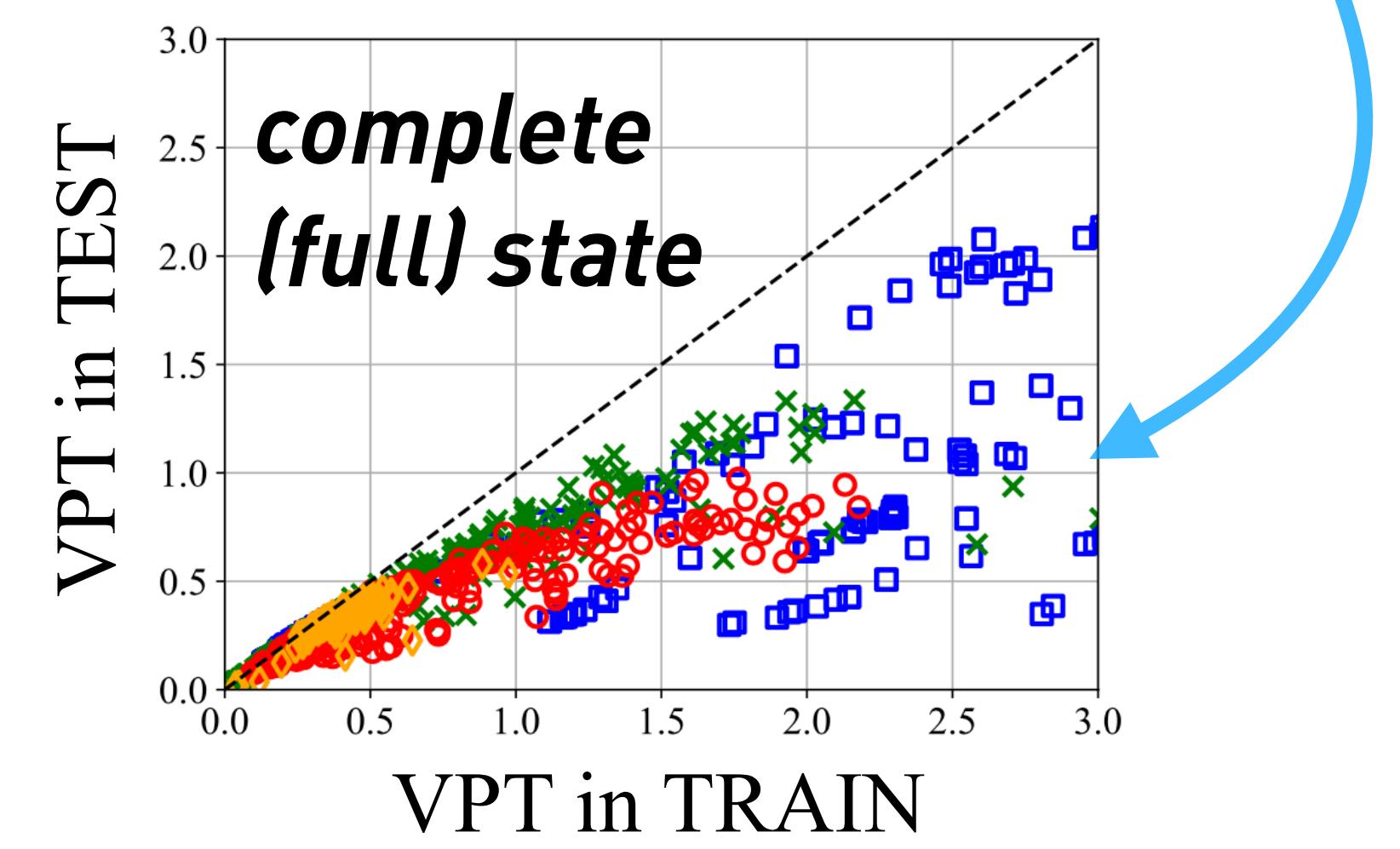
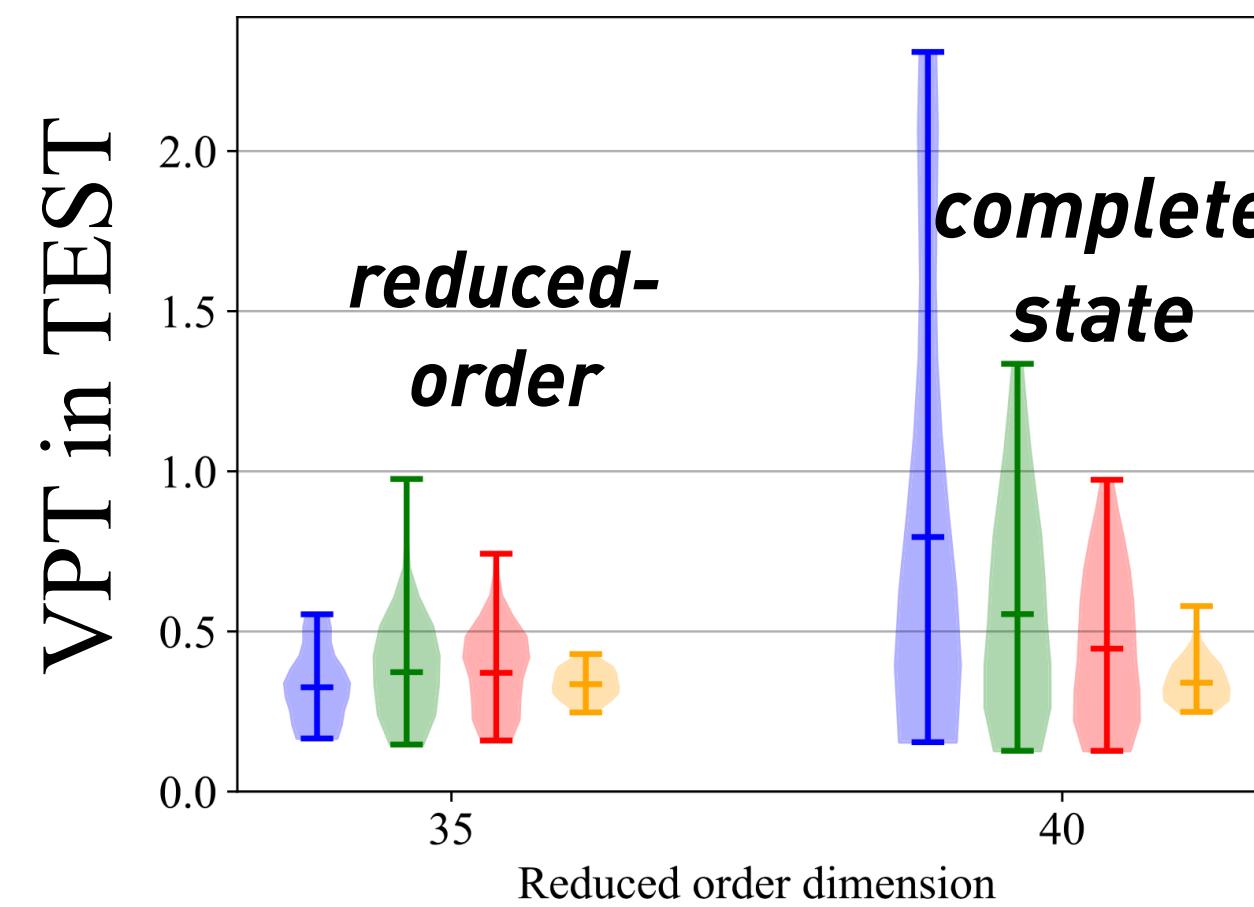
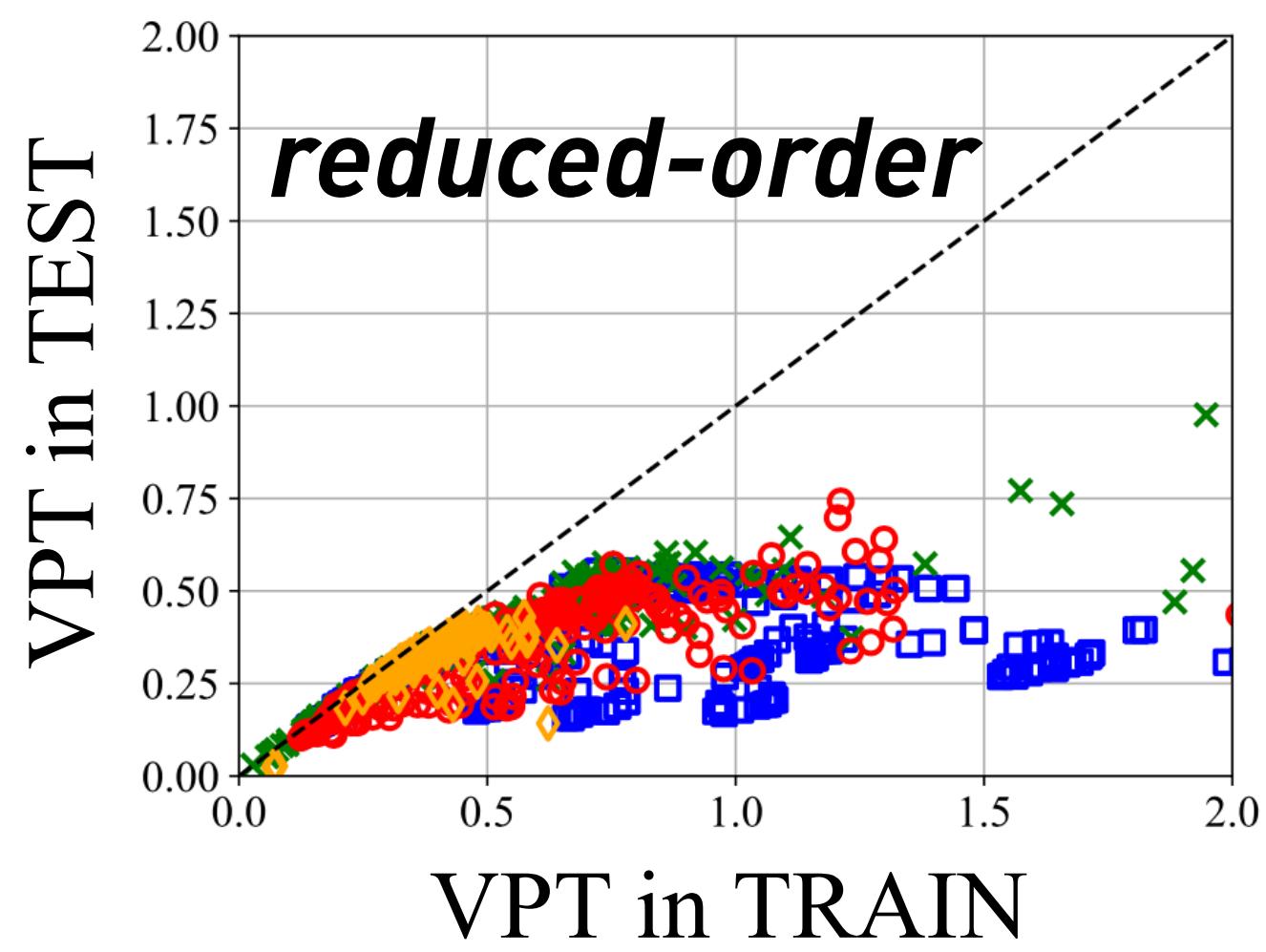


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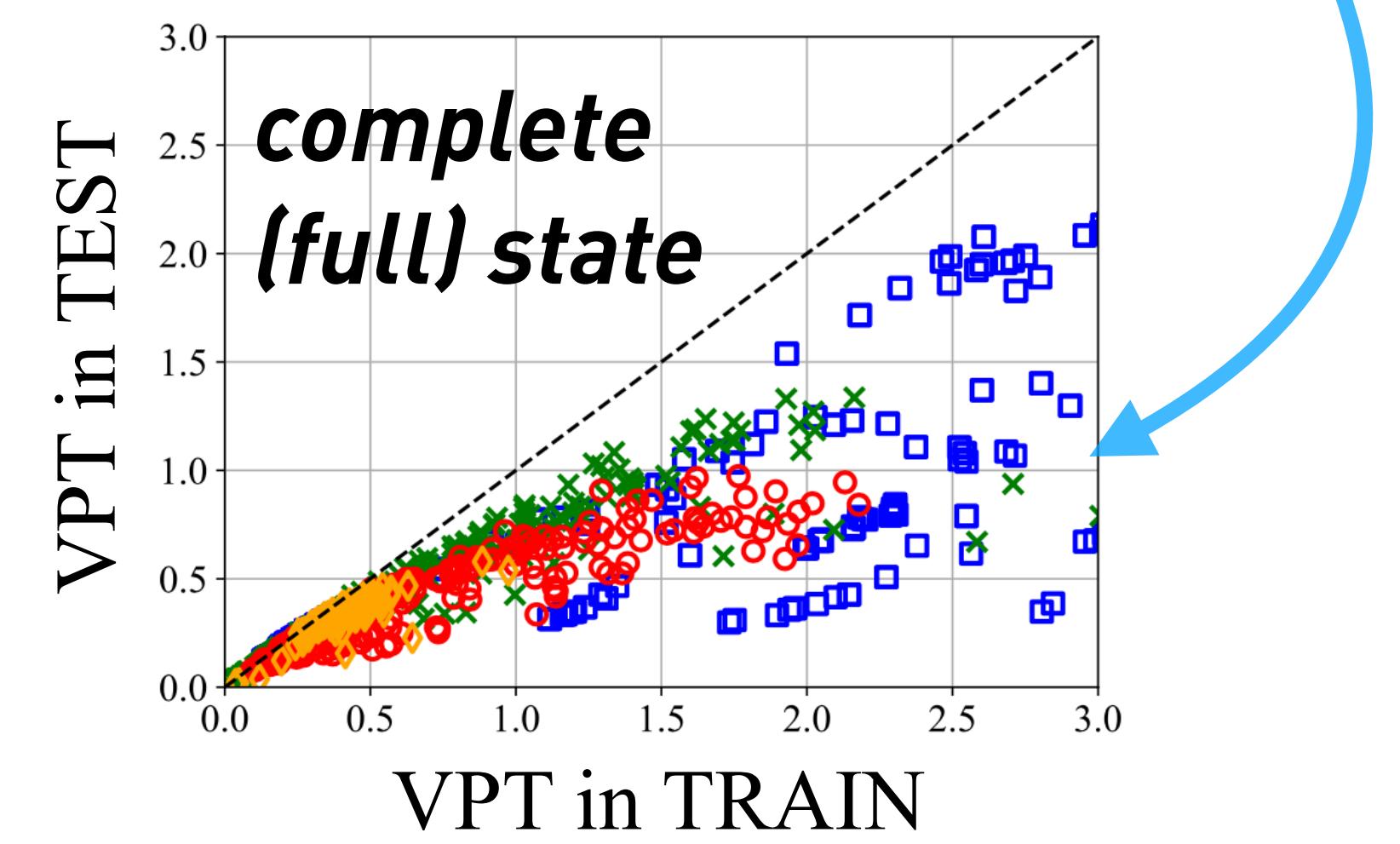
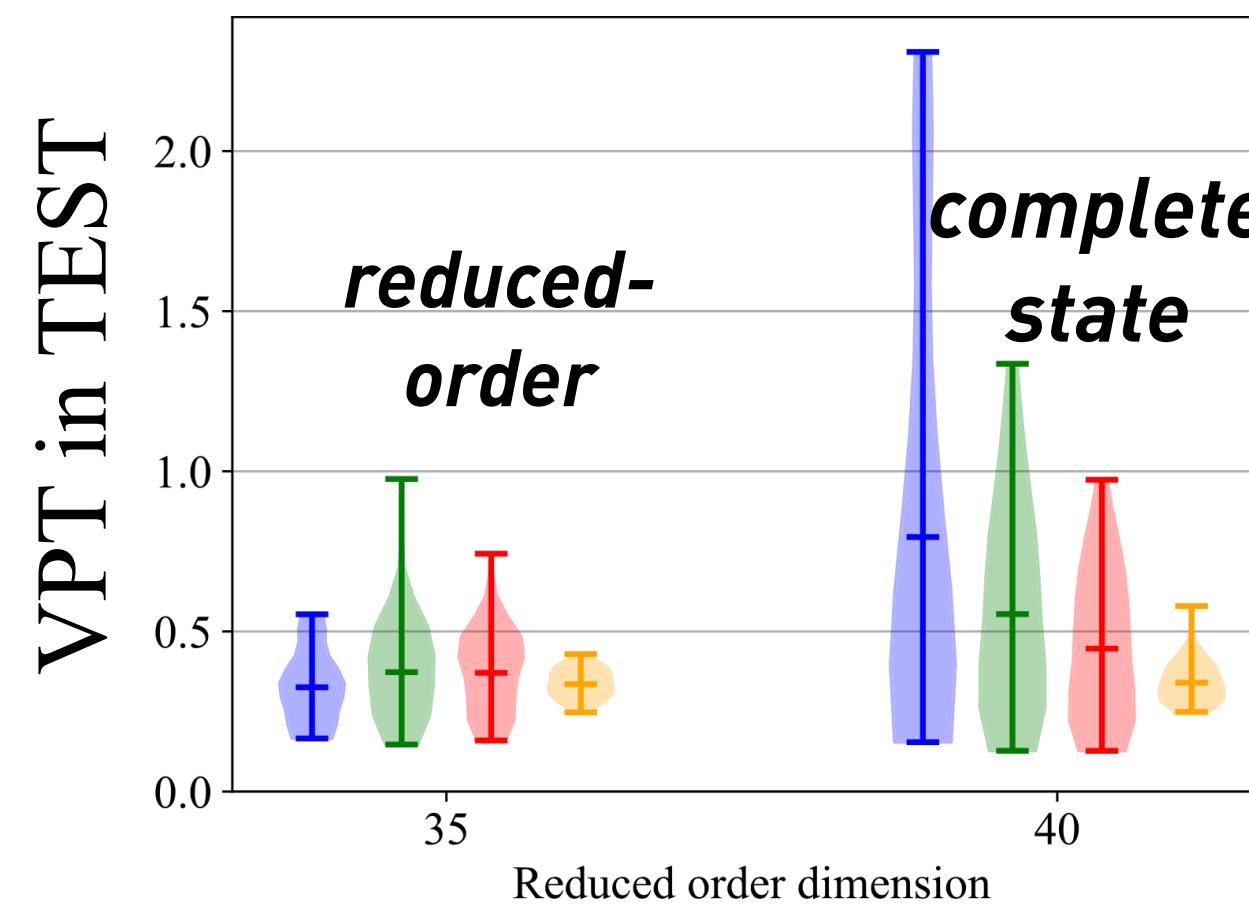
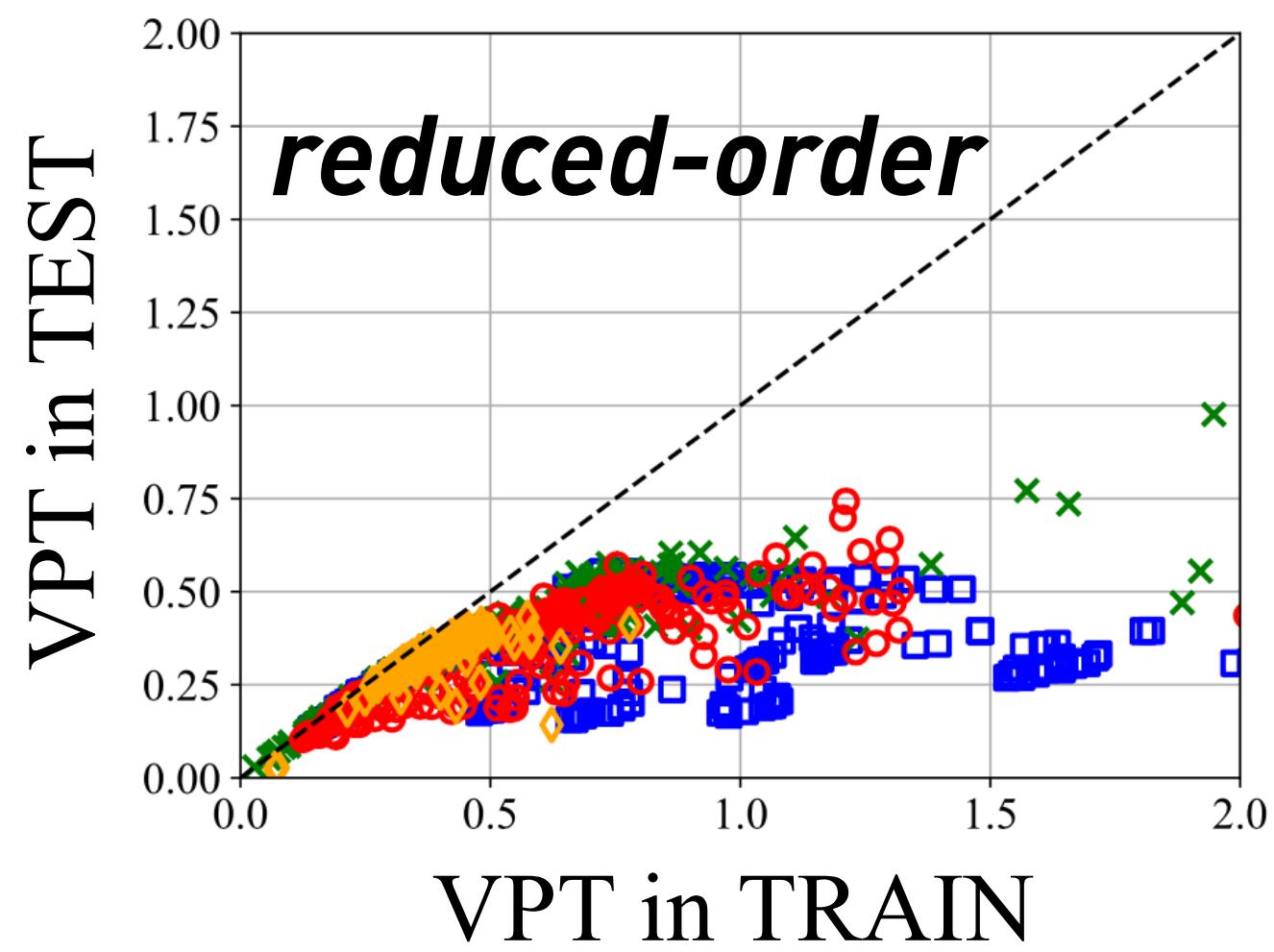
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every marker is a trained model !

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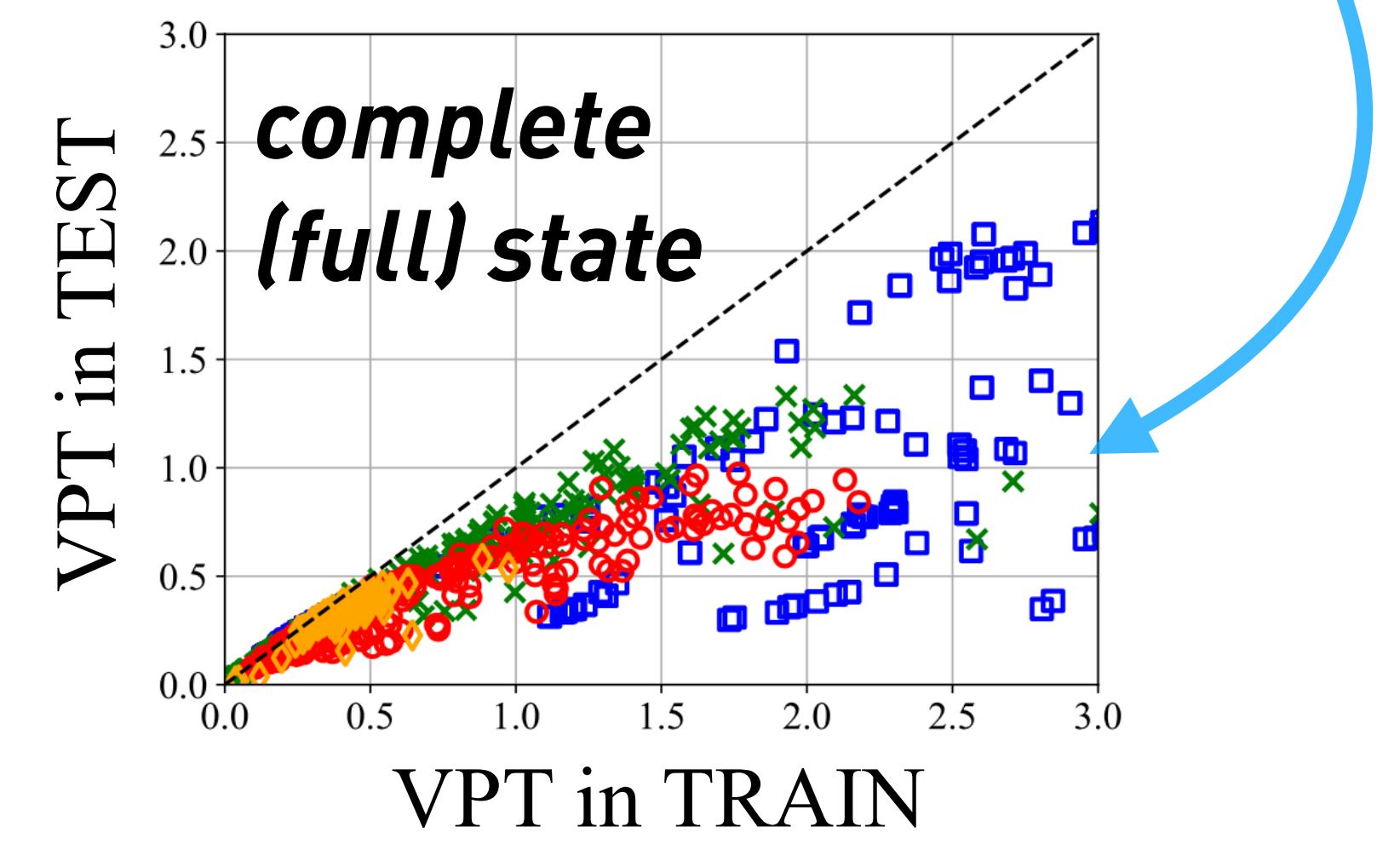
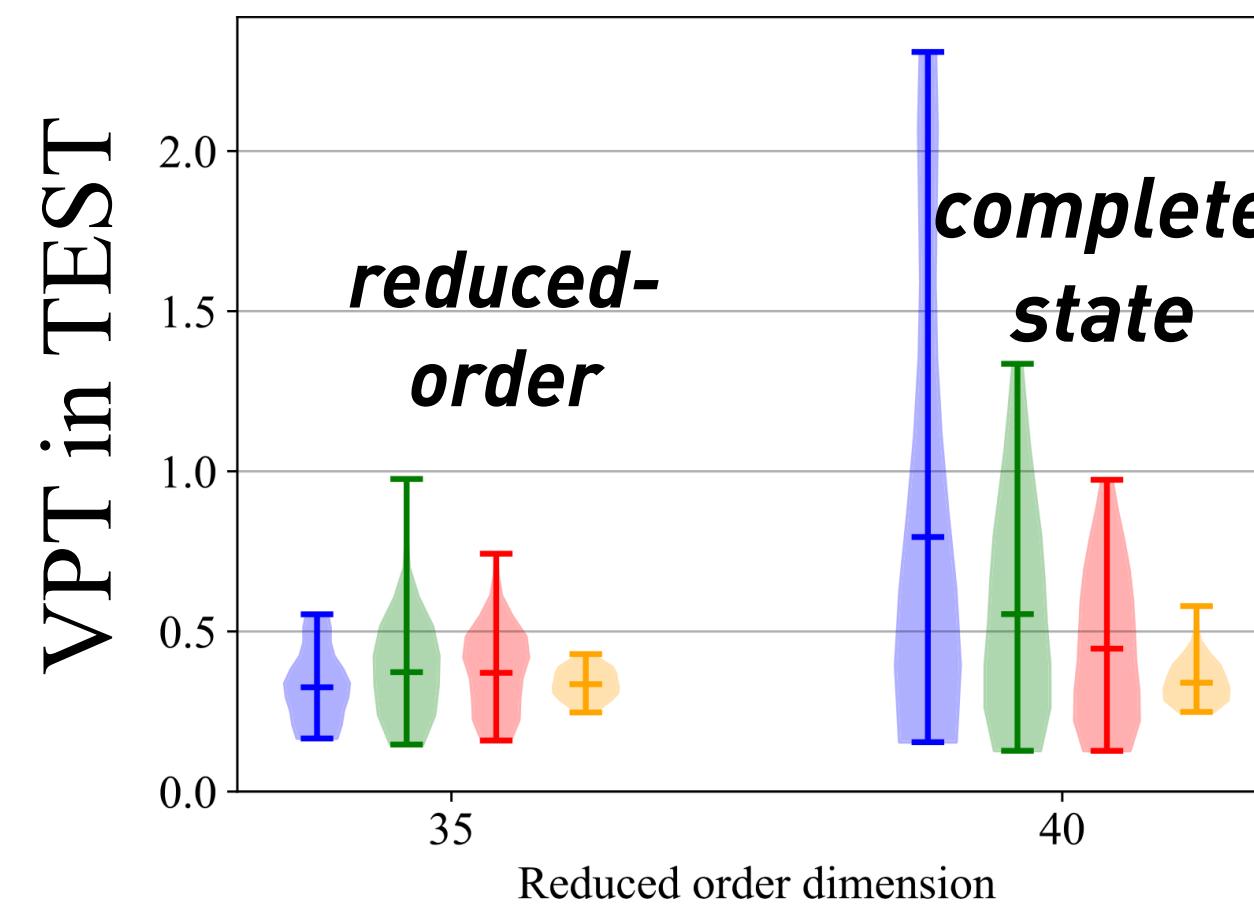
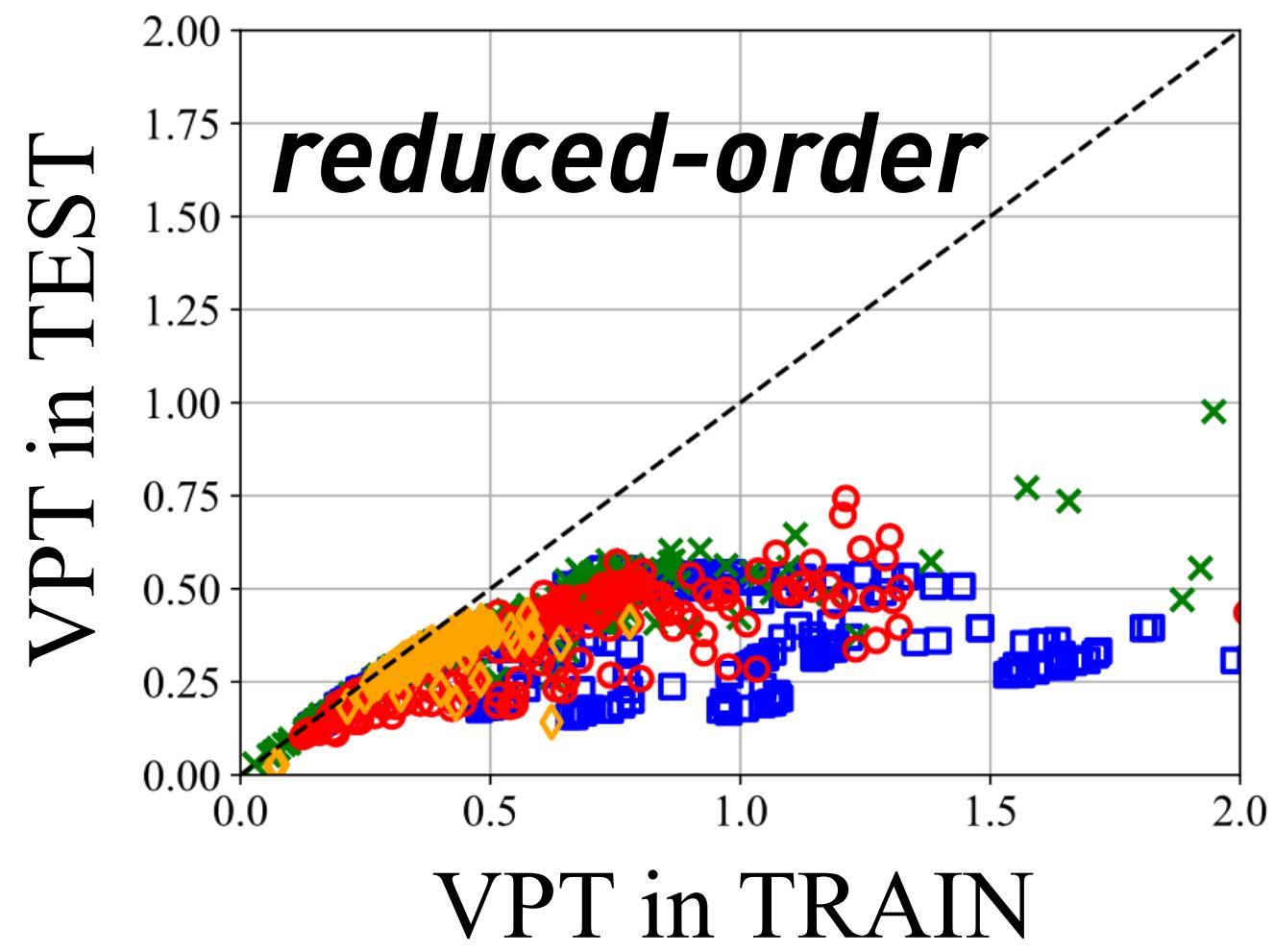


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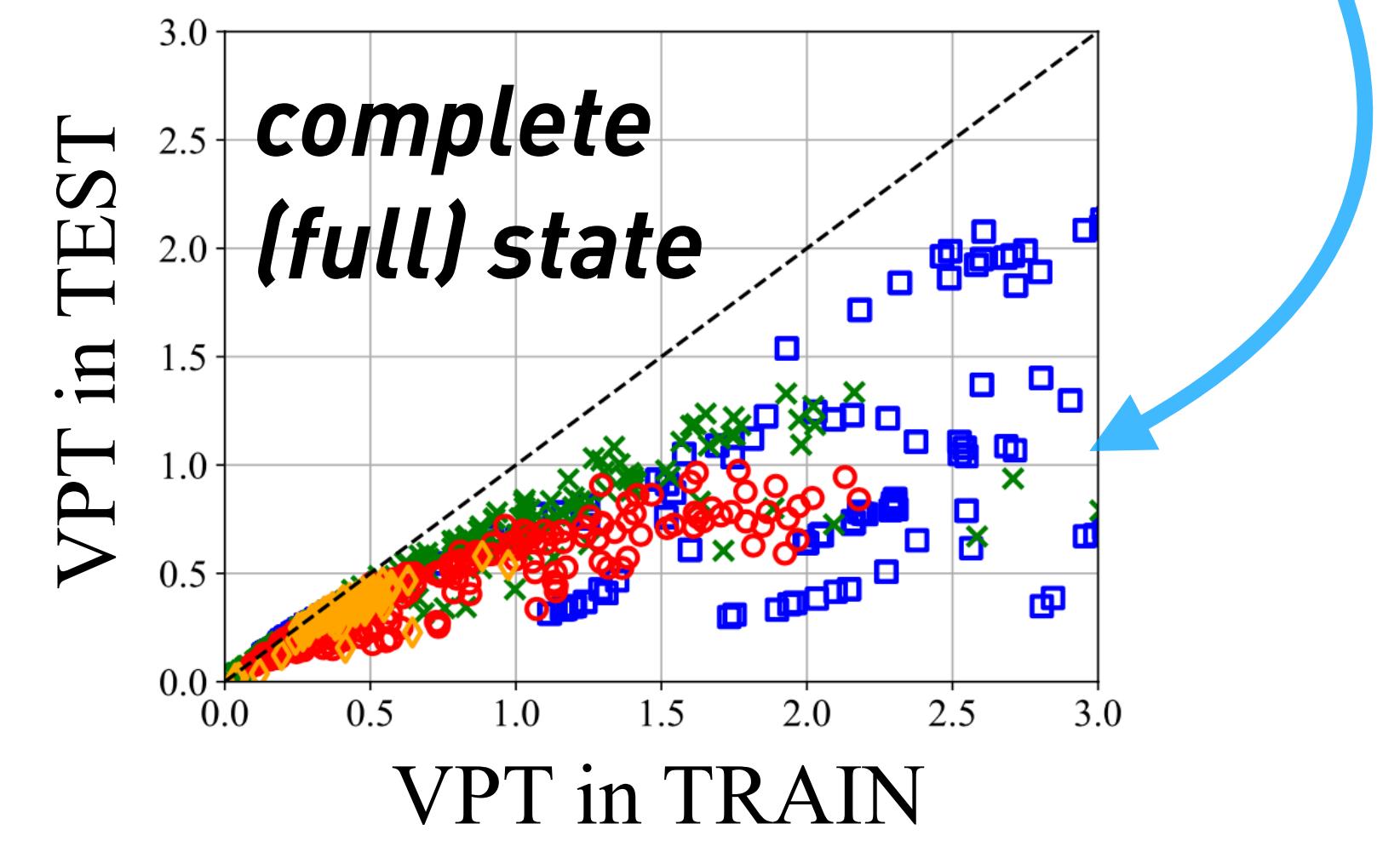
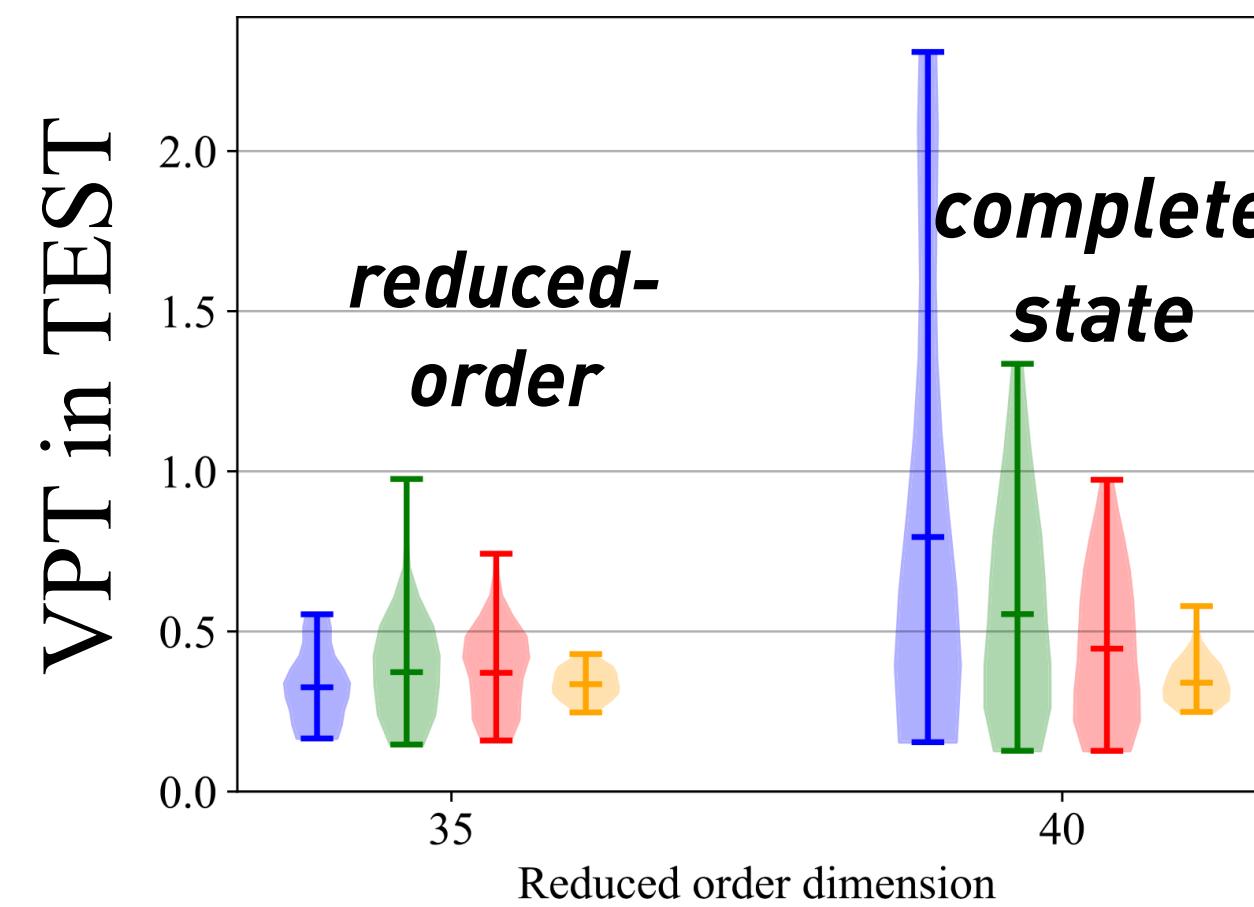
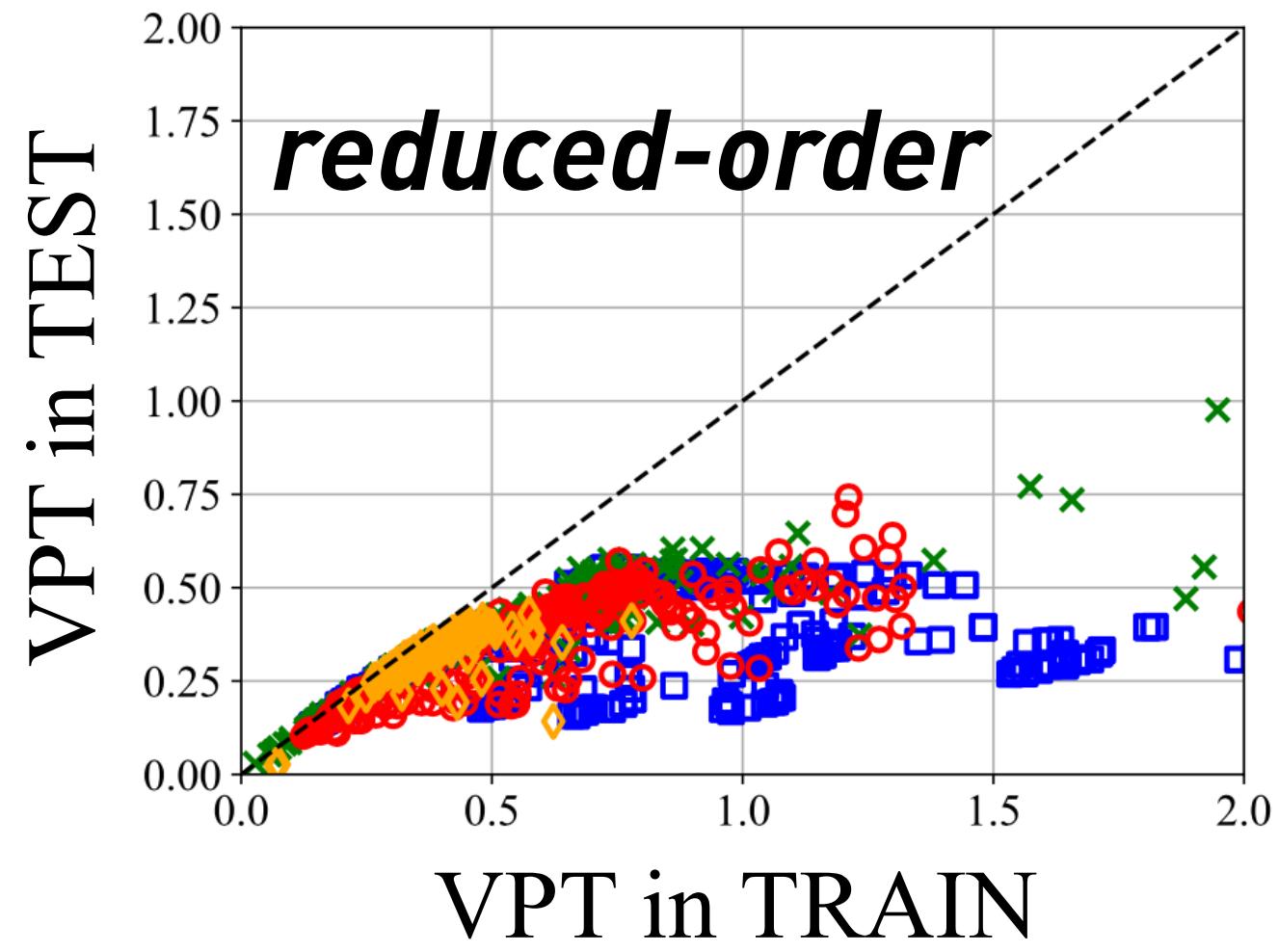


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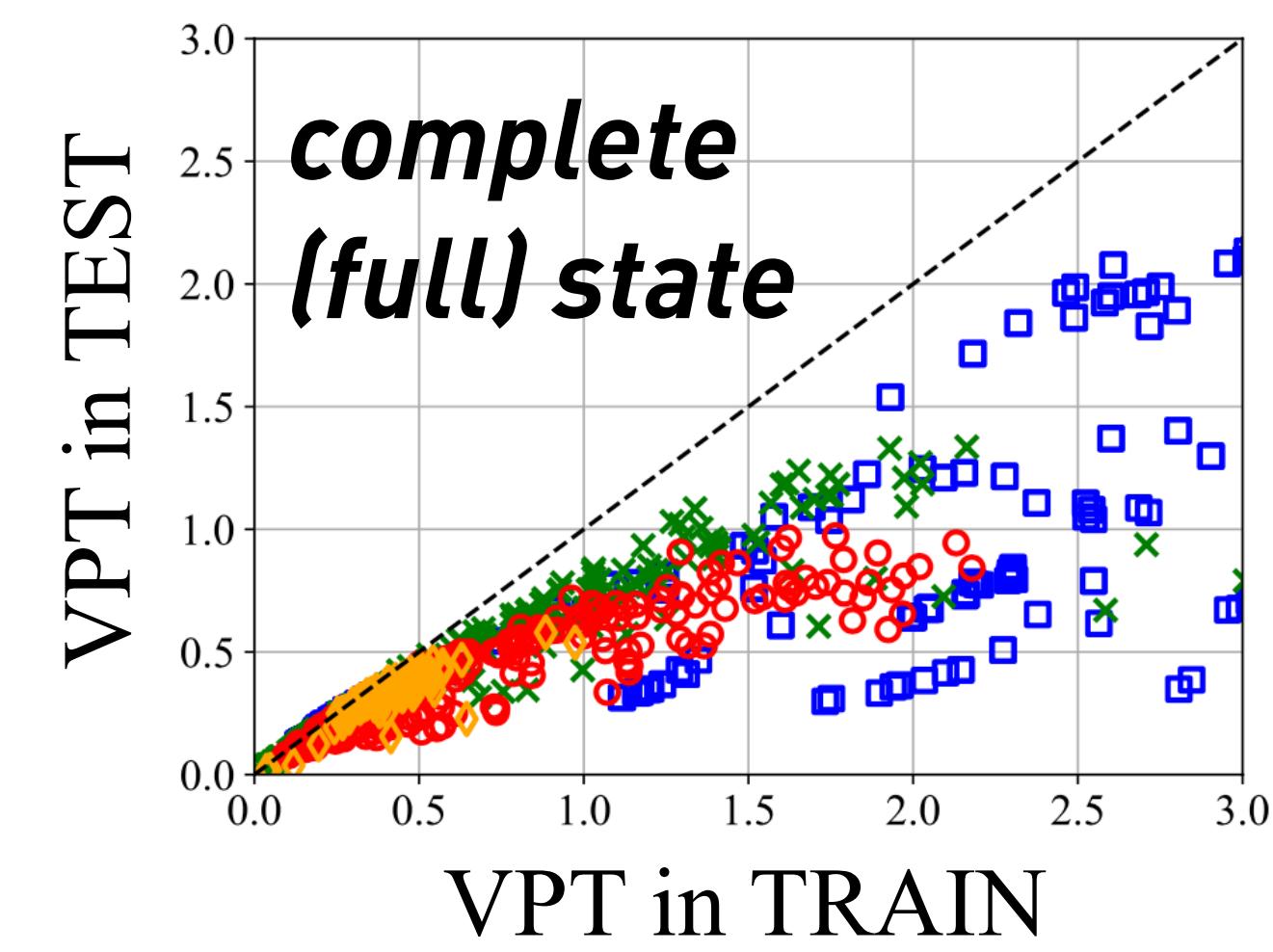
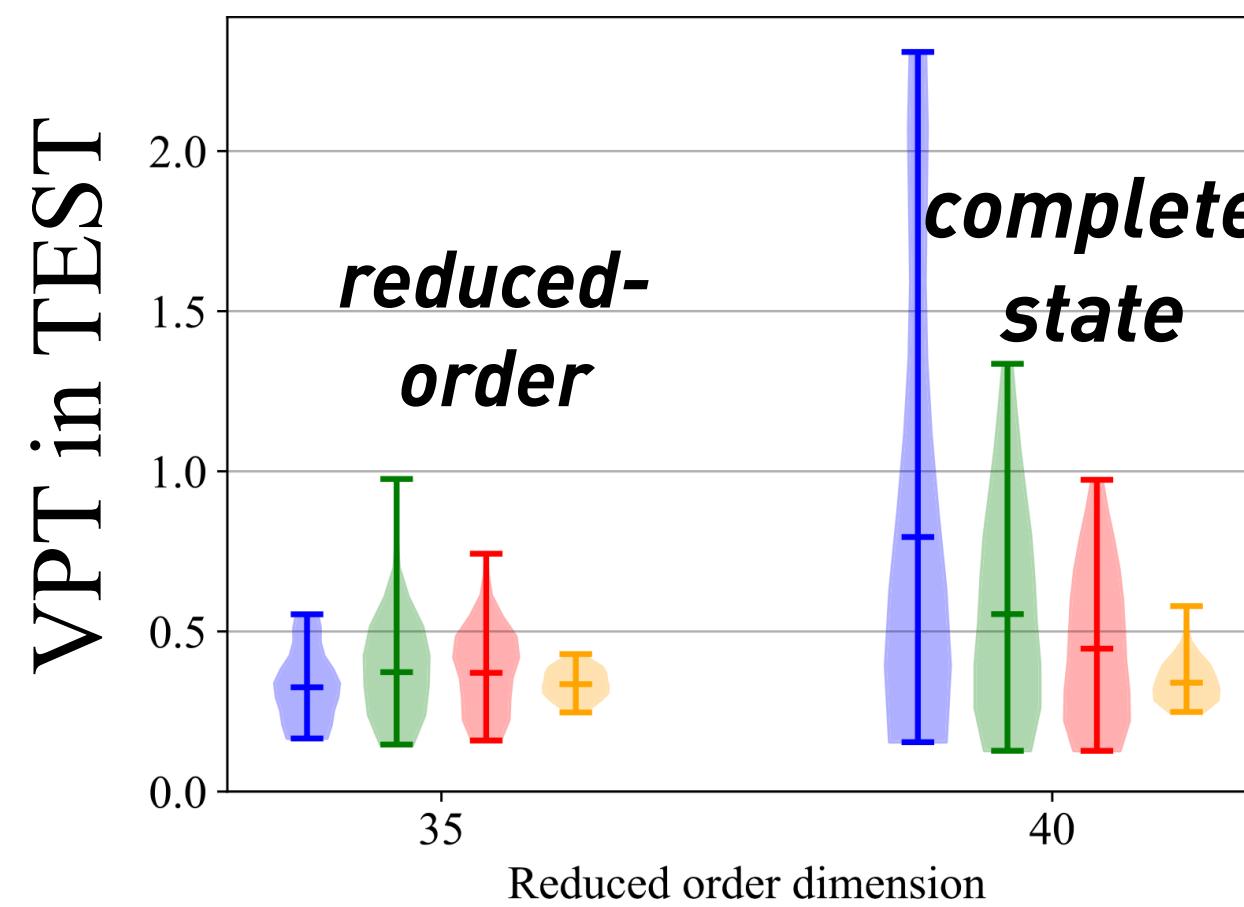
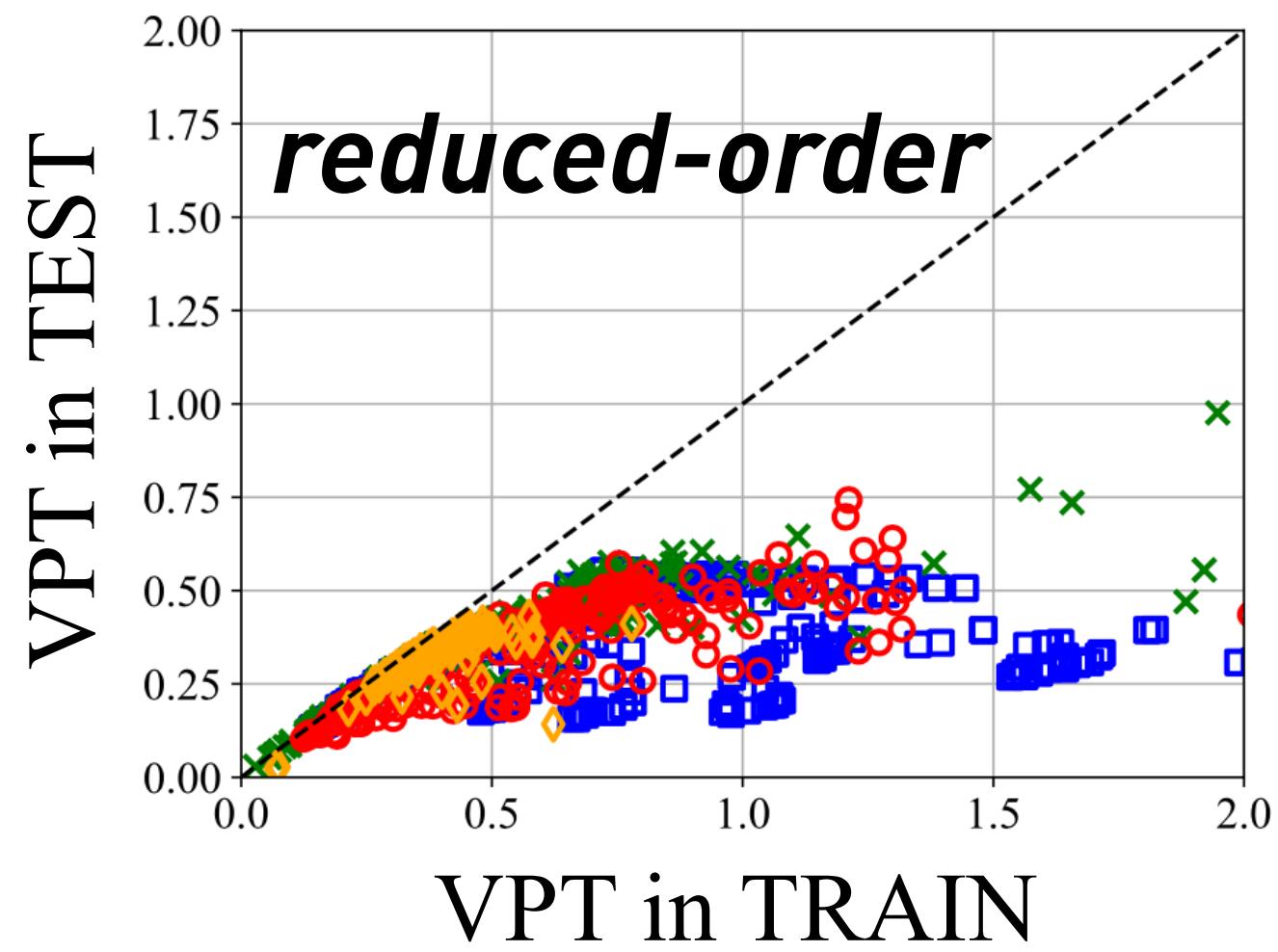


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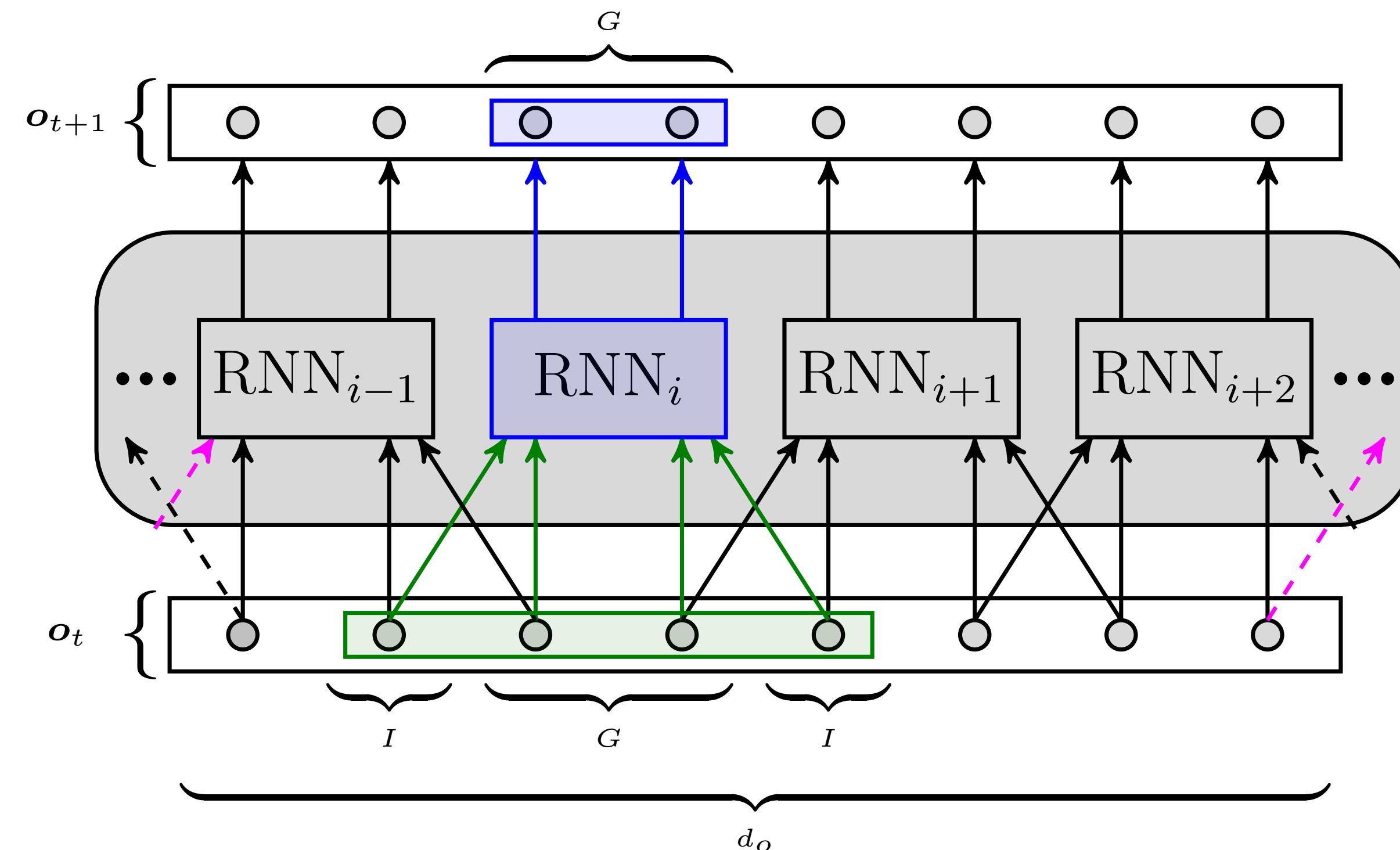
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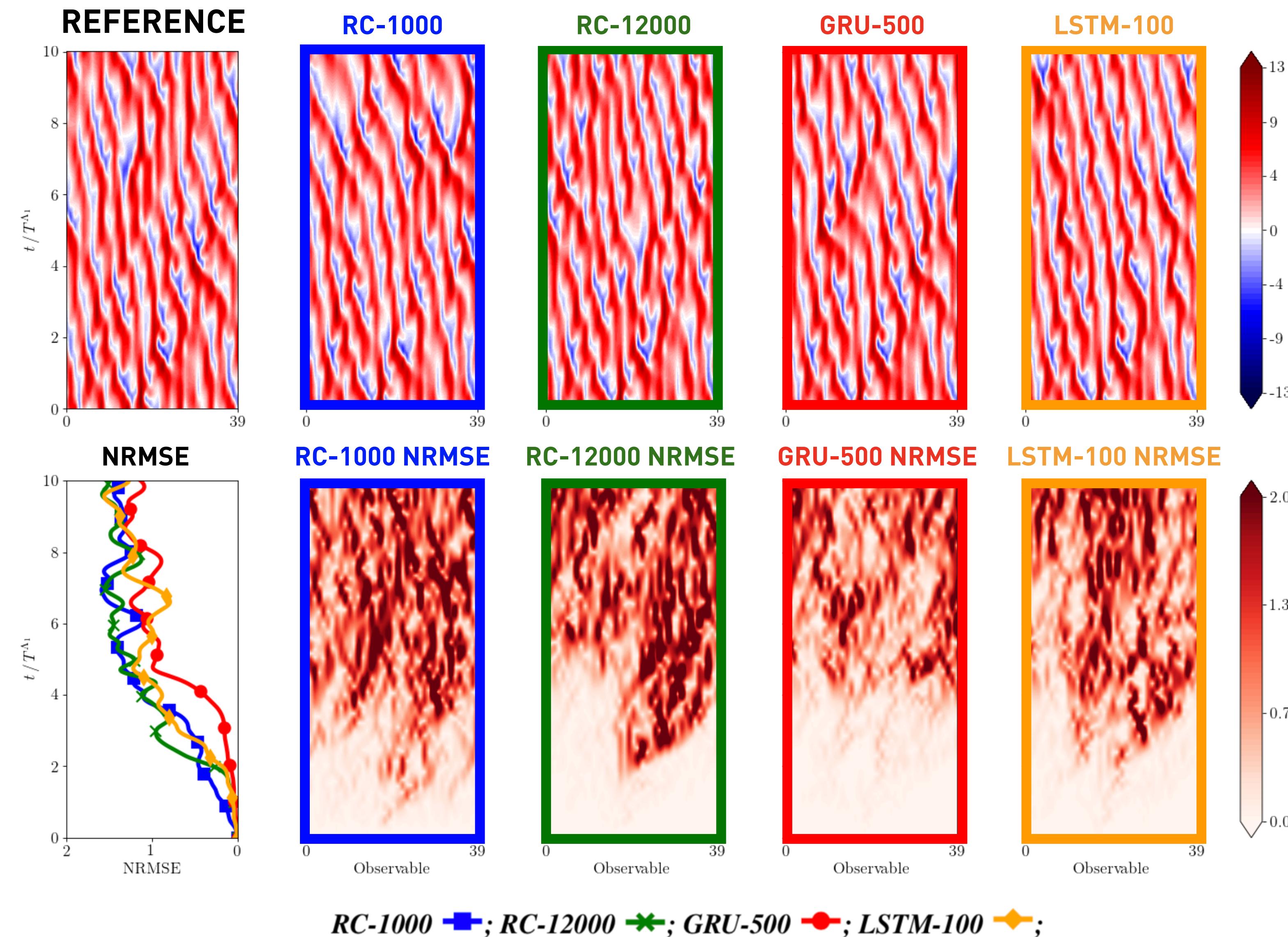


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# Lorenz 96, $F = 8$ , full state information & parallelism



# Lorenz 96, $F = 8$ , full state information & parallelism



*II*

*Learning Effective Dynamics*

# Equation-Free Framework (EFF) - Kevrekidis et. al.

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# Equation-Free Framework (EFF) - Kevrekidis et. al.

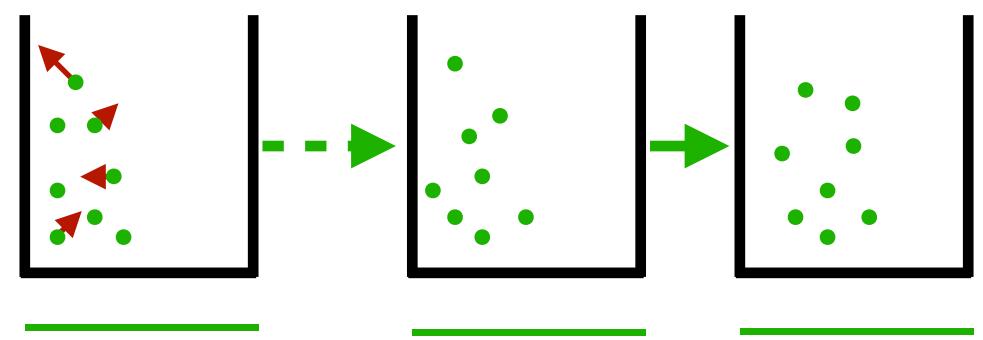
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- Complex Multiscale systems: **Micro** scale (“particles”) and **Macro** scale (“continuum”) dynamics
  - **Microscale simulations:** accurate **but** expensive to evaluate/not available
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- C Theodoropoulos, YH Qian, IG Kevrekidis, *Coarse stability and bifurcation analysis using time-steppers: a reaction-diffusion example*, Proc. Natl. Acad. Sci., 2000
  - CW Gear, IG Kevrekidis, C Theodoropoulos, *Coarse integration/bifurcation analysis via microscopic simulators: micro-Galerkin methods*, Computers and Chemical Engineering, 2002

AND MANY MANY MORE ...

# *Equation Free Framework*

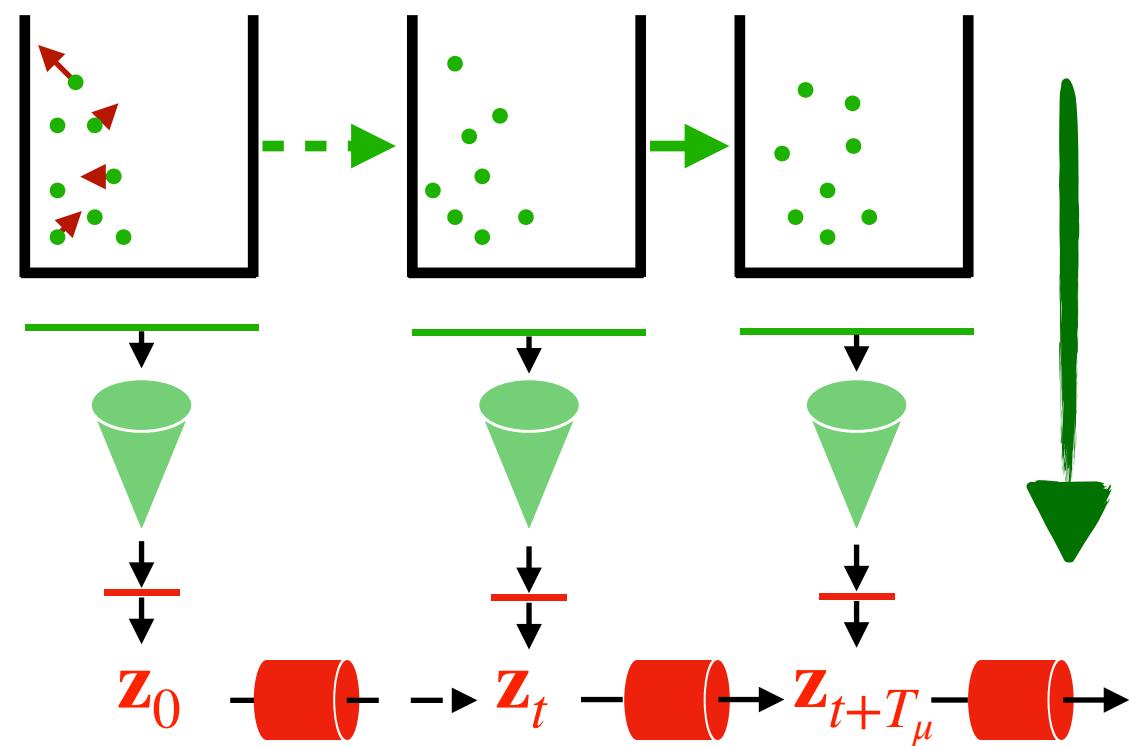
**A<sub>0</sub>** propagate  
(short times)  
**micro scale**



**A**

*Equation Free  
Framework*

**A<sub>0</sub>** propagate  
(short times)  
**micro scale**



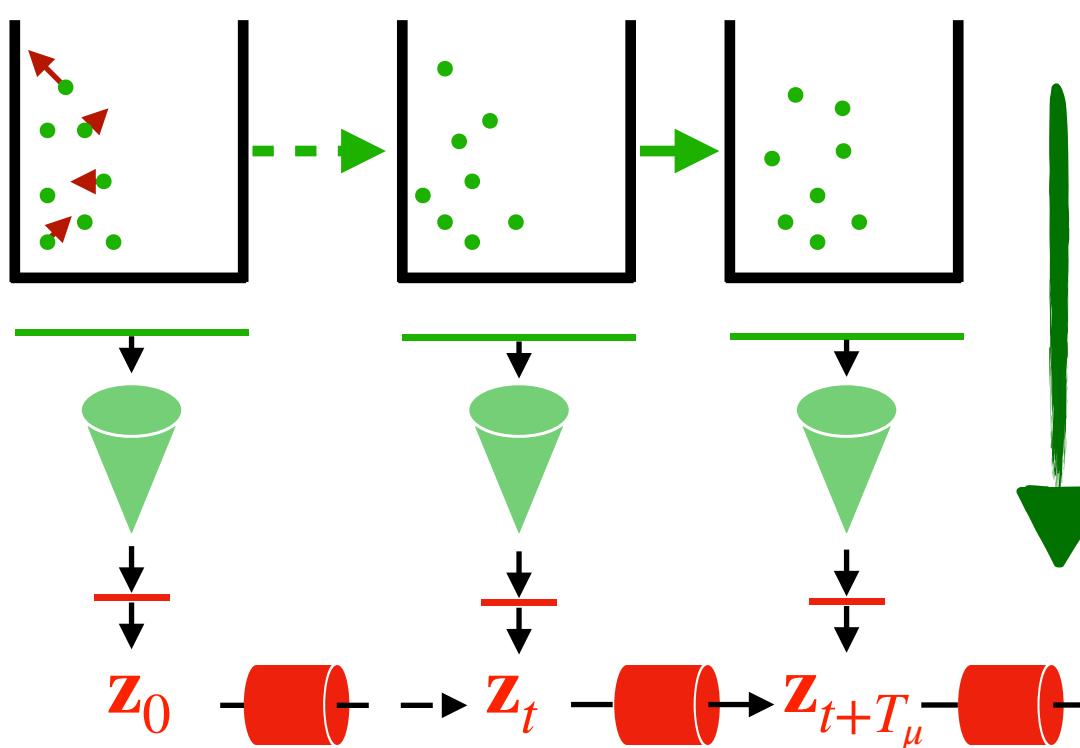
**B<sub>0</sub>** initialise  
**macro scale**

▼ **RESTRICTING /AVERAGING**  
**(micro → macro)**  
e.g. PCA / DiffMaps / analytic

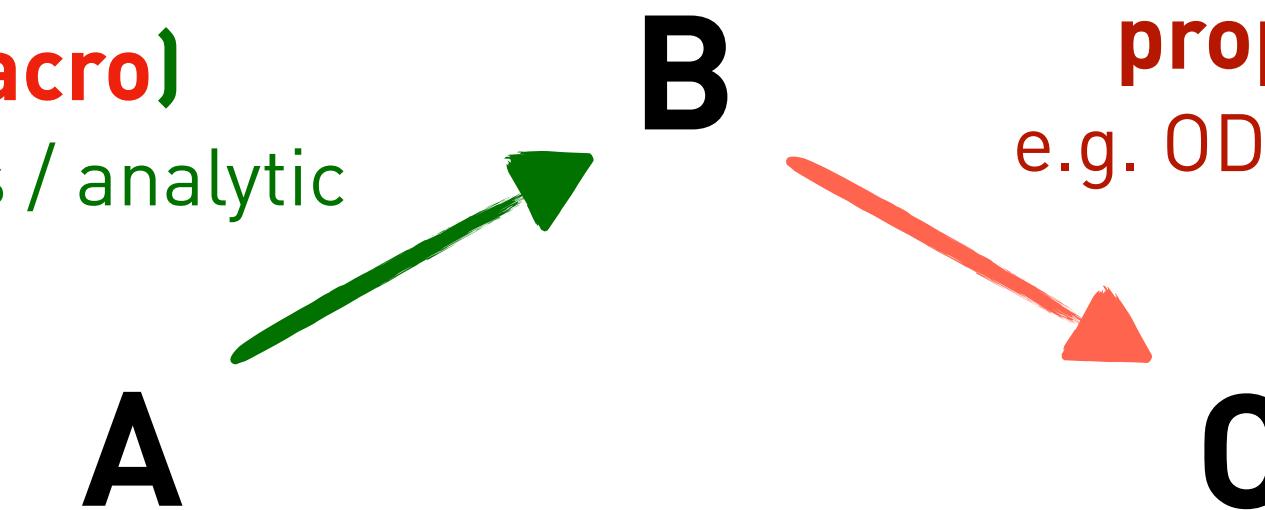


***Equation Free  
Framework***

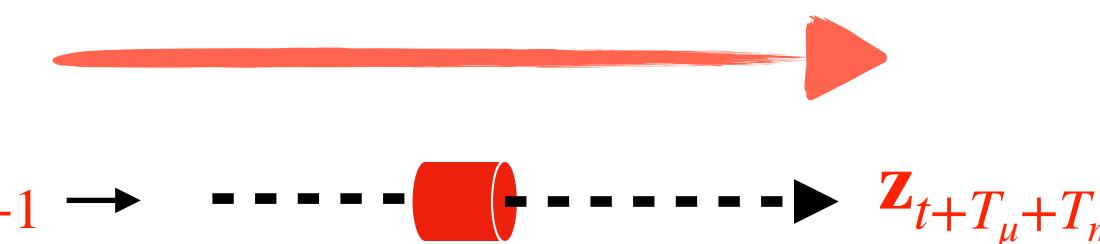
**A<sub>0</sub>** propagate  
(short times)  
**micro scale**



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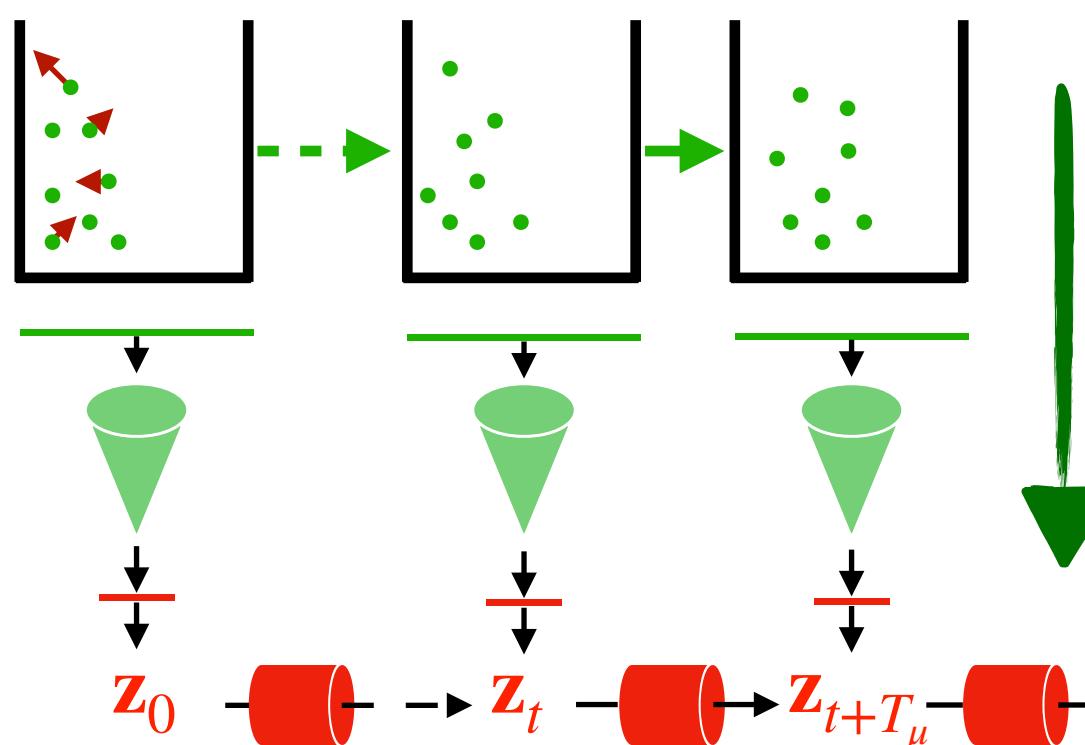
**C** propagate  
(long times)  
**macro scale**



**B<sub>0</sub>** initialise  
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*Equation Free  
Framework*

**A<sub>0</sub>** propagate  
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RESTRICTING /AVERAGING  
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**C** propagate  
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**macro scale**

→

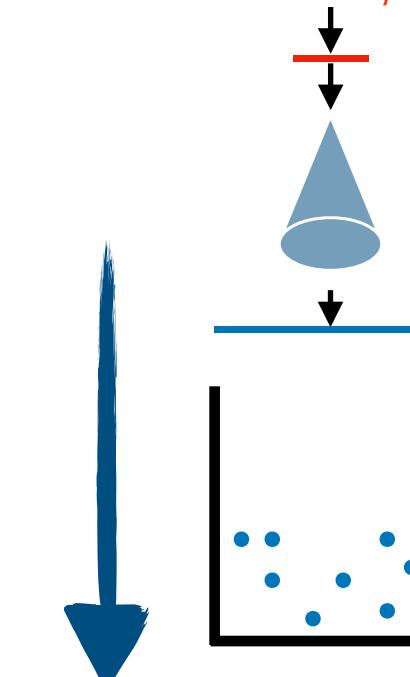


macro dynamics  
propagator  
e.g. ODE / analytic

LIFTING  
(macro → micro)

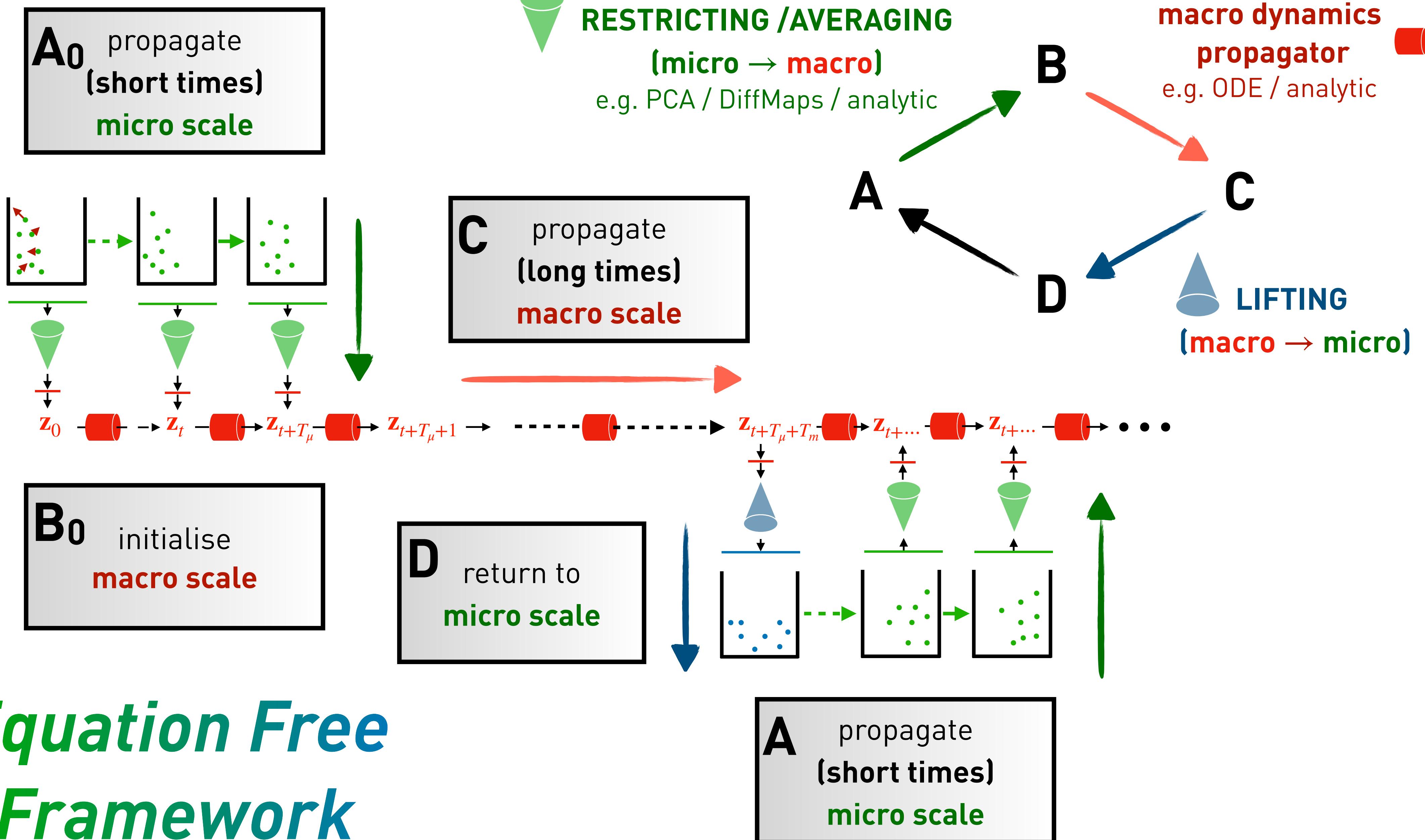


**D** return to  
**micro scale**

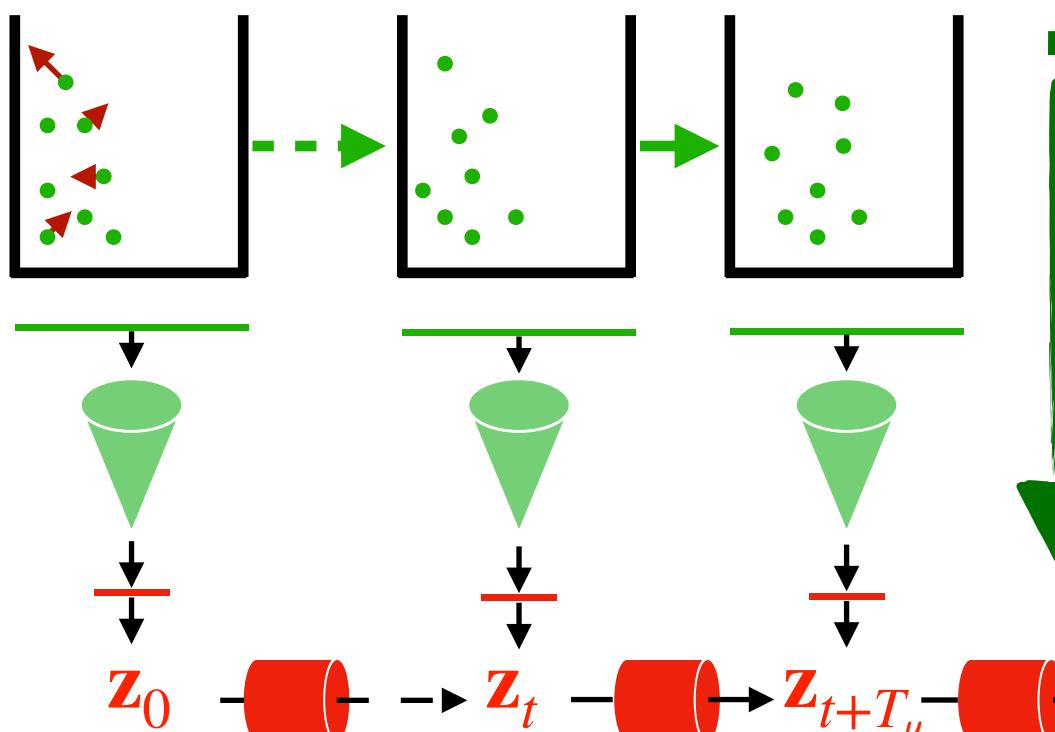


*Equation Free  
Framework*

# *Equation Free Framework*



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**micro scale**

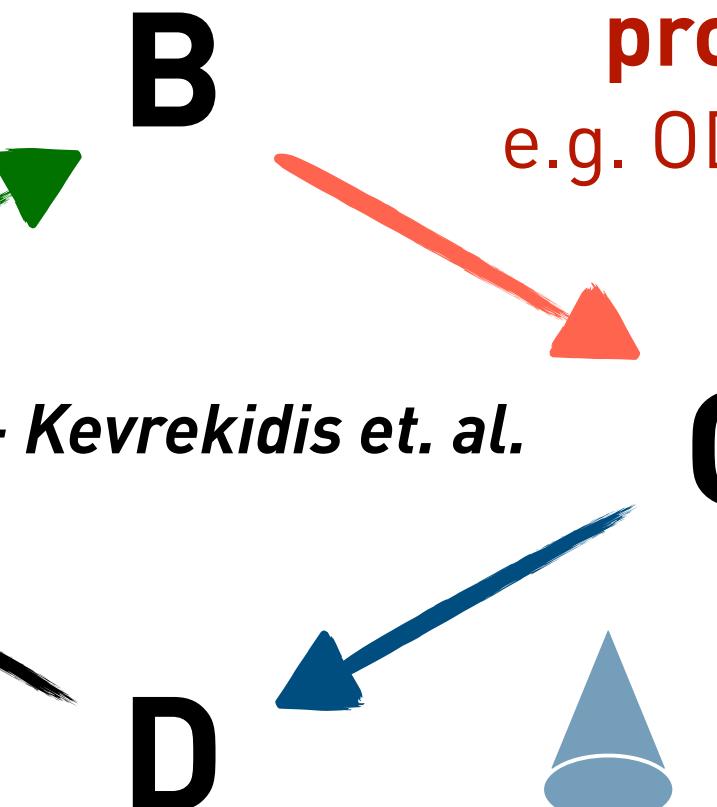
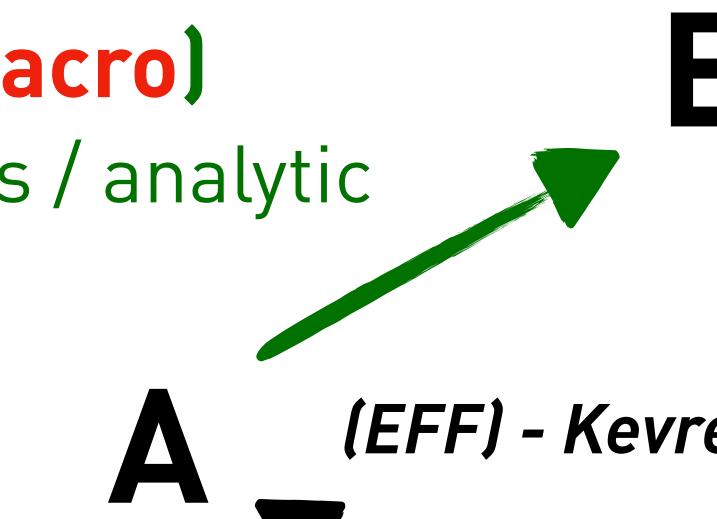


RESTRICTING / AVERAGING

(micro → macro)

e.g. PCA / DiffMaps / analytic

**C** propagate  
(long times)  
**macro scale**



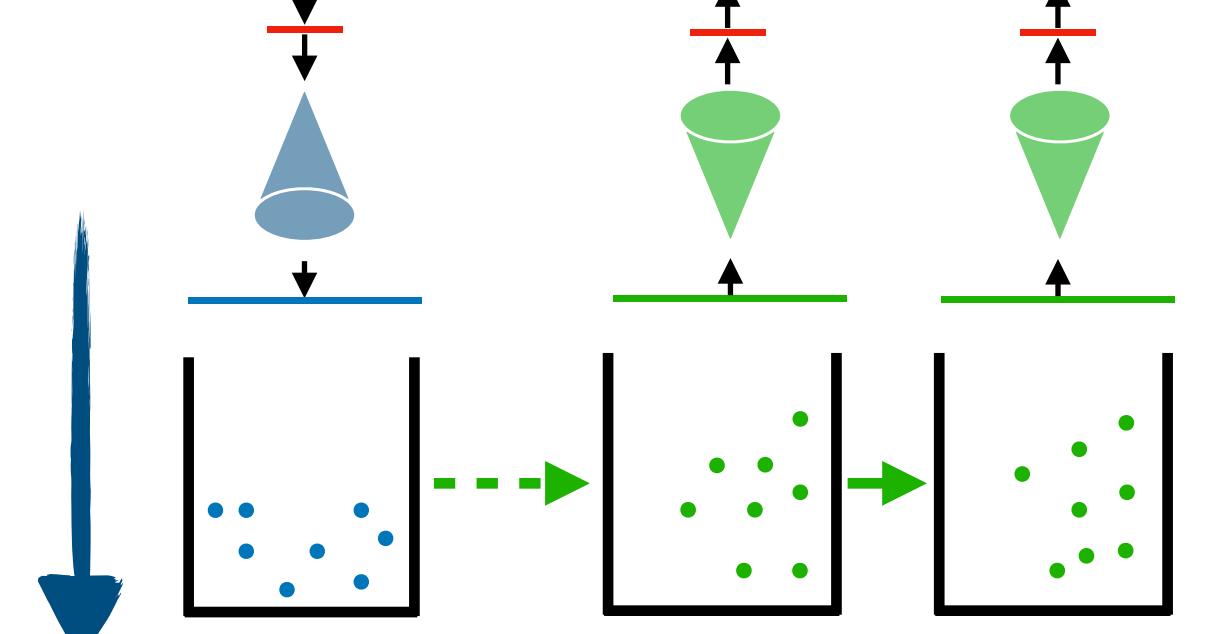
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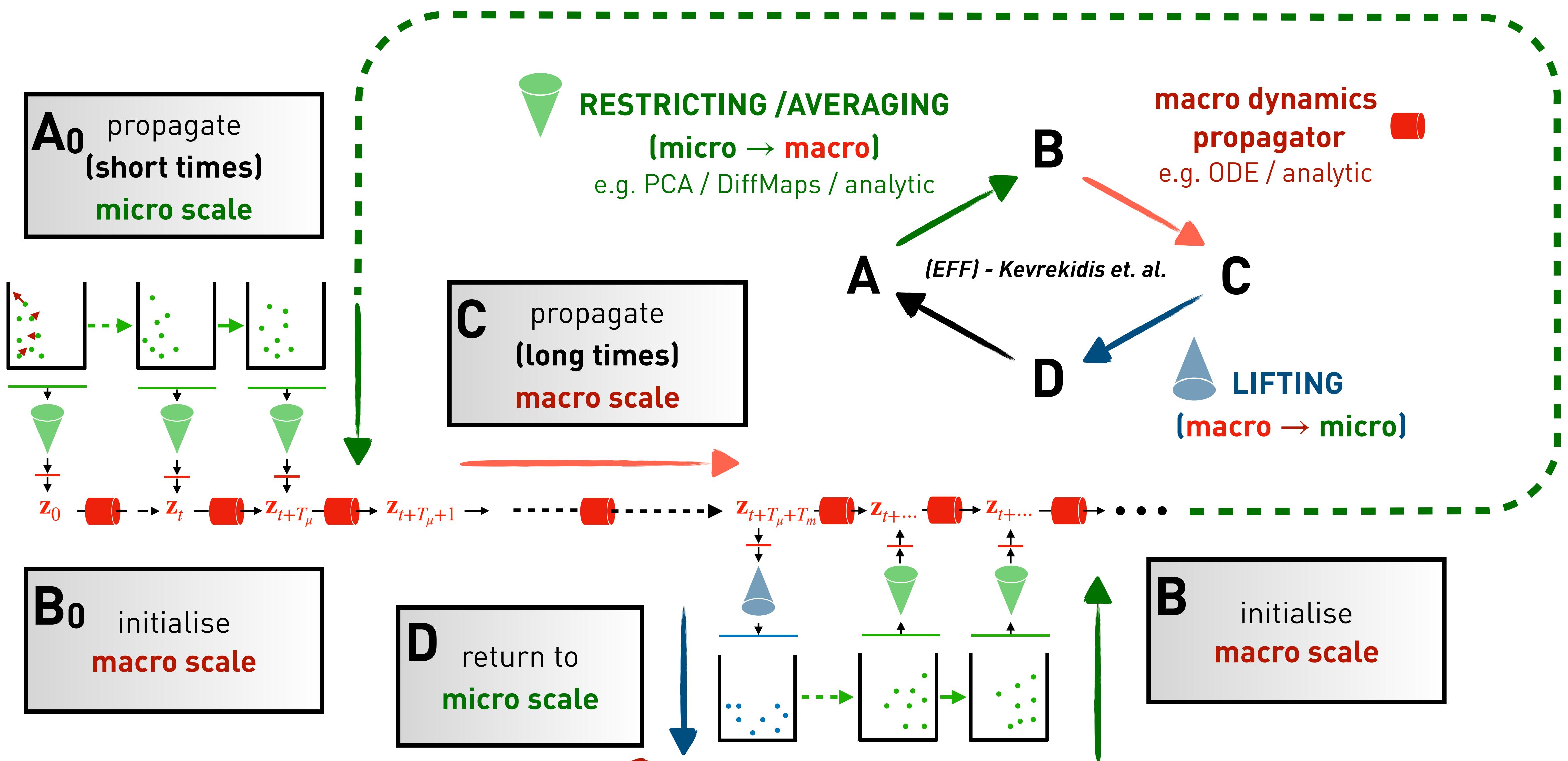
**B<sub>0</sub>** initialise  
**macro scale**

**D** return to  
**micro scale**

**A** propagate  
(short times)  
**micro scale**



# Equation Free Framework



# *Generalization to complex problems hindered*

- A. Macro dynamics propagators
  - B. **macro → micro** operators

**A** propagate  
**(short times)**  
**micro scale**

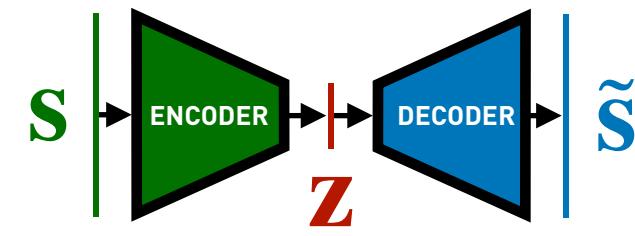
# Operators from Machine Learning

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# Operators from Machine Learning

## (CONVOLUTIONAL) AUTOENCODERS

High dimensional state



Low dimensional latent space

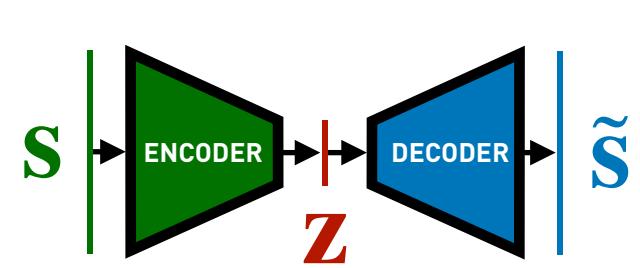
Reconstruction

- Full high dimensional description of dynamical system system  $s$
- e.g. positions of atoms / micro scale / angles, bonds
- Loss Function  $\mathcal{L} = \|s - \tilde{s}\|_2^2$
- Ideally after training  $s \approx \tilde{s}$

# Operators from Machine Learning

## (CONVOLUTIONAL) AUTOENCODERS

High dimensional state

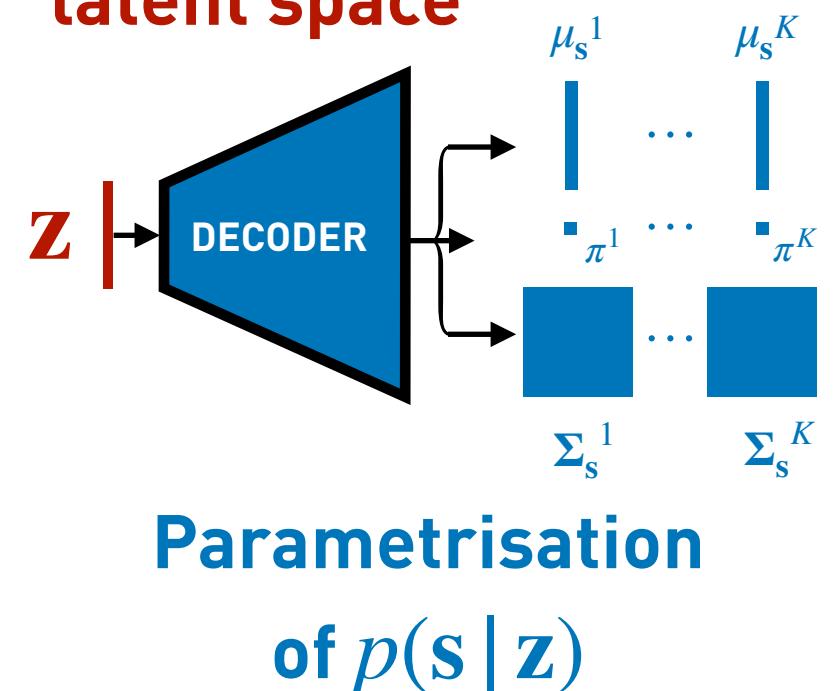


Low dimensional latent space

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## MIXTURE DENSITY NETWORKS

Low dimensional latent space



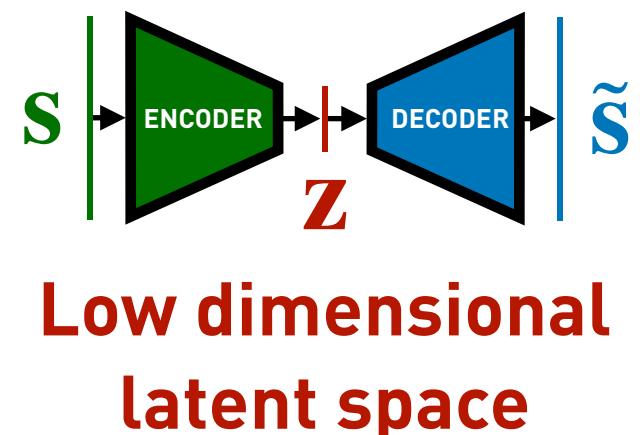
- Coarse (latent) representation has limited information
- Mapping  $\mathbf{z} \rightarrow \mathbf{s}$  can be probabilistic !
- Generative network
- $p(\mathbf{s} | \mathbf{z})$  as **mixture model**
- $$p(\mathbf{s} | \mathbf{z}) = \sum_{k=1}^K \pi_k \mathcal{N}(\mu_s^k, \Sigma_s^k)$$

# Operators from Machine Learning

## (CONVOLUTIONAL) AUTOENCODERS

High dimensional state

Reconstruction



Low dimensional latent space

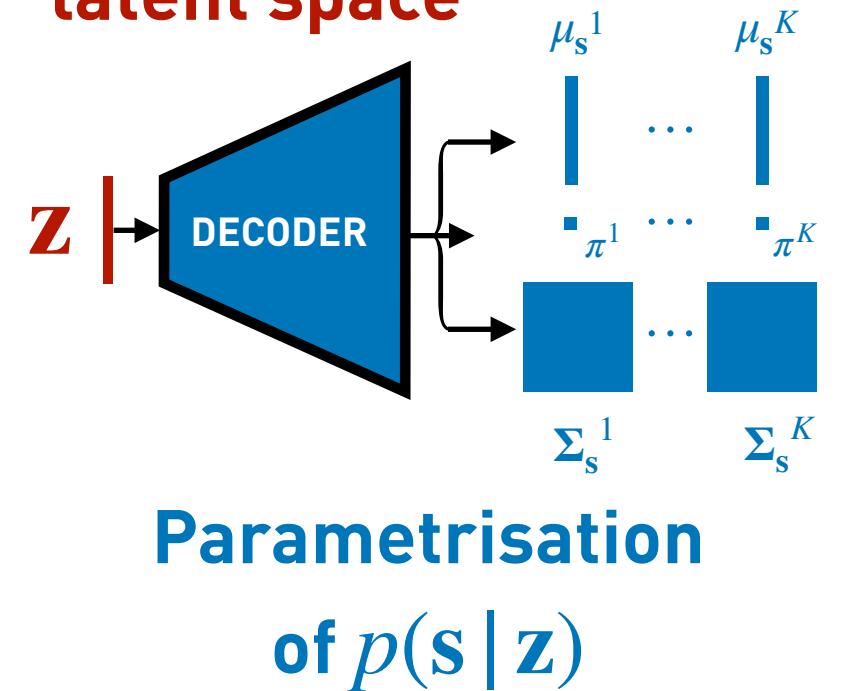
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## RECURRENT NEURAL NETWORKS

- Non-linear non-Markovian dynamics  $z$  (**macro dynamics**)
- **Forecasting** using **RNNs**
- Tracking the **history** of the low order state  $z$  to model **non-Markovian** dynamics
- Forecasting  $z_{t+\Delta t}$  from short-term history
- $\Delta t$  timestep of RNN,  $\delta t$  time step of micro dynamics  
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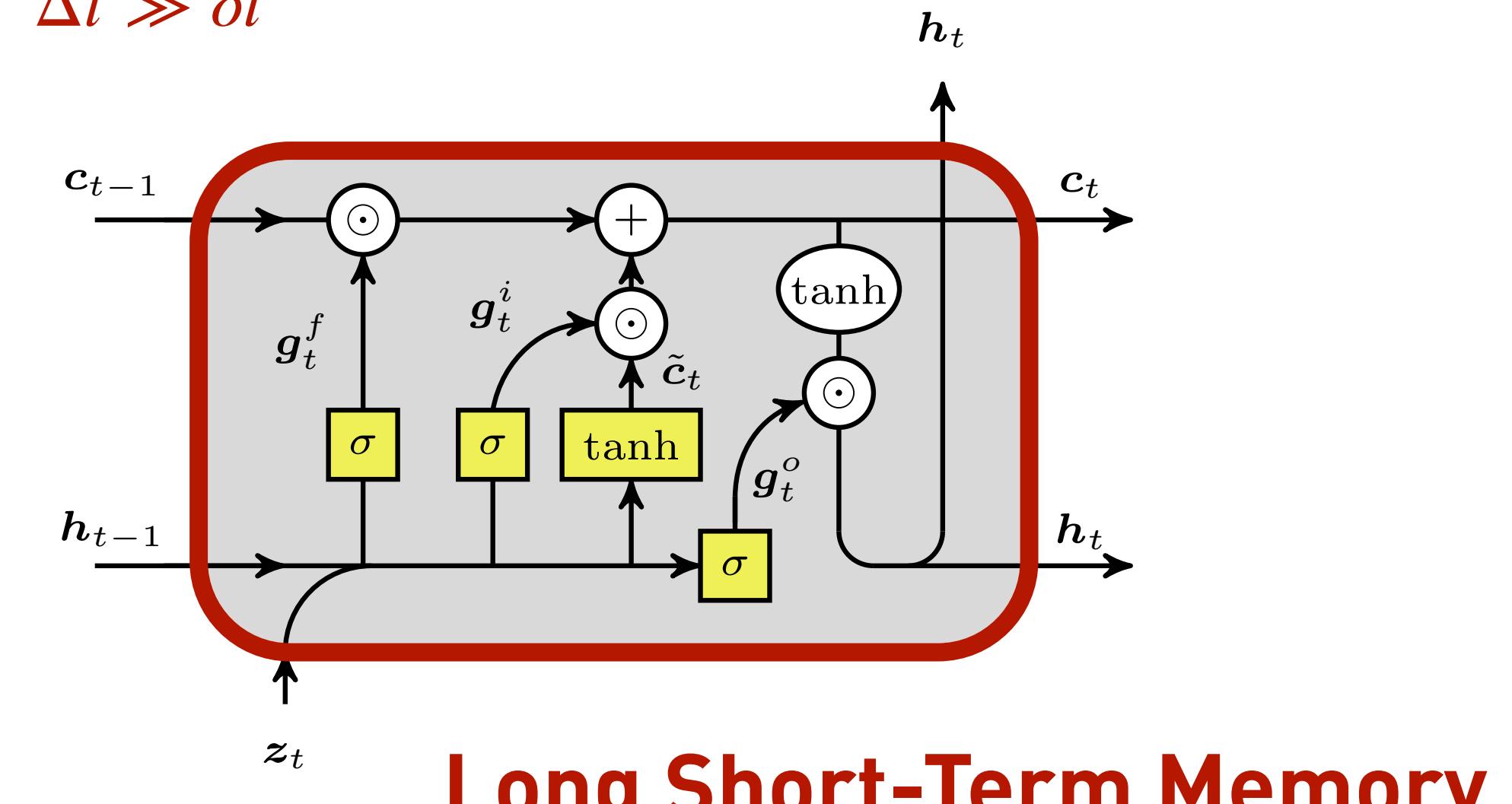
## MIXTURE DENSITY NETWORKS

Low dimensional latent space



Parametrisation of  $p(s|z)$

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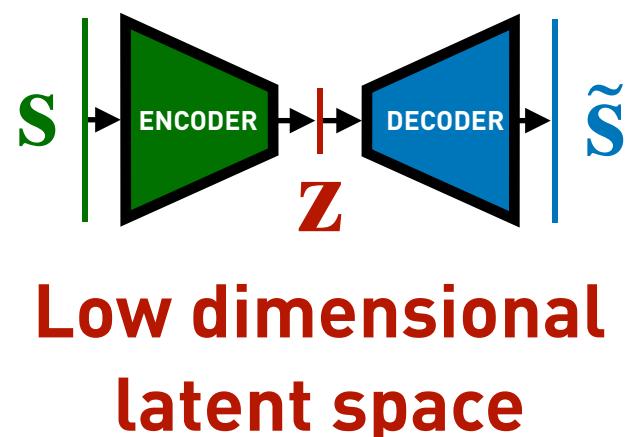
Long Short-Term Memory

# Operators from Machine Learning

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High dimensional state

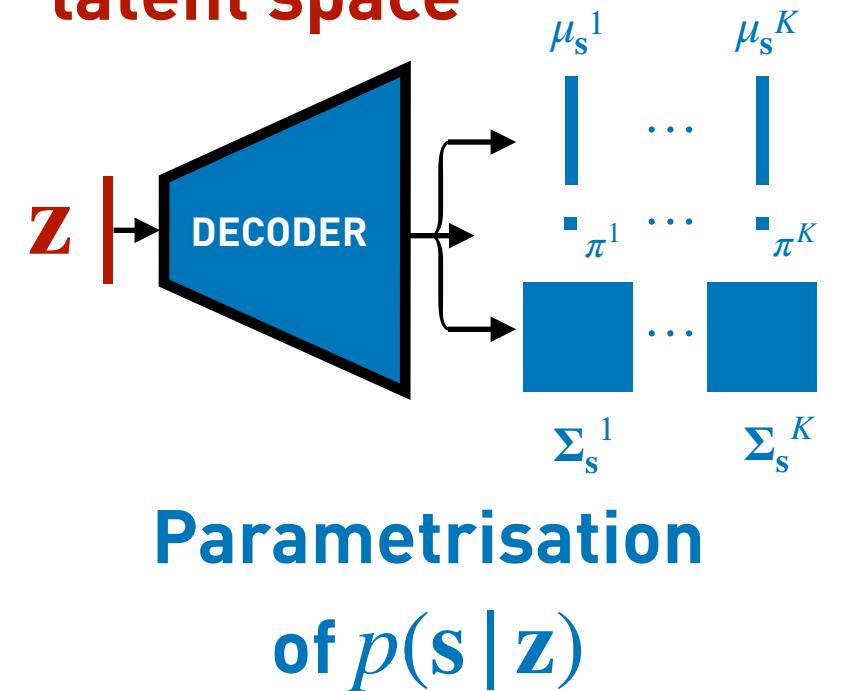
Reconstruction



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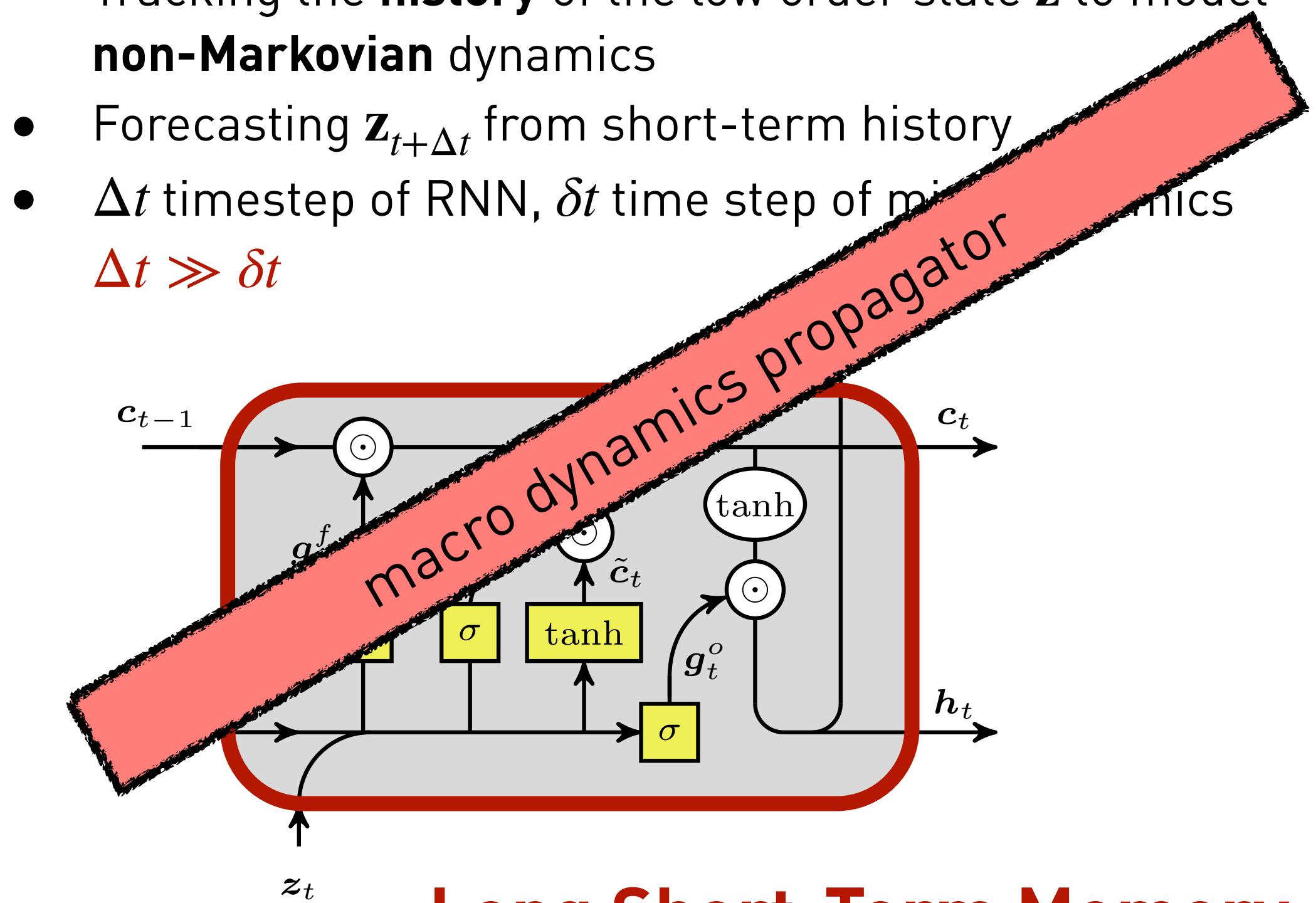
Low dimensional latent space



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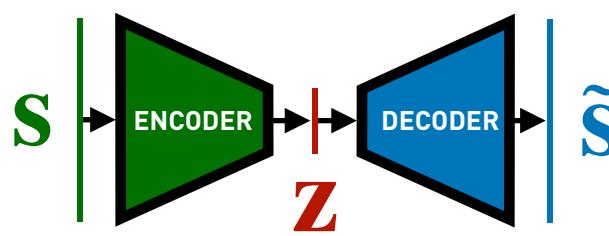
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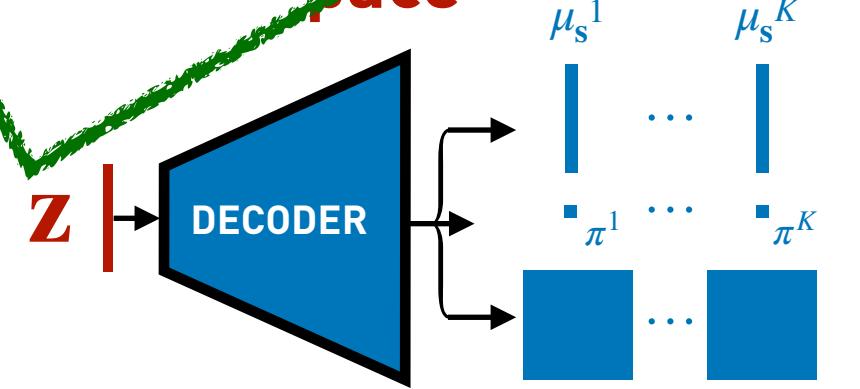
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**RESTRICTING/AVERAGING**  
(micro  $\rightarrow$  macro)

## STATE DENSITY NETWORKS

Latent space

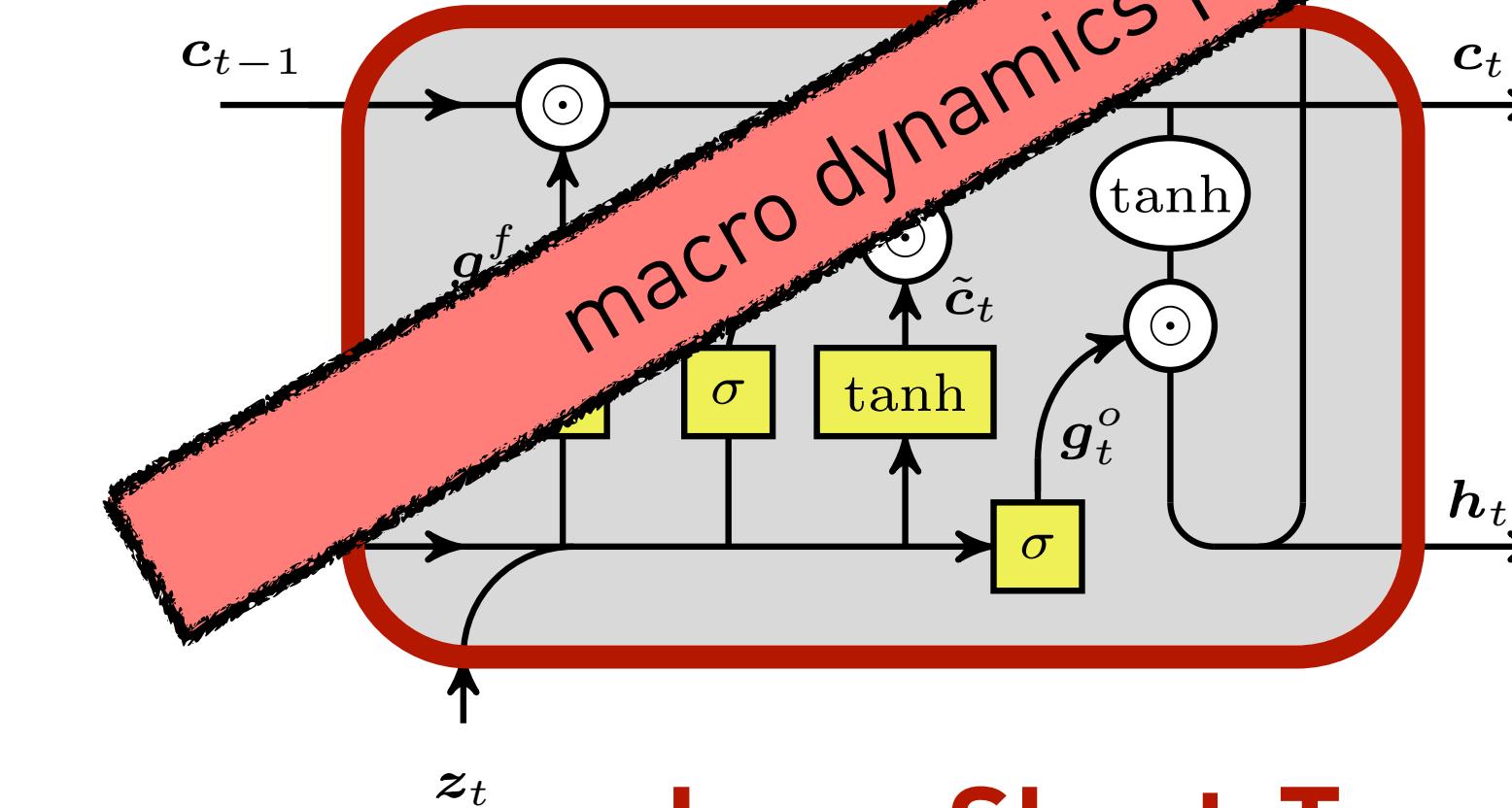


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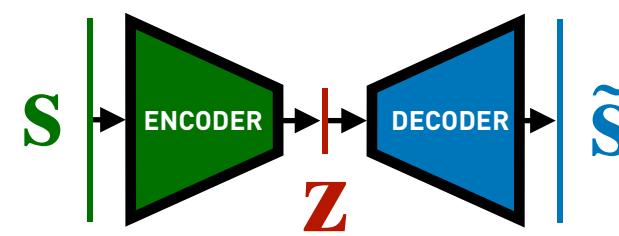


**Long Short-Term Memory**

# Operators from Machine Learning

## (CONVOLUTIONAL) AUTOENCODERS

High dimensional state



Reconstruction

- Full high dim description

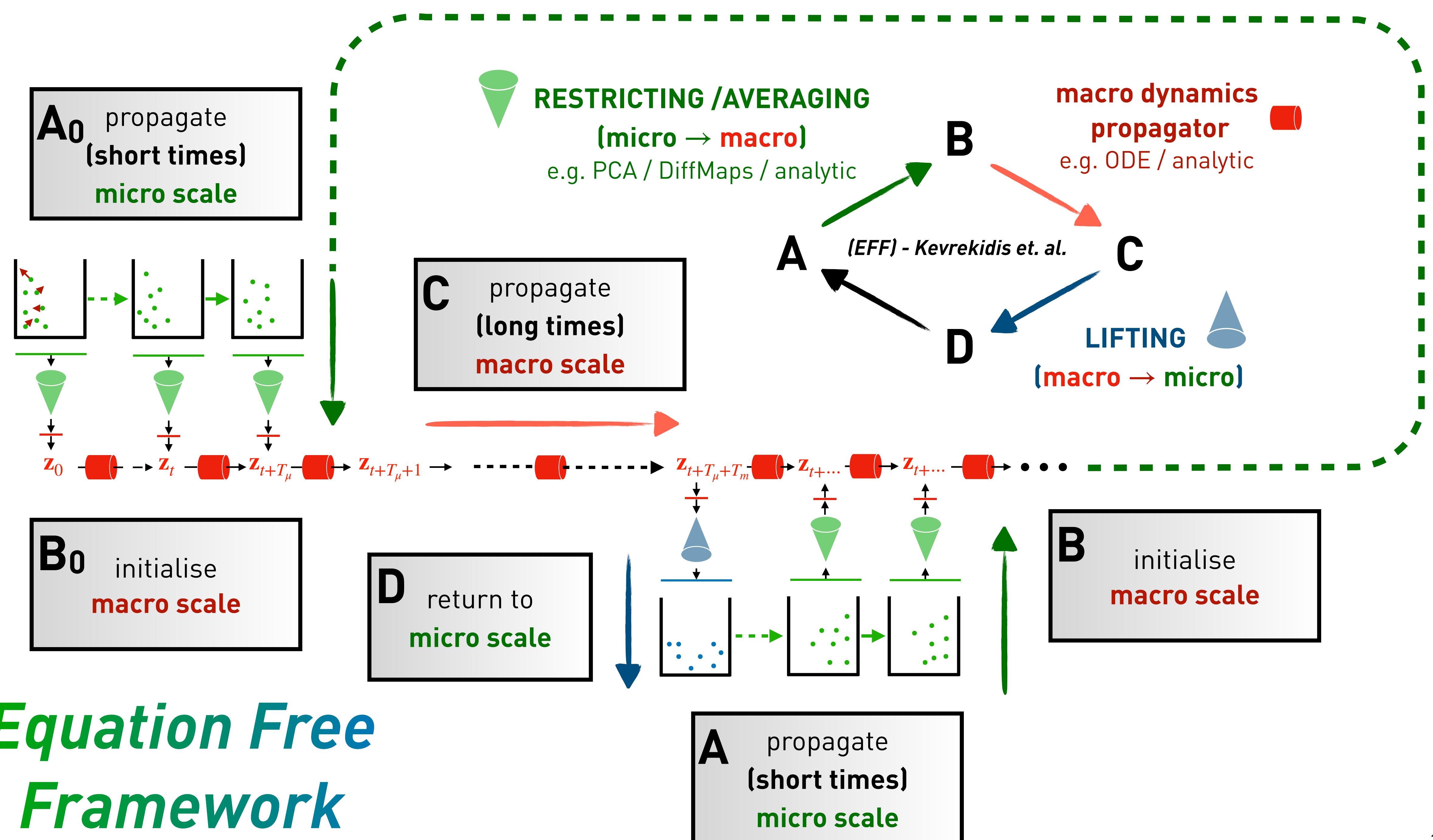
Low dimensional latent space

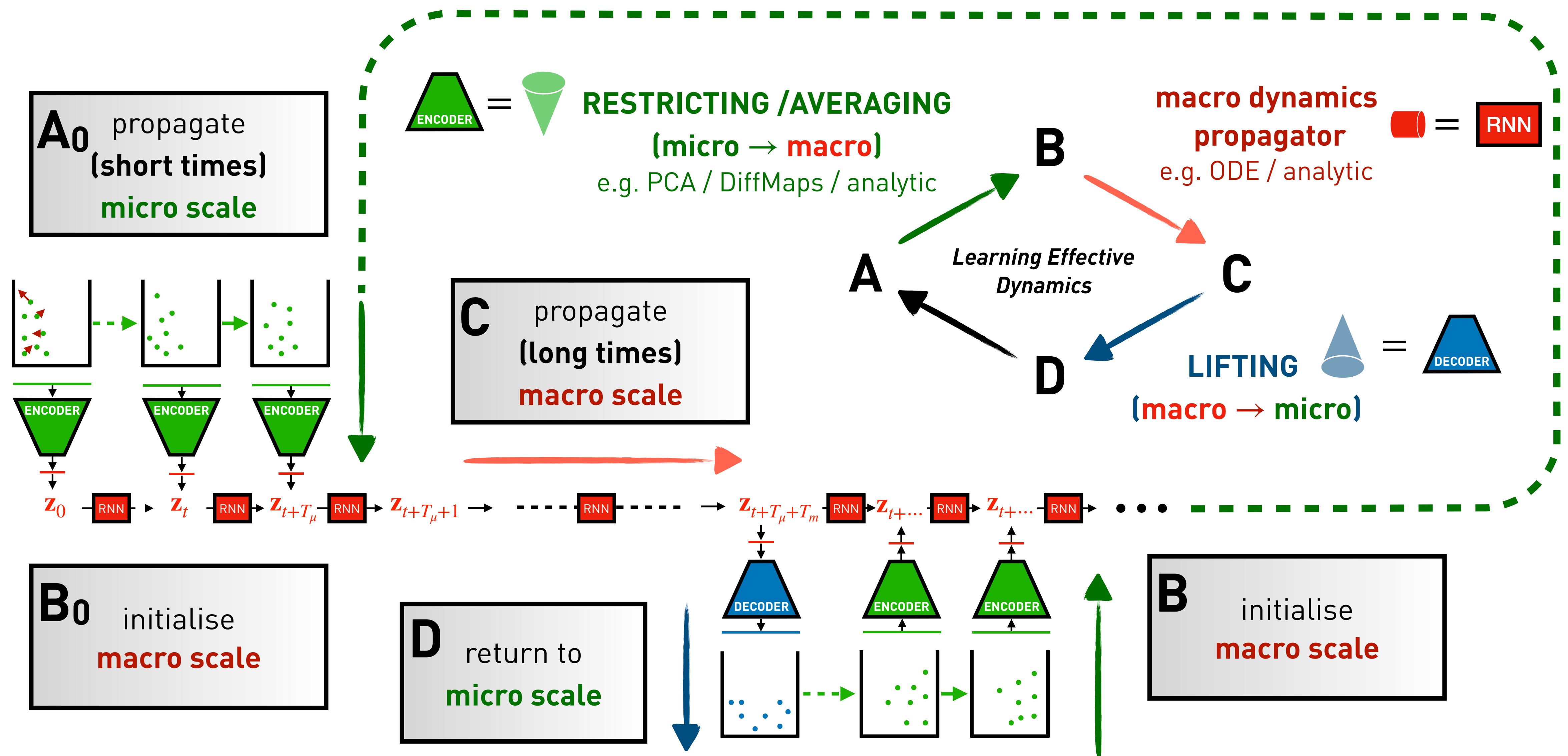


Space

Time

Space

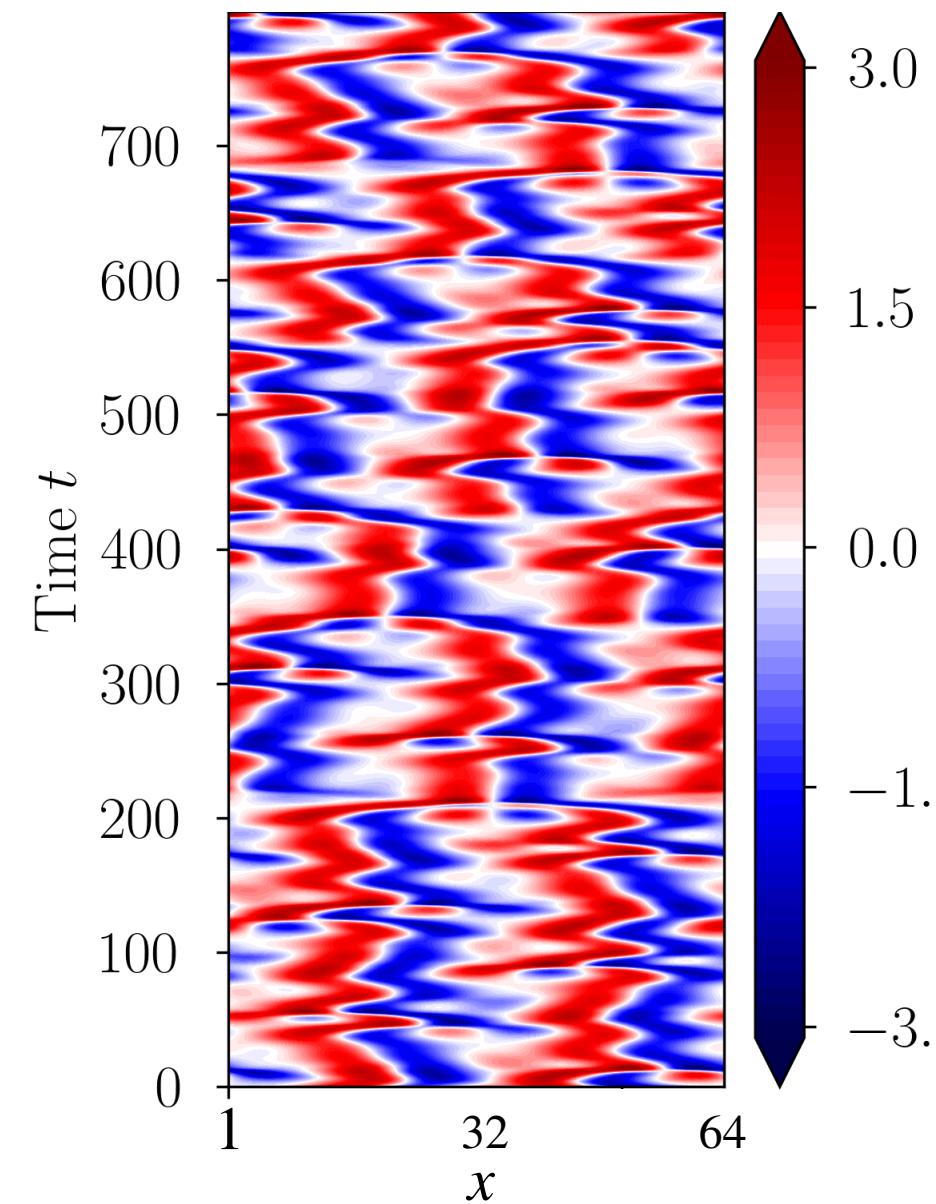




# Learning Effective Dynamics (LED)

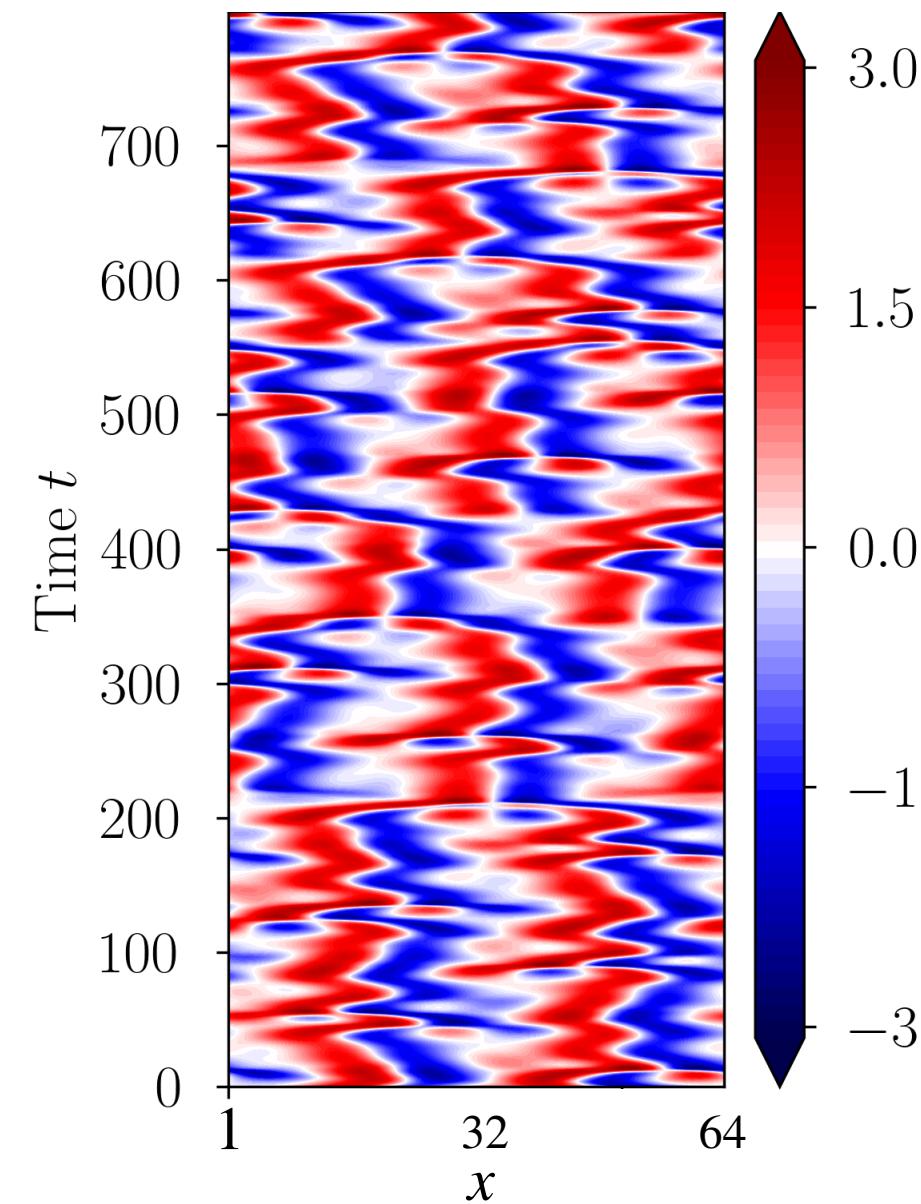
# Kuramoto-Sivashinsky ( $\tilde{L} \approx 3.5$ )

REFERENCE



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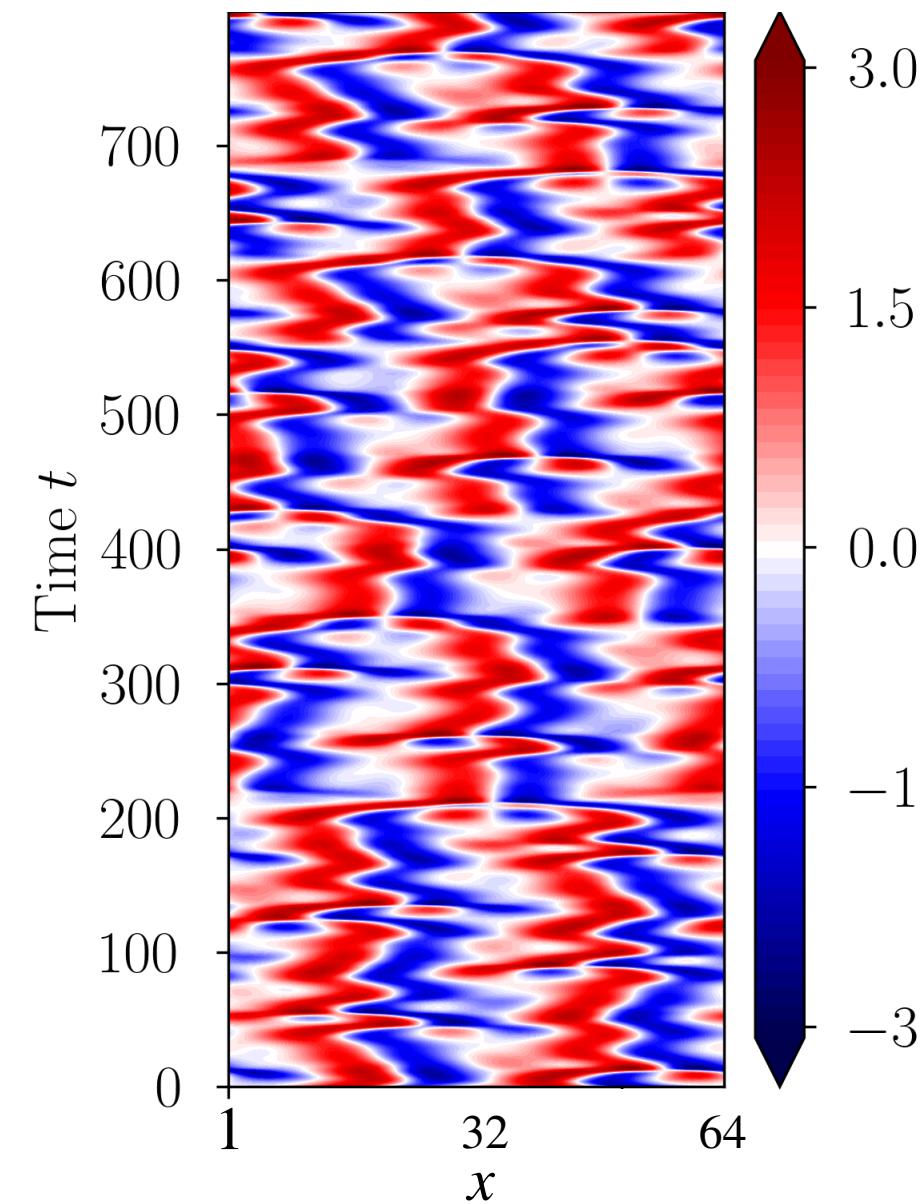
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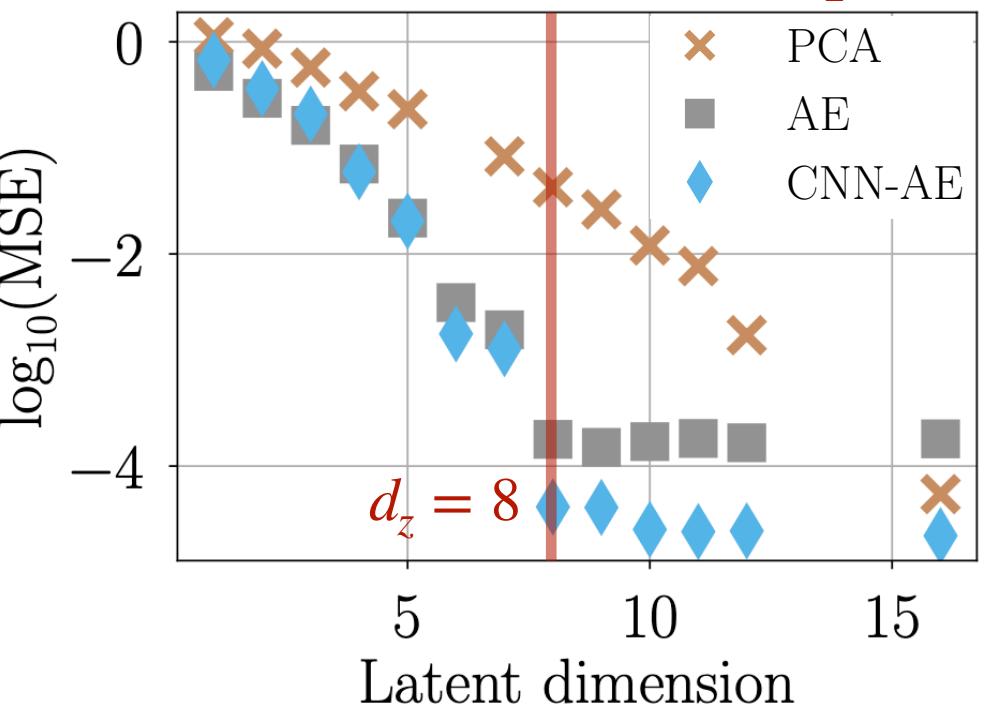
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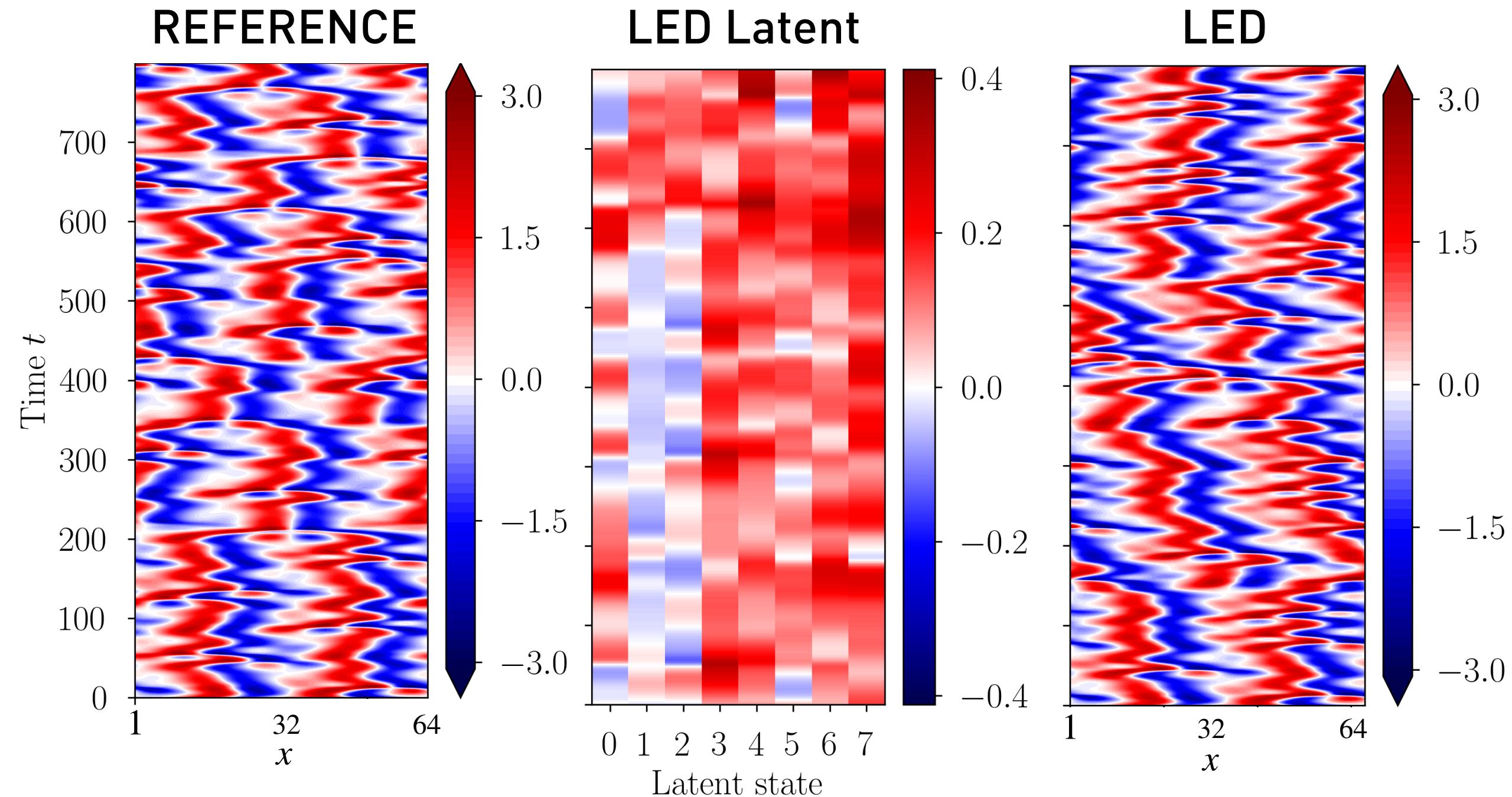
The AE error saturates after  $d_z = 8$



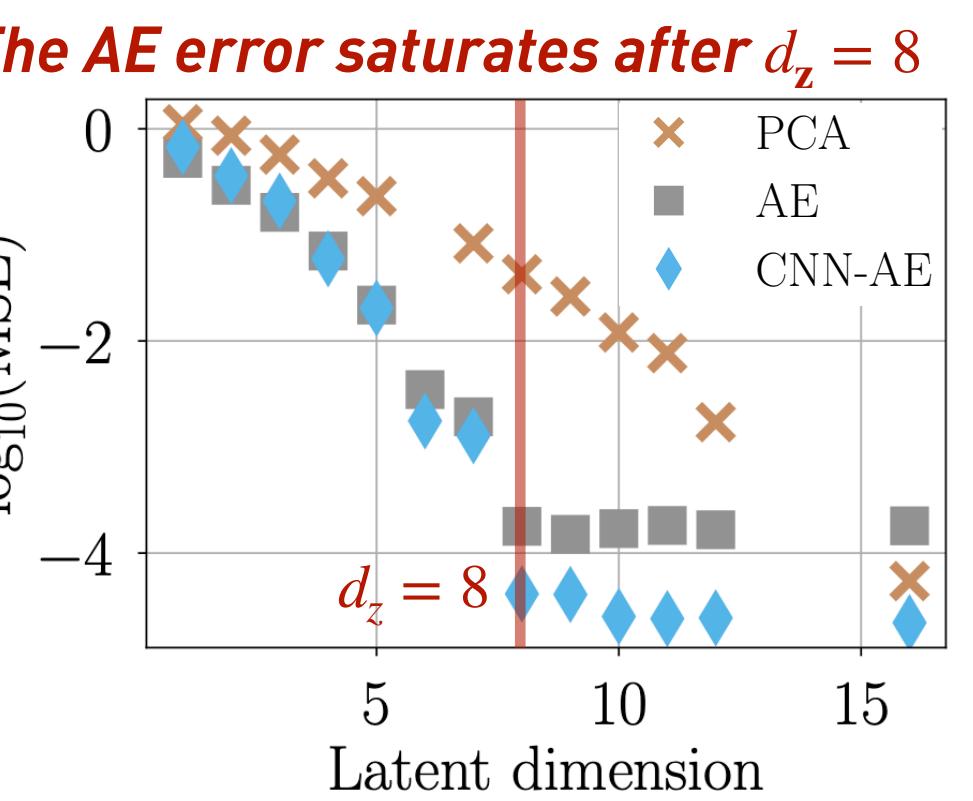
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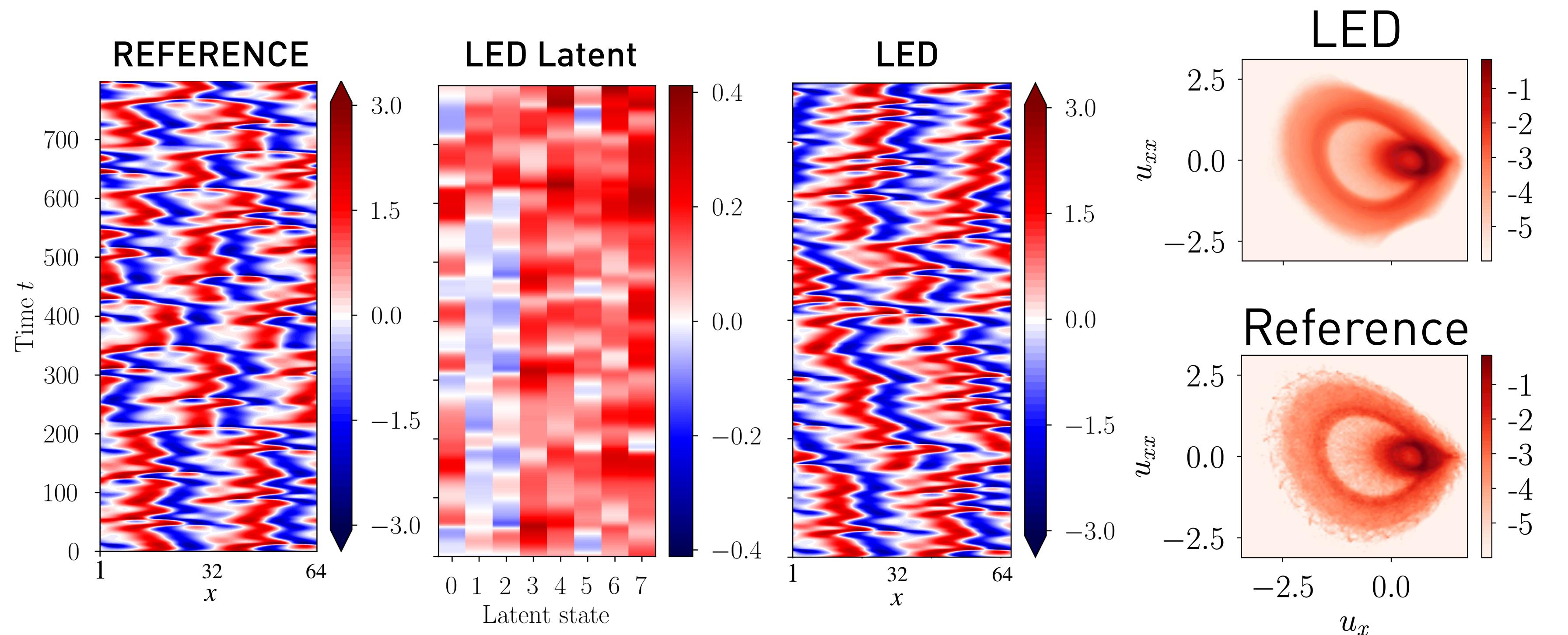
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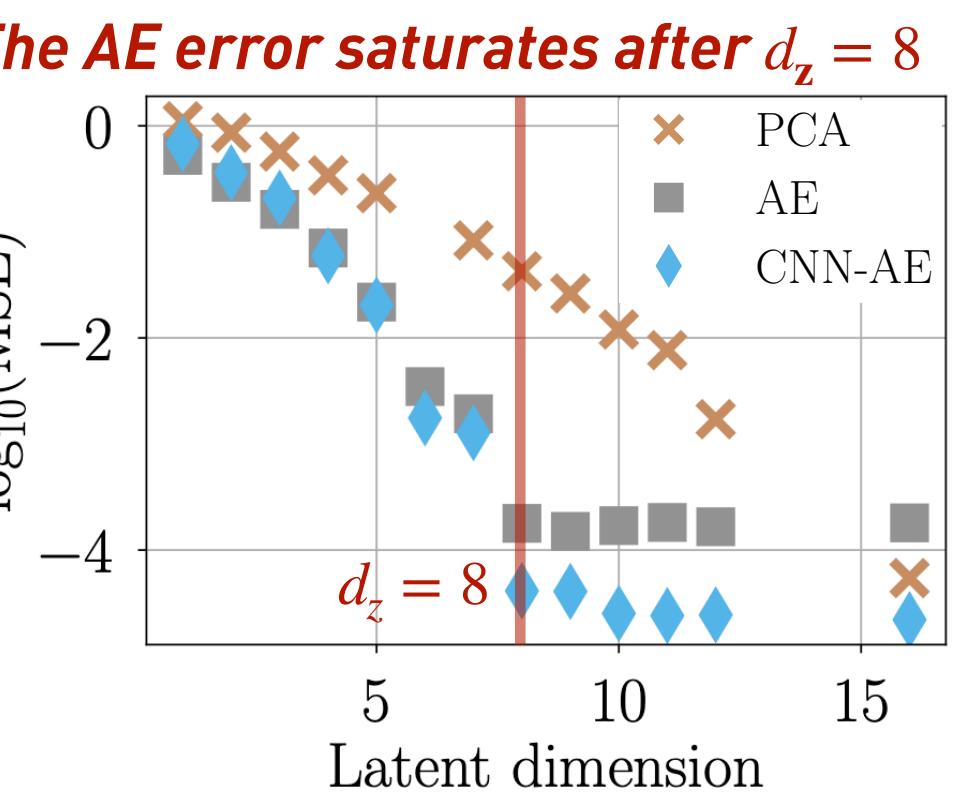
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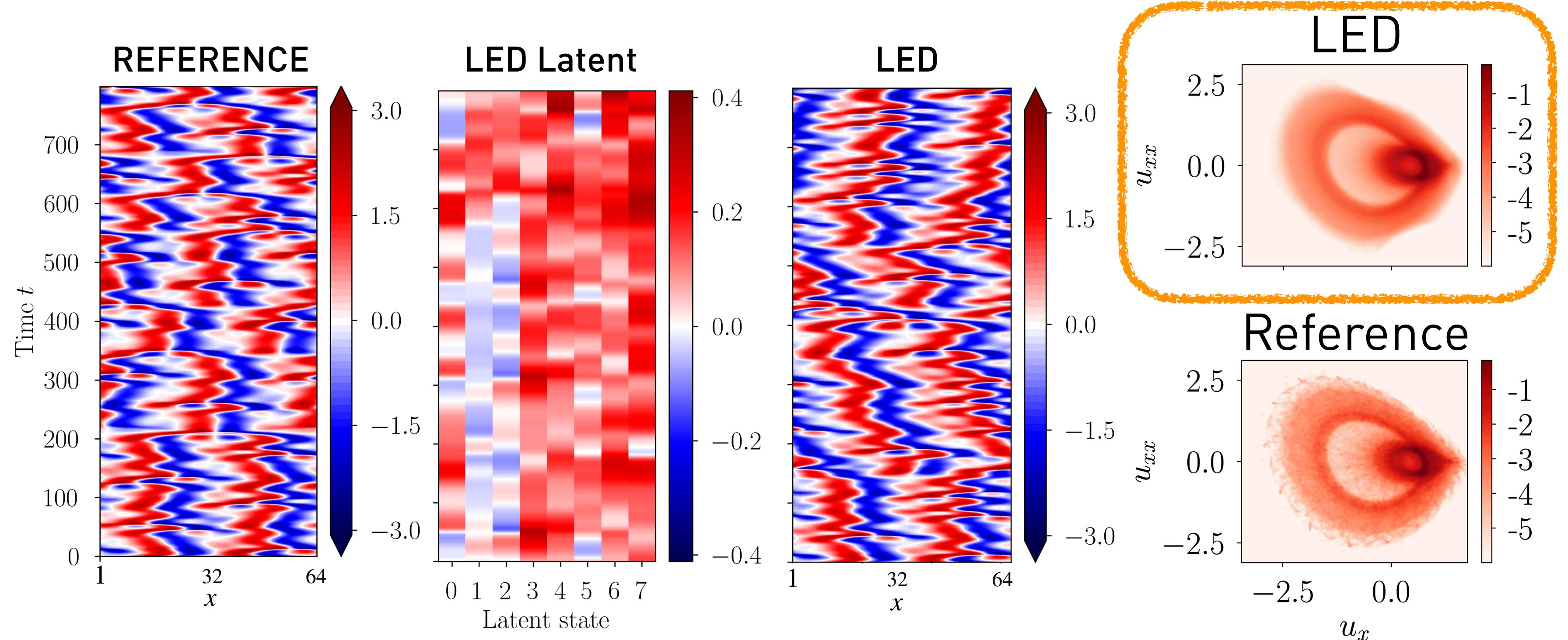
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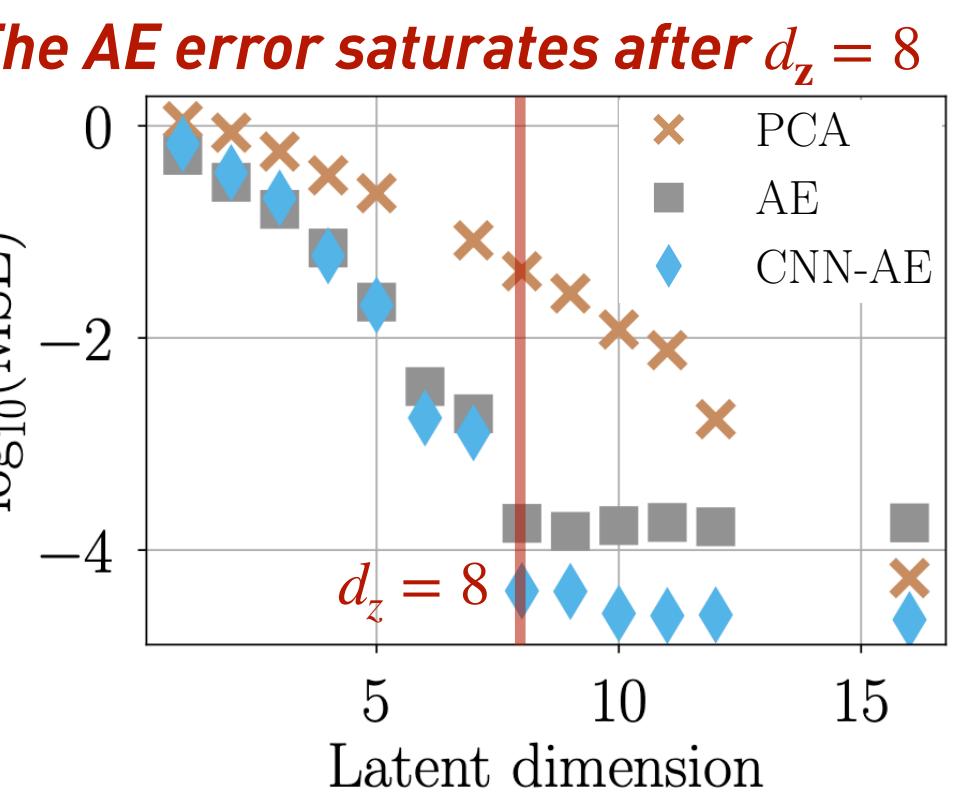
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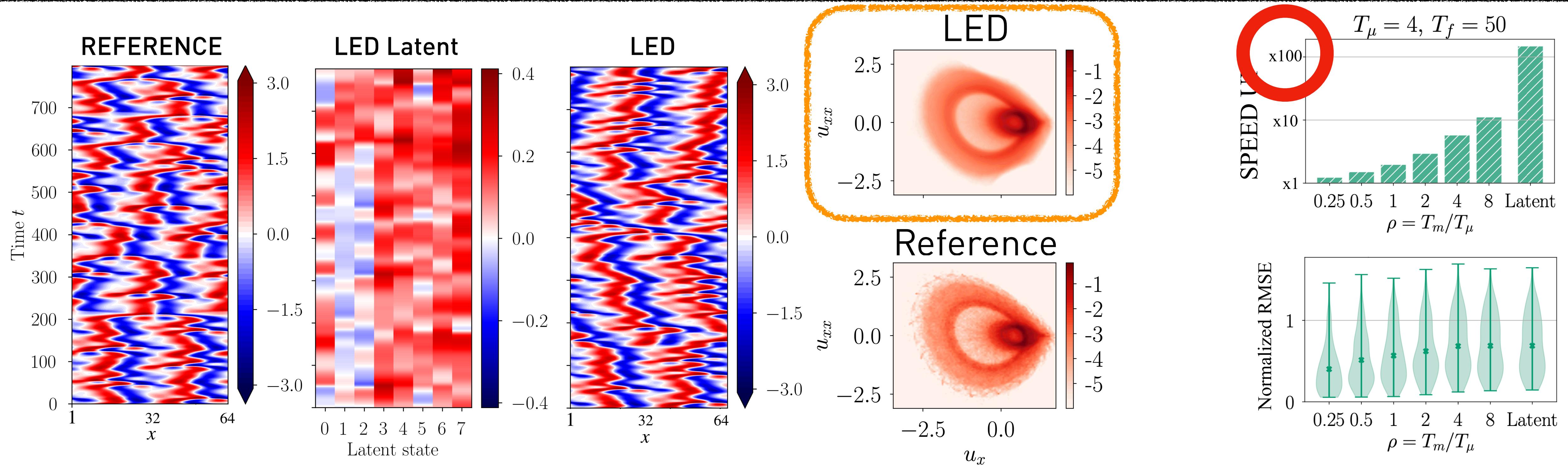
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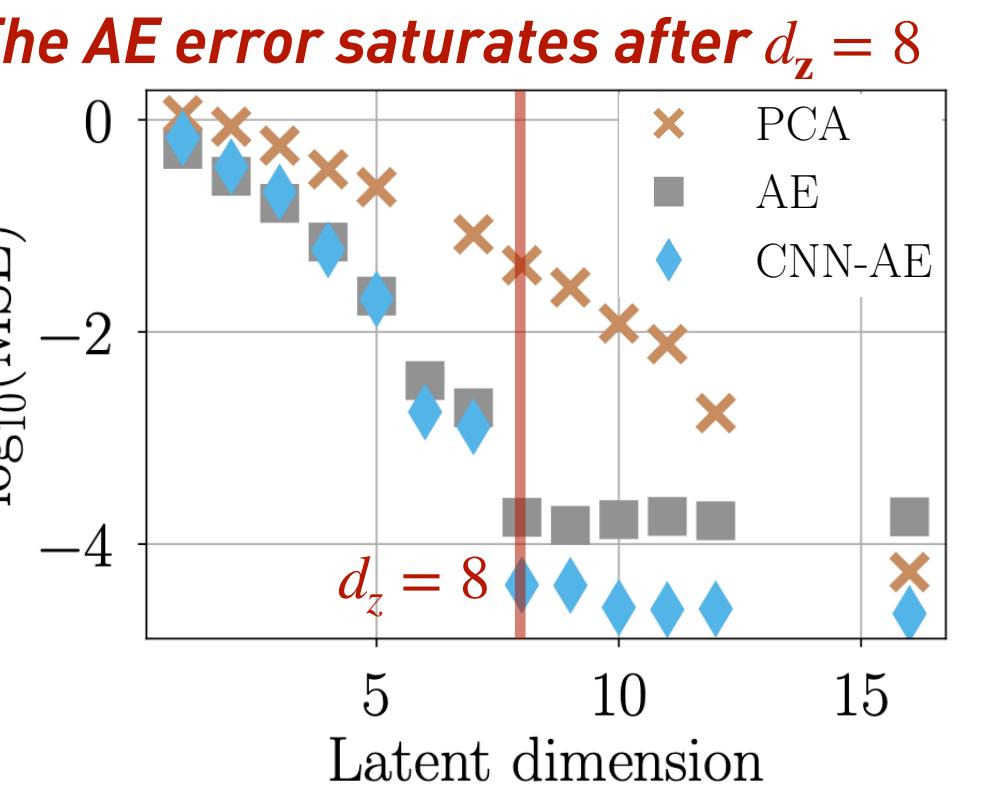
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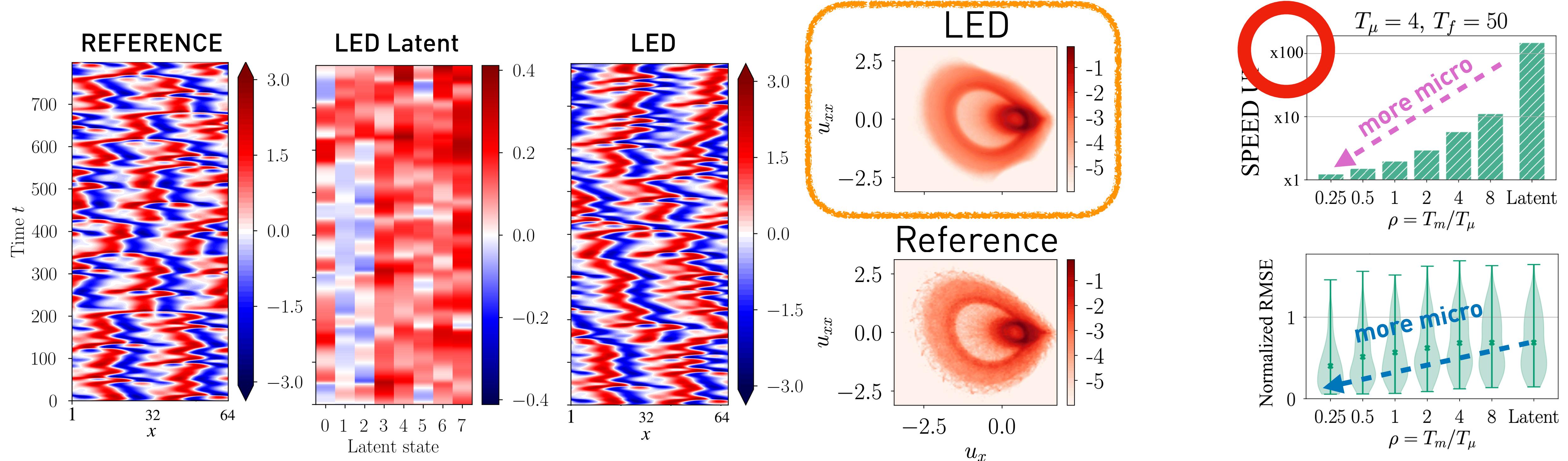
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- Reproducing the **statistics/long-term climate** accurately
- **Two orders** of magnitude faster compared to the stiff ODE solver used



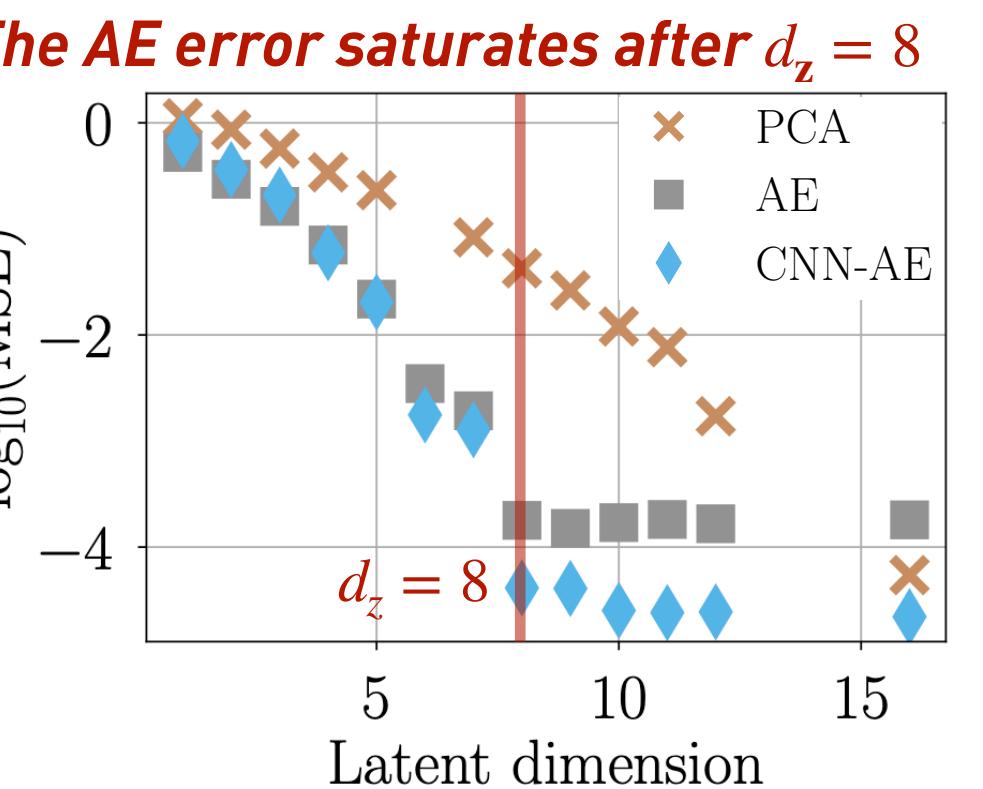
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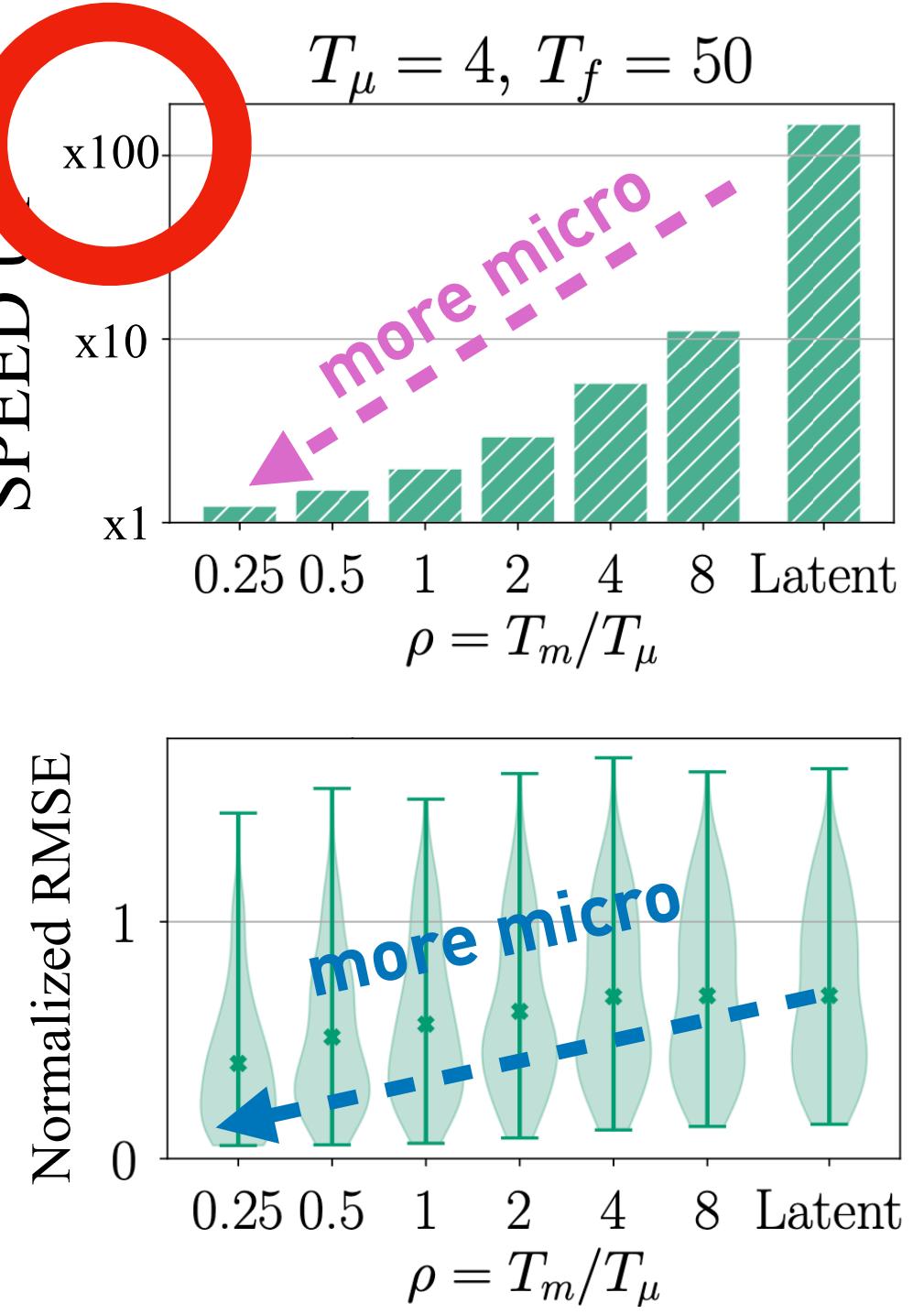
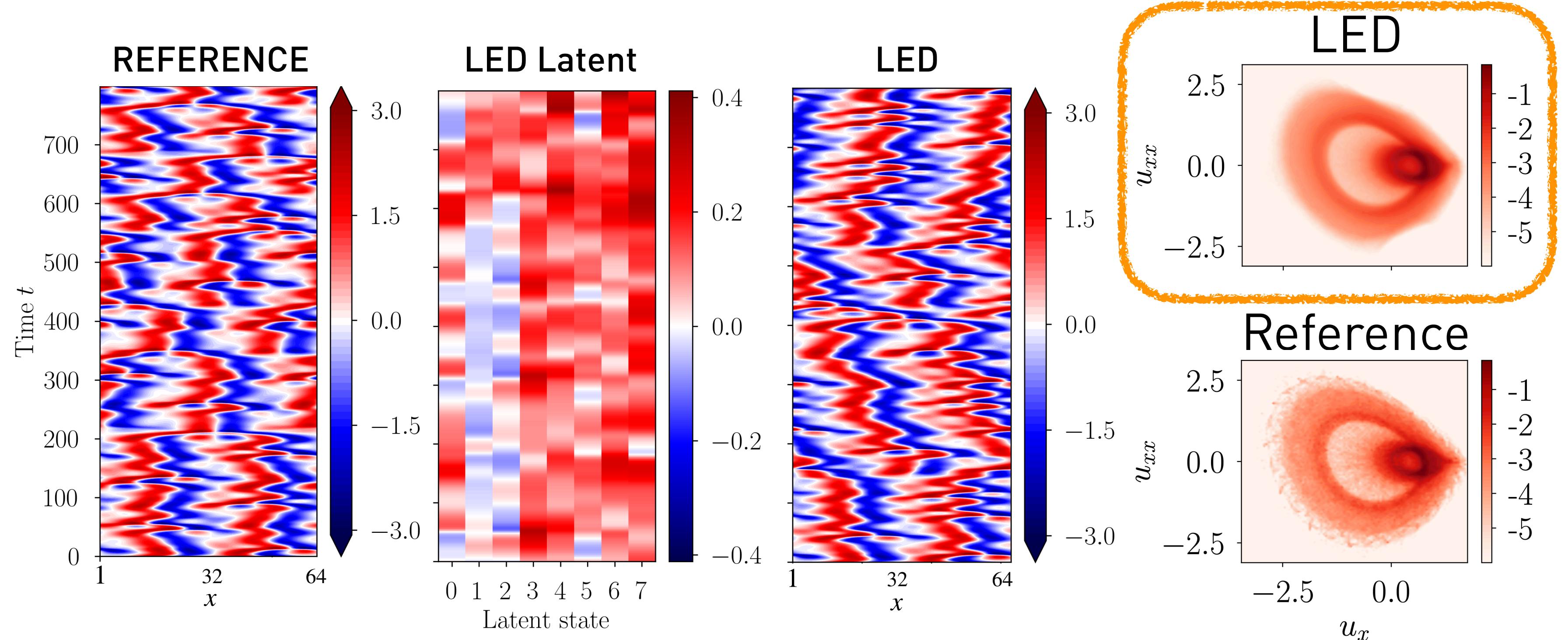
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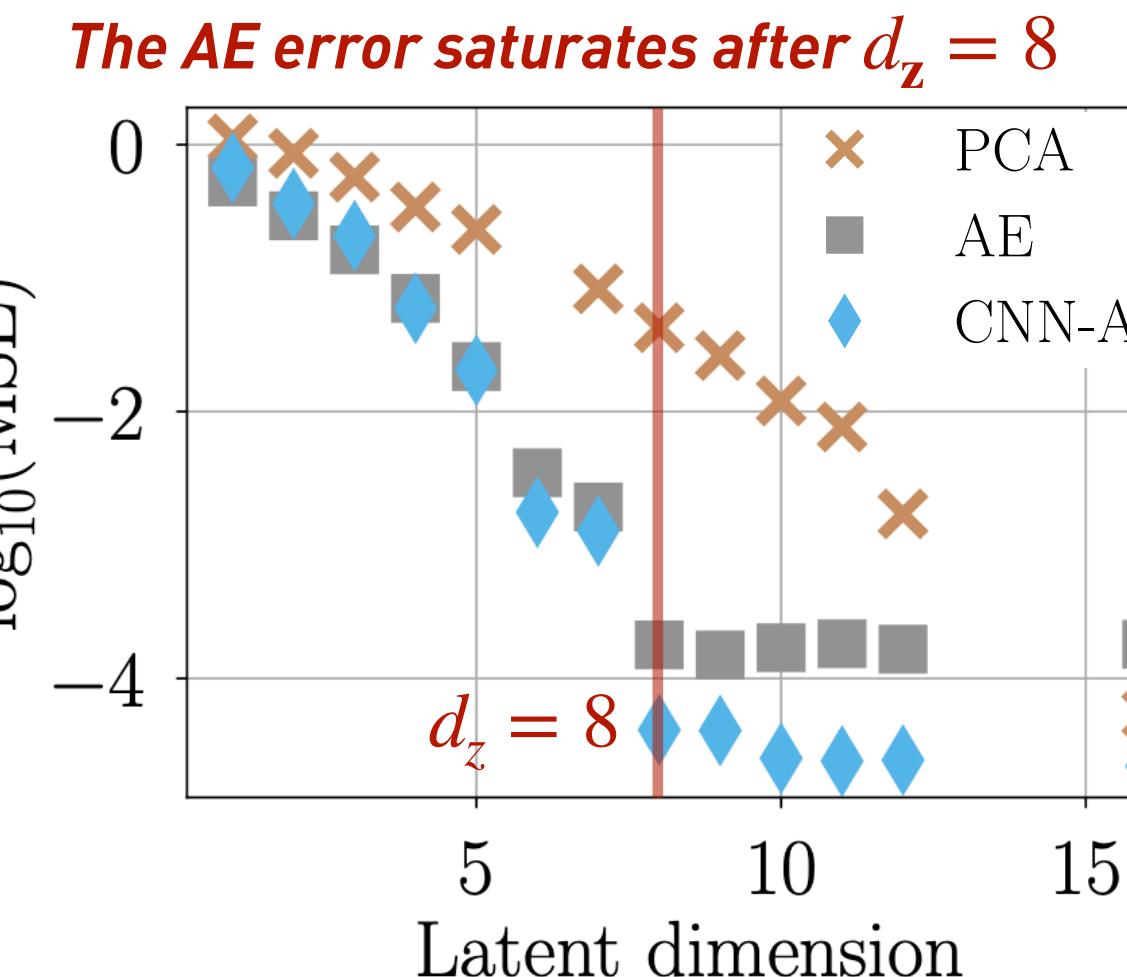
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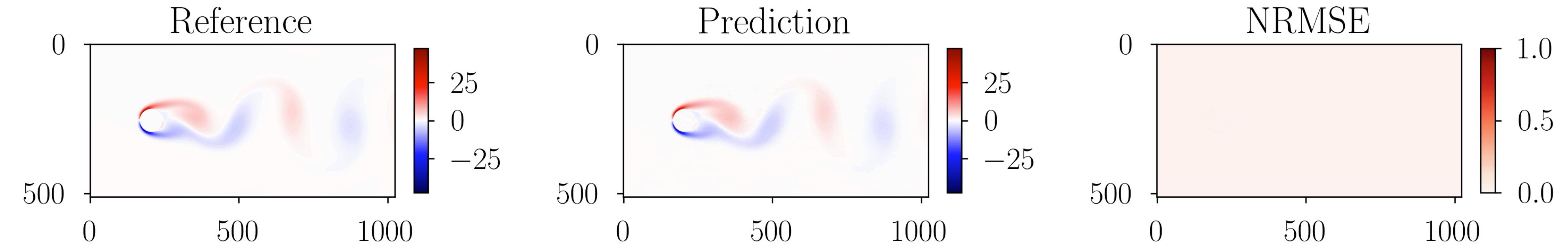
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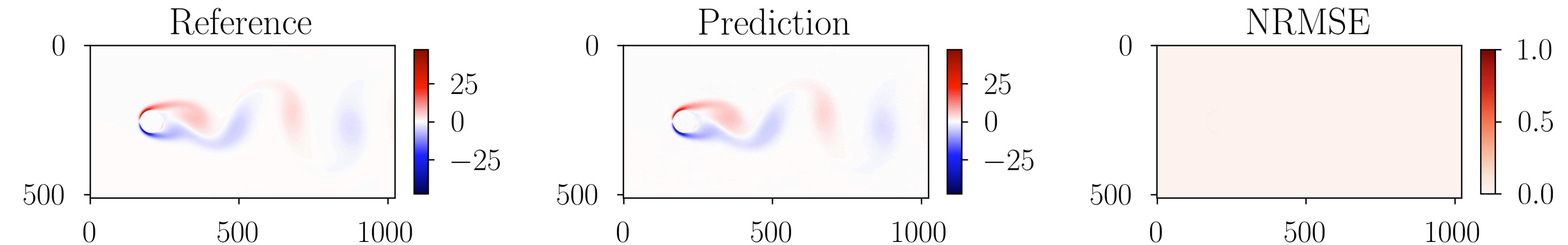
[1] Robinson, J. C. "Inertial manifolds for the kuramoto-sivashinsky equation." *Physics Letters A* **184**, 190–193 (1994).

[2] Linot, A. J. & Graham, M. D. "Deep learning to discover and predict dynamics on an inertial manifold." *Physical Review E* **101**, 062209 (2020).

# Cylinder at $Re = 100$ - (LED $d_z = 4$ )

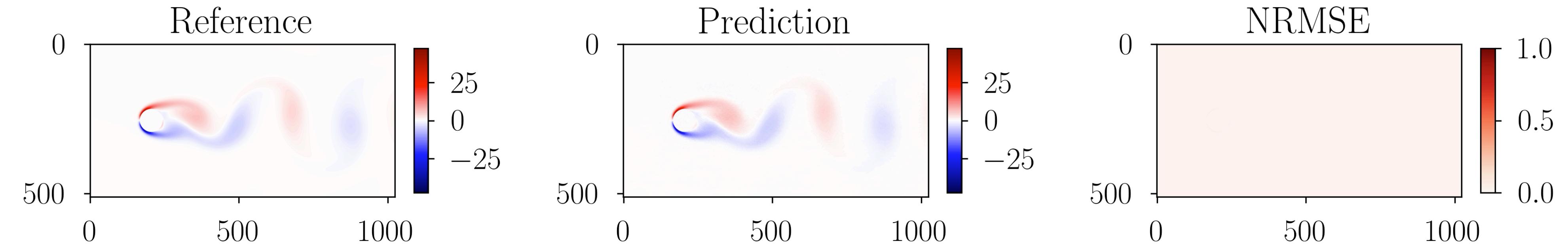


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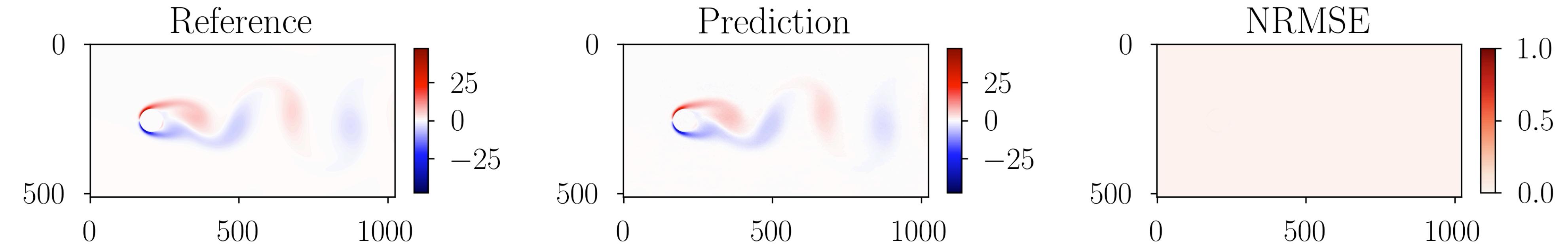
- Micro solver: Finite Differences (CubimUP2D) employing 12 cores

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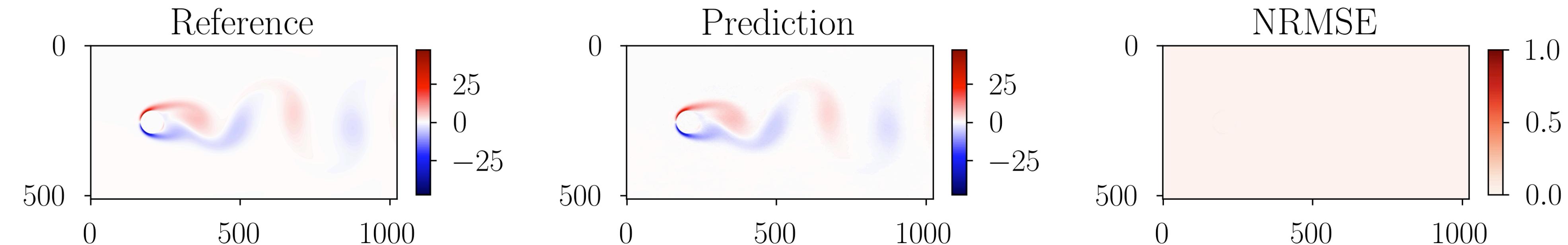
- Micro solver: Finite Differences (CubimUP2D) employing 12 cores
- State: velocity in x- and y- direction, pressure, and **vorticity**  $s_t \in \mathbb{R}^{4 \times 512 \times 1024}$

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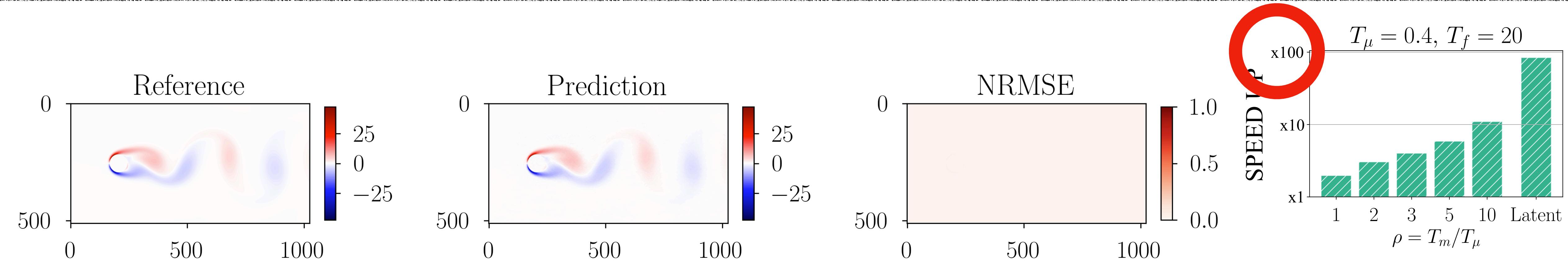
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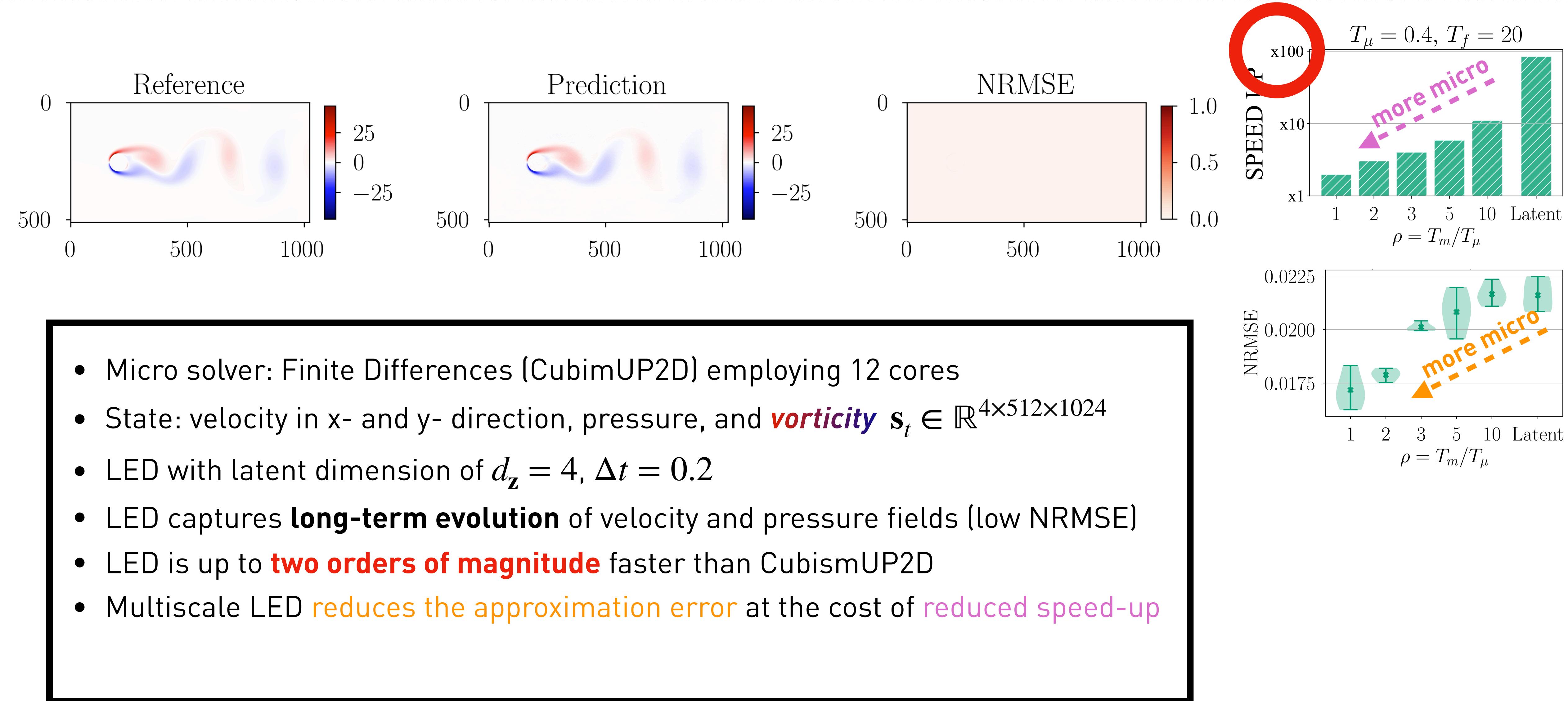
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- LED captures **long-term evolution** of velocity and pressure fields (low NRMSE)

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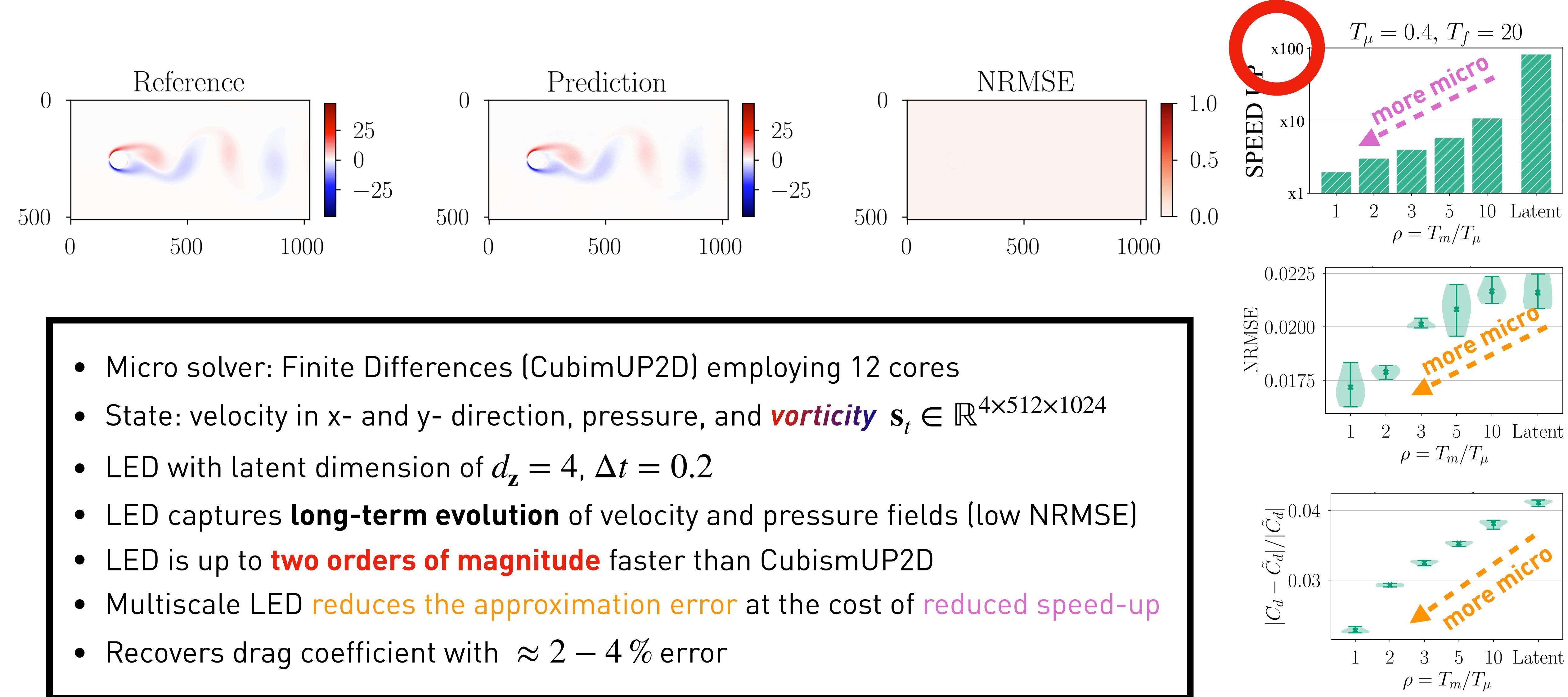


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- LED with latent dimension of  $d_z = 4$ ,  $\Delta t = 0.2$
- LED captures **long-term evolution** of velocity and pressure fields (low NRMSE)
- LED is up to **two orders of magnitude** faster than CubismUP2D

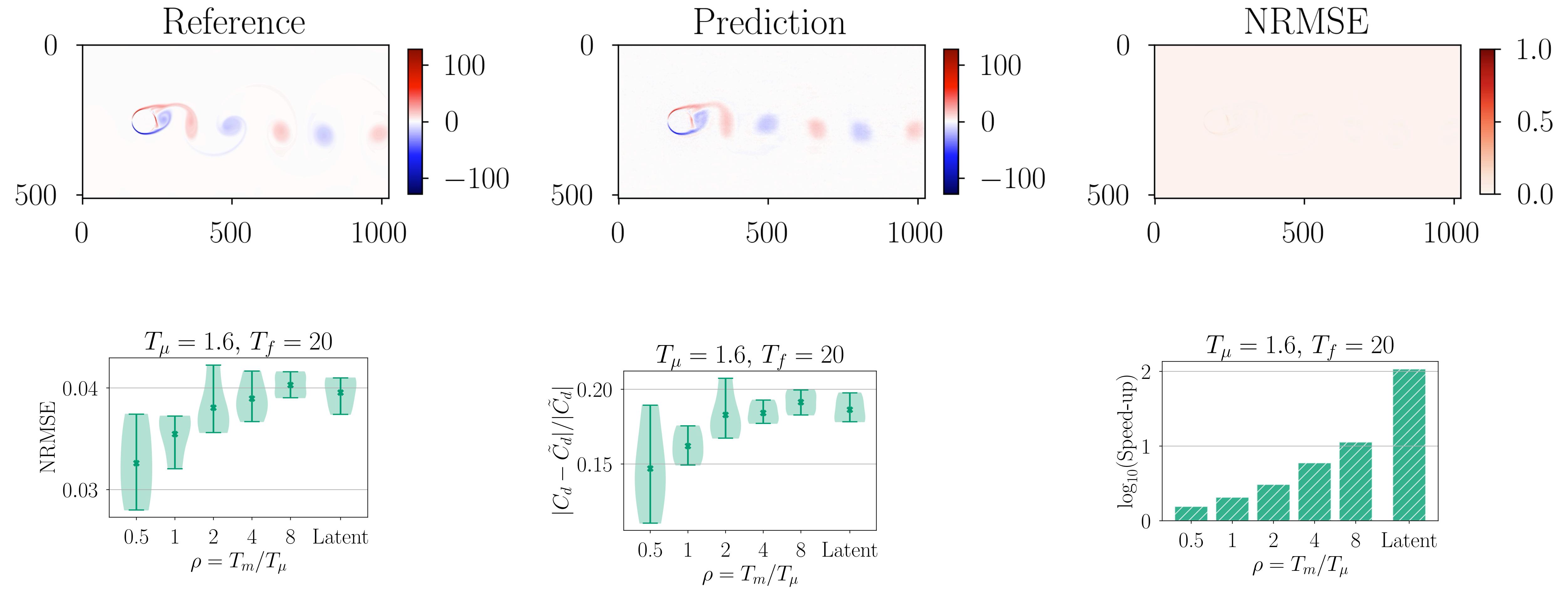
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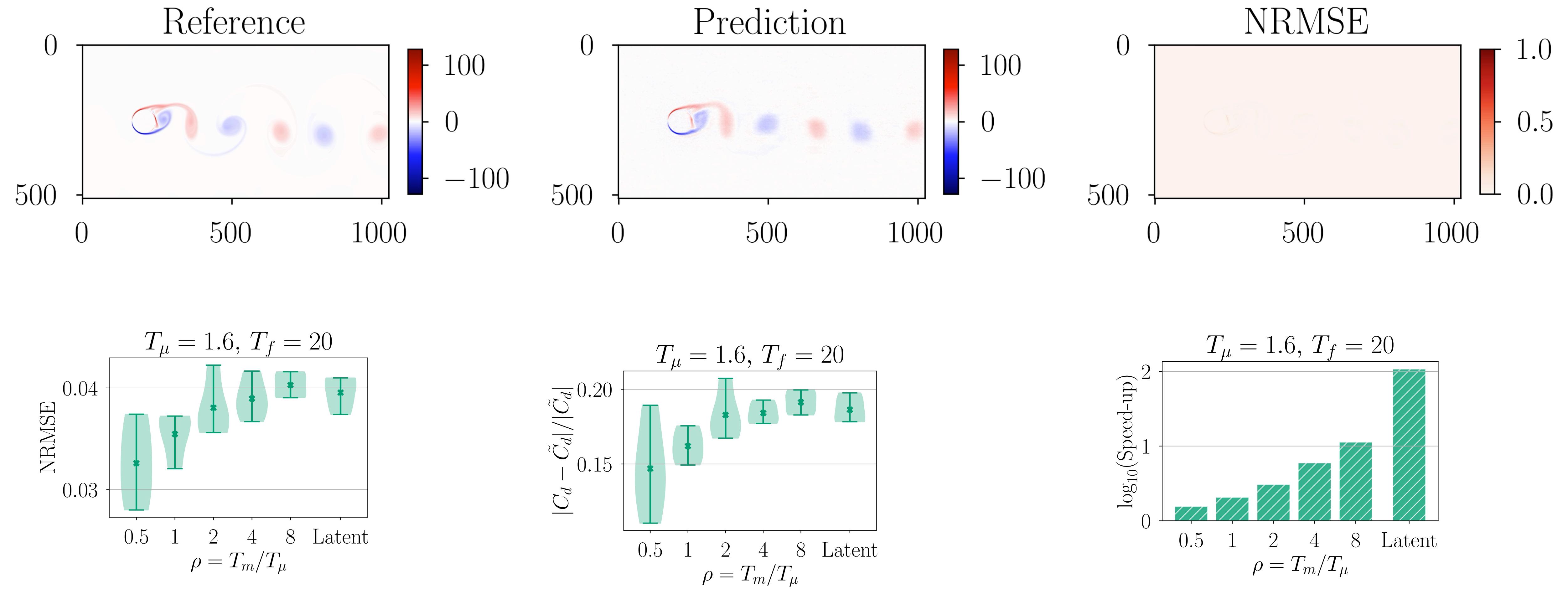
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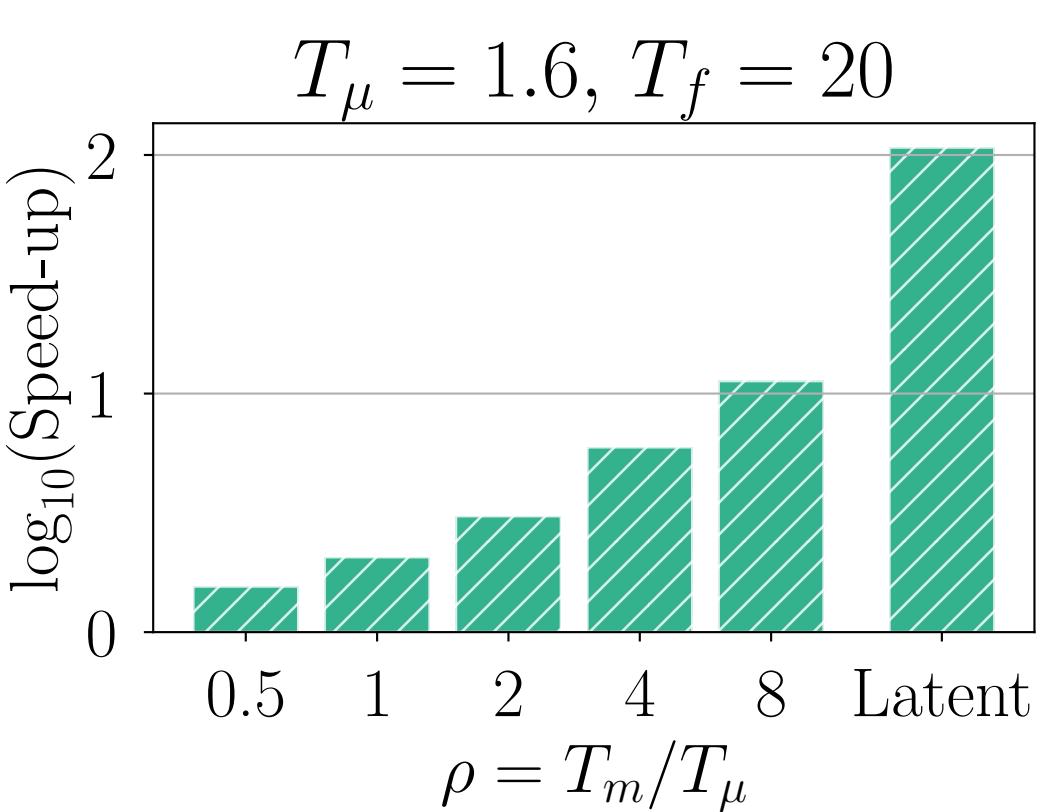
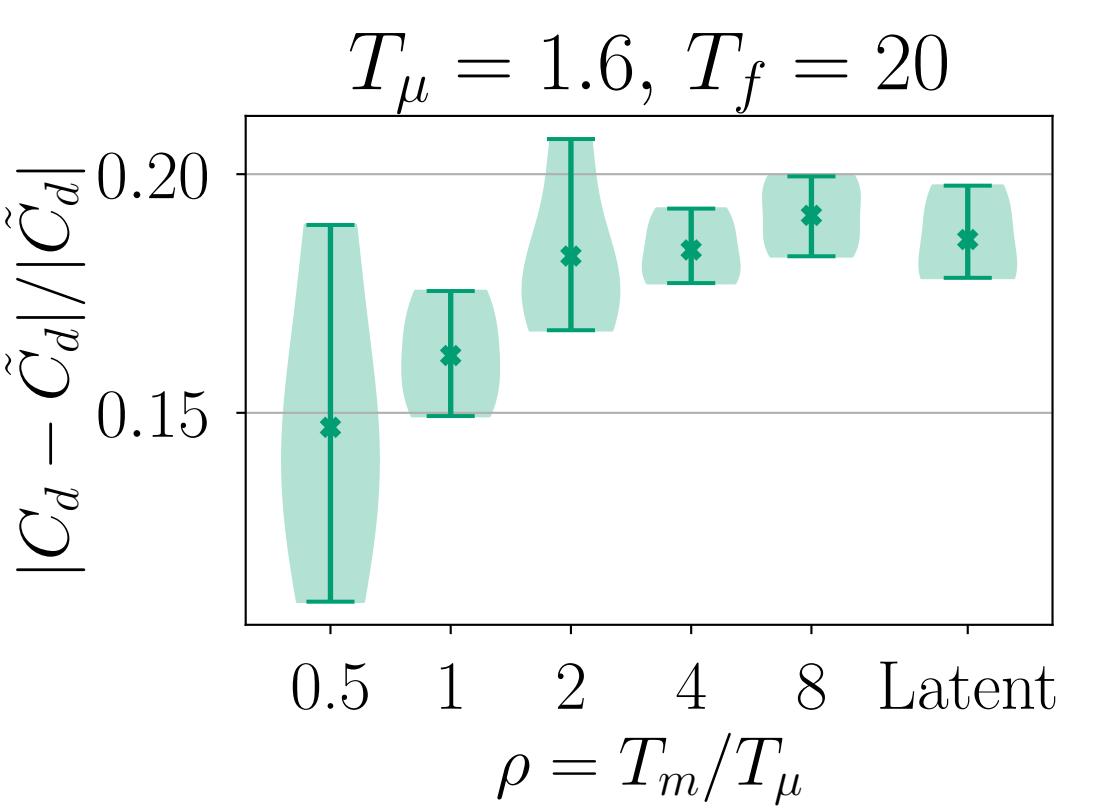
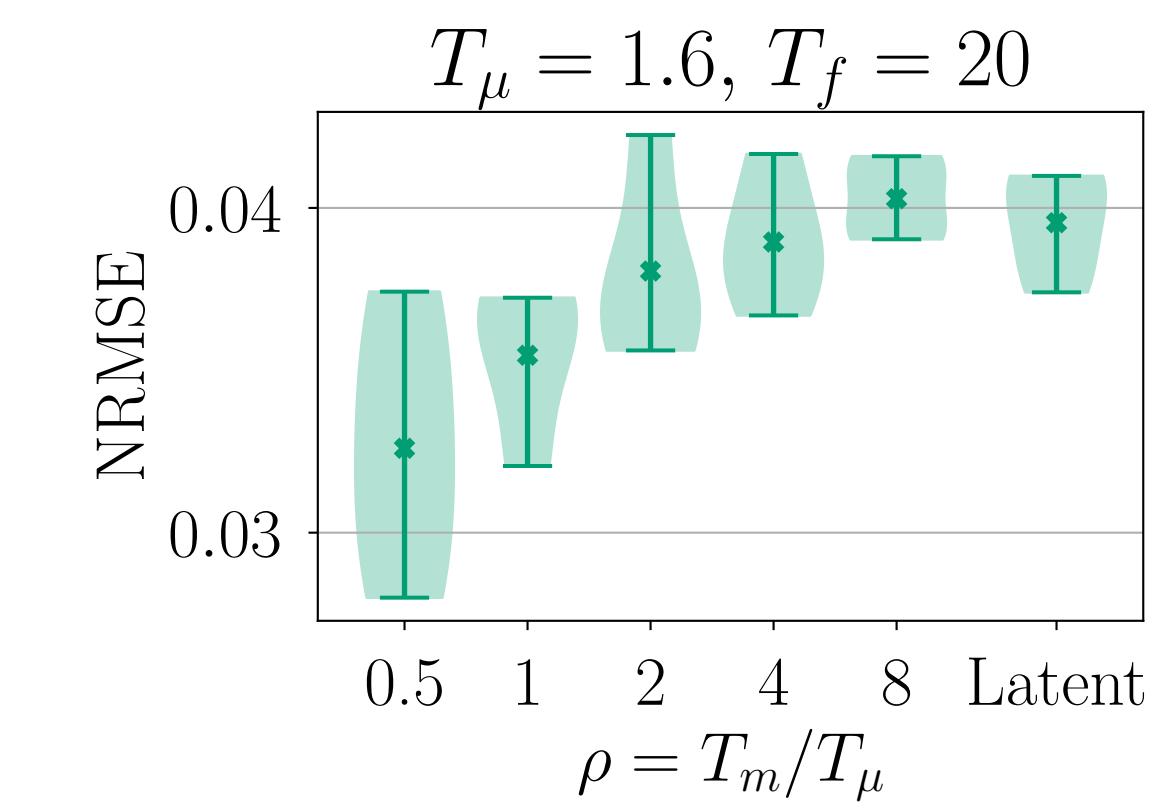
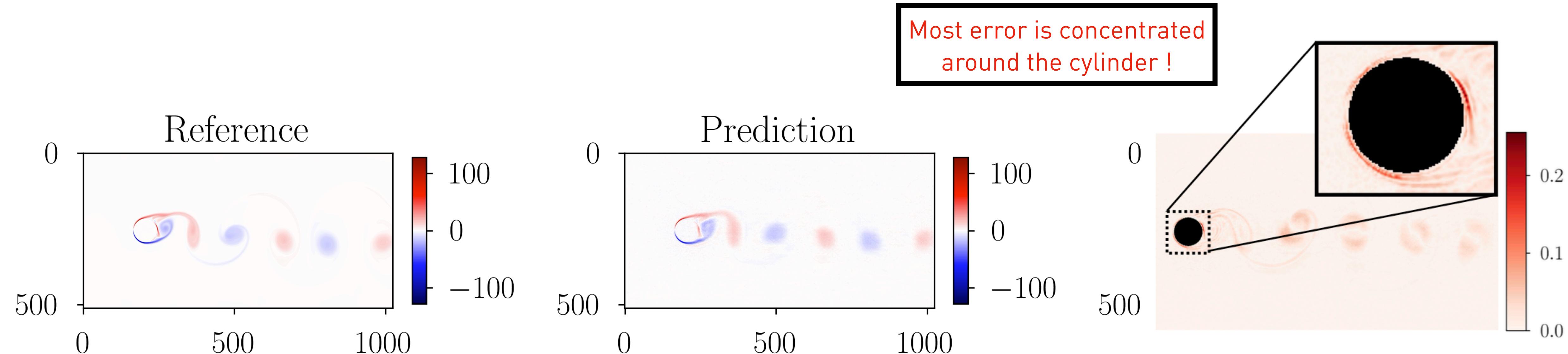
# Cylinder at $Re = 1000$ (LED $d_z = 10$ )



# Cylinder at $Re = 1000$ (LED $d_z = 10$ )



# Cylinder at $Re = 1000$ (LED $d_z = 10$ )



# Comparisons of Latent Propagators

PR Vlachas, G Arampatzis, C Uhler, P Koumoutsakos,  
*Multiscale Simulations of Complex Systems  
by Learning their Effective Dynamics,*  
Nature Machine Intelligence, (to appear 2022)

**SINDy**

SL Brunton, JL Proctor, JN Kutz,  
*Discovering governing equations from  
data by sparse identification of  
nonlinear dynamical systems,*  
PNAS (2016)

**RC**

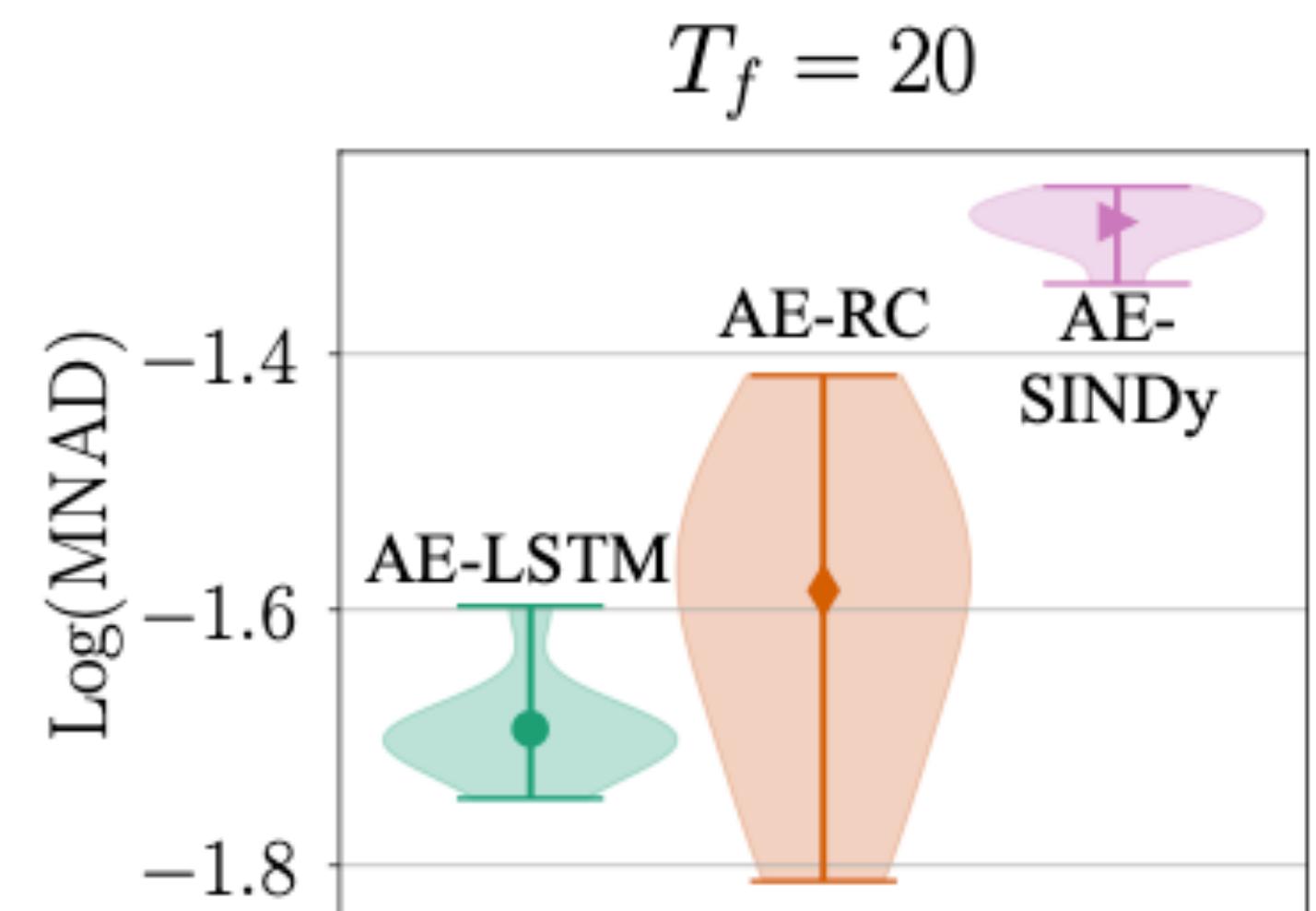
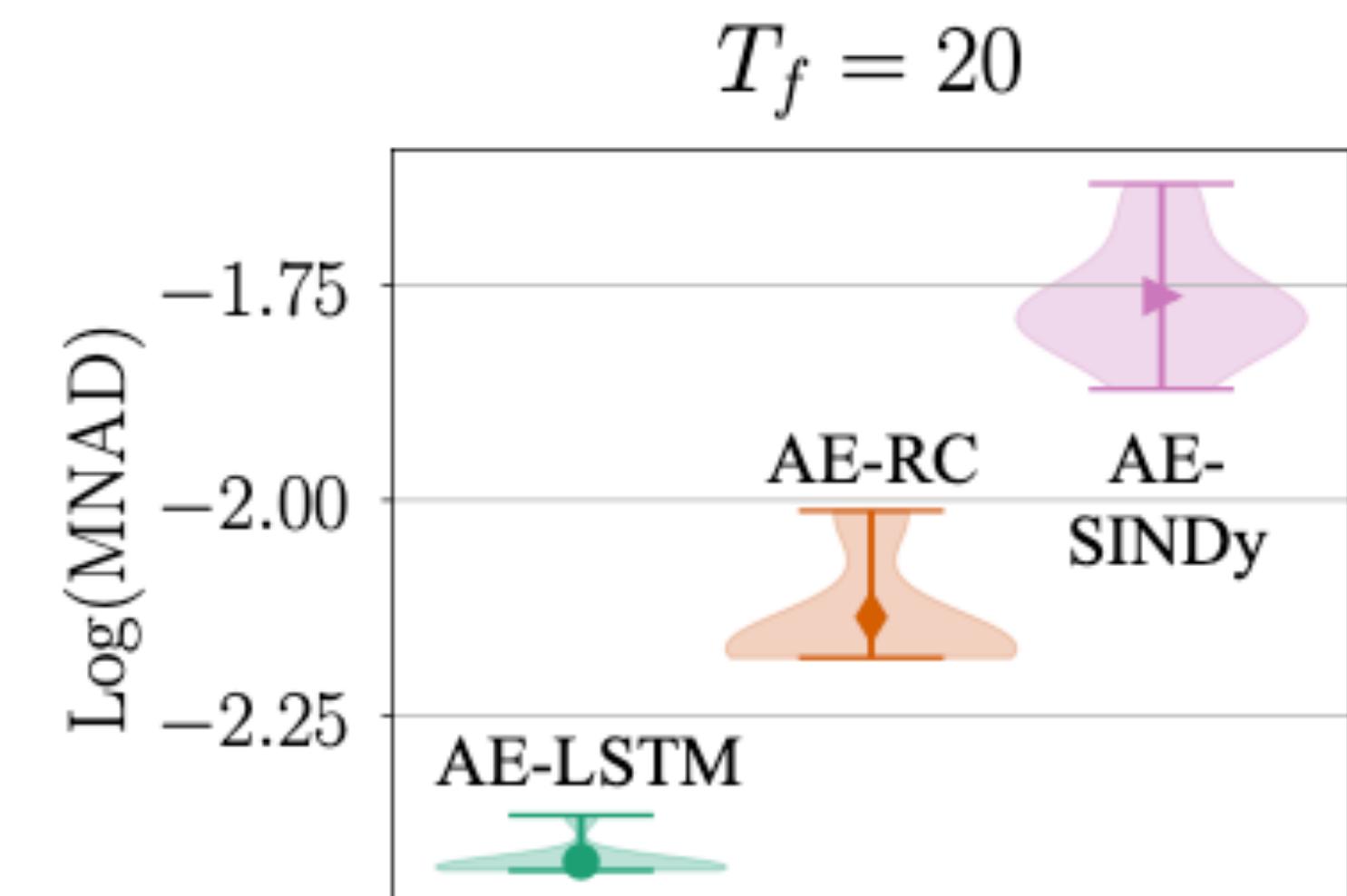
J Pathak, B Hunt, M Girvan, Z  
Lu, E Ott, *Model-free prediction of  
large spatiotemporally chaotic  
systems from data: A reservoir  
computing approach,*  
Physical review letters, 2018

**LSTM**

S Hochreiter, J Schmidhuber,  
*Long short-term memory,*  
Neural Computation, 1997

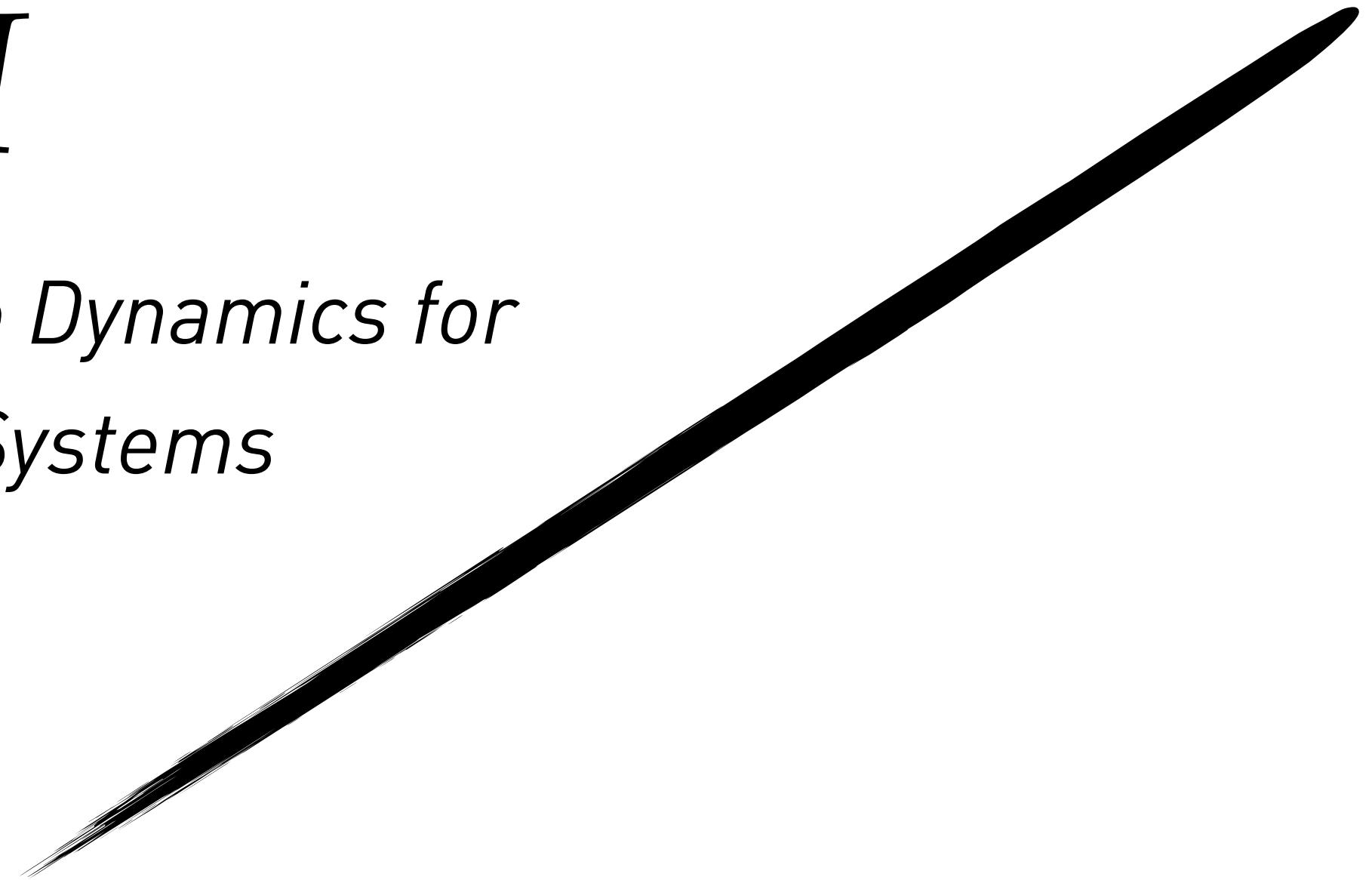
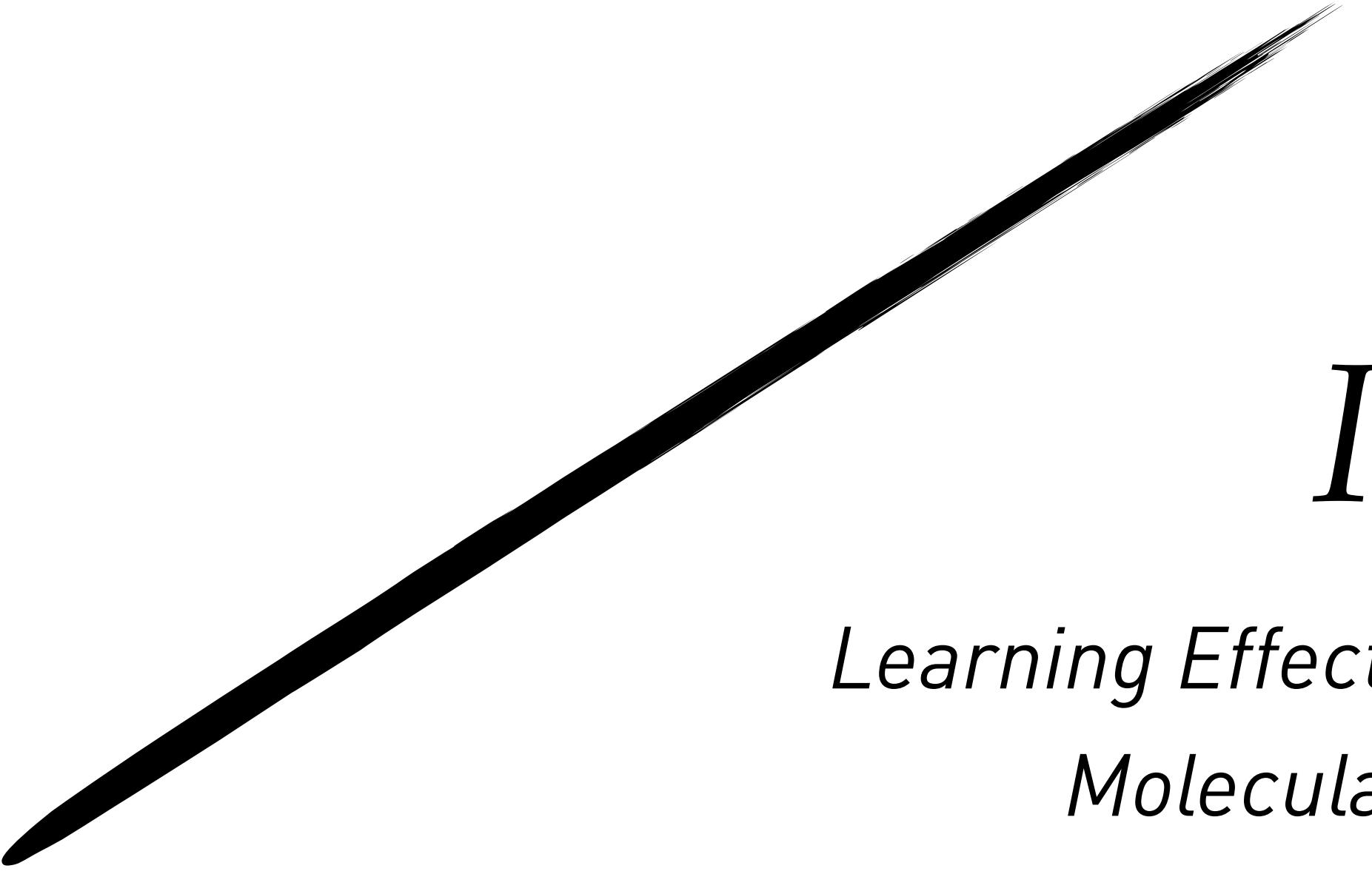
Mean normalised absolute difference:

$$\text{NAD}(t_j) = \frac{1}{N_x} \sum_{i=1}^{N_x} \frac{|y(x_i, t_j) - \hat{y}(x_i, t_j)|}{\max_{i,j}(y(x_i, t_j)) - \min_{i,j}(y(x_i, t_j))}$$
$$\text{MNAD} = \frac{1}{N_T} \sum_{j=1}^{N_T} \text{NAD}(t_j)$$



$Re = 100$

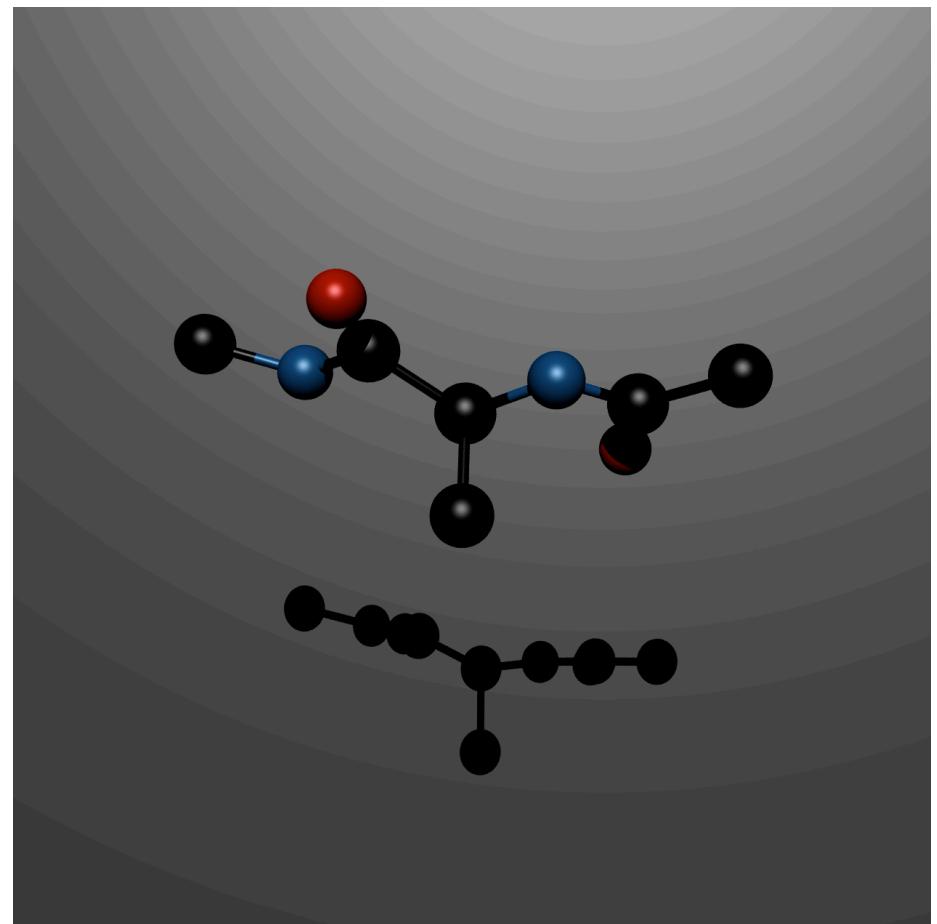
$Re = 1000$



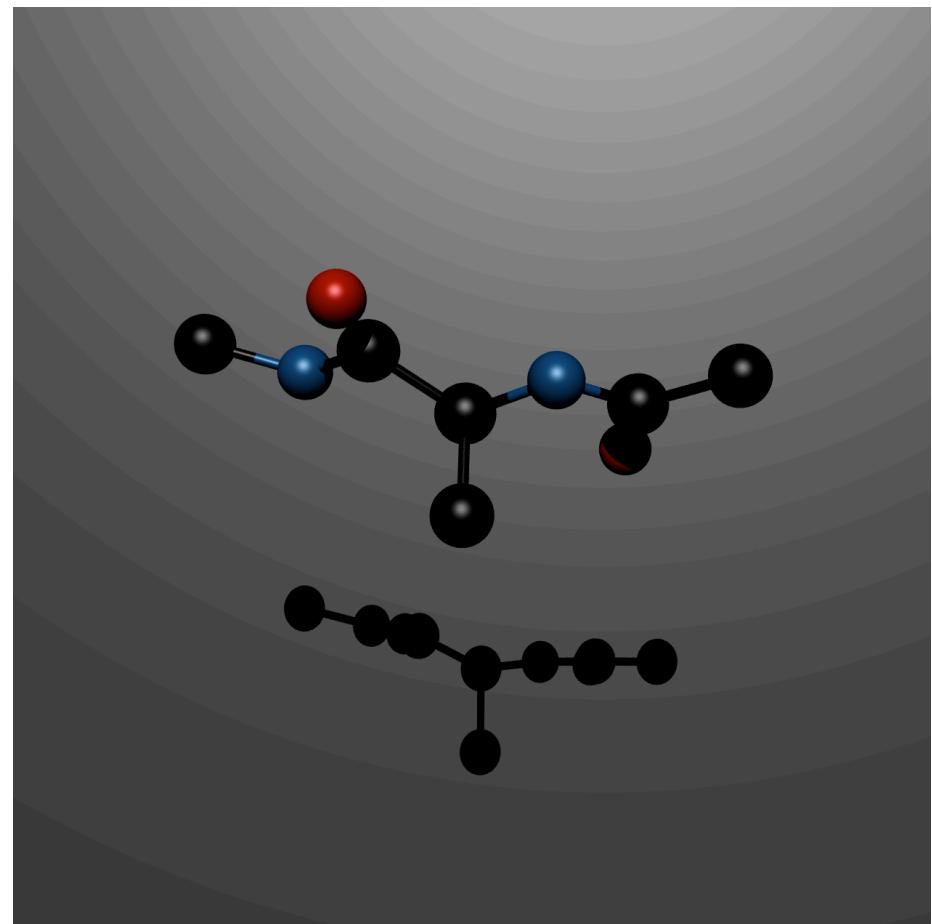
*III*

*Learning Effective Dynamics for  
Molecular Systems*

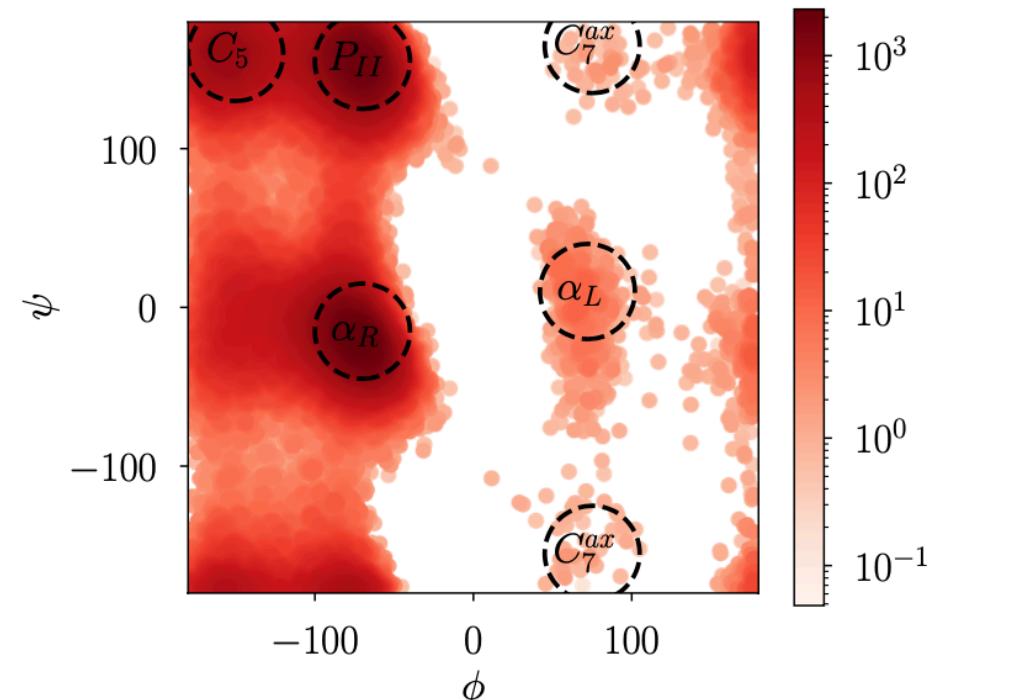
# Alanine Dipeptide



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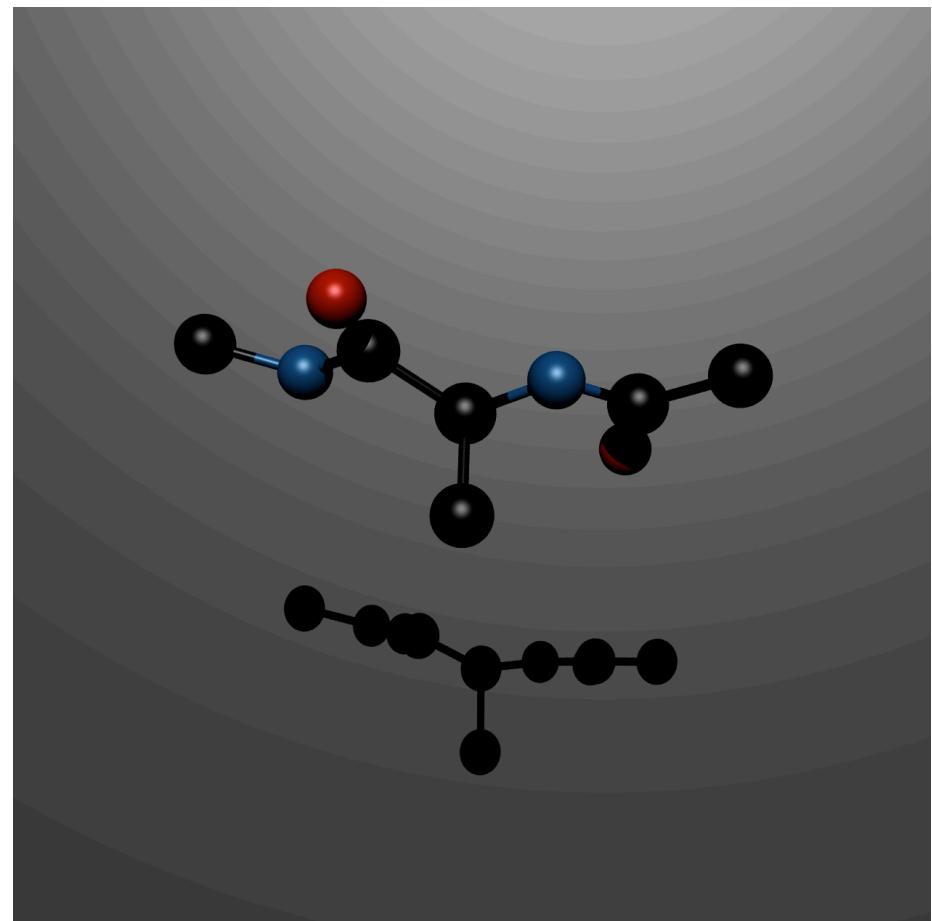


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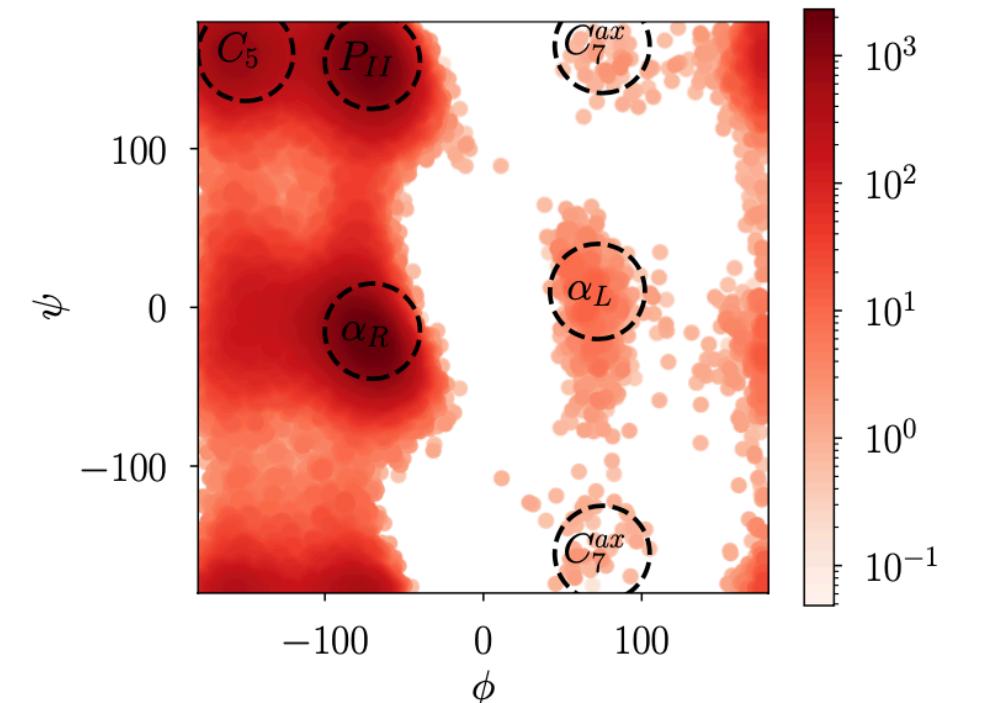


- Alanine dipeptide dynamics in water solved with Molecular Dynamics (MD solver)

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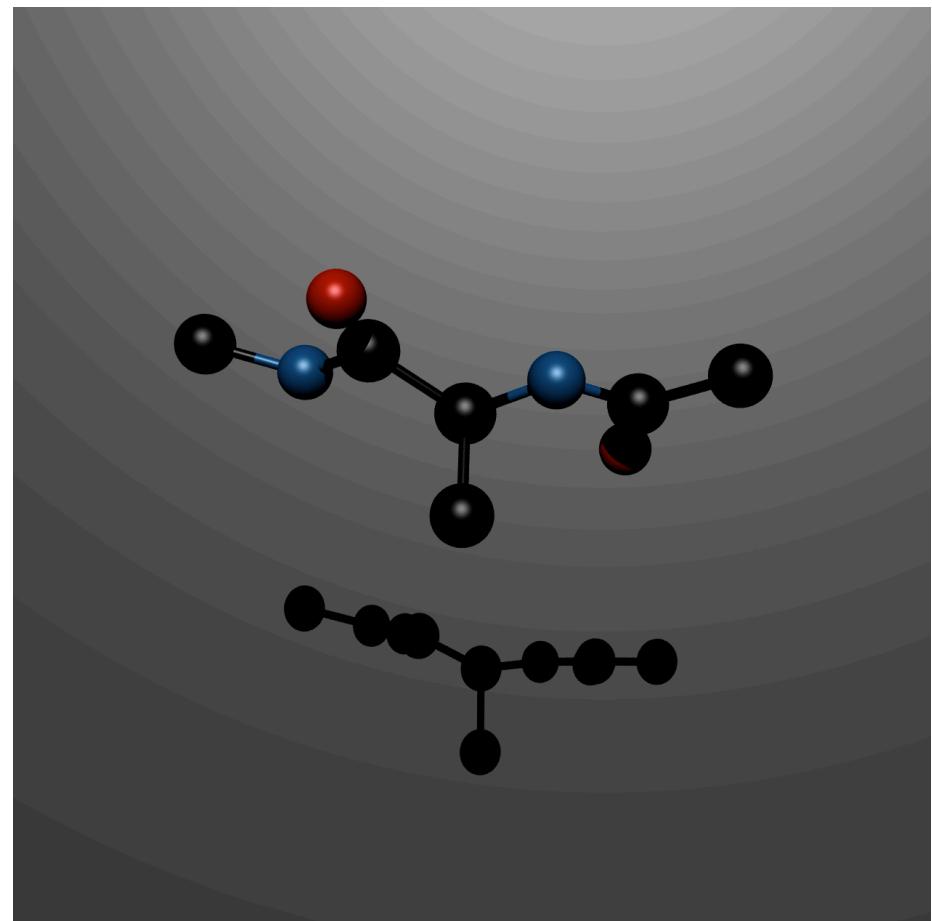


## Reference

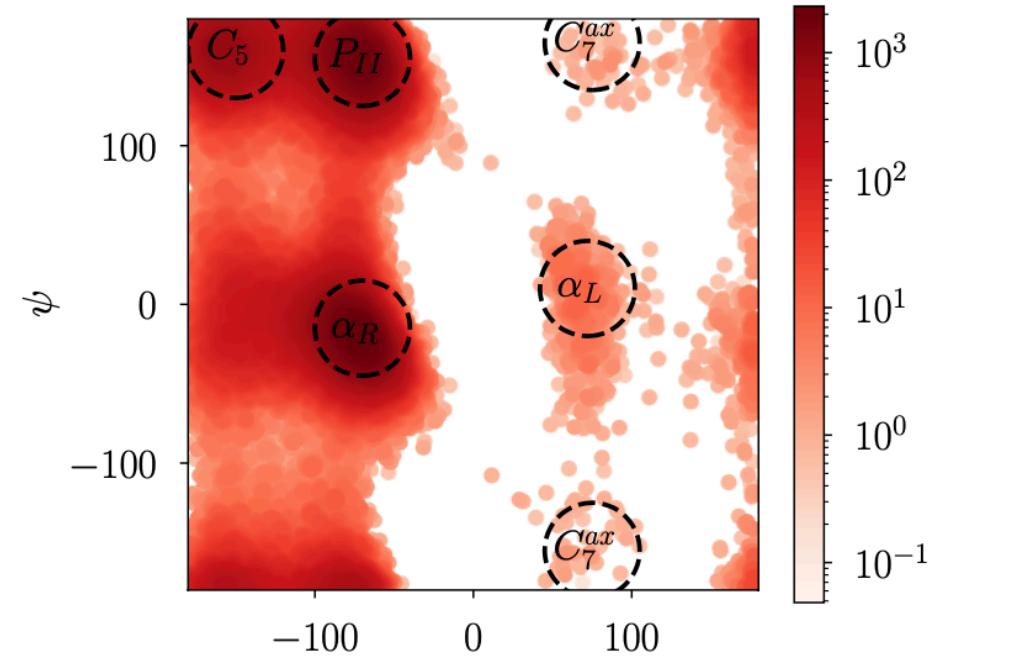


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- Stochastic transitions between **5 meta-stable states**  $\{P_{II}, C_5, \alpha_R, \alpha_L, C_7^{ax}\}$

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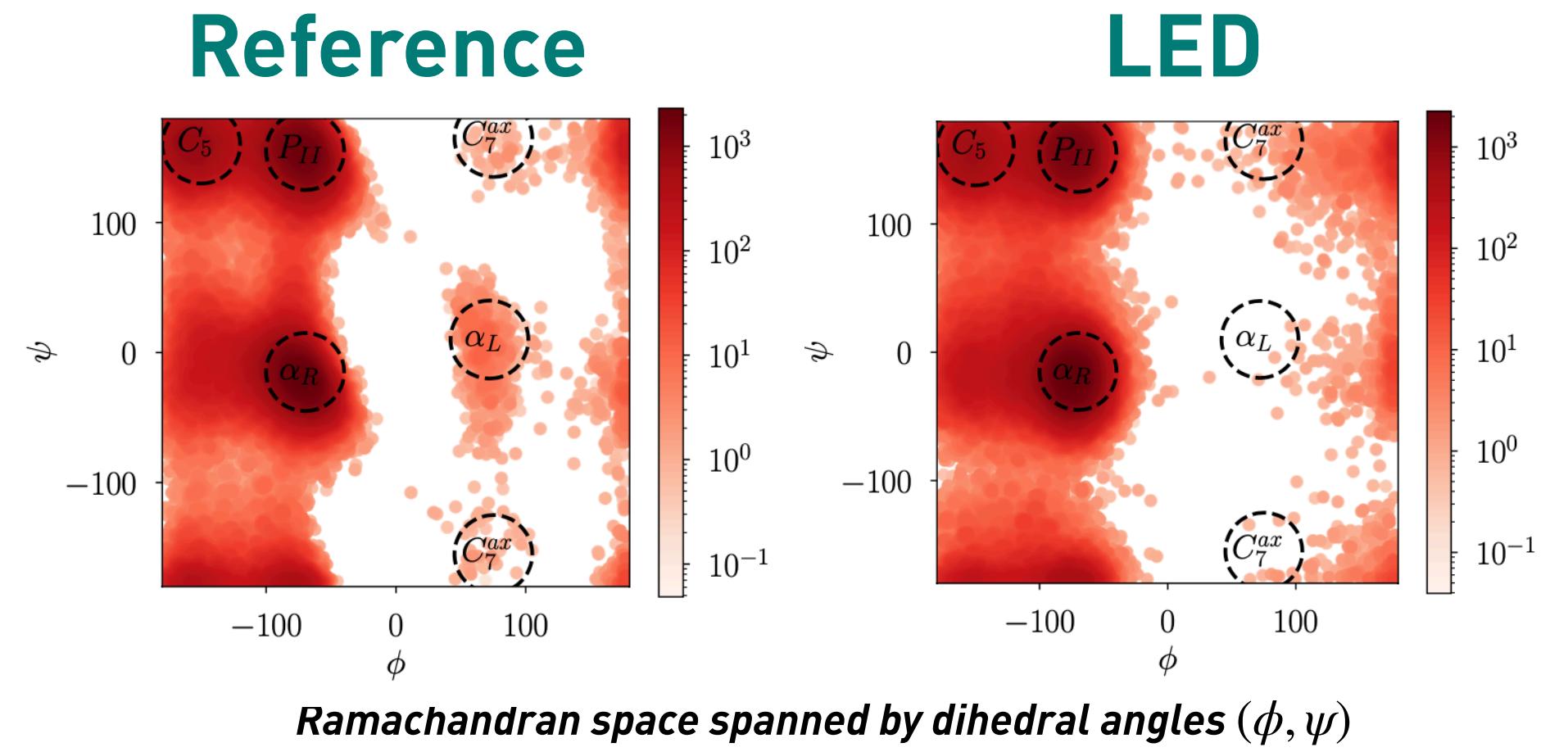
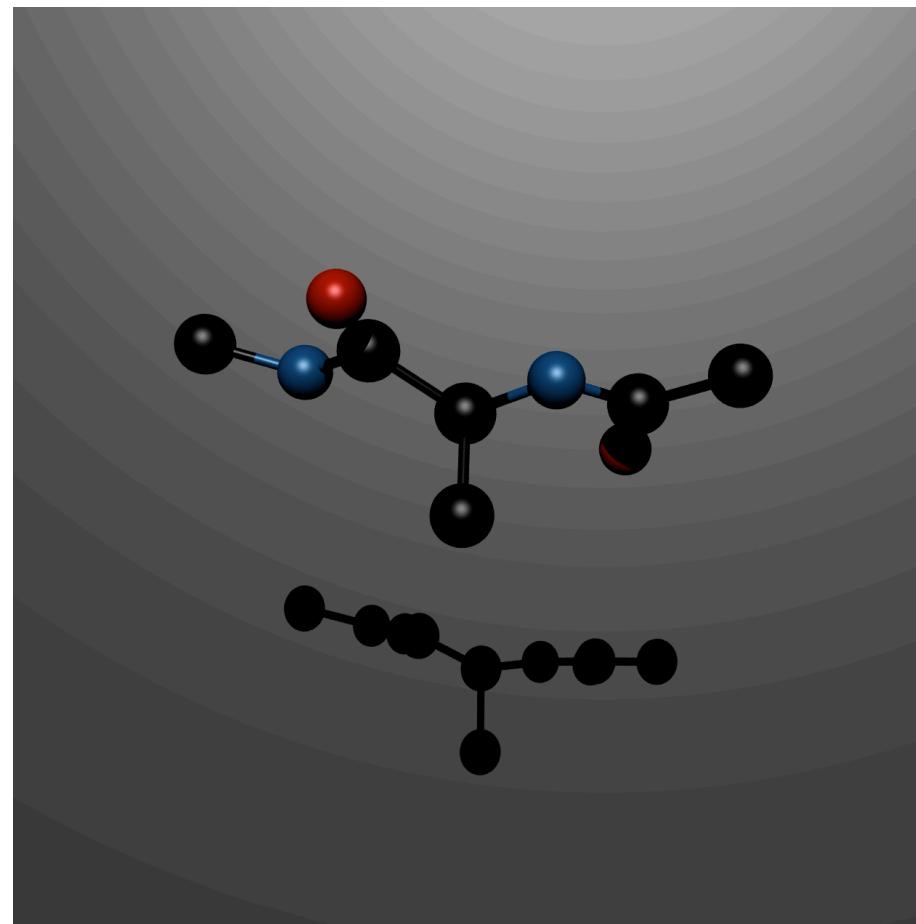
## Reference



Ramachandran space spanned by dihedral angles ( $\phi, \psi$ )

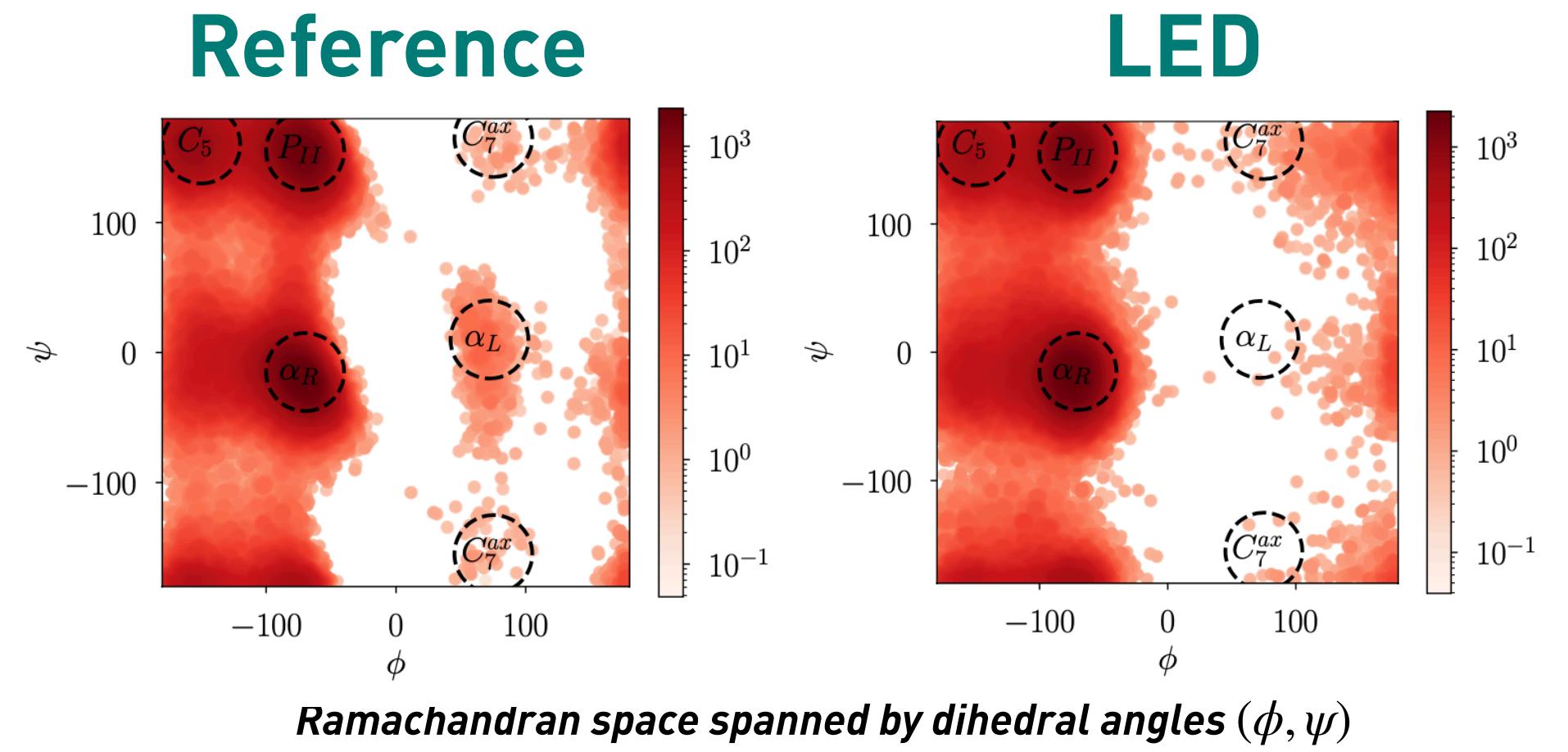
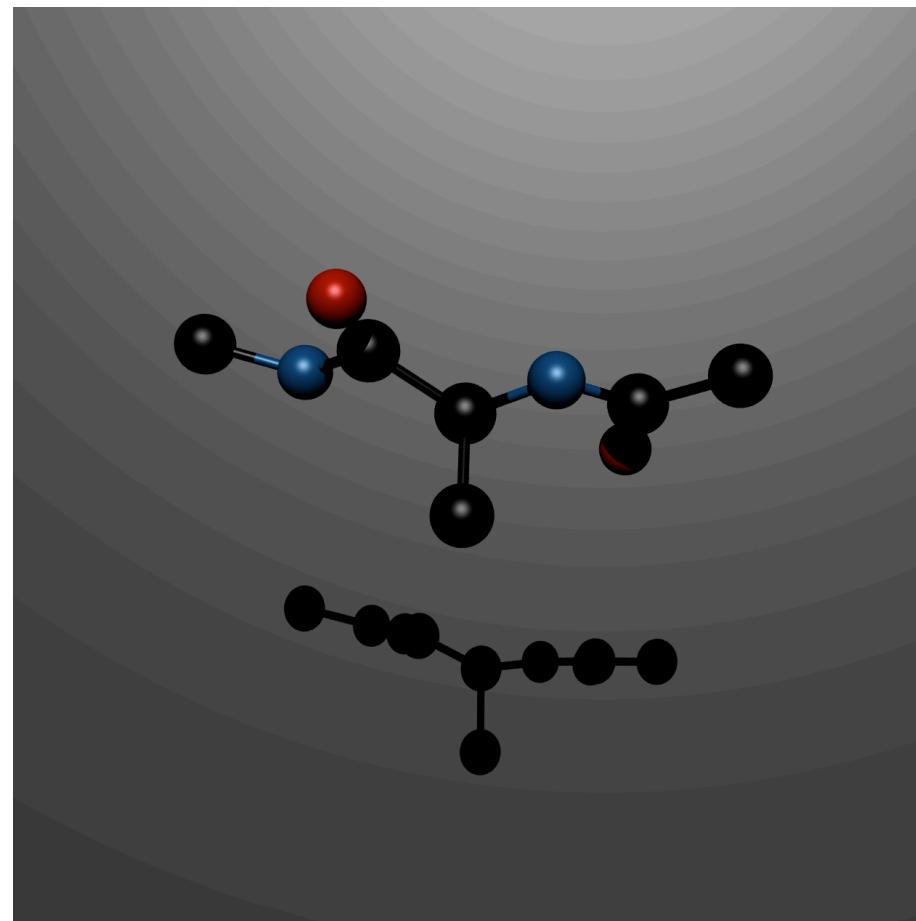
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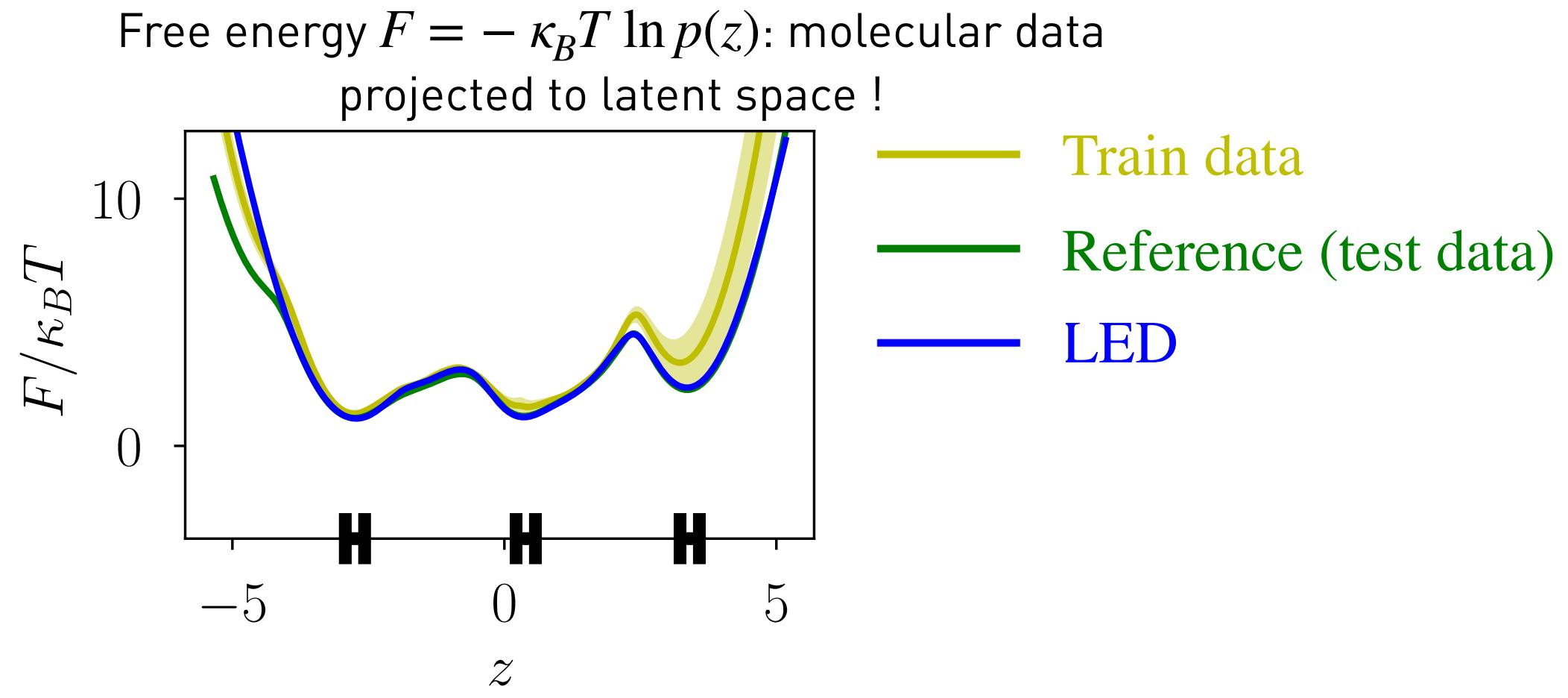
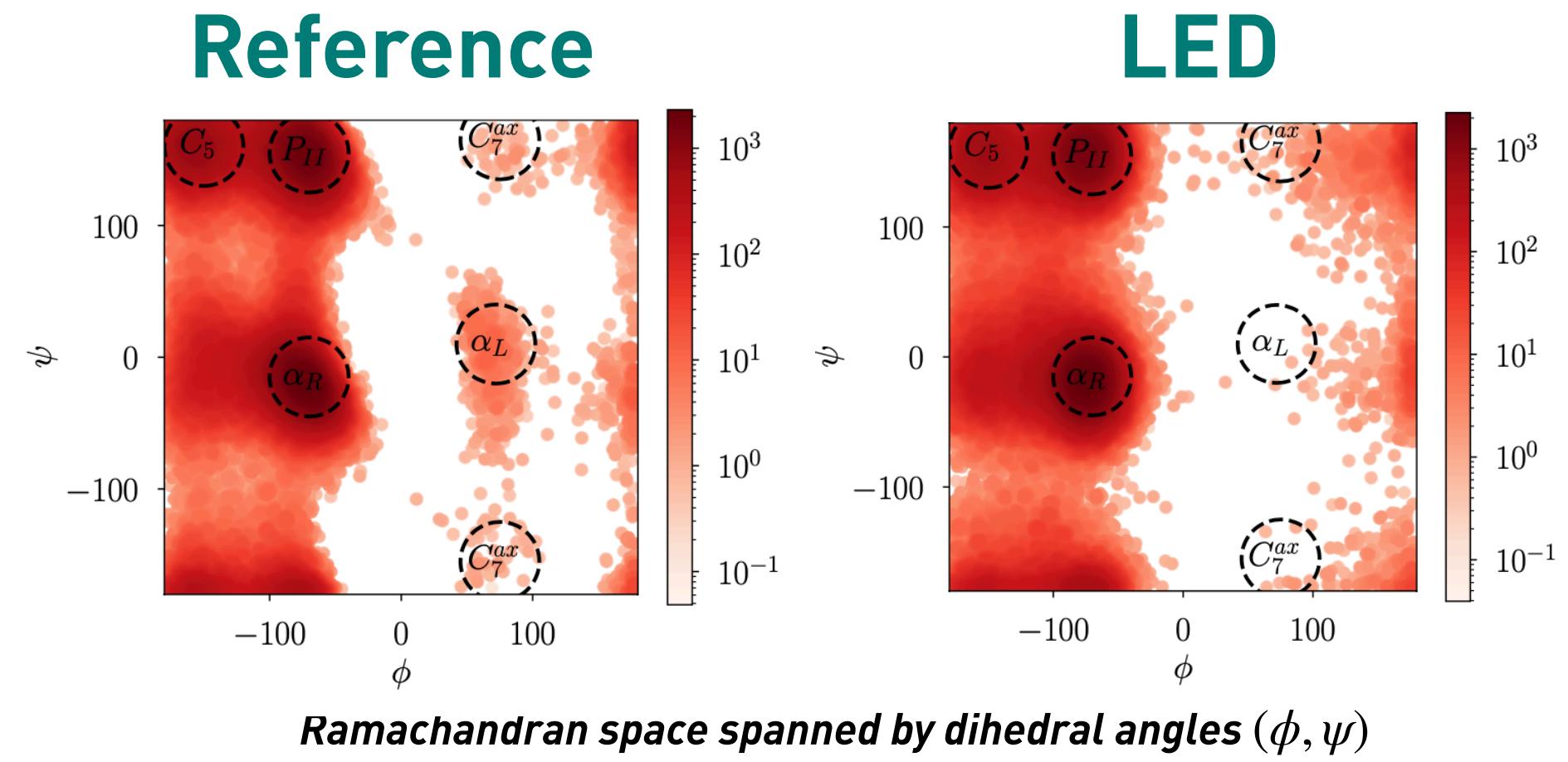
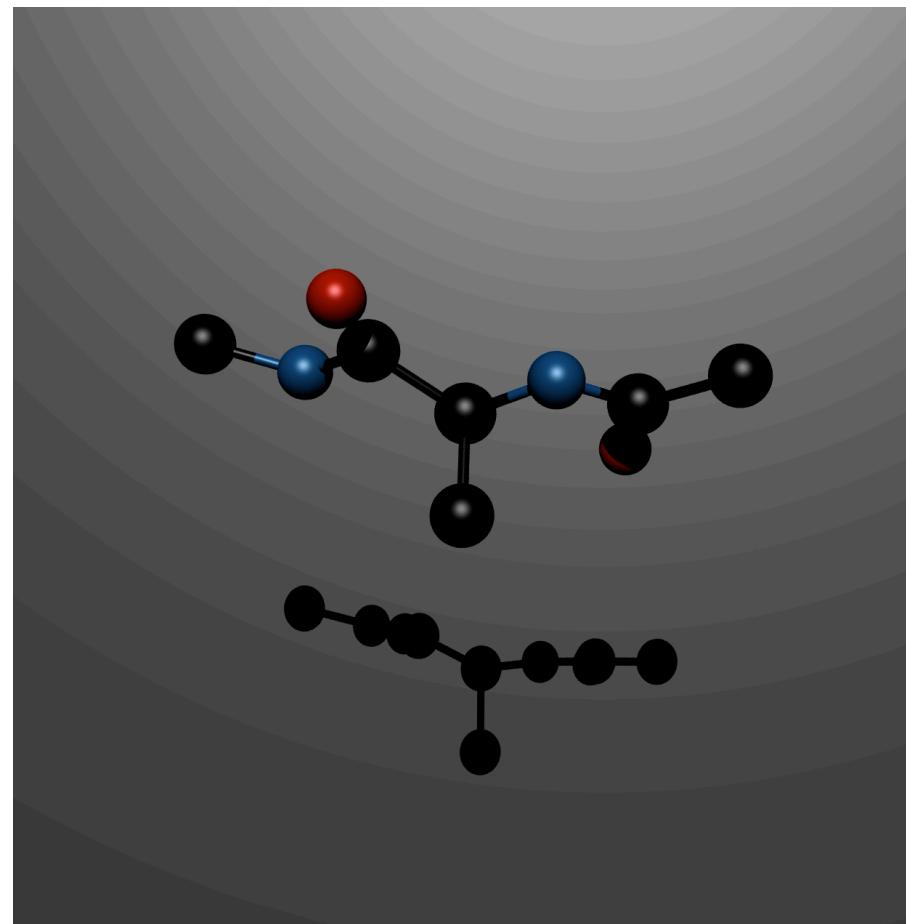
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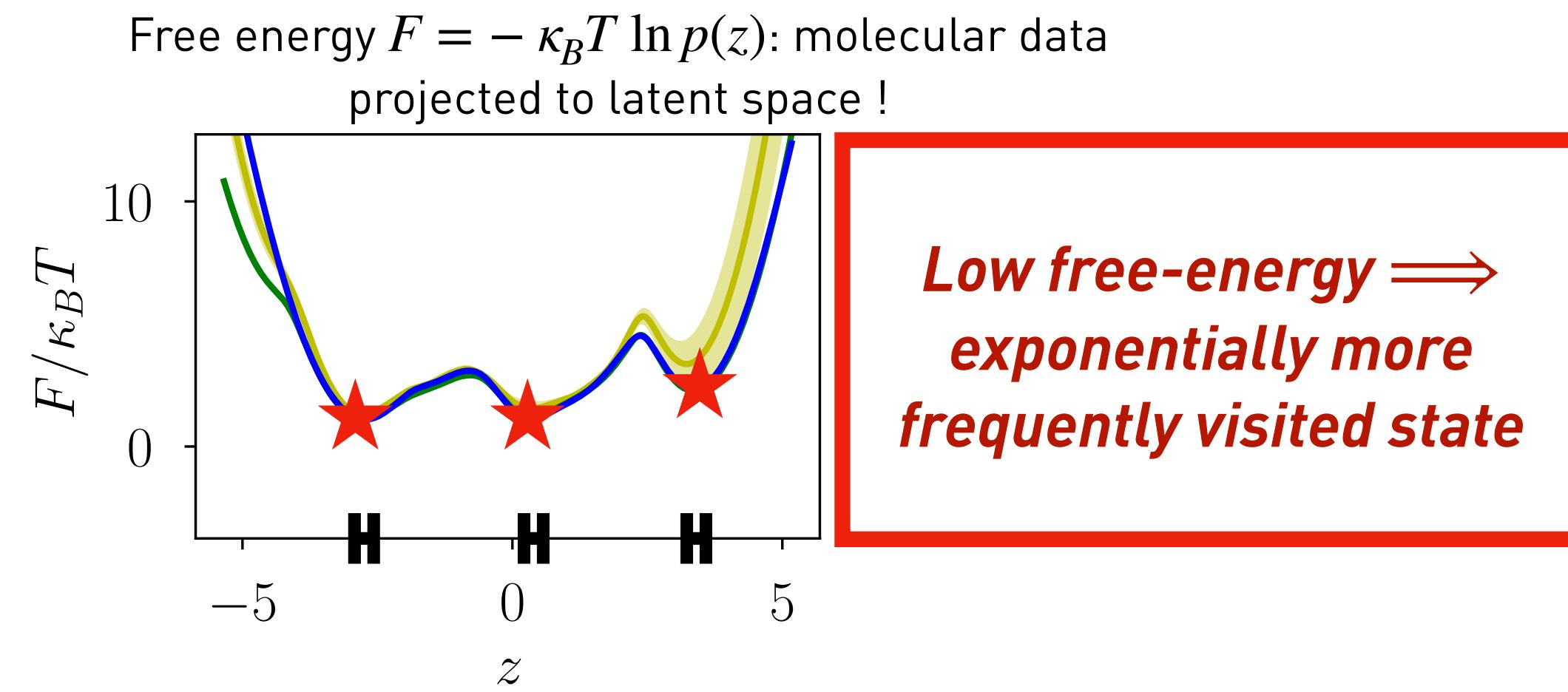
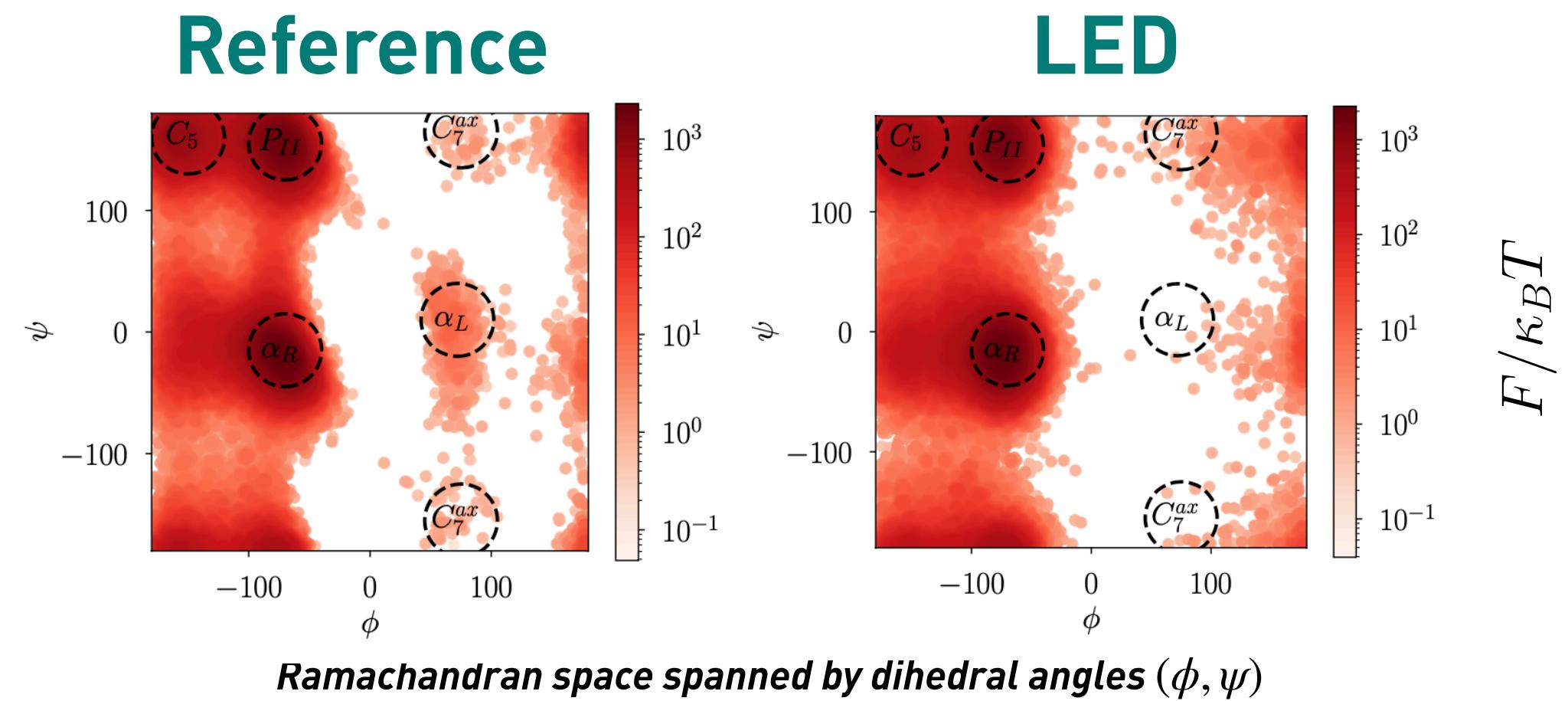
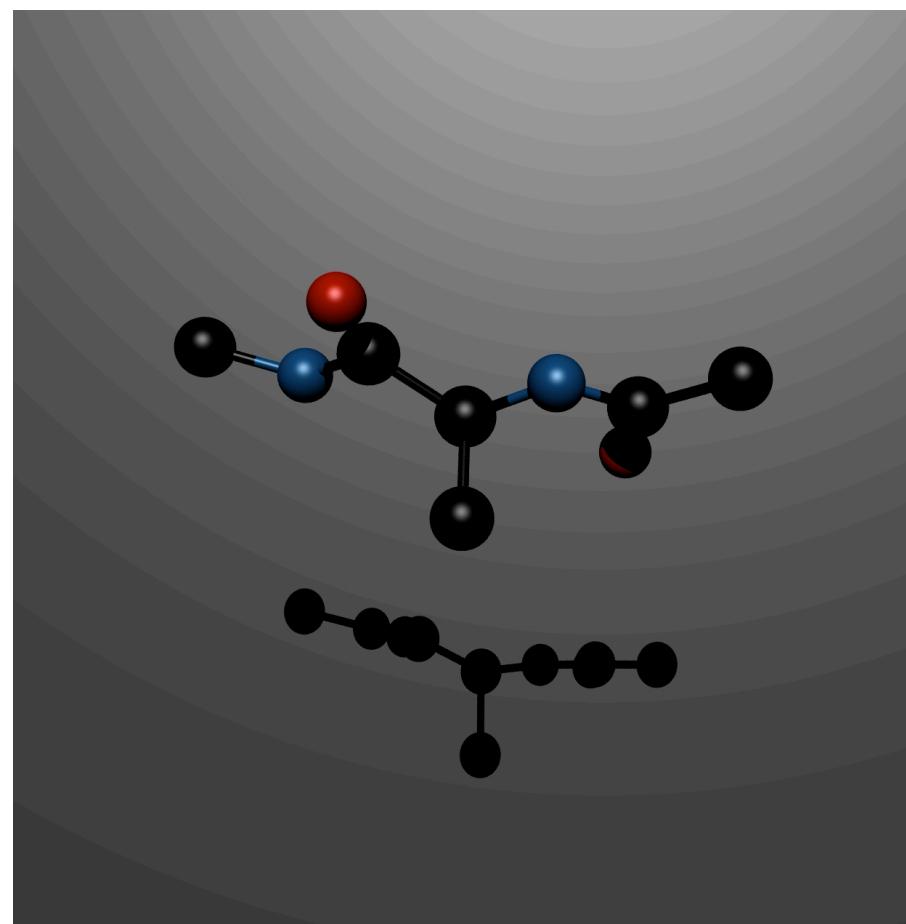
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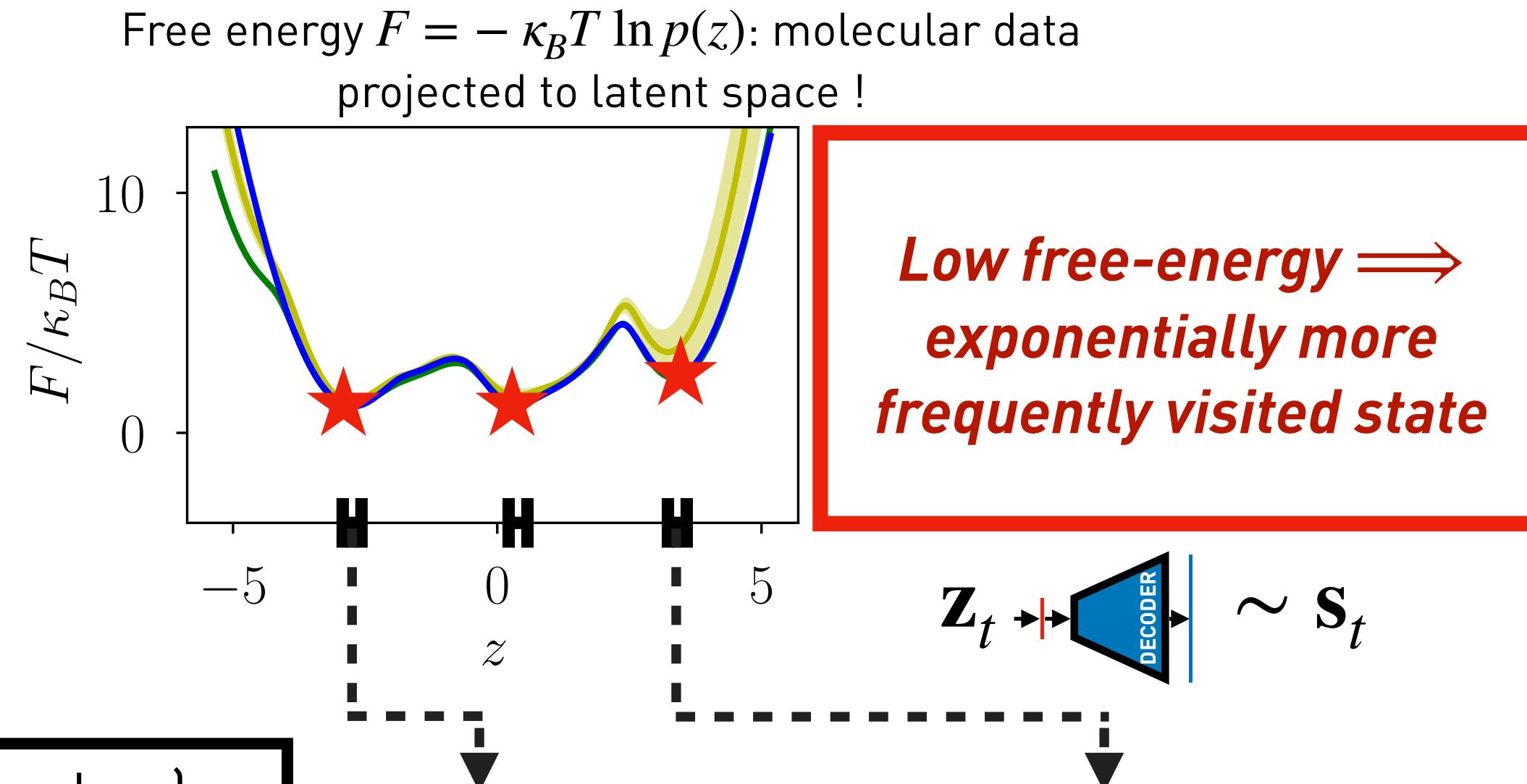
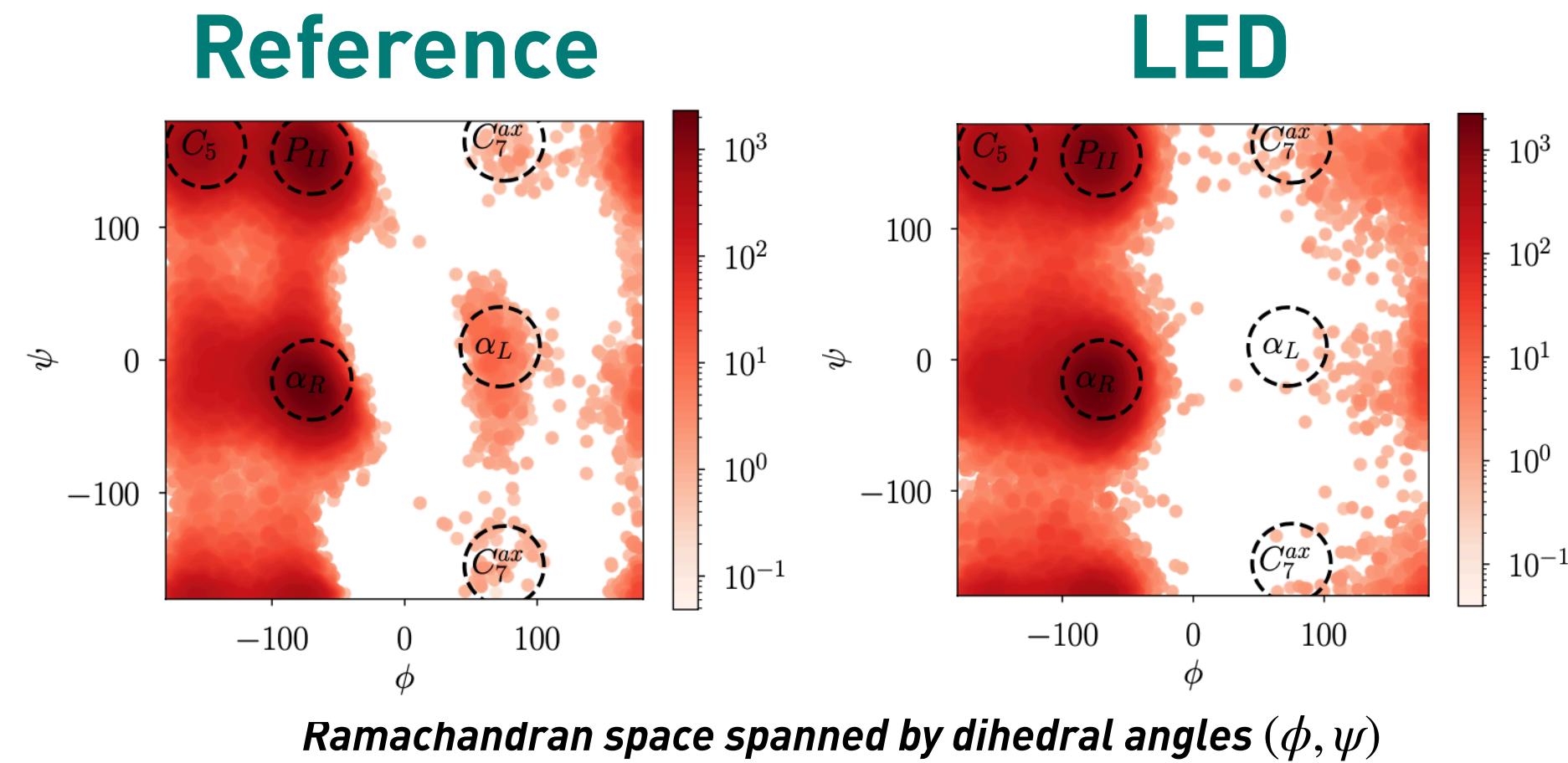
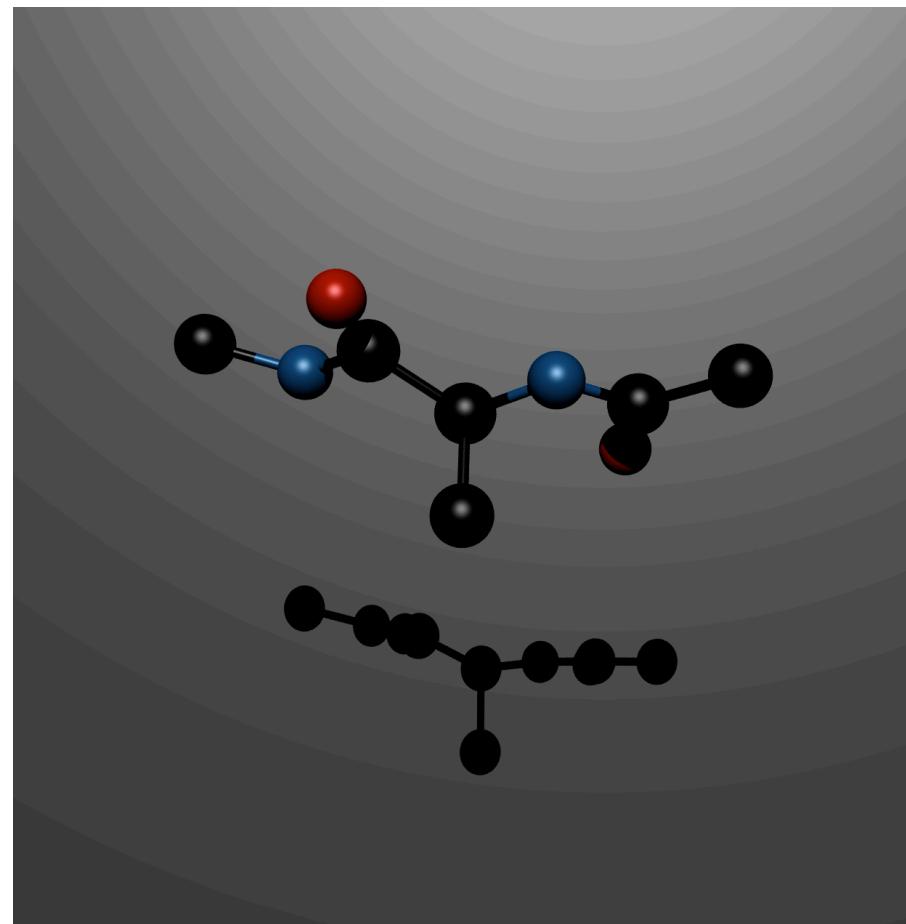
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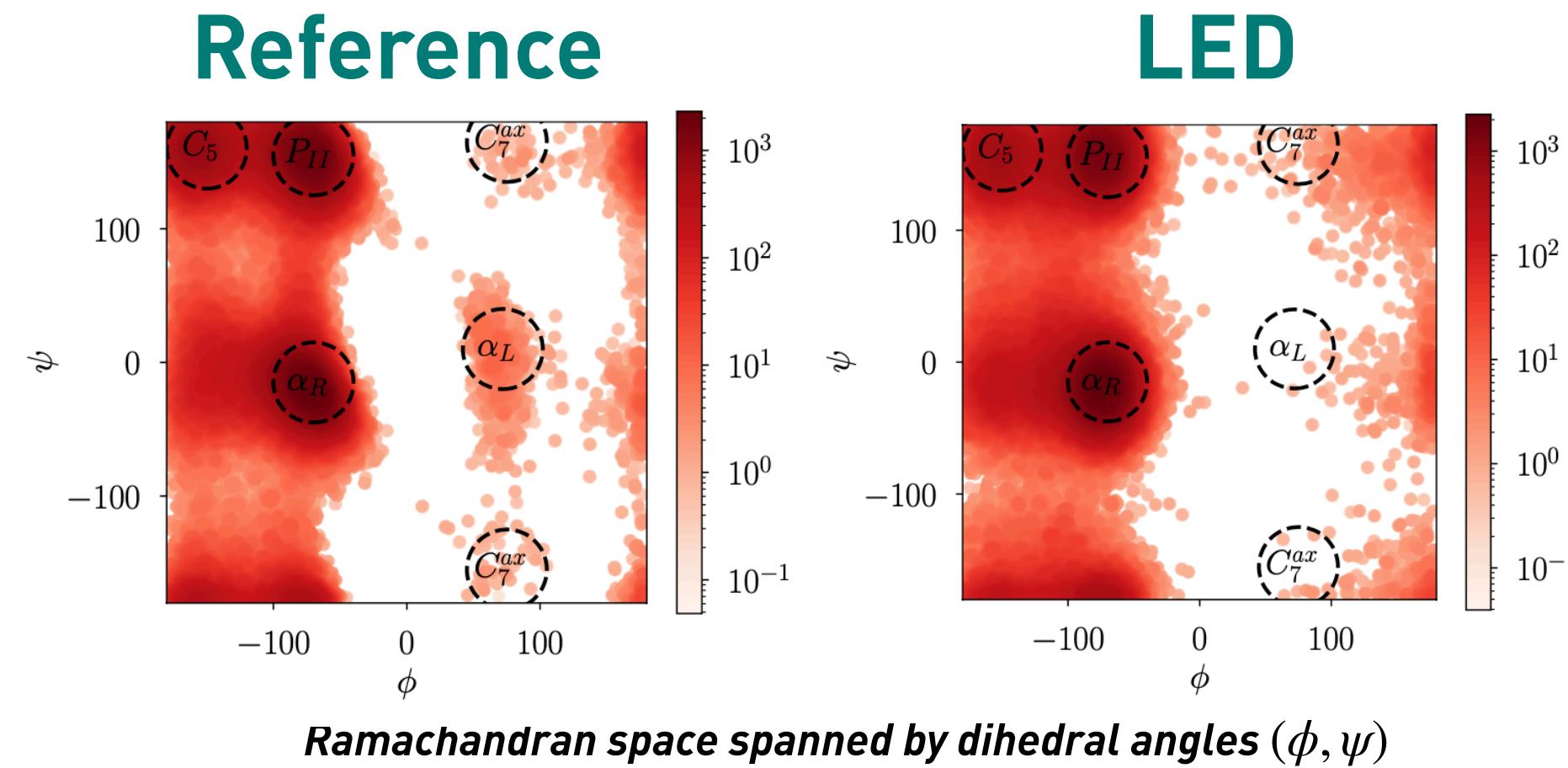
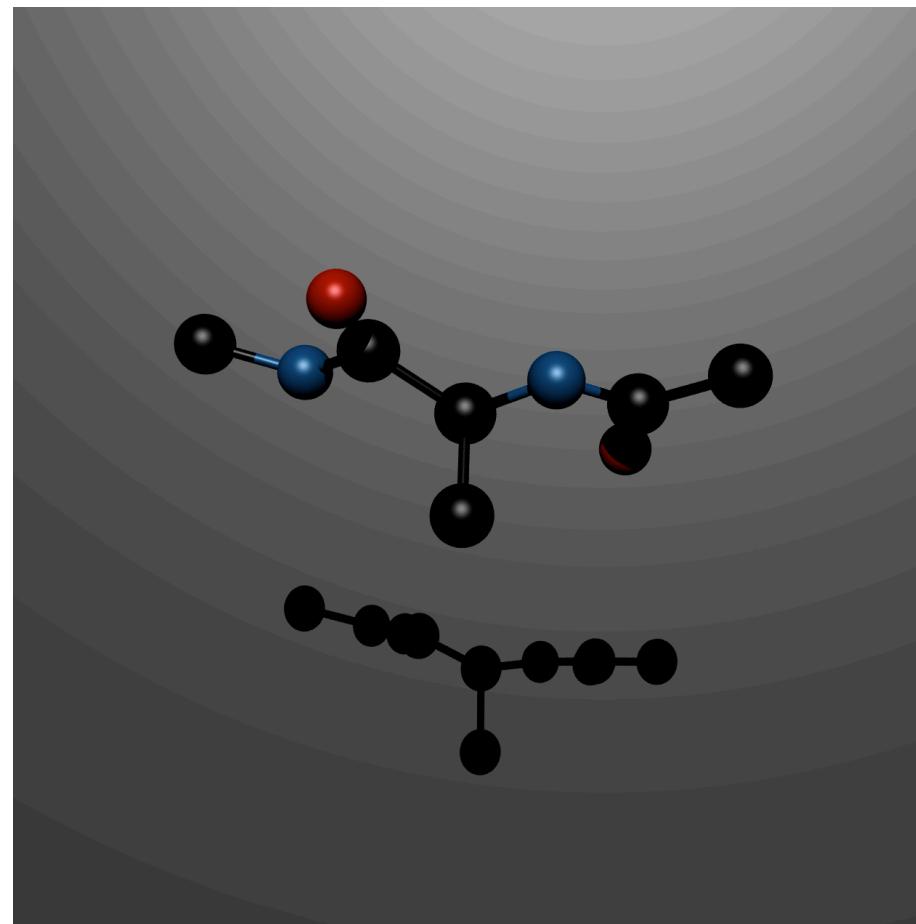
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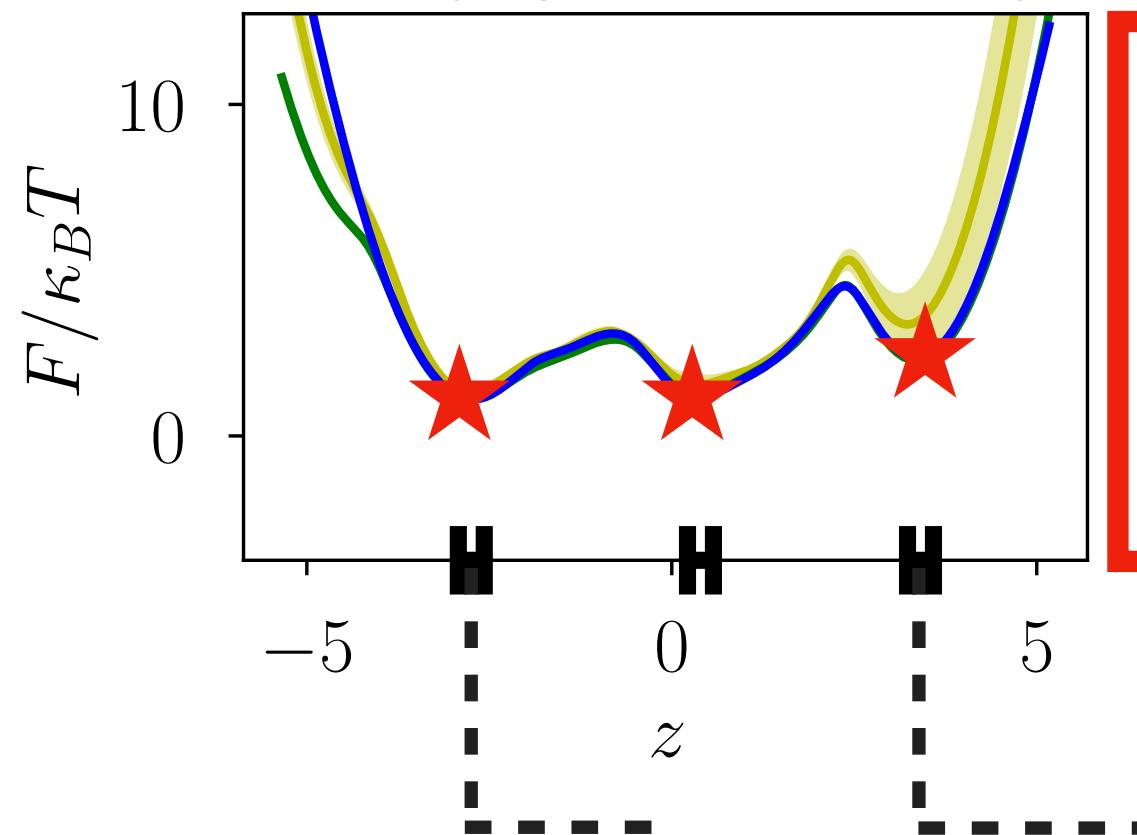


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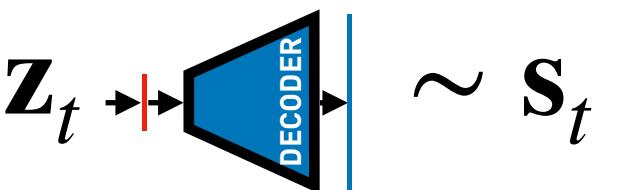
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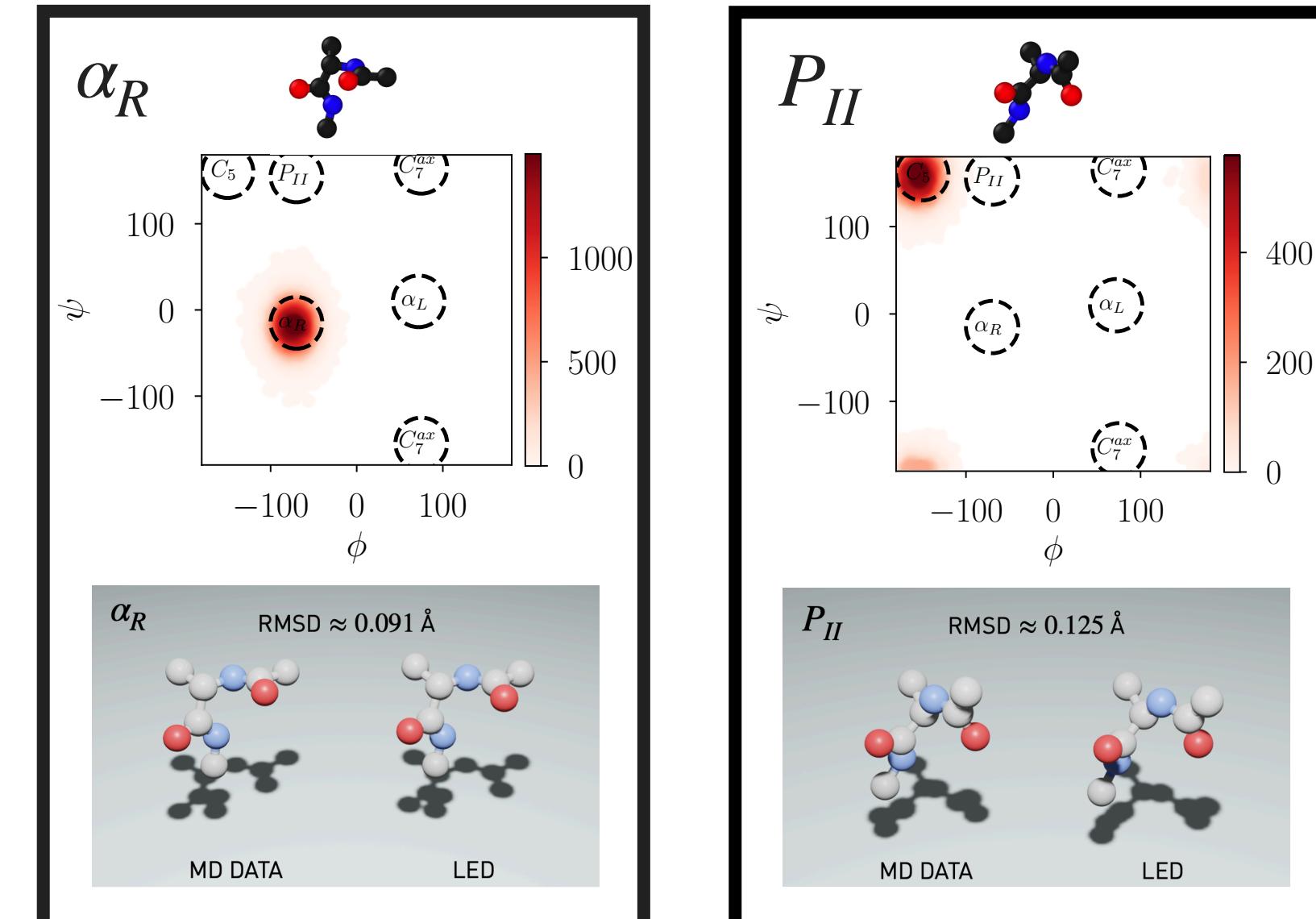
Free energy  $F = -\kappa_B T \ln p(z)$ : molecular data projected to latent space !



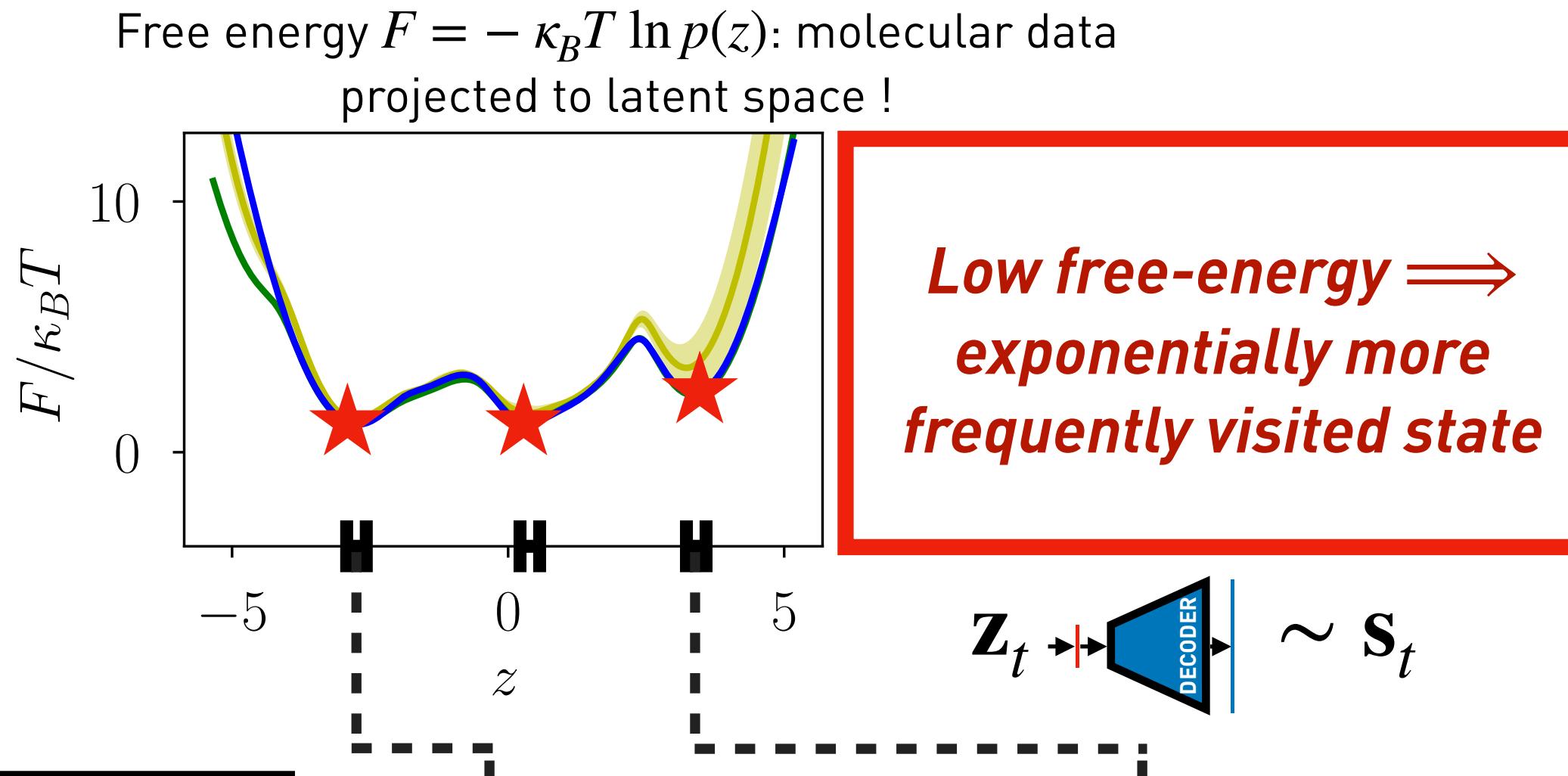
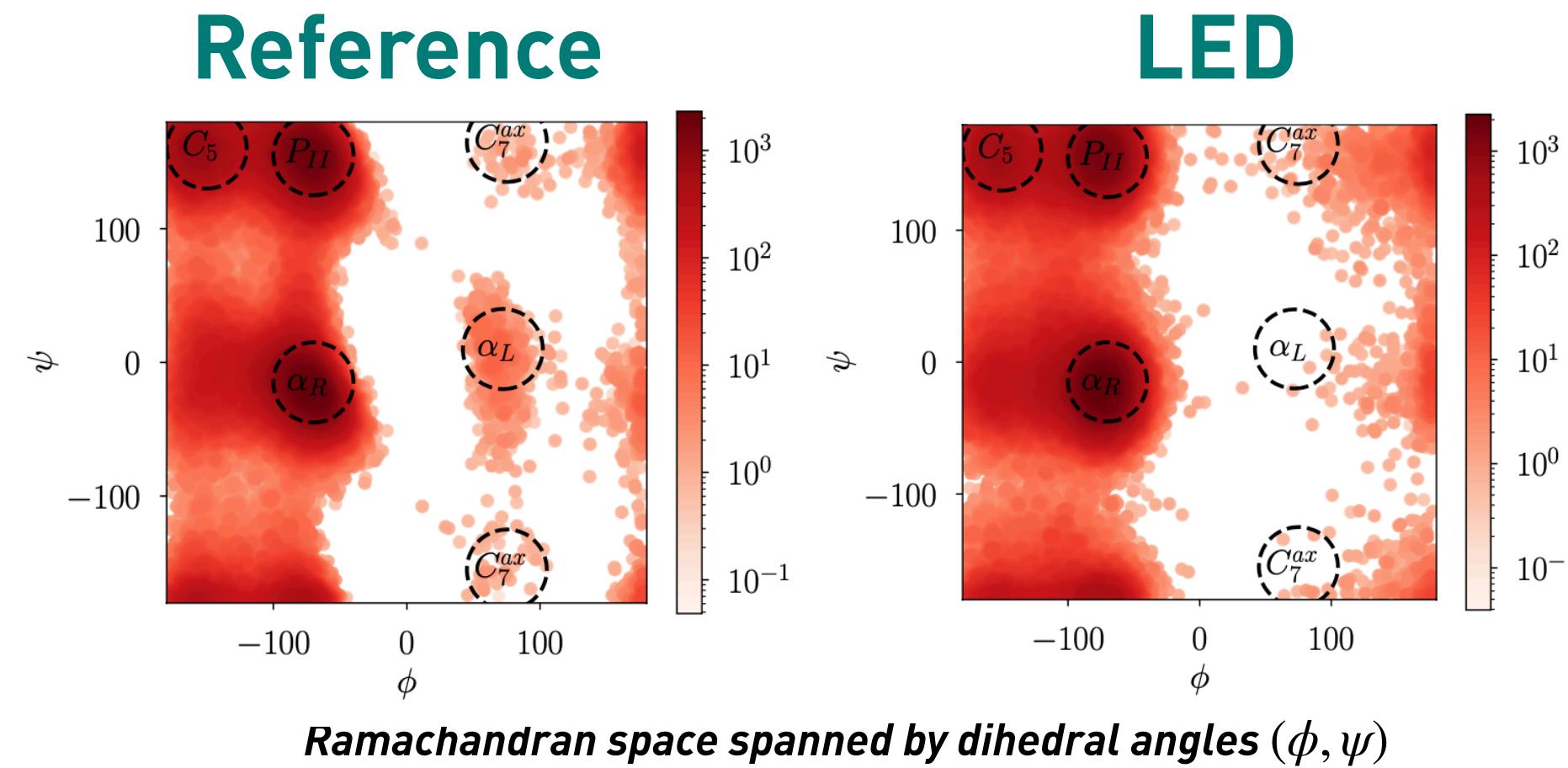
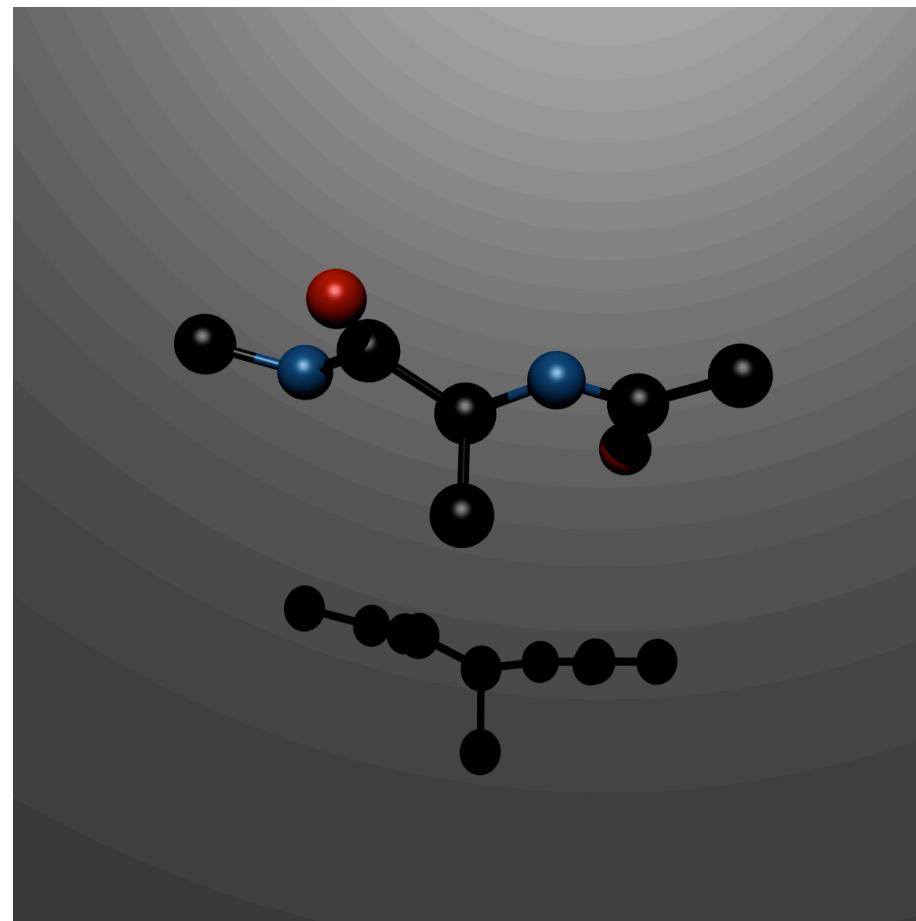
**Low free-energy  $\Rightarrow$  exponentially more frequently visited state**



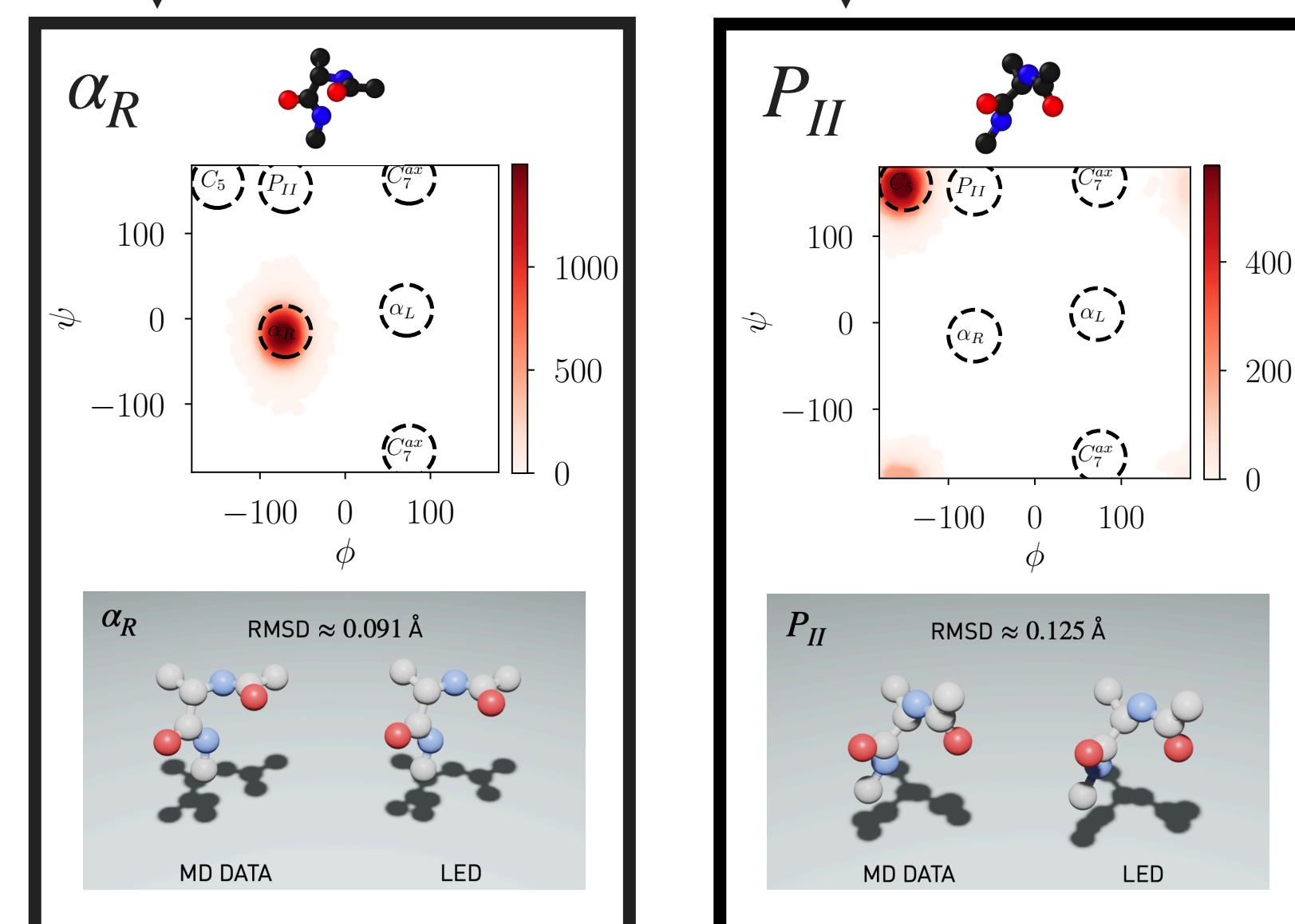
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  - reproduces coarsely the statistics
  - reproduces kinetics, and mean transition times
  - free energy profile **minima** are mapped to configurations of meta stable states



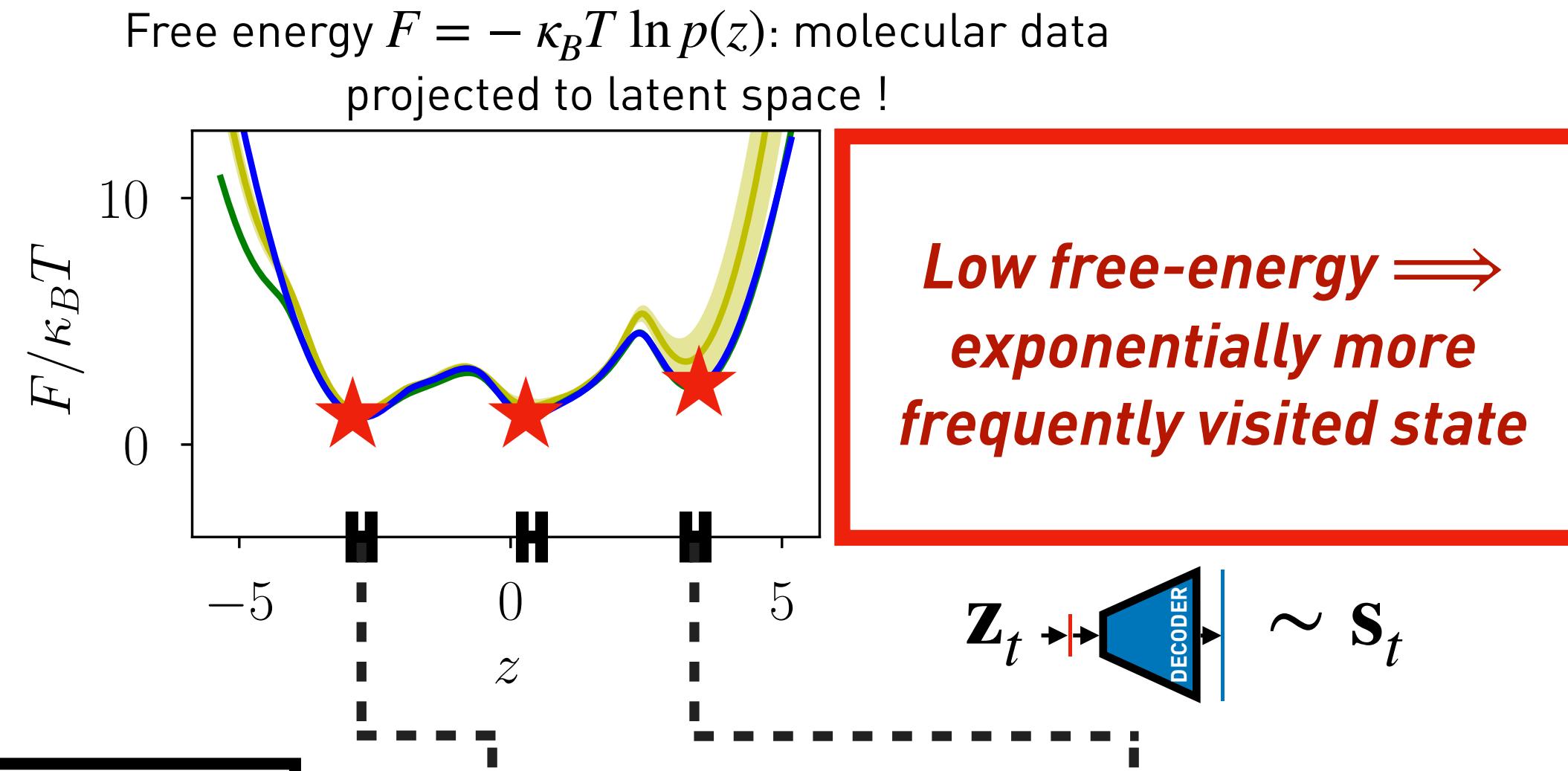
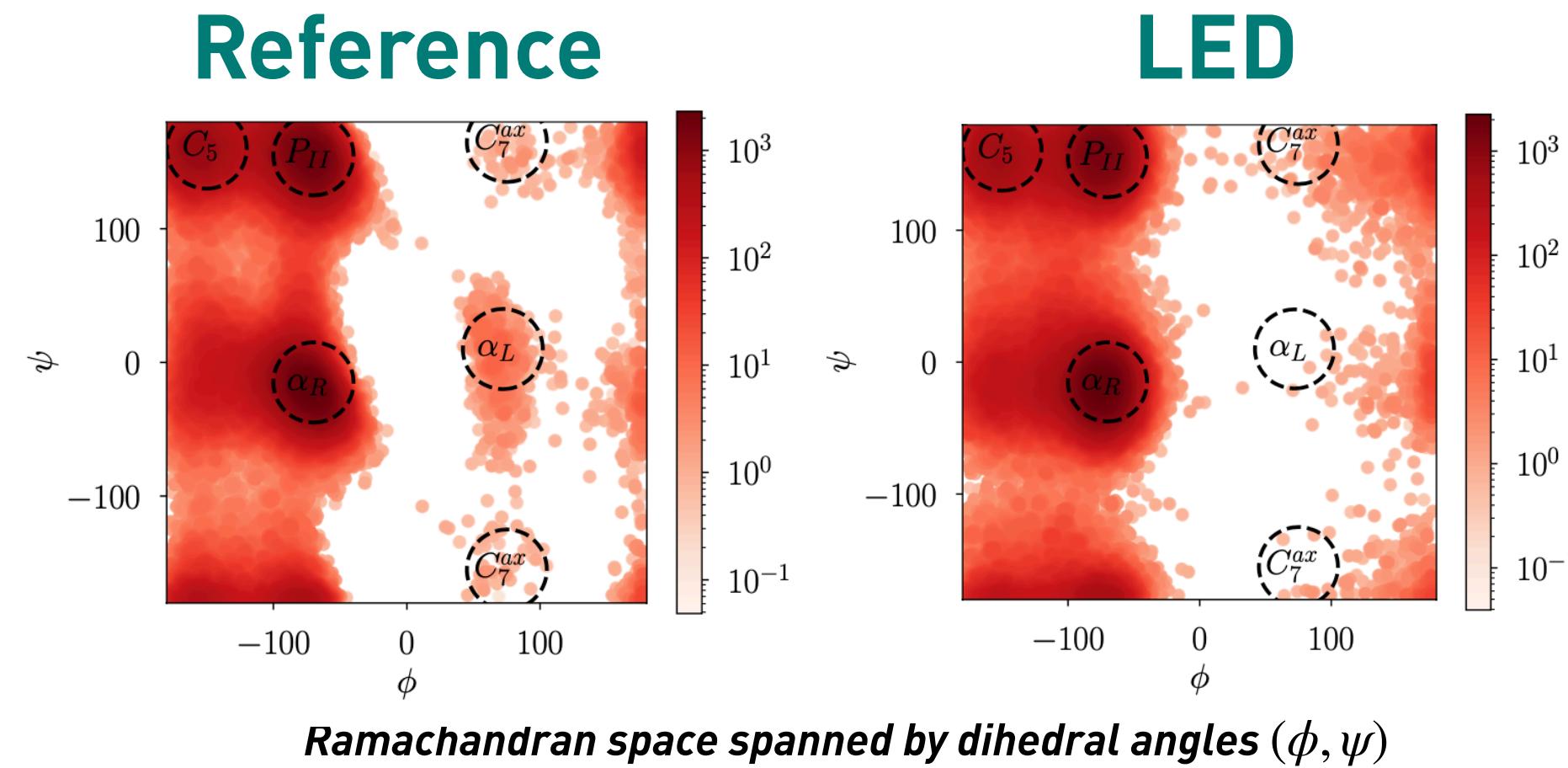
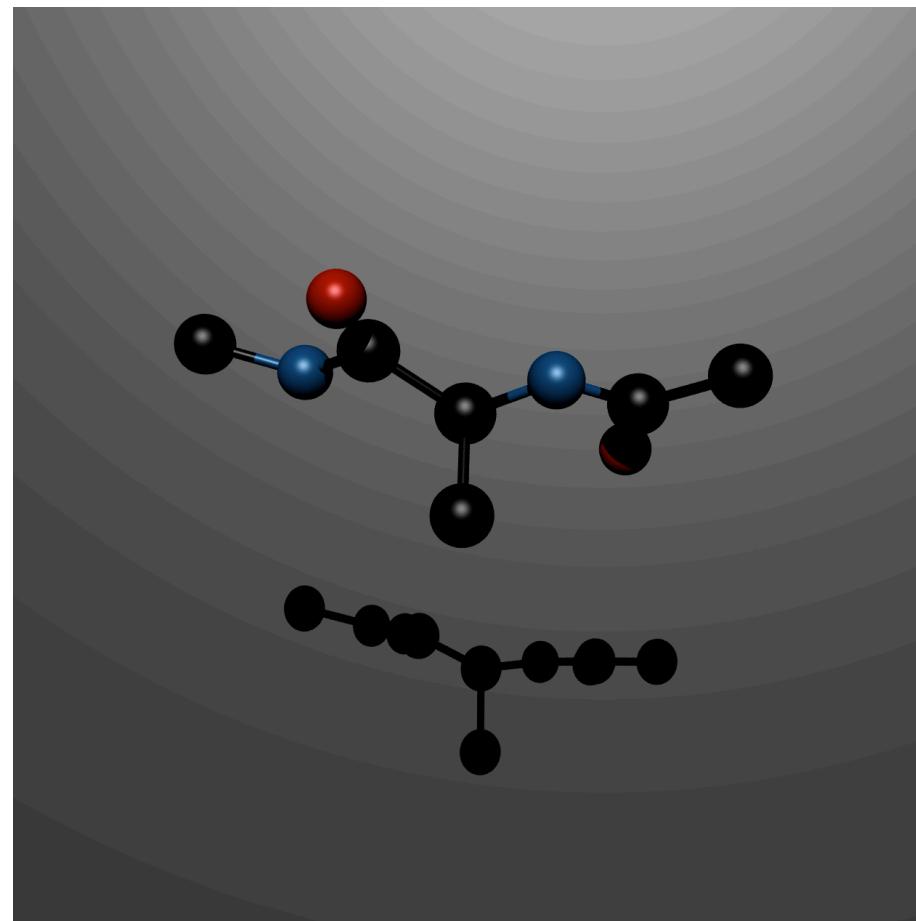
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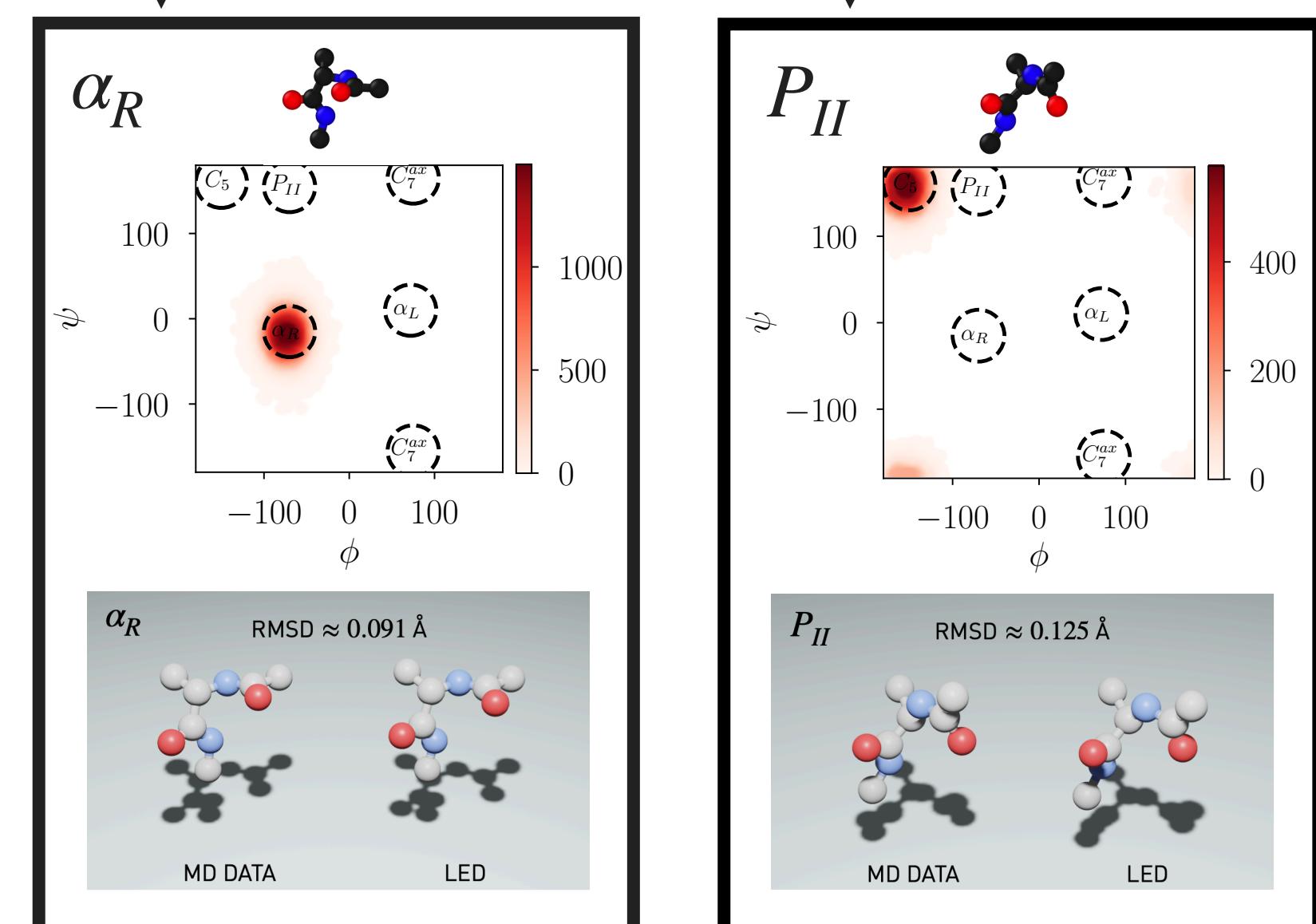
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- LED is at least **three orders faster (x1000)** than MD solver



# Avenues for Future Research

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  - AdaLED on real world experiments (challenge: how to reinitialise experiment from micro-scale)

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Ivica Kičić

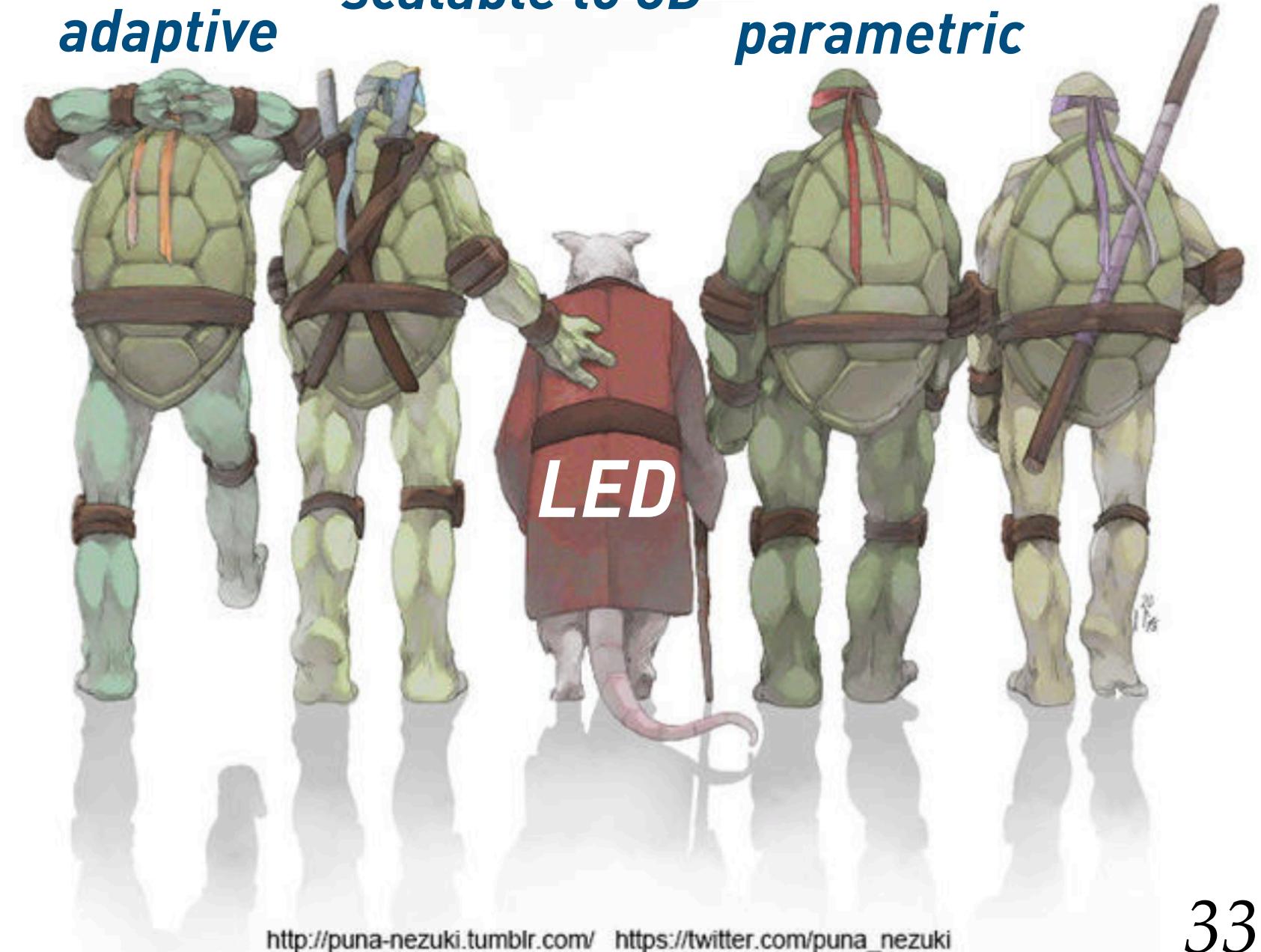
George Arampatzis

**AdaLED**

scalable to 3D

parametric

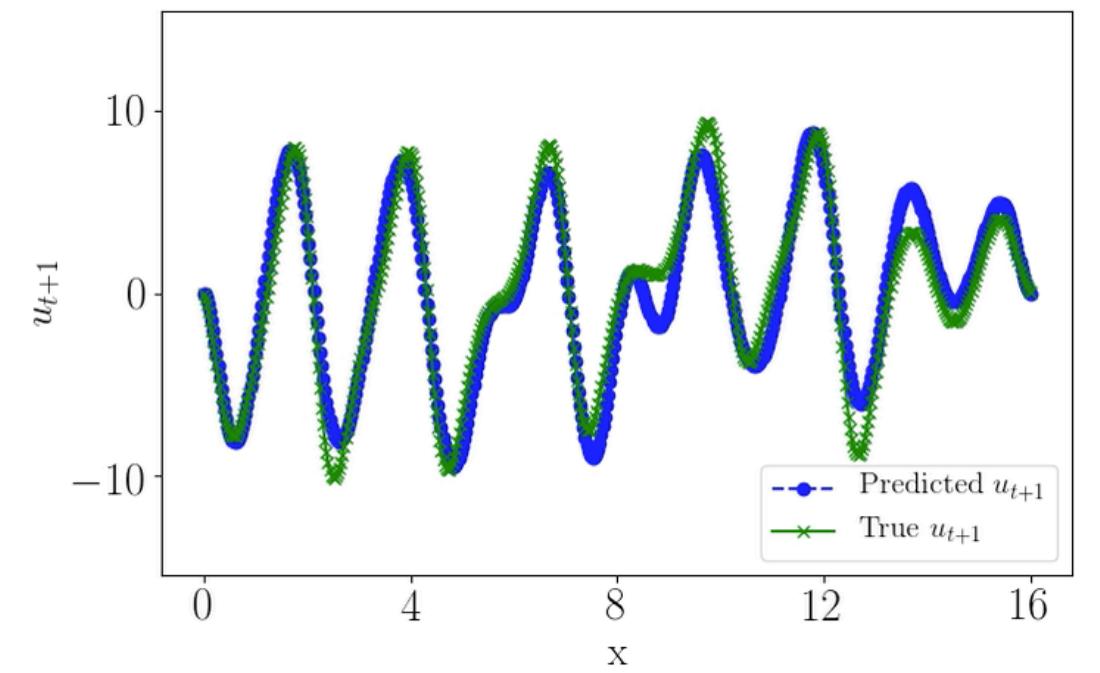
uncertainty  
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## HYBRID LSTM - MSM

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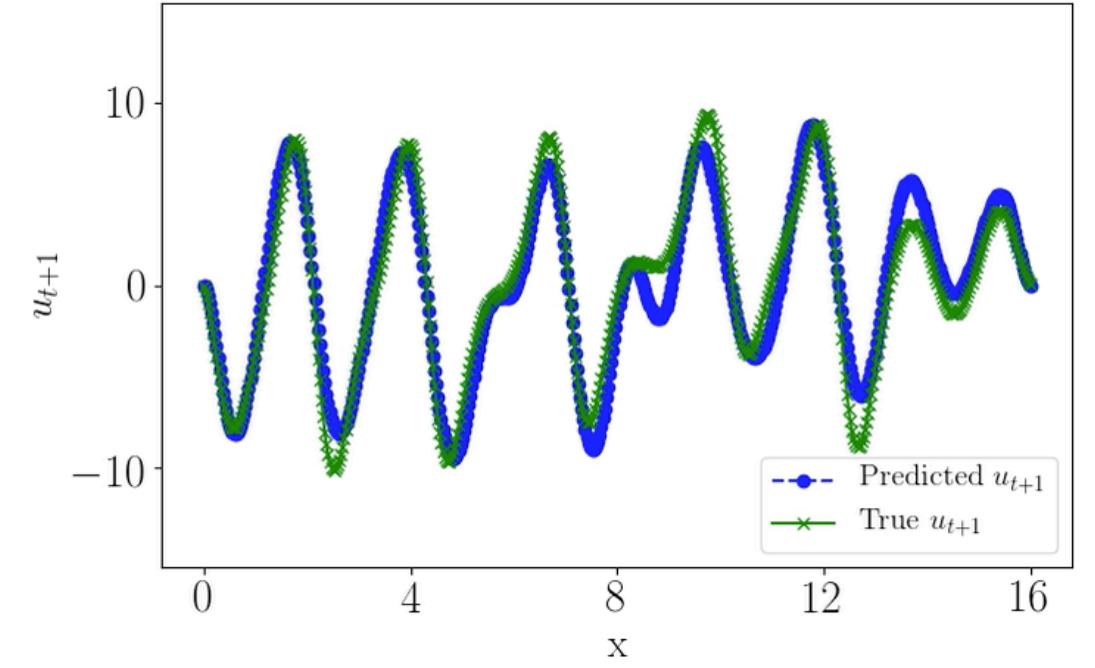


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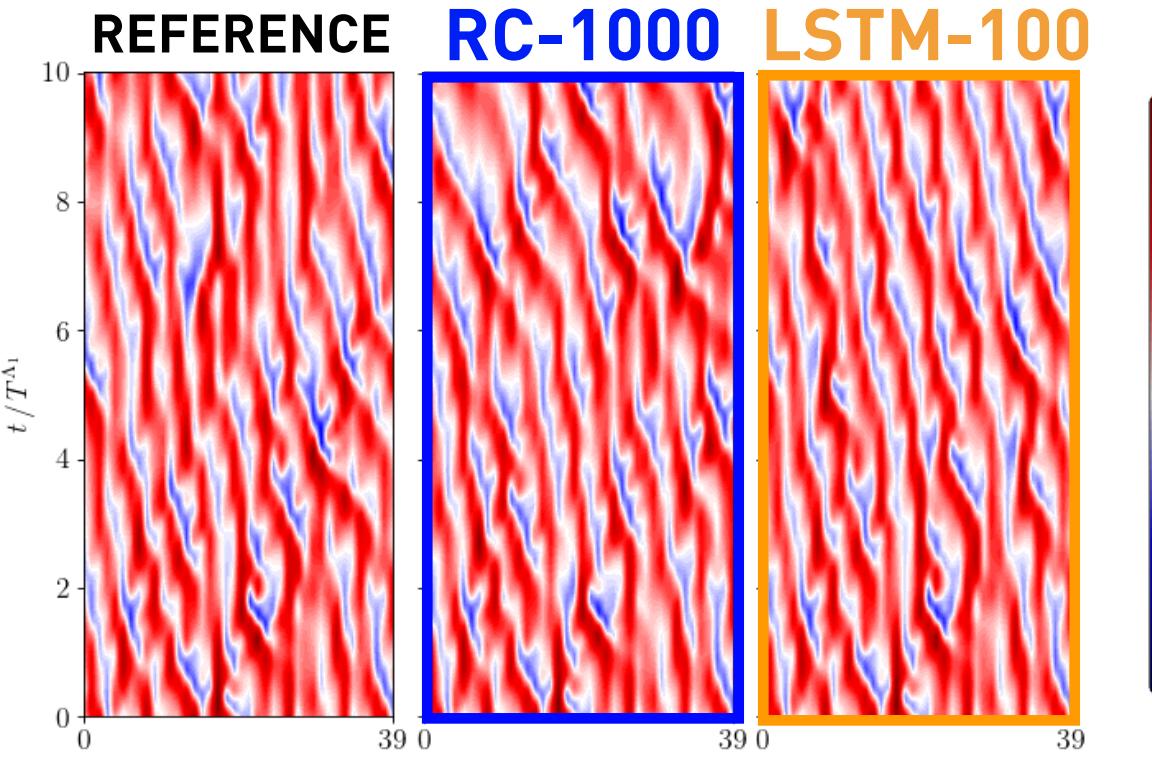
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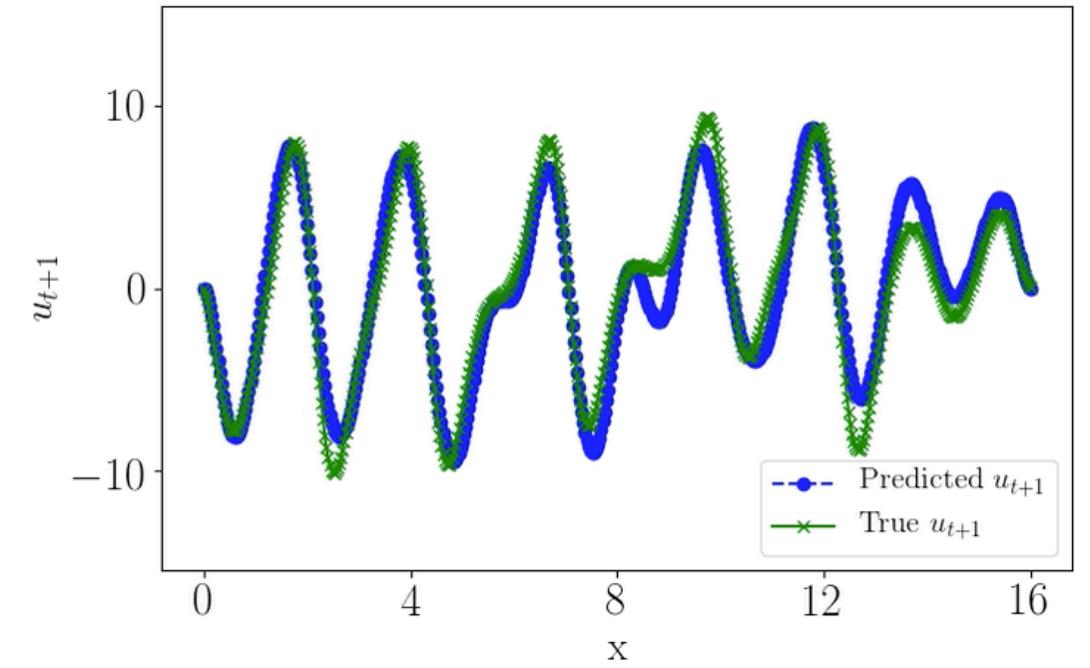
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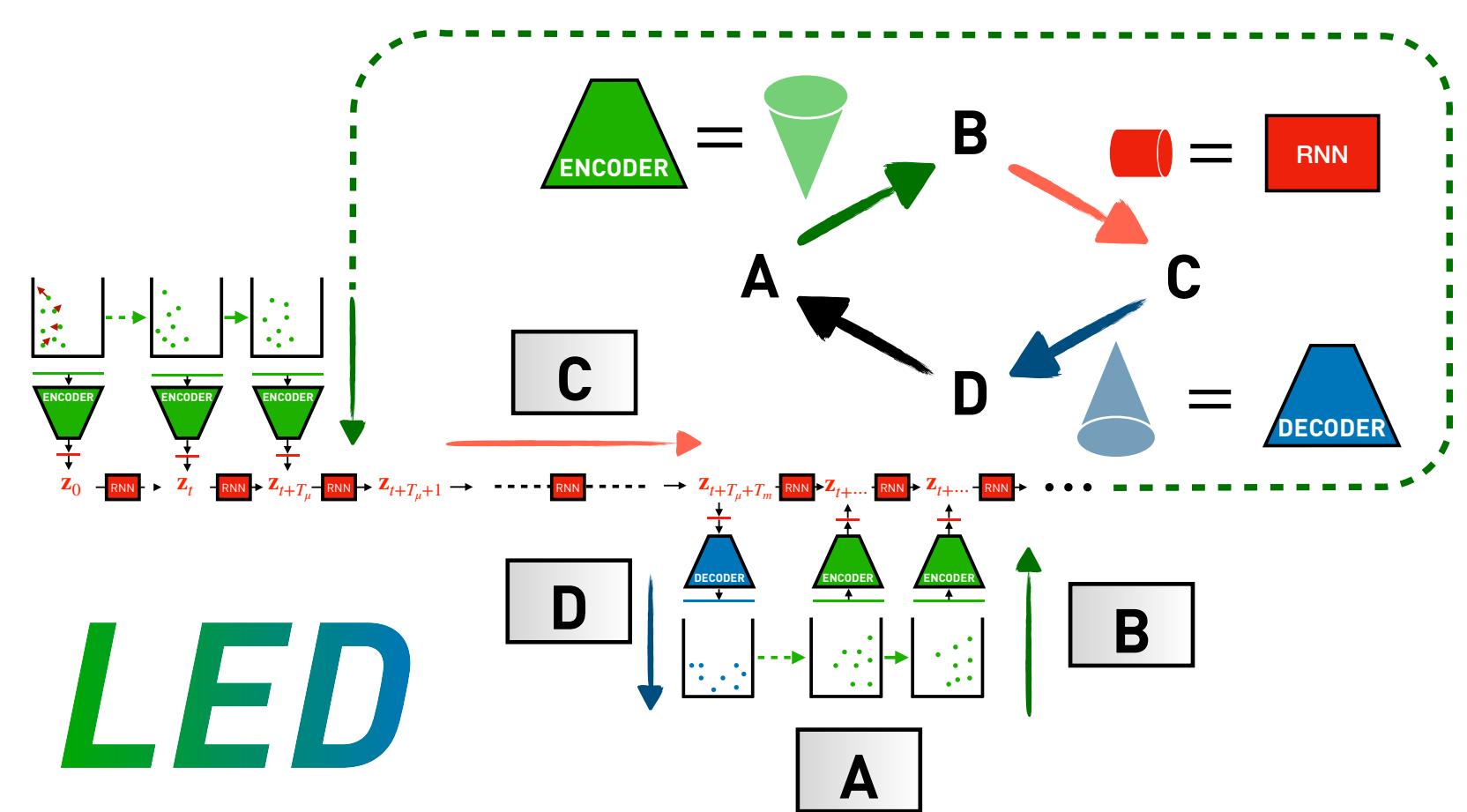
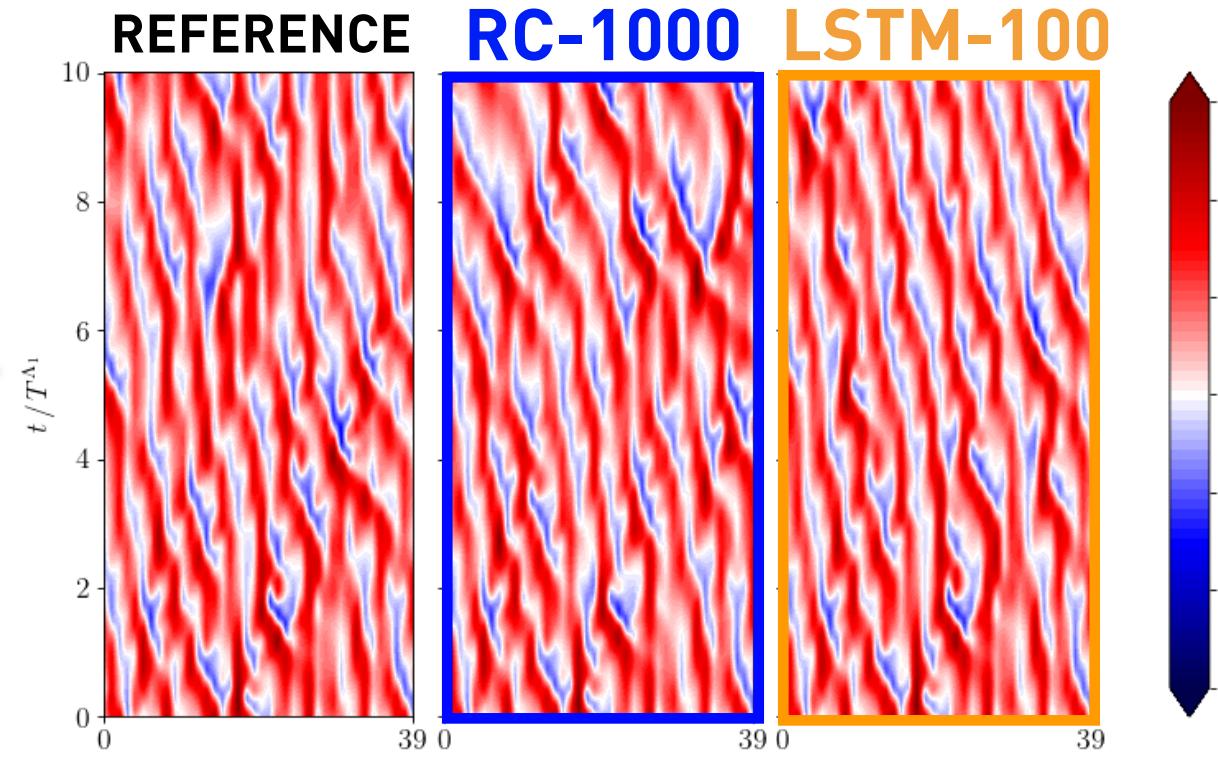
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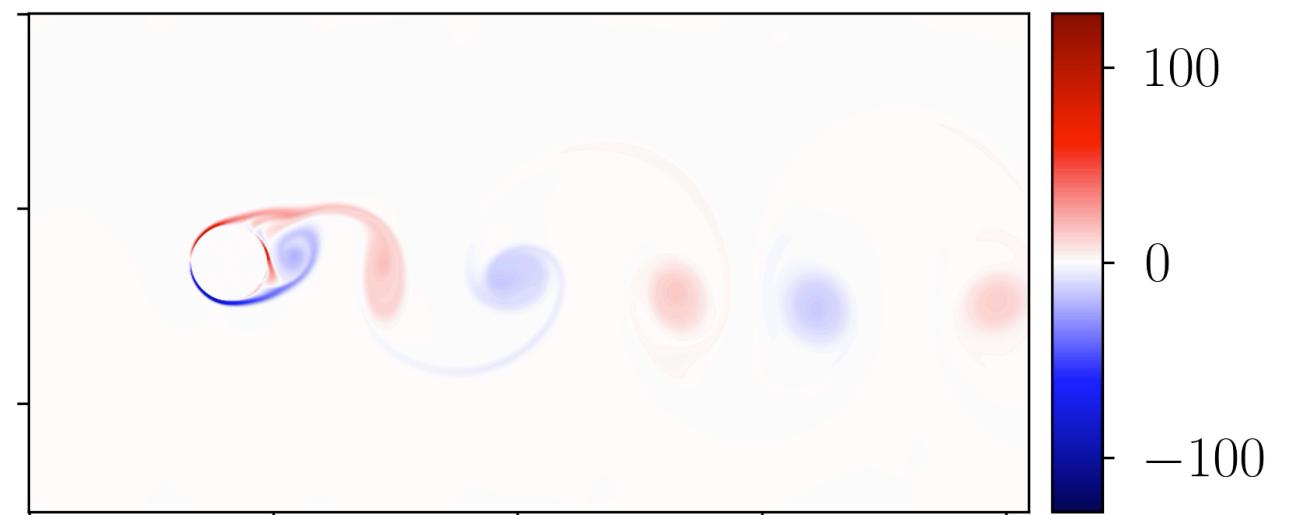
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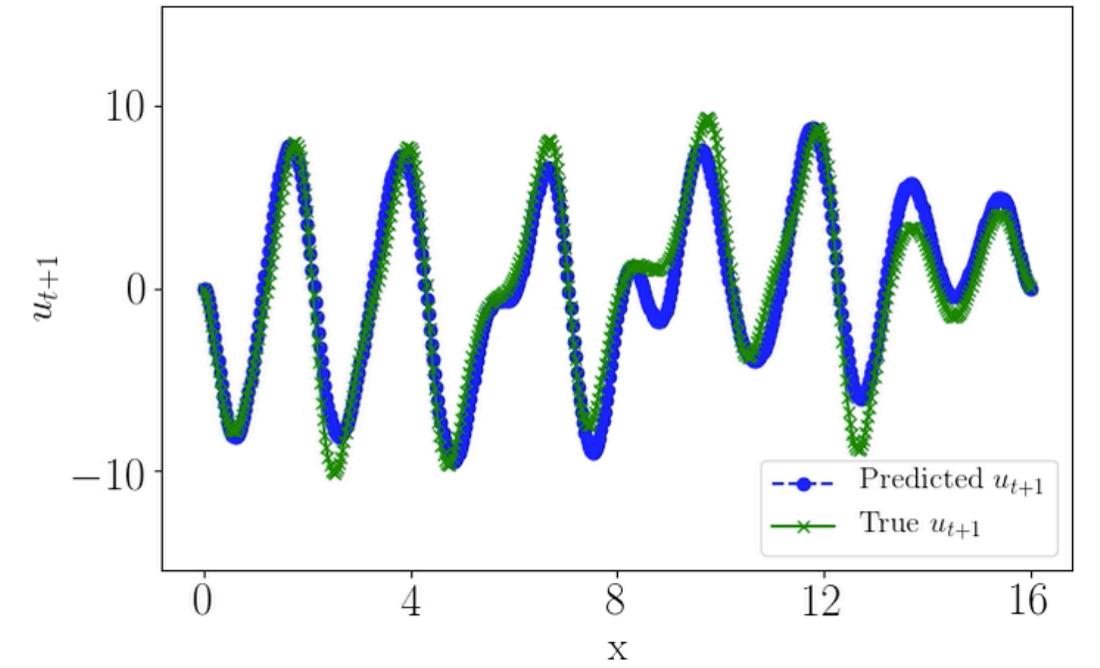
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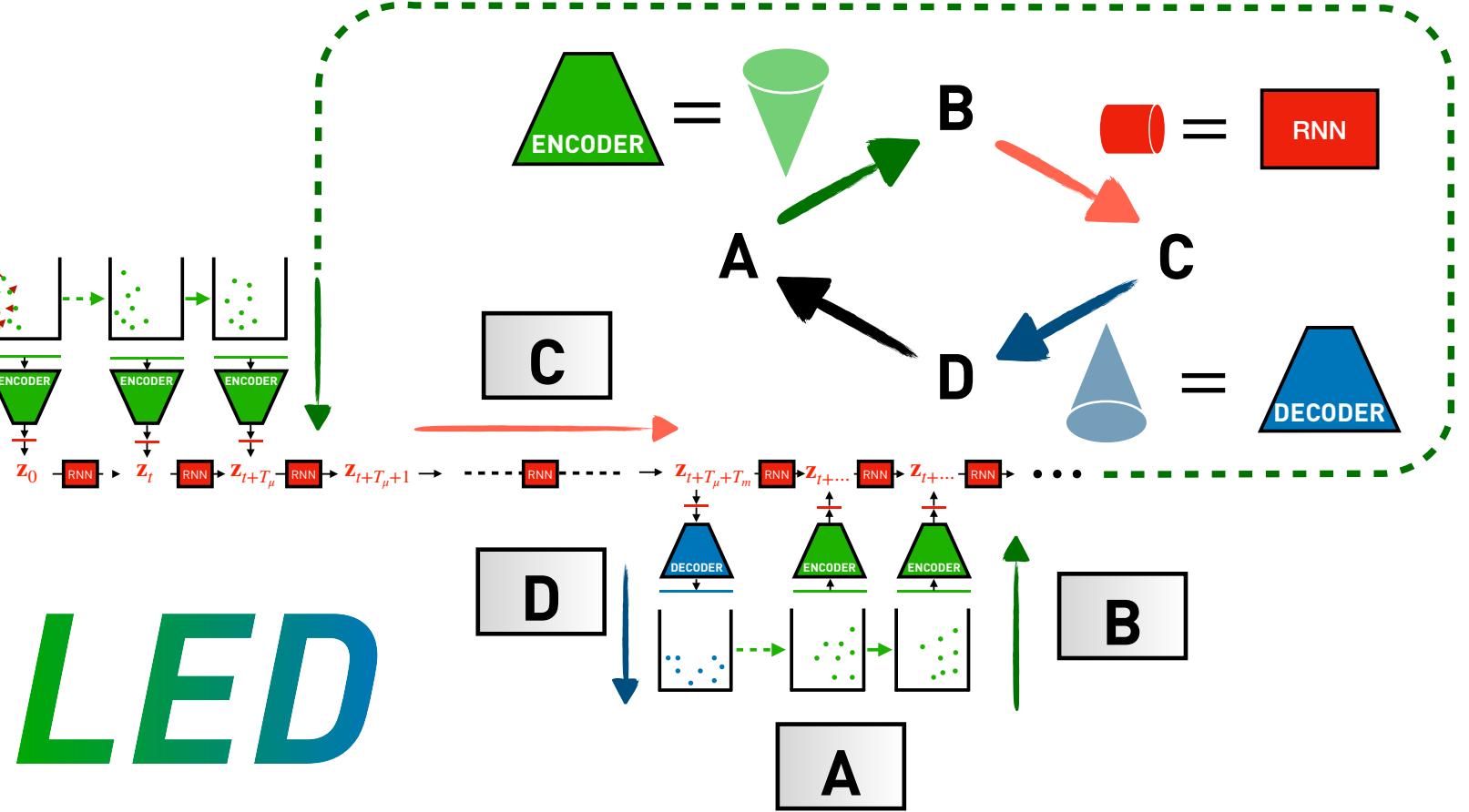
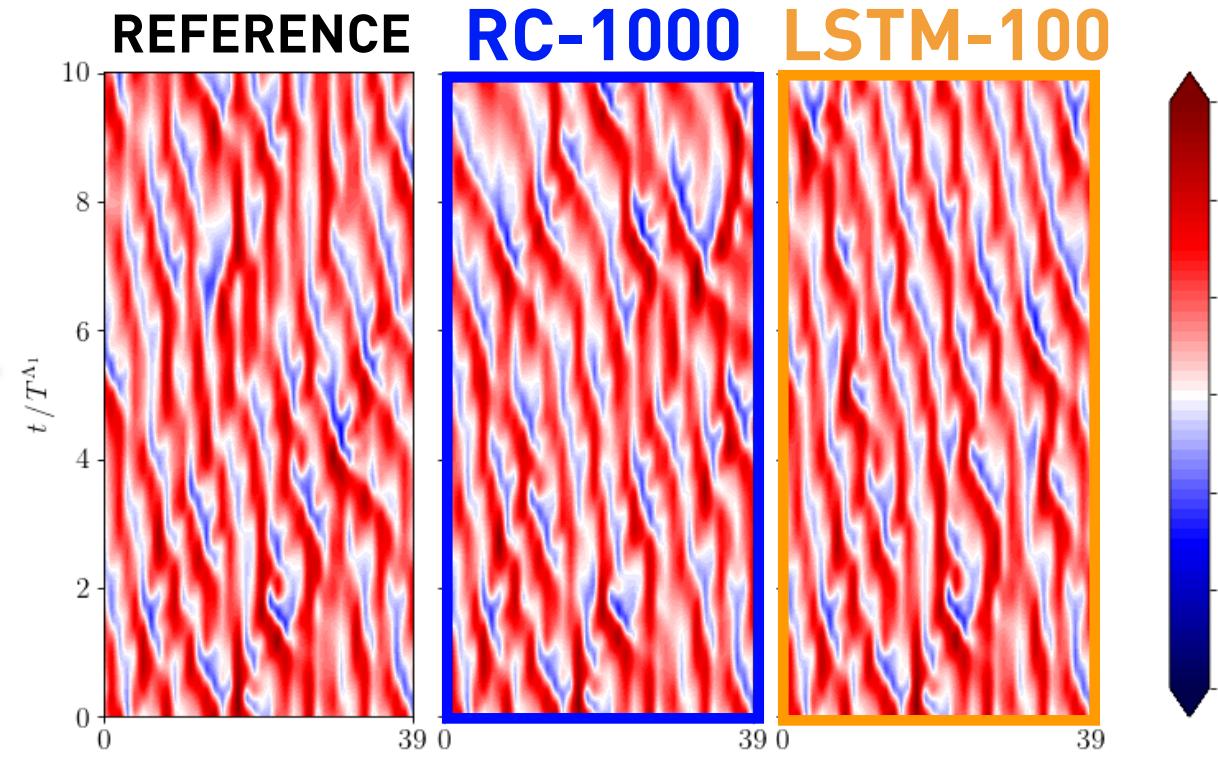
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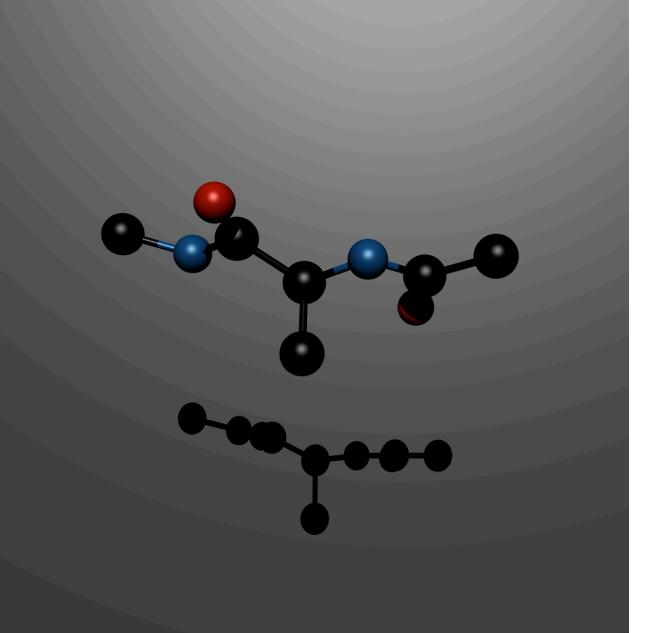
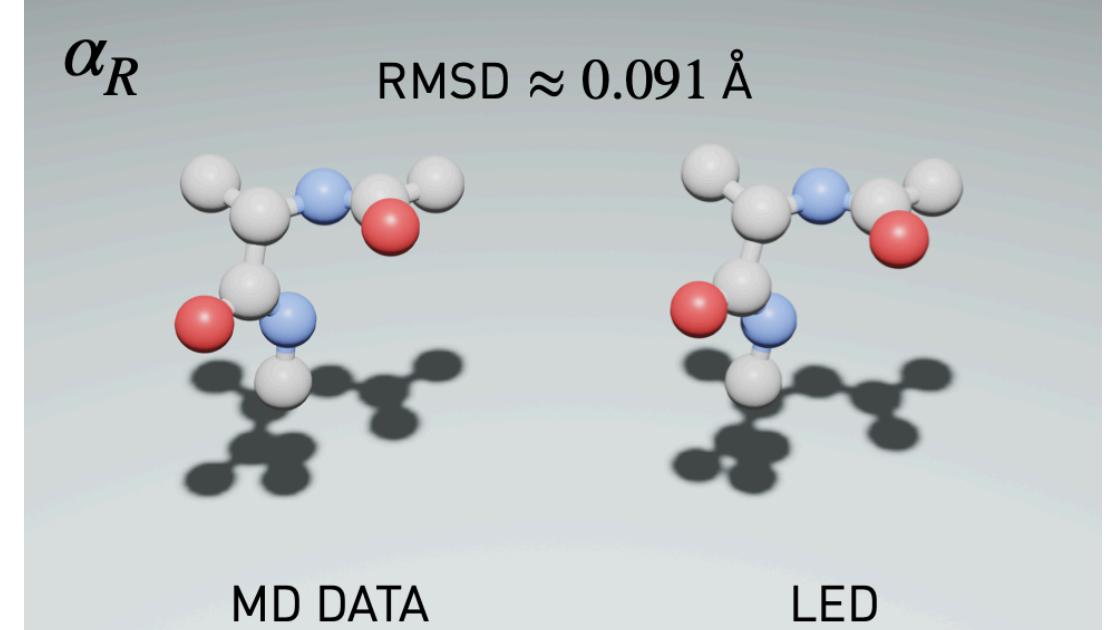
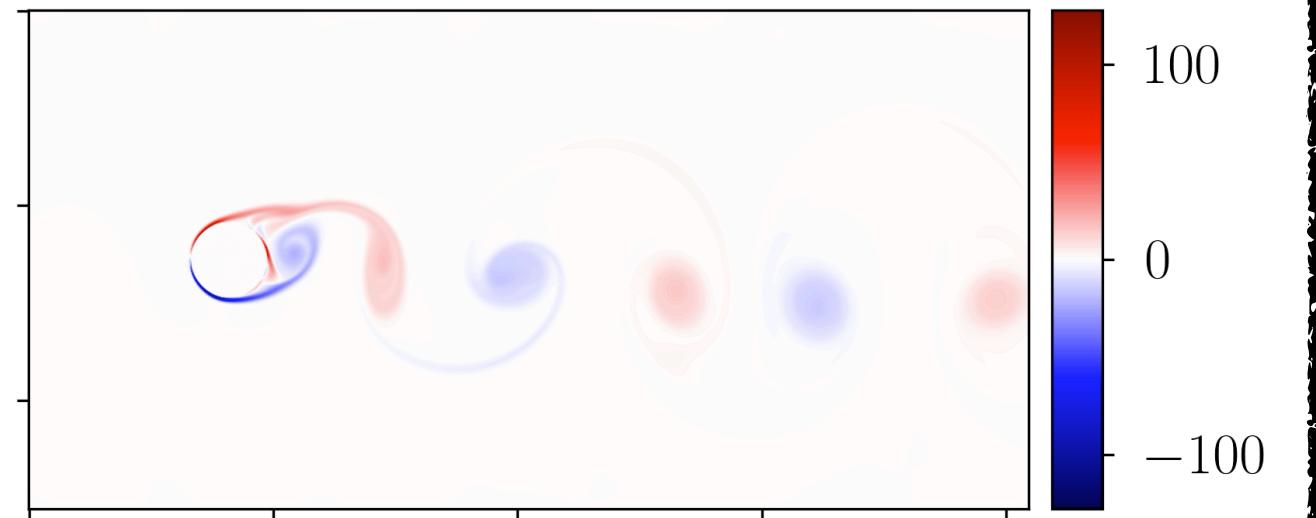
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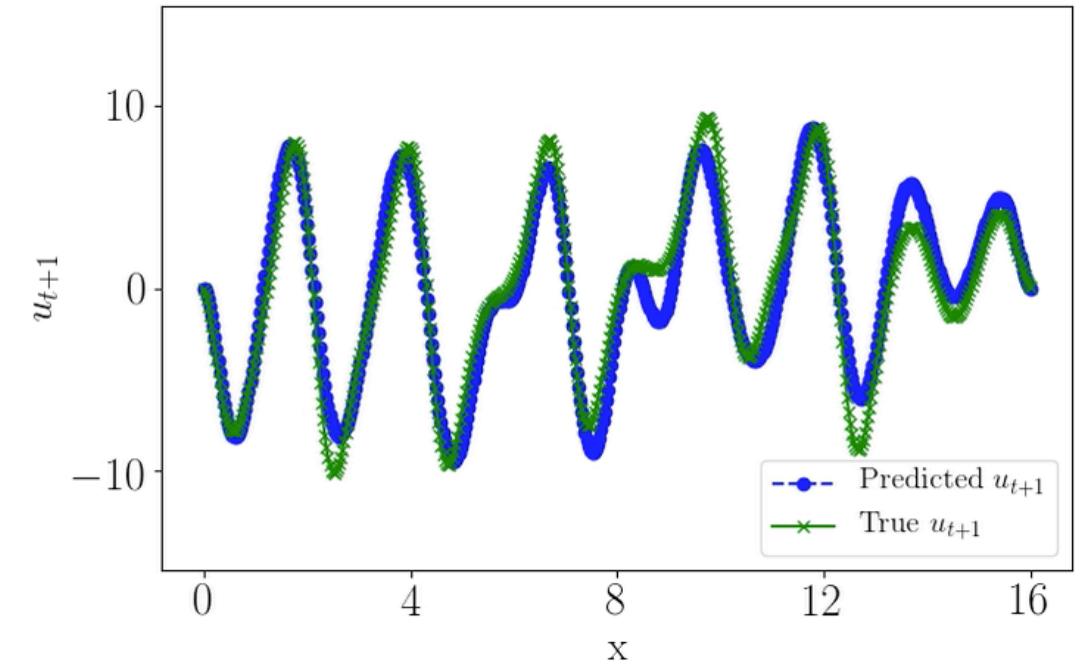


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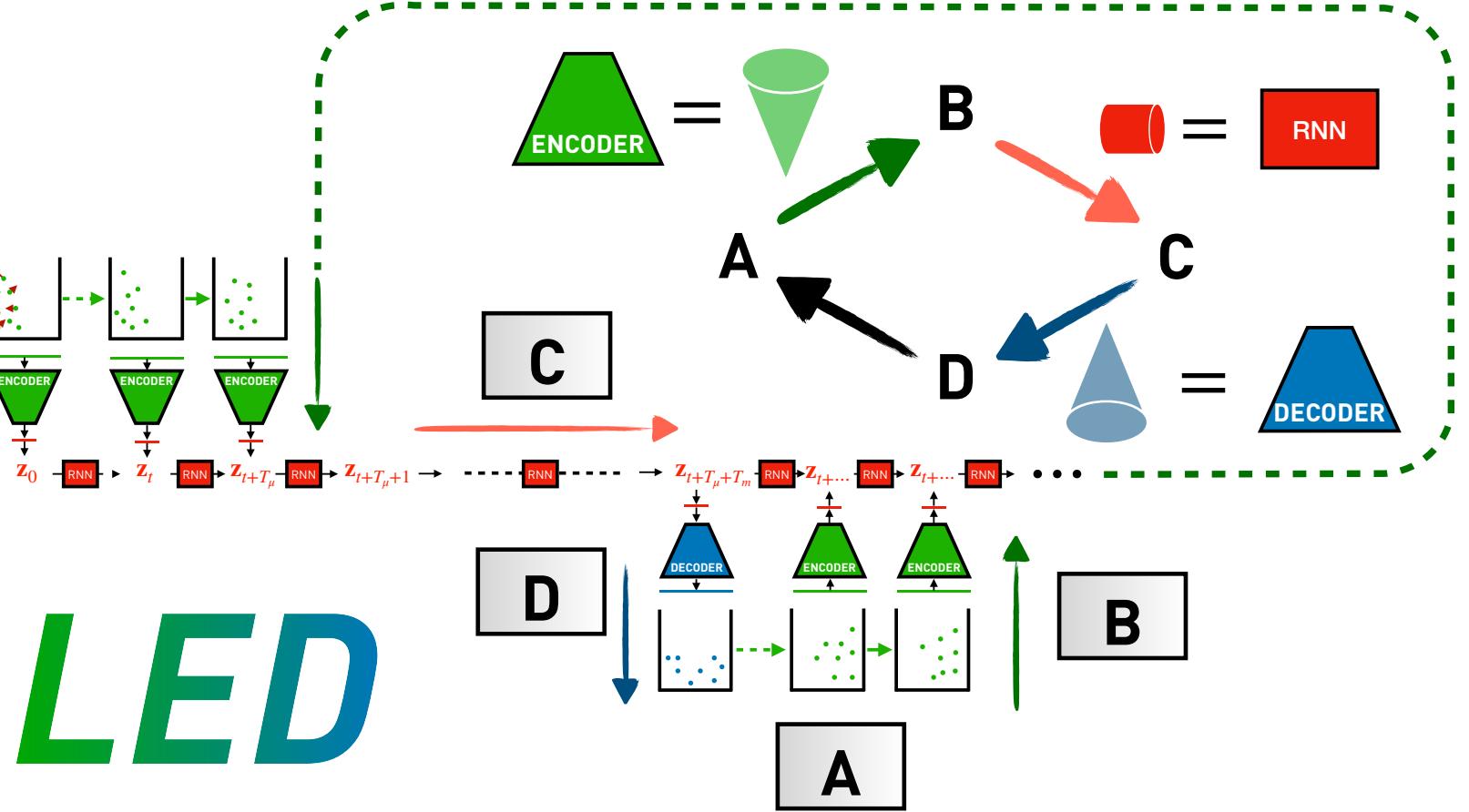
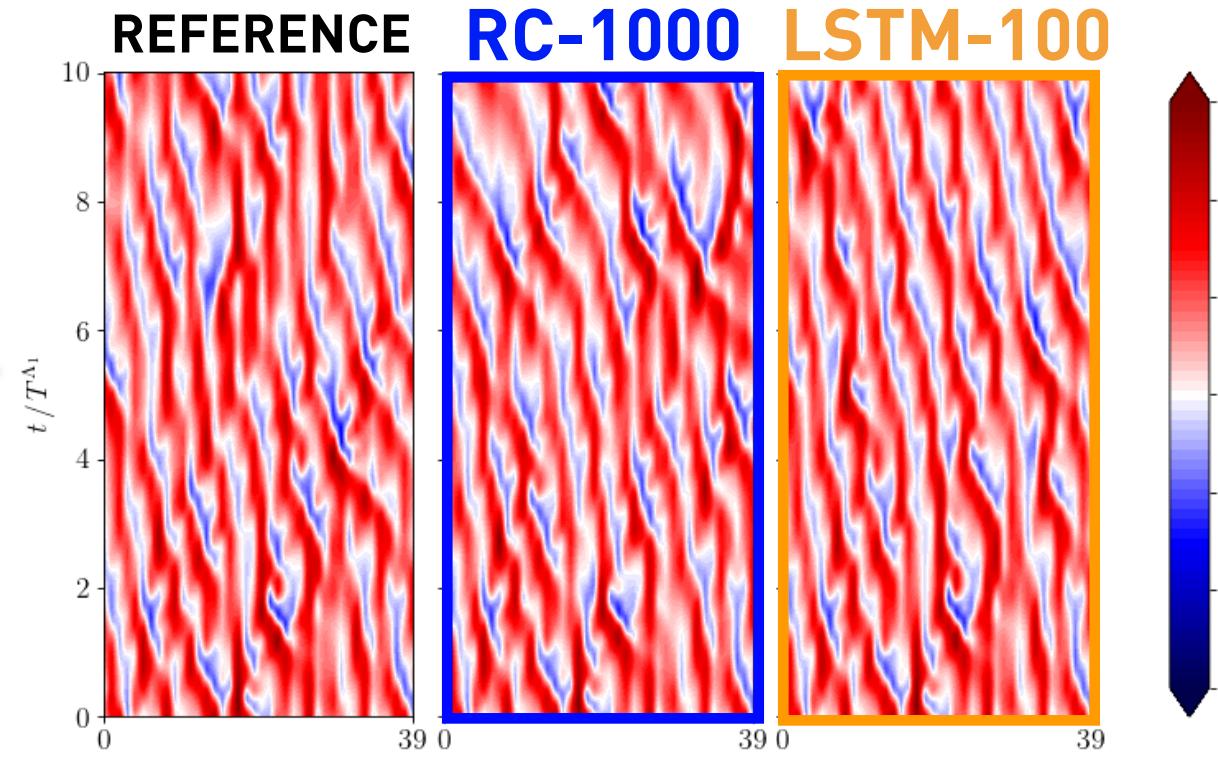
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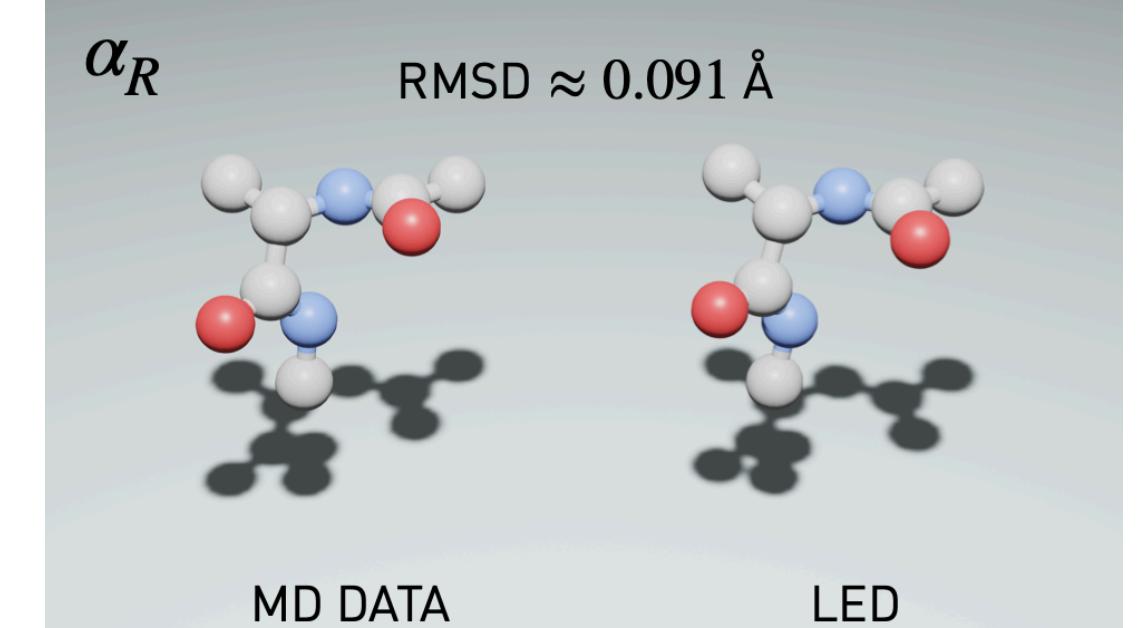
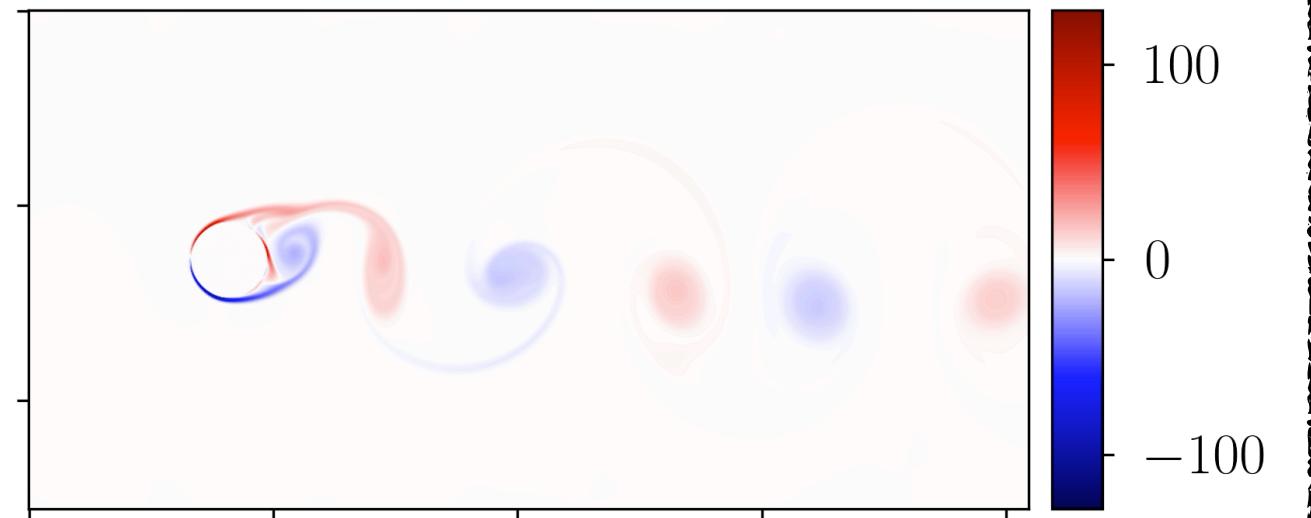
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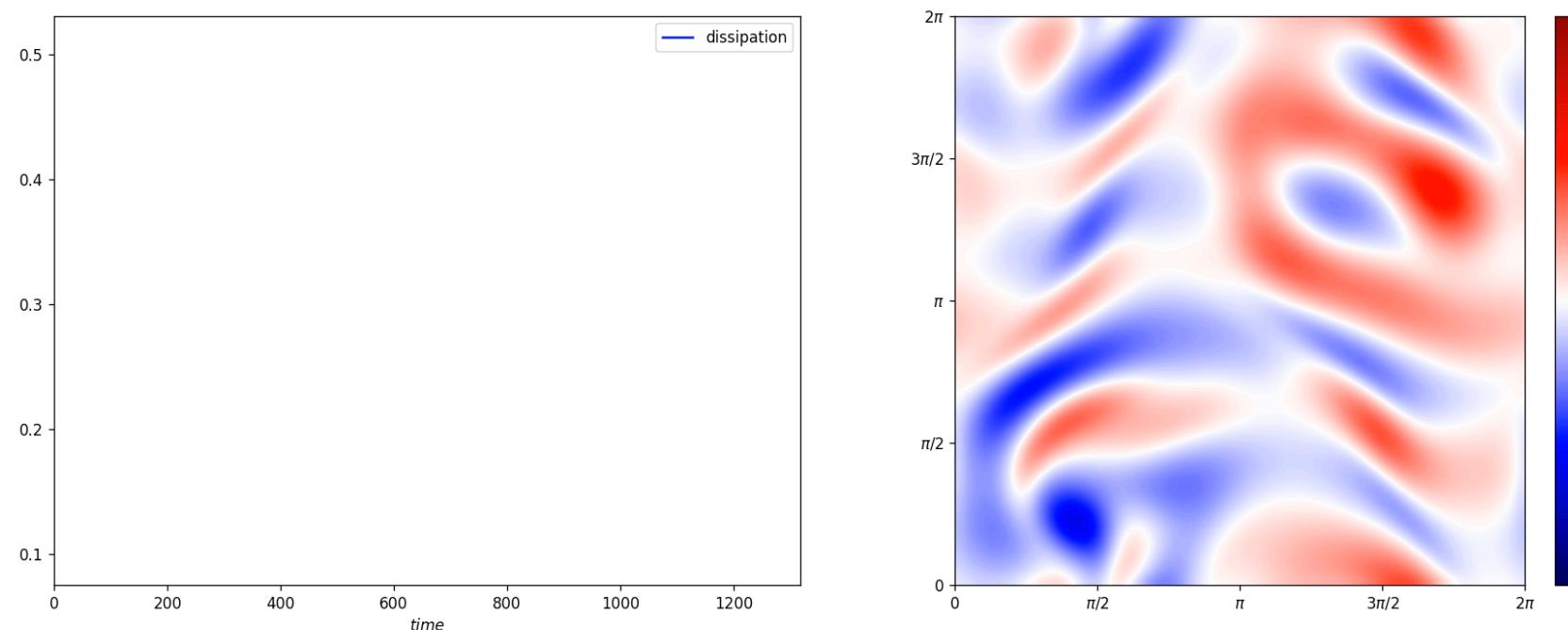
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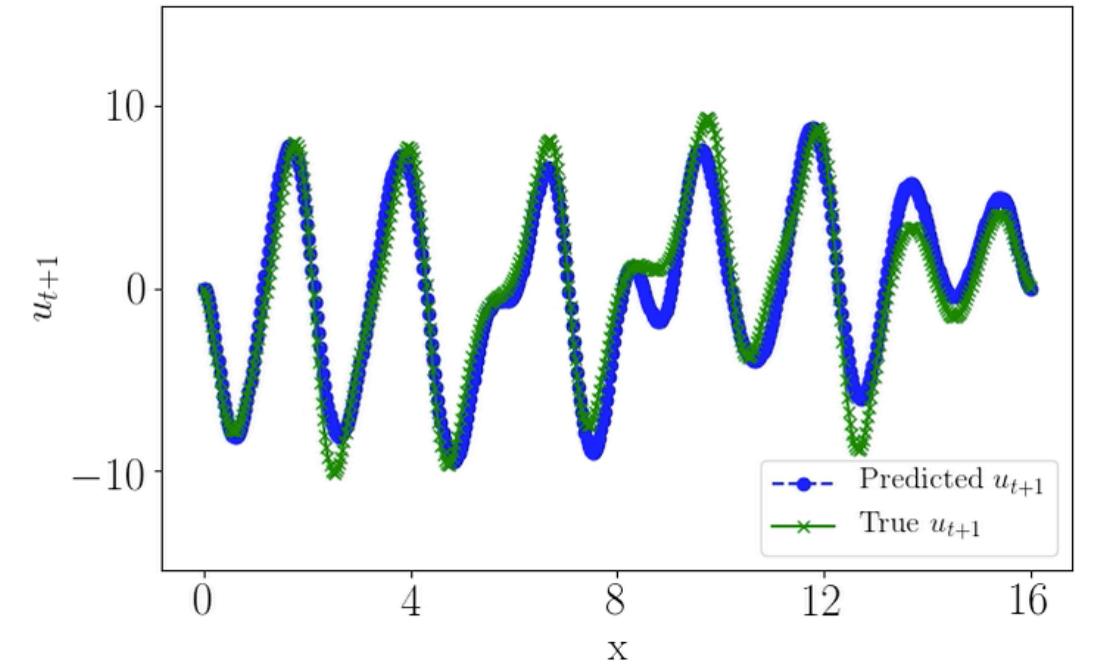
**ZY Wan, P Vlachas,  
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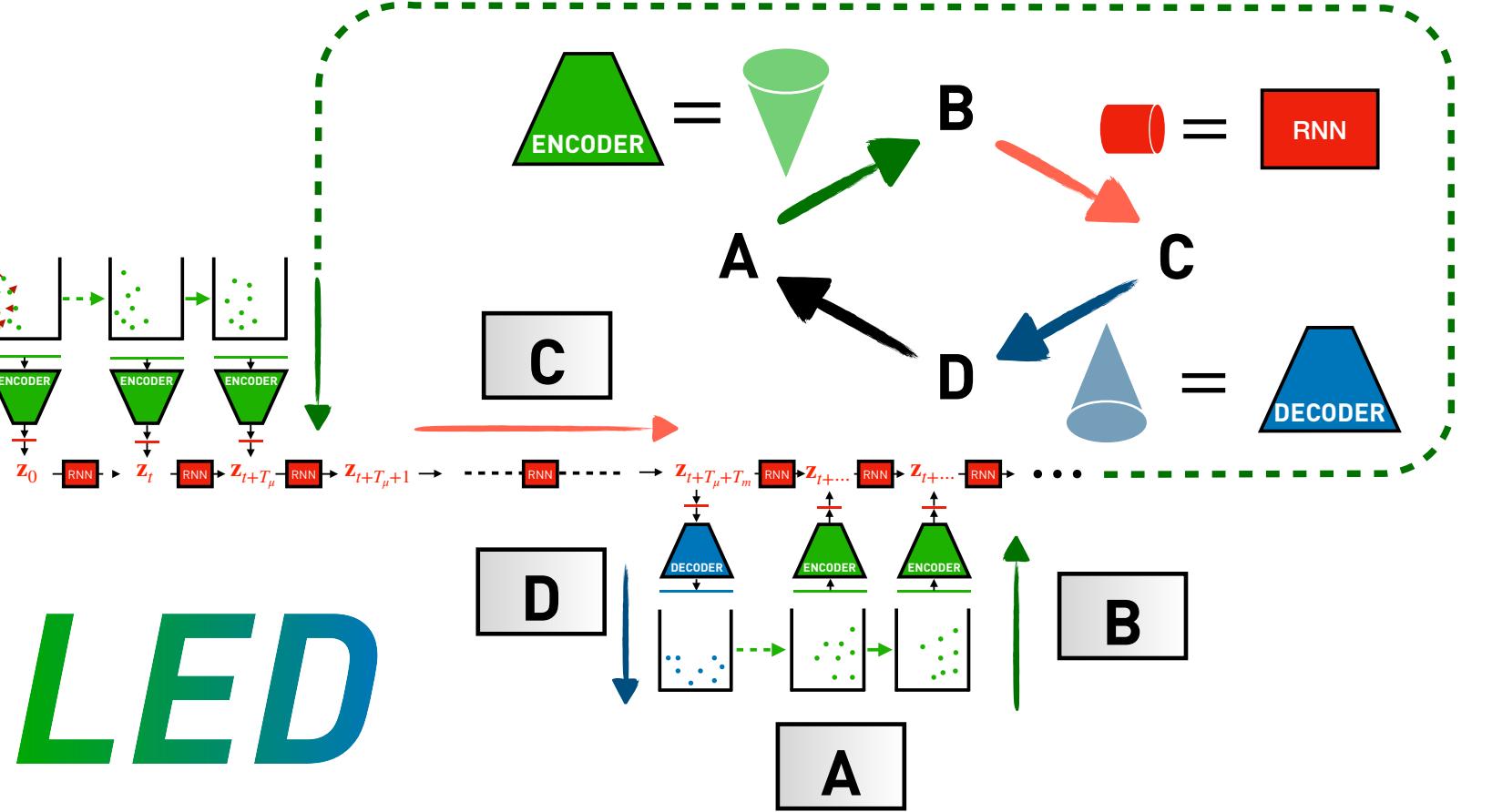
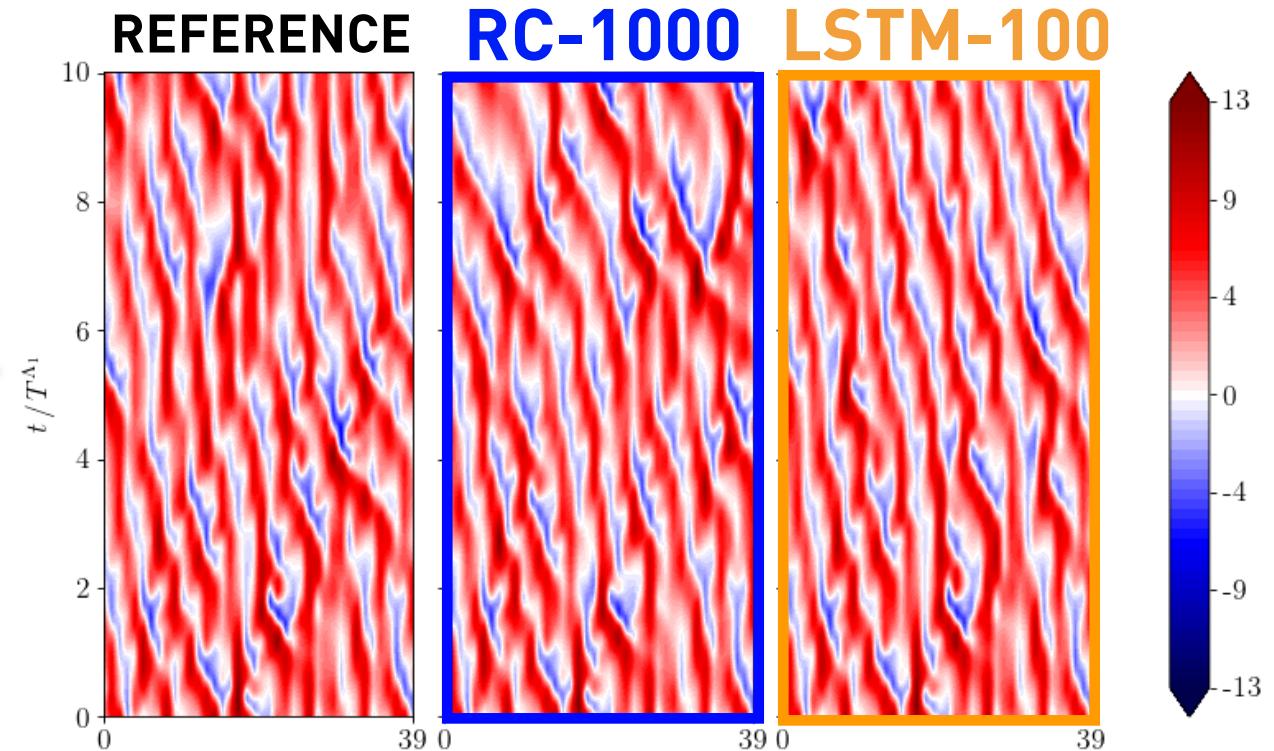
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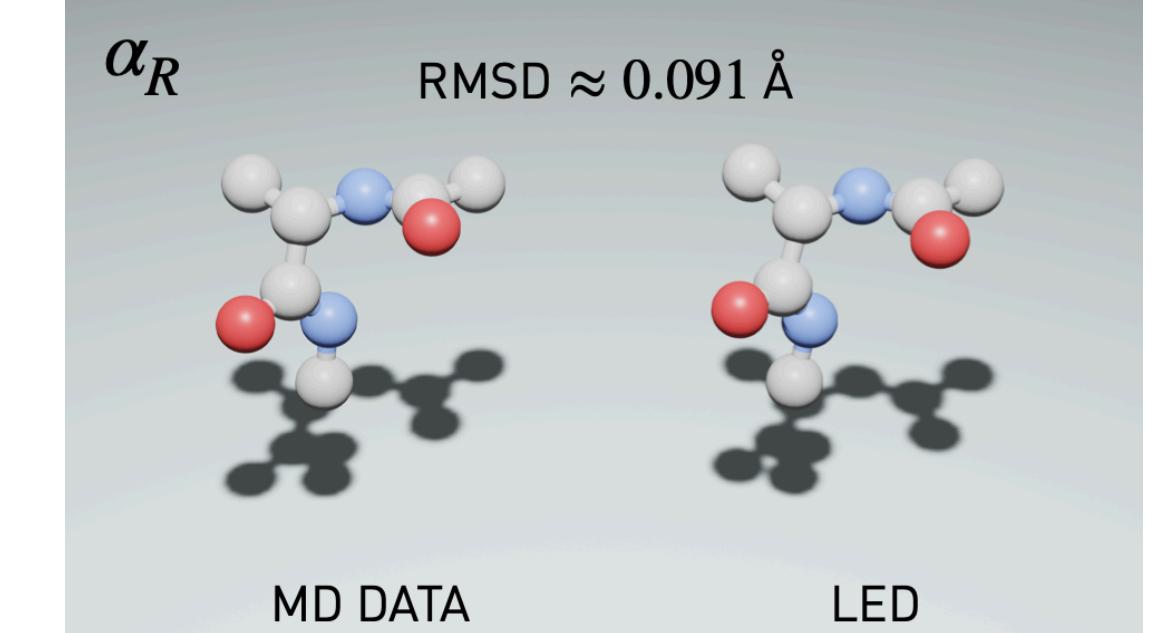
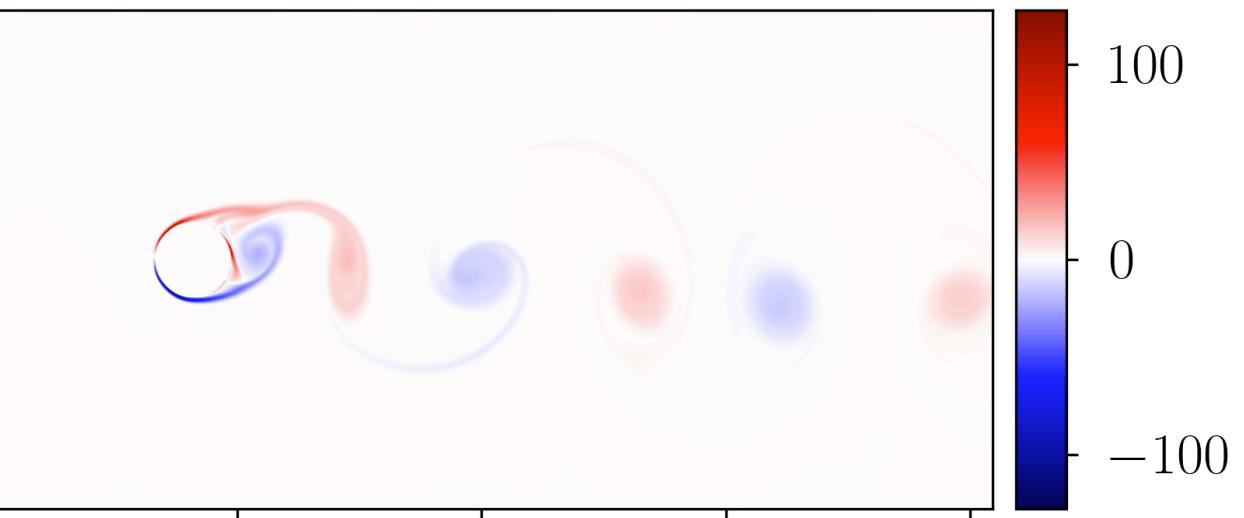
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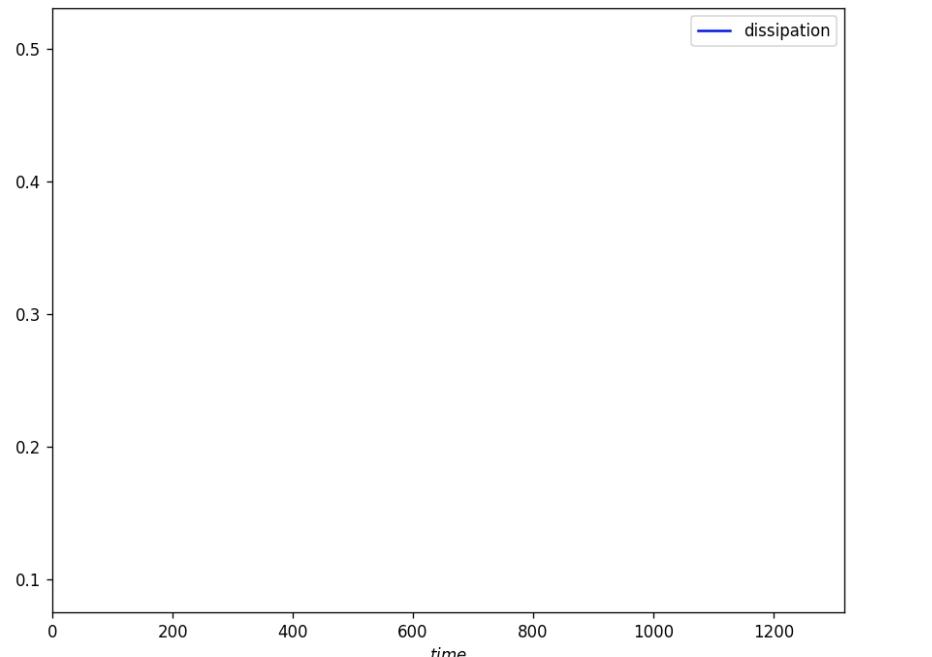
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**PR Vlachas, P Koumoutsakos,** Scheduled Autoregressive Backpropagation Through Time for Long-Term Forecasting, (in preparation)

