

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

Pantelis R. Vlachas  
Computational Science and Engineering Lab



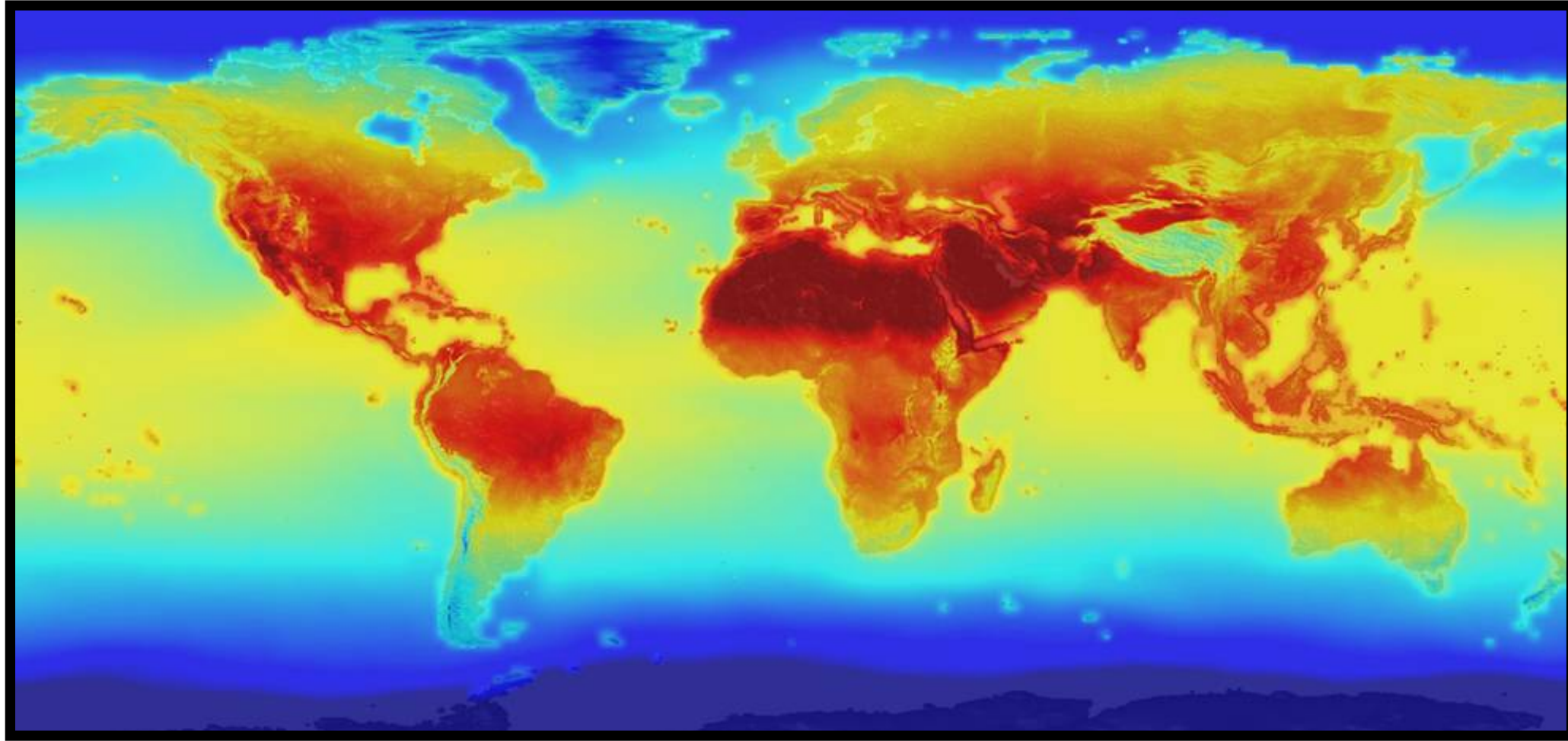
# Motivation

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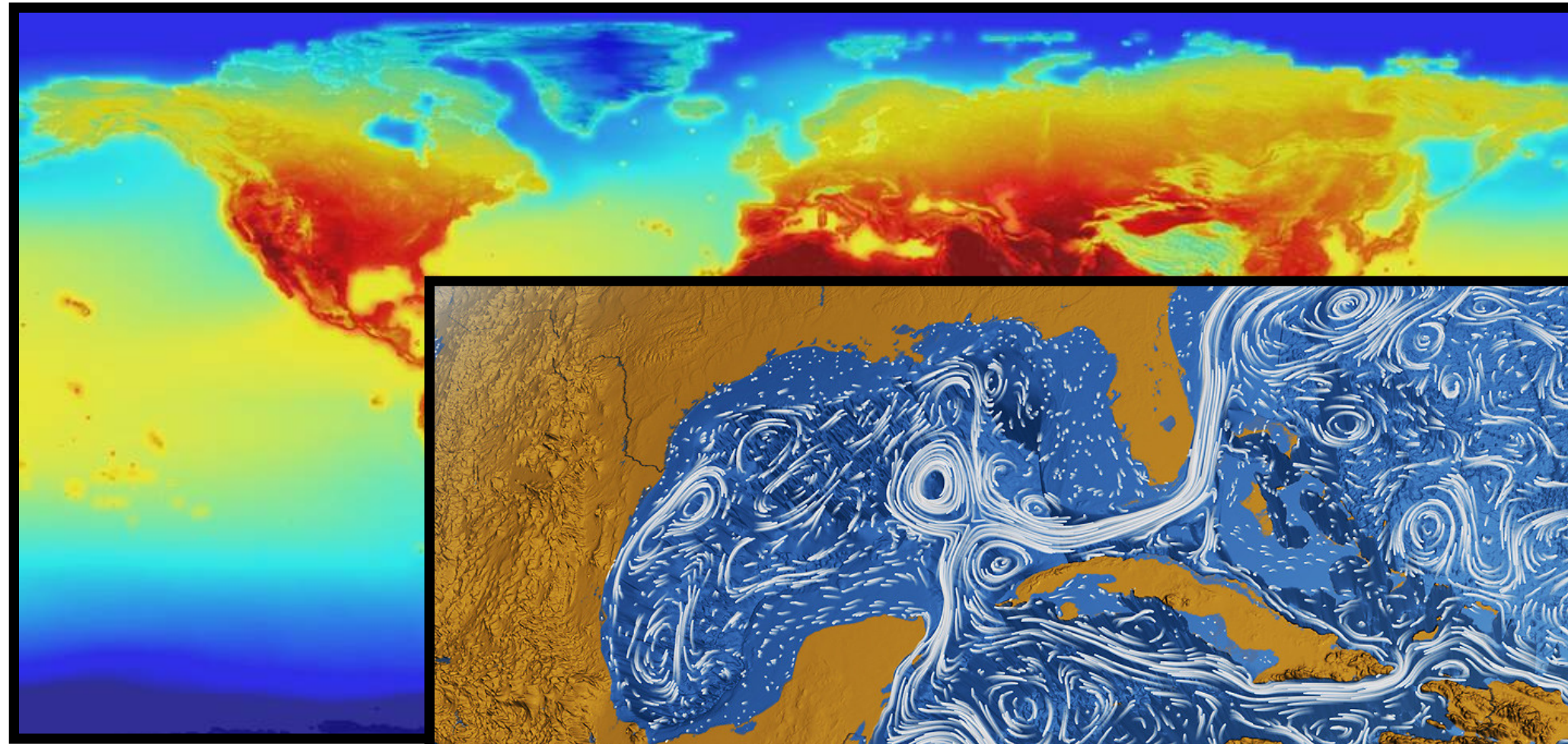


Climate

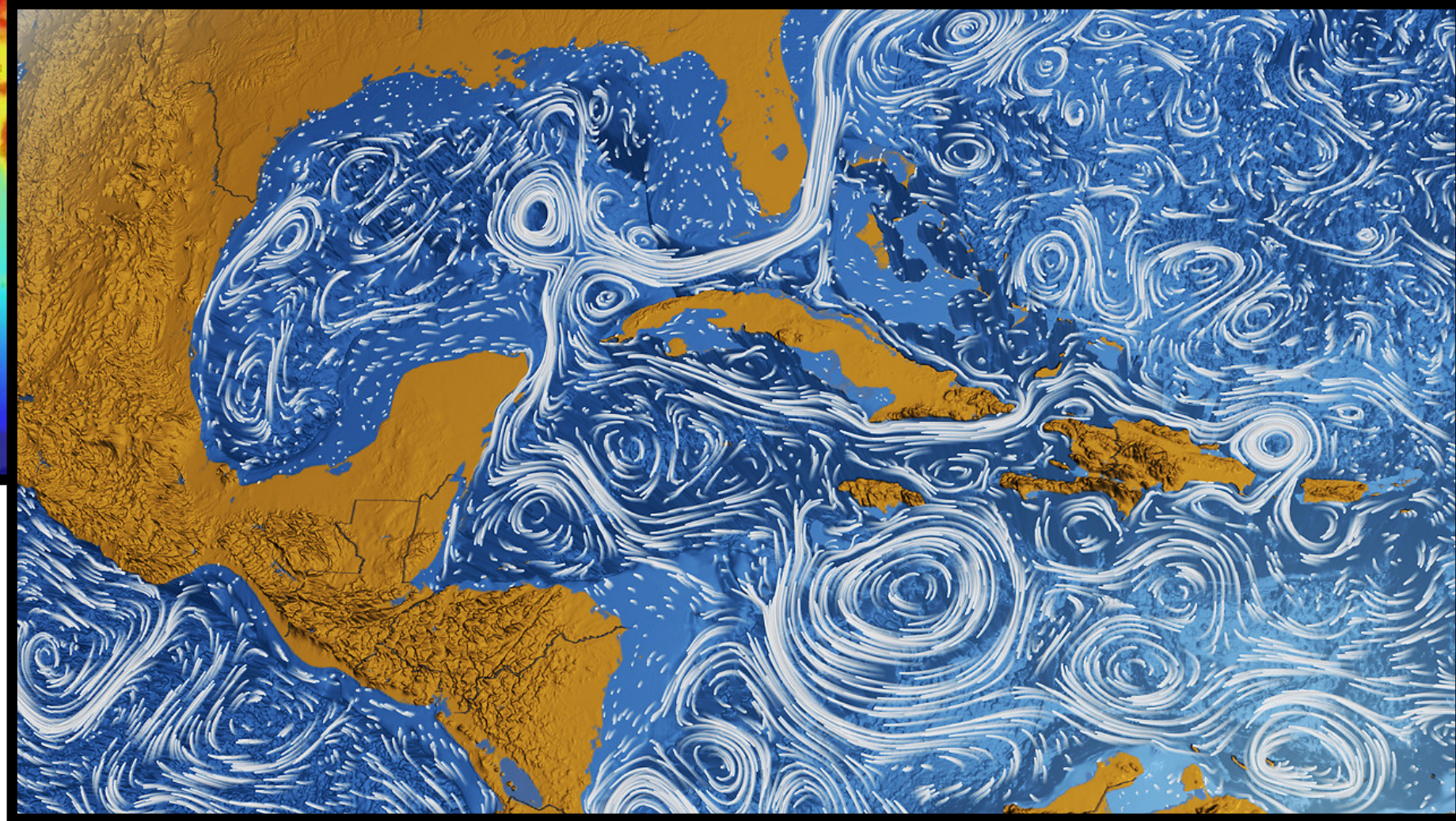
- Complex multiscale systems  
(deterministic, stochastic, chaotic)



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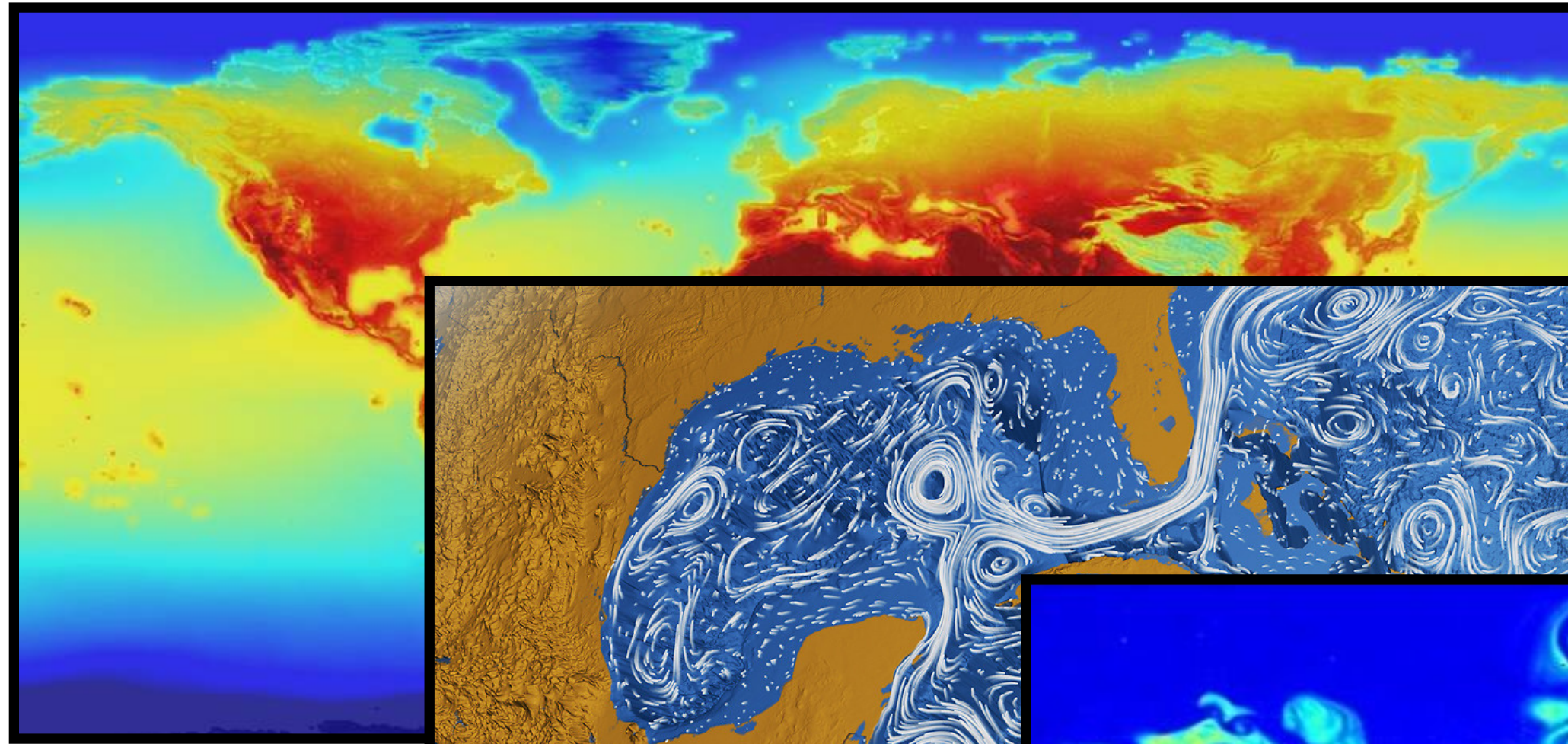
Ocean currents

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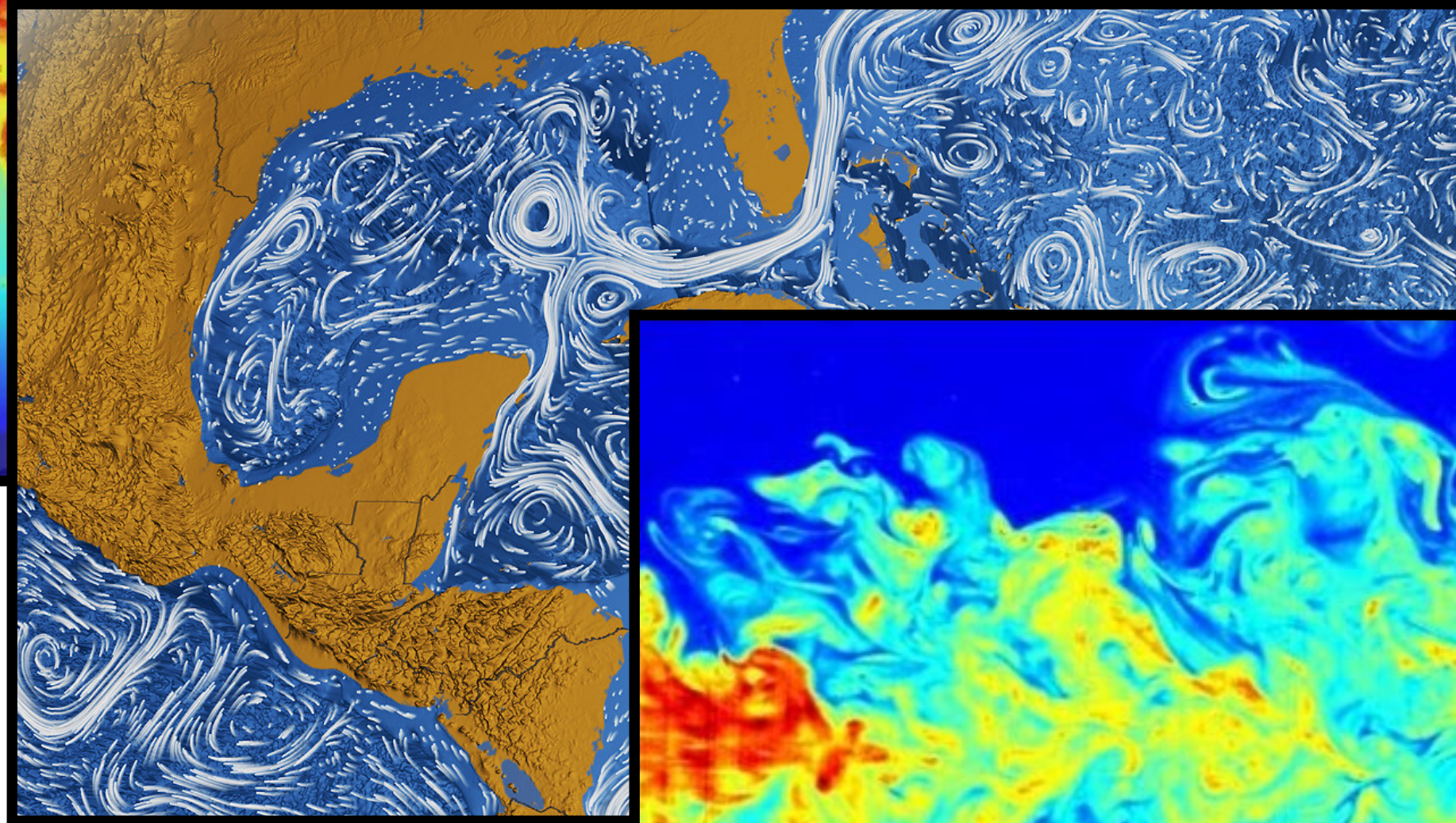


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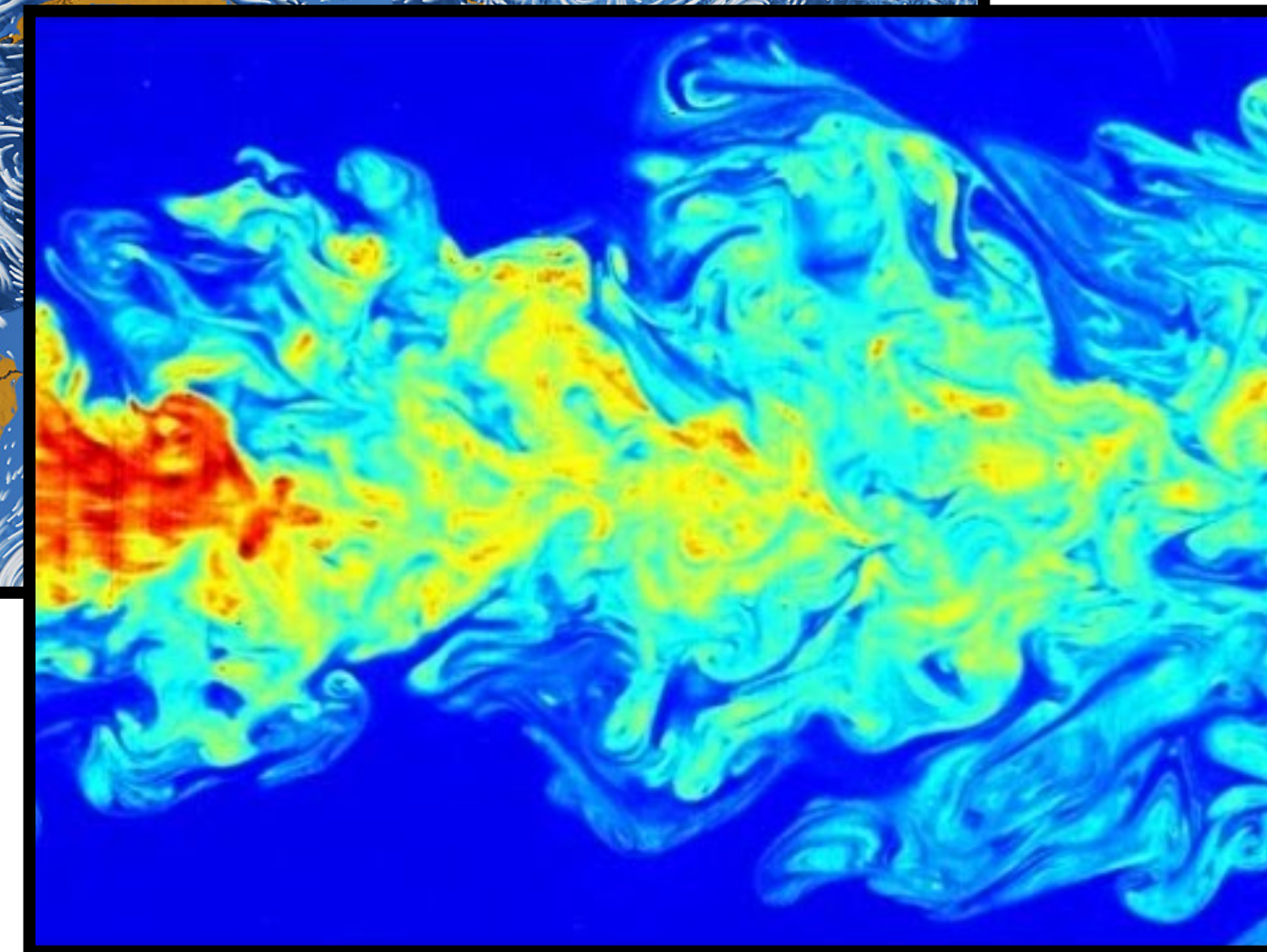
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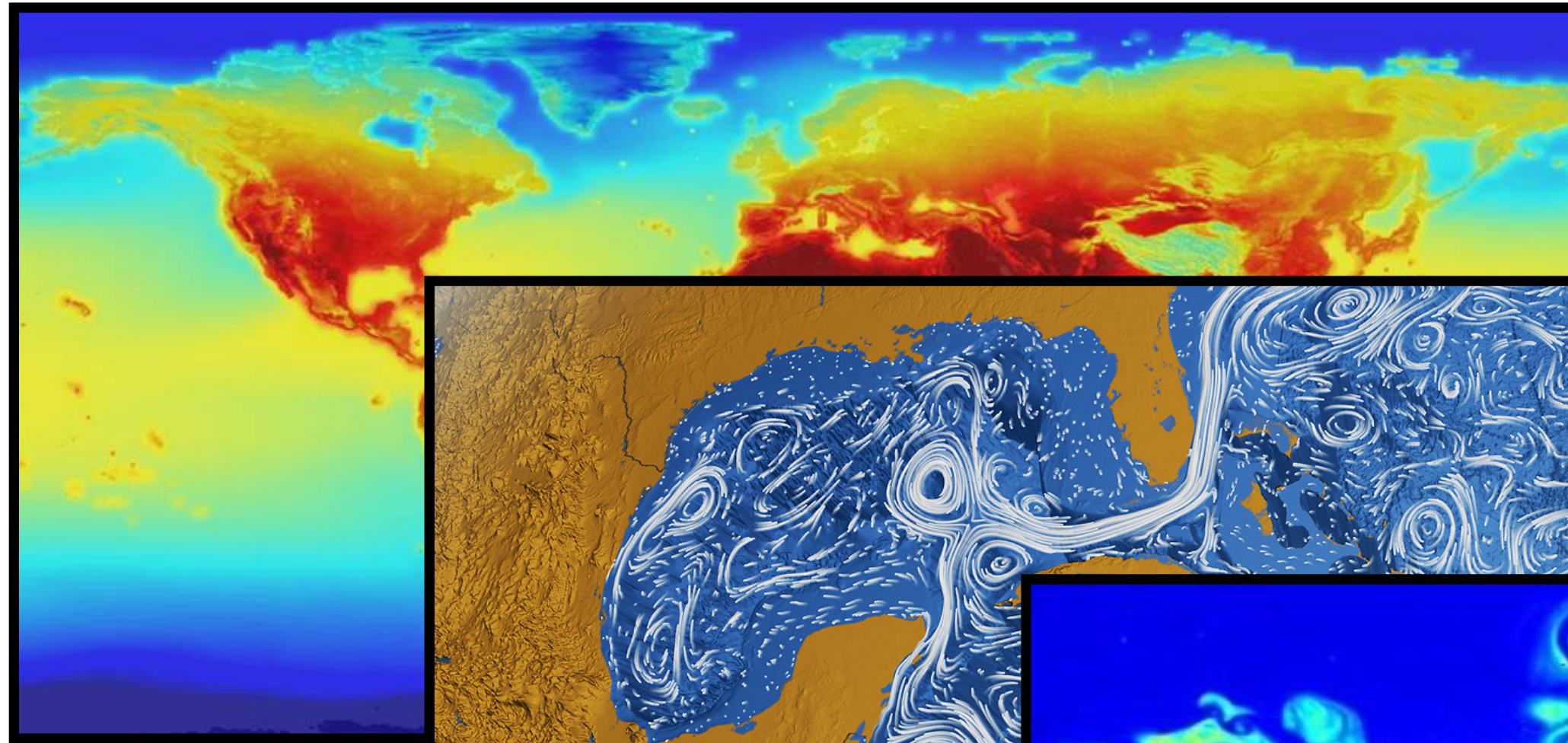


Turbulence

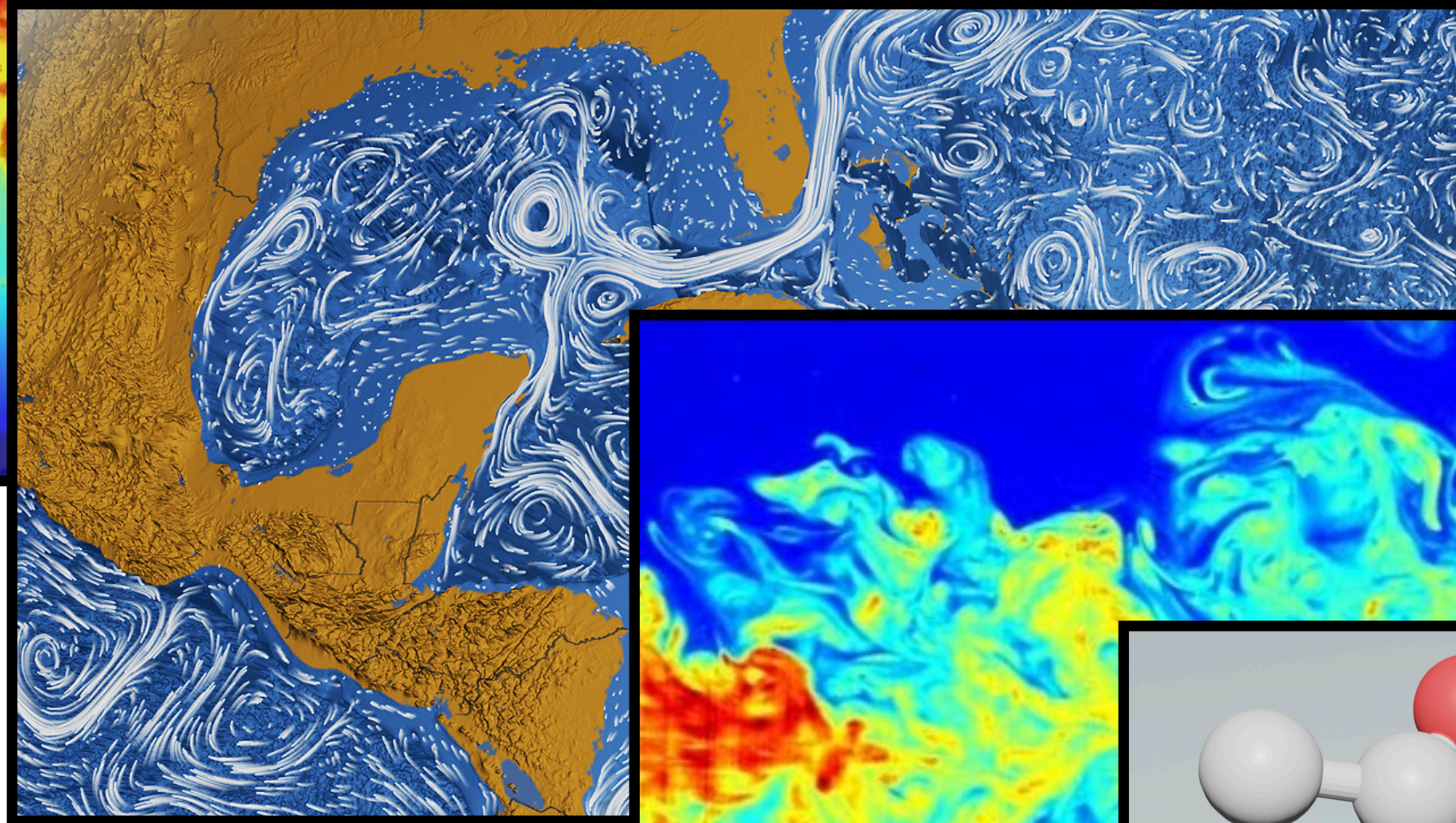


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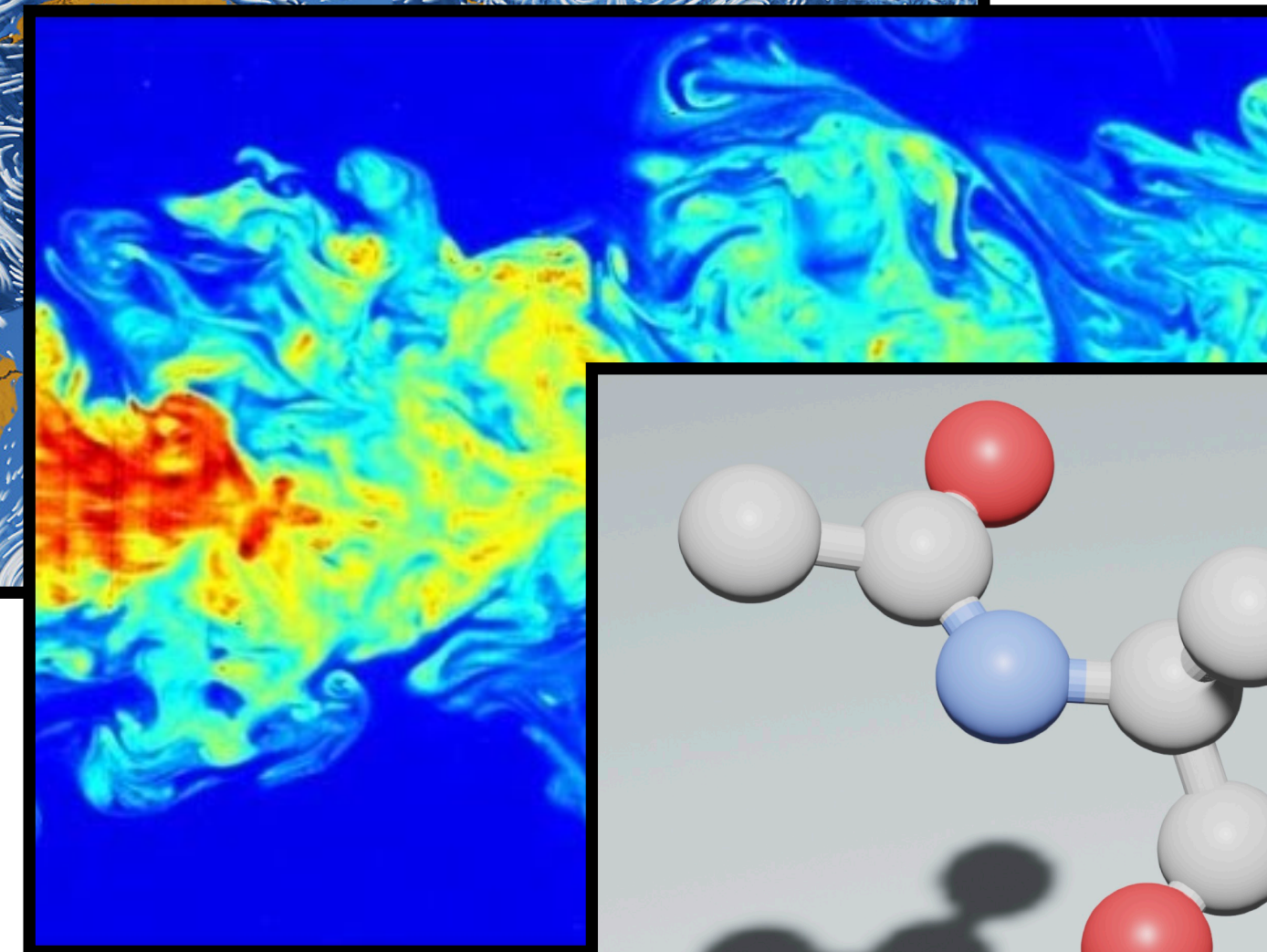
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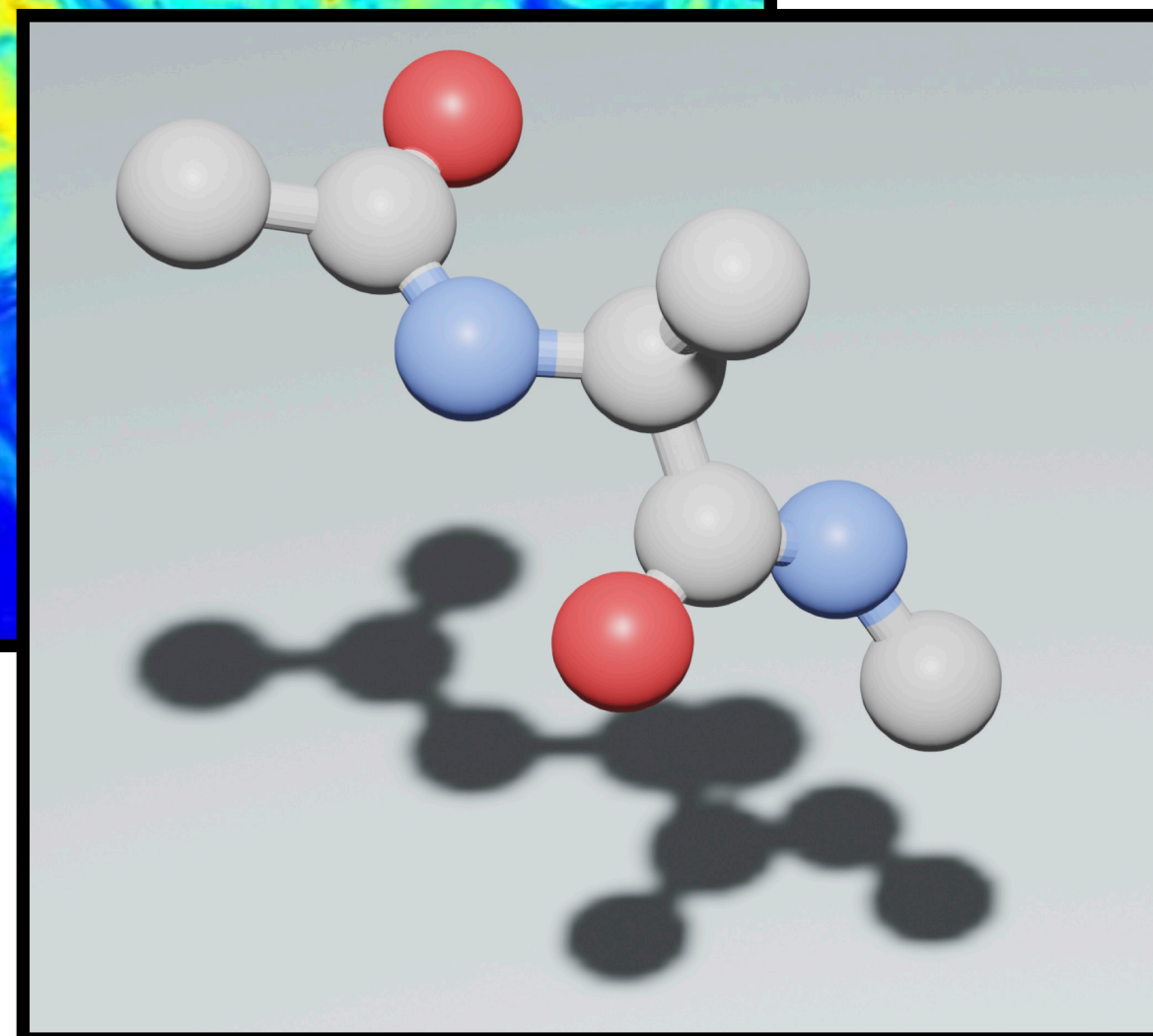
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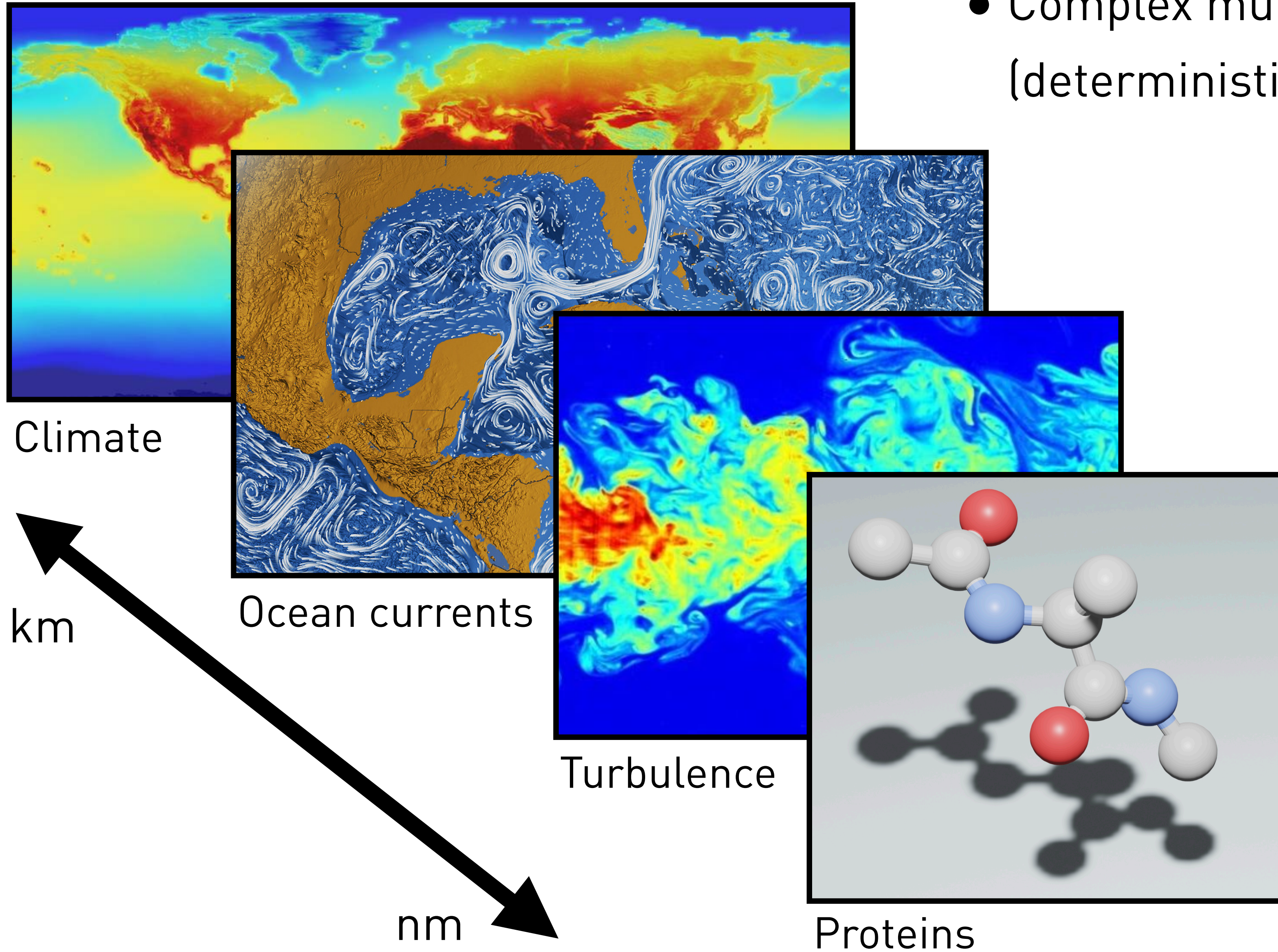


Proteins



# Motivation

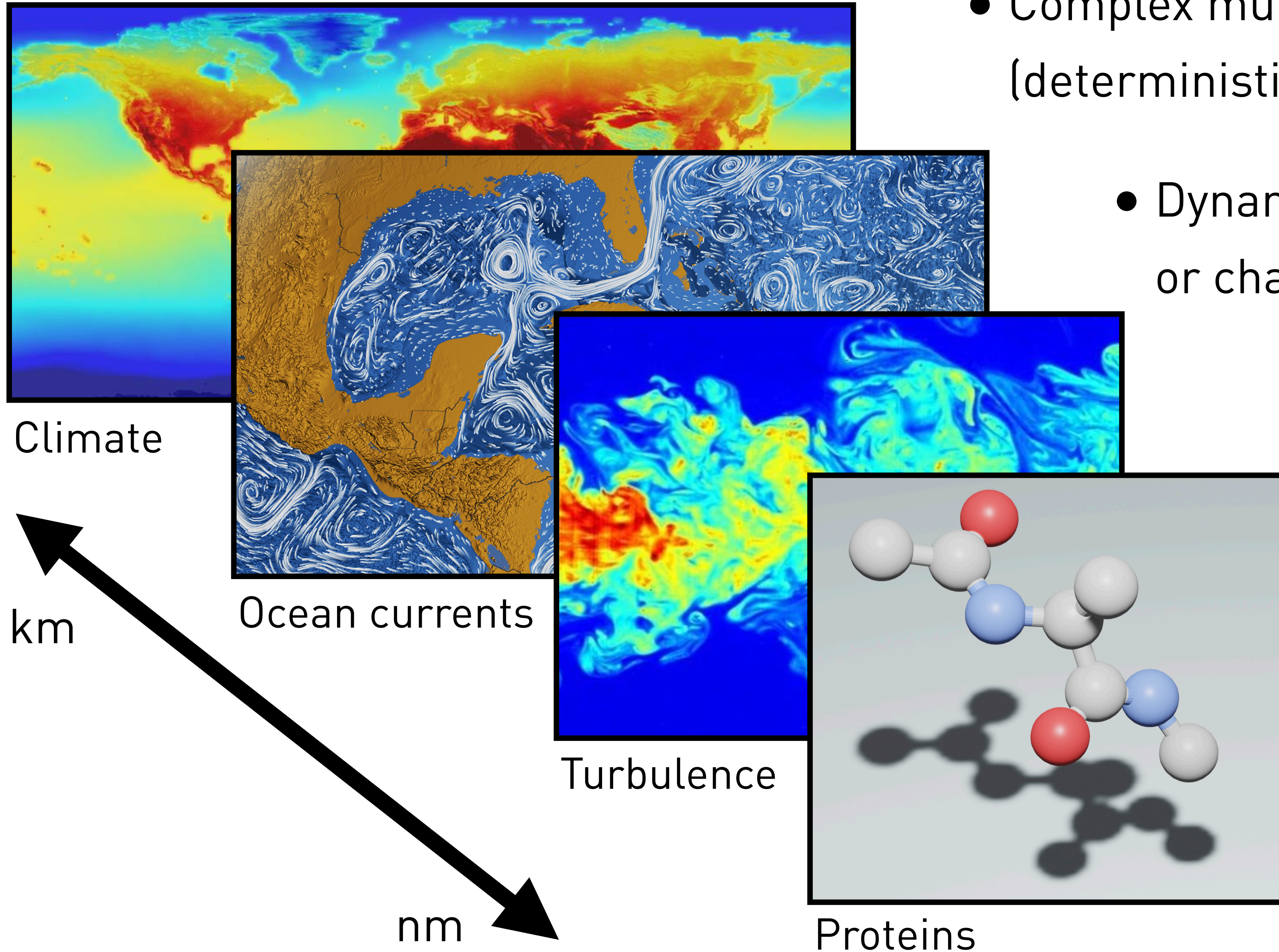
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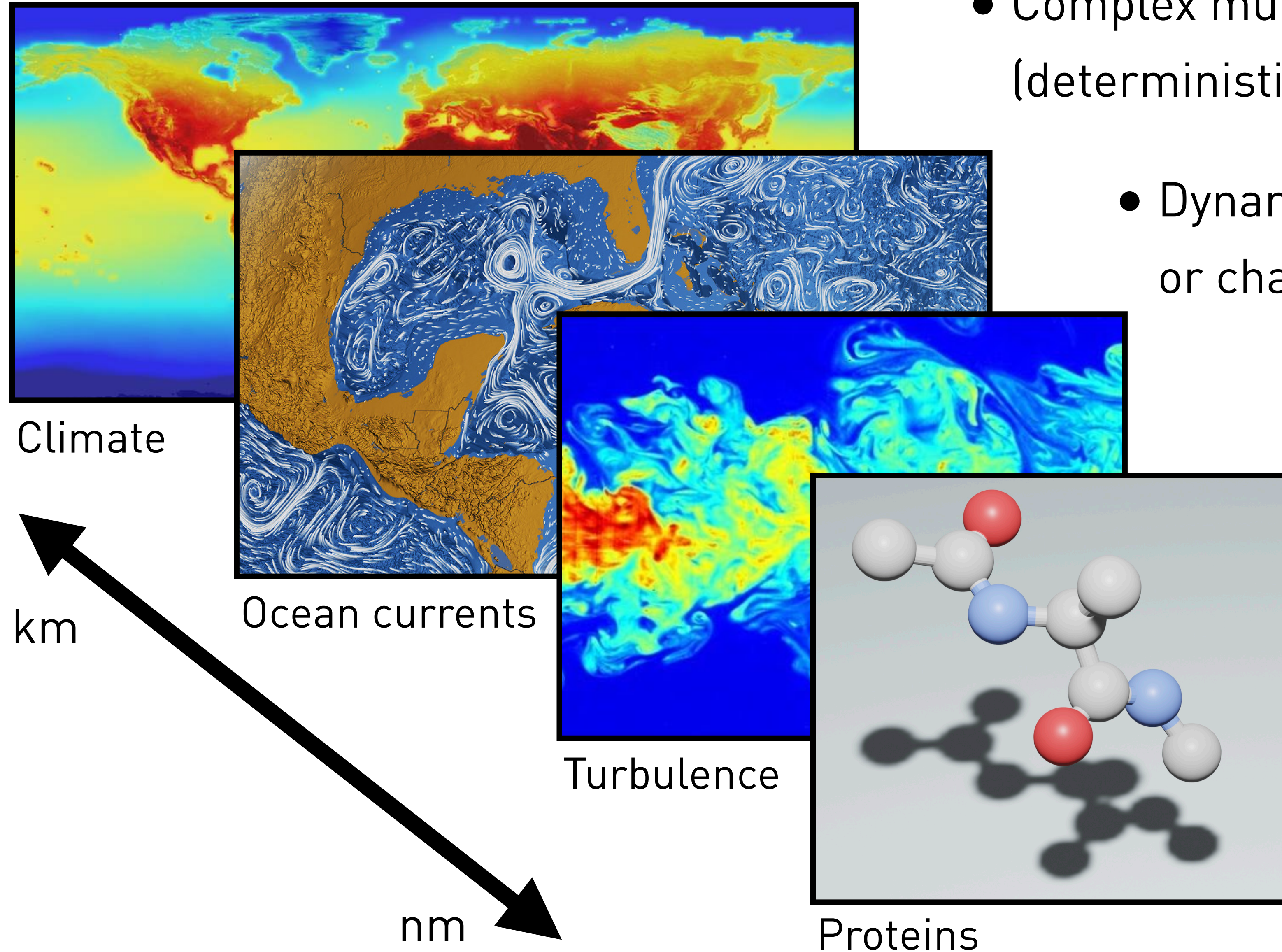
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- Dynamics expensive to simulate and/  
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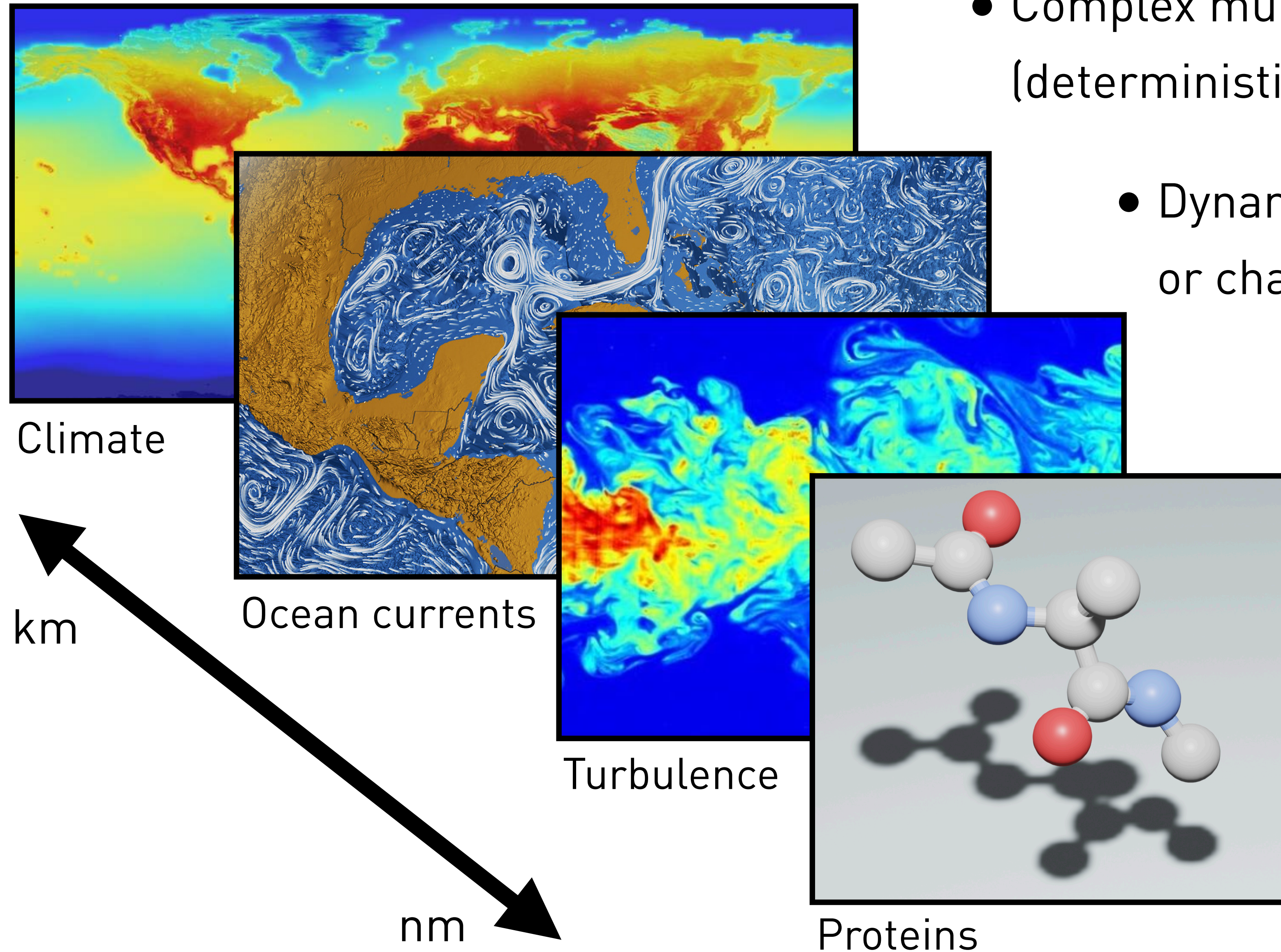
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- Can we design fast (multiscale)  
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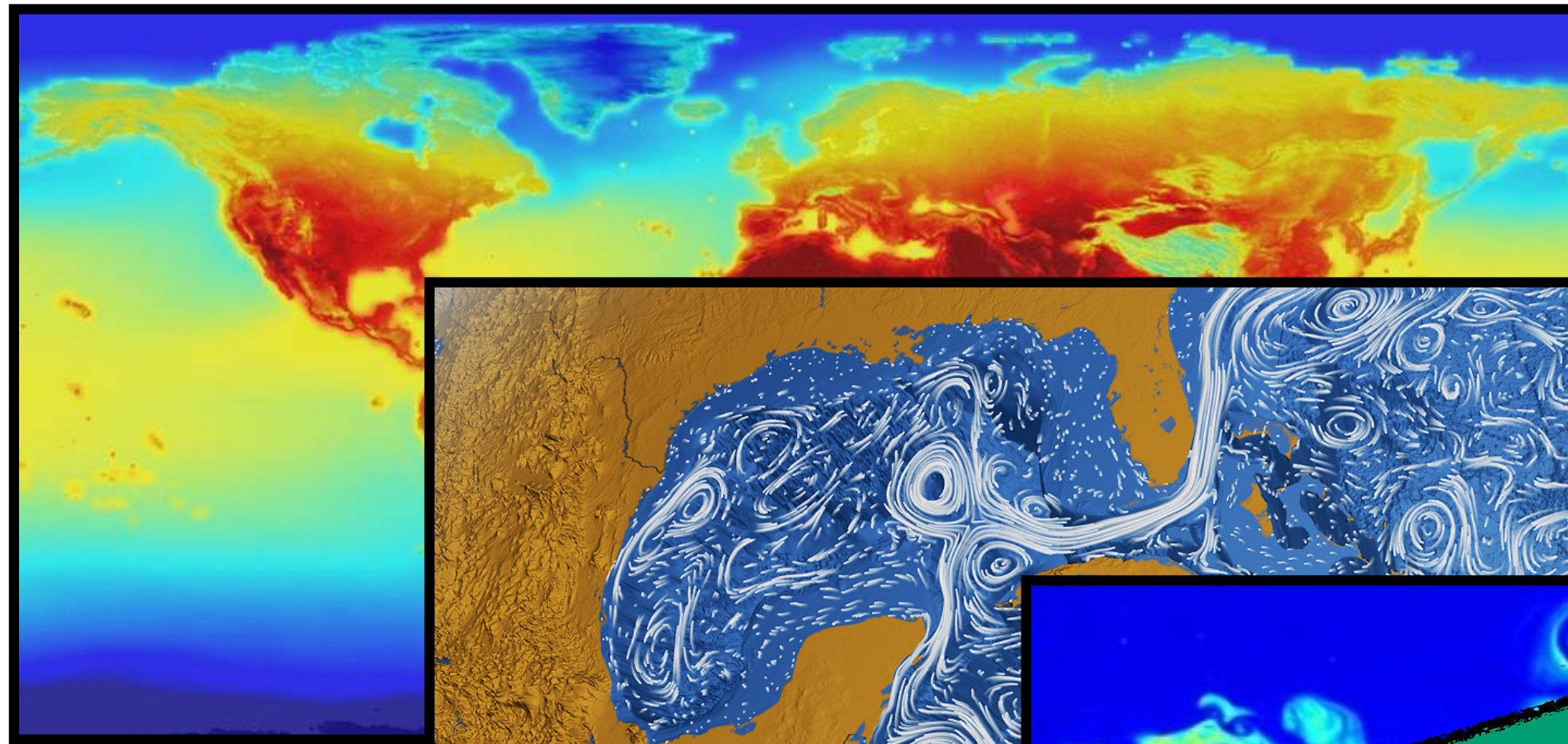
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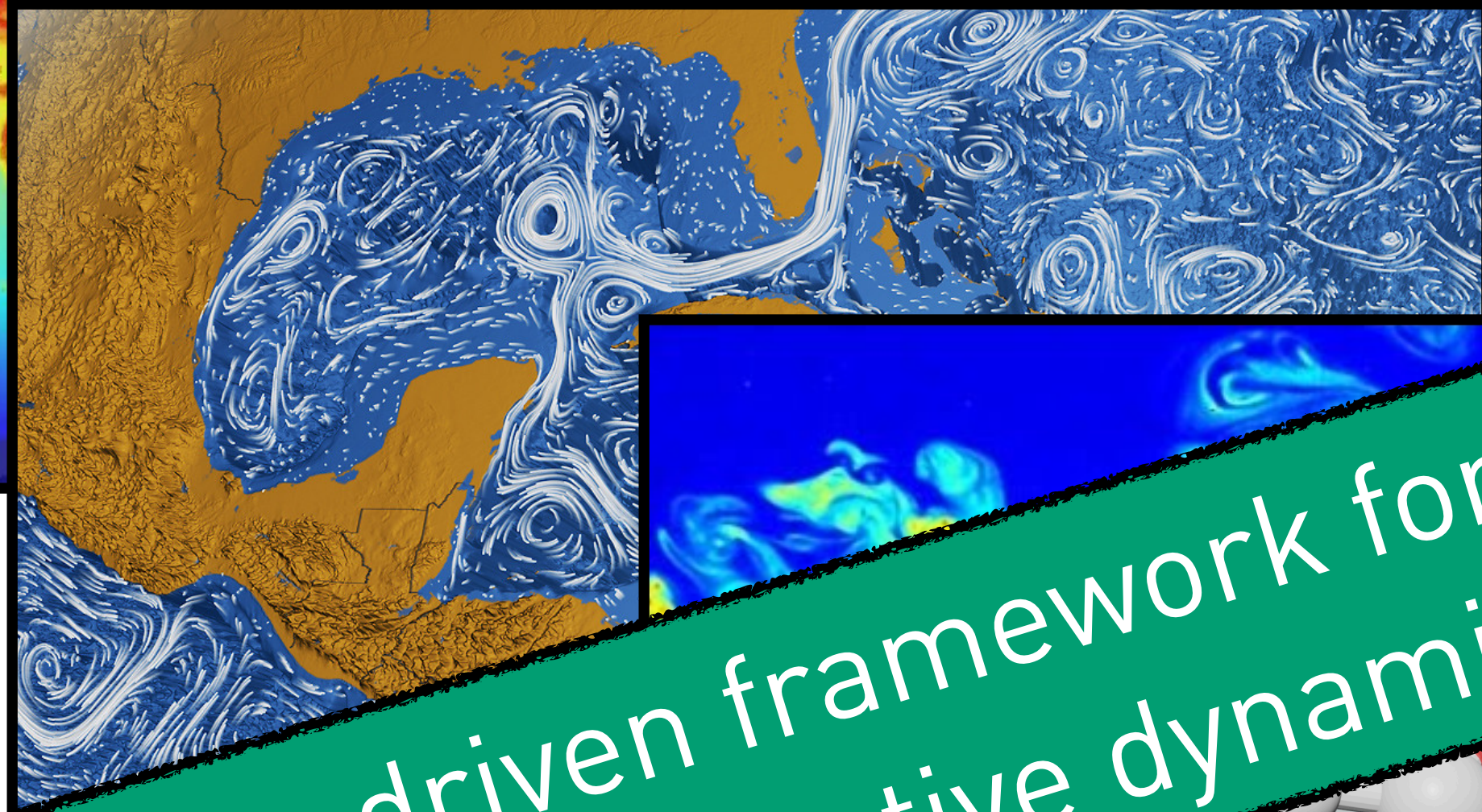
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  - Examples:
    - LES/RANS
    - Surrogate models / DMD
    - Coarse graining models of  
molecular systems



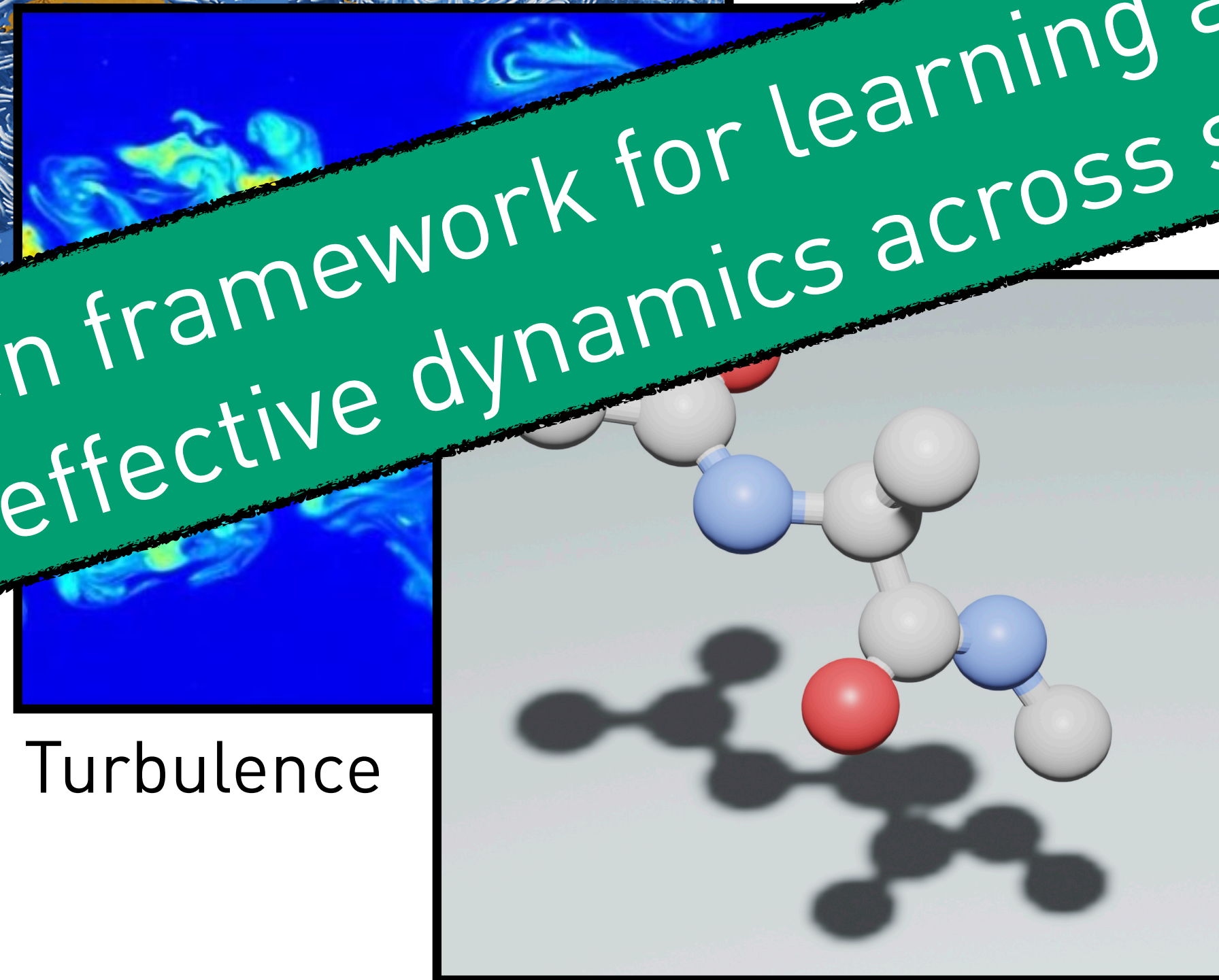
# Motivation



Climate



Turbulence



Proteins

- Complex multiscale systems  
(deterministic, stochastic, chaotic)

- Dynamics exhibit extreme variability and/or

Data-driven framework for learning and forecasting effective dynamics across scales

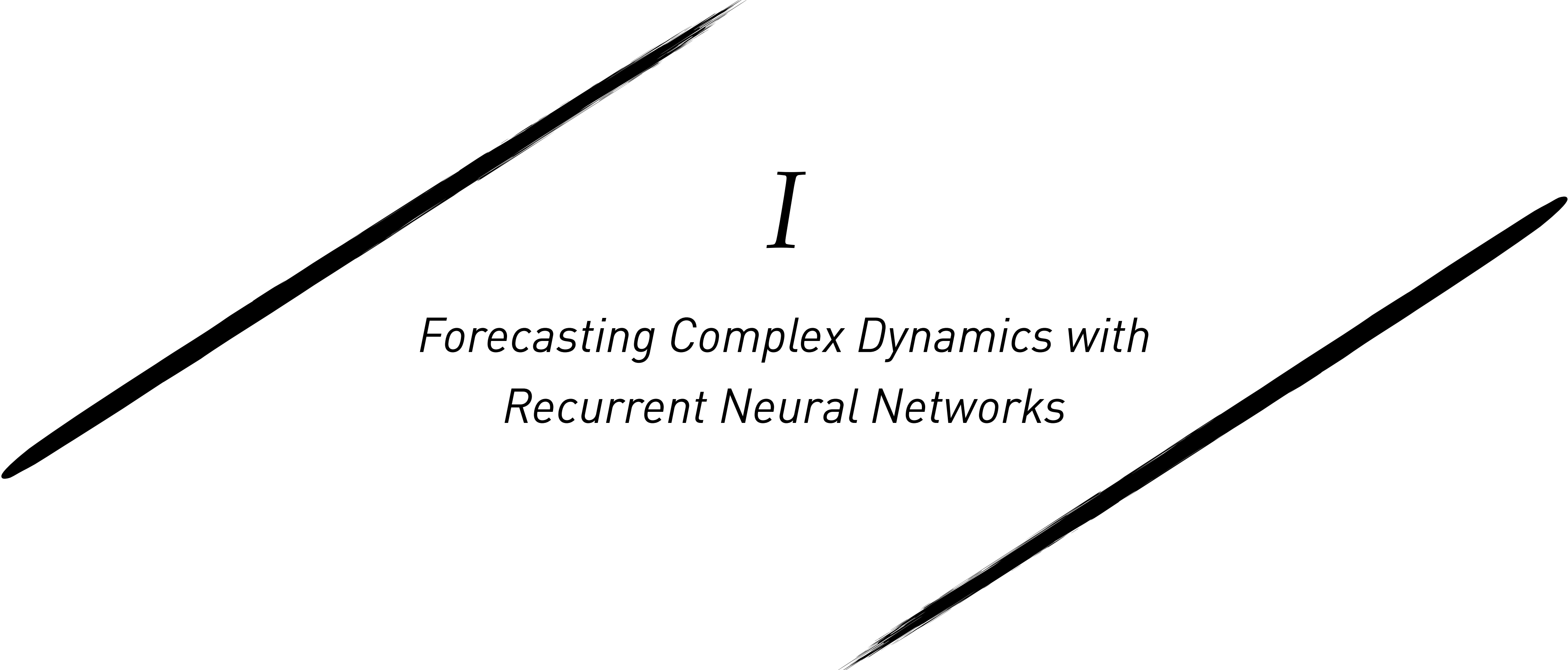
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nm





*I*

*Forecasting Complex Dynamics with  
Recurrent Neural Networks*

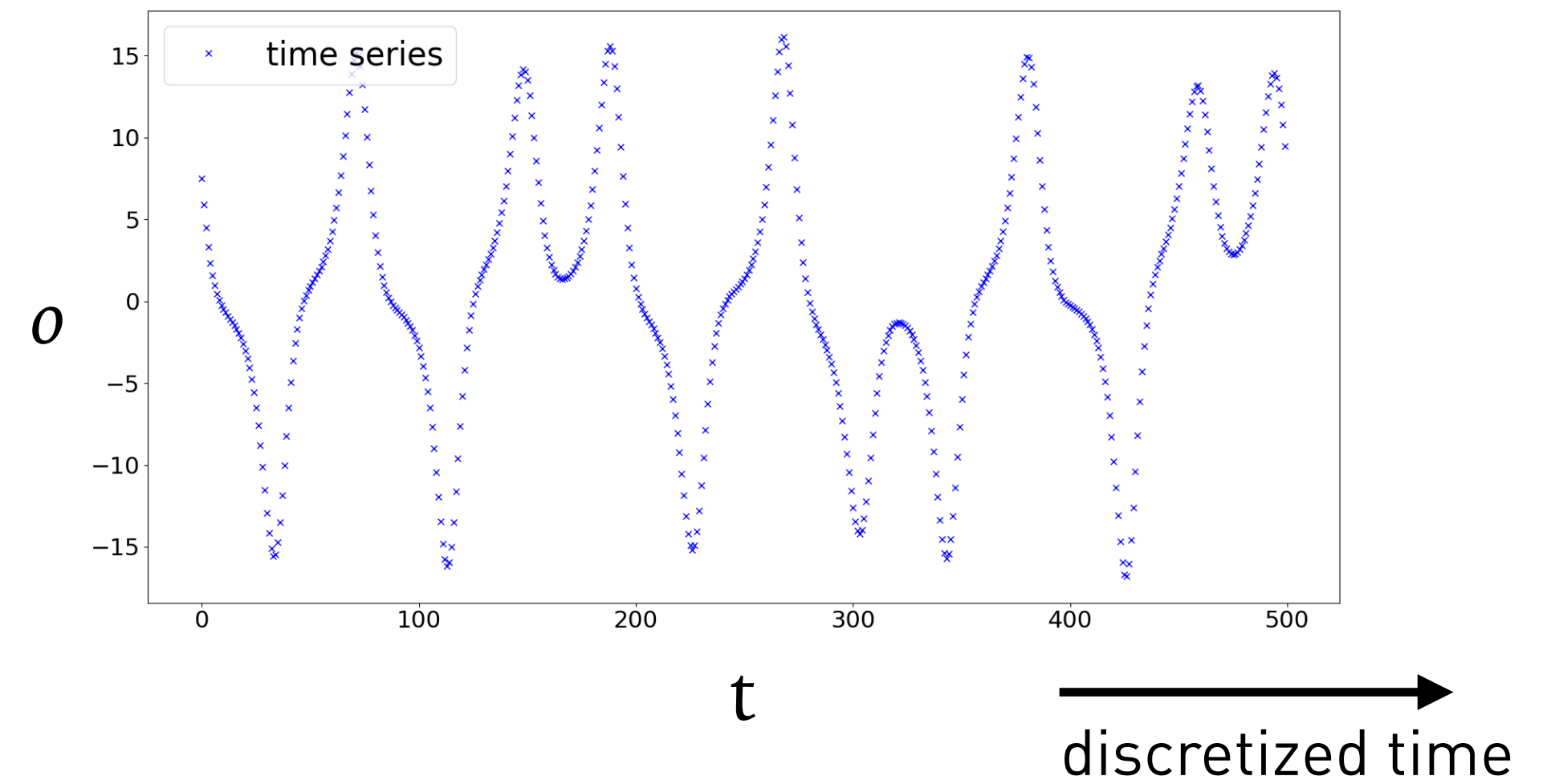


# Recurrent Neural Networks (RNNs)

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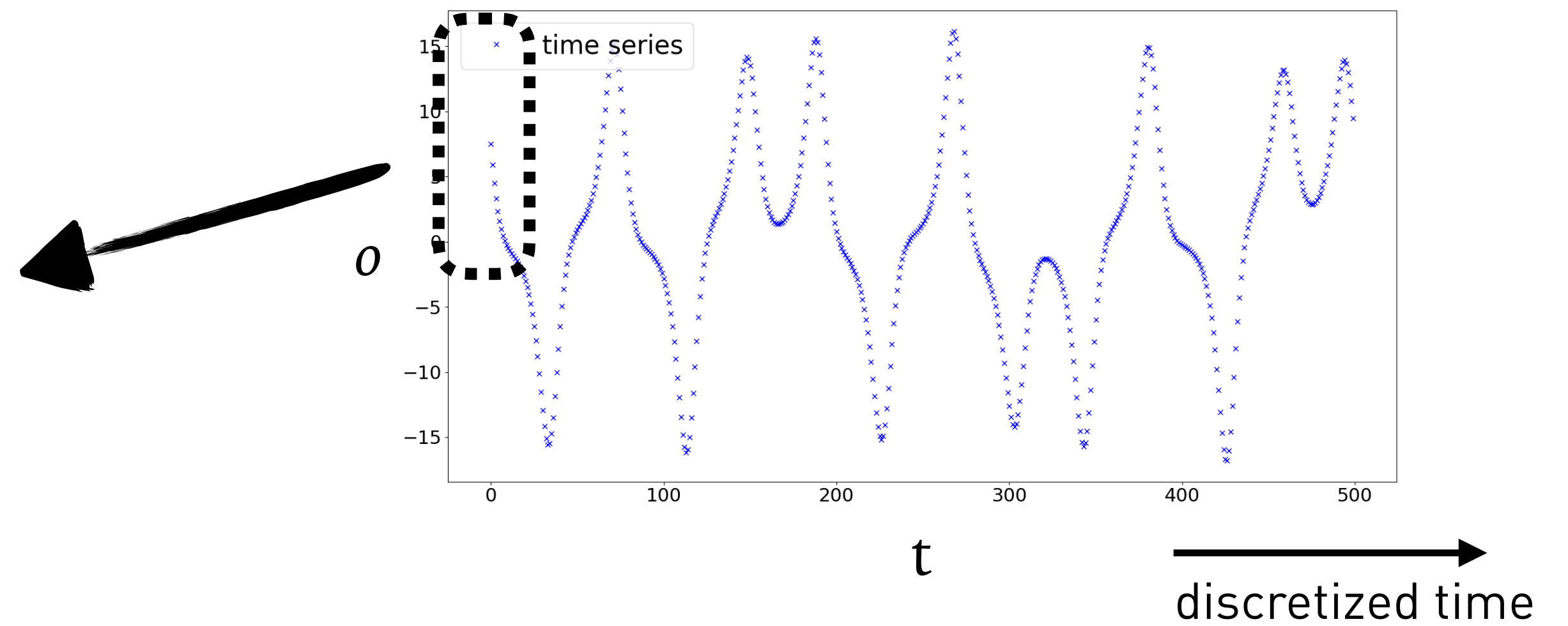


## Data from trajectories

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



# Recurrent Neural Networks (RNNs)

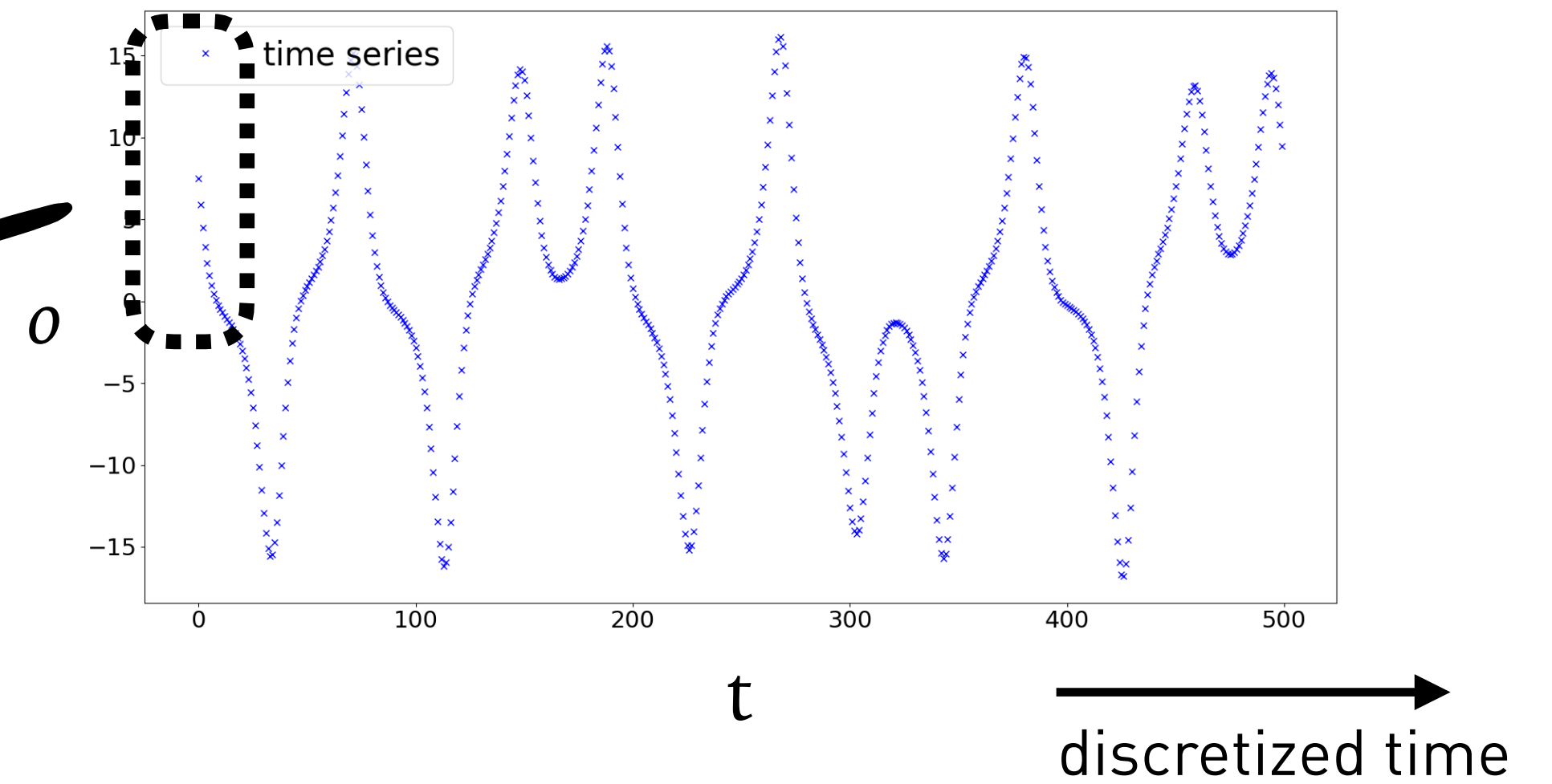
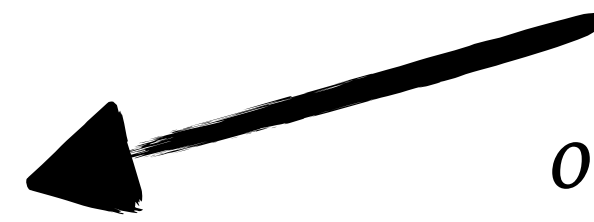
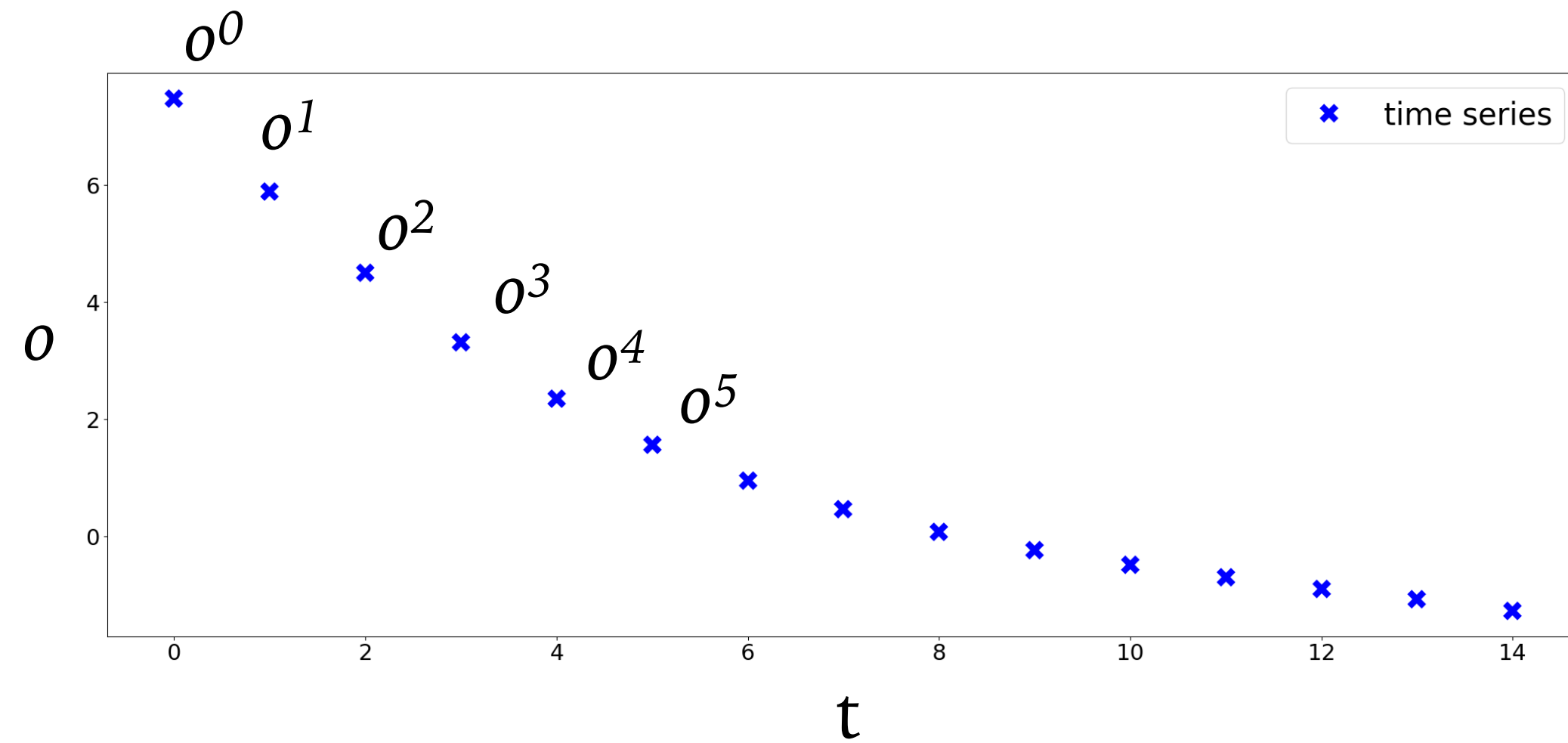


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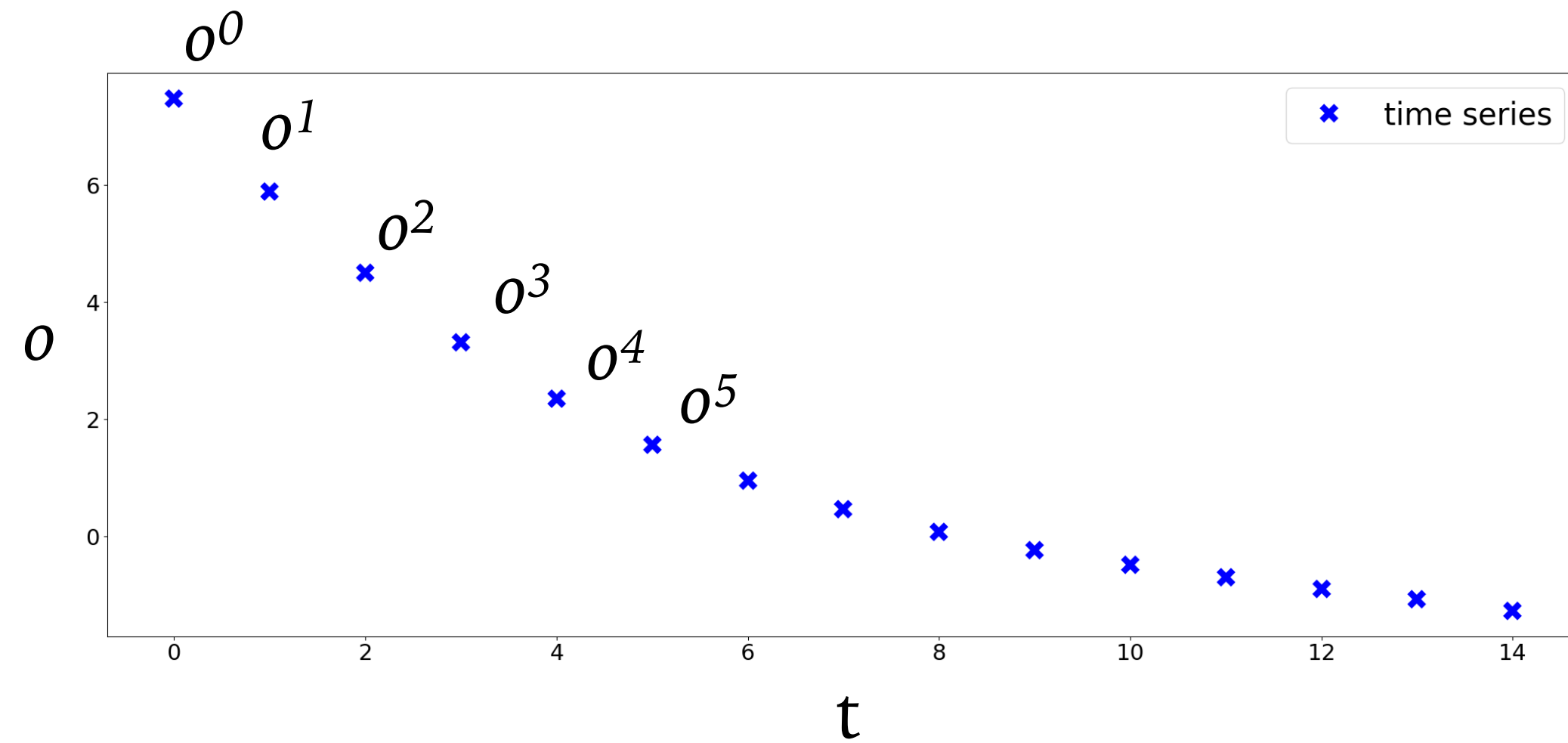


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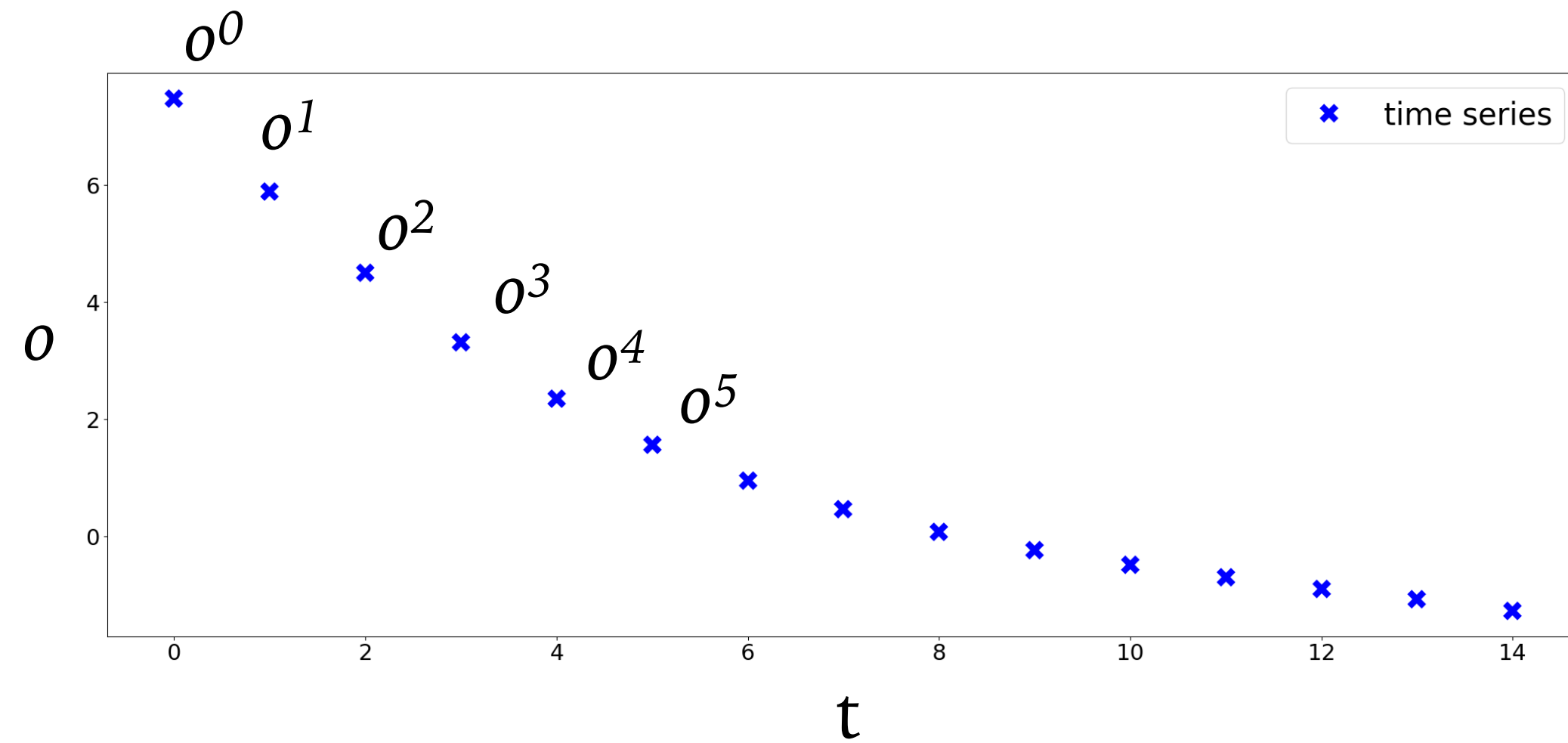
# Recurrent Neural Networks (RNNs)



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




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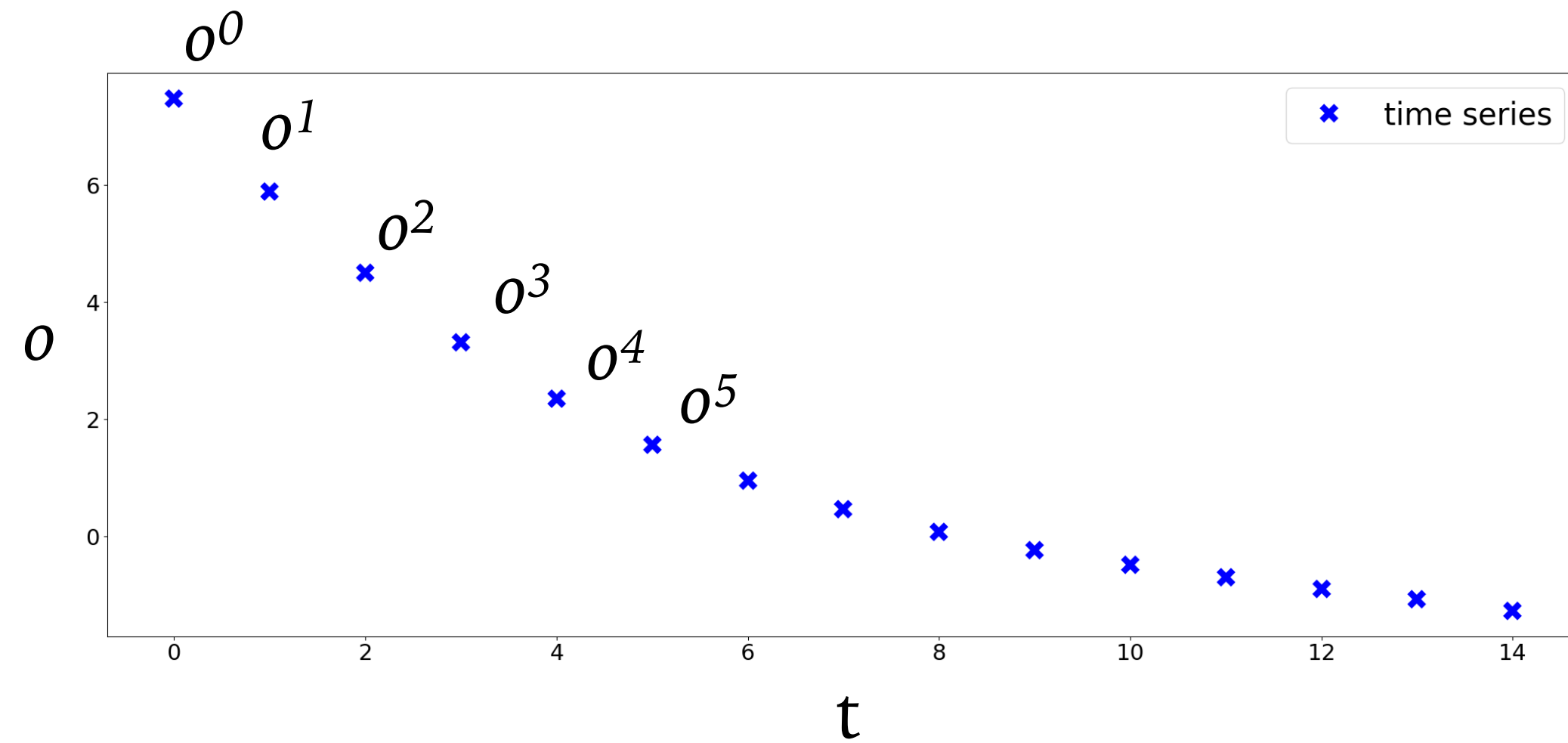
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history  
encoded in  $h^{t-1}$



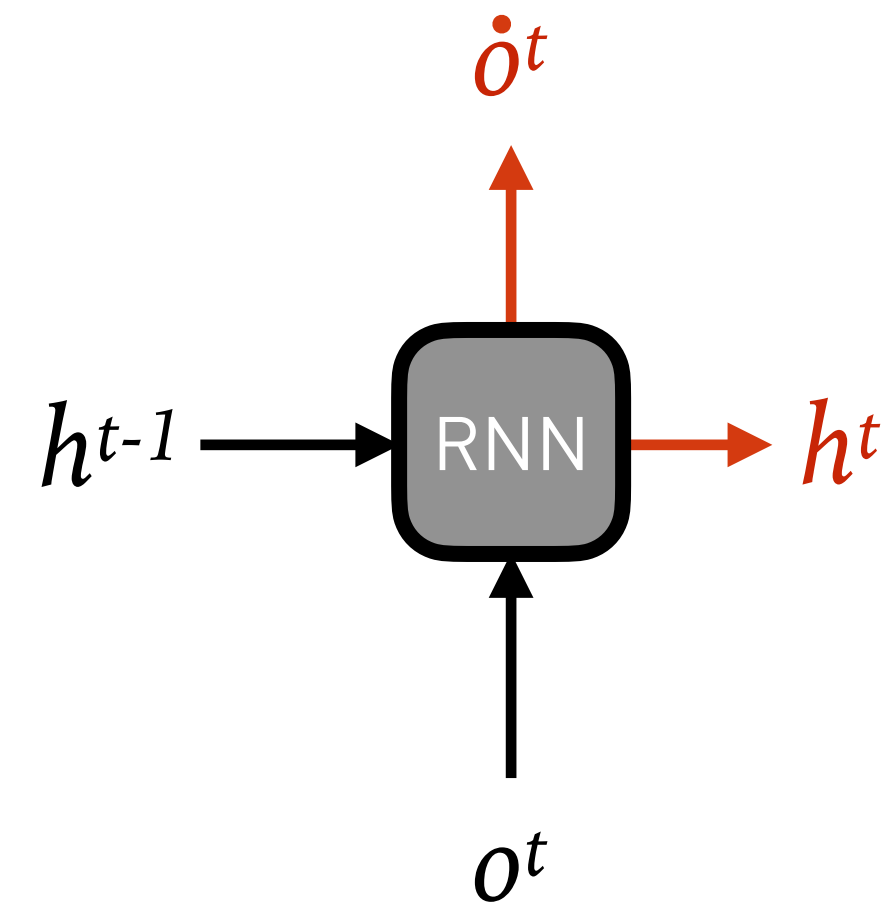


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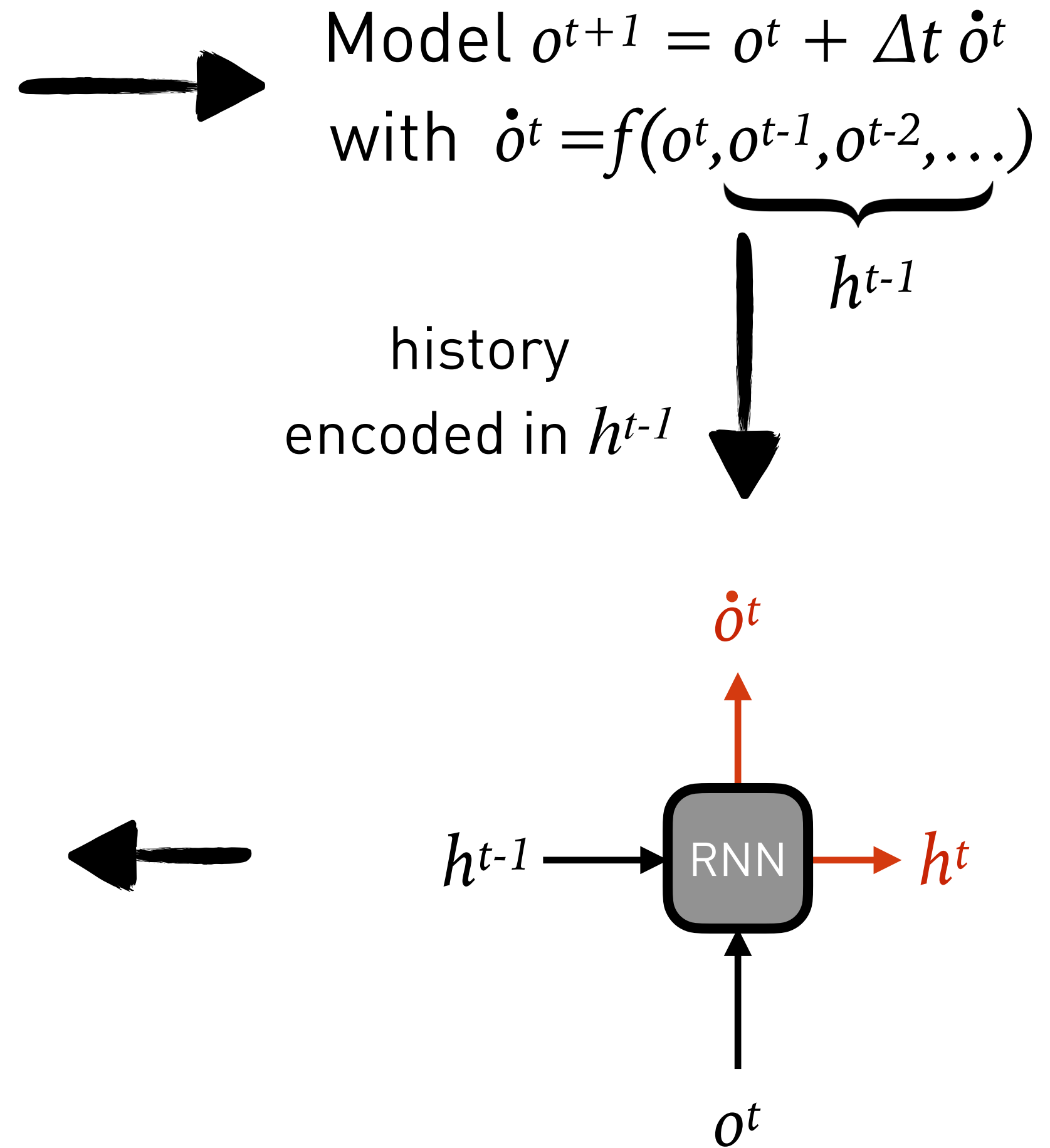
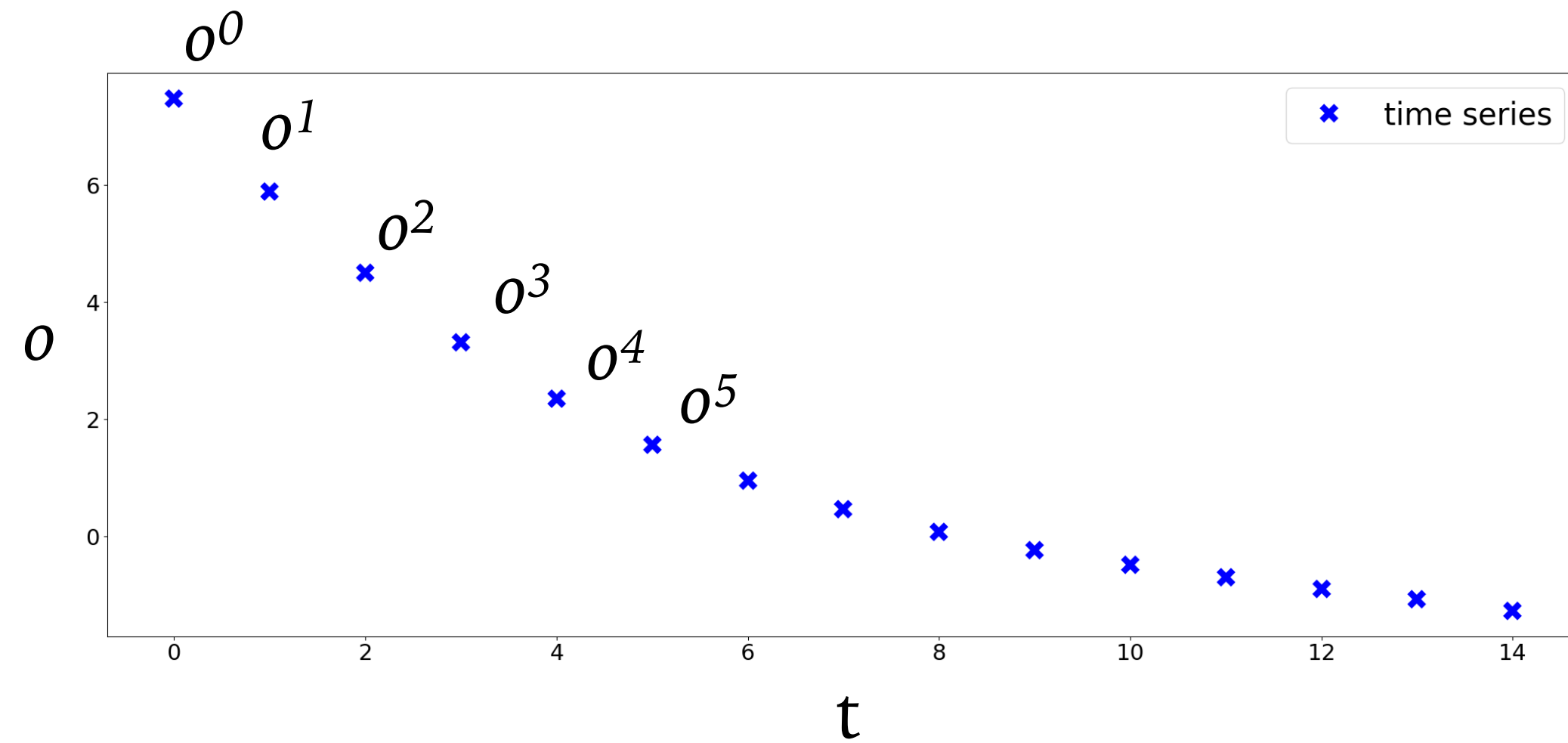
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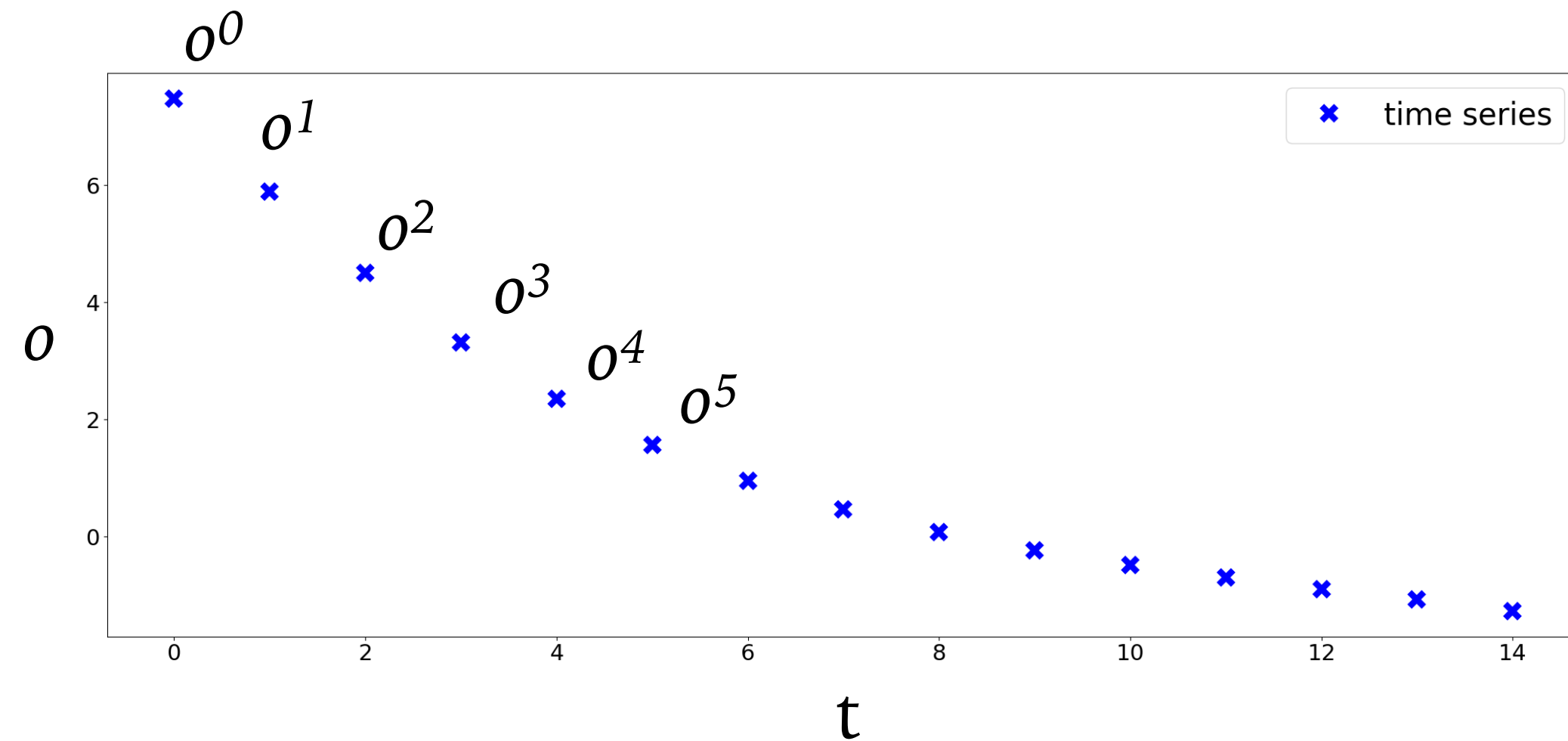


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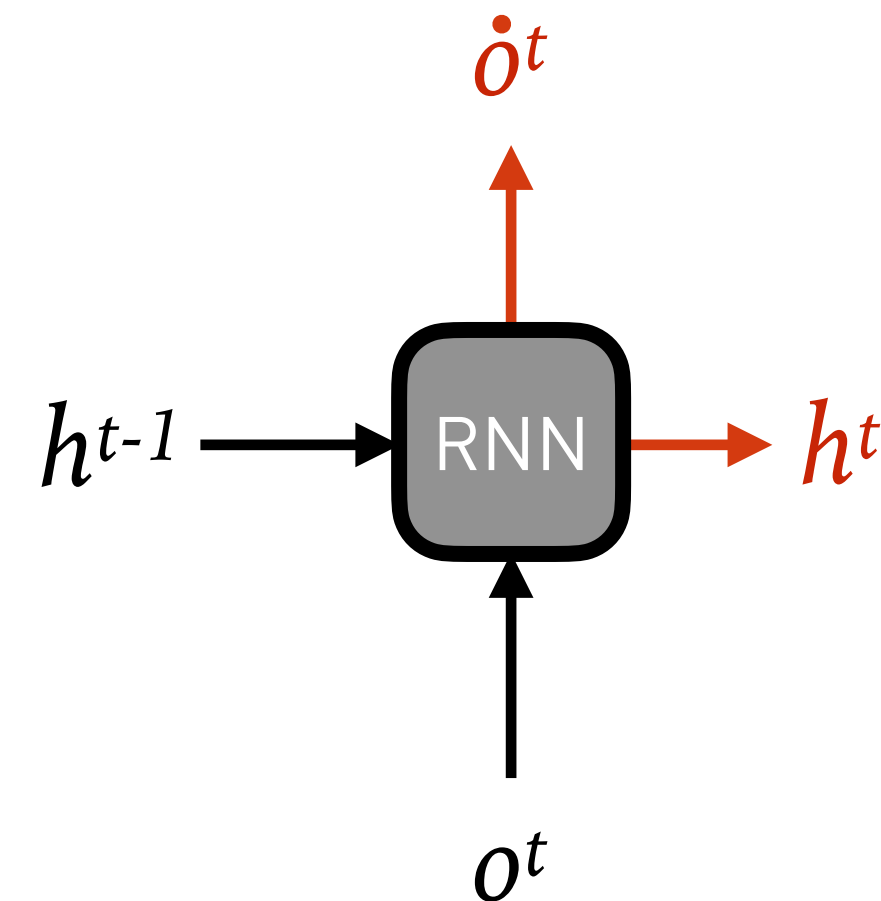
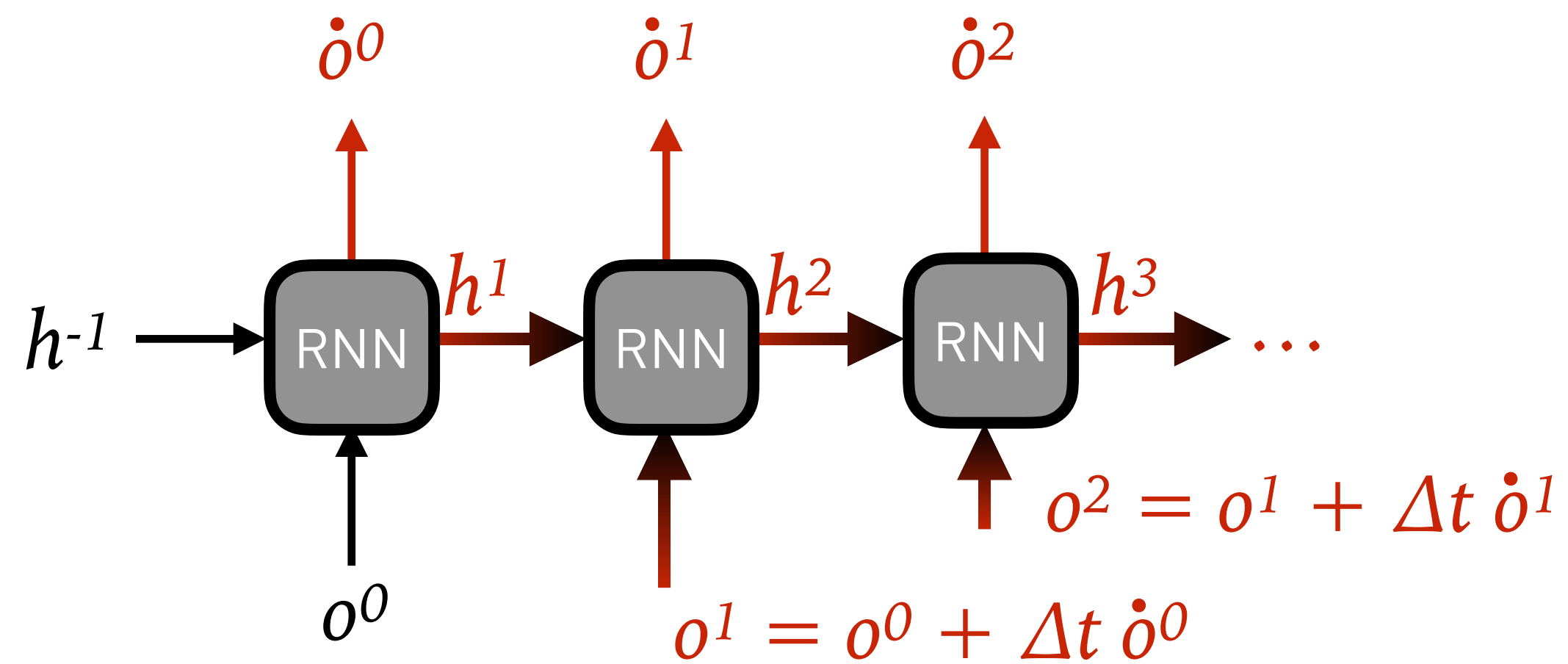


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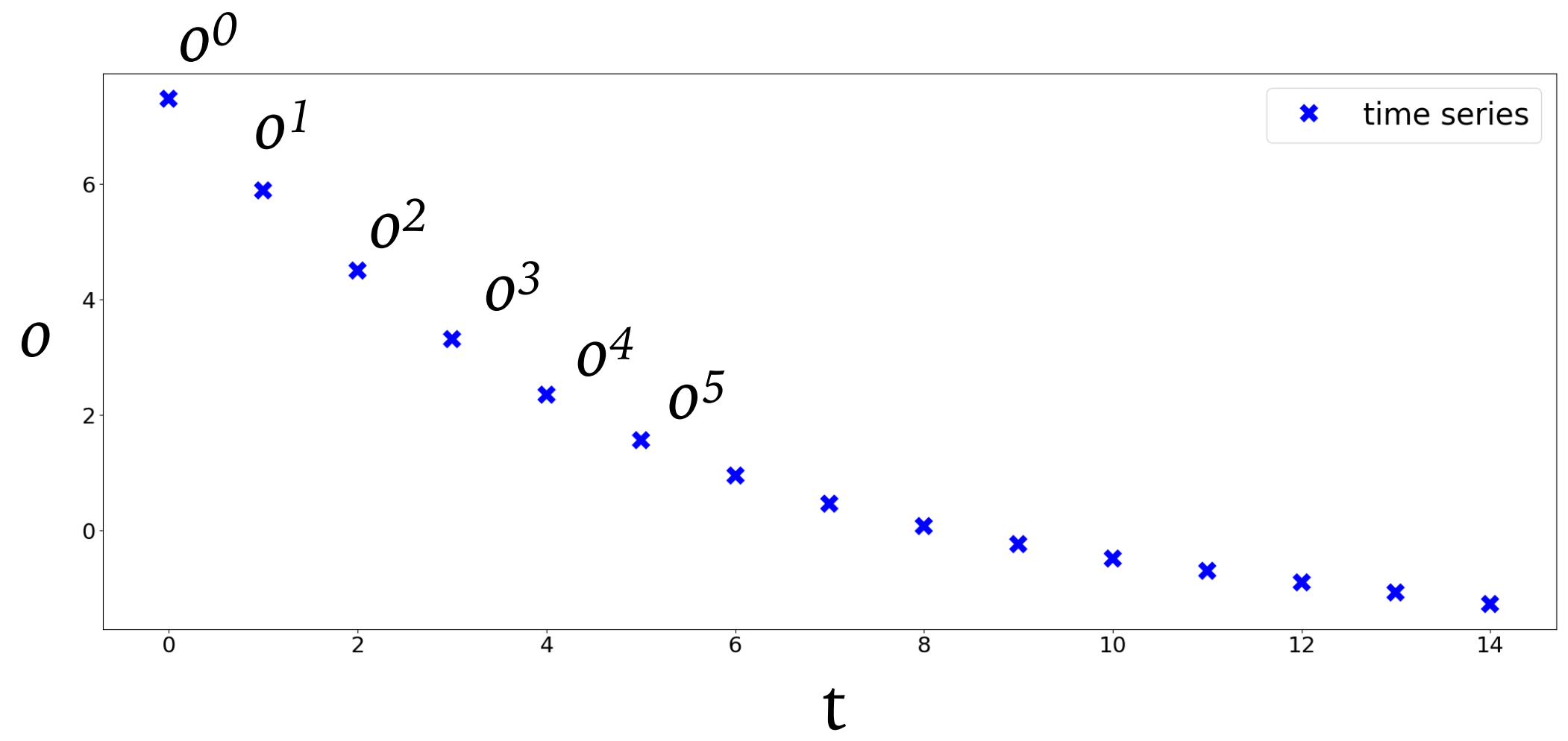
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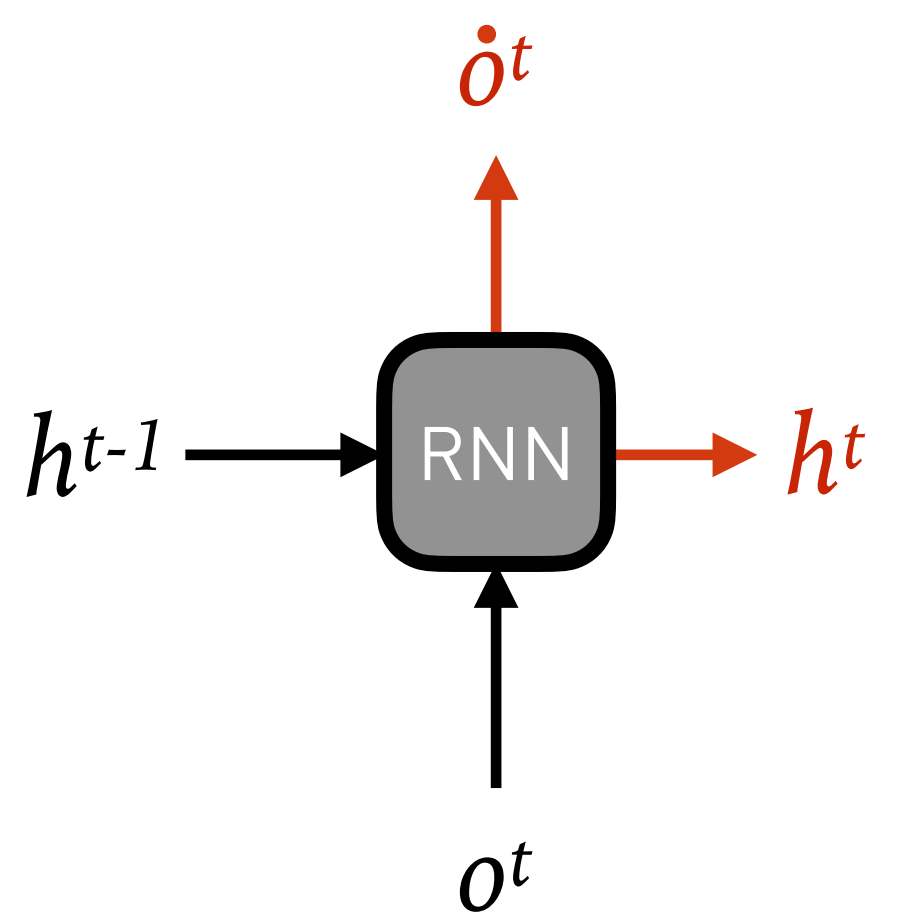
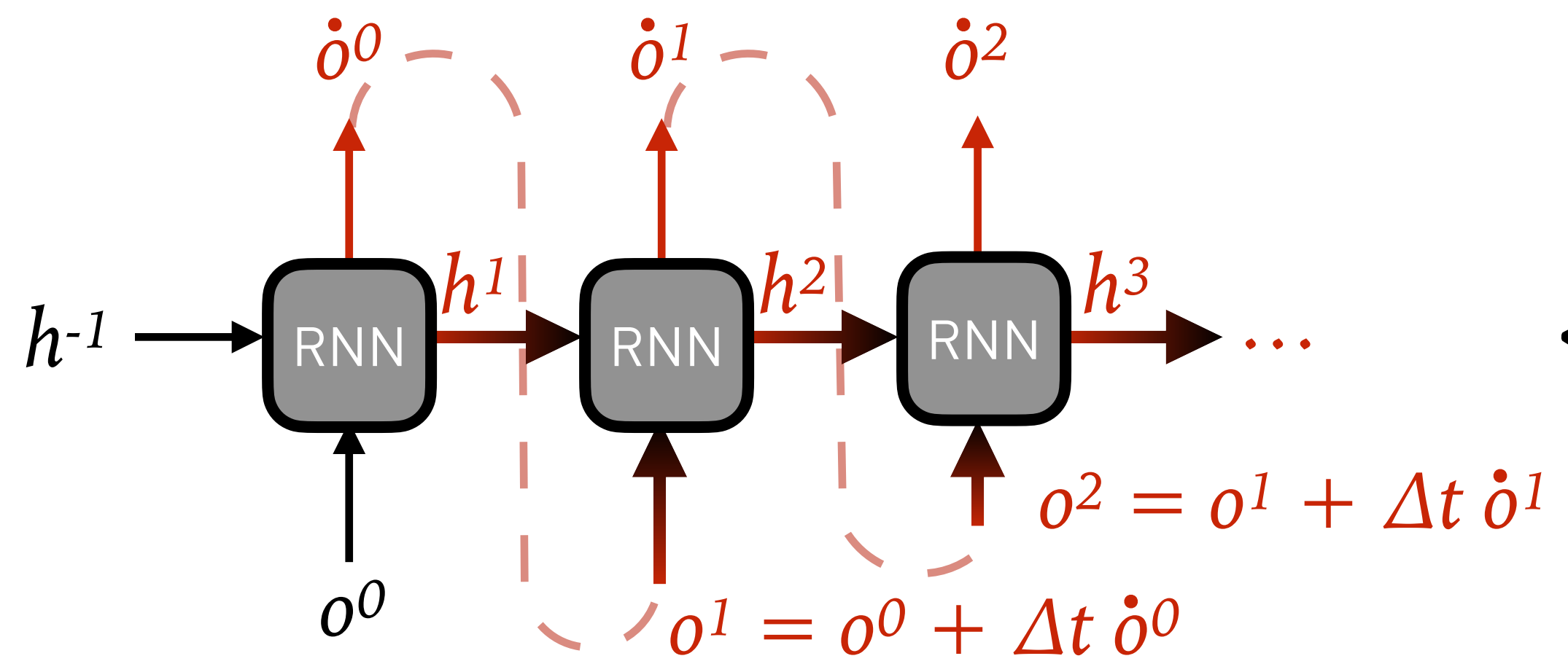


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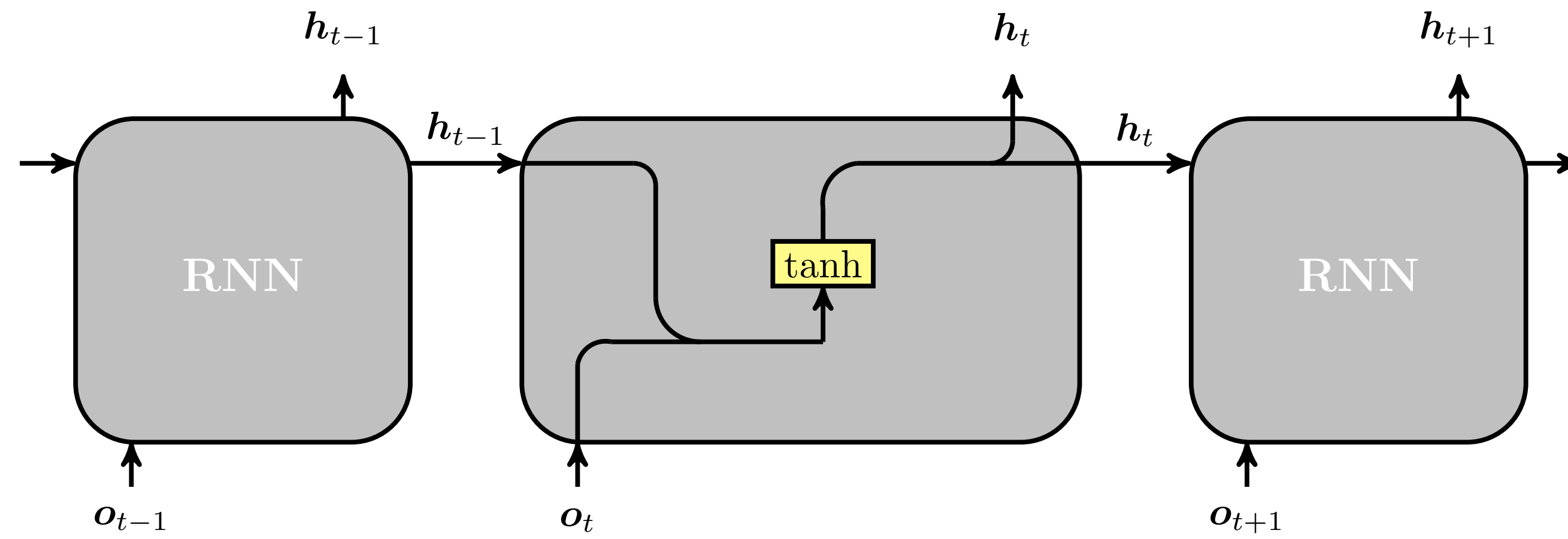
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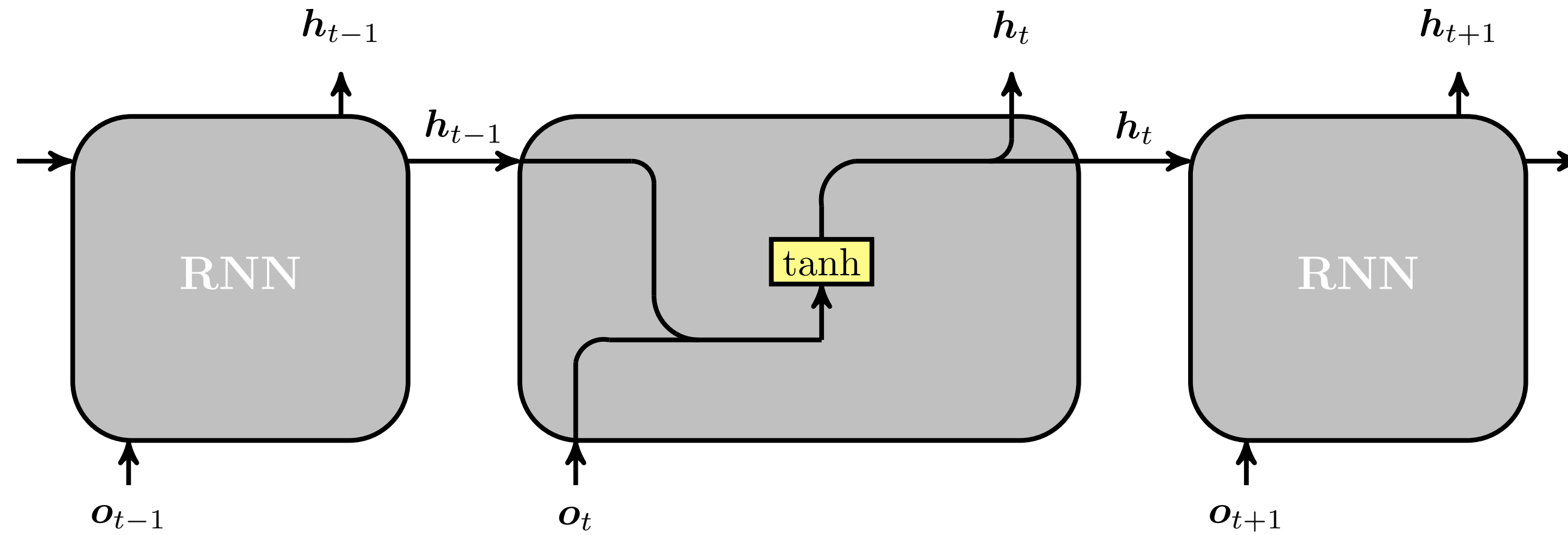


# Elman RNN (1990)





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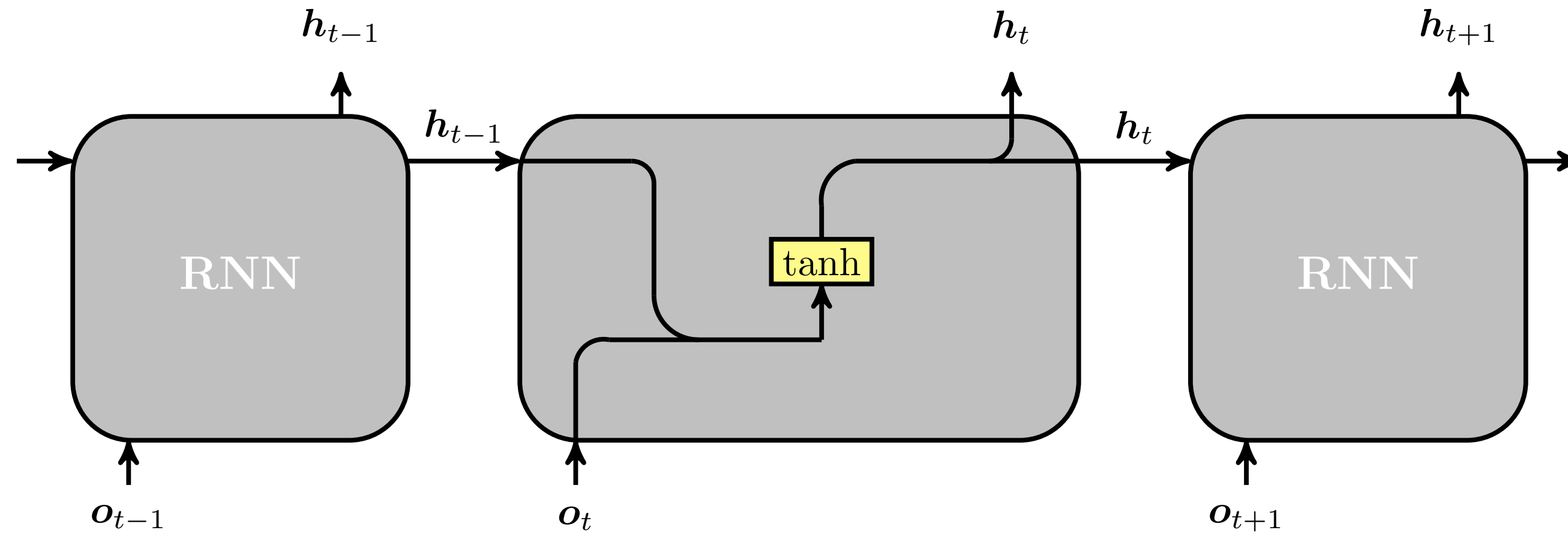


Hidden-to-hidden mapping

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



# Elman RNN (1990)



Hidden-to-hidden mapping

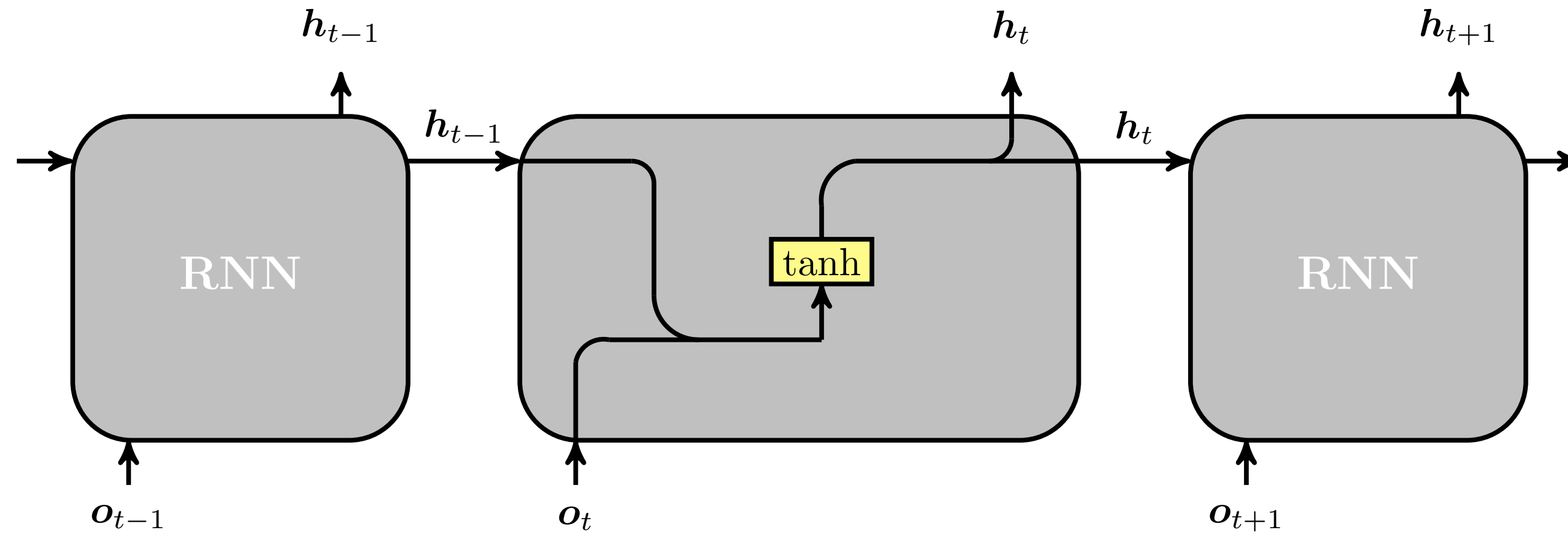
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Hidden-to-output mapping

$$y_t = W_{oh} h_t \begin{cases} \hat{=} o_{t+1} \\ \text{or} \\ \hat{=} \dot{o}_t \end{cases}$$



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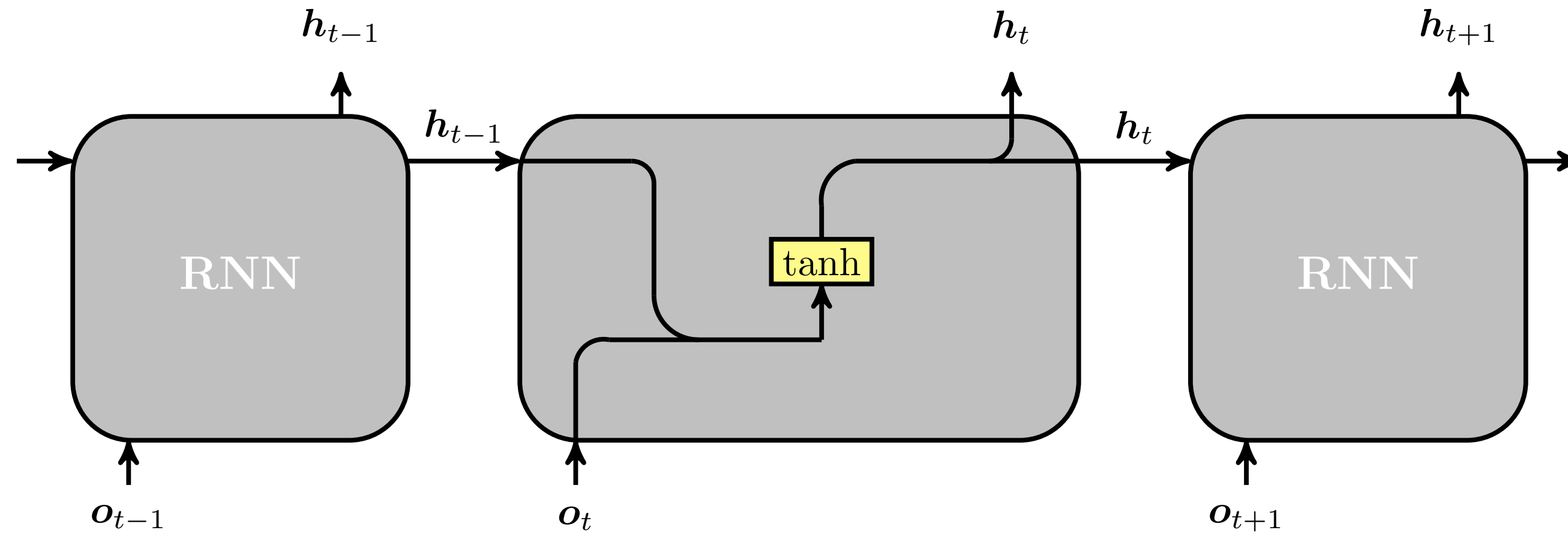
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Parameters (WEIGHTS) to be learned:

$$W_{ho}, W_{hh}, b_h, W_{oh}$$



# Elman RNN (1990)



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

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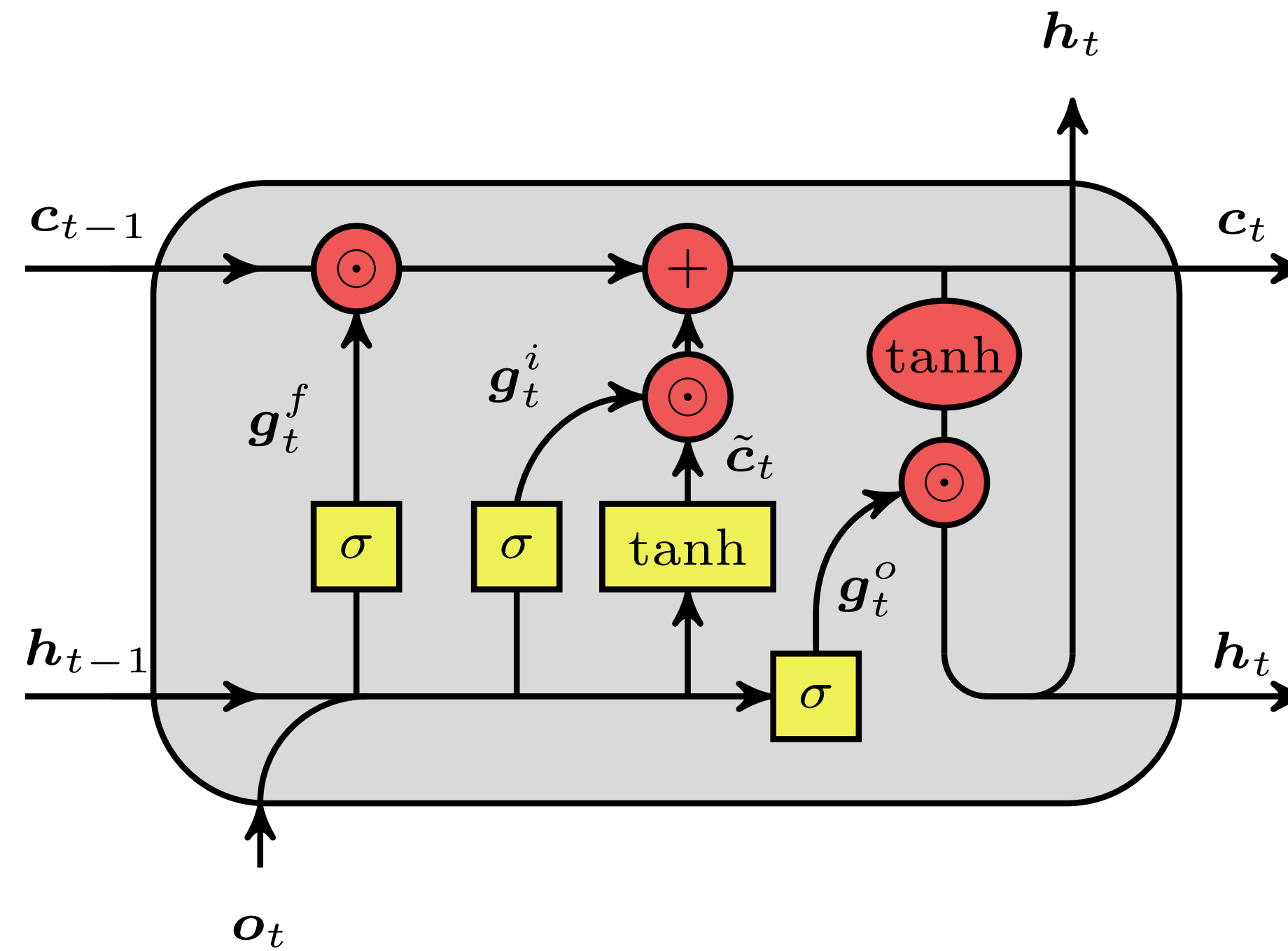
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# Long Short-Term Memory (LSTM) S. Hochreiter and J. Schmidhuber (1997)



Long Short-Term Memory Cell



# Kuramoto-Sivashinsky

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



# Kuramoto-Sivashinsky

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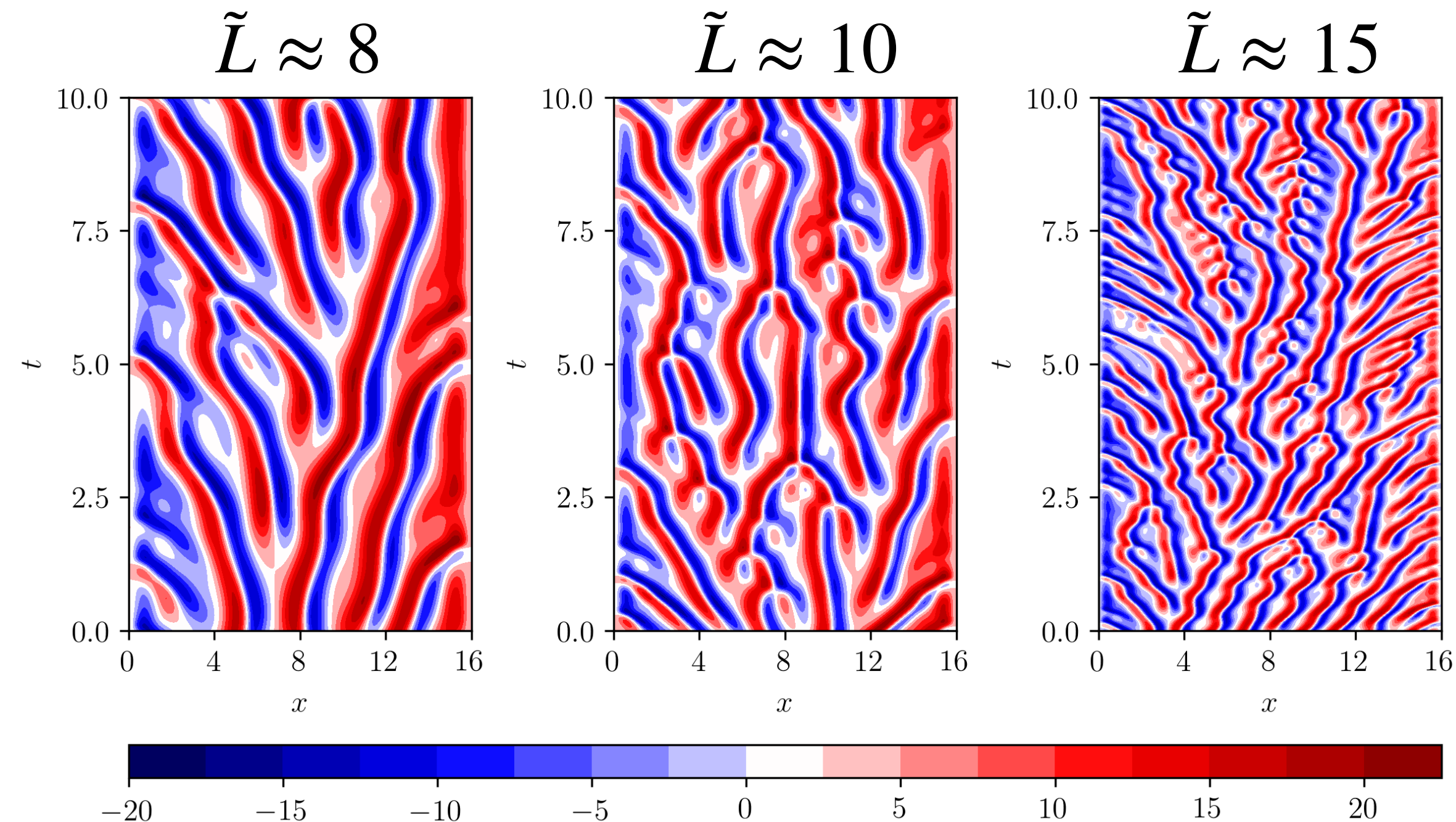
- Fourth order PDE, negative viscosity  $\nu$
- Dirichlet & second order boundary conditions
- Domain  $x \in [0, L]$ ,  $L = 16$
- **Chaoticity scales with bifurcation parameter**

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



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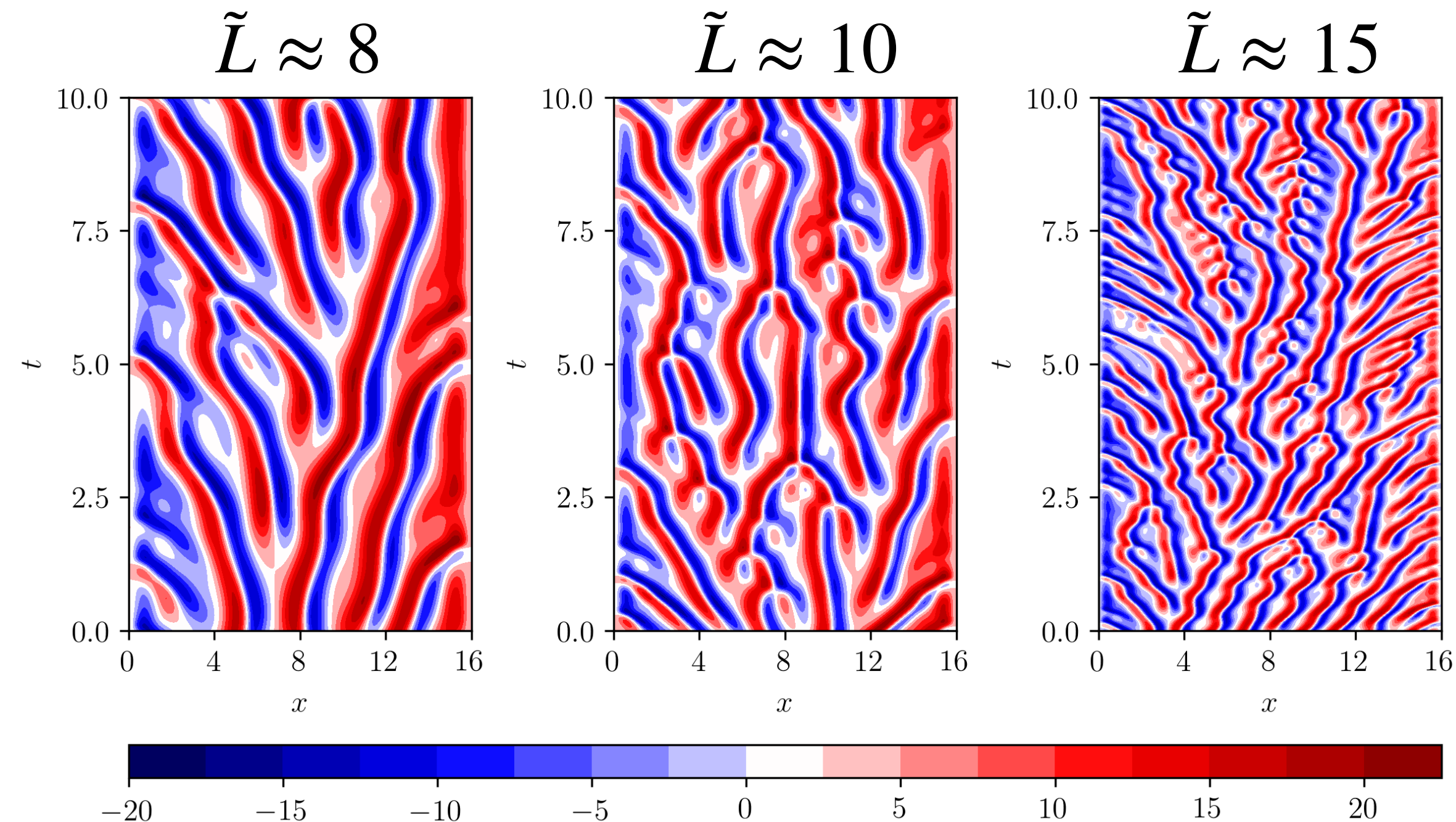
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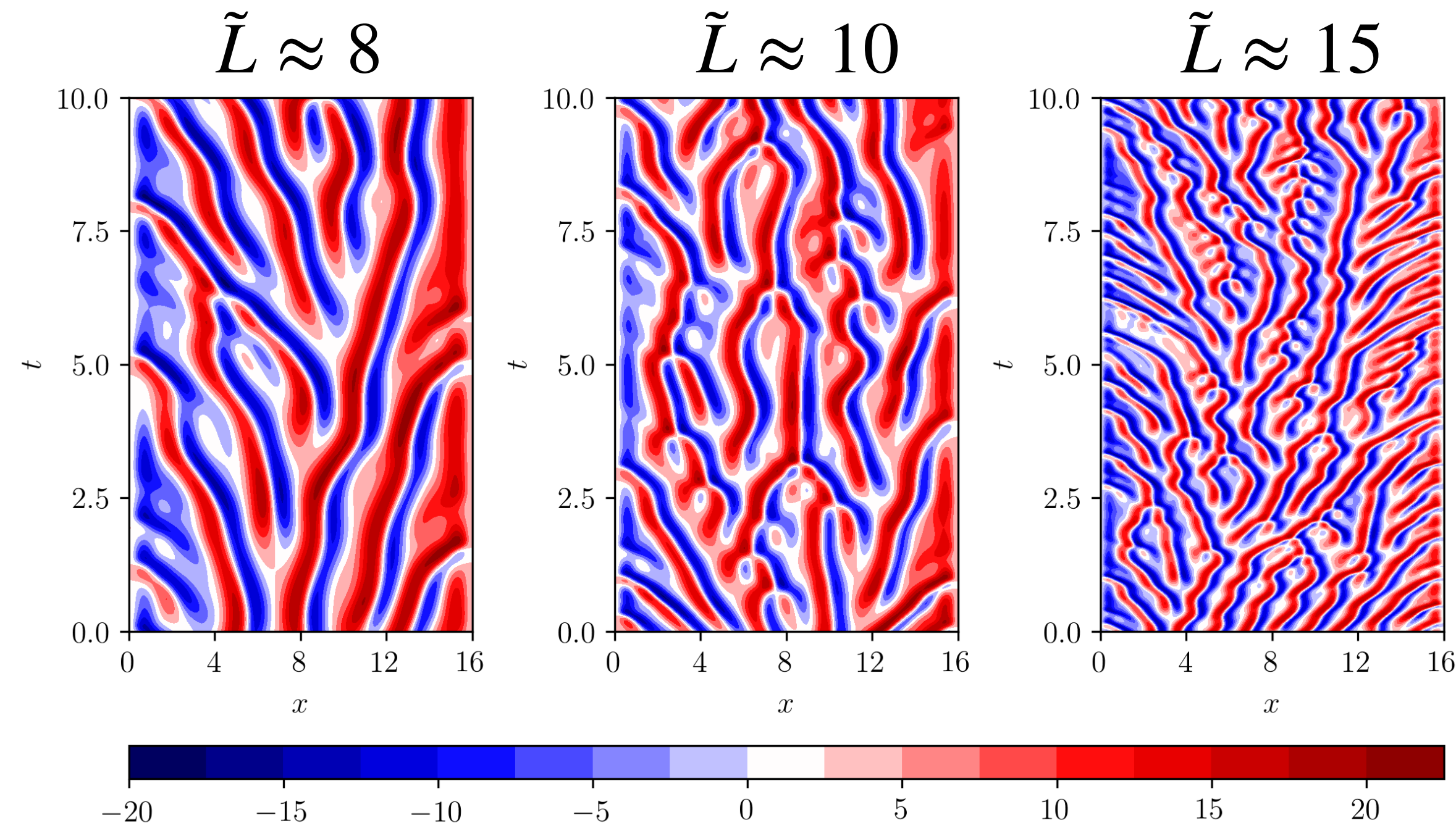
Discretization with  
 $d_u = 512$  gridpoints

$$d_u = \frac{L}{\Delta x}$$



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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

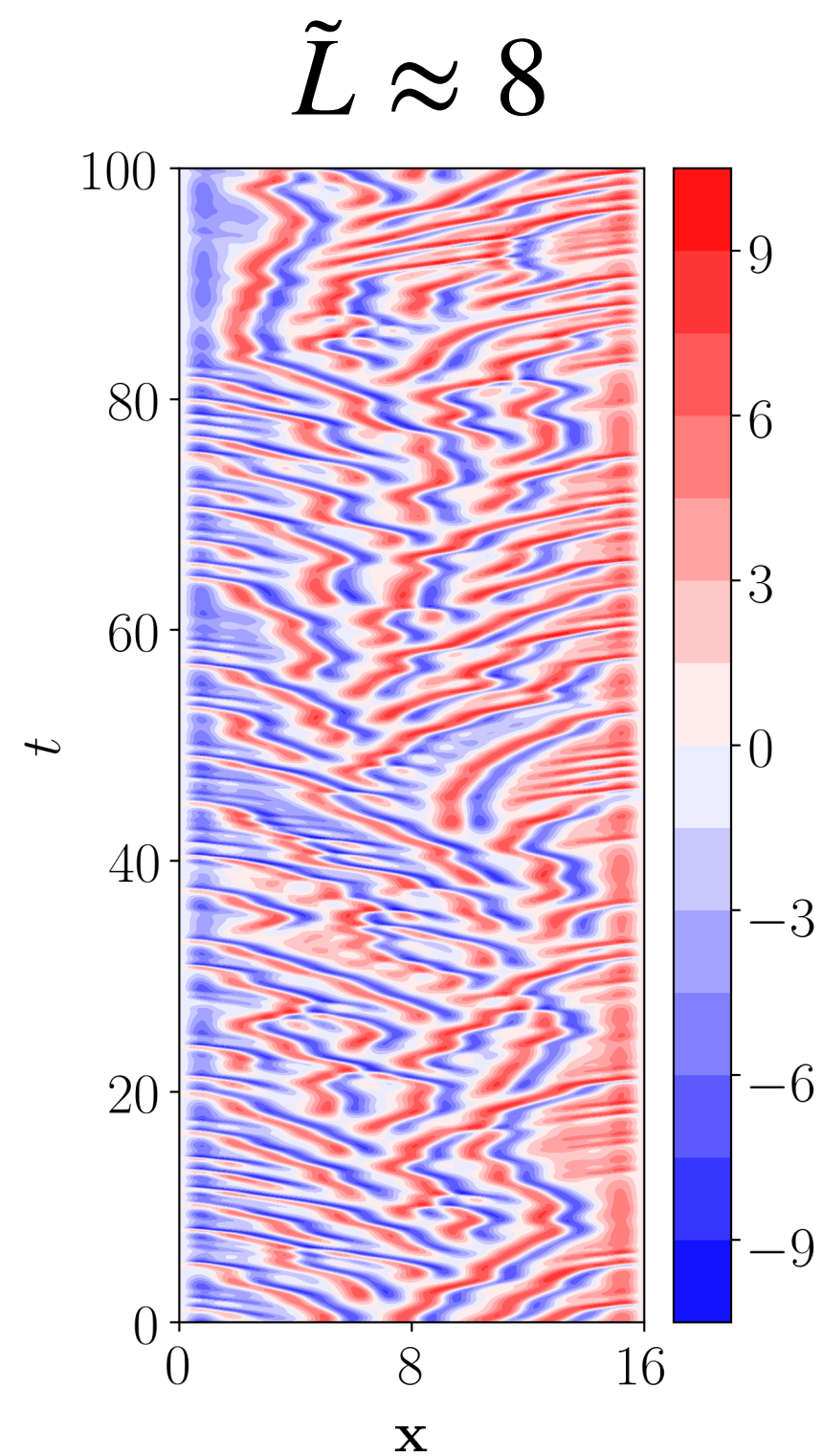
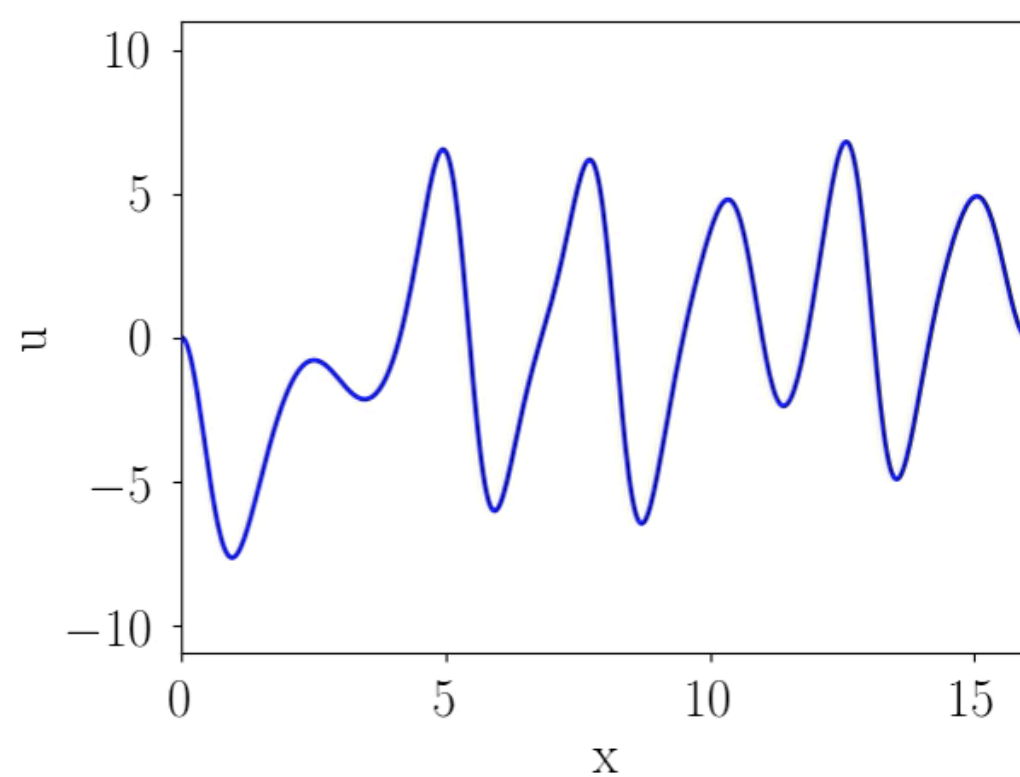


# Constructing the observable - training data

*High dimensional*

High dimensional  
simulation data

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



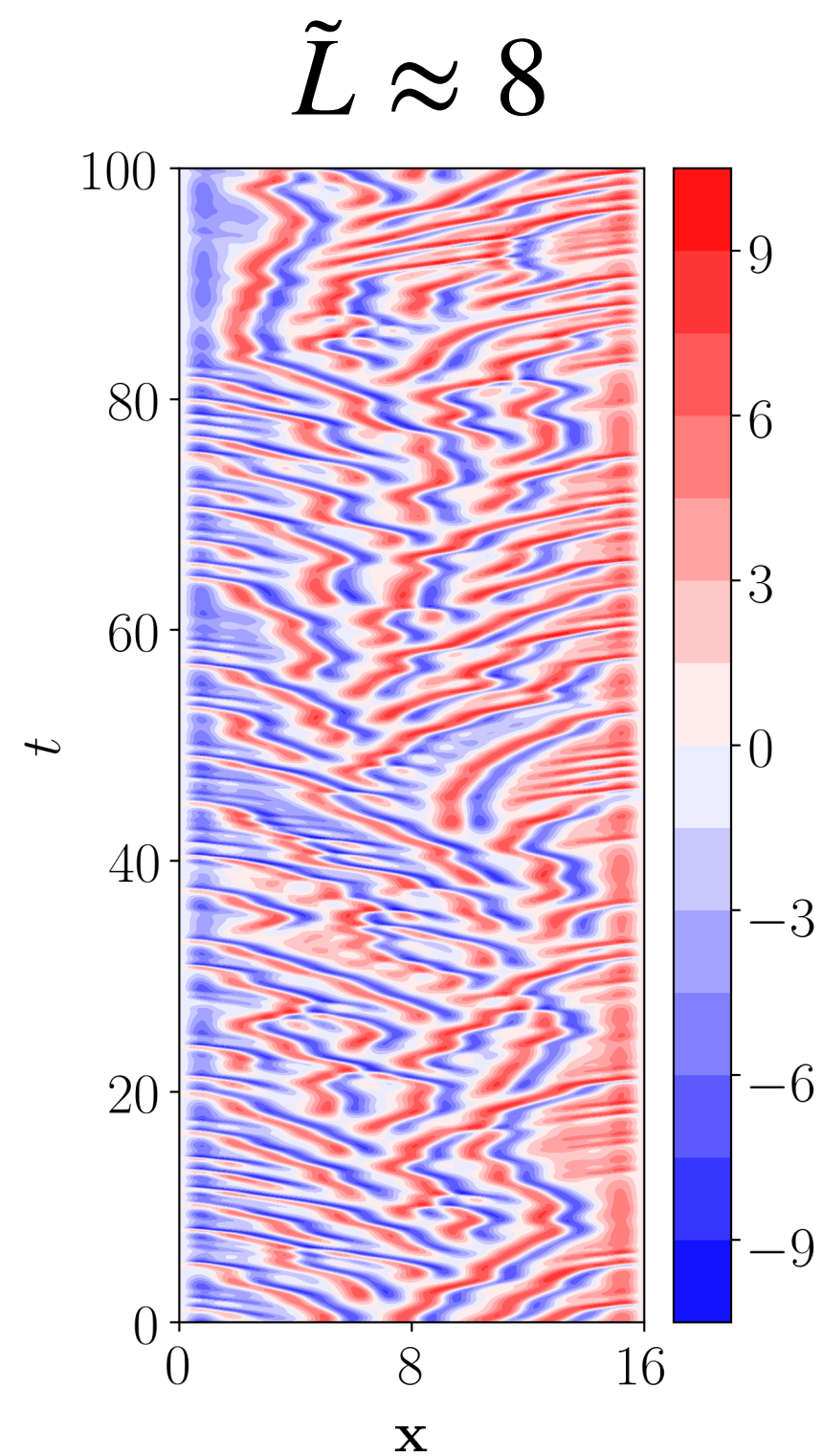
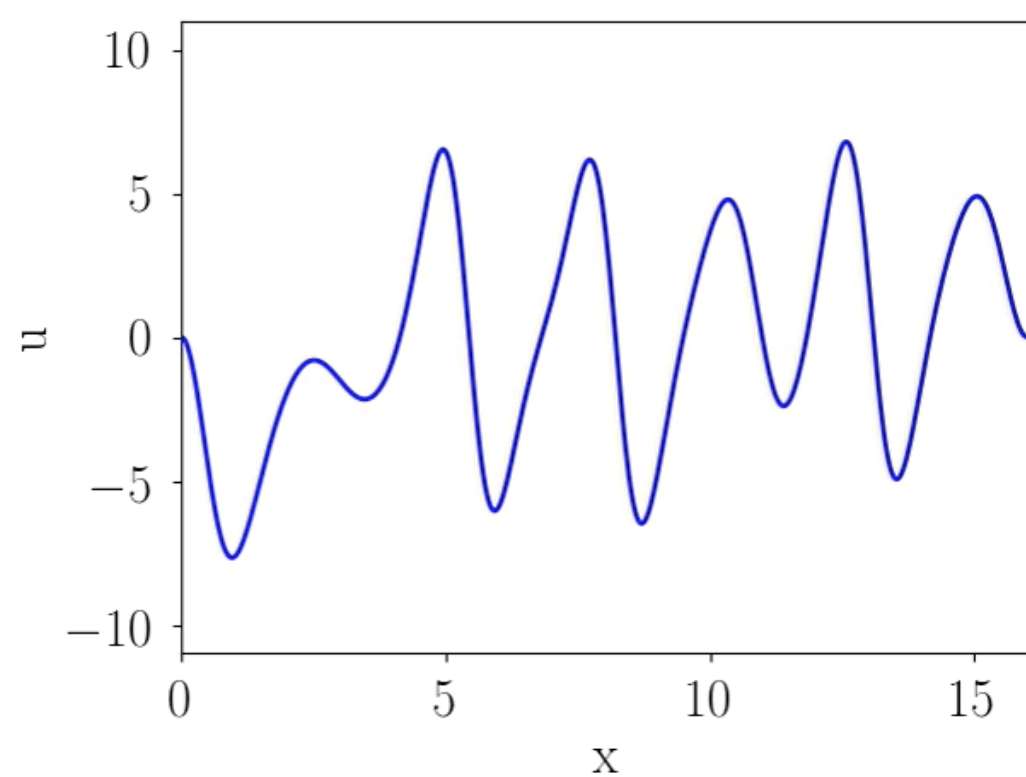


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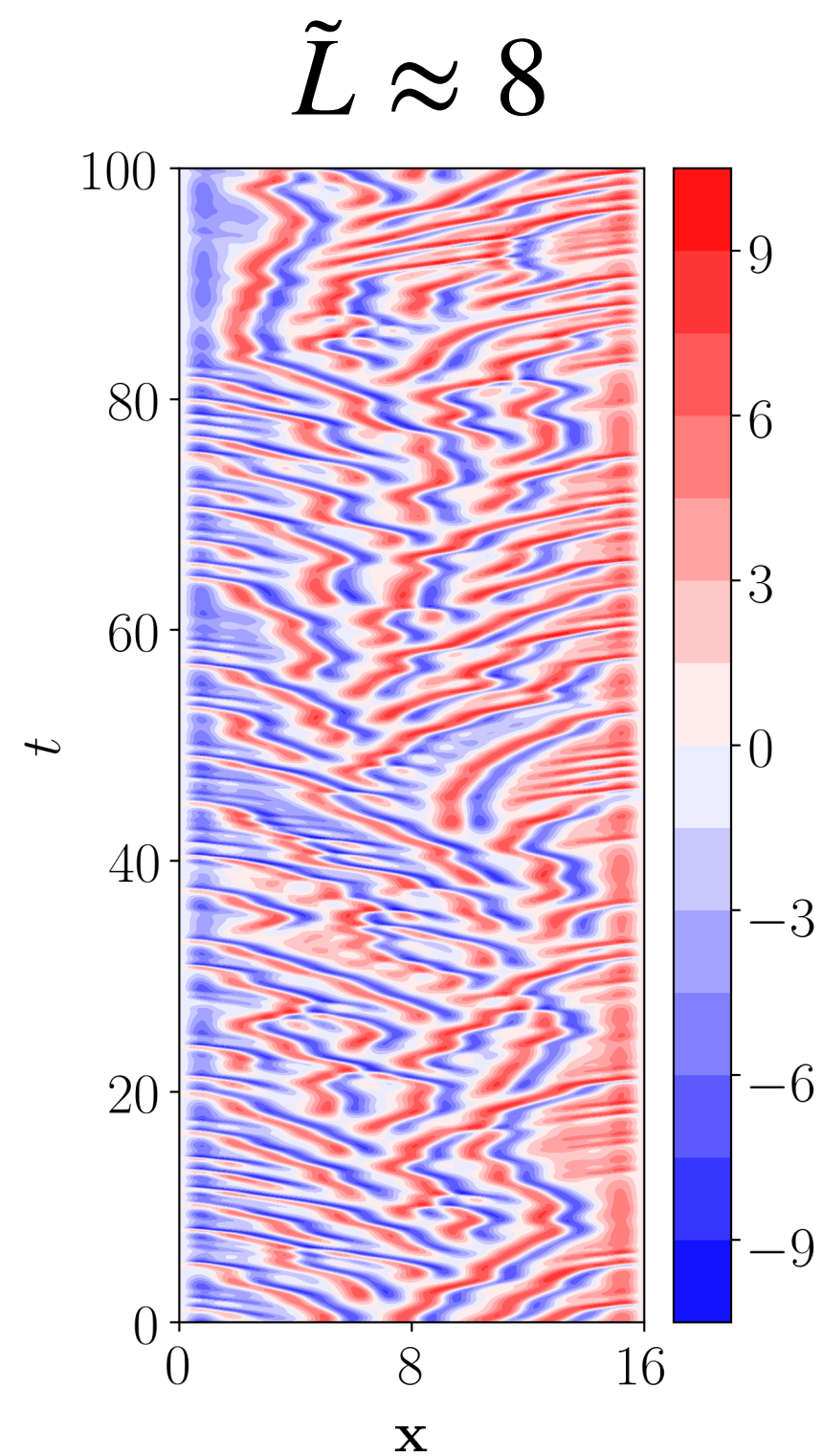
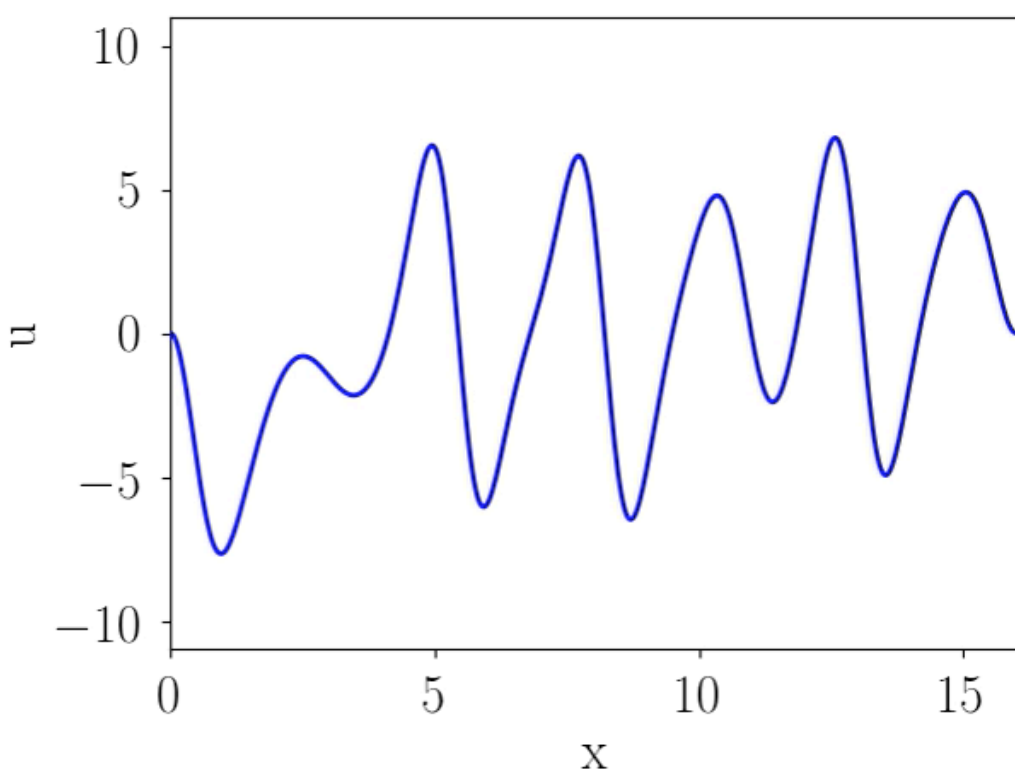


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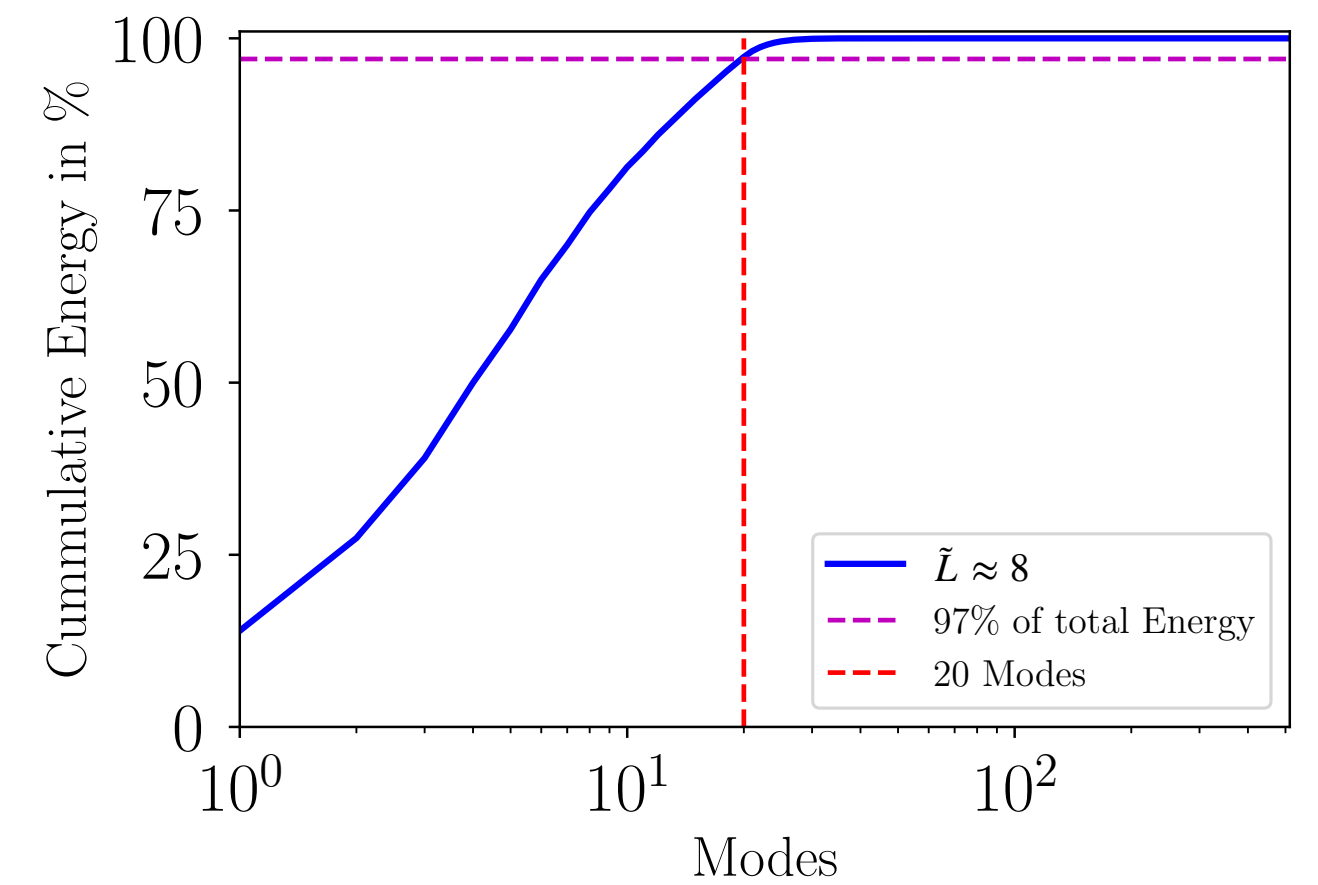
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$\tilde{L} \approx 8$

SVD / PCA

Singular Value  
Decomposition



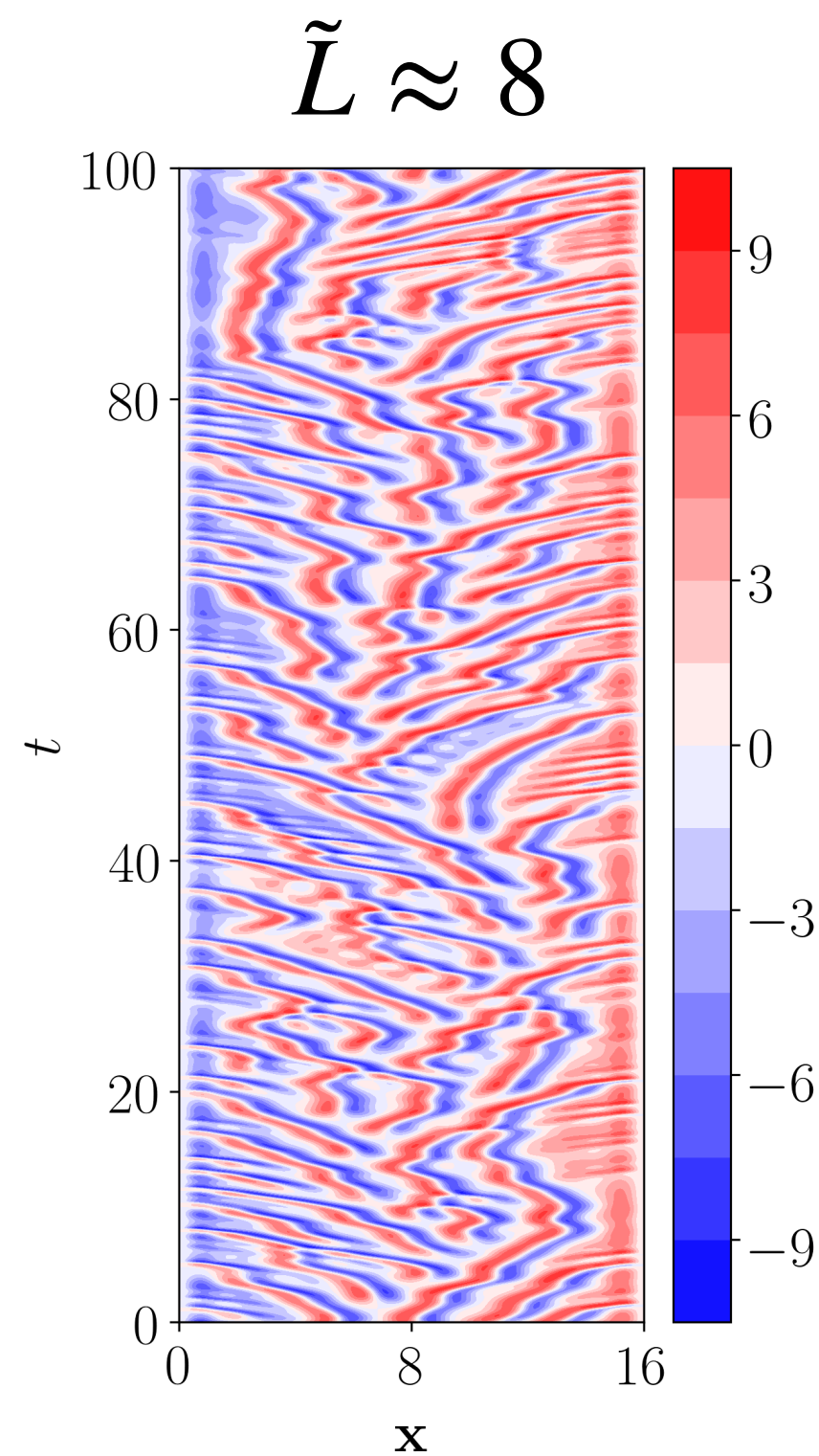
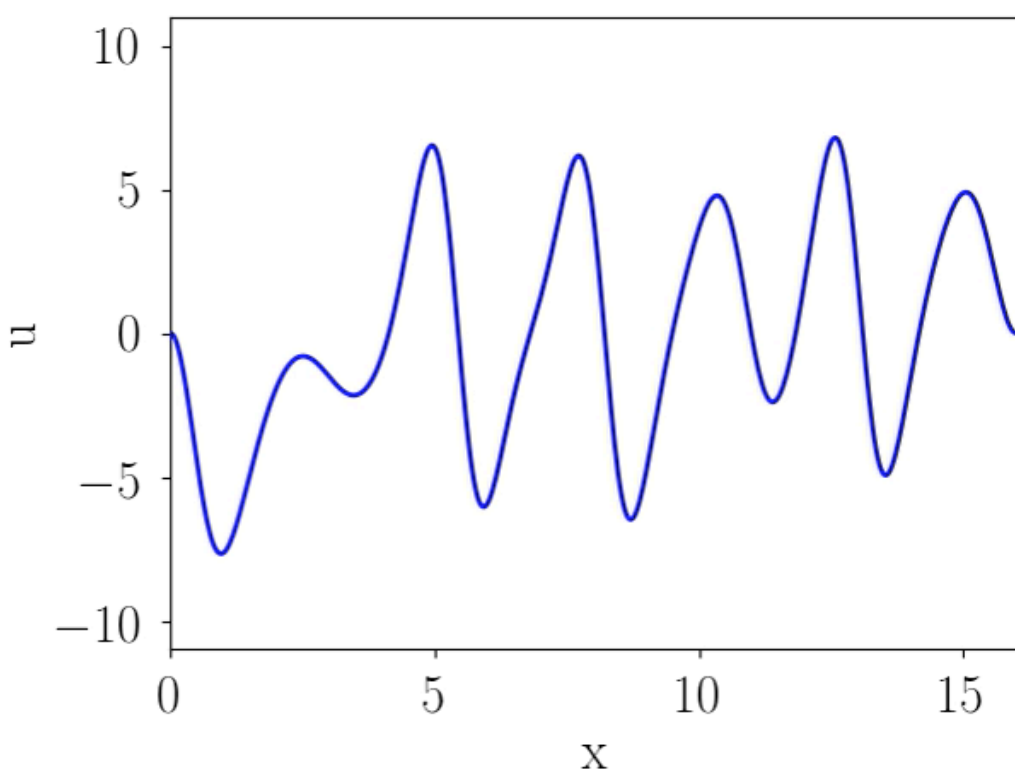


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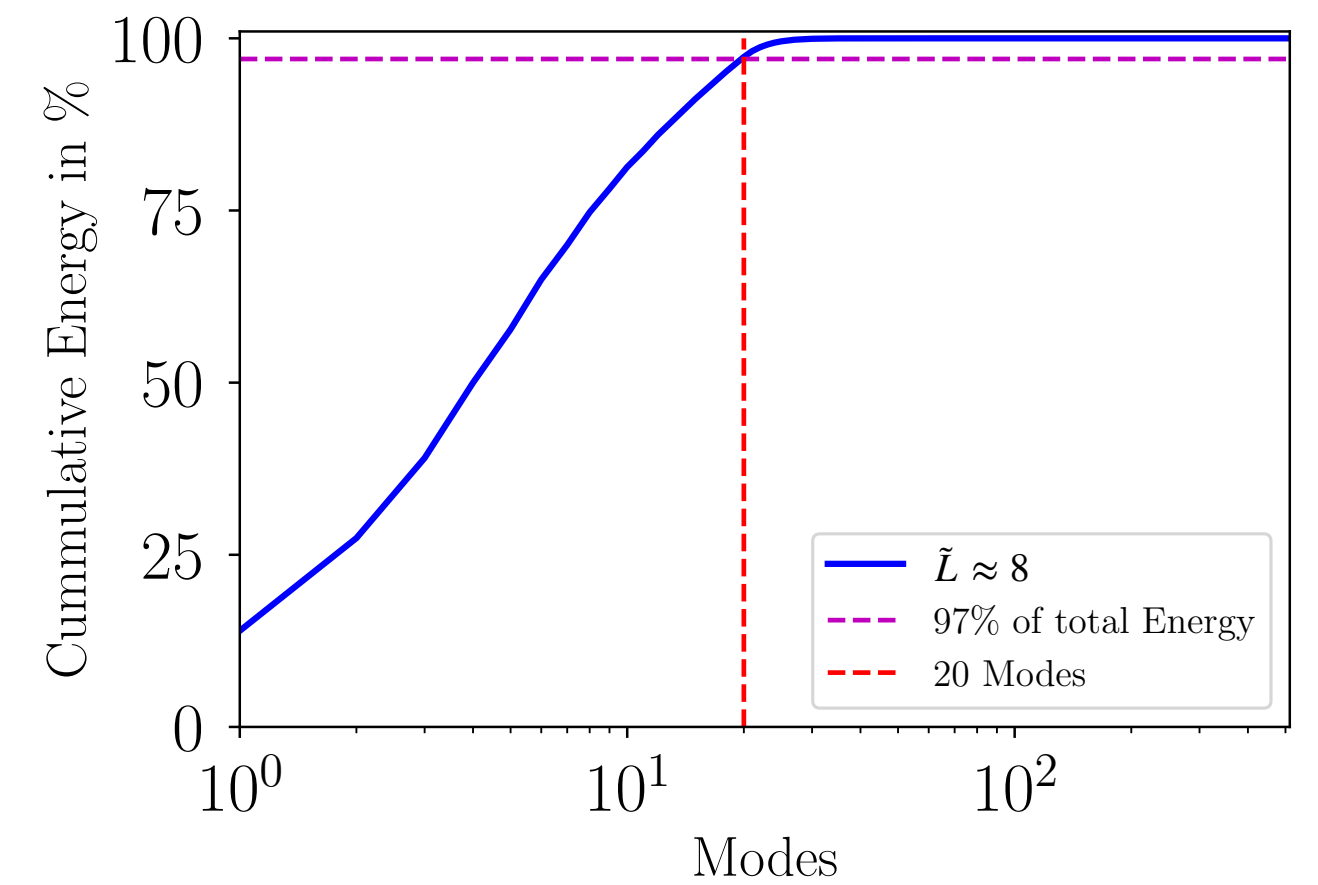


**SVD / PCA**

Singular Value  
Decomposition



*Throw away  
modes with  
low energy*



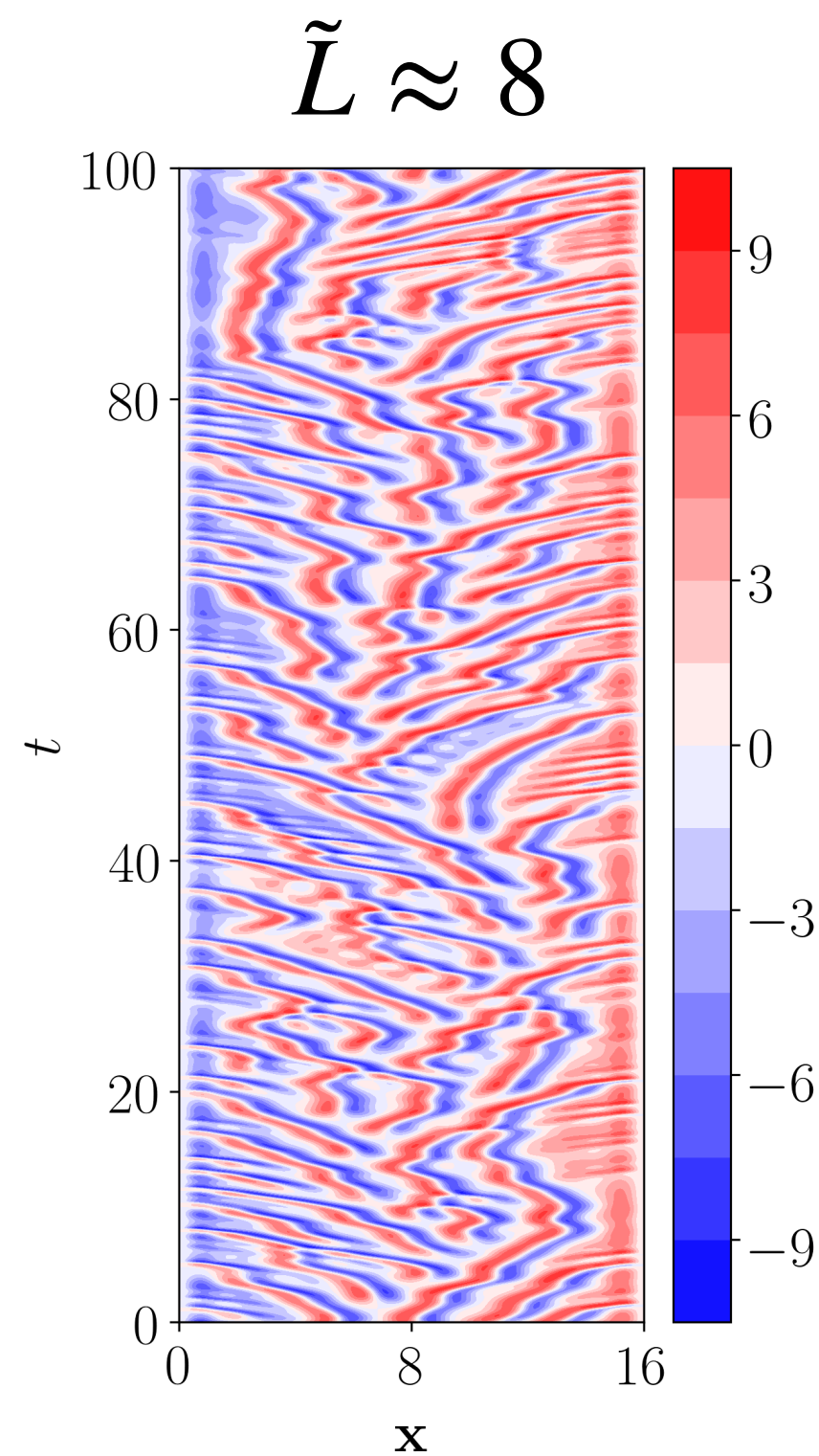
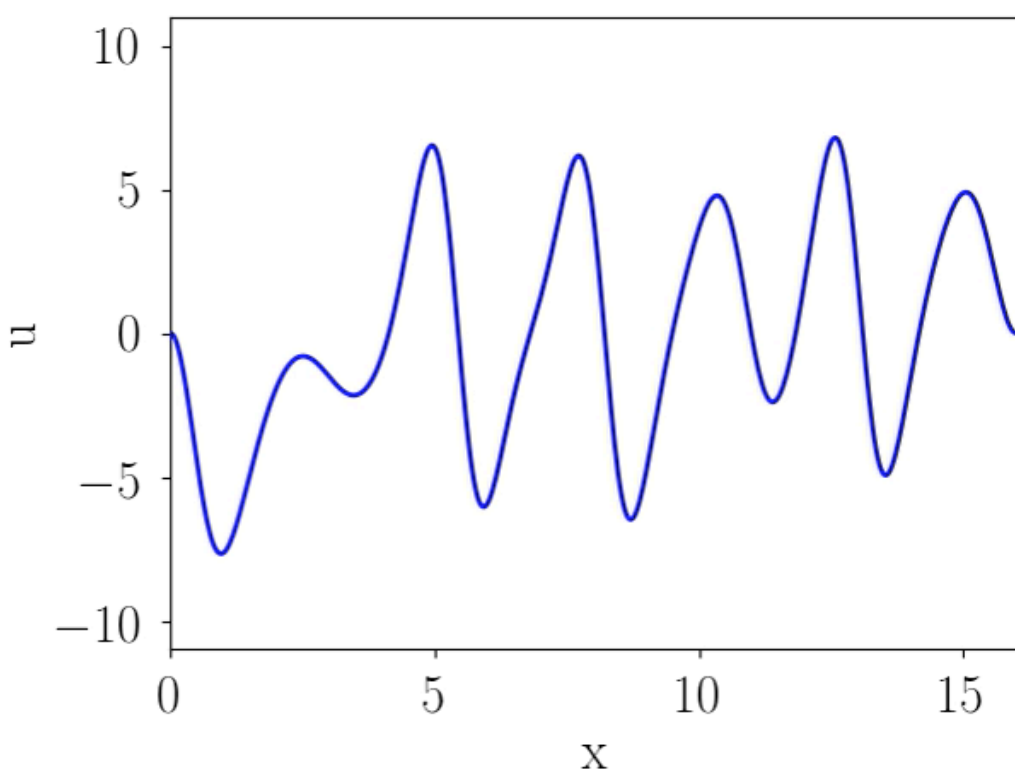


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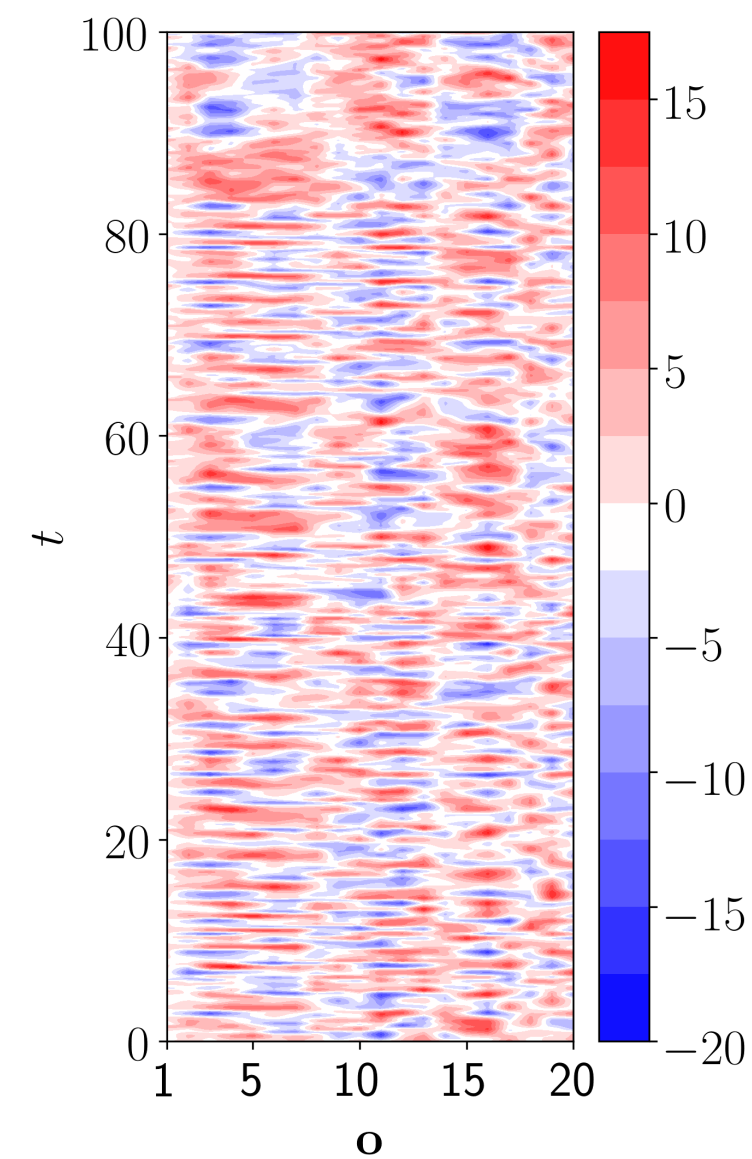
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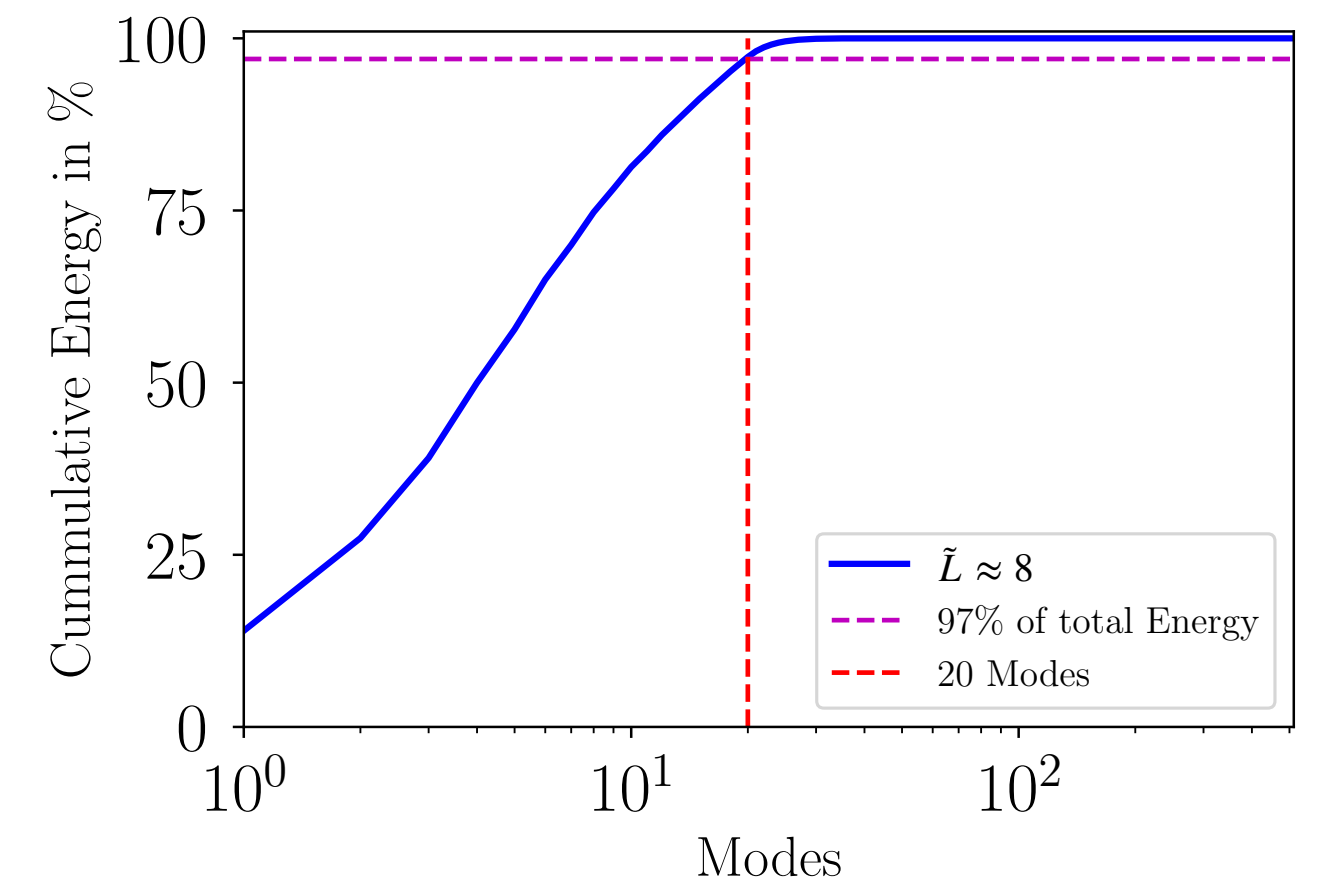
**Throw away  
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$\nu = 1/10$



20 Modes (observable)

$$o_t \in \mathbb{R}^{20}$$



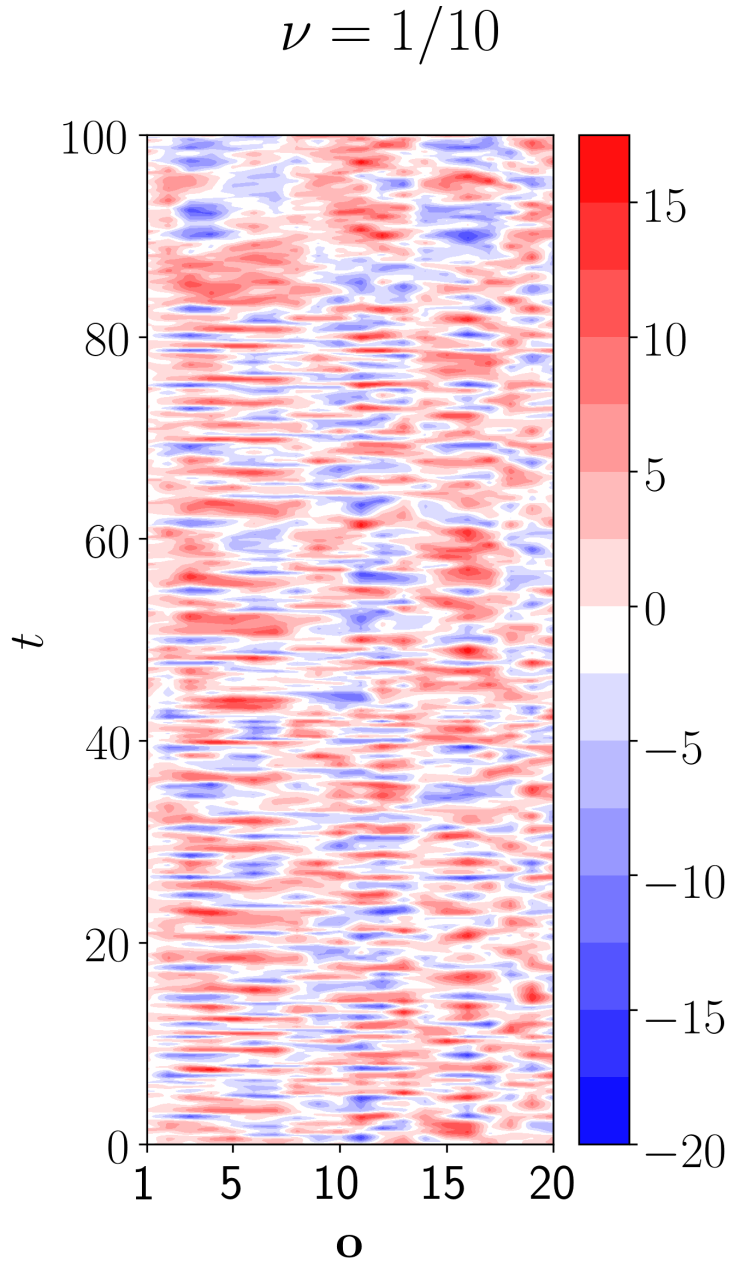
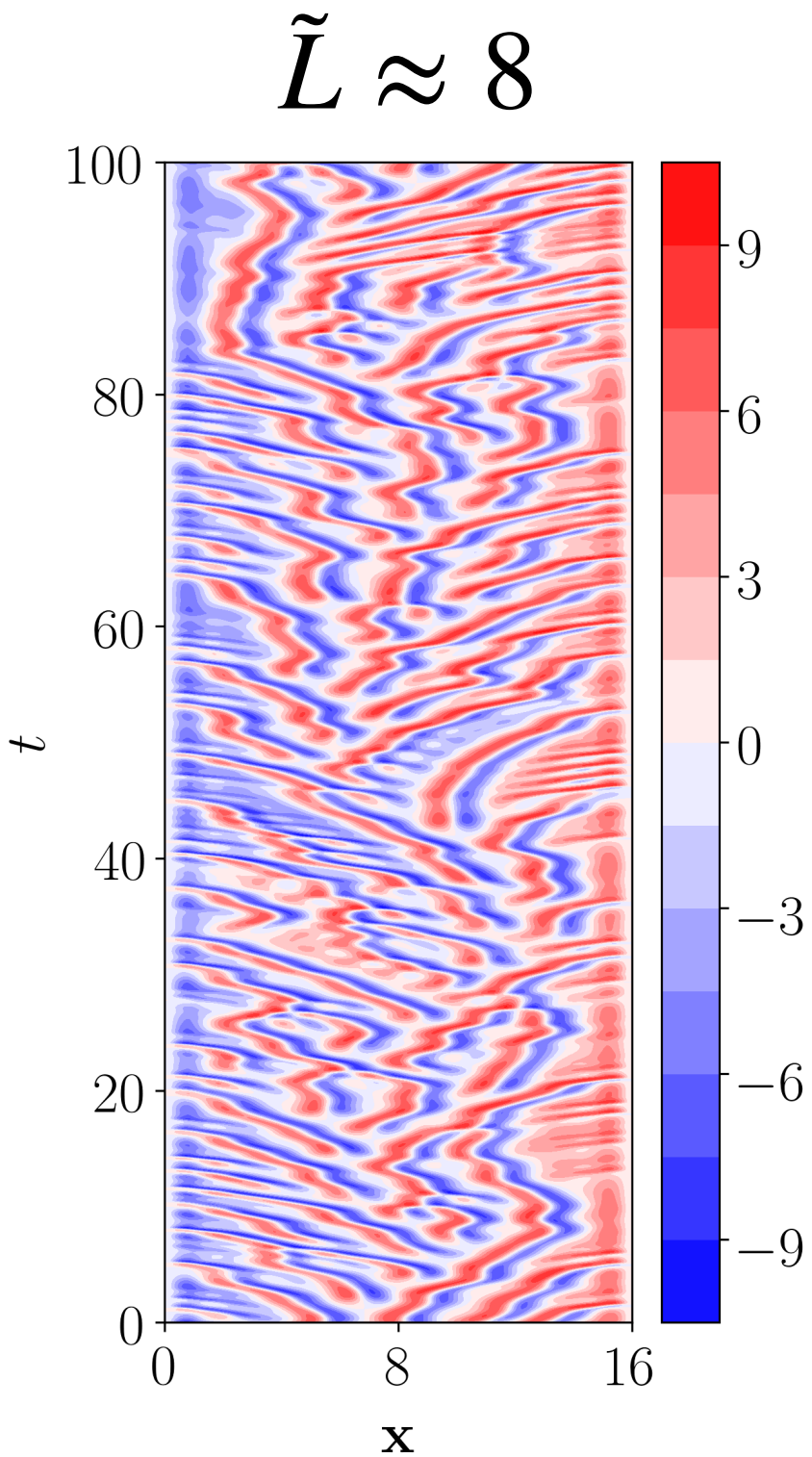
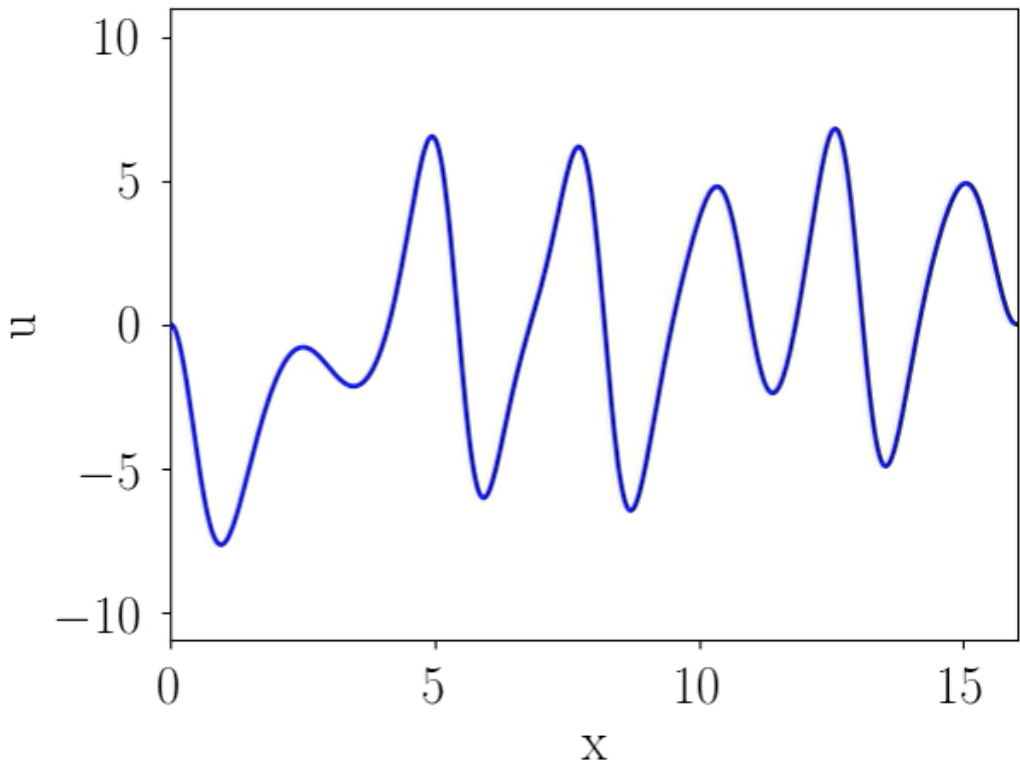


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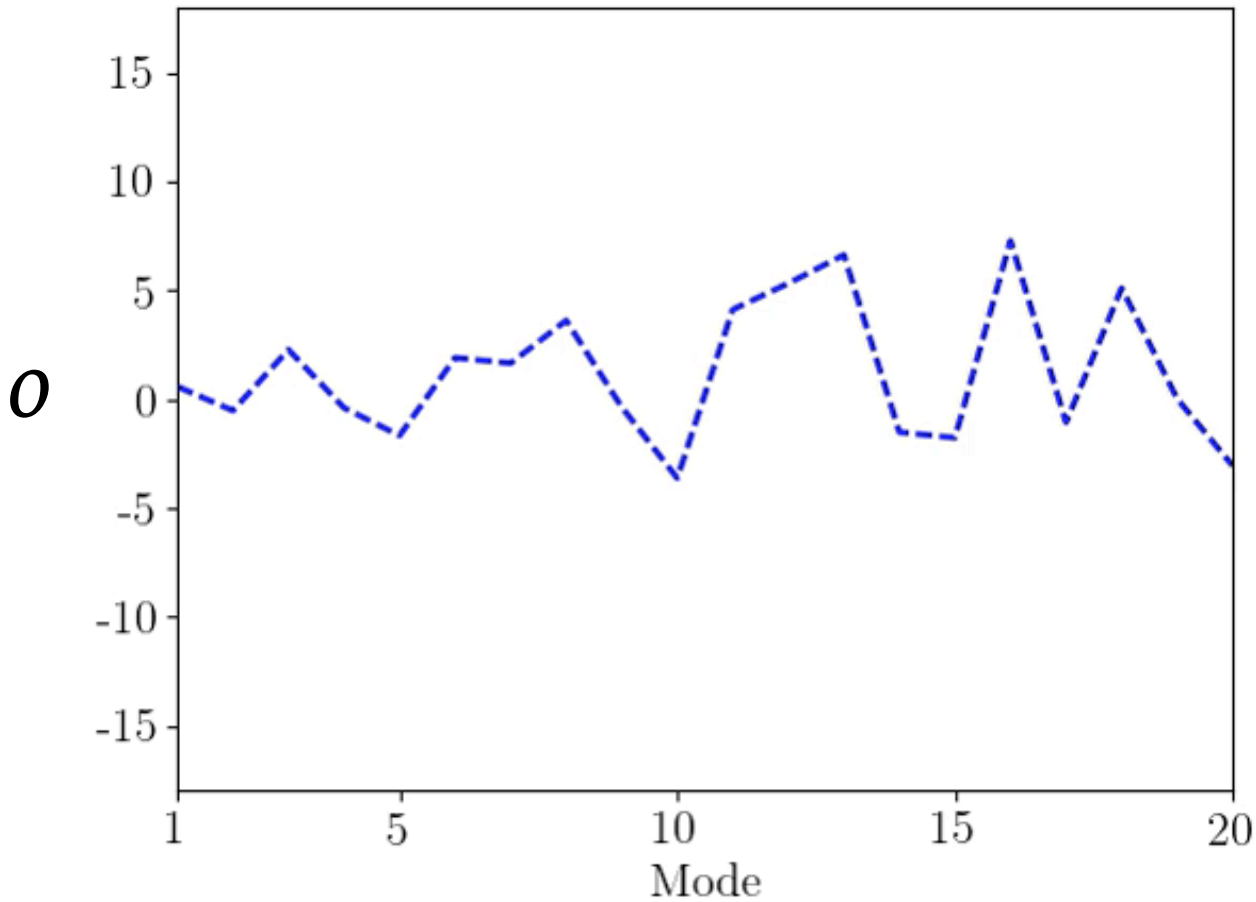
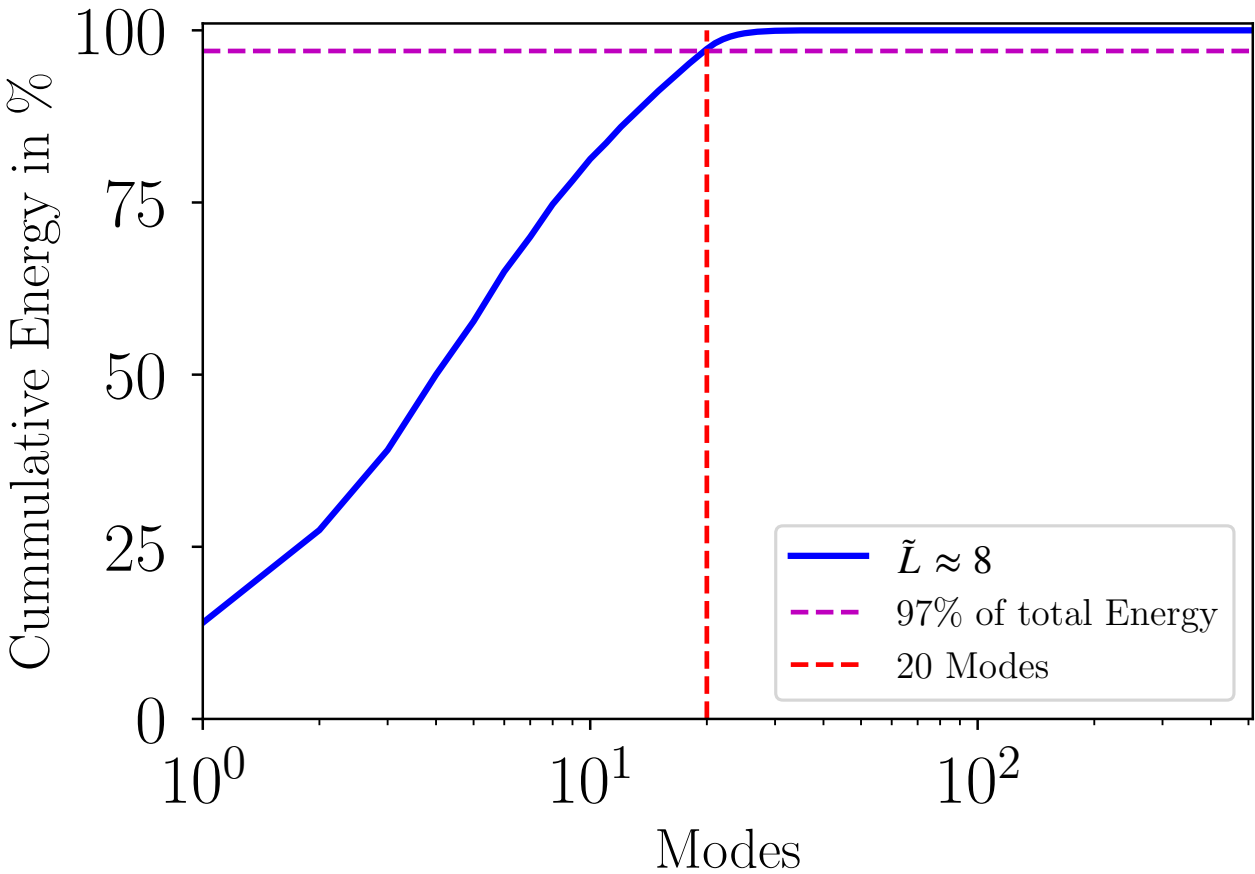
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- $T = 10^4$
- half a million samples
- $u_t \in \mathbb{R}^{512}$



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



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

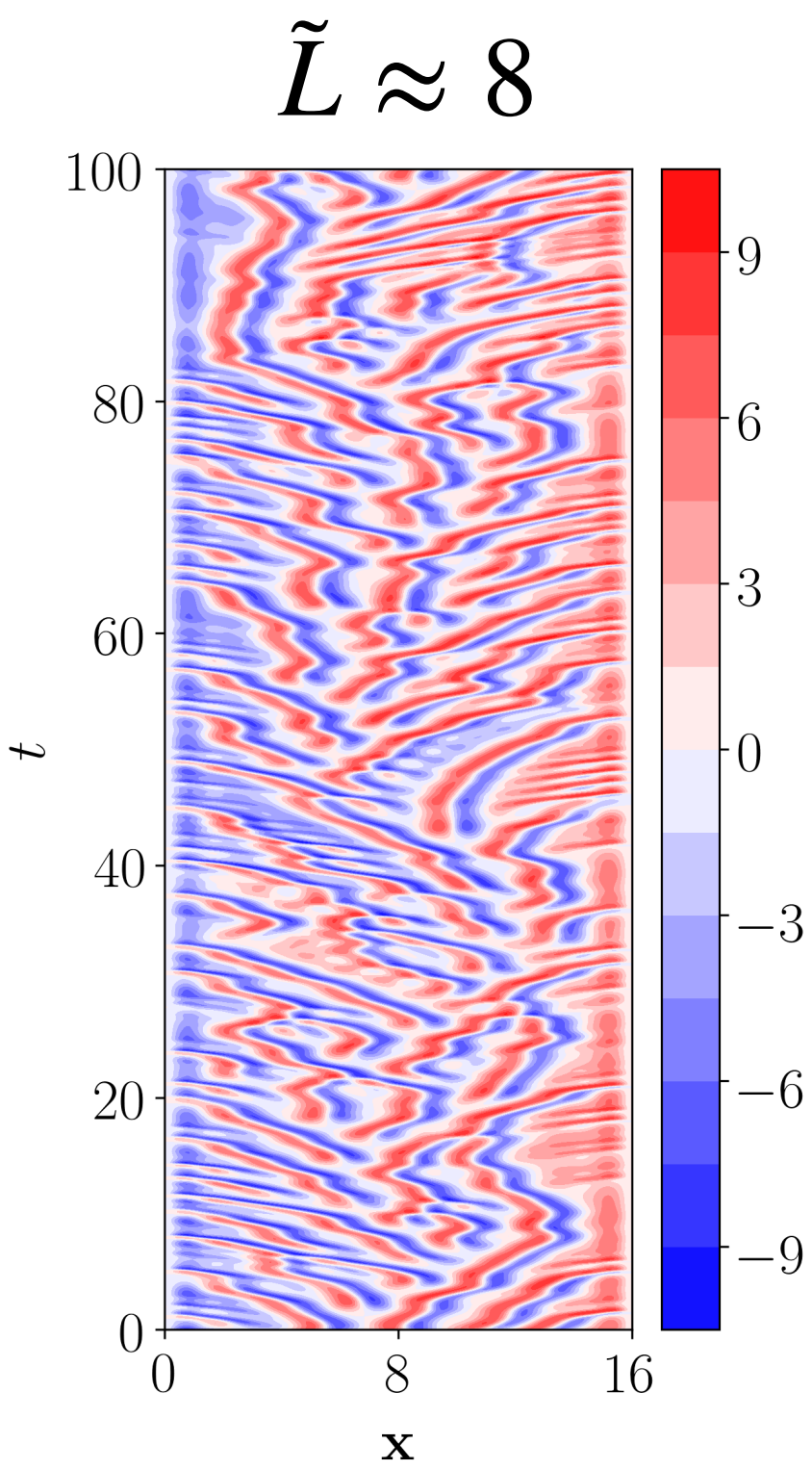
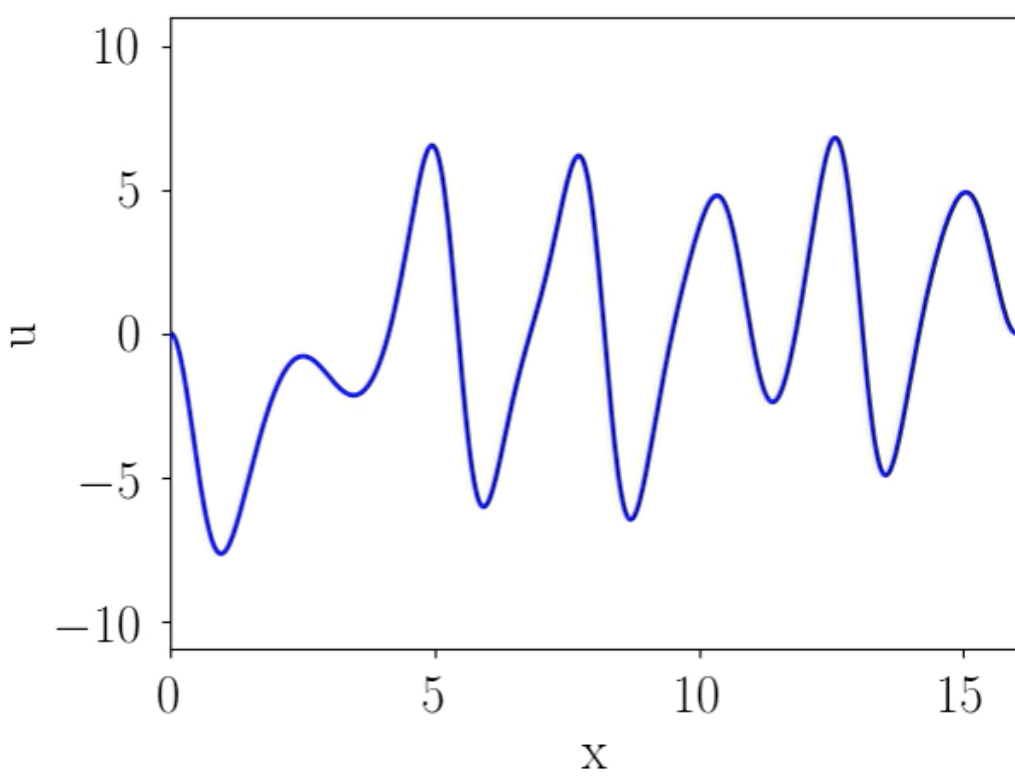


# Constructing the observable - training data

*High dimensional*

High dimensional simulation data

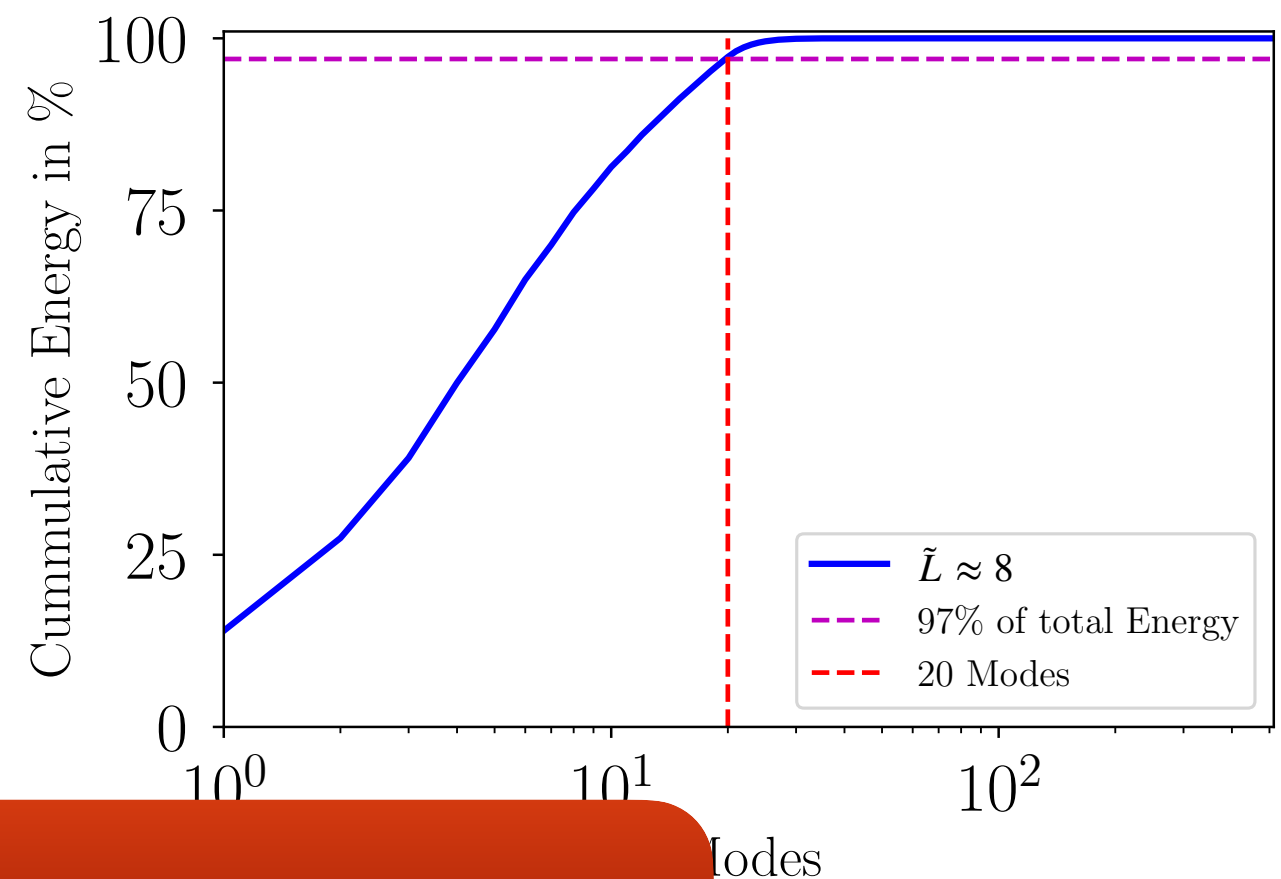
- $T = 10^4$
- half a million samples
- $u_t \in \mathbb{R}^{512}$



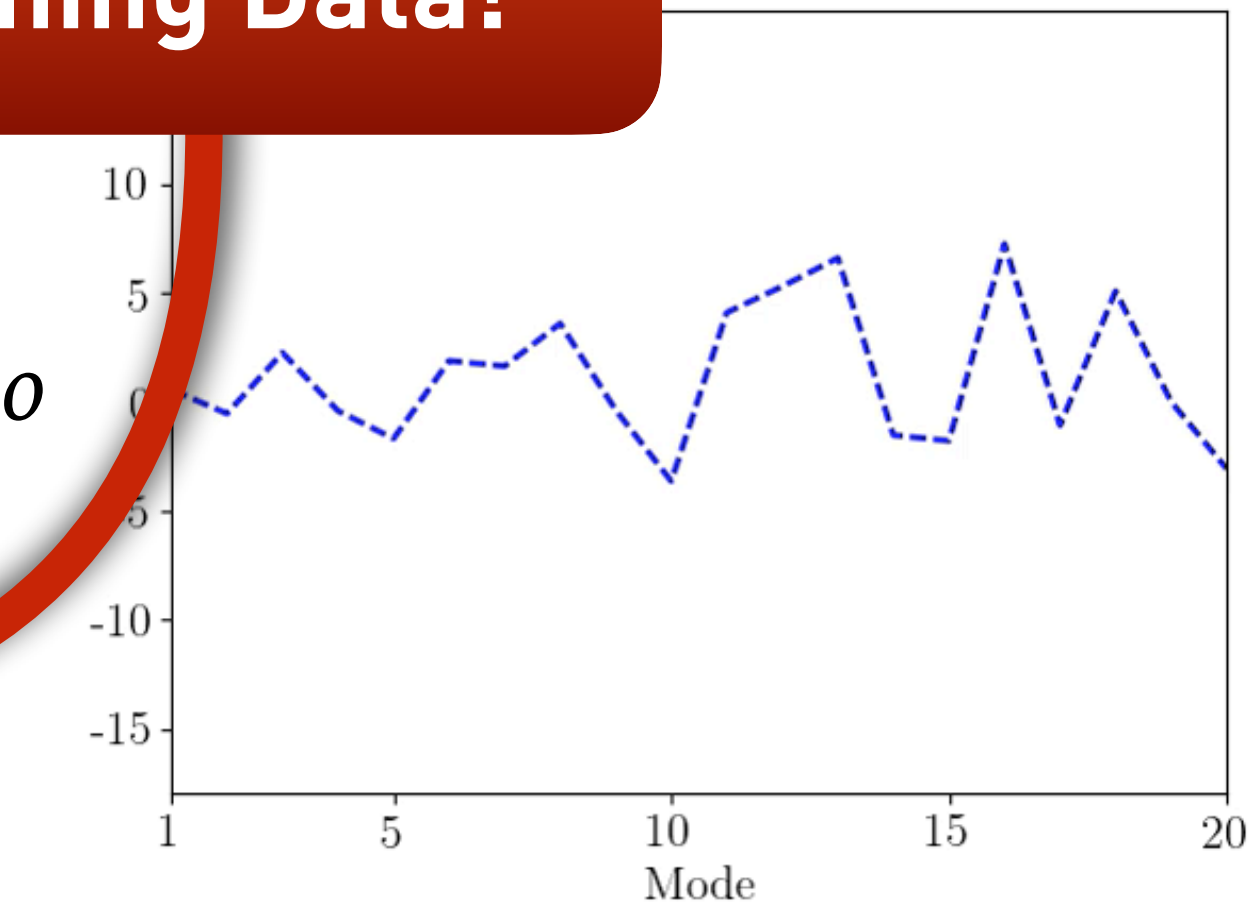
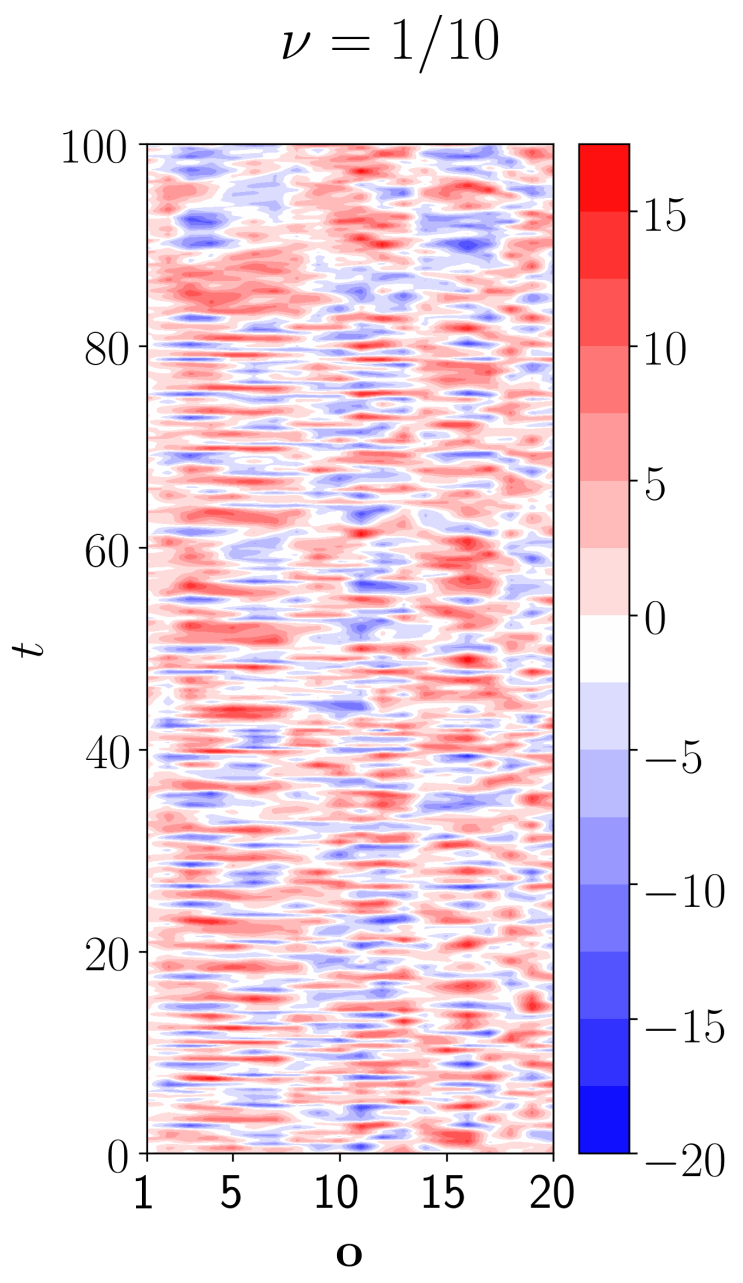
**SVD / PCA**

Singular Value Decomposition

*Throw away modes with low energy*



**Training Data!**



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

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



# Forecasting on UNSEEN data - Iterative prediction in practice

---



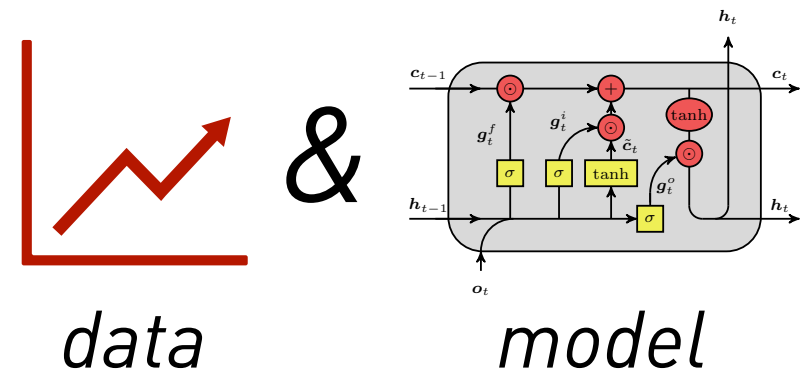
# Forecasting on UNSEEN data - Iterative prediction in practice

---



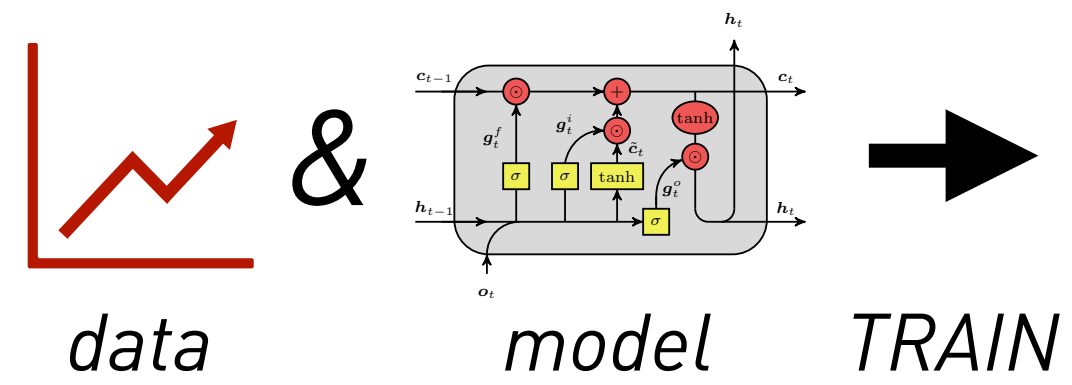


# Forecasting on UNSEEN data - Iterative prediction in practice



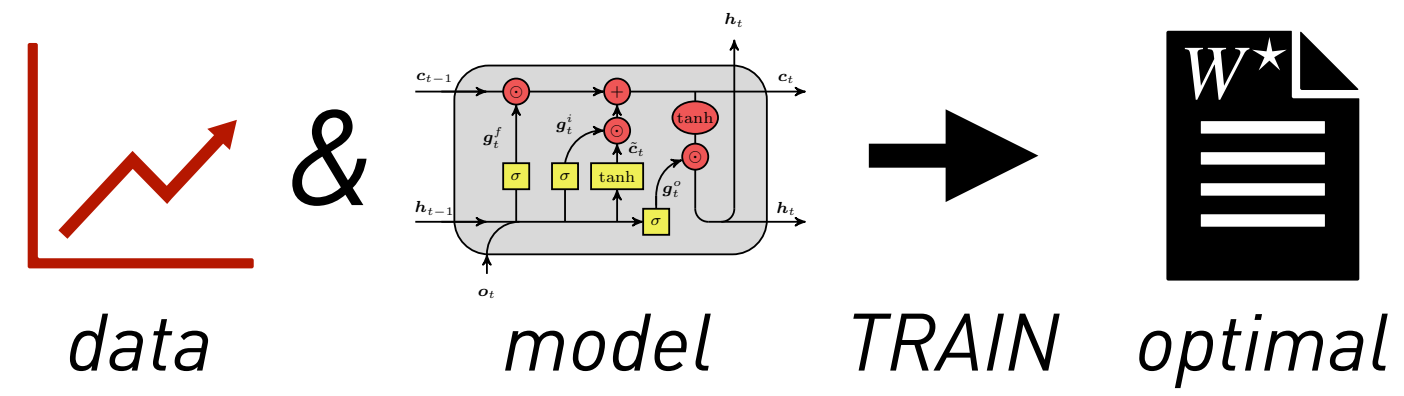


# Forecasting on UNSEEN data - Iterative prediction in practice



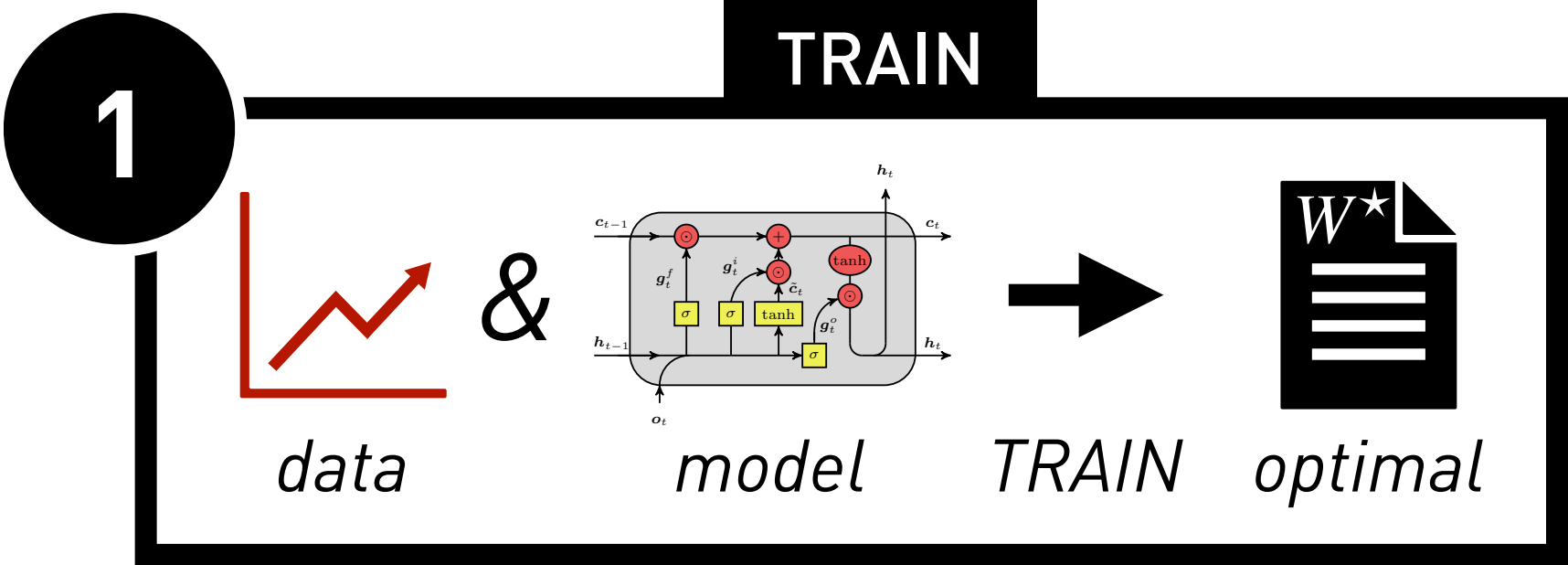


# Forecasting on UNSEEN data - Iterative prediction in practice





# Forecasting on UNSEEN data - Iterative prediction in practice

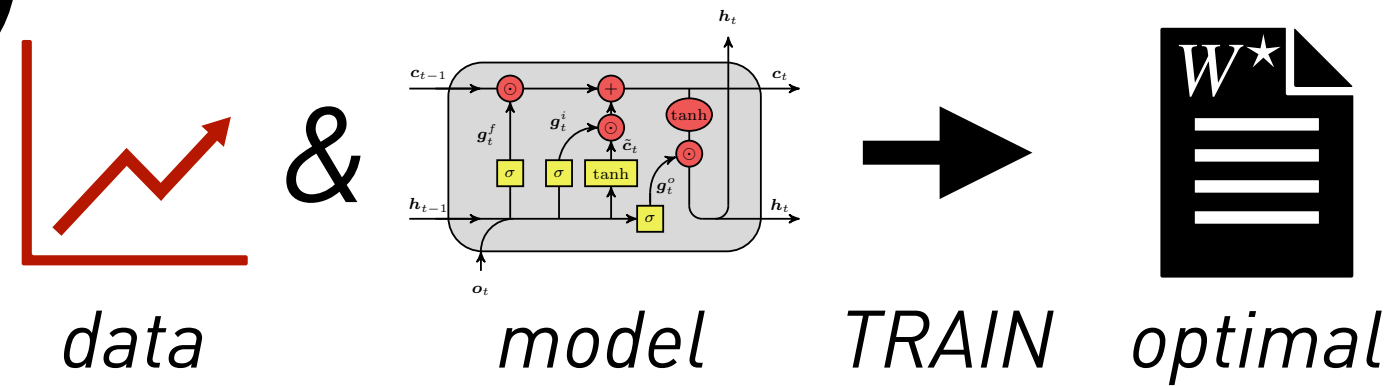




# Forecasting on UNSEEN data - Iterative prediction in practice

1

TRAIN



2

TEST

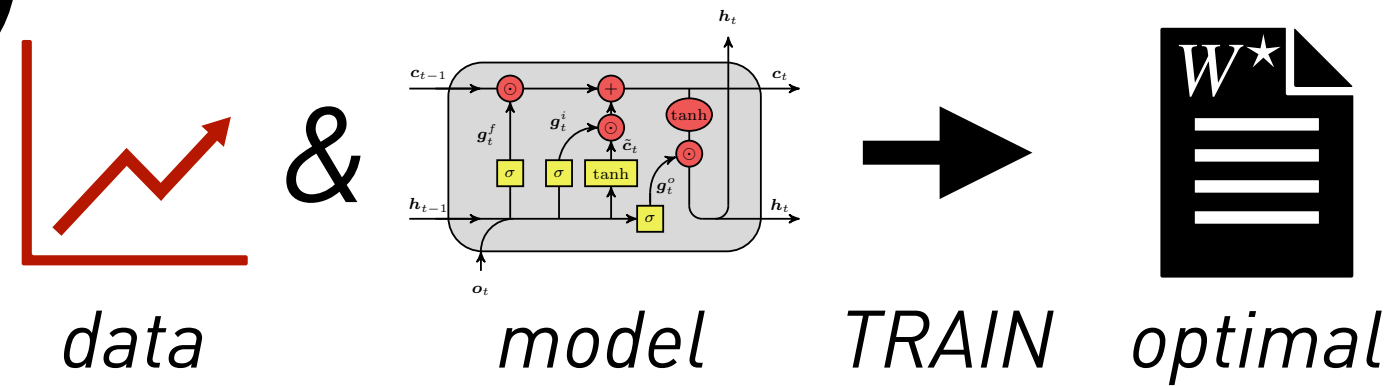
How to predict the dynamics of TEST (unseen) data?



# Forecasting on UNSEEN data - Iterative prediction in practice

1

TRAIN

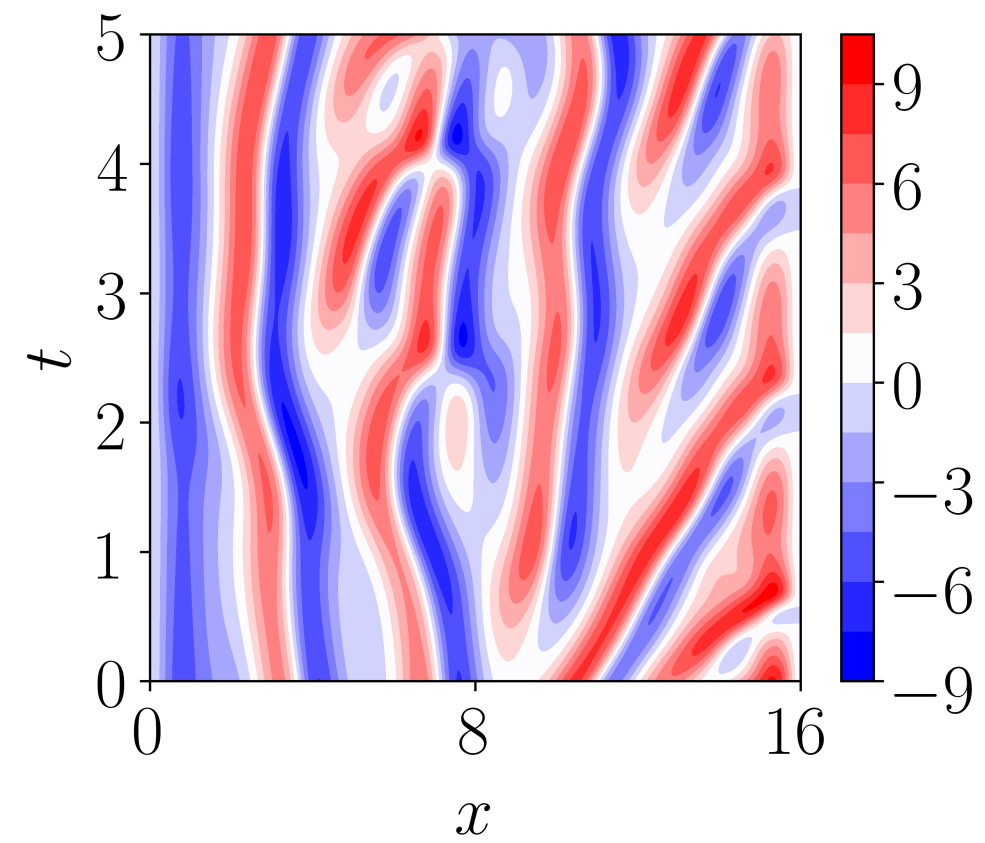


2

TEST

How to predict the dynamics of TEST (unseen) data?

TEST: *UNKNOWN* state dynamics (reference)

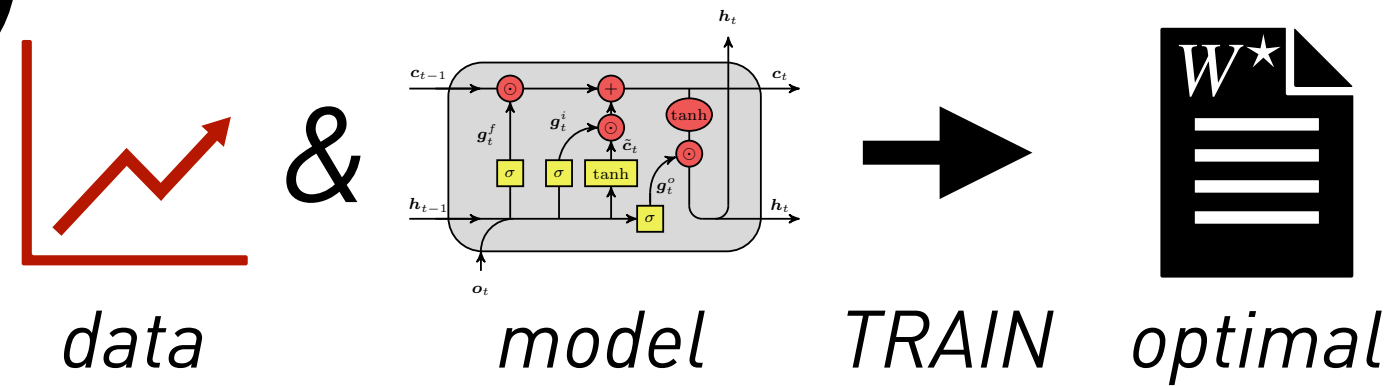




# Forecasting on UNSEEN data - Iterative prediction in practice

1

TRAIN

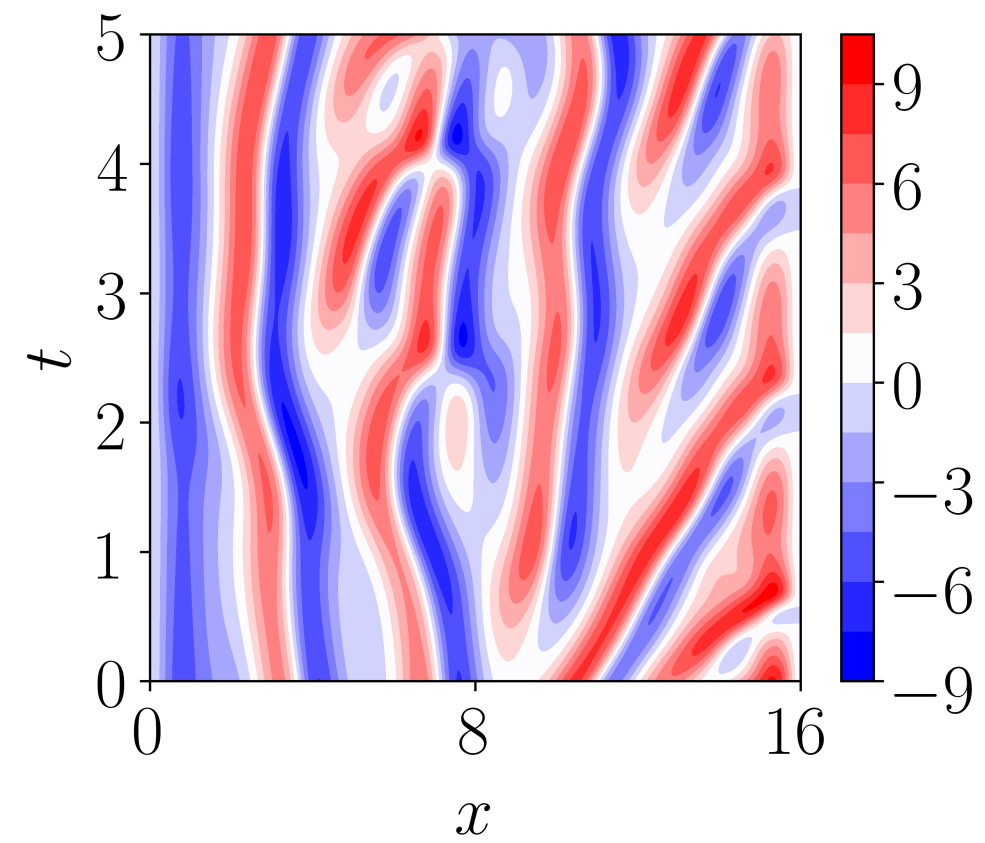


2

TEST

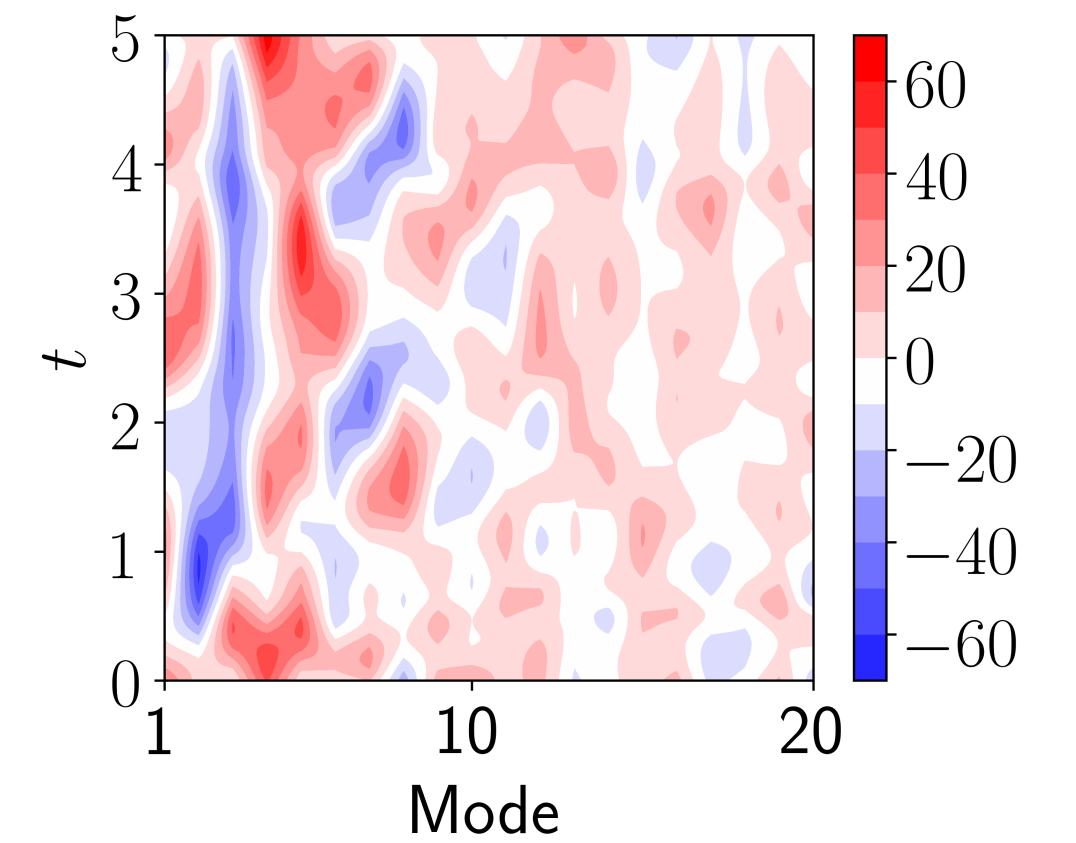
How to predict the dynamics of TEST (unseen) data?

TEST: *UNKNOWN* state dynamics (reference)



SVD

*SVD Mode* dynamics (reference)

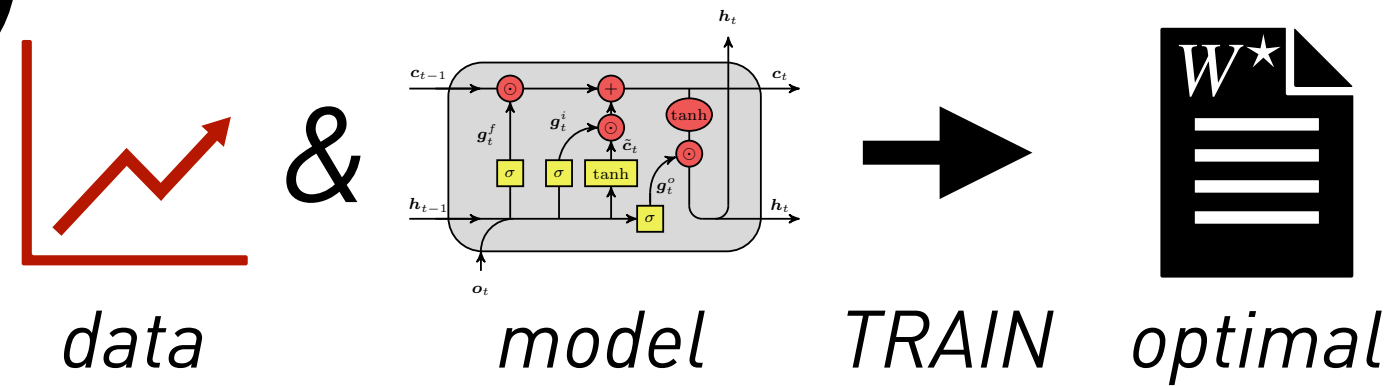




# Forecasting on UNSEEN data - Iterative prediction in practice

1

TRAIN

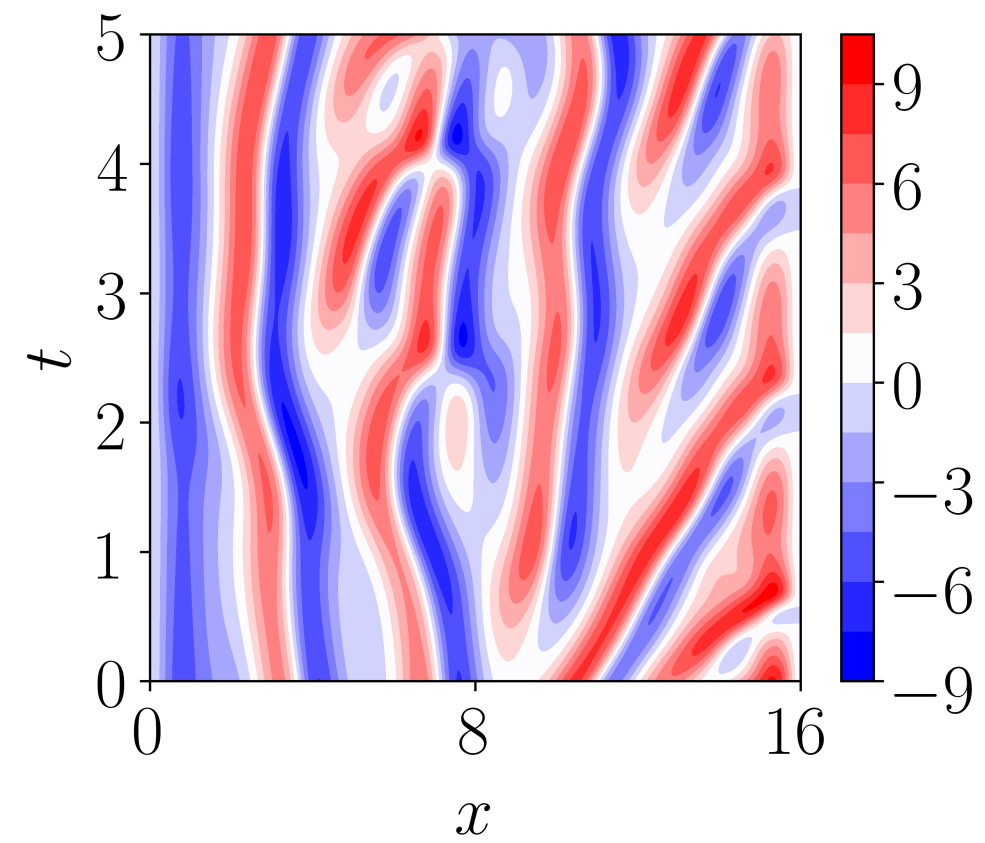


2

TEST

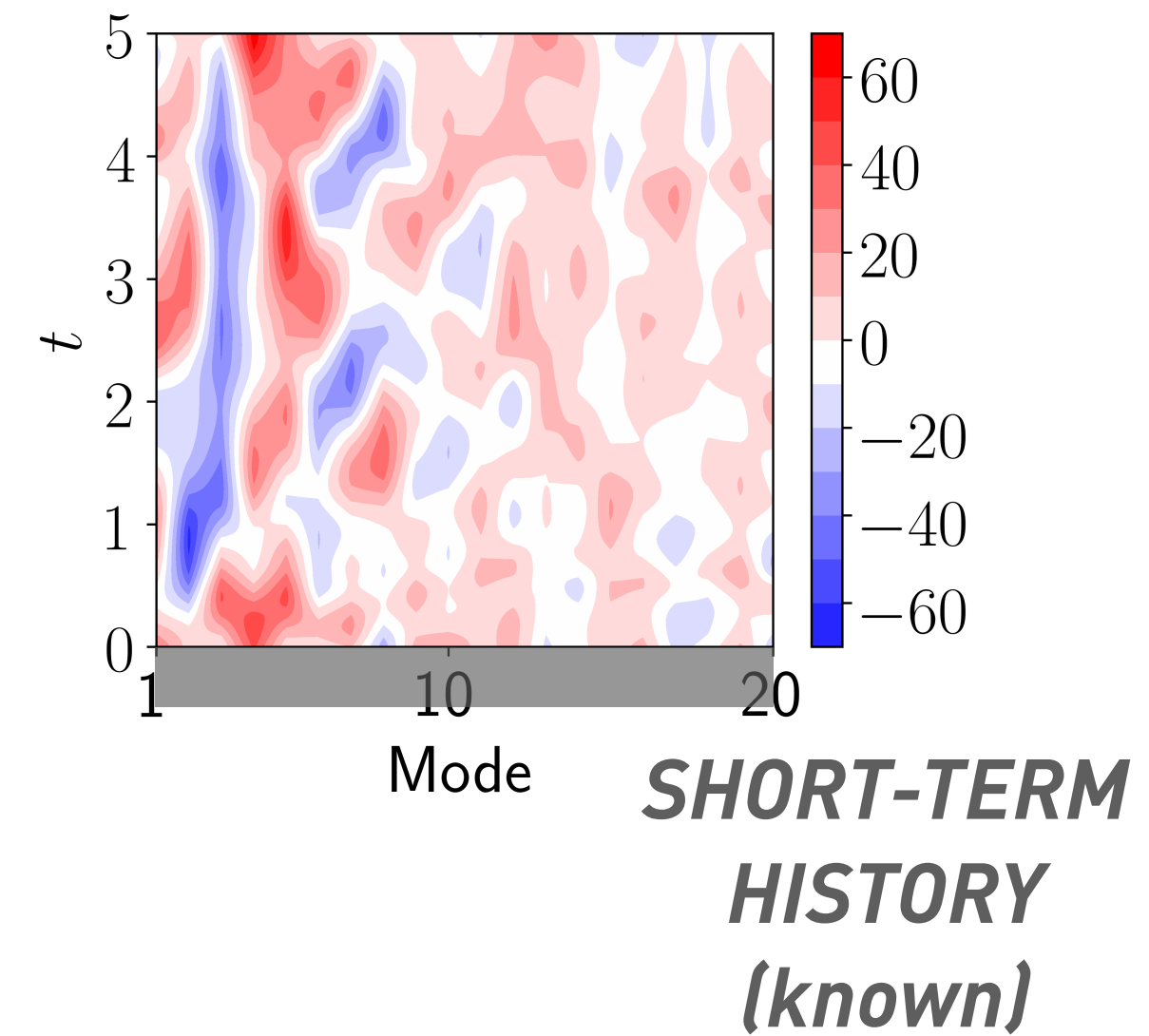
How to predict the dynamics of TEST (unseen) data?

TEST: *UNKNOWN* state dynamics (reference)



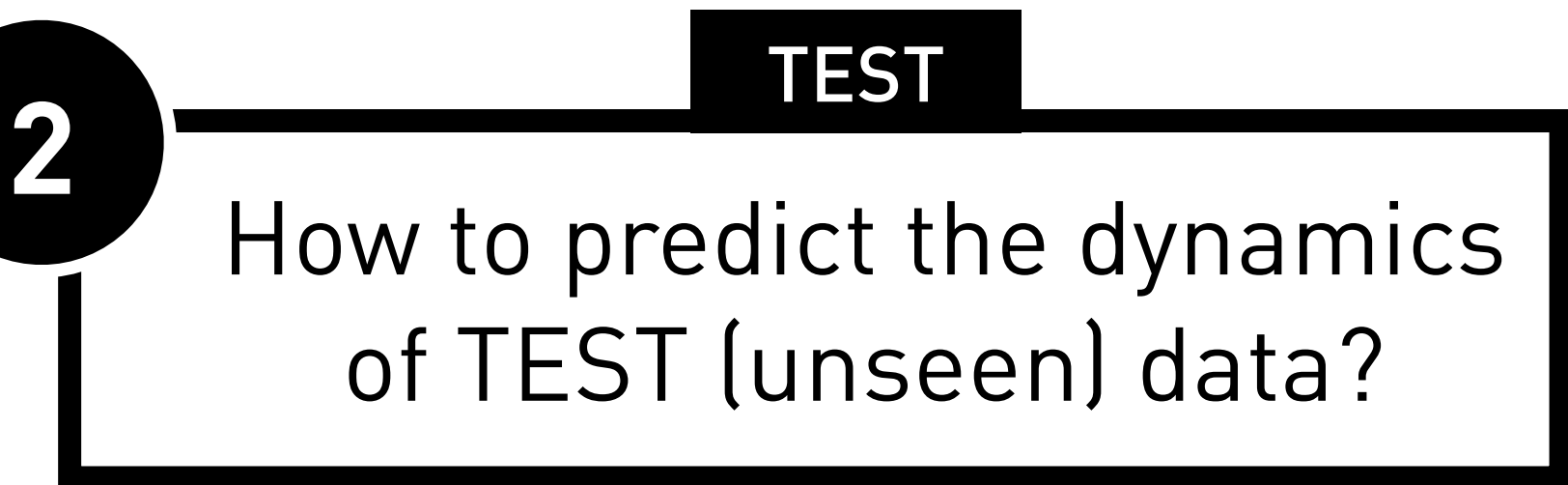
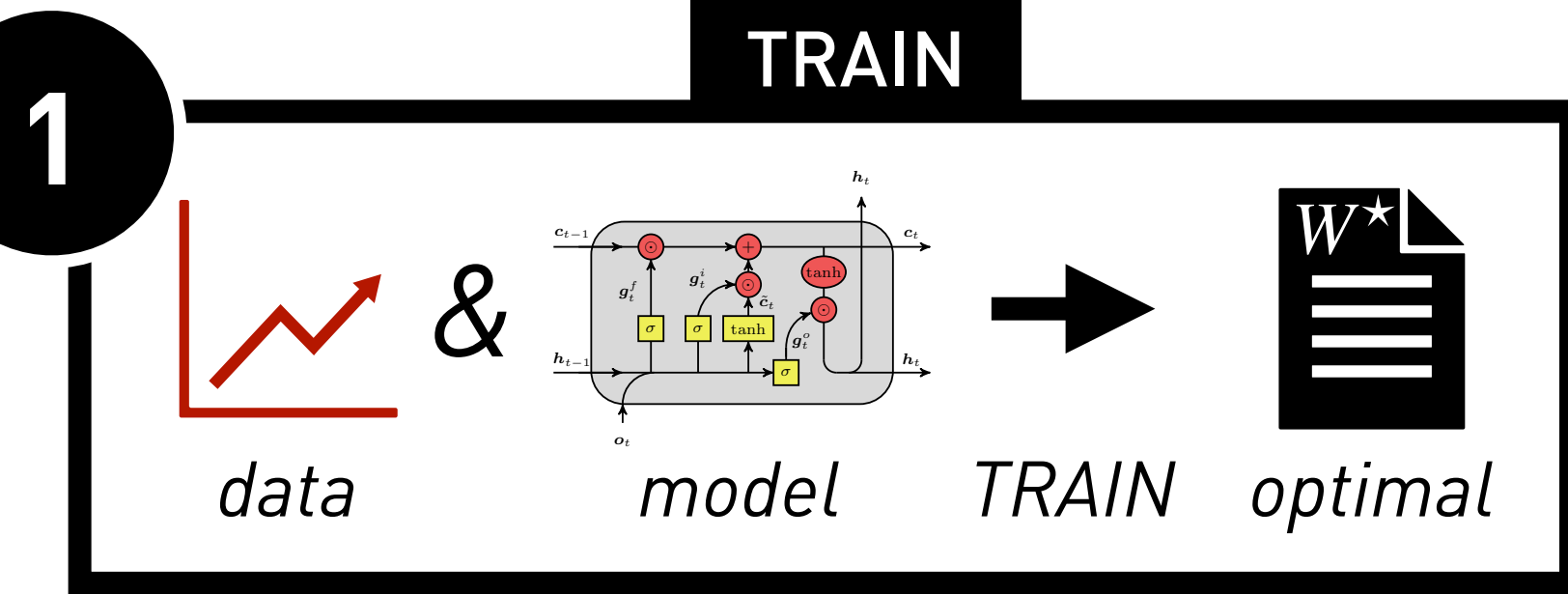
SVD

*SVD Mode* dynamics (reference)

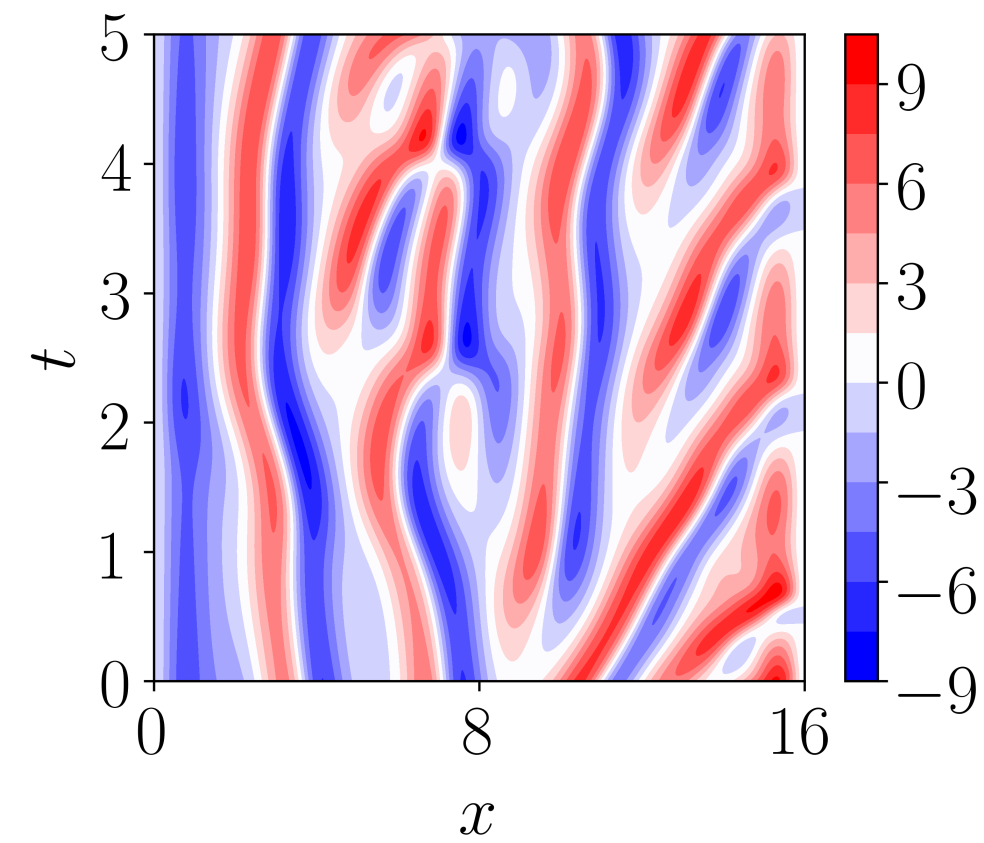




# Forecasting on UNSEEN data - Iterative prediction in practice

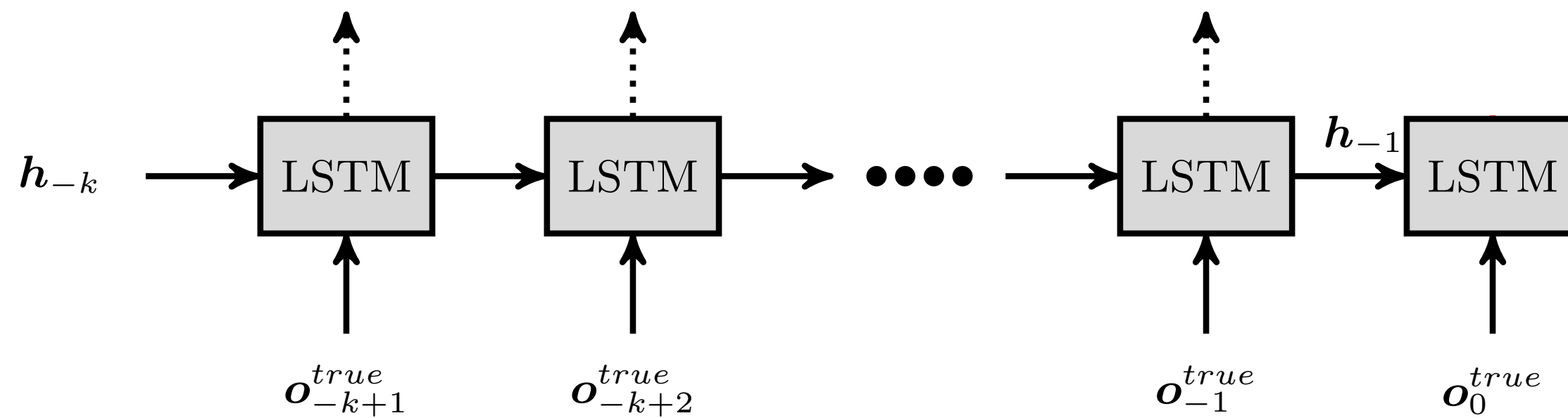
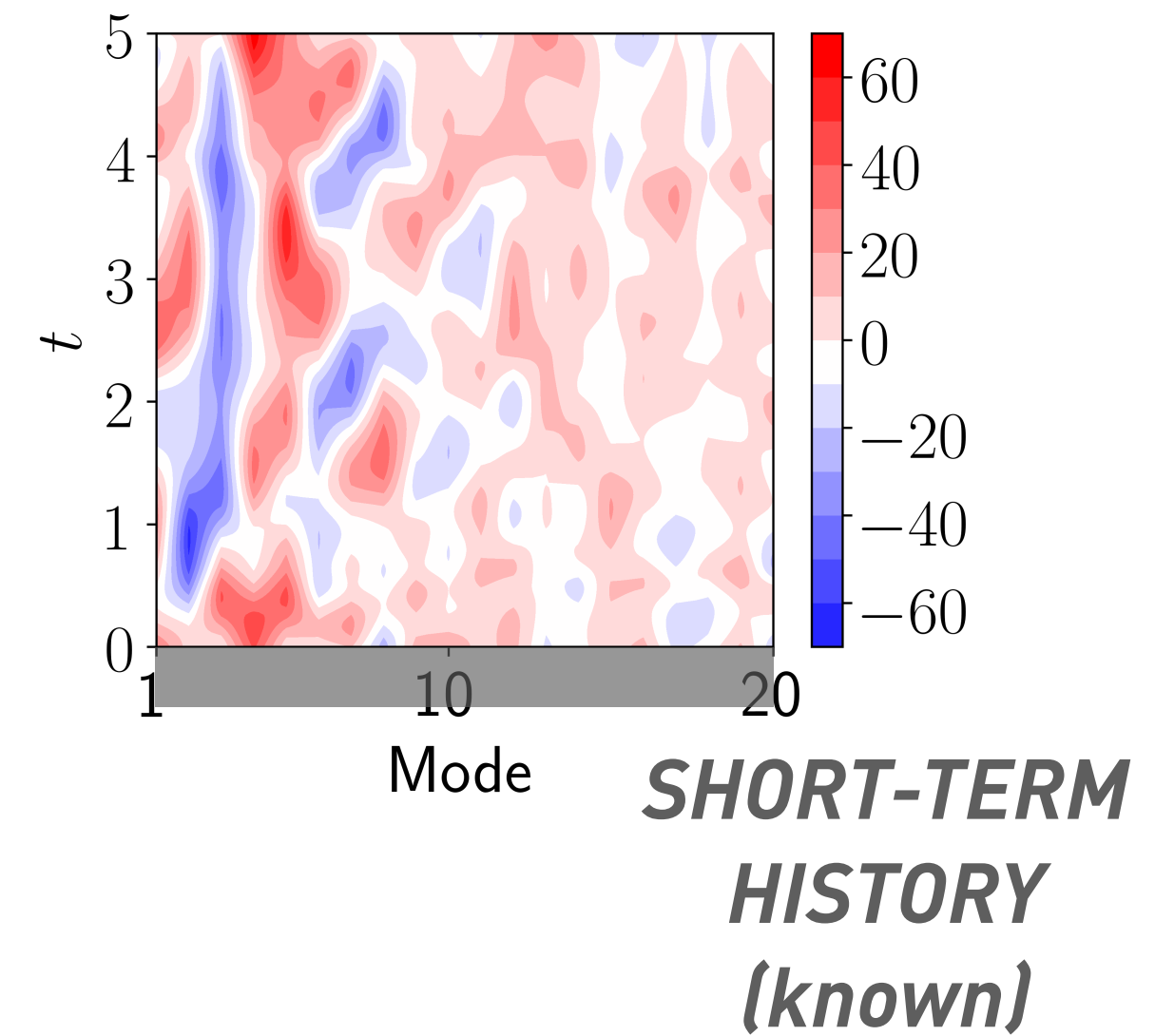


**TEST: *UNKNOWN* state dynamics (reference)**



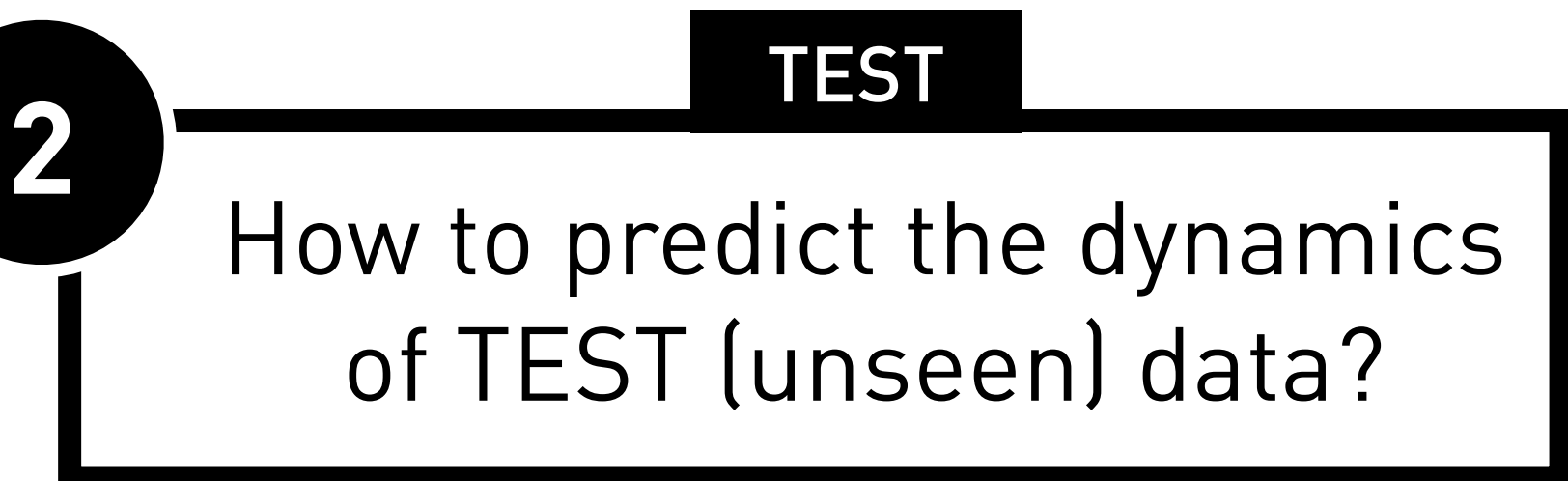
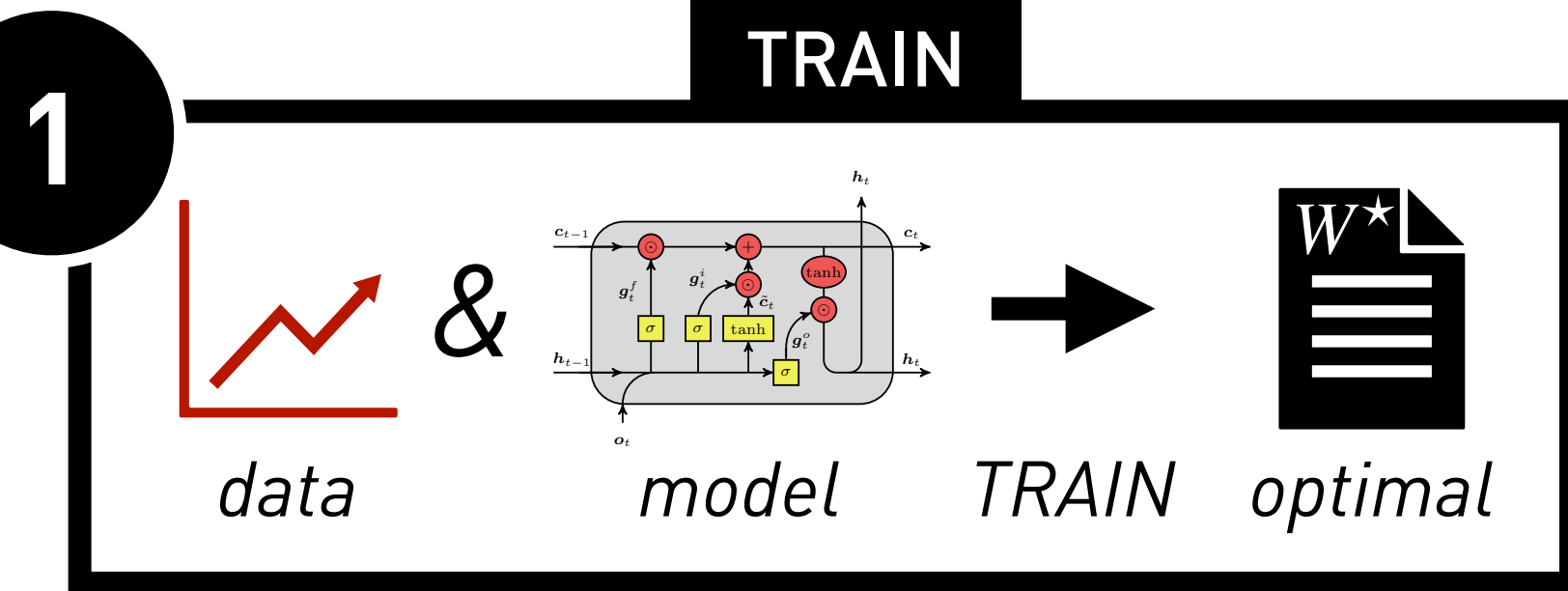
**SVD**

***SVD Mode* dynamics (reference)**

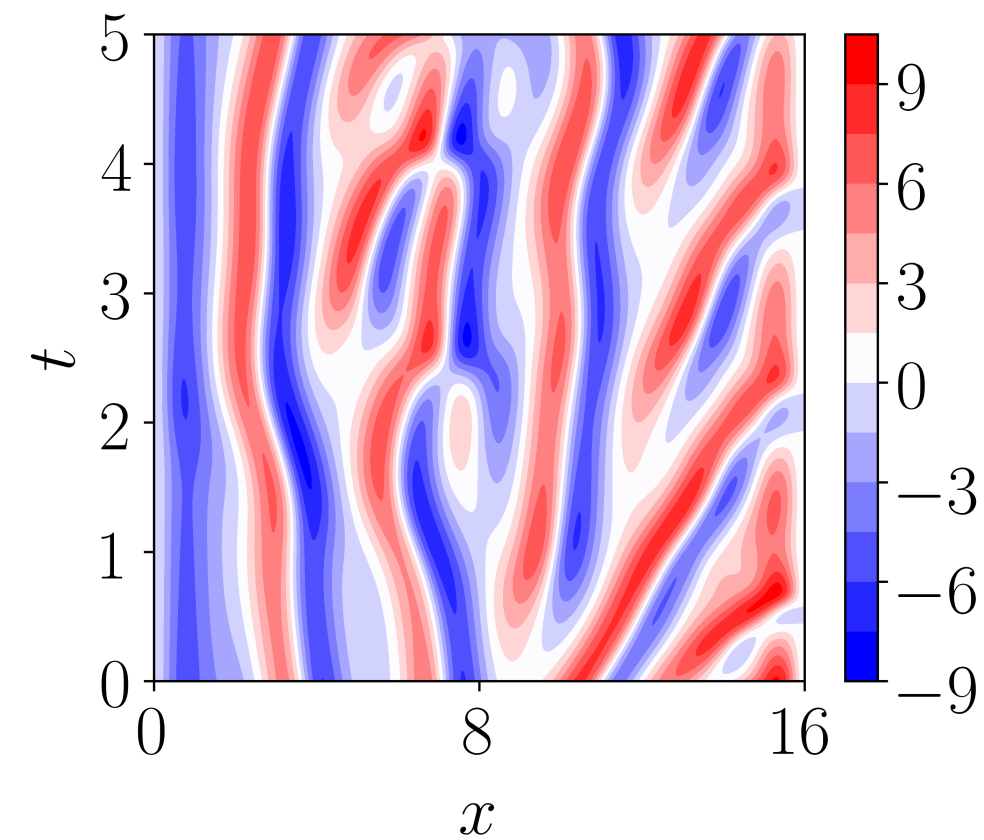




# Forecasting on UNSEEN data - Iterative prediction in practice

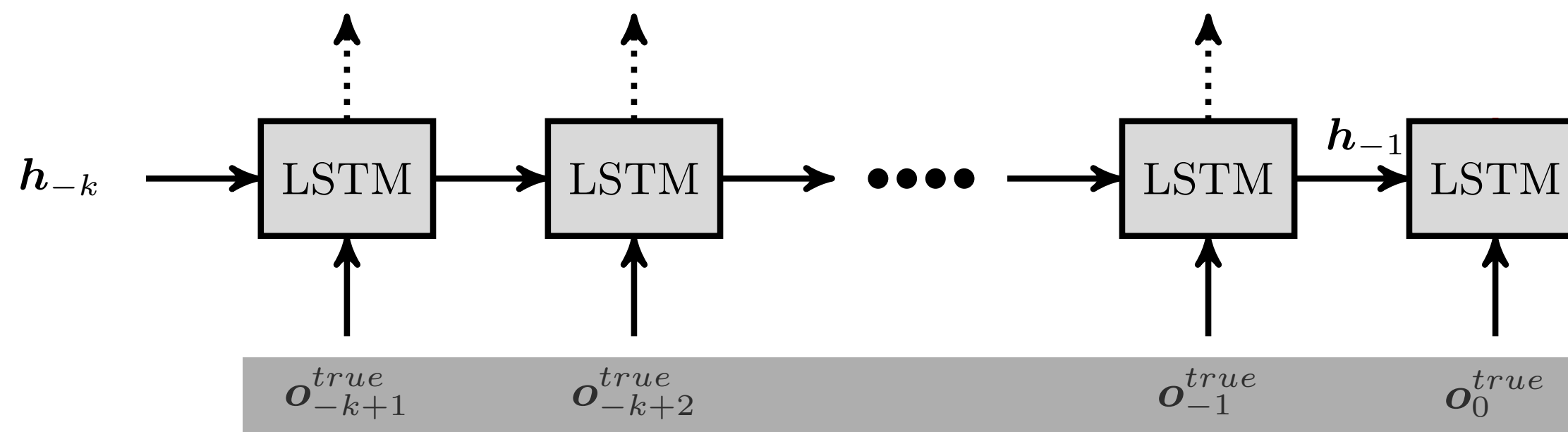
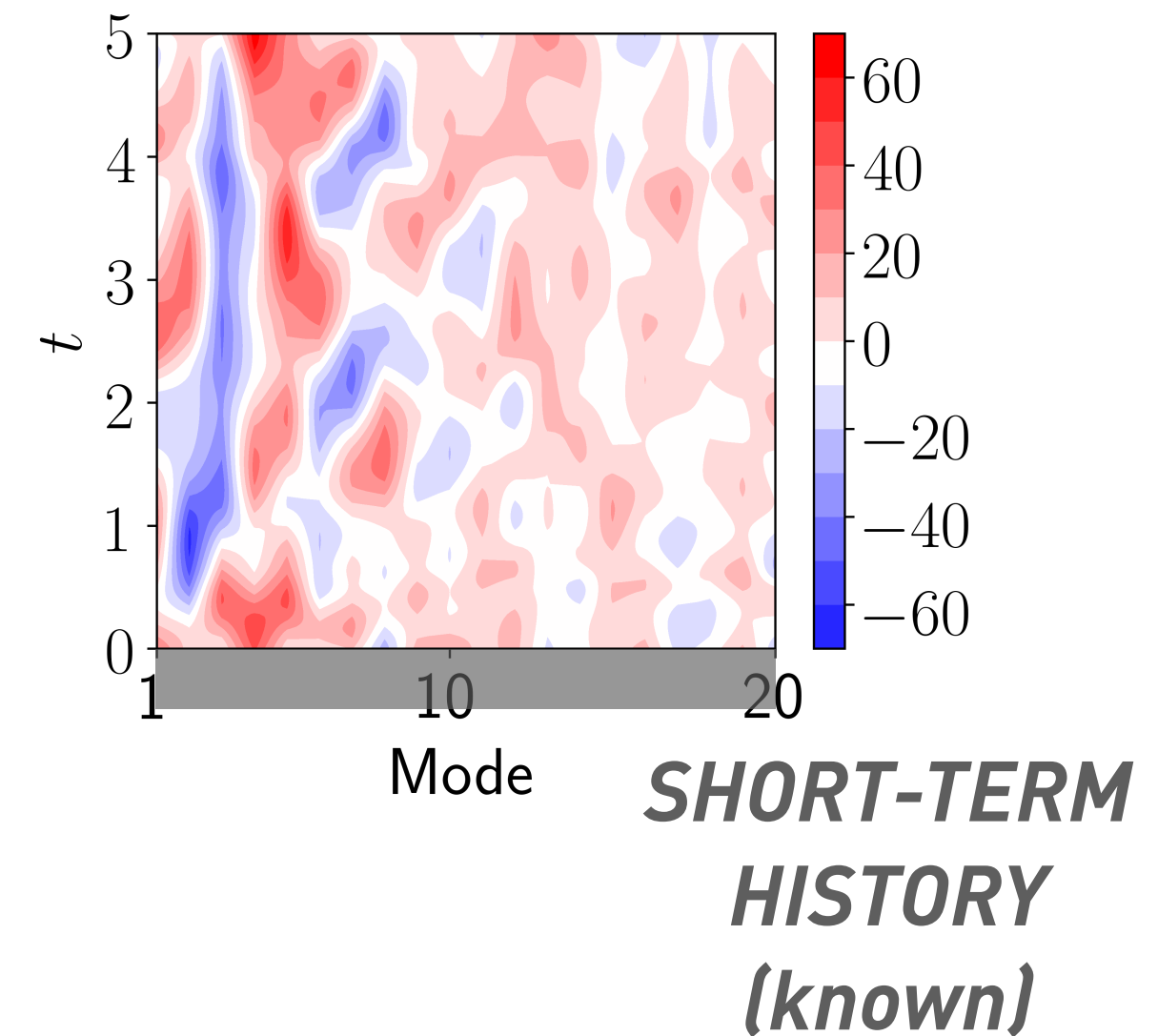


**TEST: UNKNOWN** state dynamics (reference)



**SVD**

**SVD Mode** dynamics (reference)



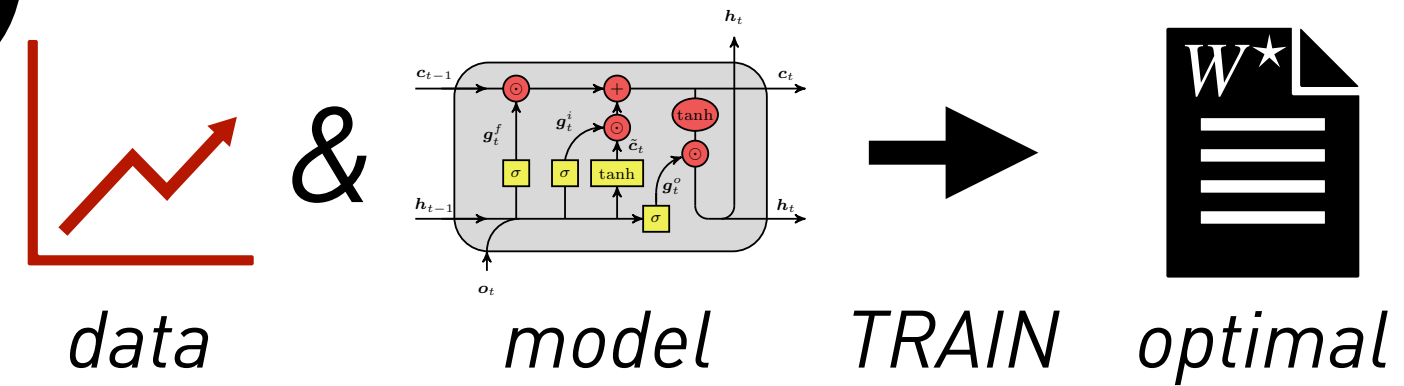
**SHORT-TERM HISTORY**  
(known)



# Forecasting on UNSEEN data - Iterative prediction in practice

1

TRAIN

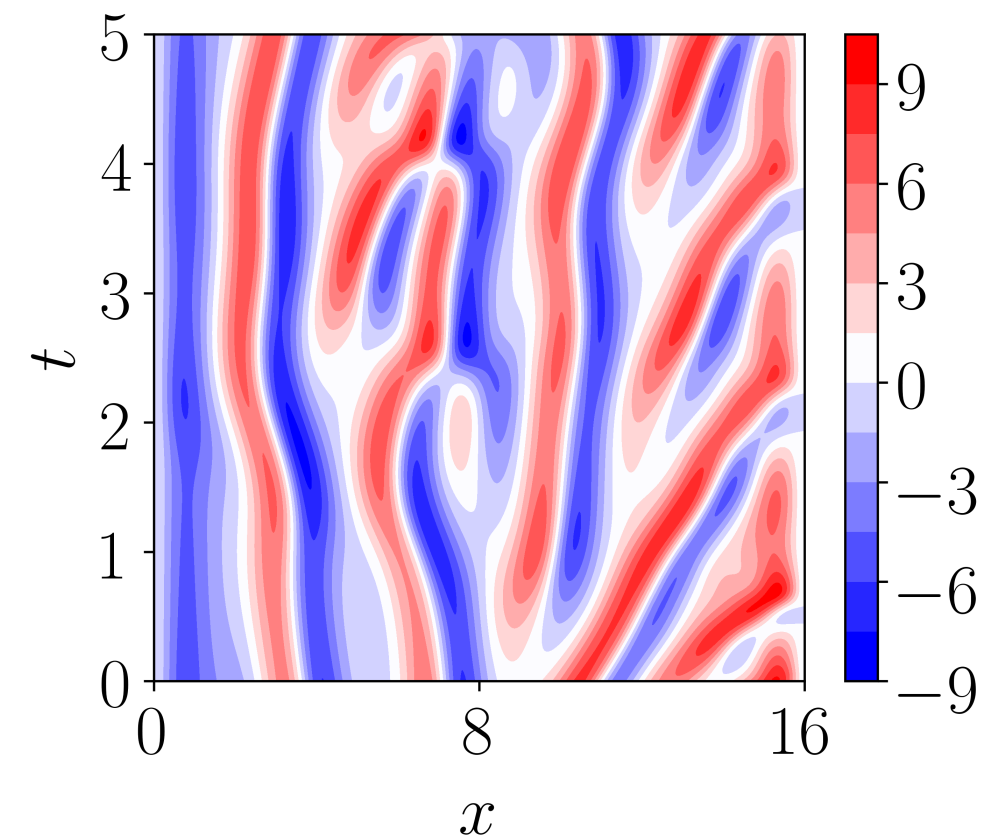


2

TEST

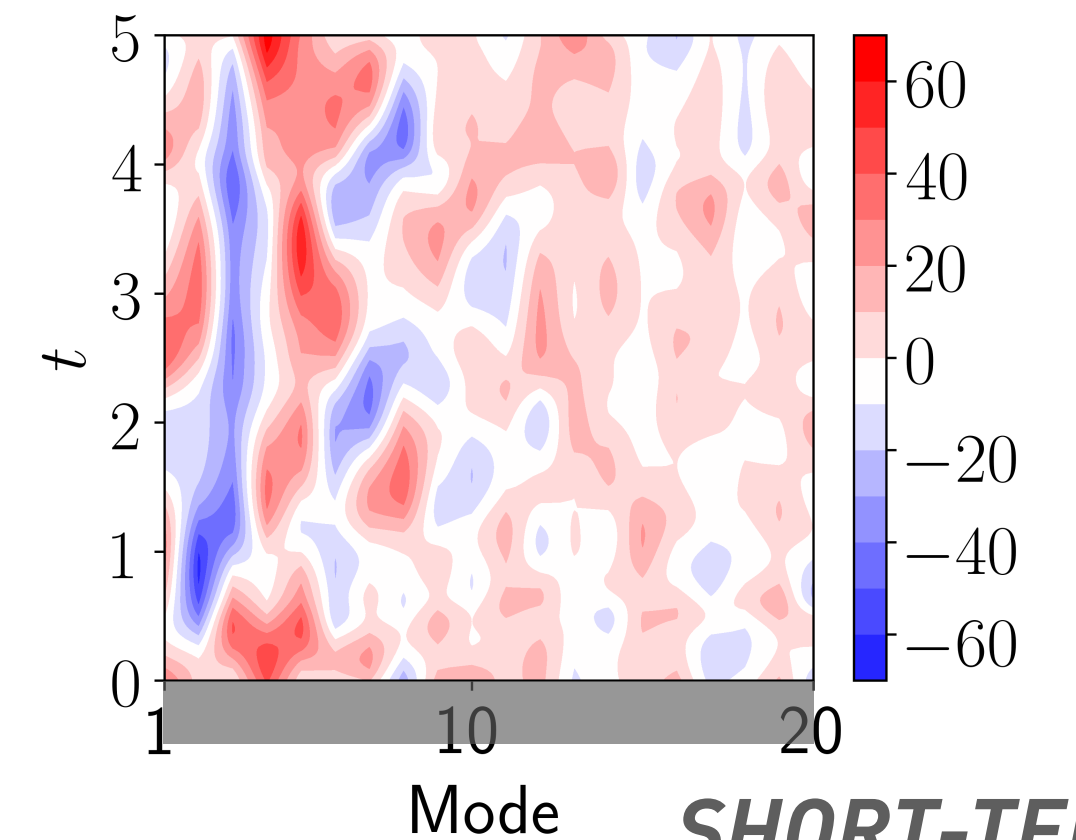
How to predict the dynamics of TEST (unseen) data?

TEST: *UNKNOWN* state dynamics (reference)

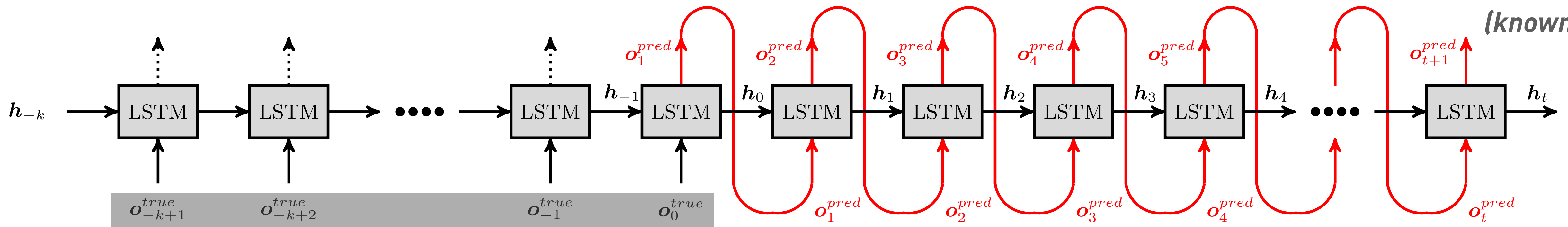


*SVD Mode* dynamics (reference)

SVD



*SHORT-TERM HISTORY (known)*



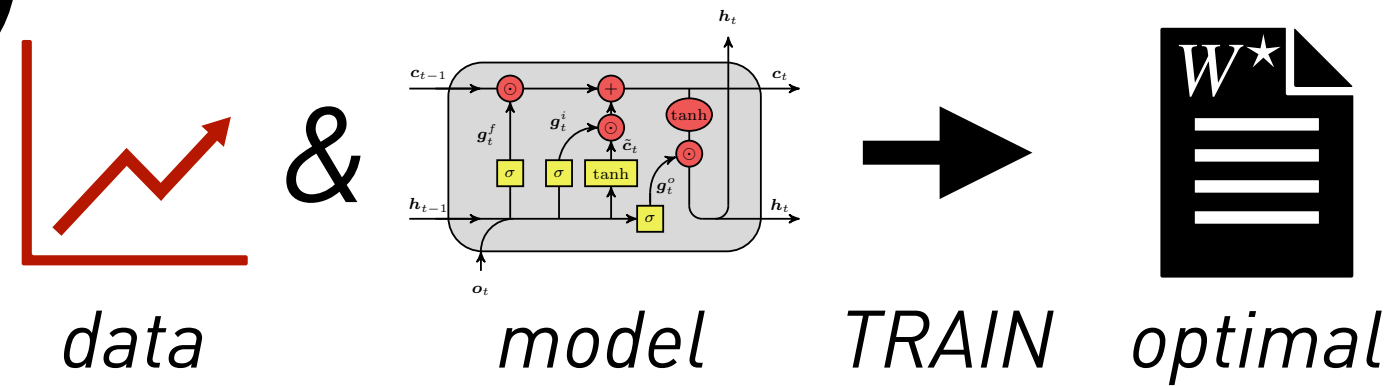
*SHORT-TERM HISTORY (known)*



# Forecasting on UNSEEN data - Iterative prediction in practice

1

TRAIN

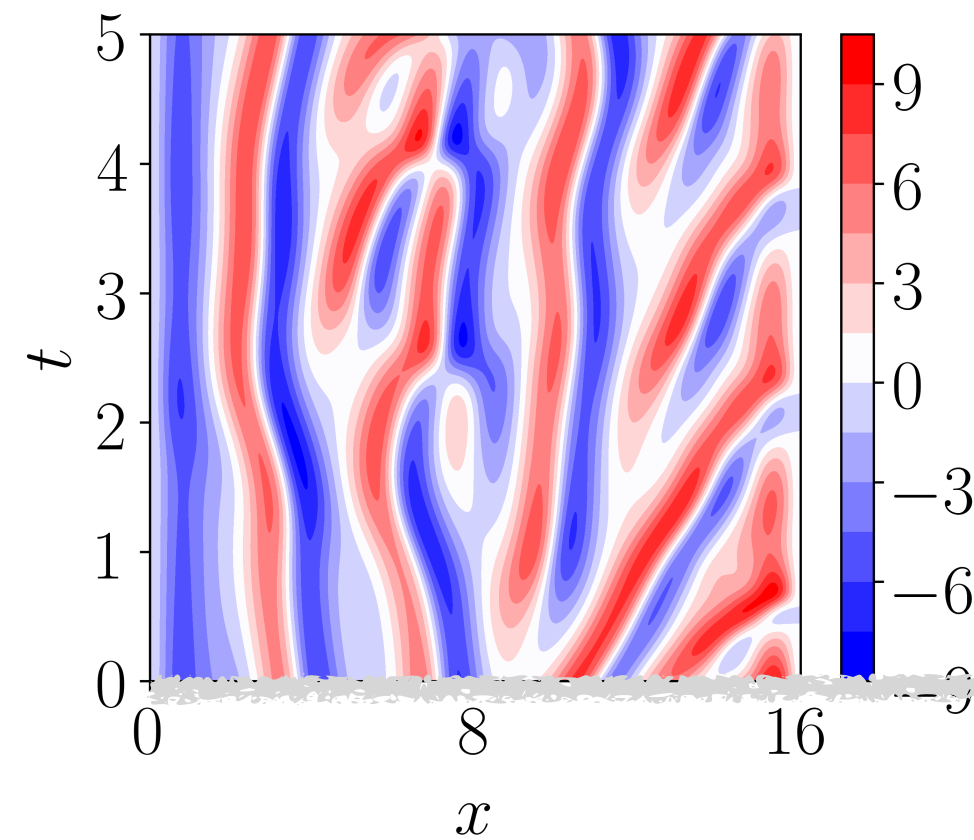


2

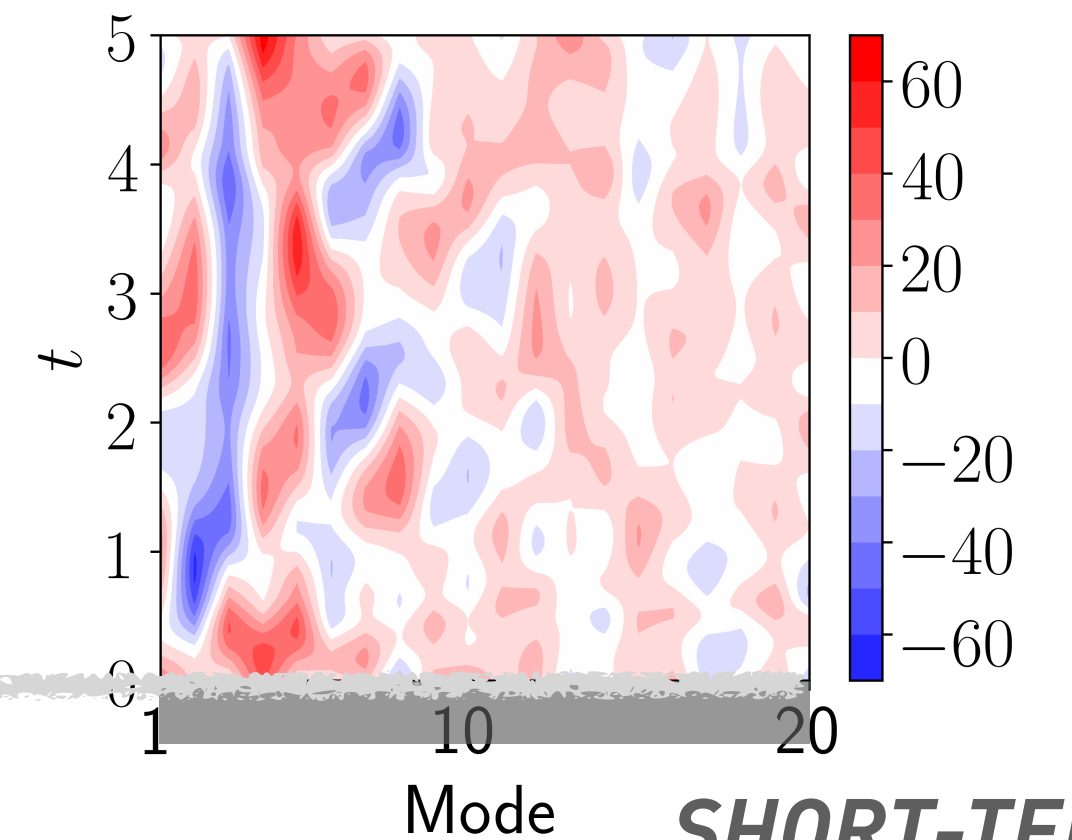
TEST

How to predict the dynamics of TEST (unseen) data?

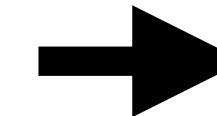
TEST: *UNKNOWN* state dynamics (reference)



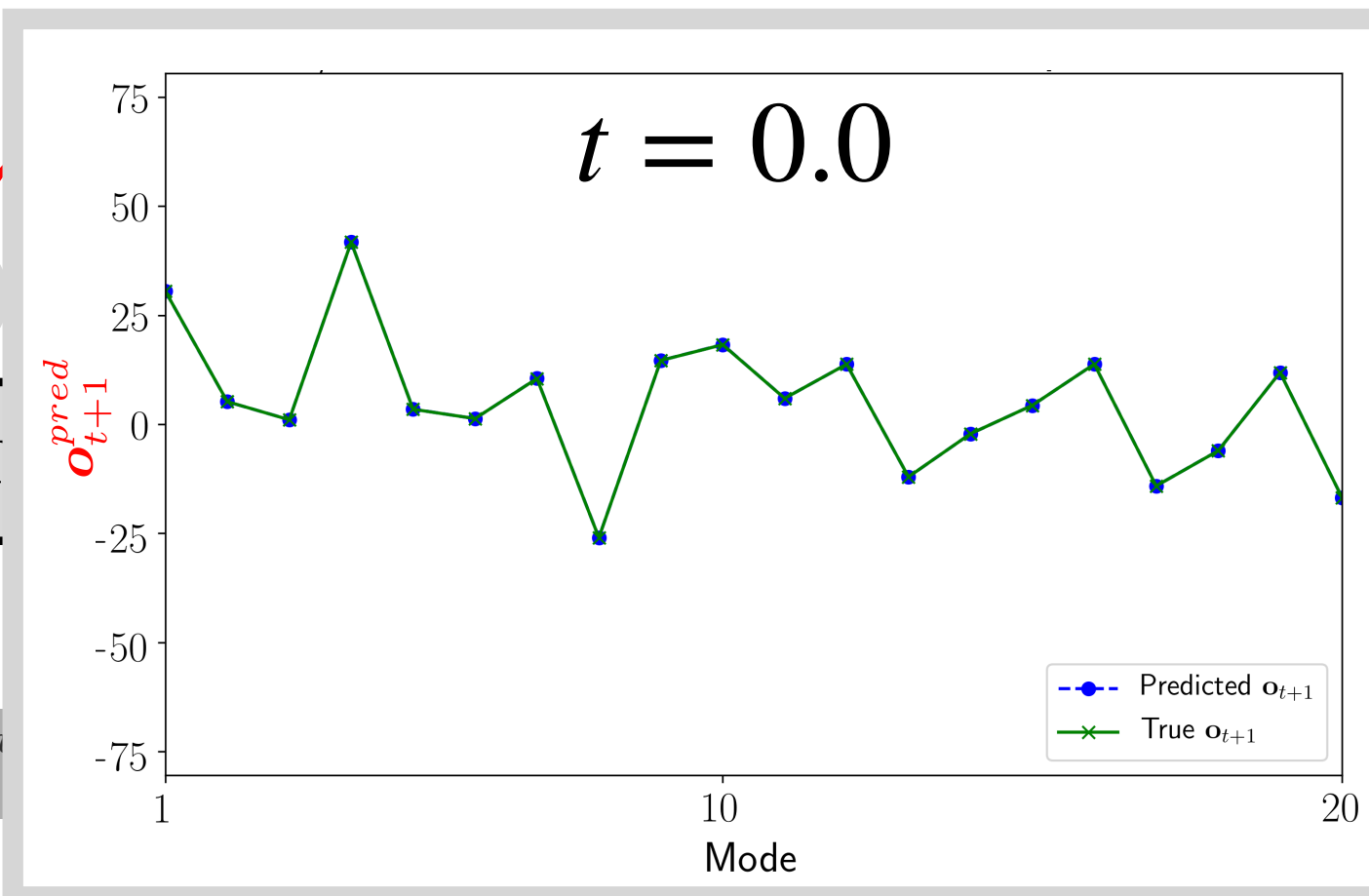
*SVD Mode* dynamics (reference)



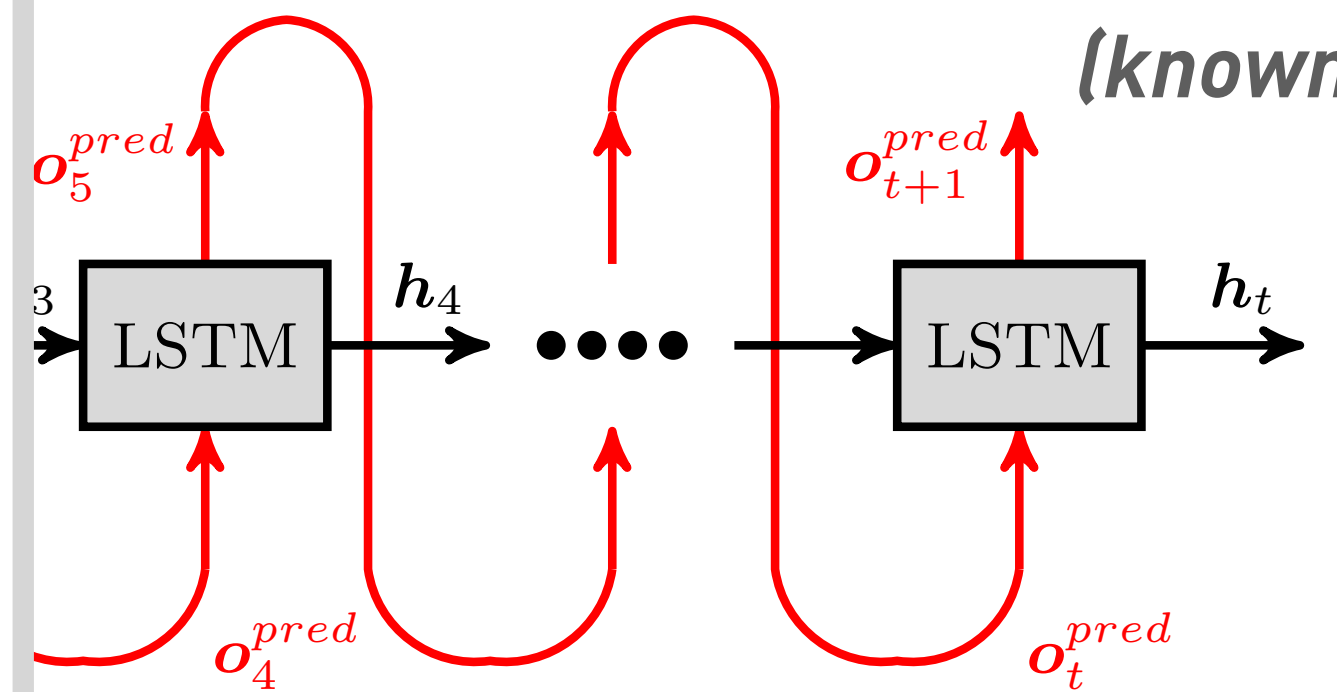
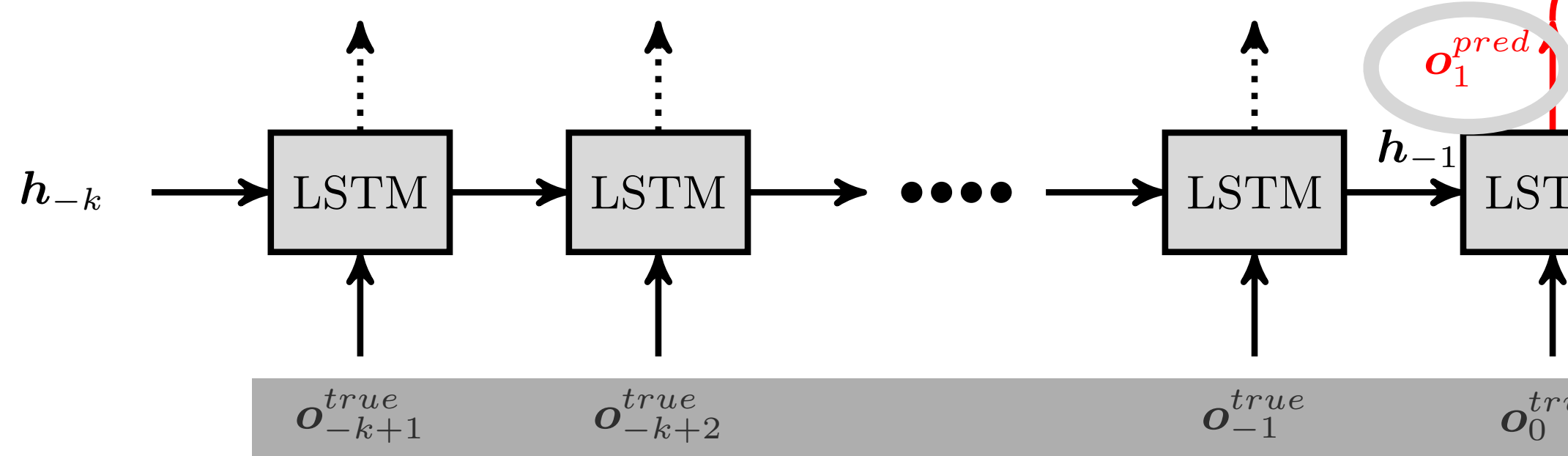
SVD



*SHORT-TERM HISTORY (known)*



*SHORT-TERM HISTORY (known)*

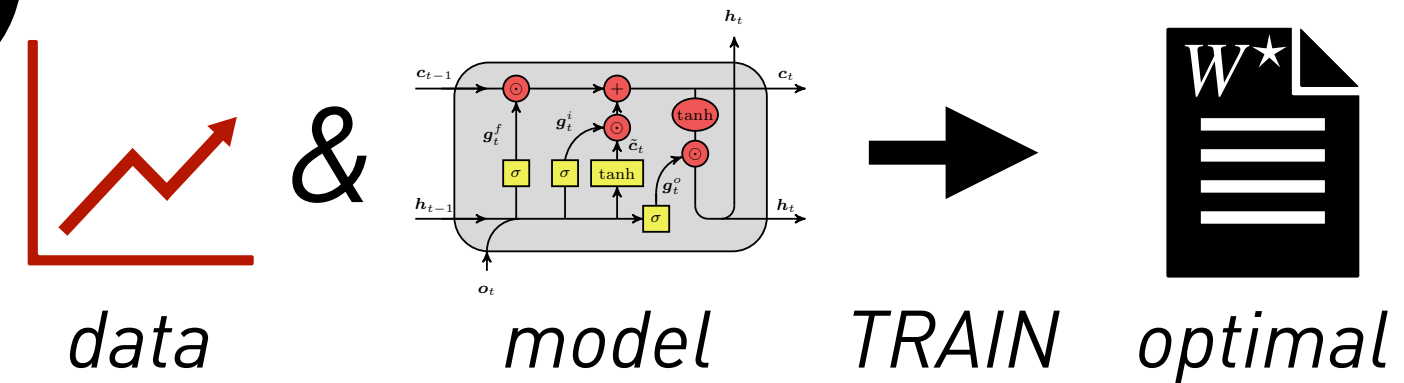




# Forecasting on UNSEEN data - Iterative prediction in practice

1

TRAIN

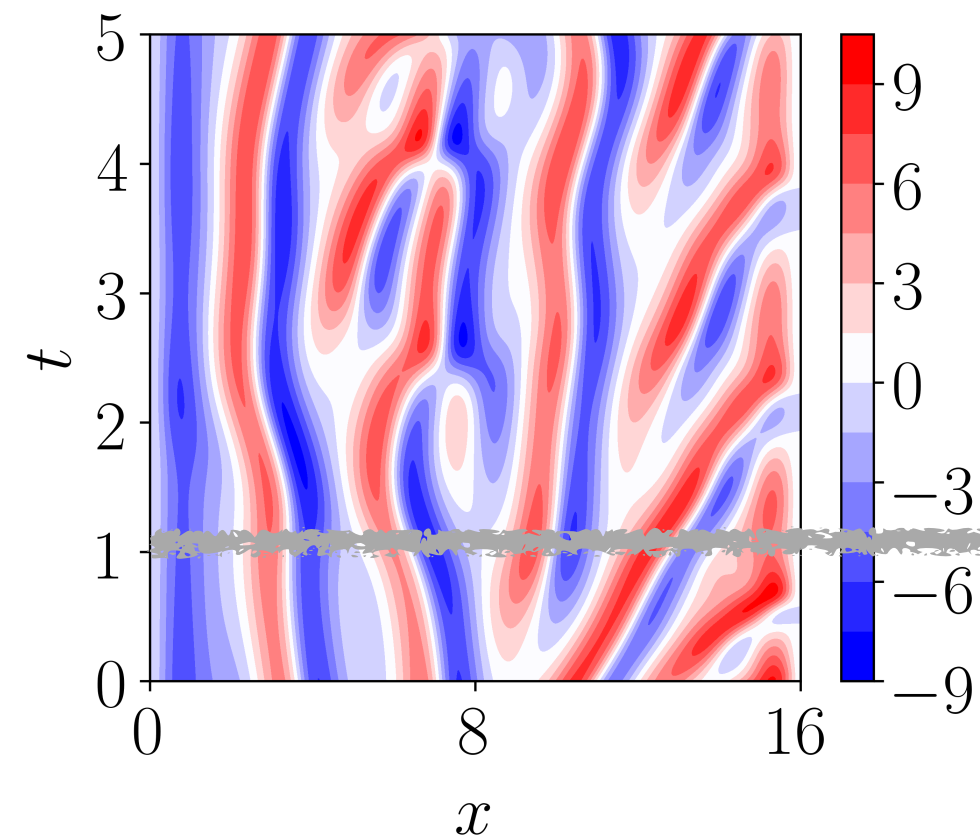


2

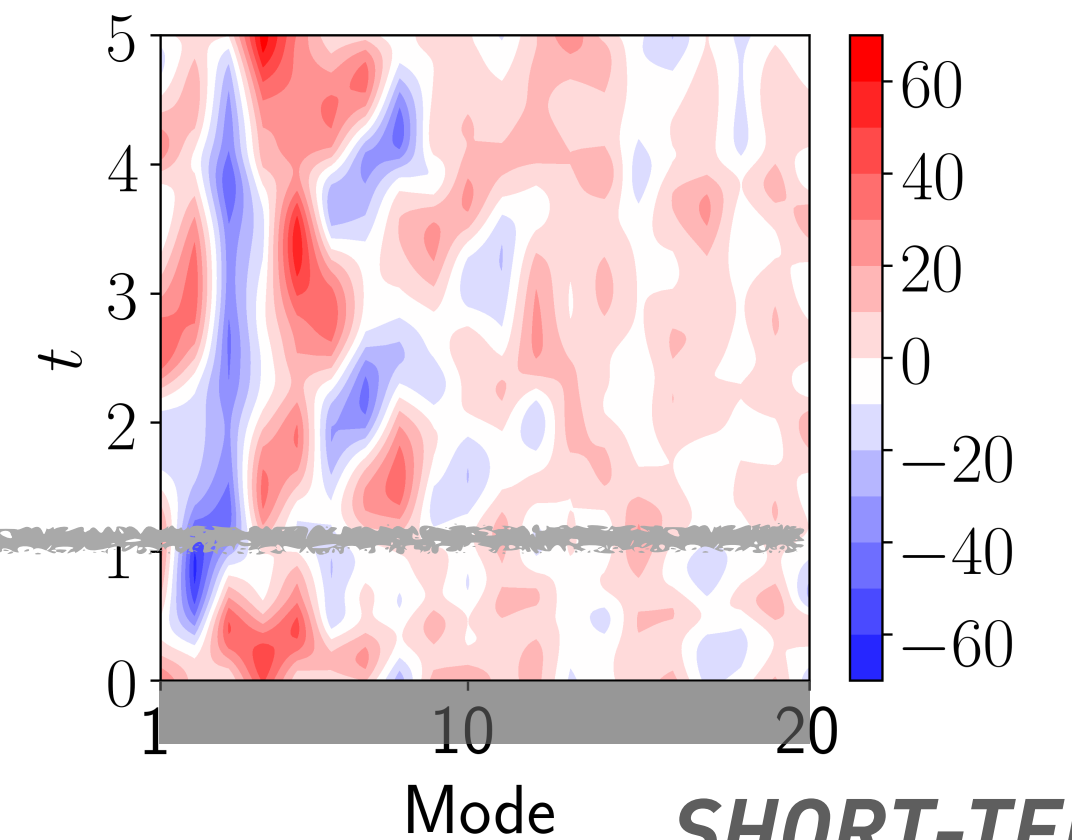
TEST

How to predict the dynamics of TEST (unseen) data?

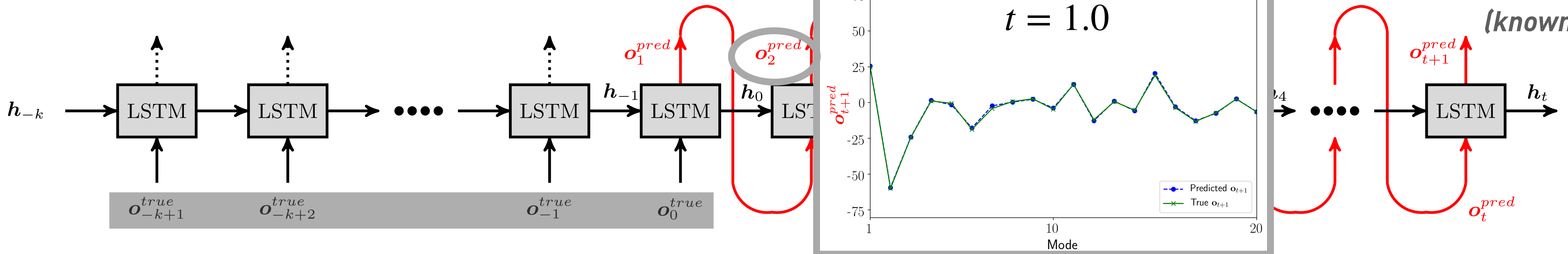
TEST: *UNKNOWN* state dynamics (reference)



*SVD Mode* dynamics (reference)



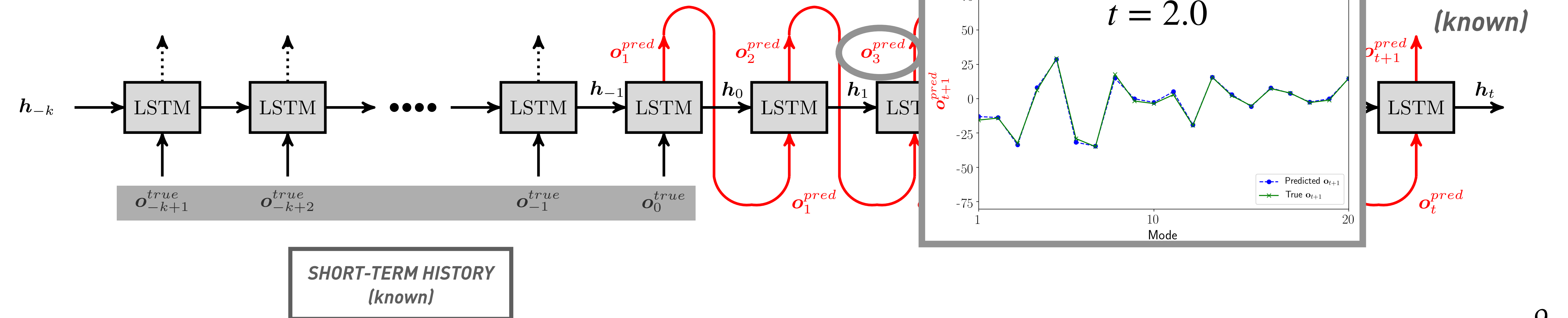
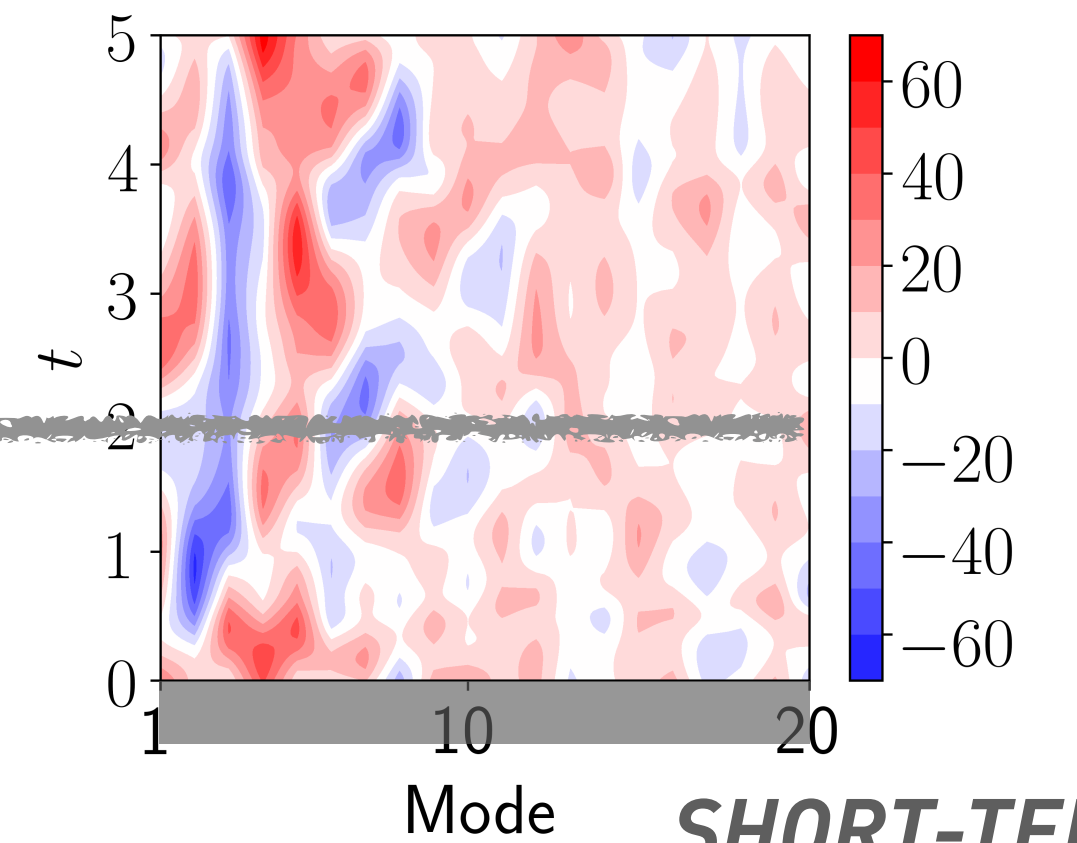
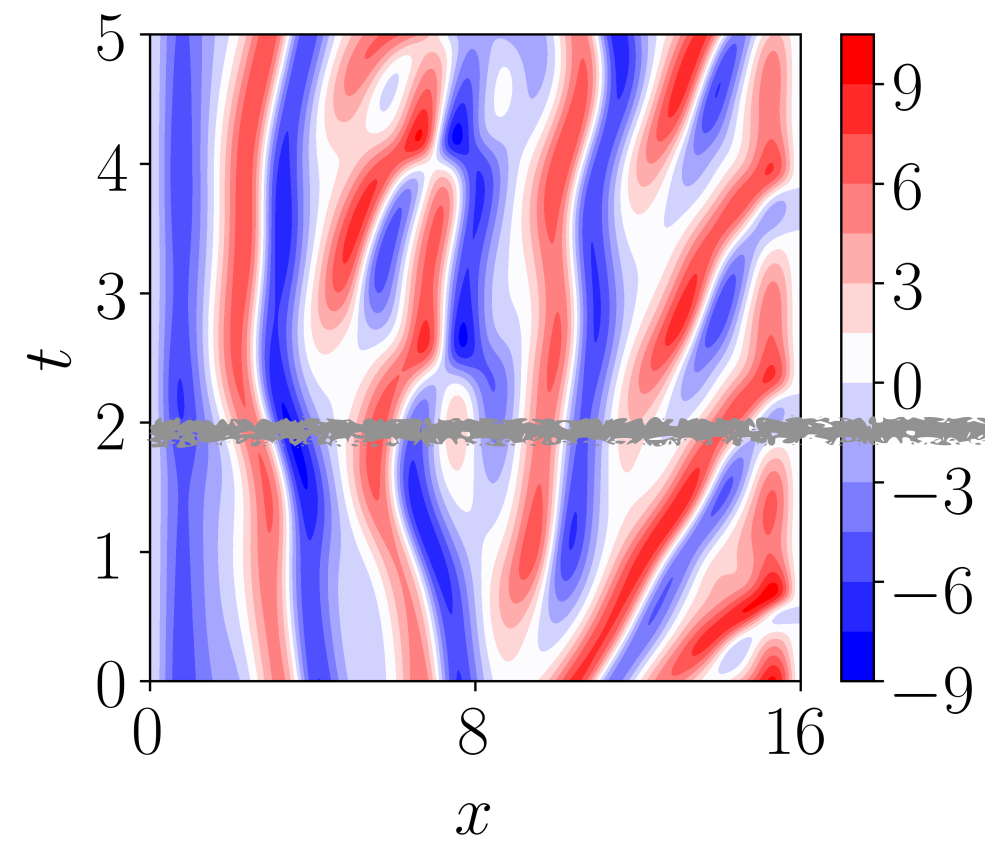
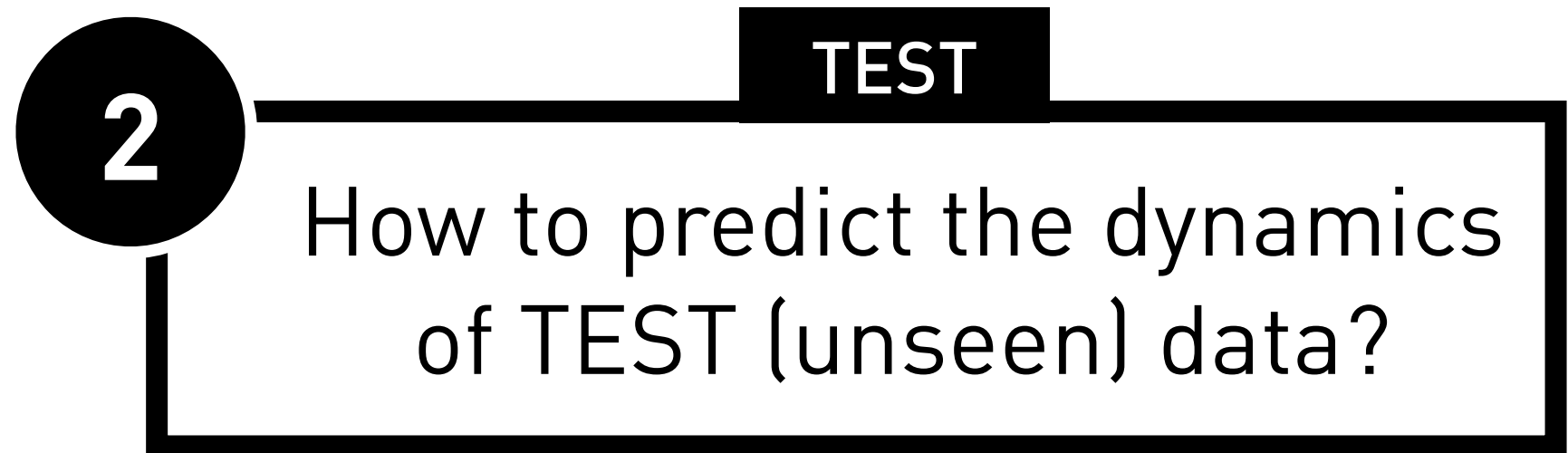
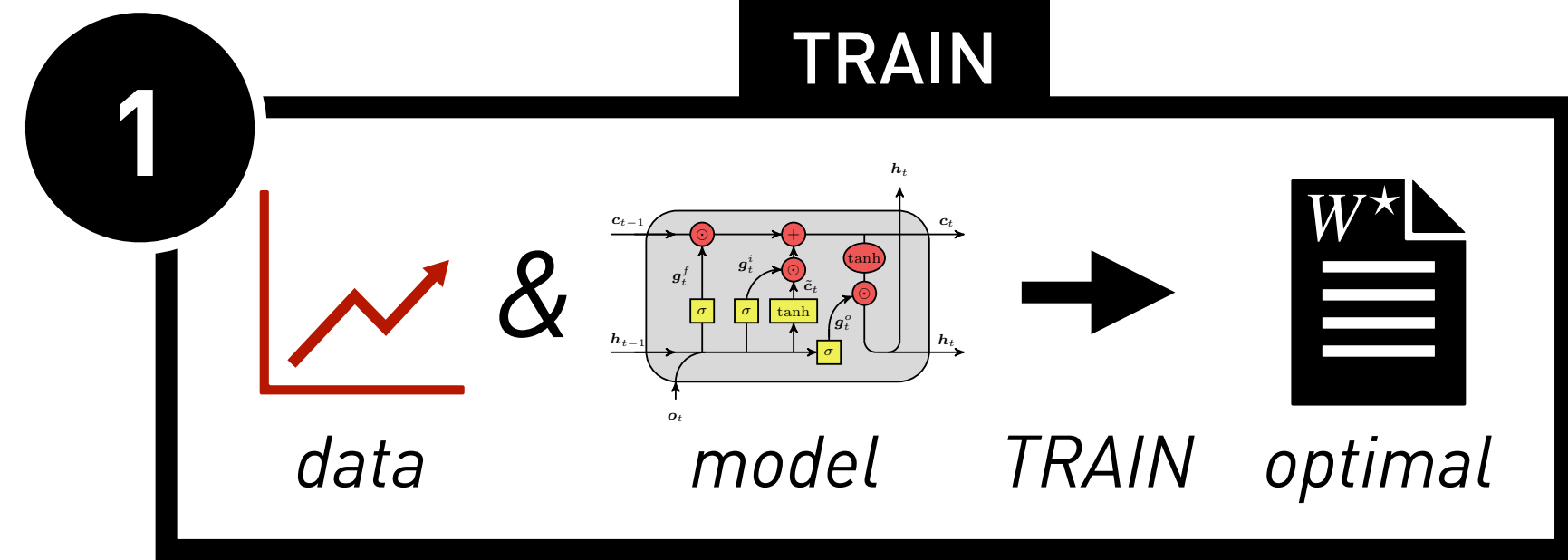
*SHORT-TERM HISTORY (known)*



*SHORT-TERM HISTORY (known)*



# Forecasting on UNSEEN data - Iterative prediction in practice

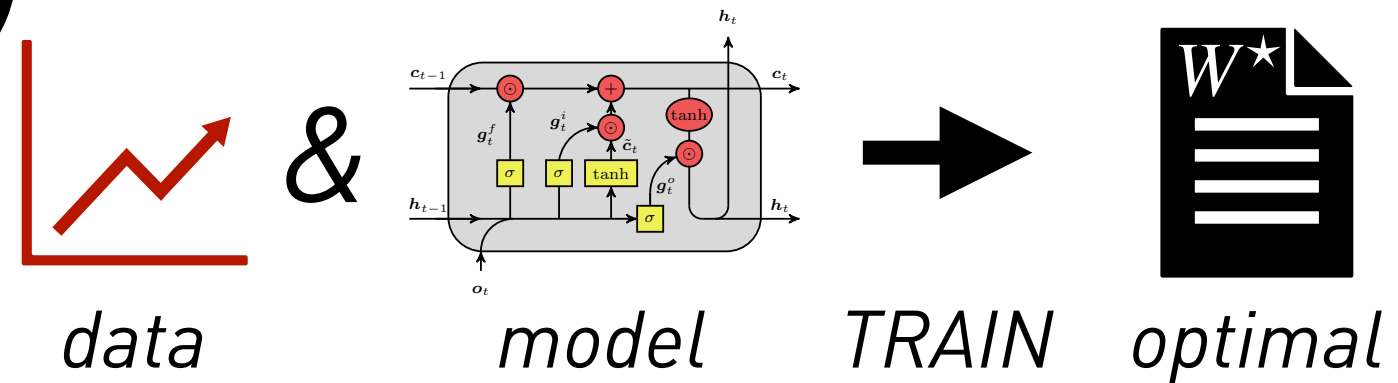




# Forecasting on UNSEEN data - Iterative prediction in practice

1

TRAIN

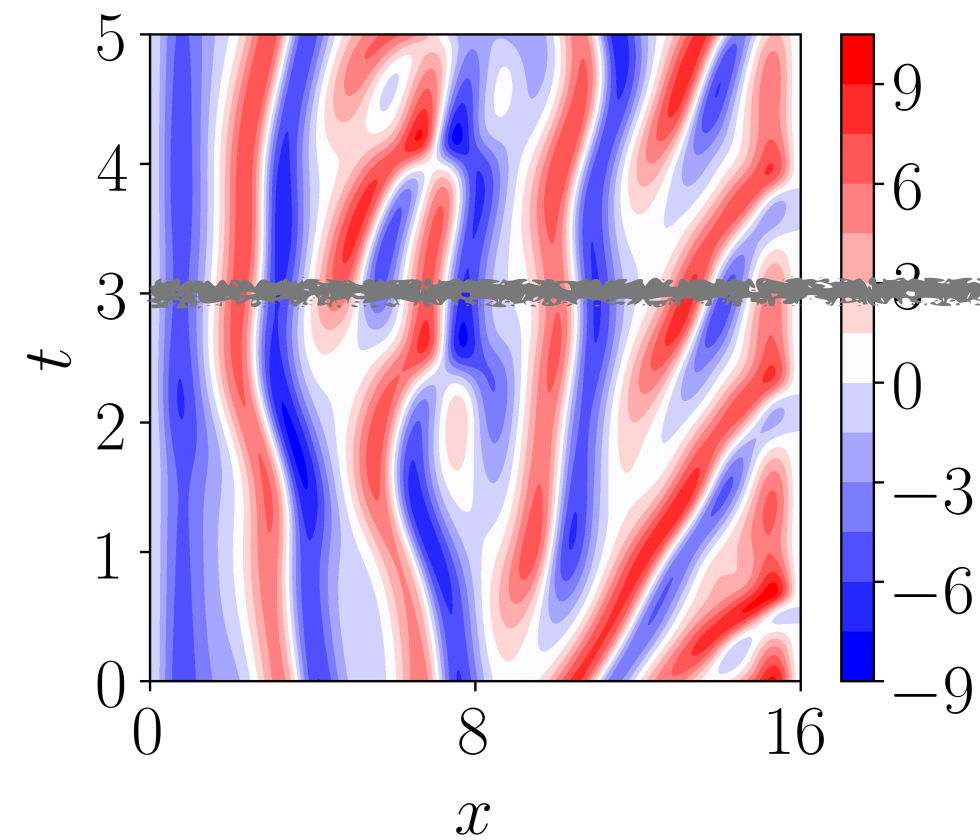


2

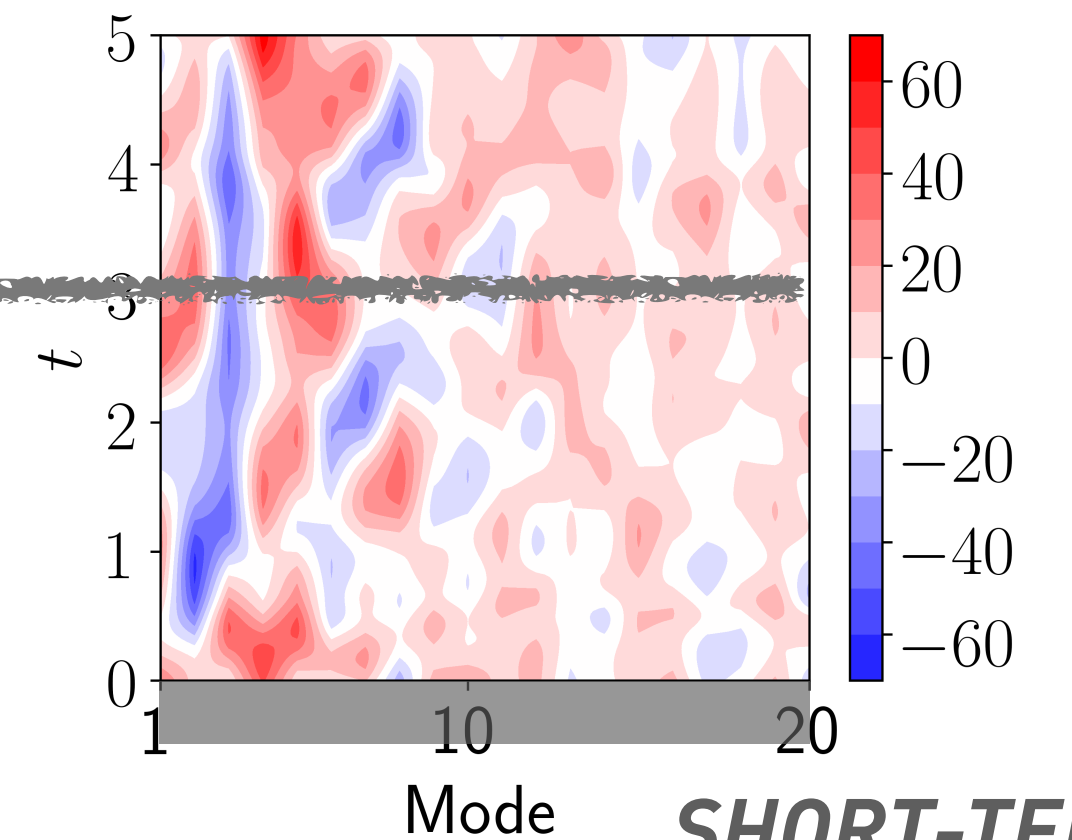
TEST

How to predict the dynamics of TEST (unseen) data?

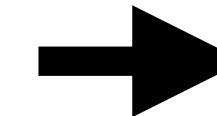
TEST: *UNKNOWN* state dynamics (reference)



*SVD Mode* dynamics (reference)

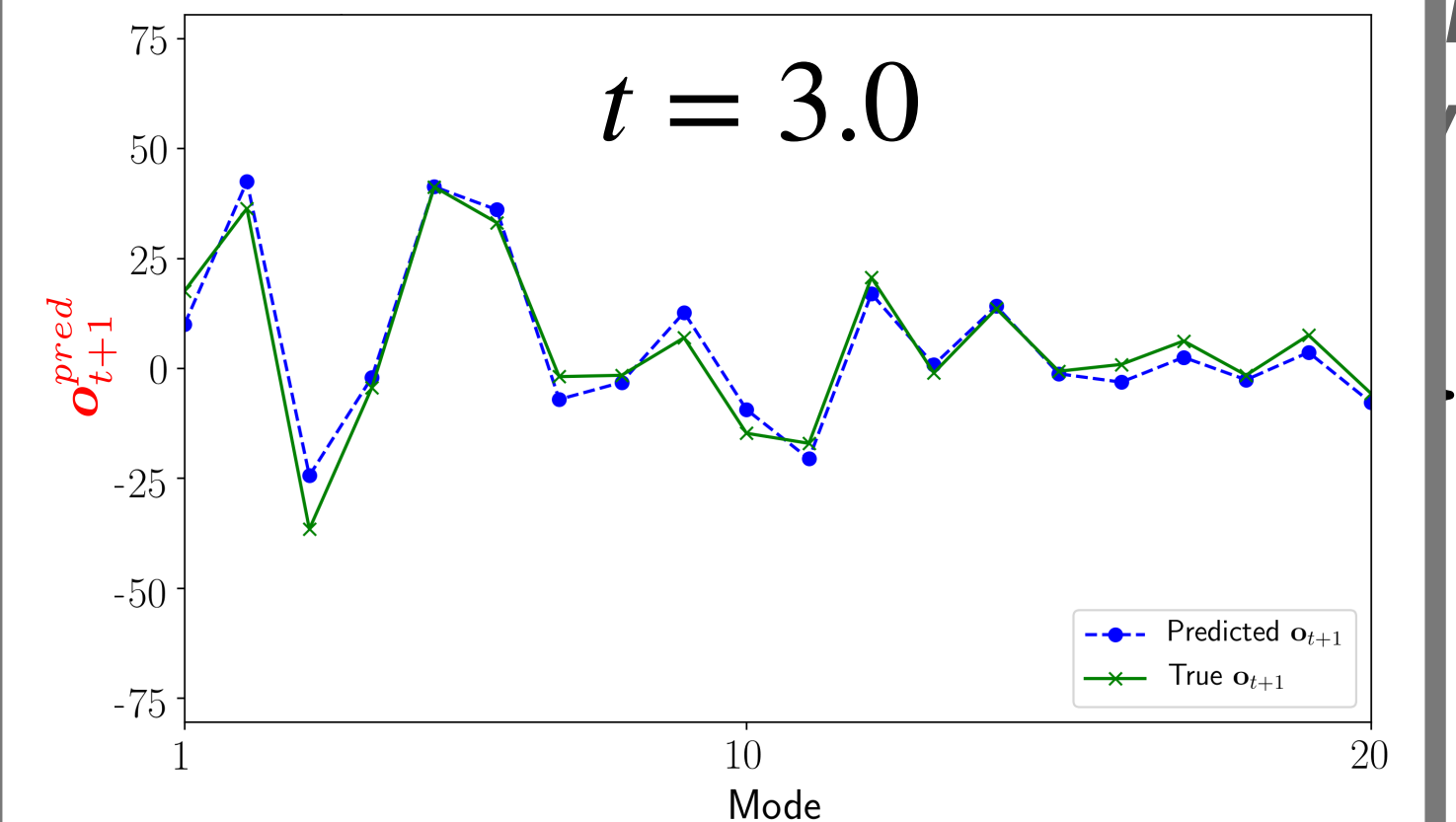


SVD



*SHORT-TERM*  
*RY*  
*(n)*

$t = 3.0$



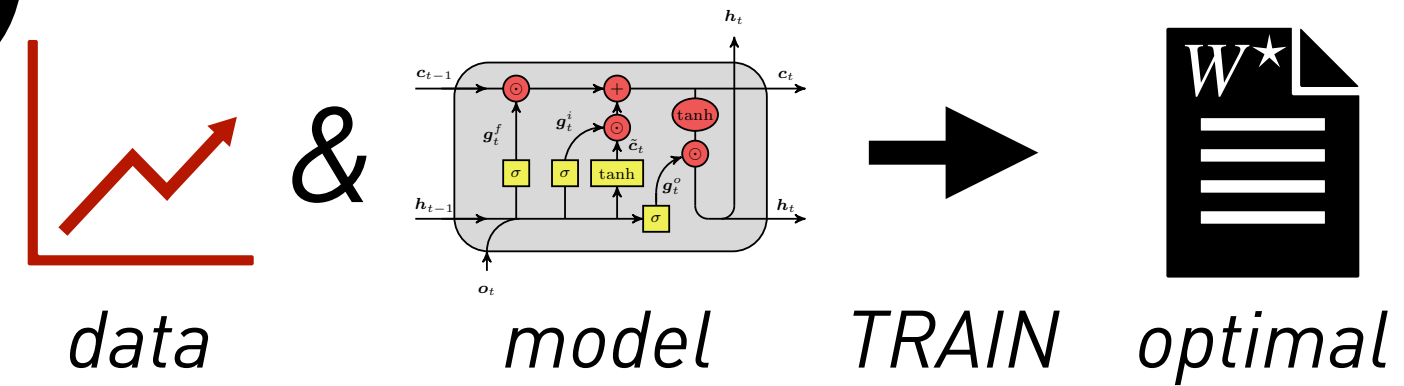
*SHORT-TERM HISTORY*  
*(known)*



# Forecasting on UNSEEN data - Iterative prediction in practice

1

TRAIN

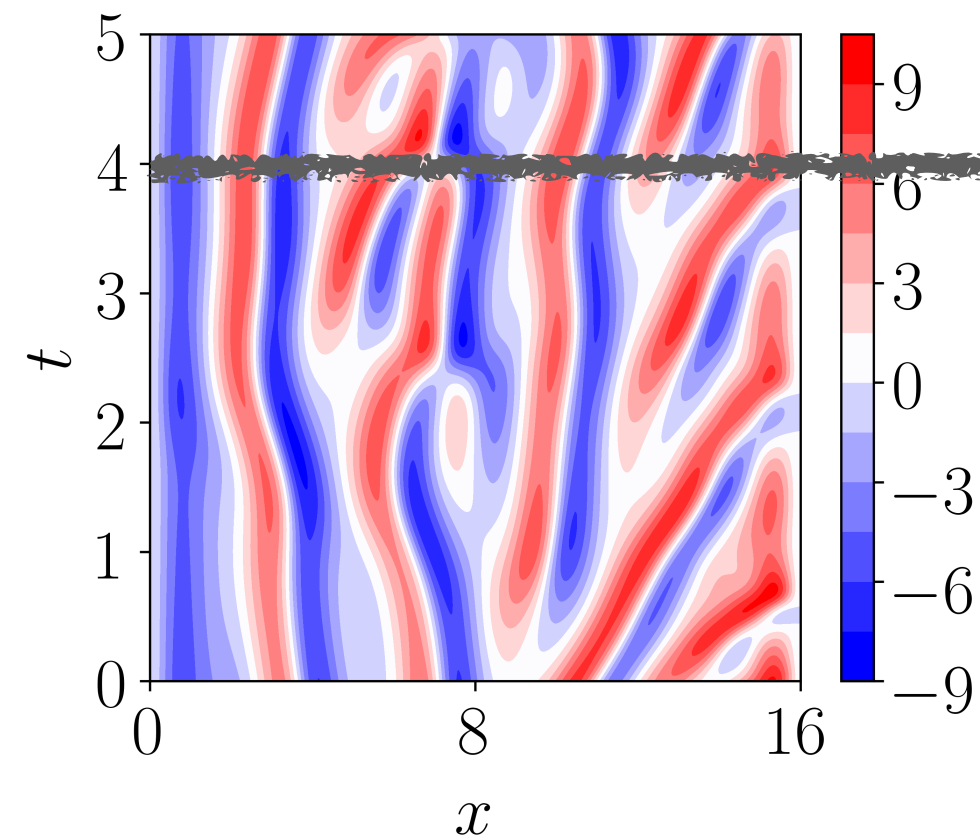


2

TEST

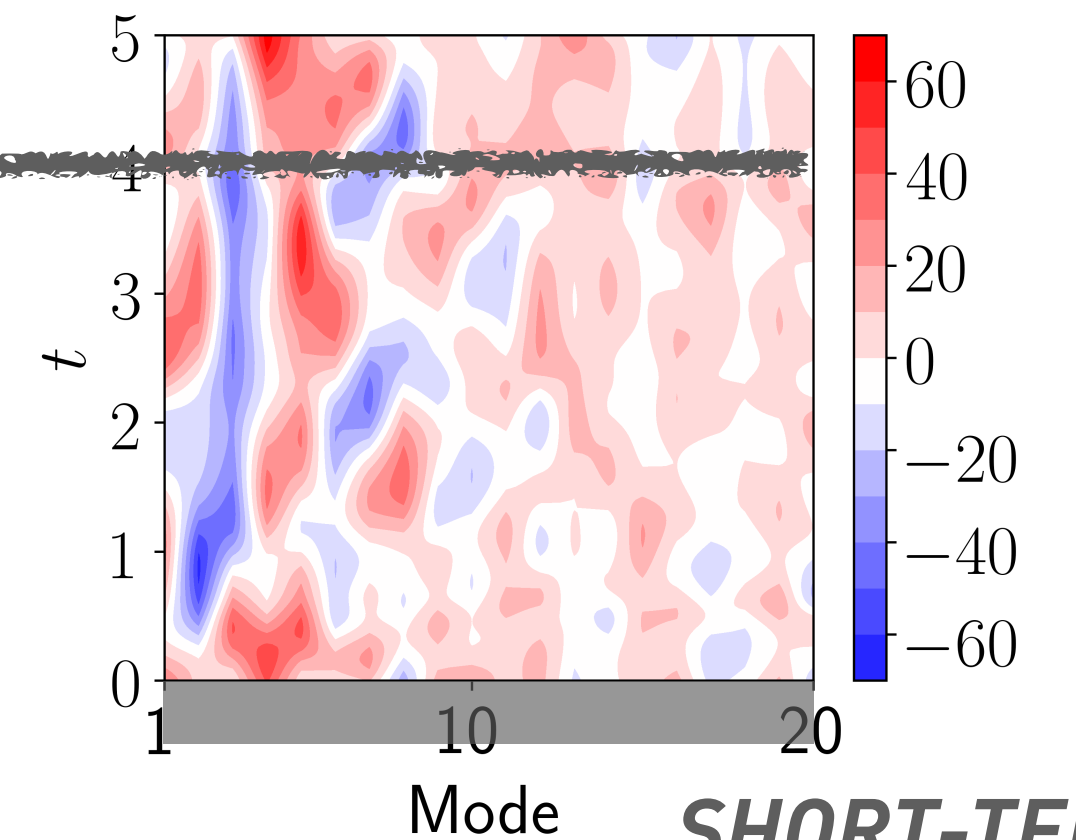
How to predict the dynamics of TEST (unseen) data?

TEST: *UNKNOWN* state dynamics (reference)



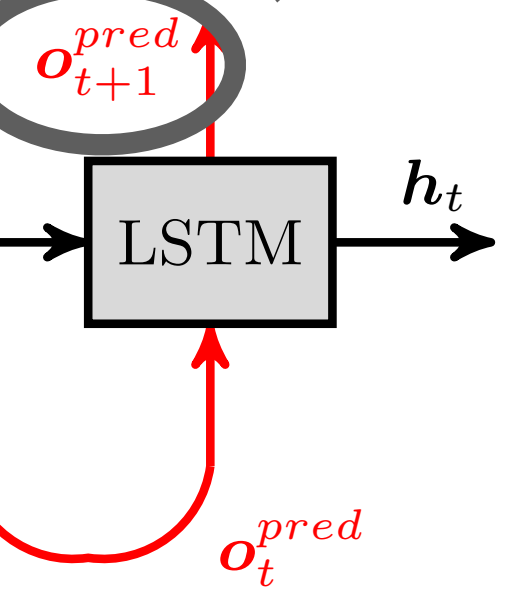
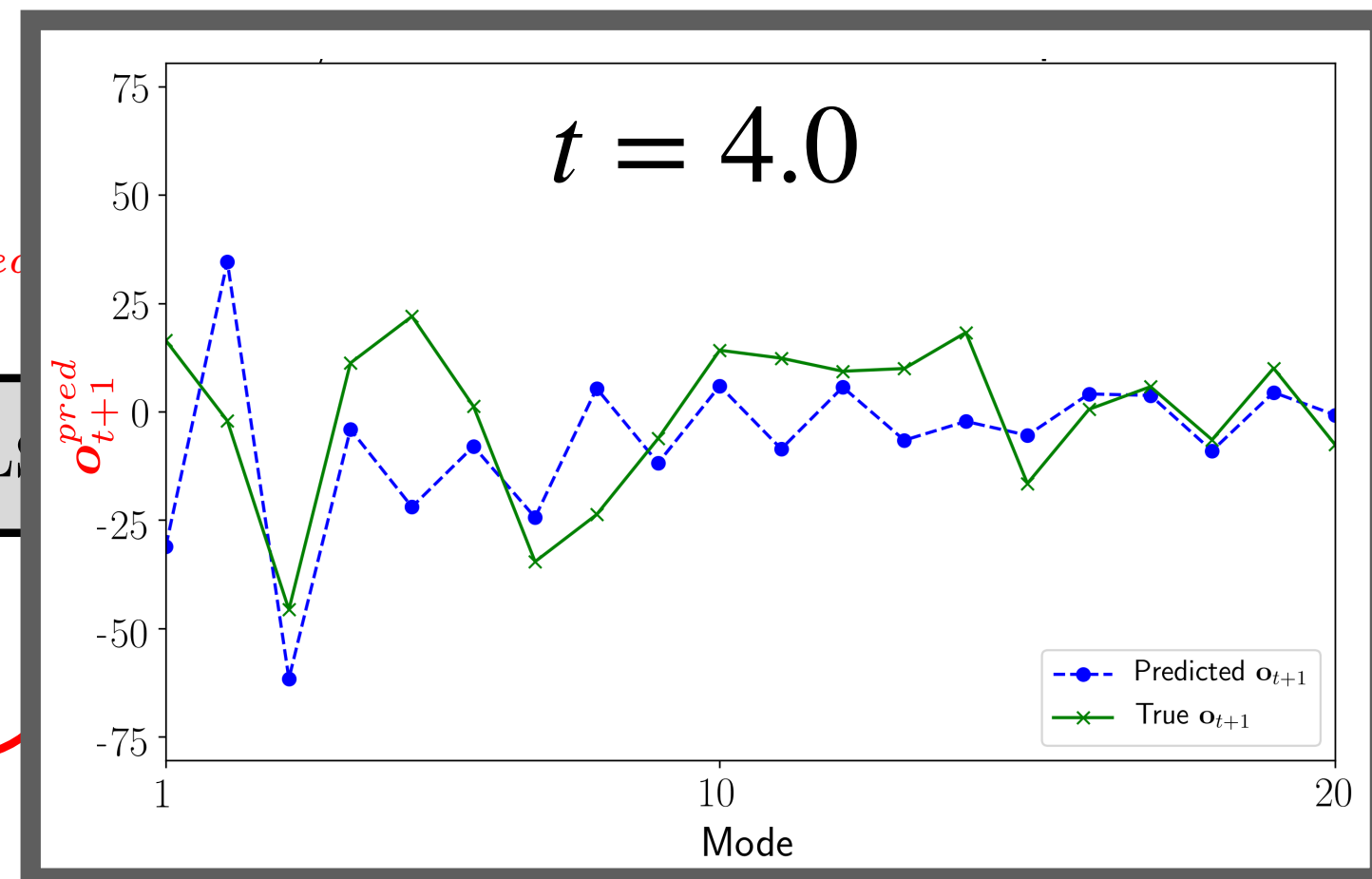
*SVD Mode* dynamics (reference)

SVD



*SHORT-TERM HISTORY (known)*

$t = 4.0$



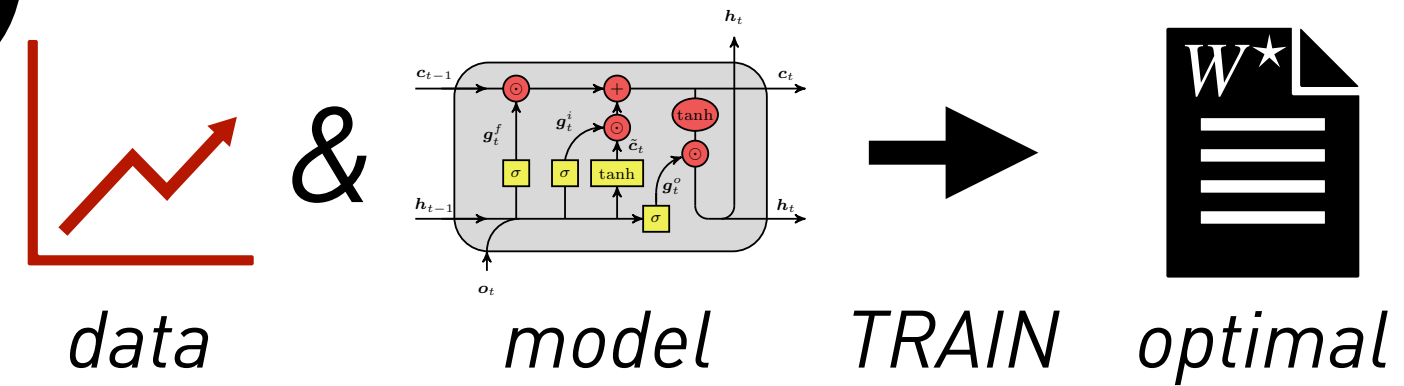
*SHORT-TERM HISTORY (known)*



# Forecasting on UNSEEN data - Iterative prediction in practice

1

TRAIN

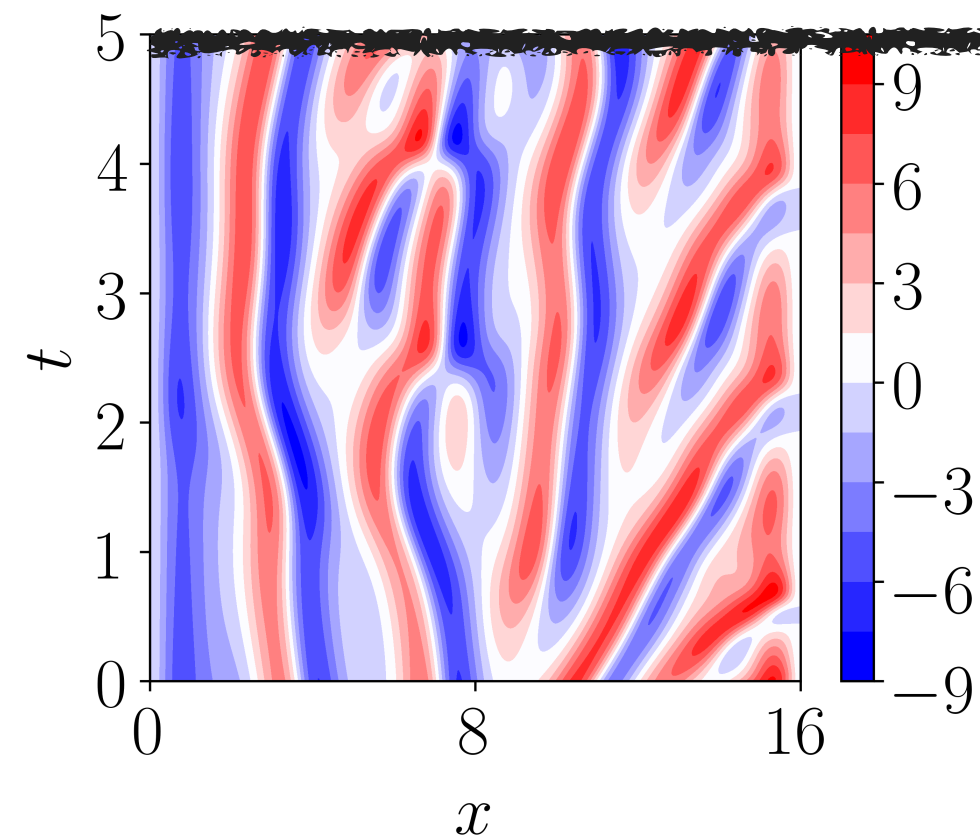


2

TEST

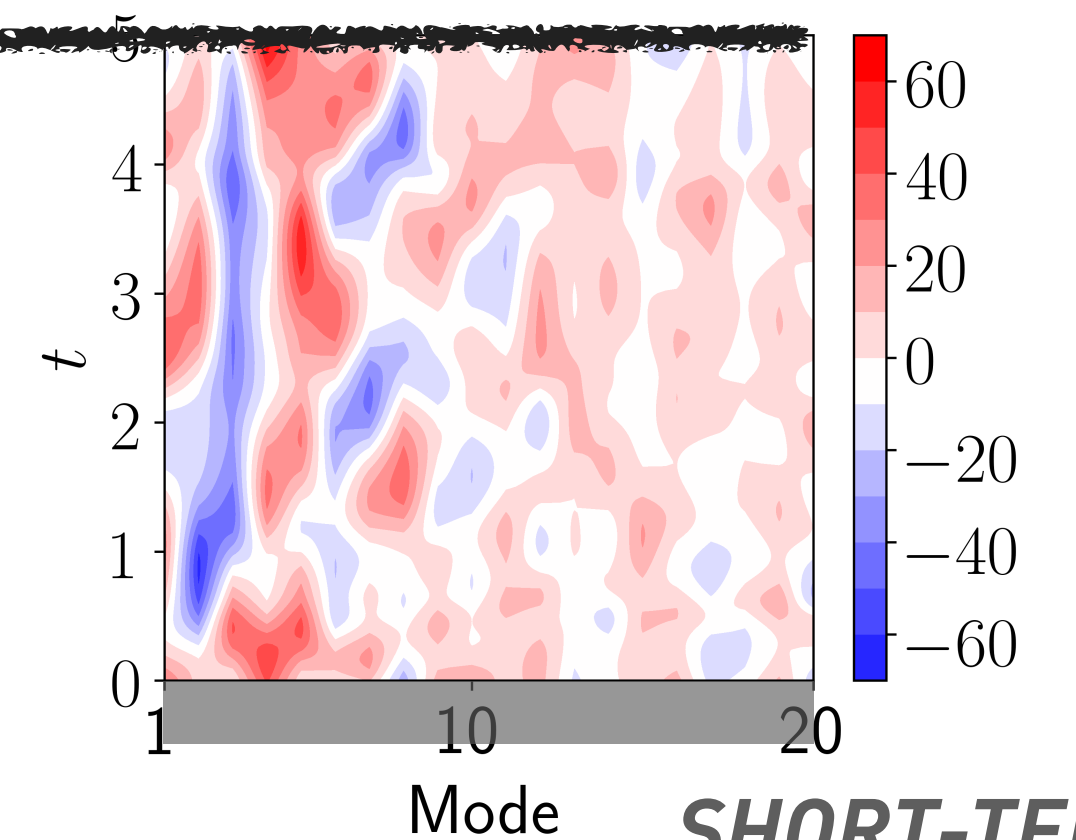
How to predict the dynamics of TEST (unseen) data?

TEST: *UNKNOWN* state dynamics (reference)

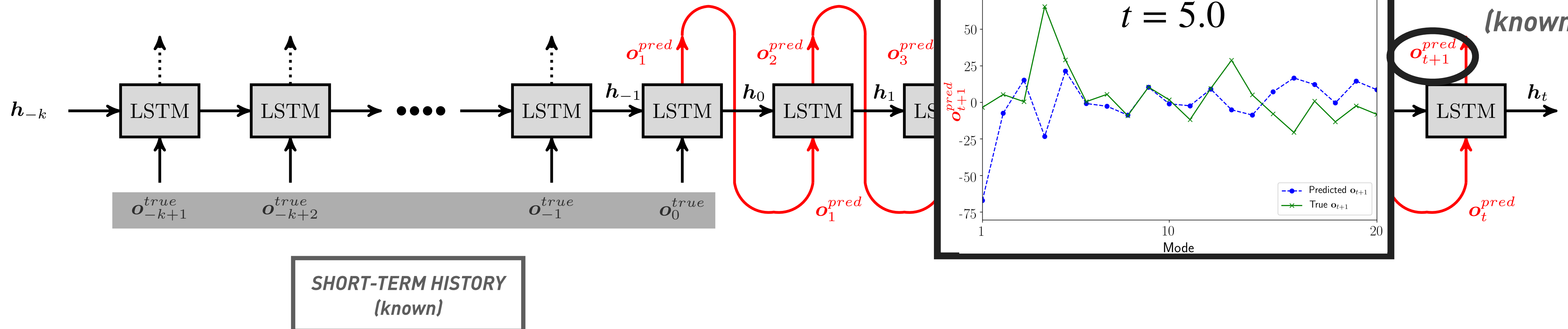


*SVD Mode* dynamics (reference)

SVD



*SHORT-TERM HISTORY (known)*



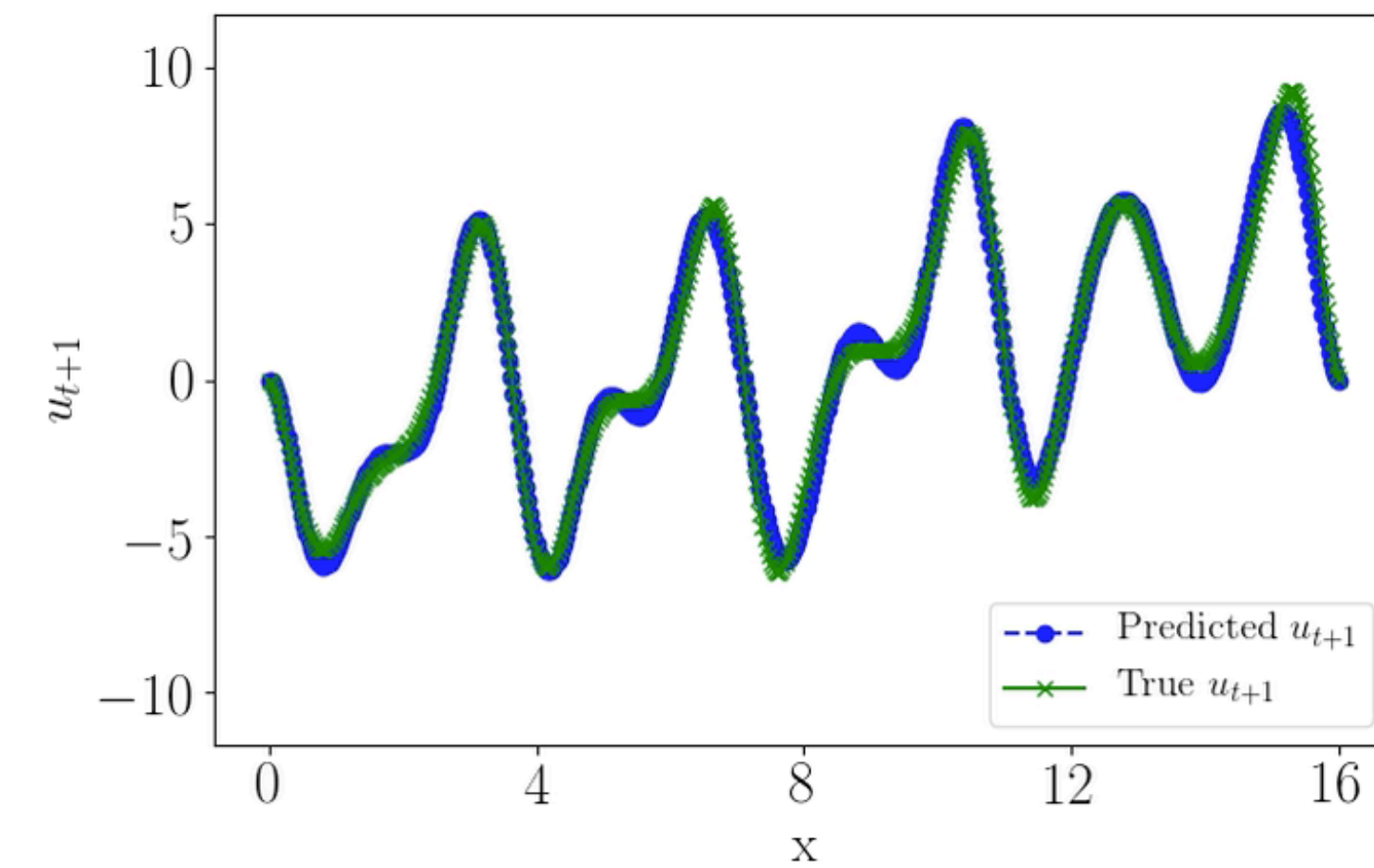
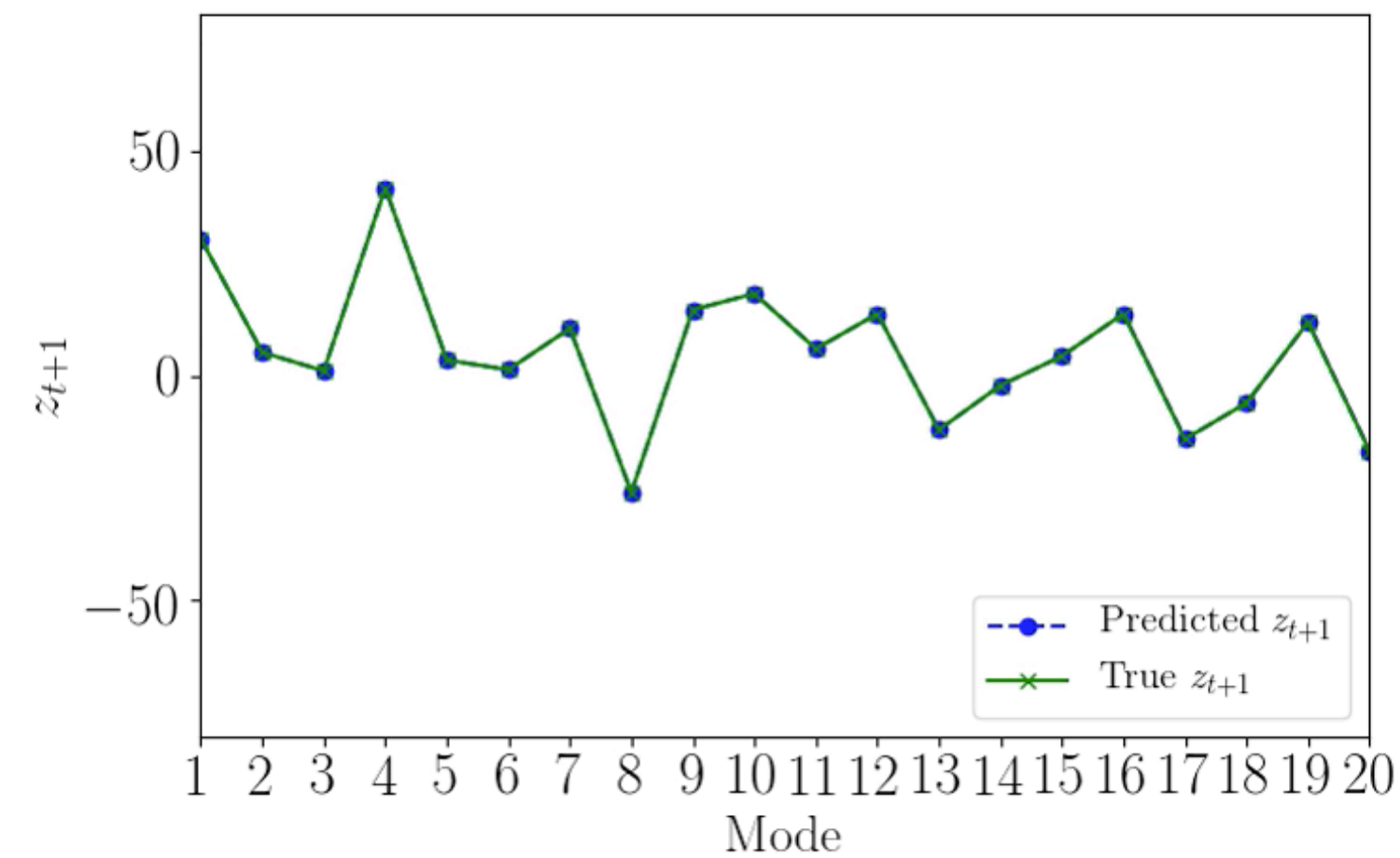


# Accumulation of prediction error

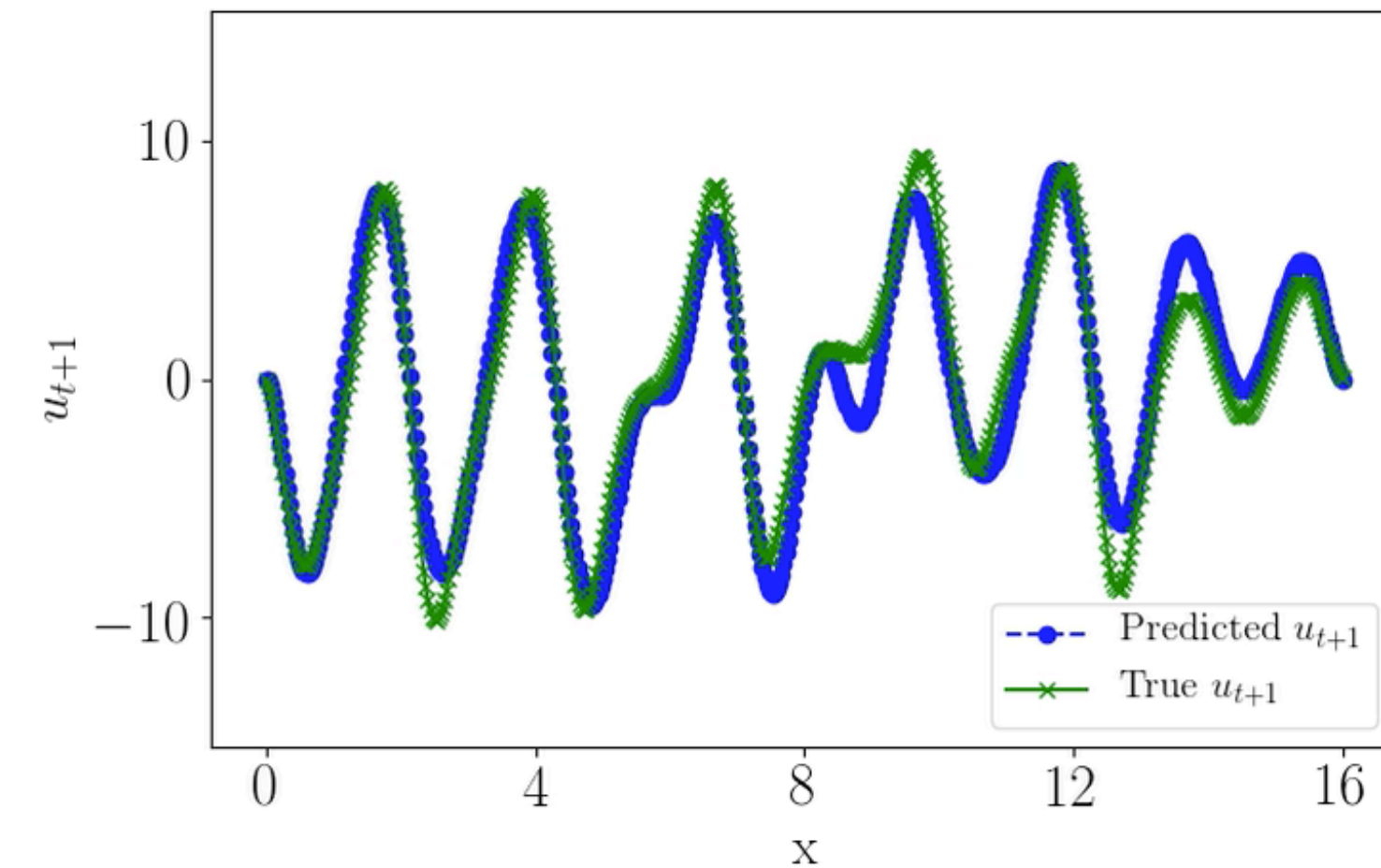
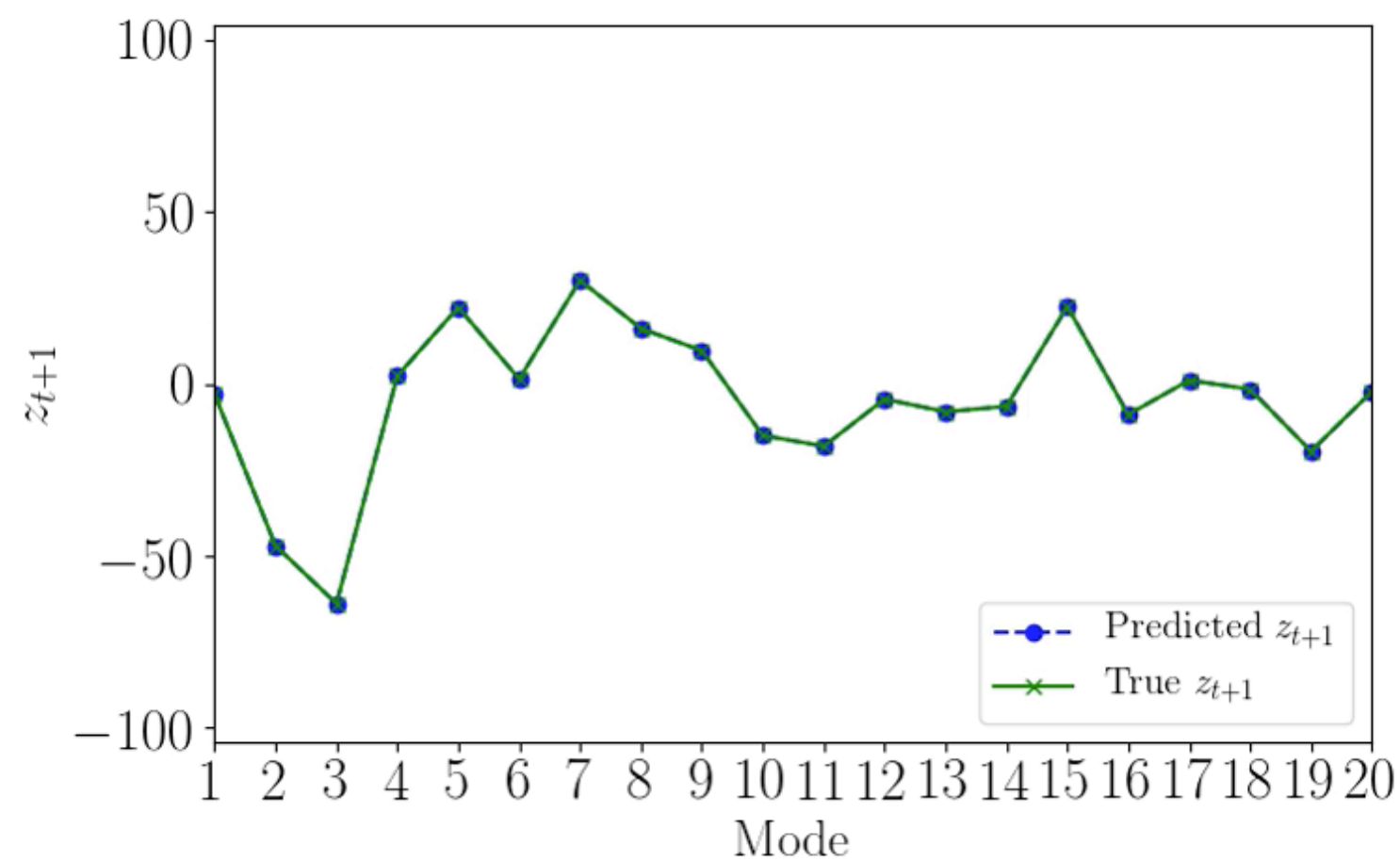
prediction in **reduced** space

expanded in **high-dimensional** space

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



$$\tilde{L} \approx 10$$



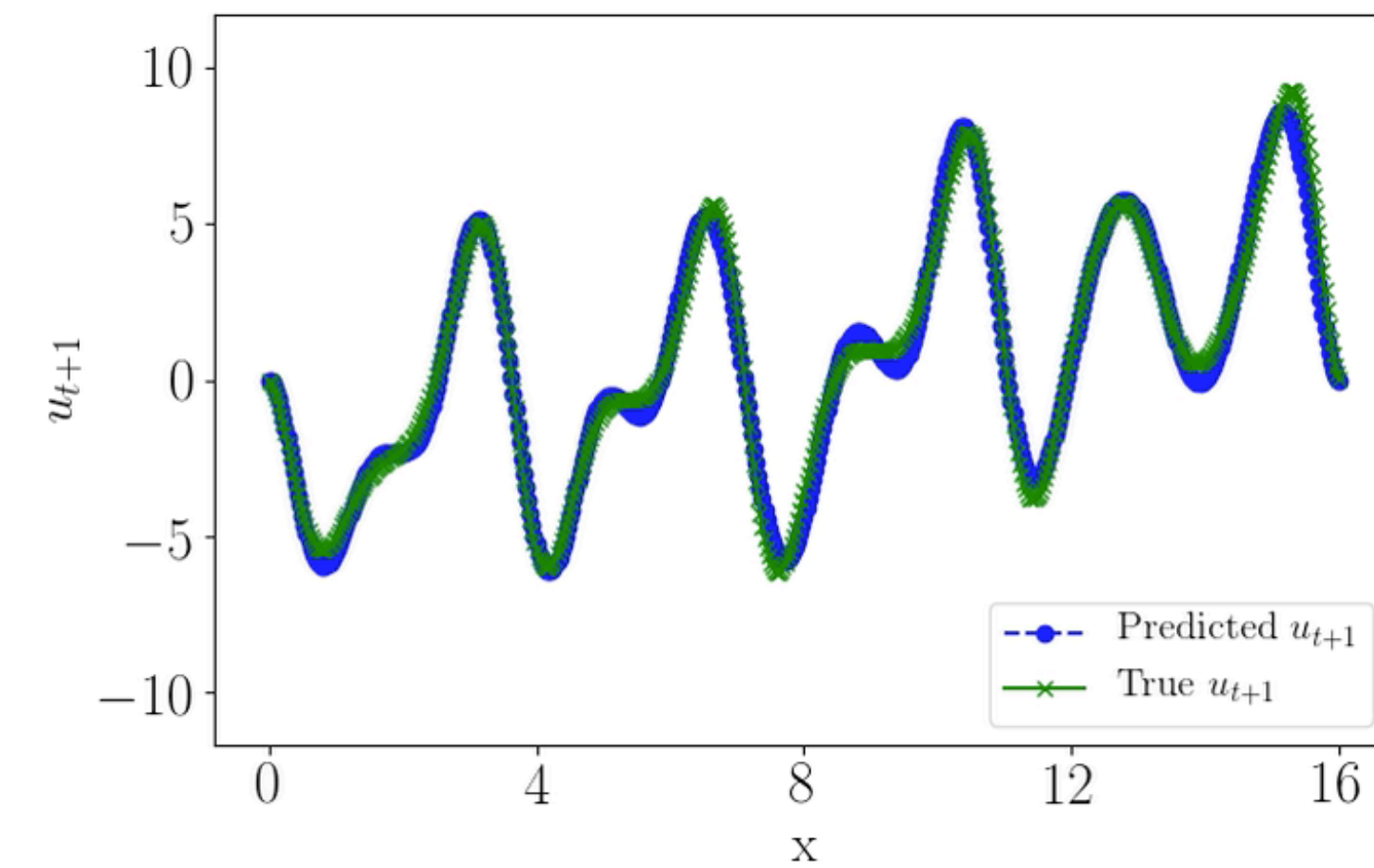
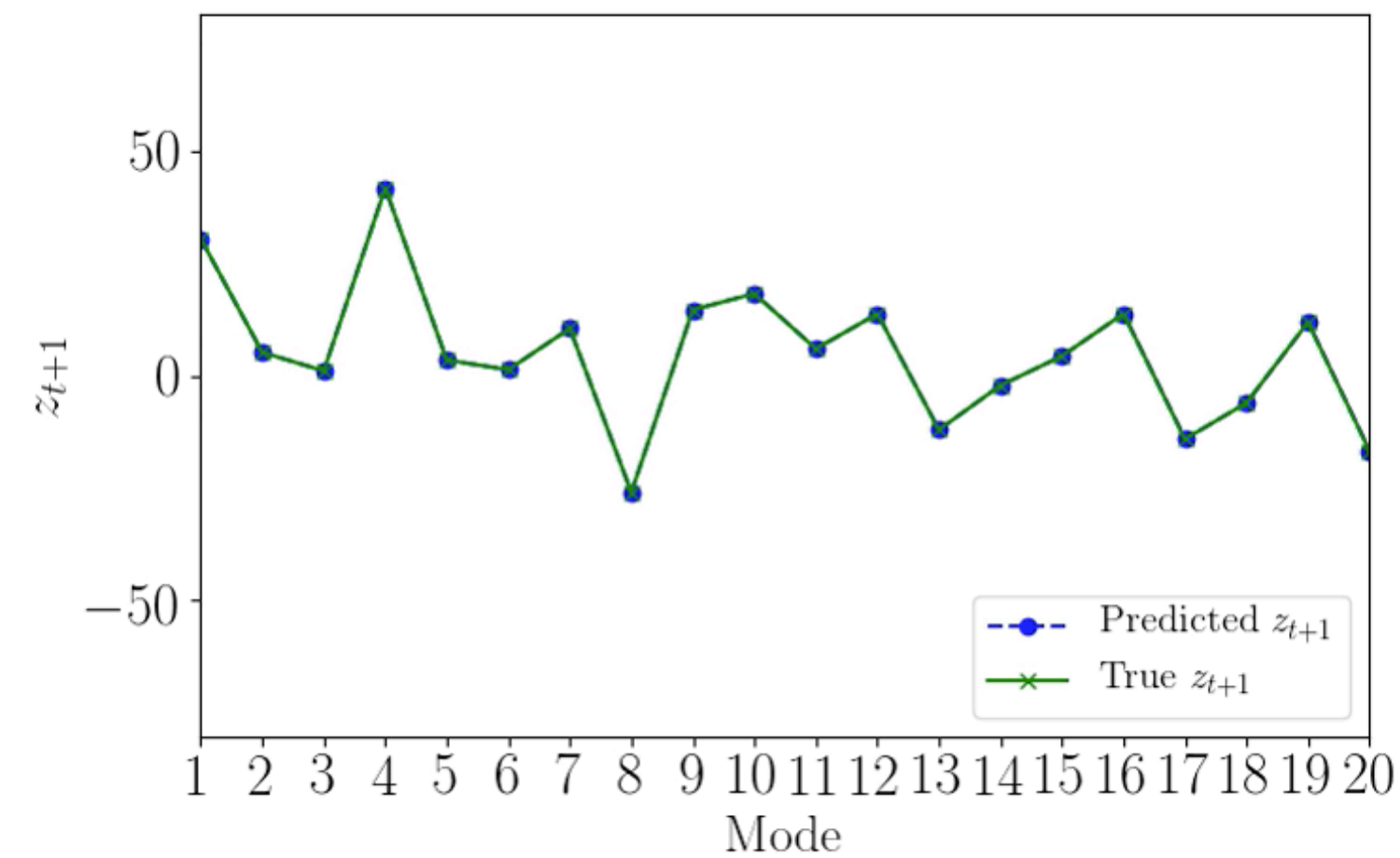


# Accumulation of prediction error

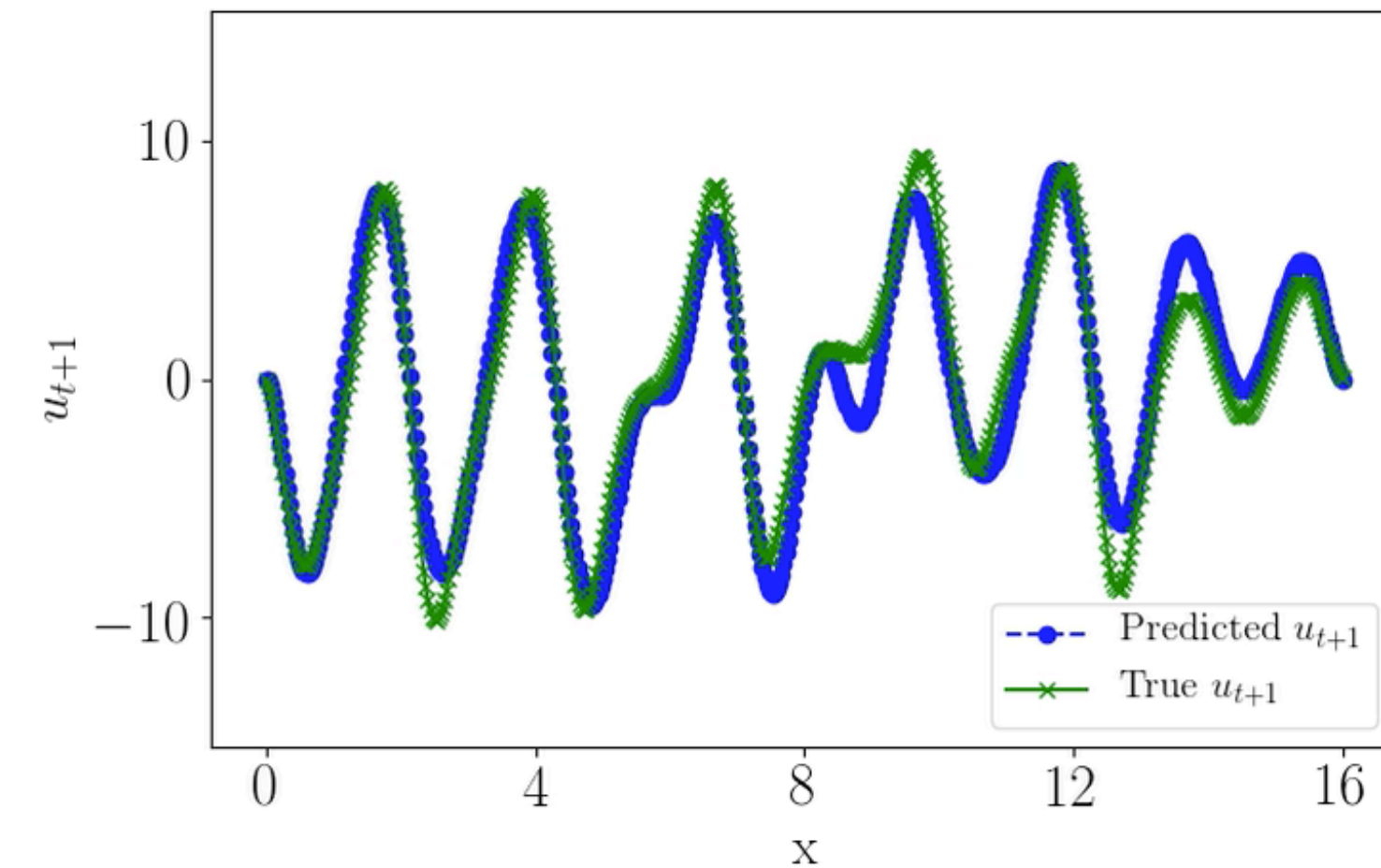
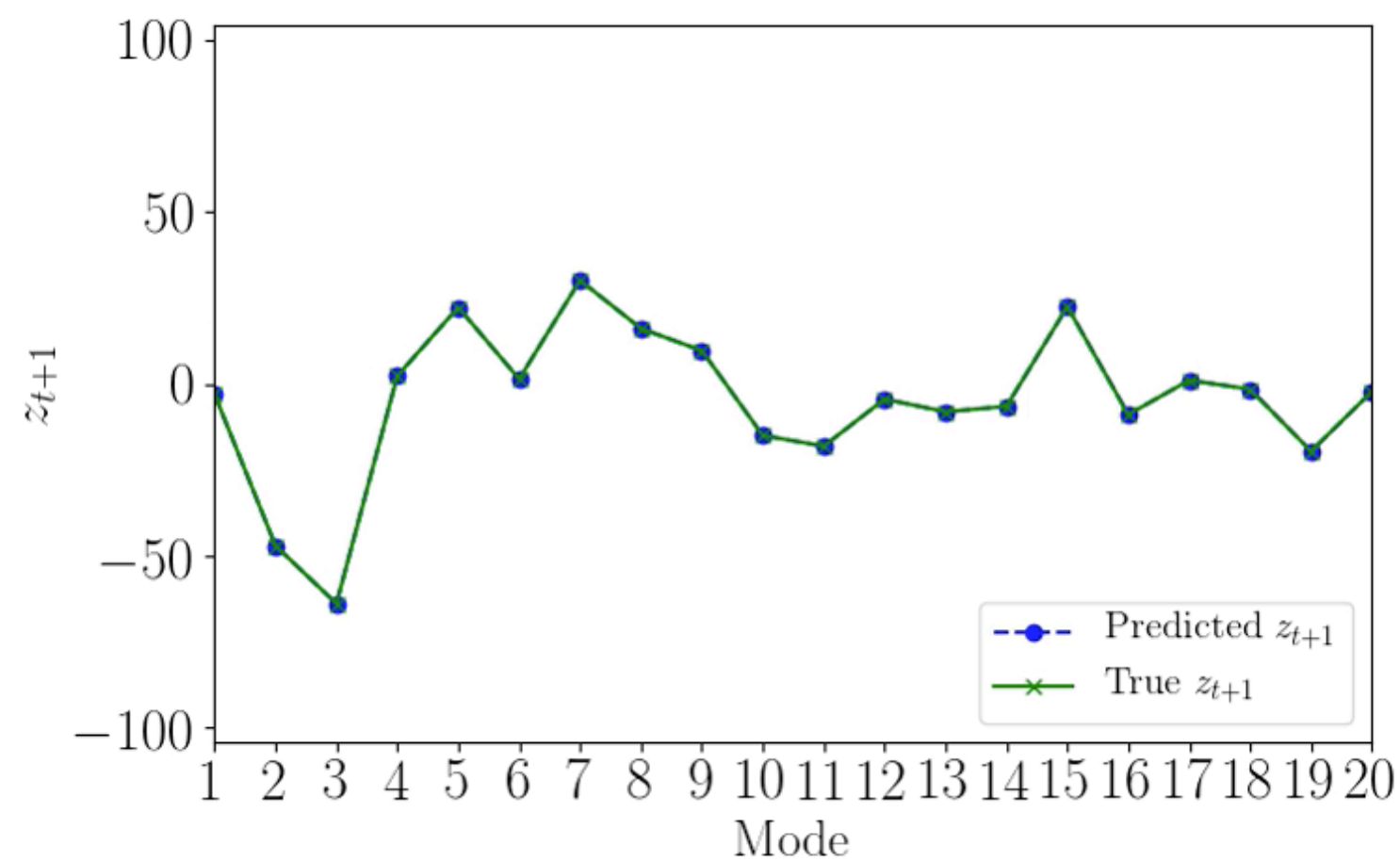
prediction in **reduced** space

expanded in **high-dimensional** space

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



$$\tilde{L} \approx 10$$





# Challenges

---



# Challenges

---

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



# Challenges

---

- 1 Iterative prediction error **accumulates** leading to unphysical predictions  
- *divergence from attractor*
  - Dynamics underrepresented in training data



# Challenges

---

- 1 Iterative prediction error **accumulates** leading to unphysical predictions  
- *divergence from attractor*
  - Dynamics underrepresented in training data
  - Scarce data in attractor boundaries



# Challenges

---

1

Iterative prediction error **accumulates** leading to unphysical predictions

- *divergence from attractor*

- Dynamics underrepresented in training data
- Under-resolved high dimensional dynamics
- Scarce data in attractor boundaries



# Challenges

---

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

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



# Challenges

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

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



# Capturing Long-Term Behavior

---

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



# Capturing Long-Term Behavior

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

**ADD - > MEAN STOCHASTIC MODEL (MSM)**

**Mean Stochastic Model**



# Capturing Long-Term Behavior

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

## ADD - > MEAN STOCHASTIC MODEL (MSM)

- Ornstein-Uhlenbeck process - computationally cheap

### Mean Stochastic Model

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



# Capturing Long-Term Behavior

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

## ADD - > MEAN STOCHASTIC MODEL (MSM)

- Ornstein-Uhlenbeck process - computationally cheap

### Mean Stochastic Model

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

parameters  
estimated from **data**

wiener  
process



# Capturing Long-Term Behavior

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

## ADD - > MEAN STOCHASTIC MODEL (MSM)

- Ornstein-Uhlenbeck process - computationally cheap

### Mean Stochastic Model

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

parameters  
estimated from **data**

wiener  
process

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

decorrelation  
time



# Capturing Long-Term Behavior

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

## ADD - > MEAN STOCHASTIC MODEL (MSM)

- Ornstein-Uhlenbeck process - computationally cheap

### Mean Stochastic Model

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

parameters  
estimated from **data**

wiener  
process

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

**data standard  
deviation**

**decorrelation  
time**

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



# Capturing Long-Term Behavior

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

## ADD - > MEAN STOCHASTIC MODEL (MSM)

- Ornstein-Uhlenbeck process - computationally cheap
- Relies on **global attractor statistics**

### Mean Stochastic Model

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

parameters  
estimated from **data**

wiener  
process

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

**data standard  
deviation**

**decorrelation  
time**

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



# Capturing Long-Term Behavior

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

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- Ornstein-Uhlenbeck process - computationally cheap
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## Hybrid LSTM - MSM

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

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

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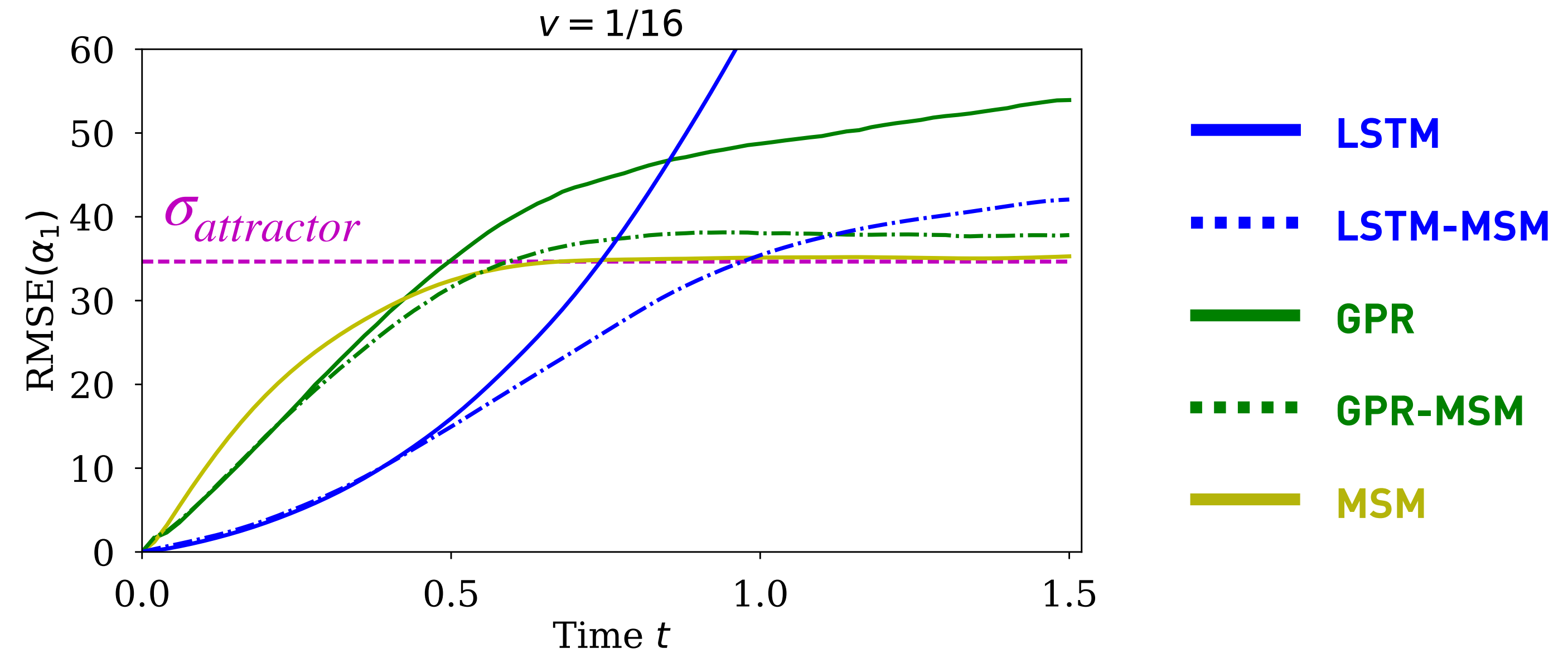


# Results on KS - *Comparison with Gaussian Process Regression (GPR)*

$V$	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:

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





# Challenges

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

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

Mitigation? **Hybrid LSTM - MSM approach**



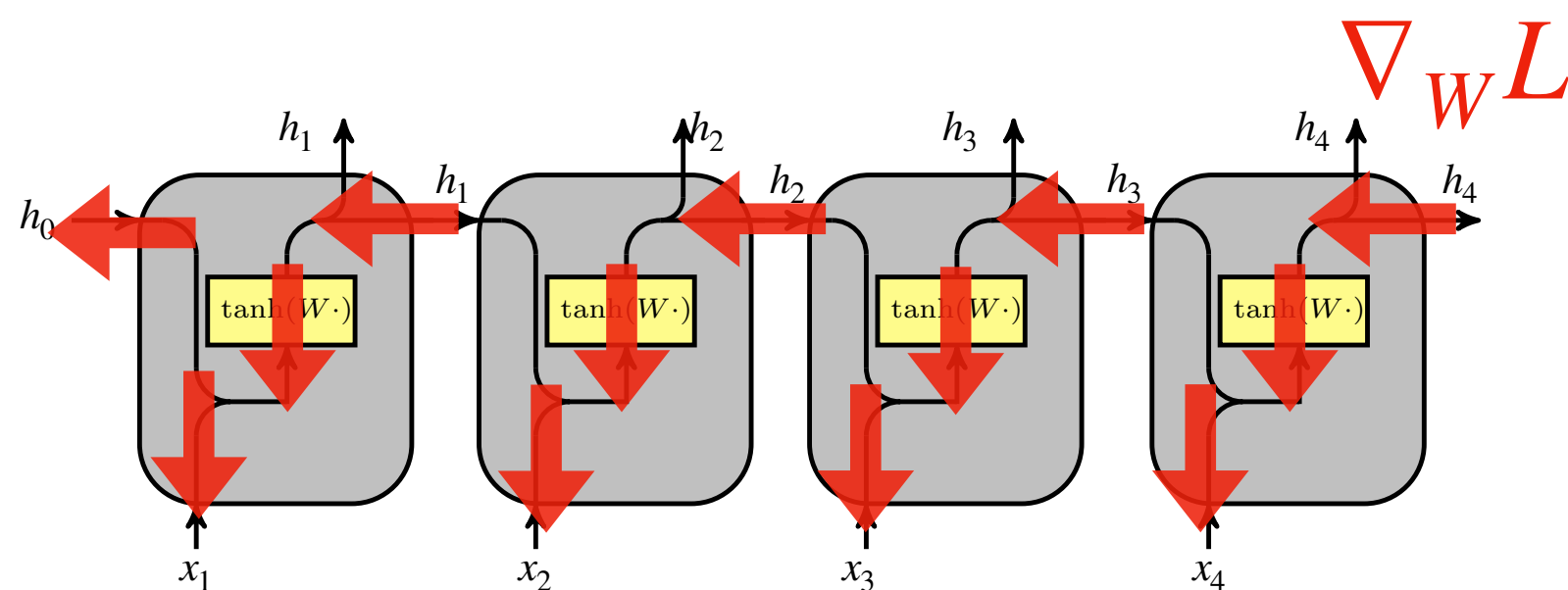
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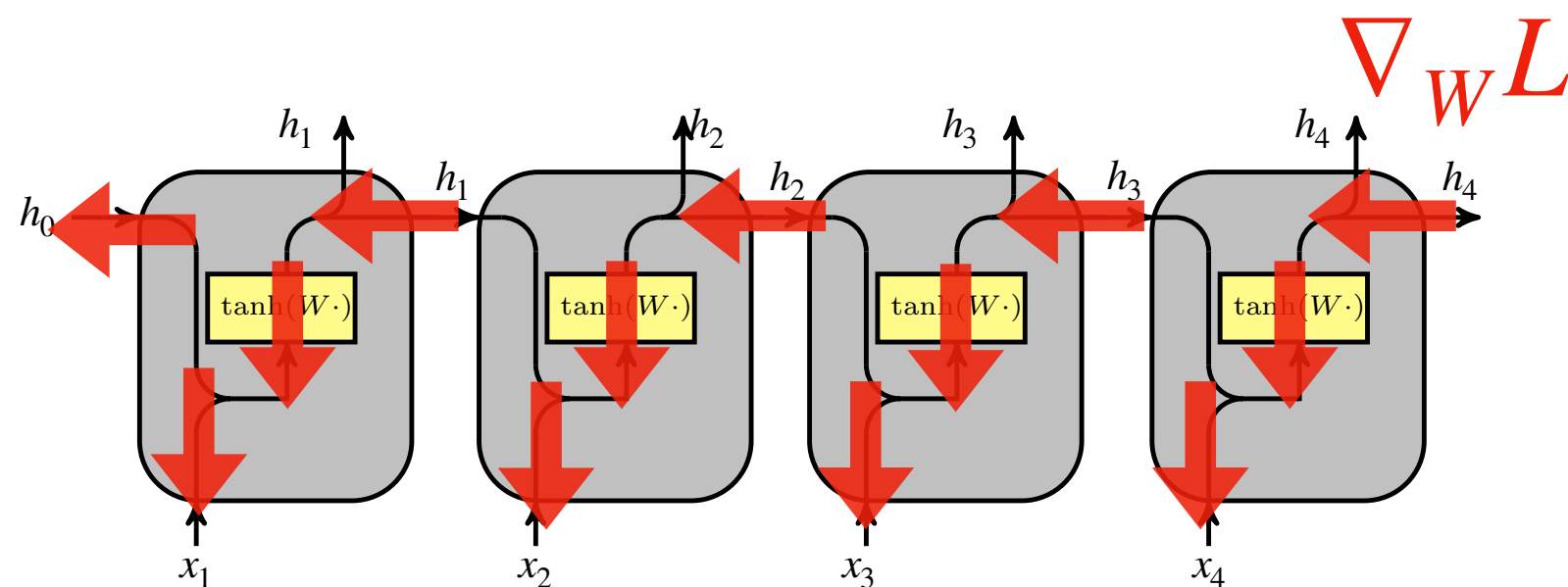
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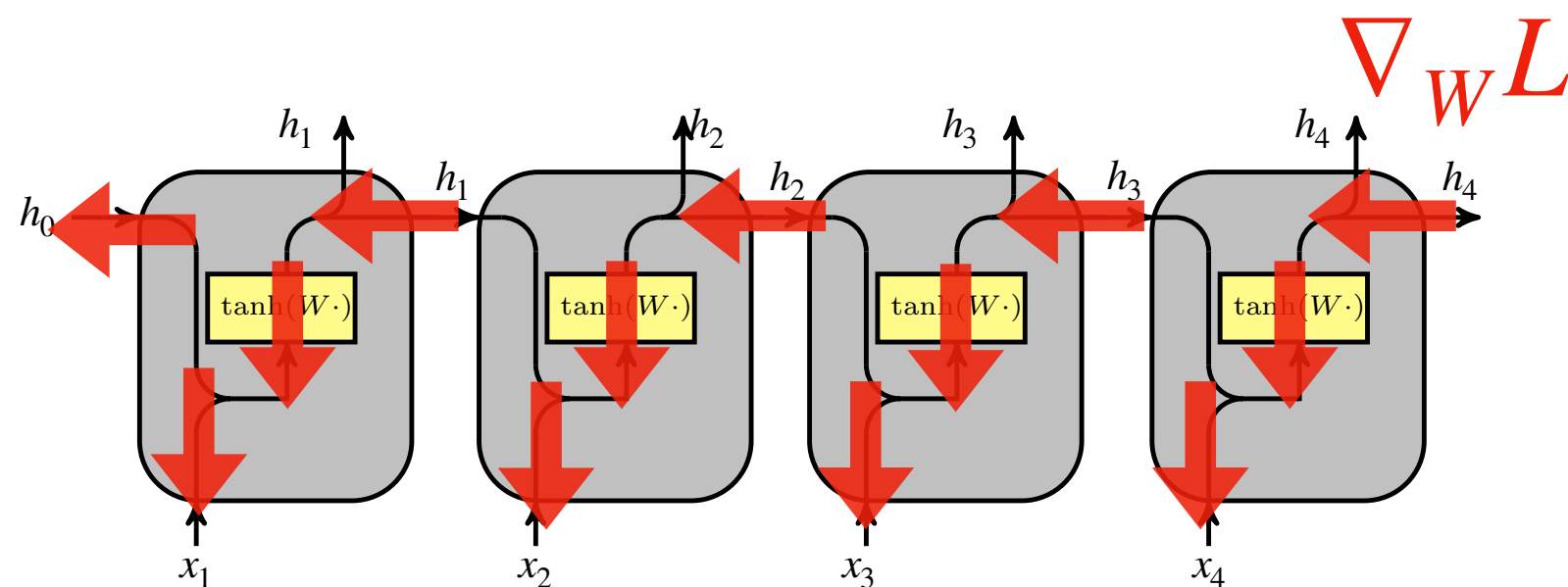
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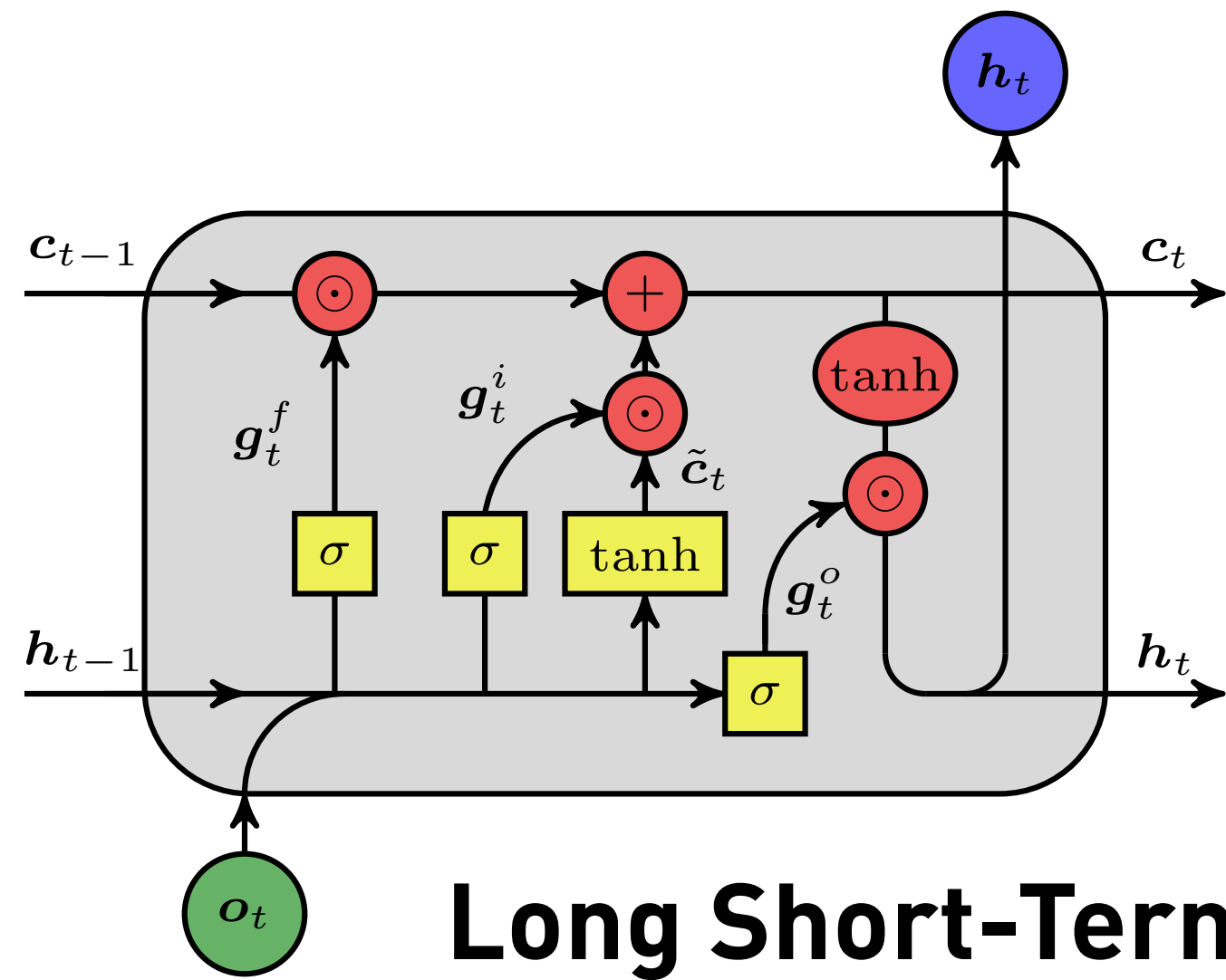
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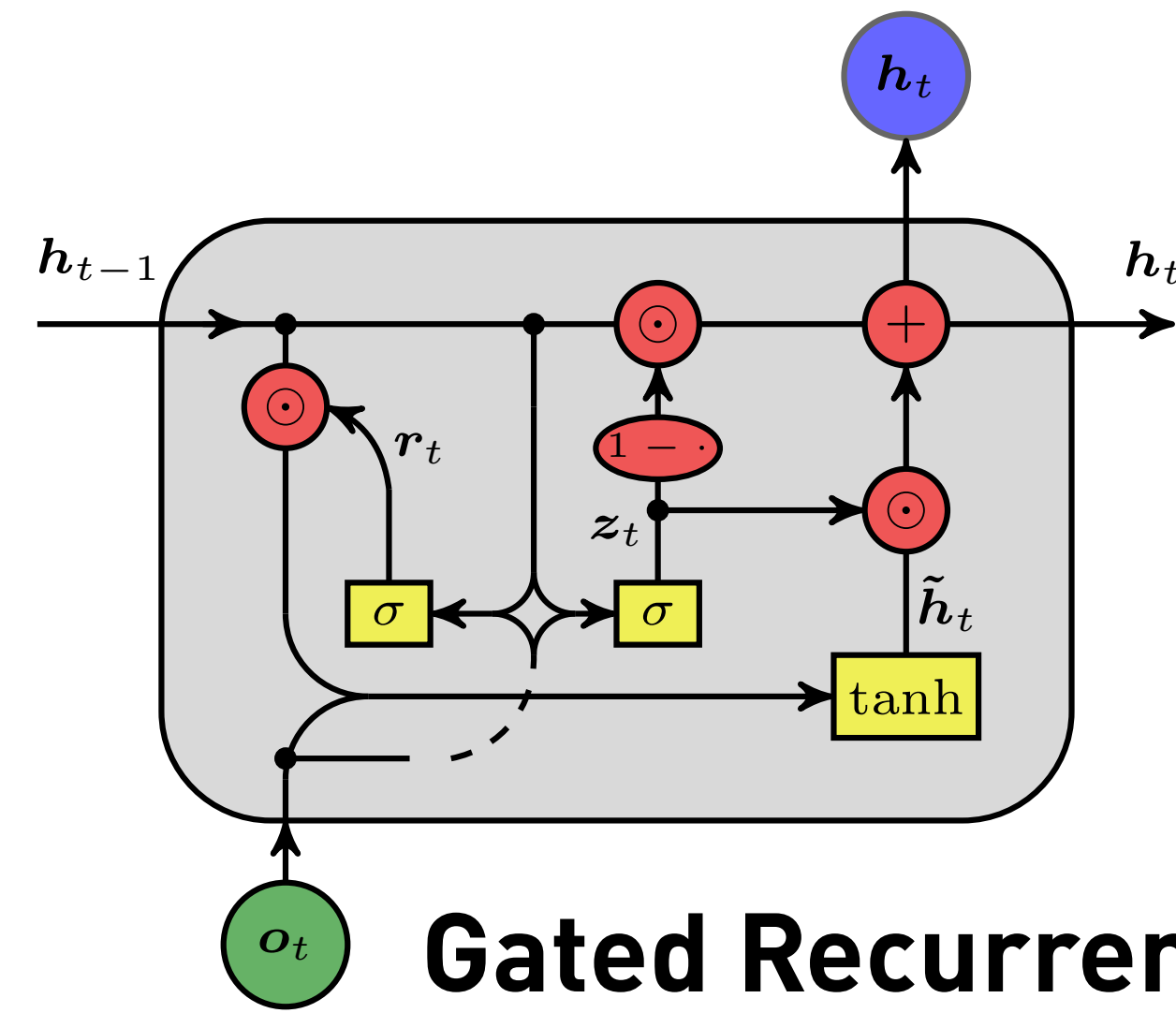
Mitigation? **Sophisticated architectures**





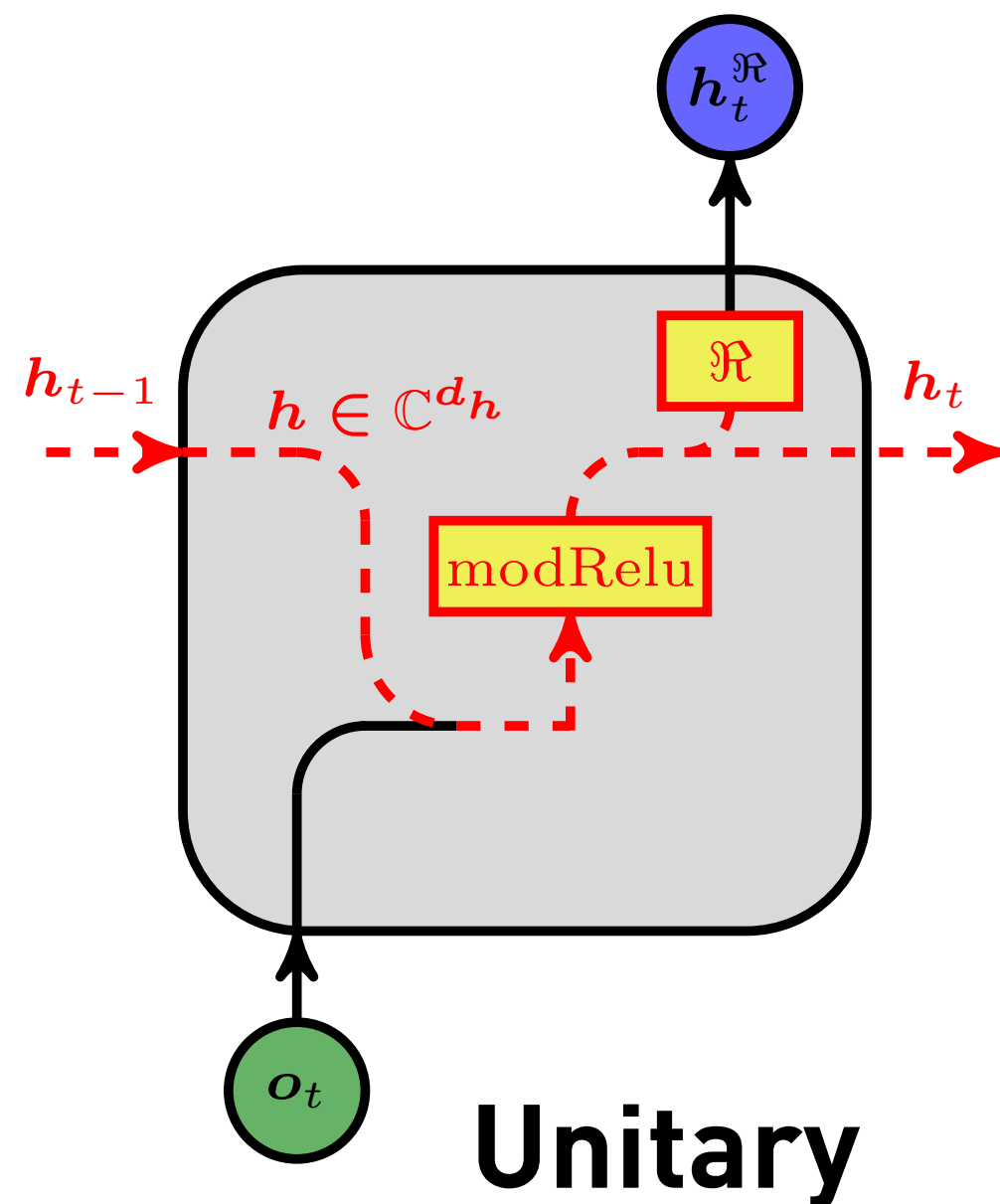
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- Gating mechanisms
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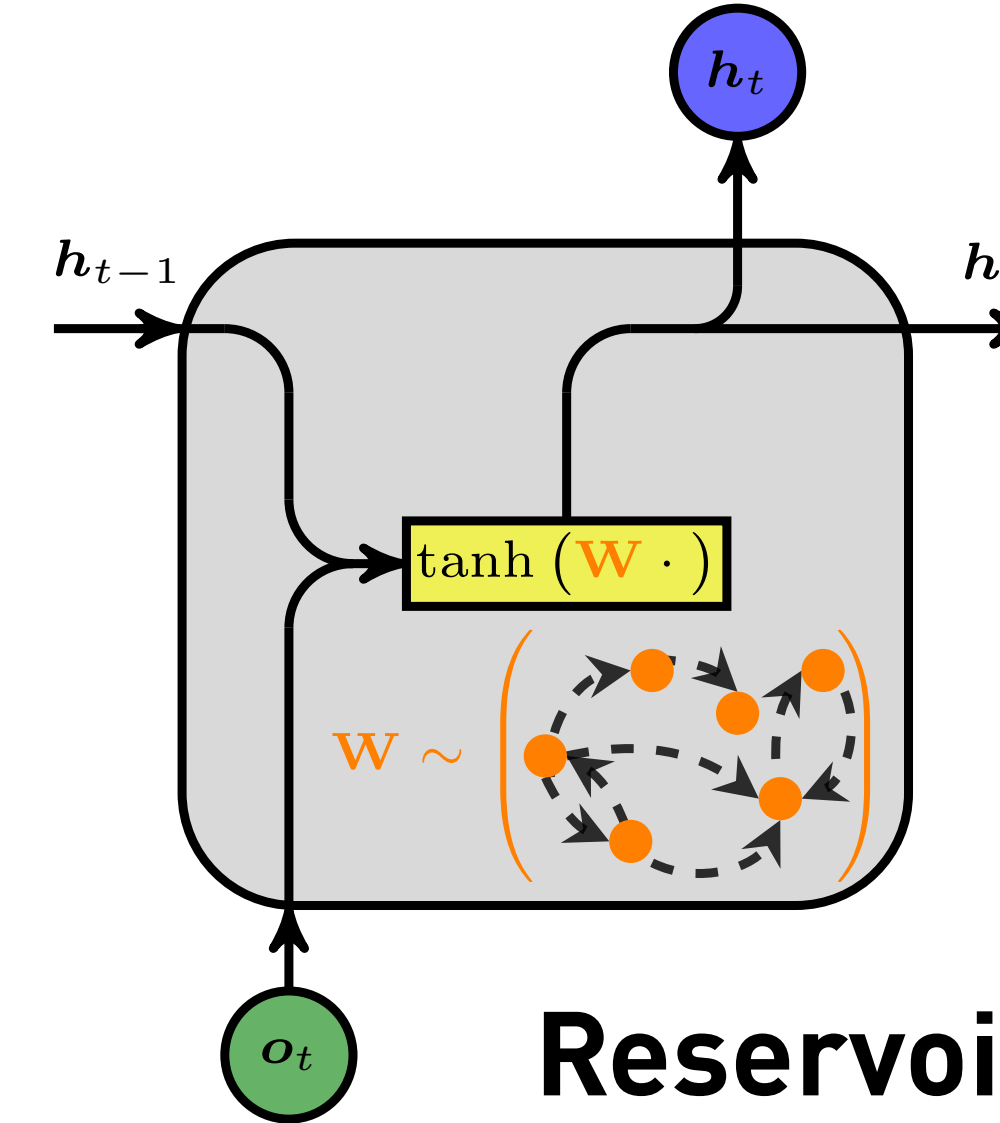
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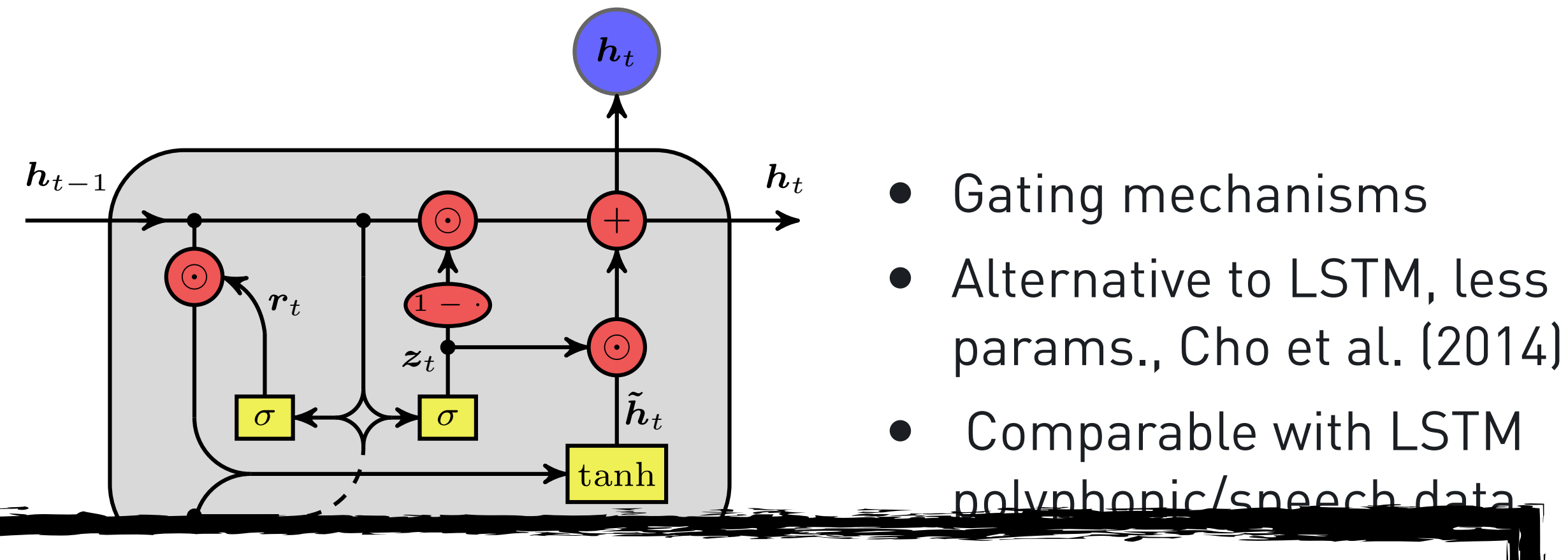
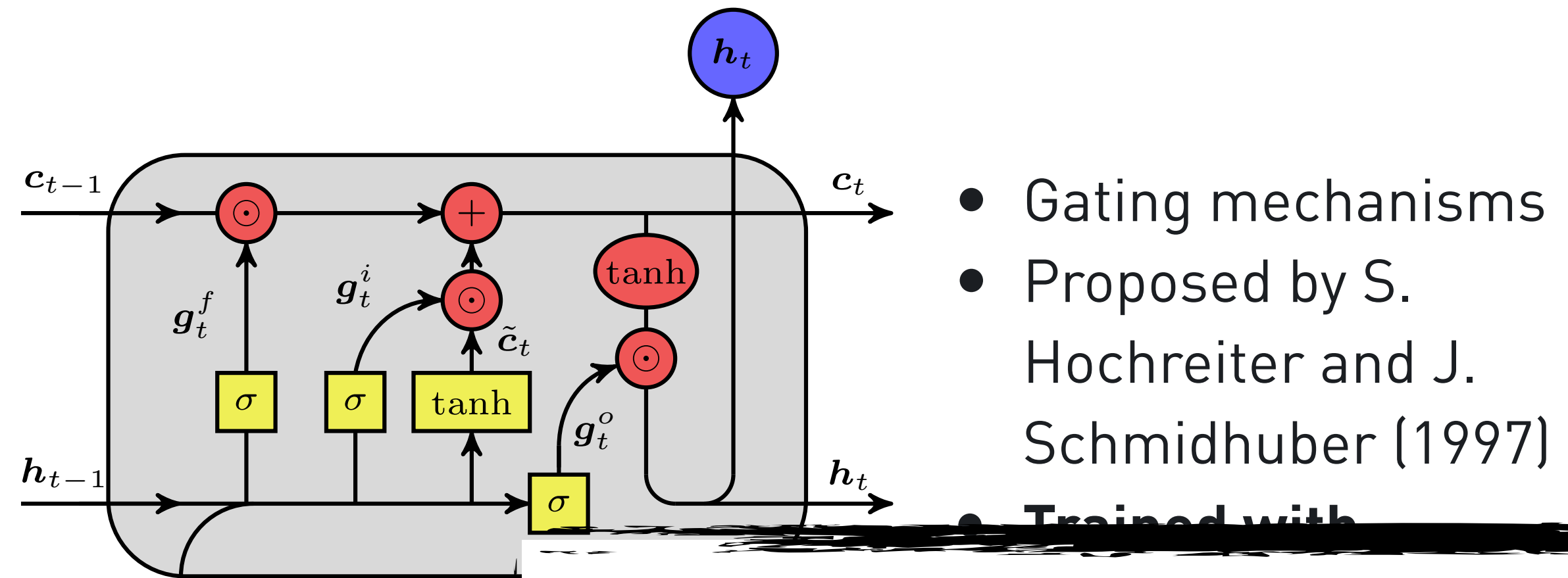
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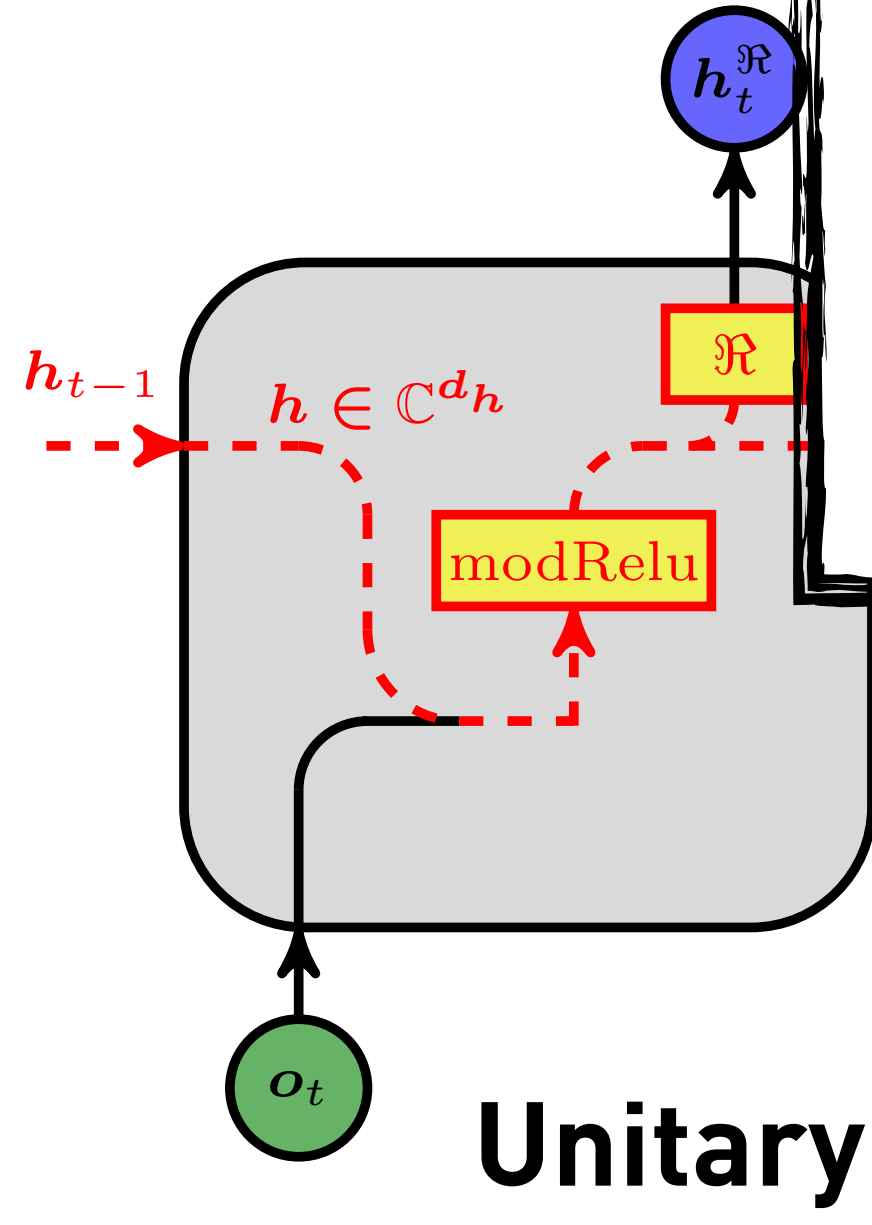
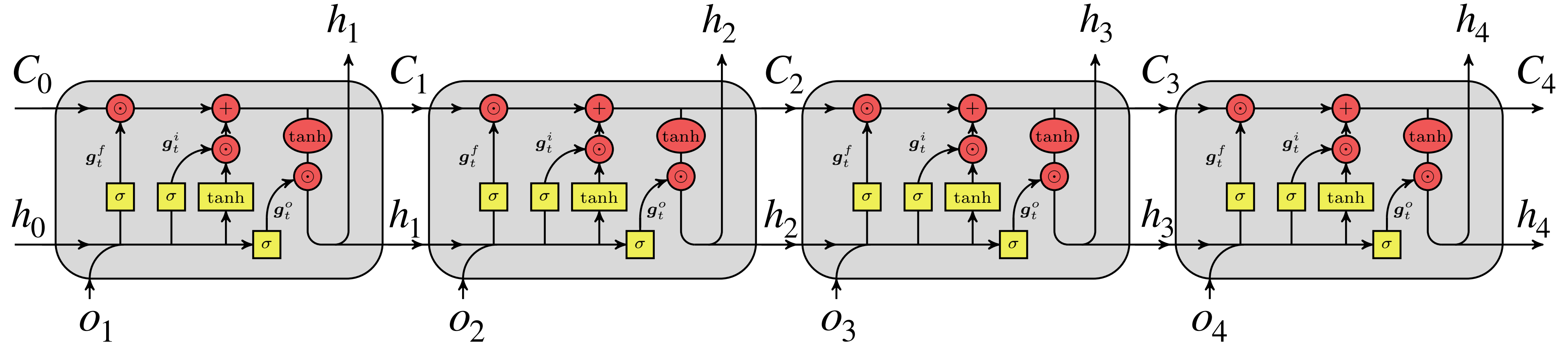
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- Pathak, Ott, et. al. (2017, 2018)
- Echo state networks, Liquid state machines, Maass et. al. (2002), Jaeger et. al. (2007)
- **Random sparse** recurrent weight matrix with **spectral radius smaller than one**
- **Train linear output layer with regularised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

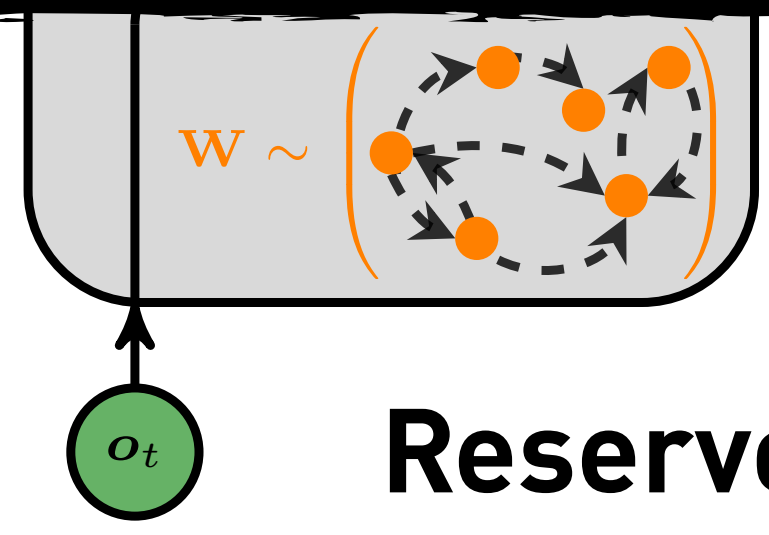




Gating architectures: **Uninterrupted gradient flow !**

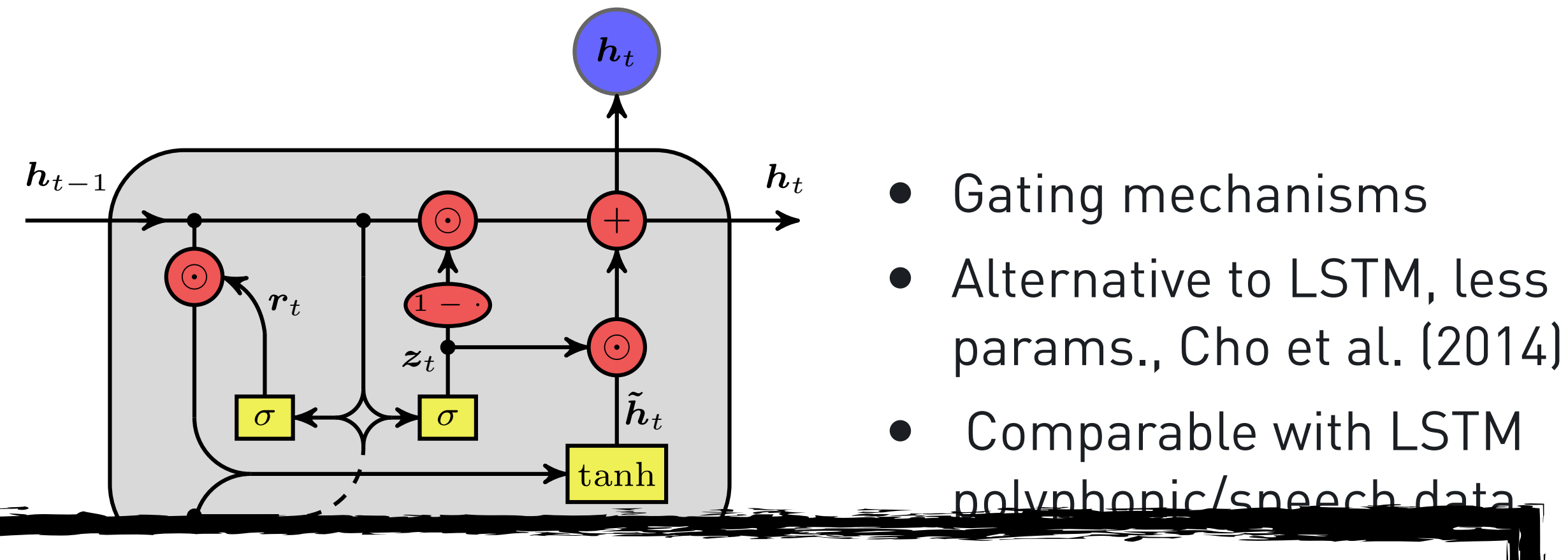
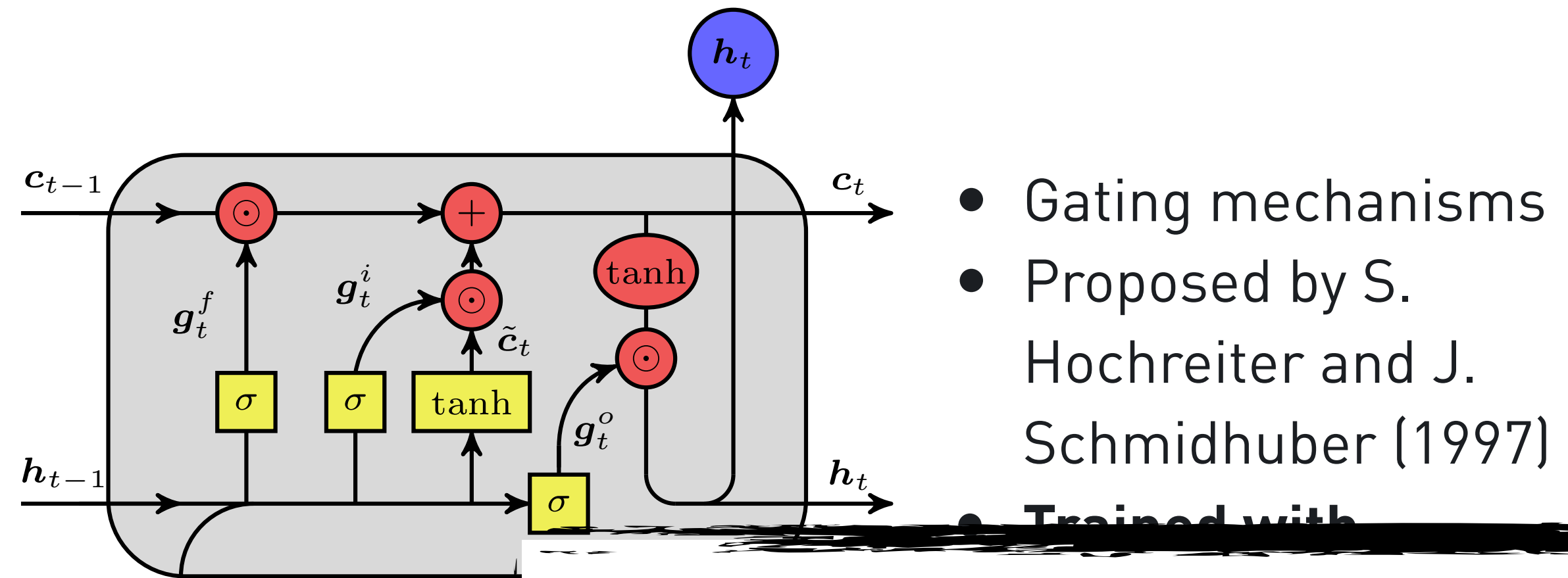


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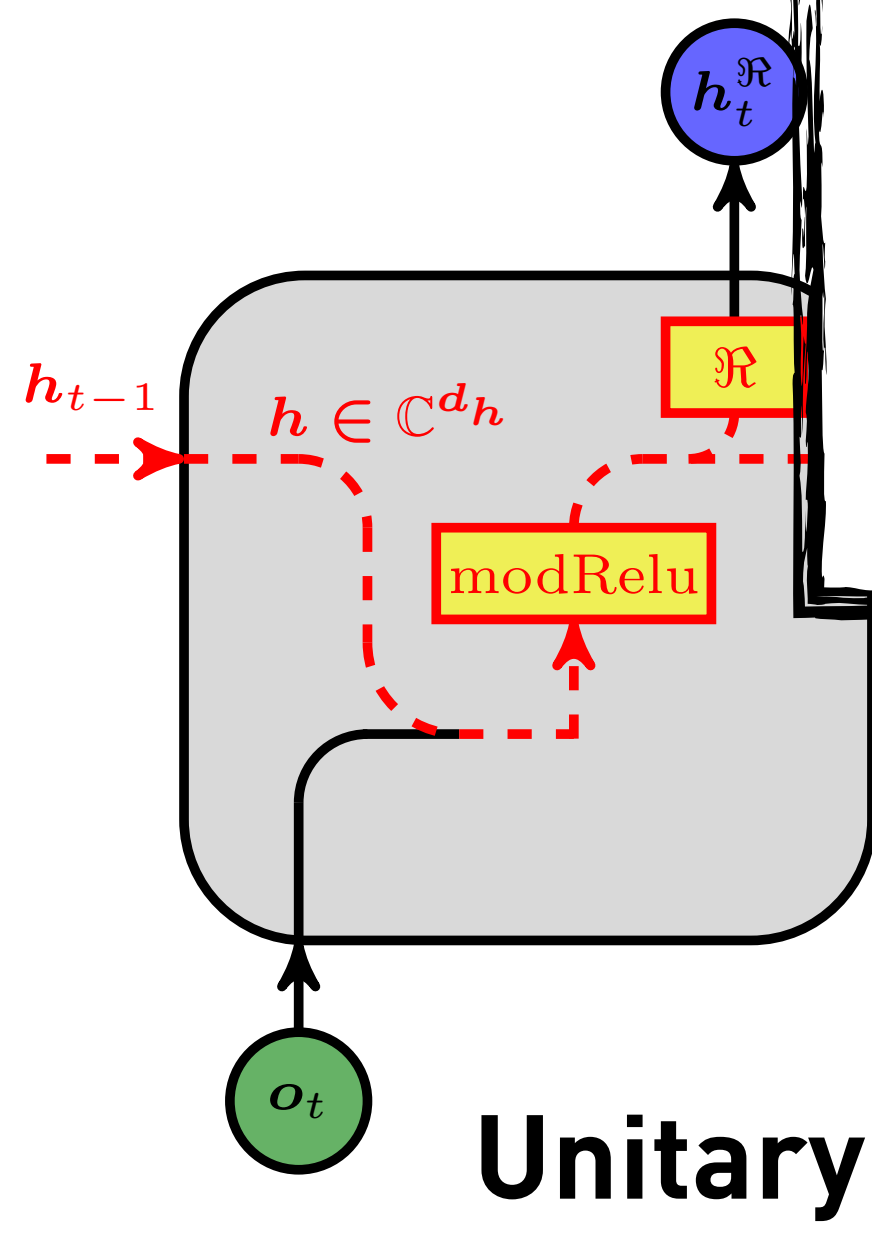
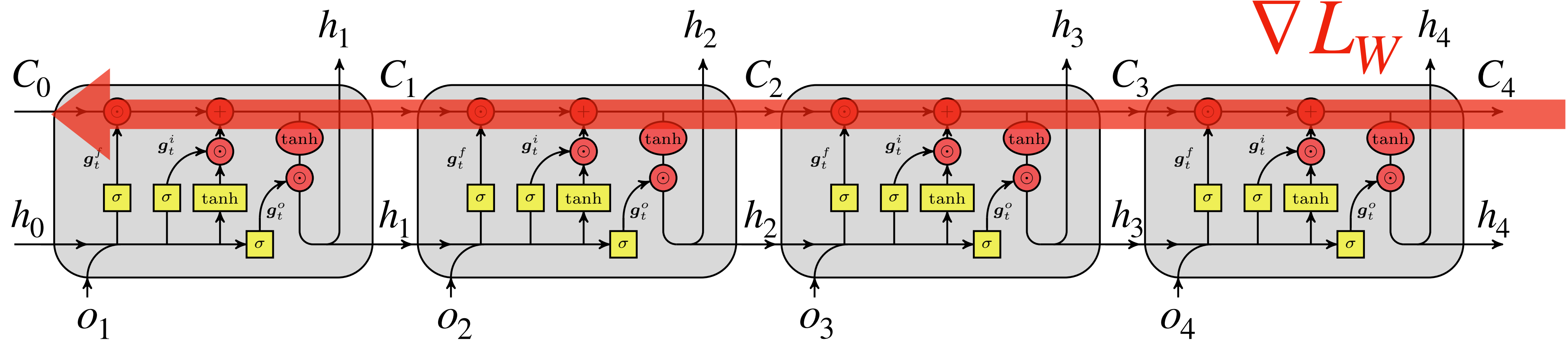


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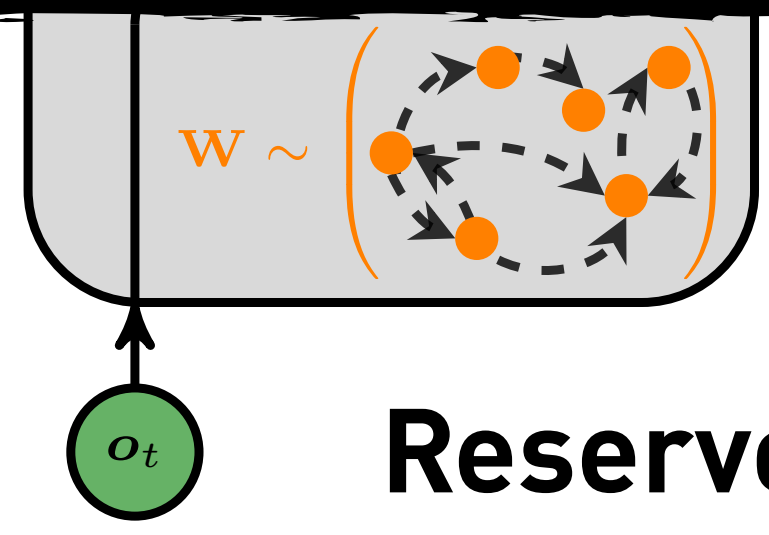




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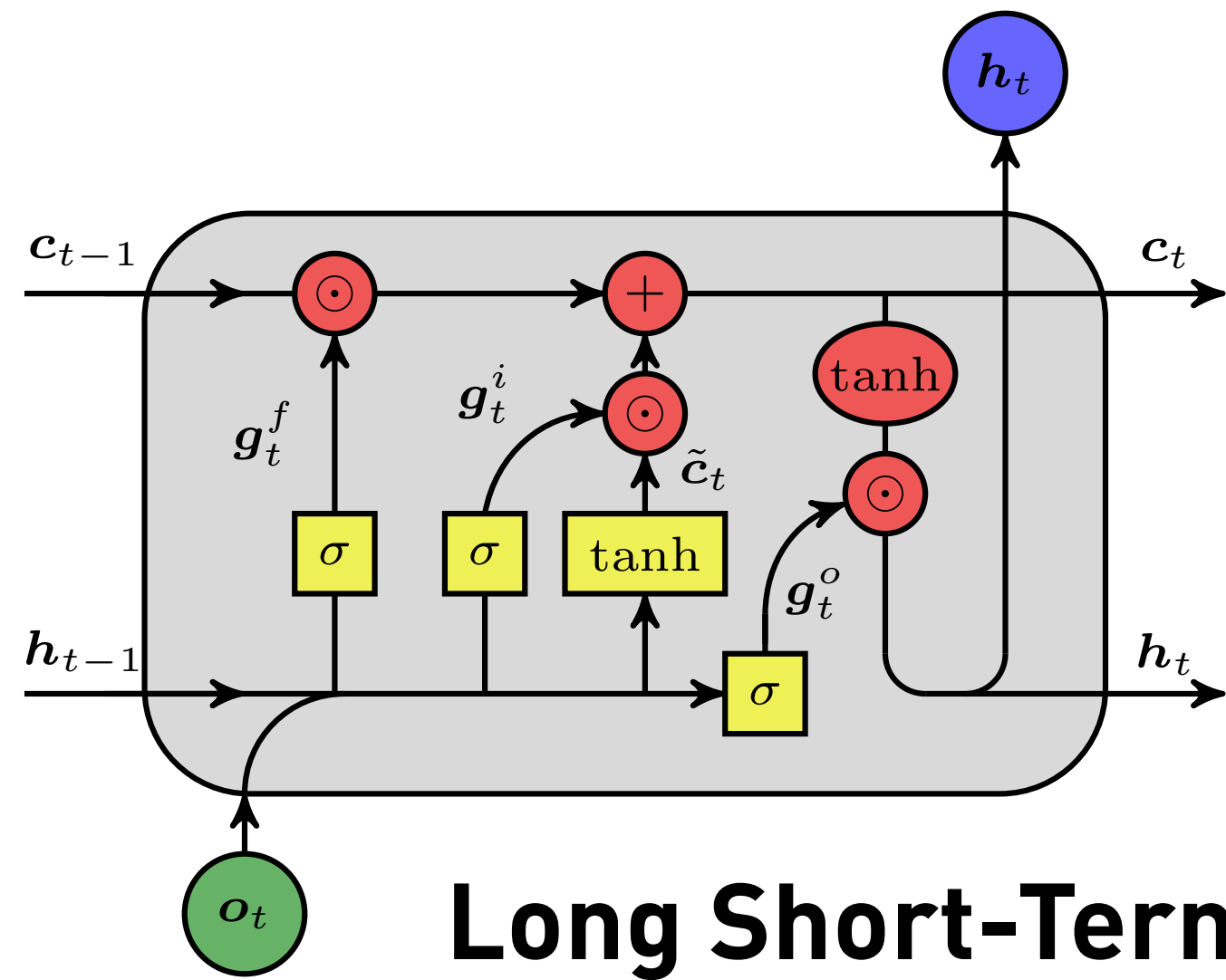


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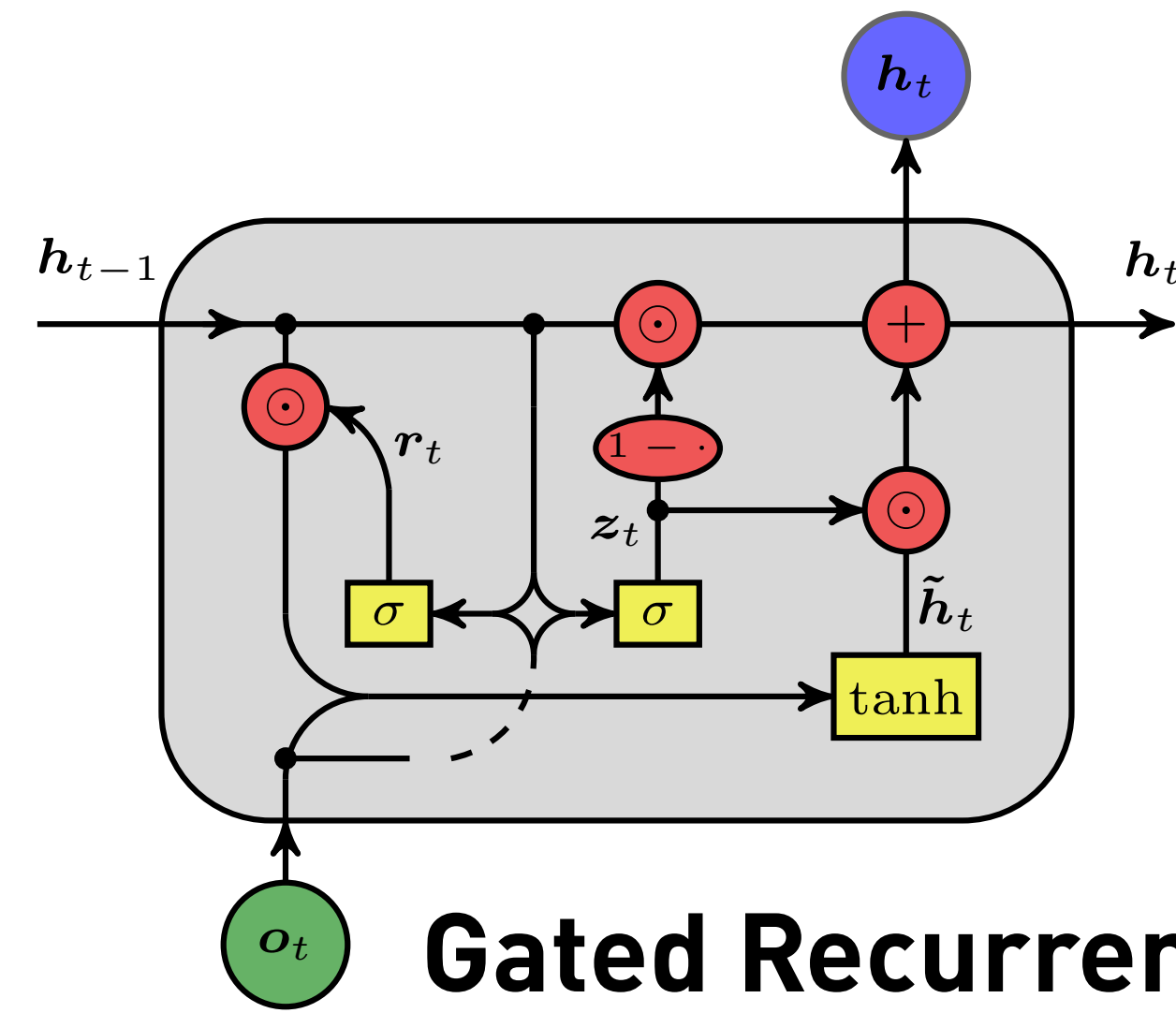
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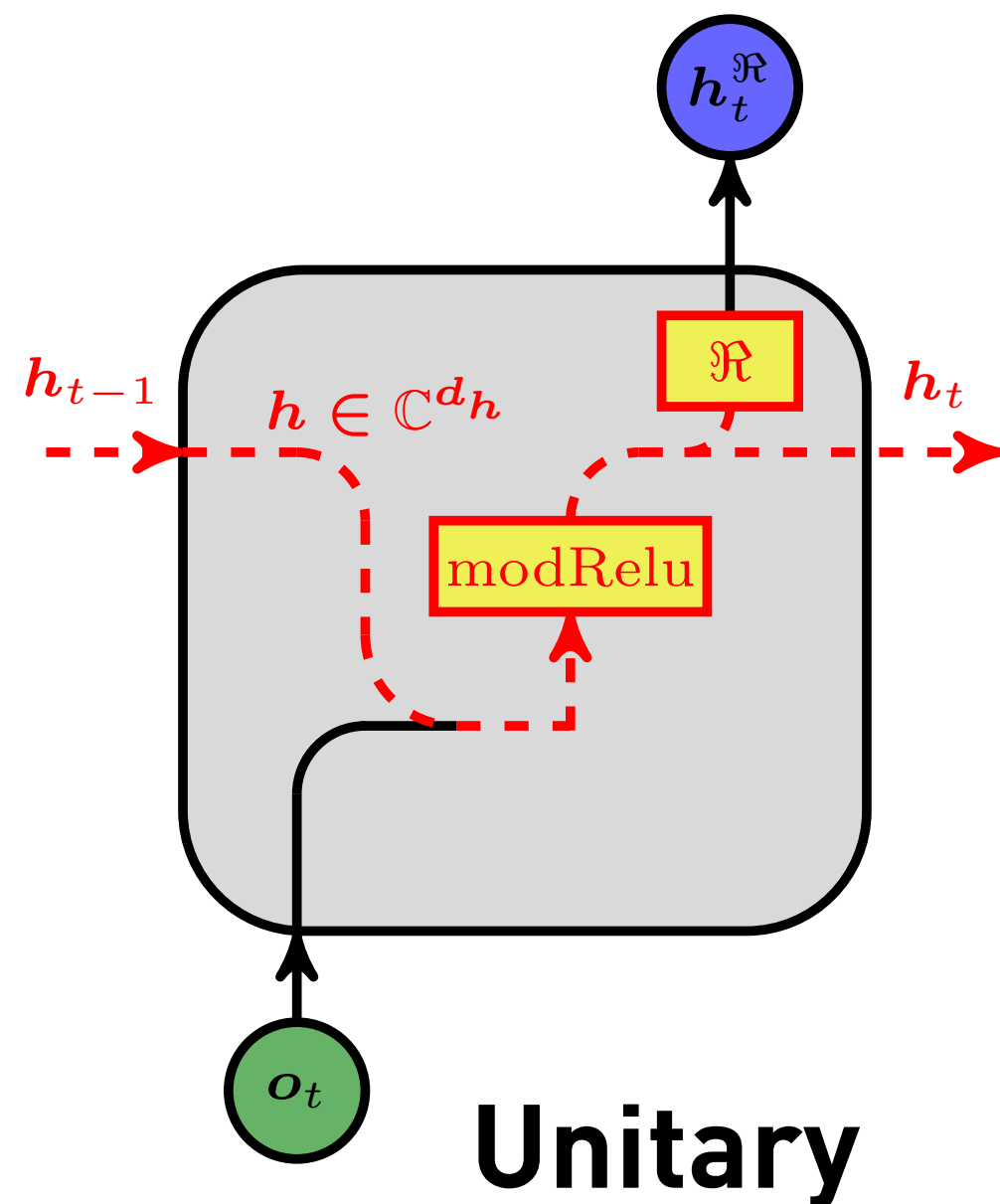
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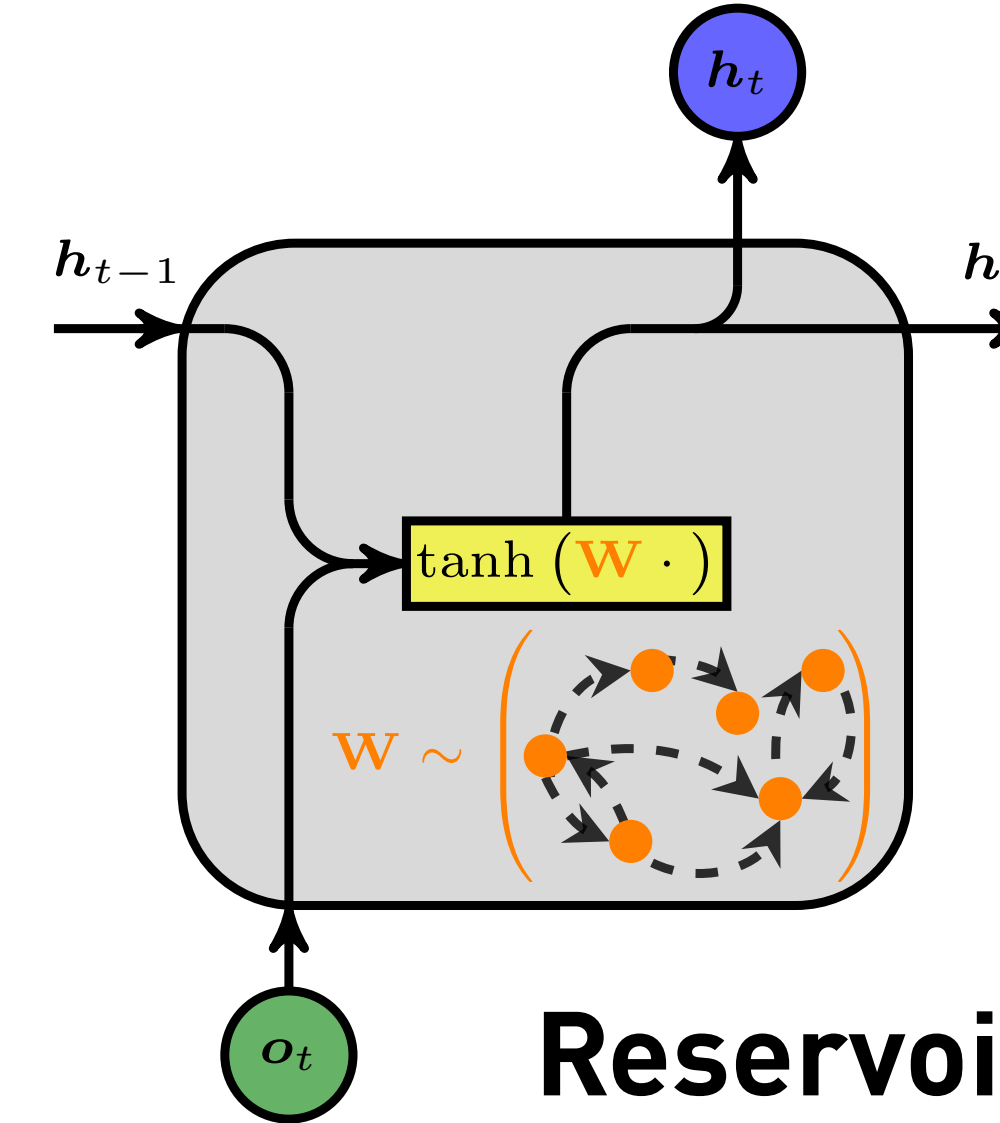
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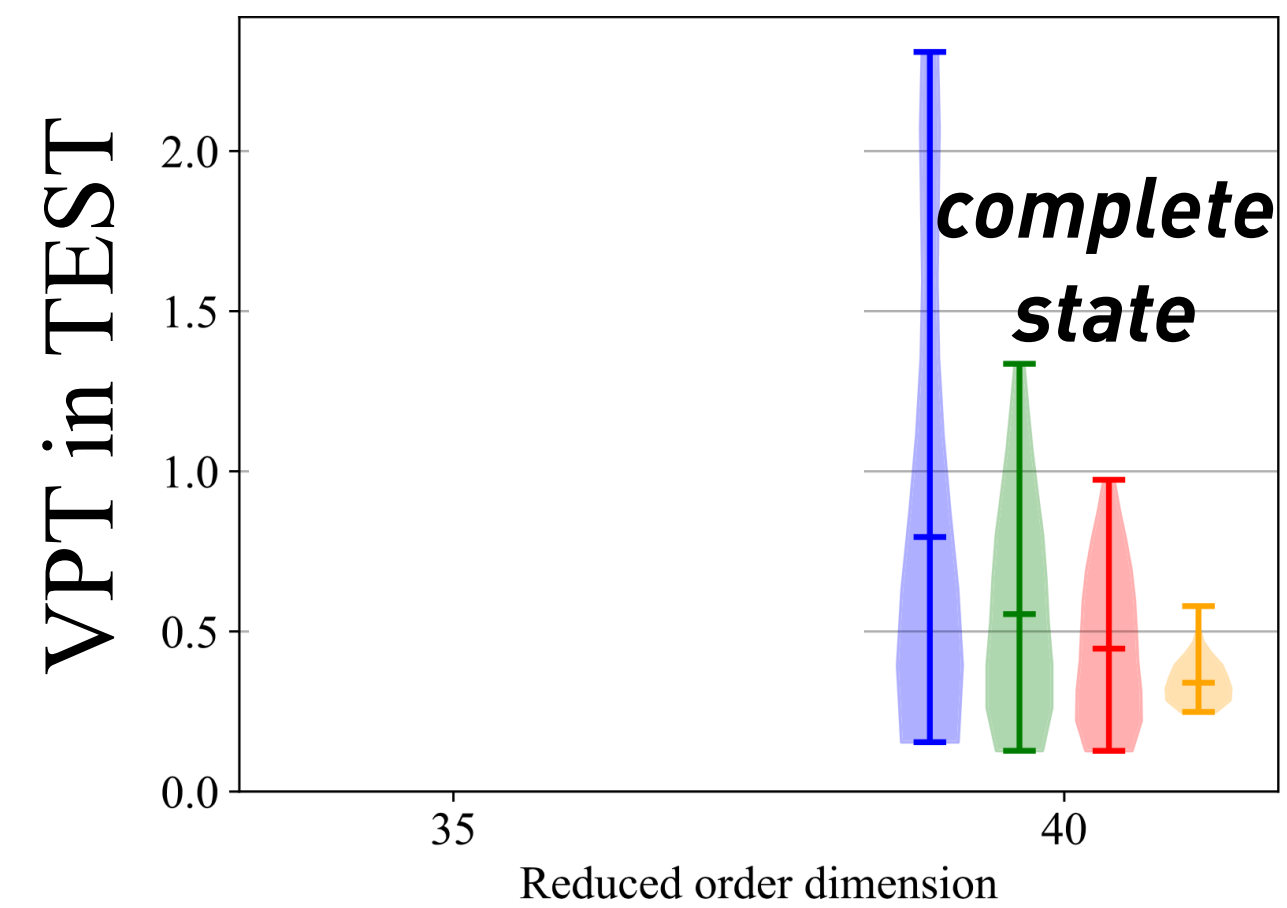
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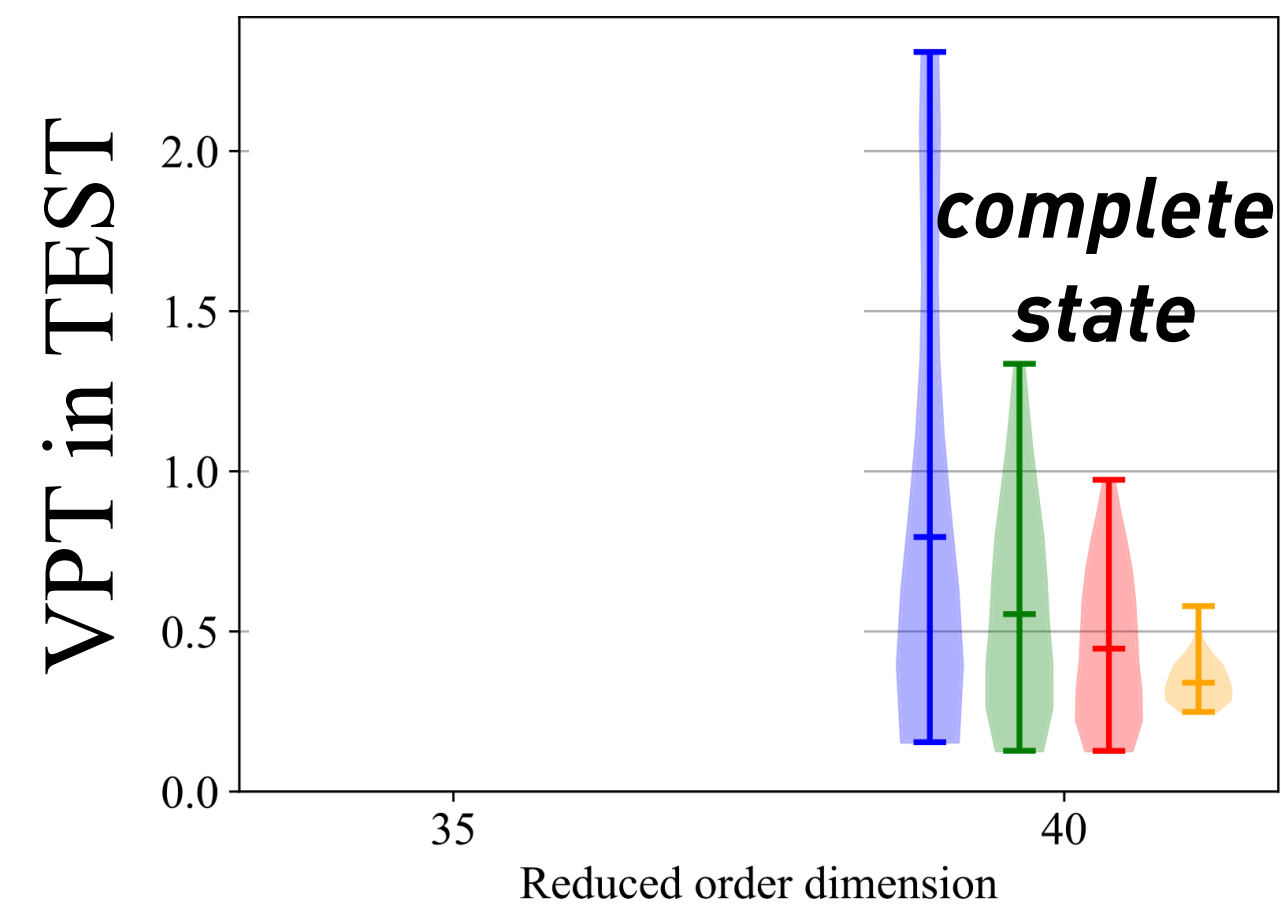
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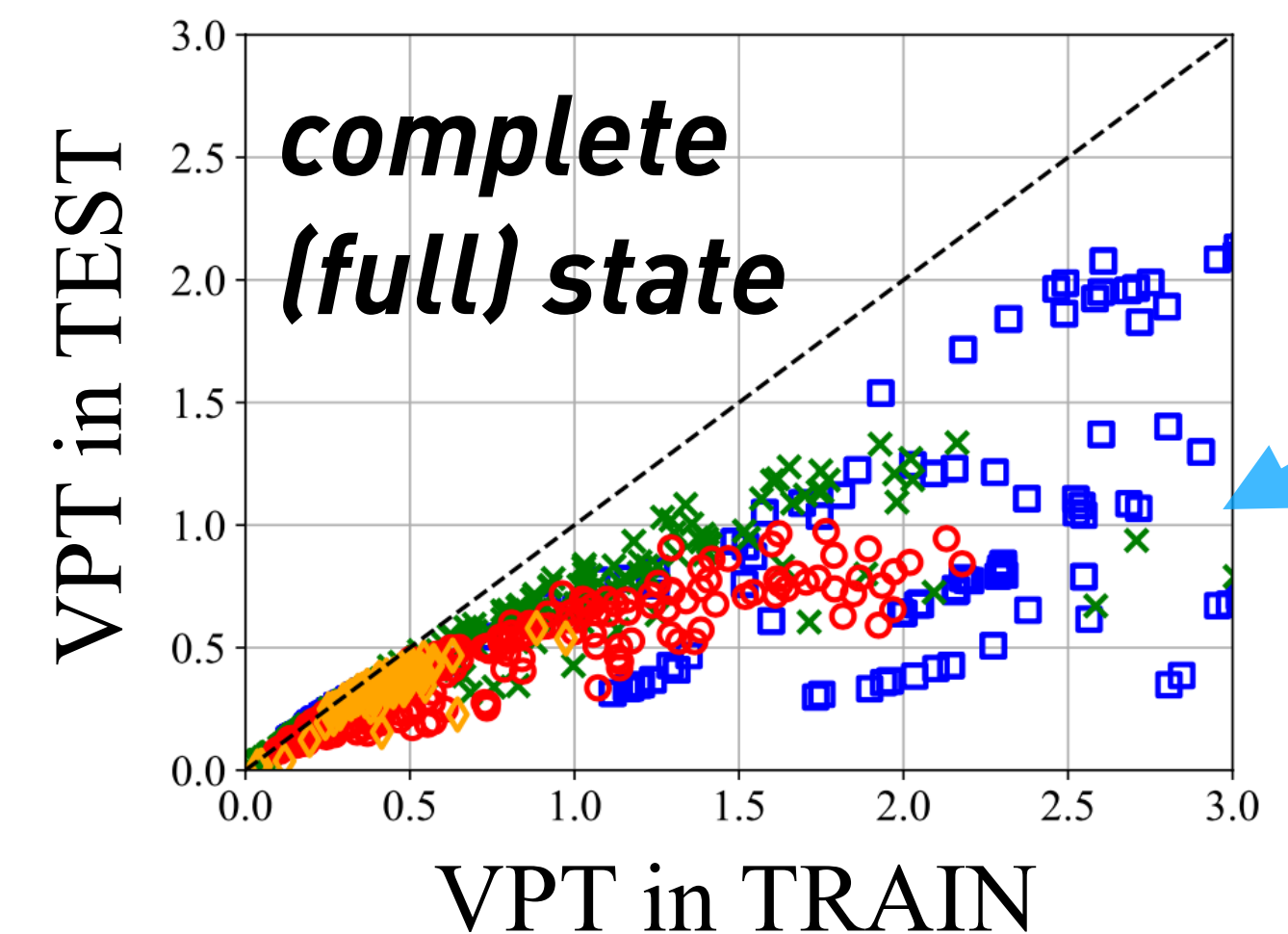
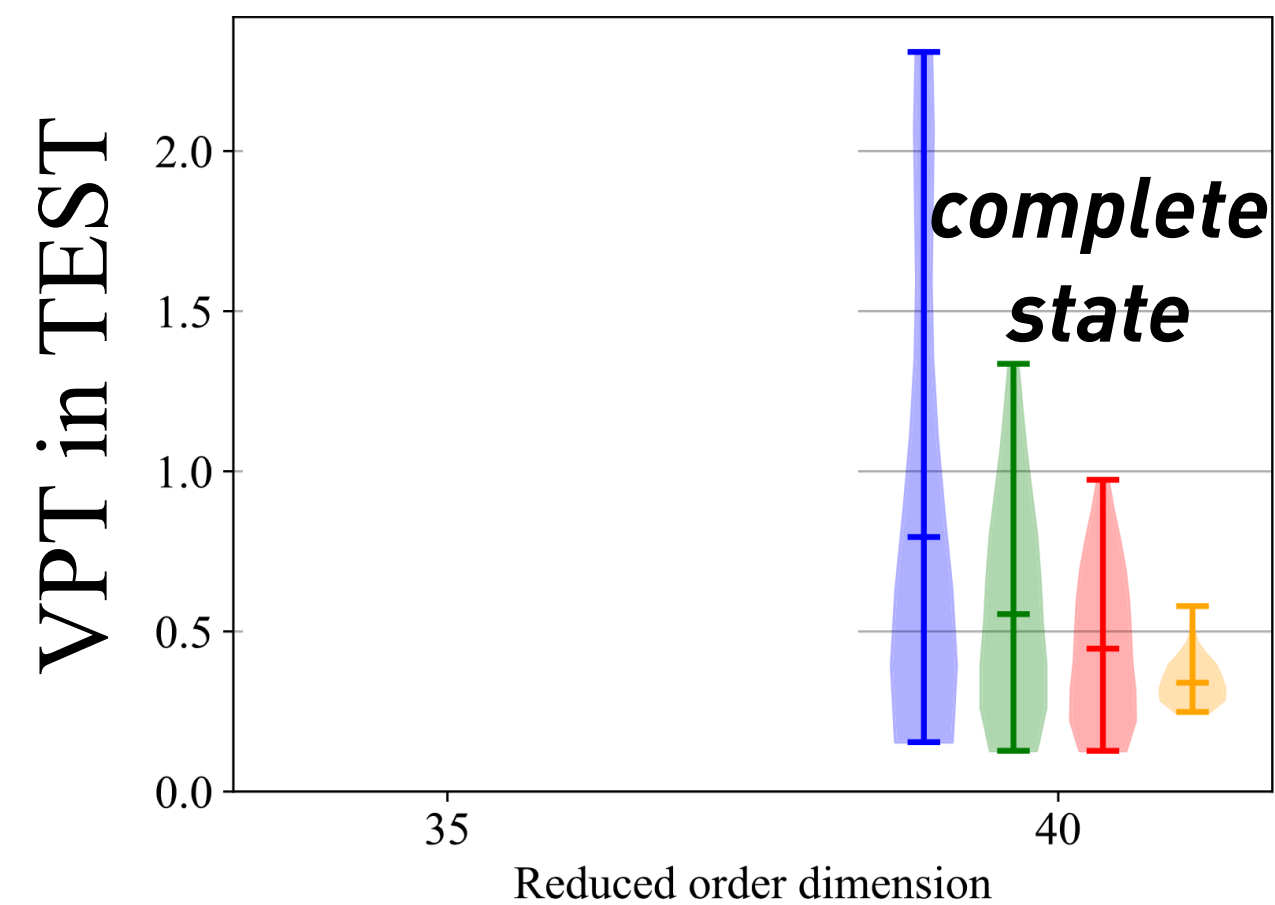
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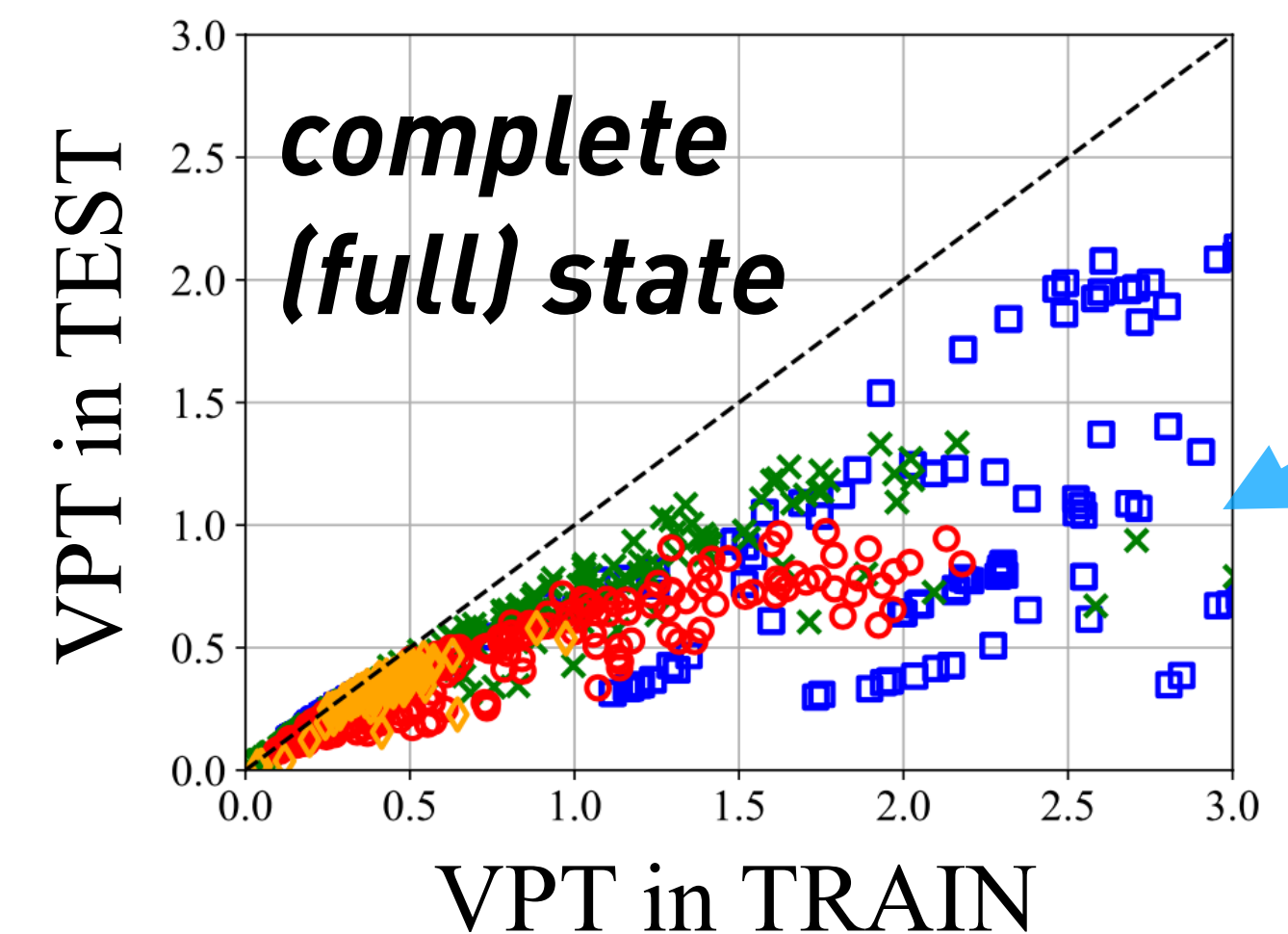
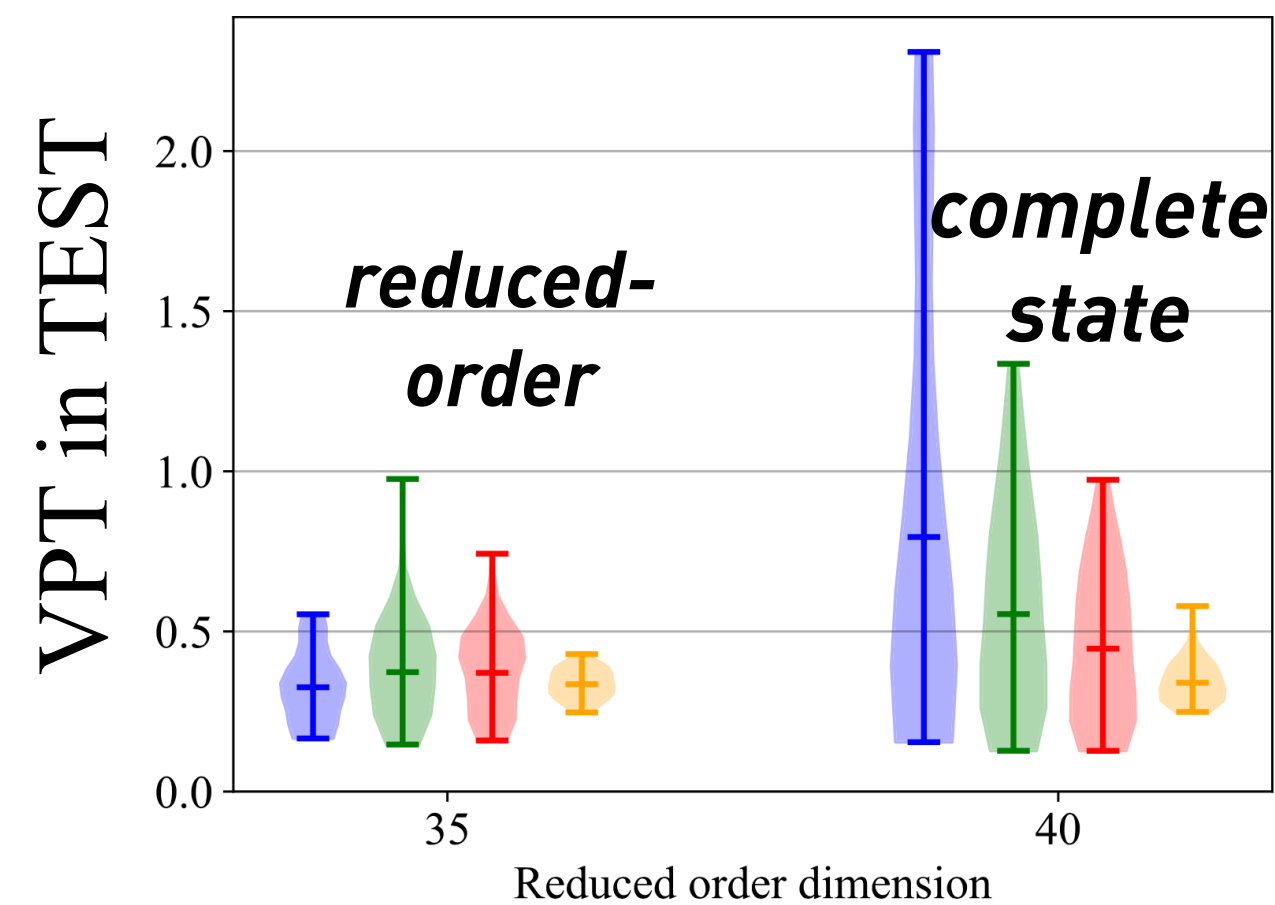
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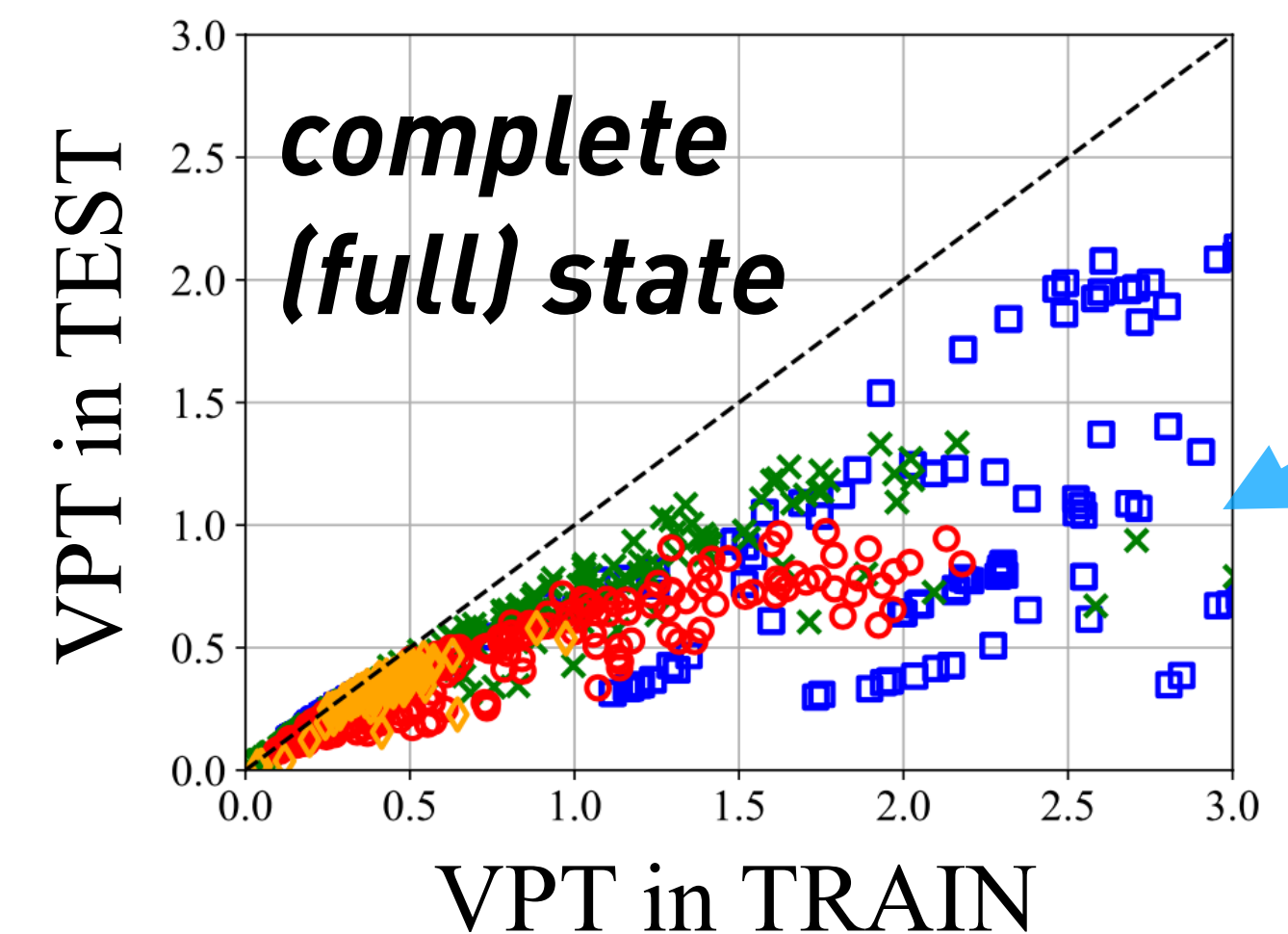
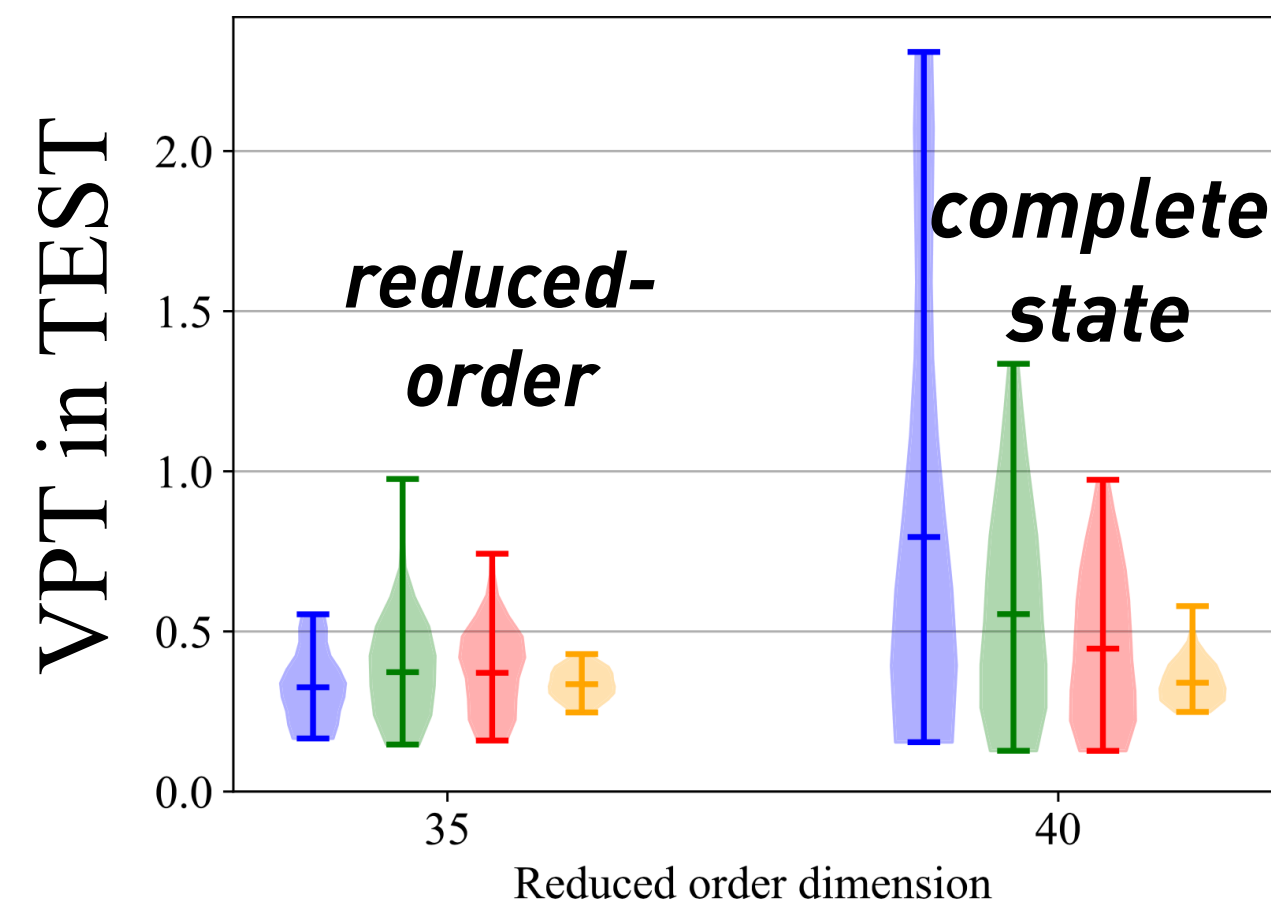
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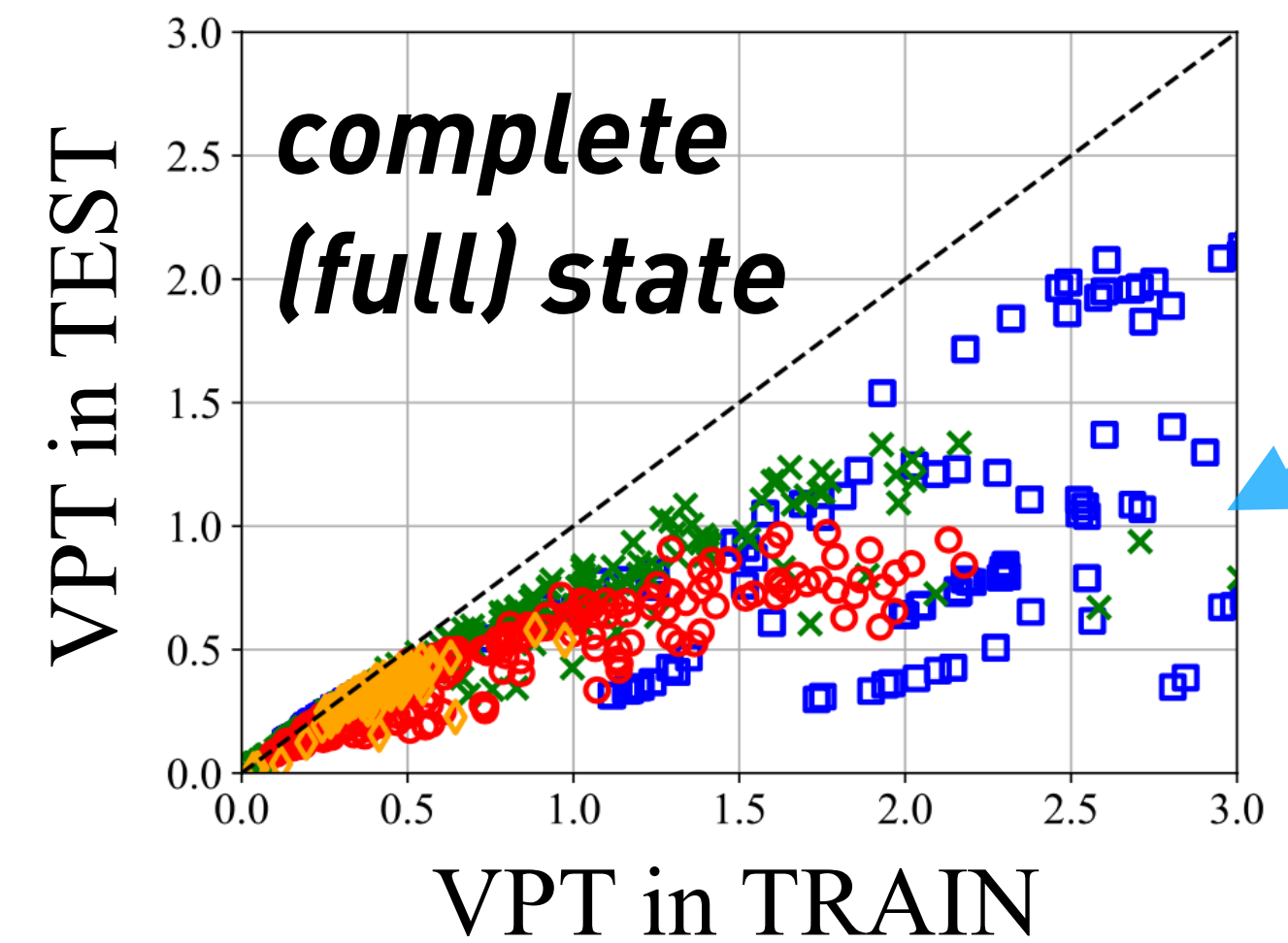
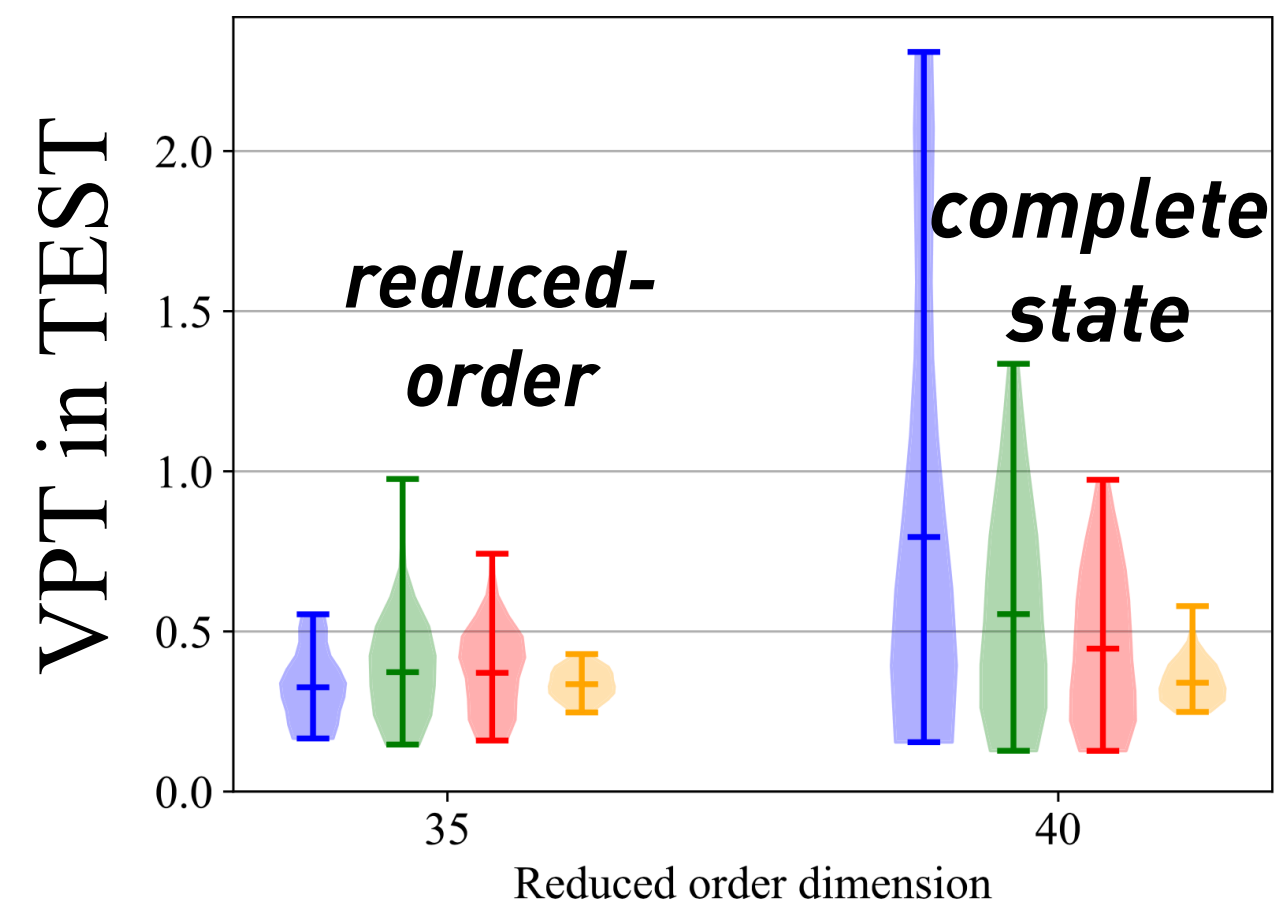
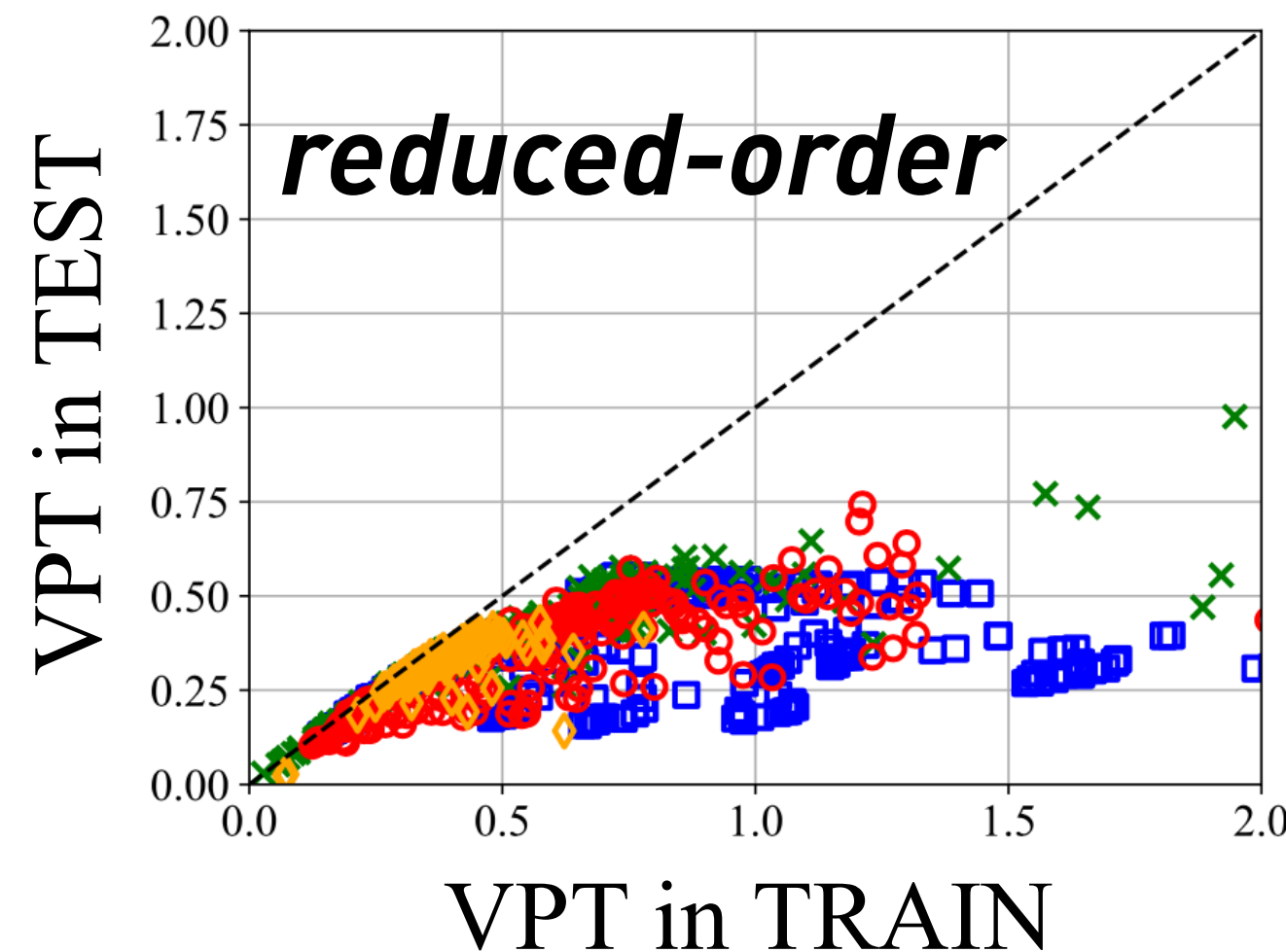
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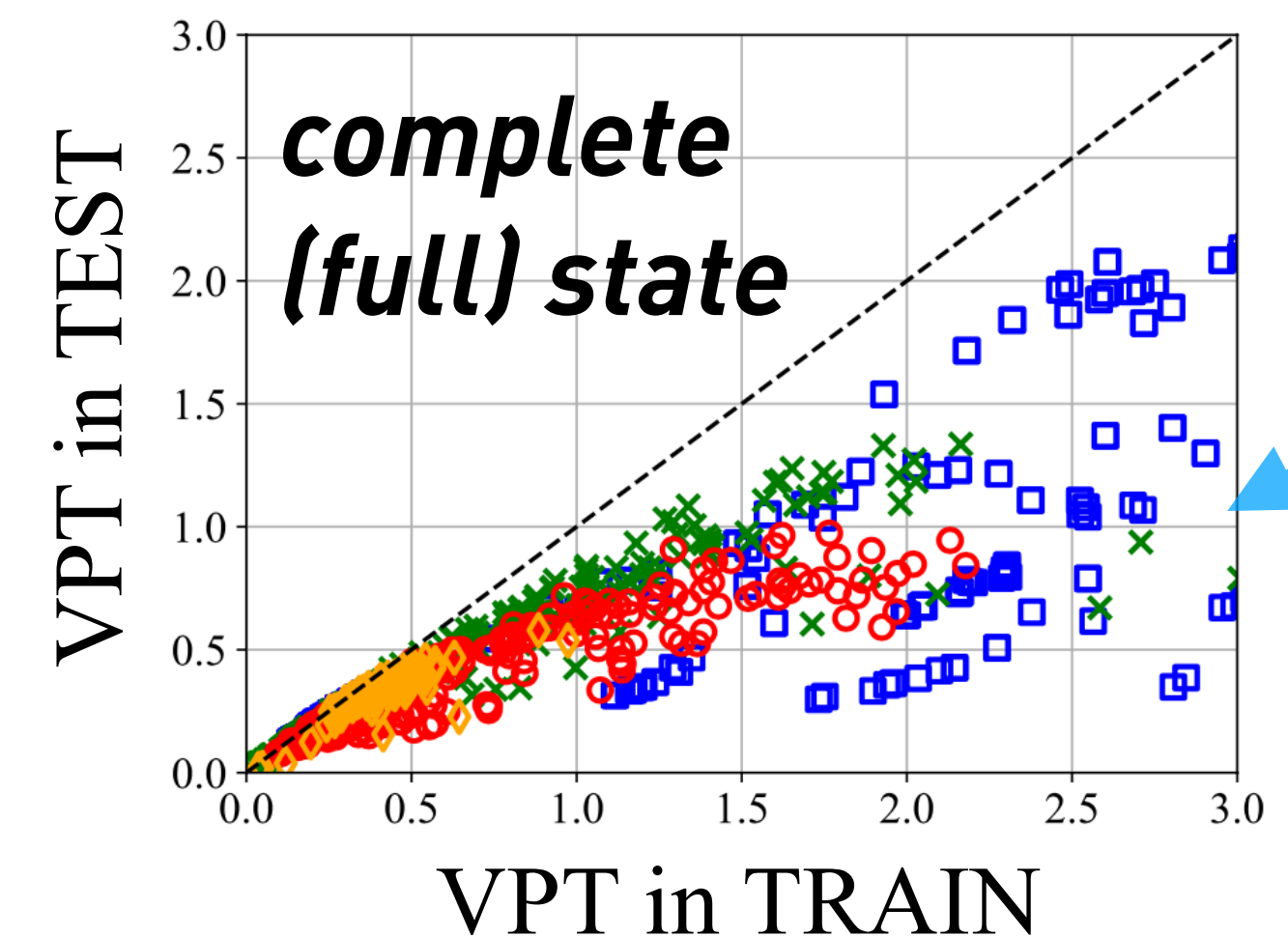
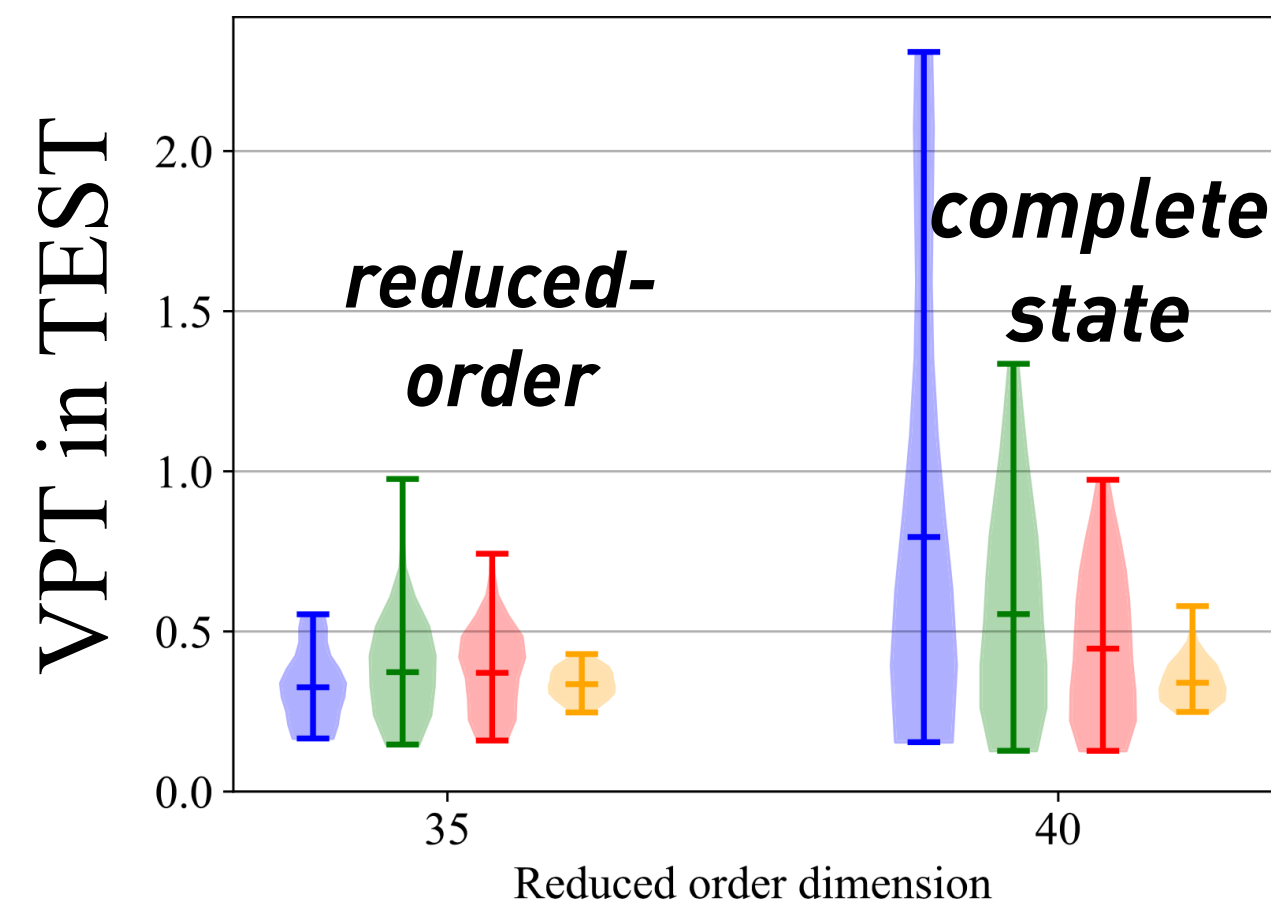
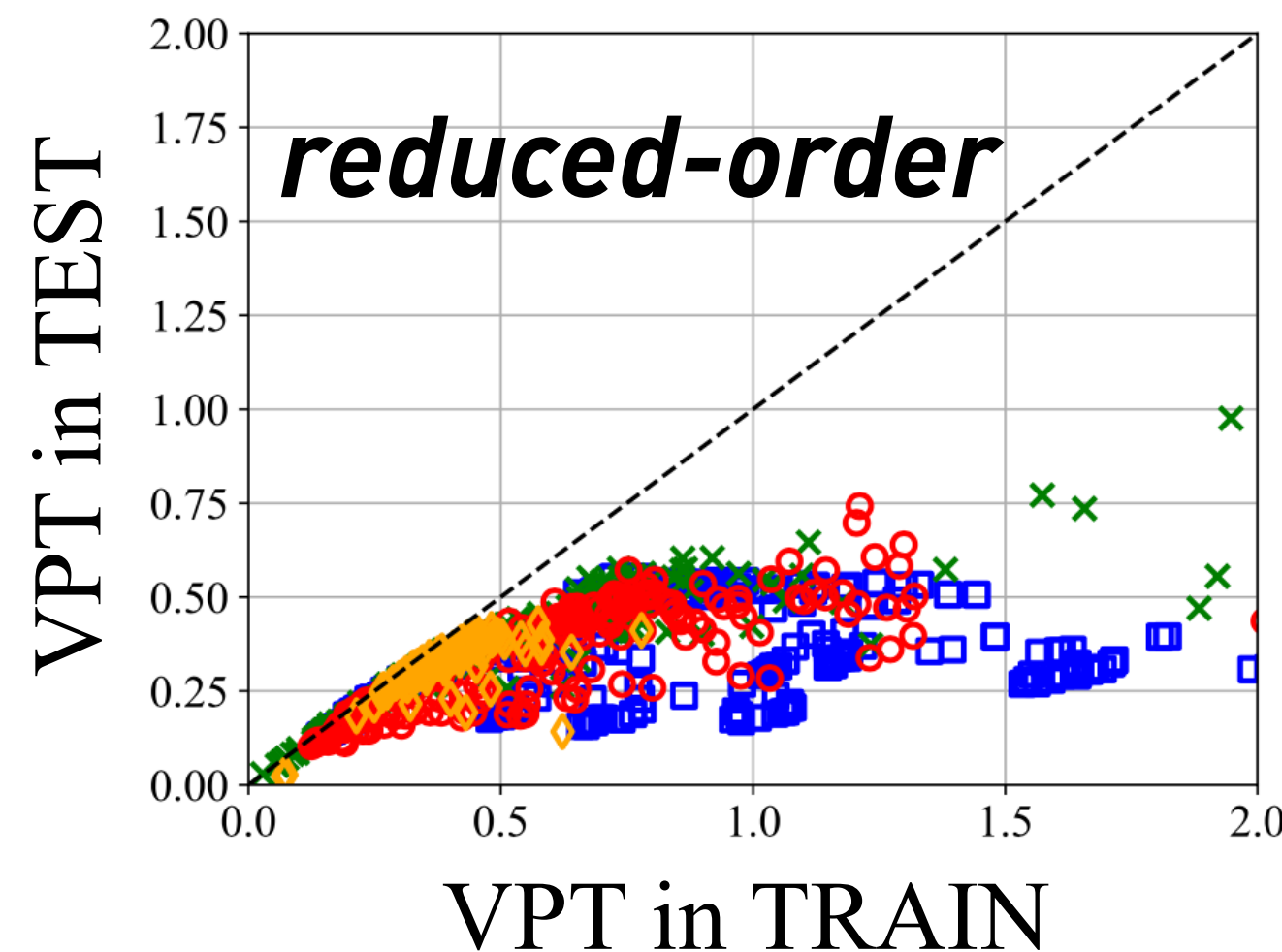
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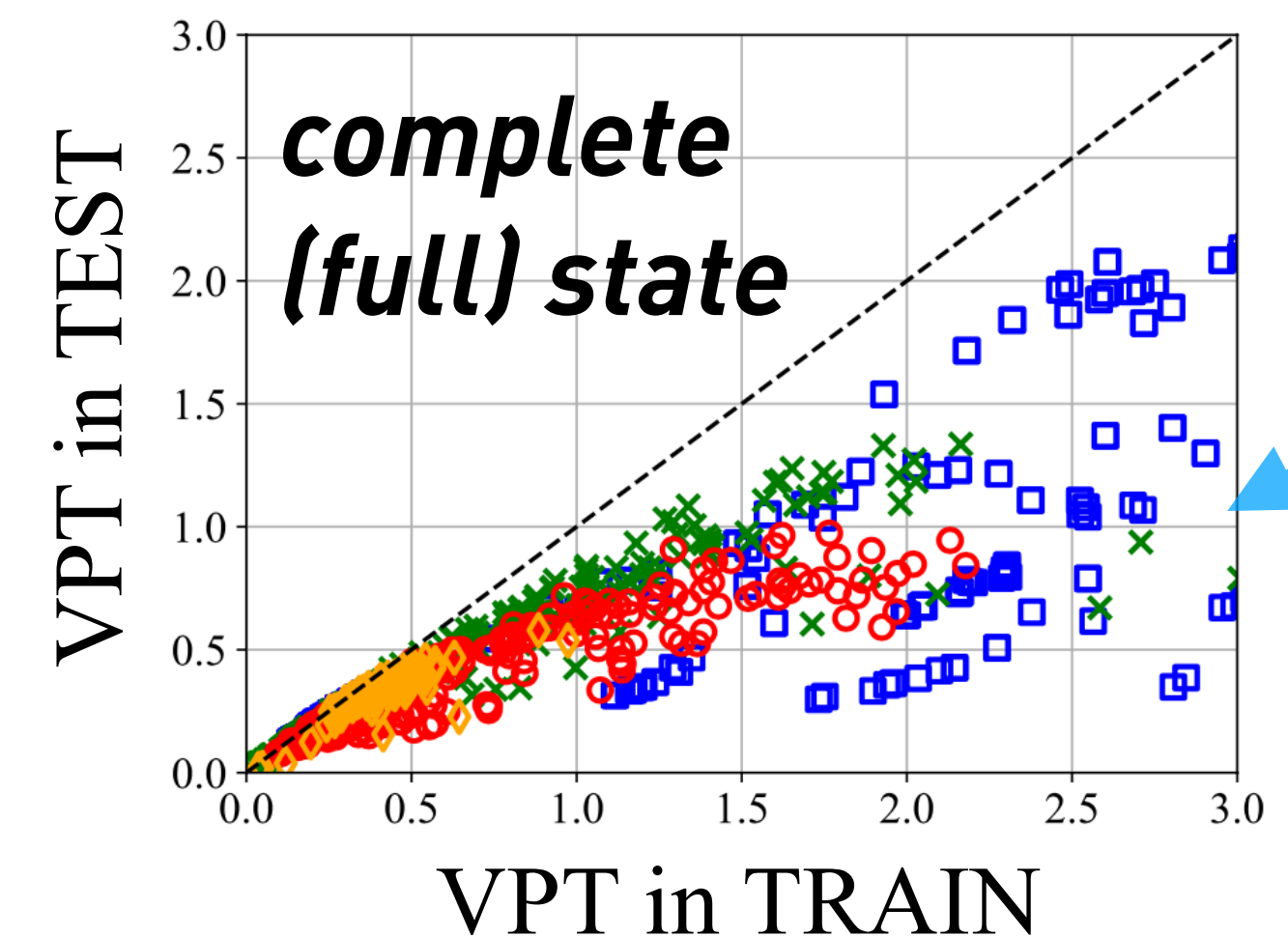
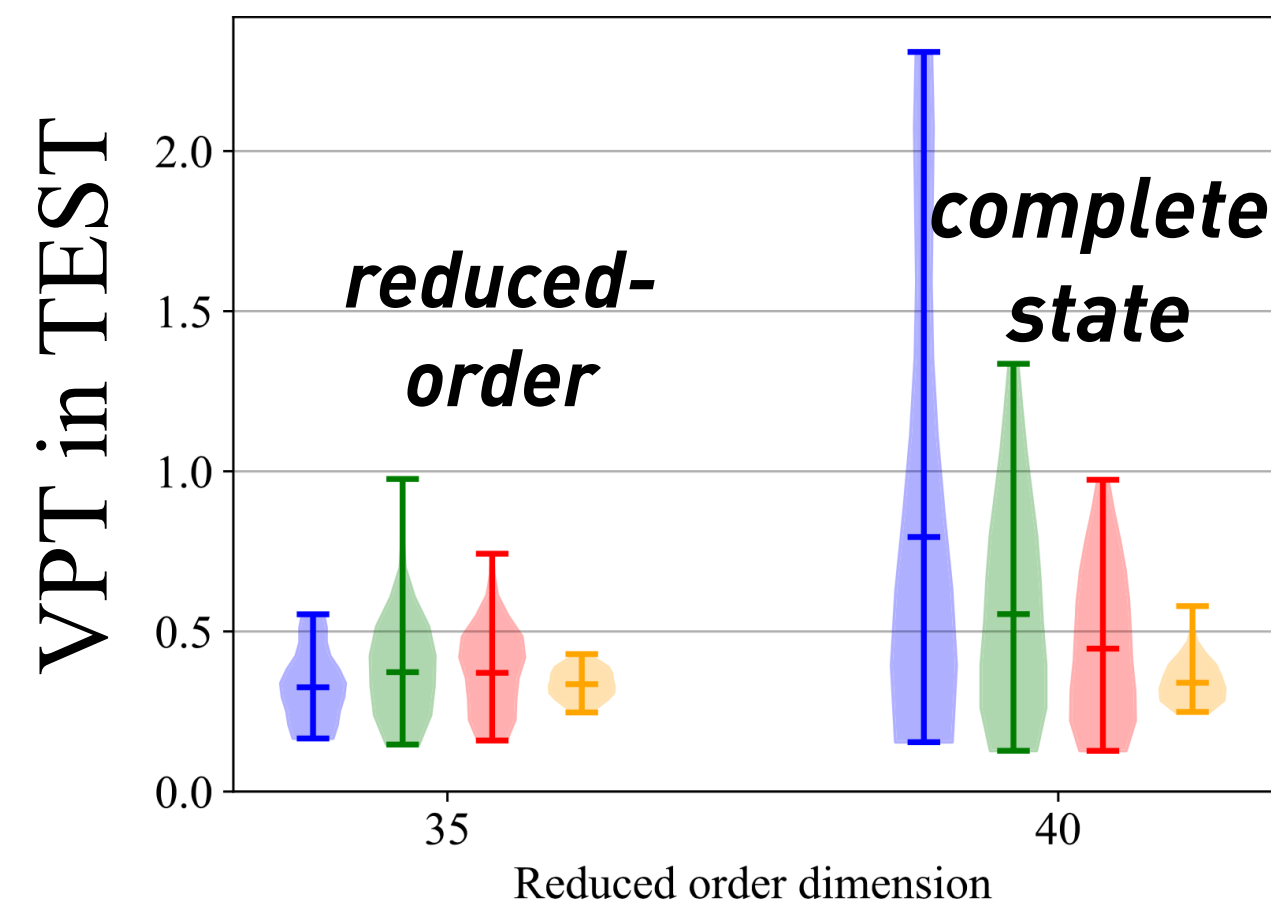
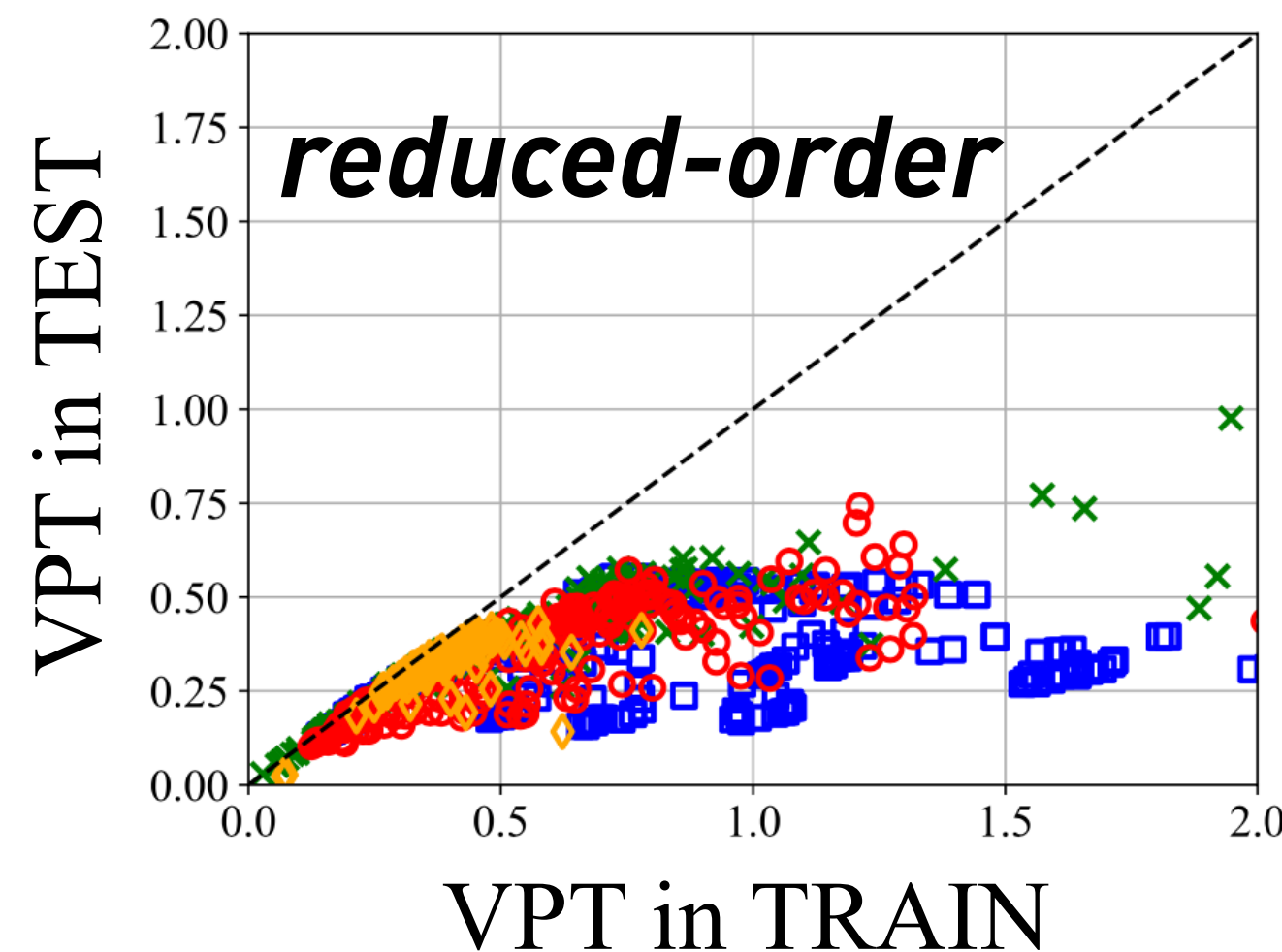
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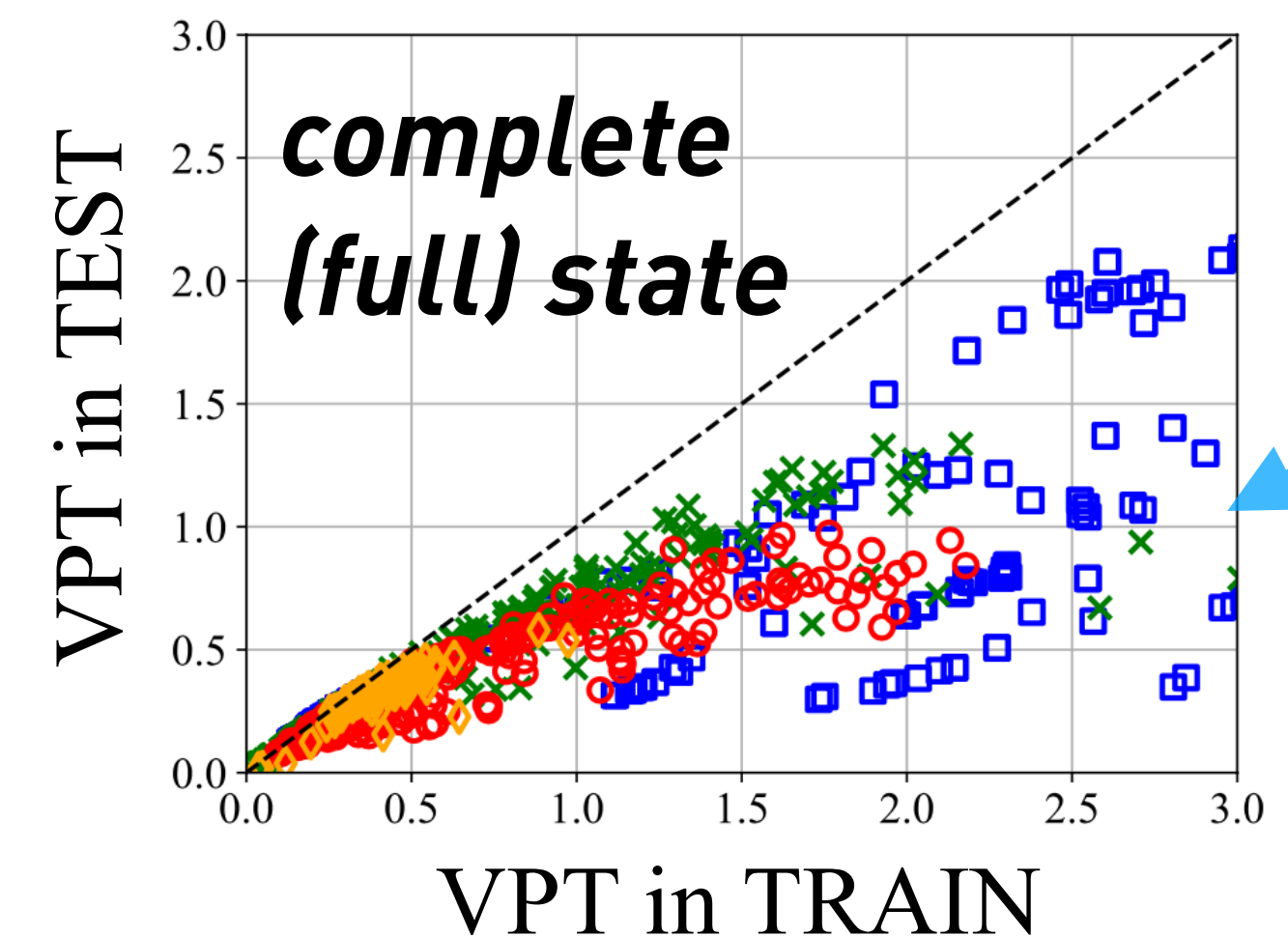
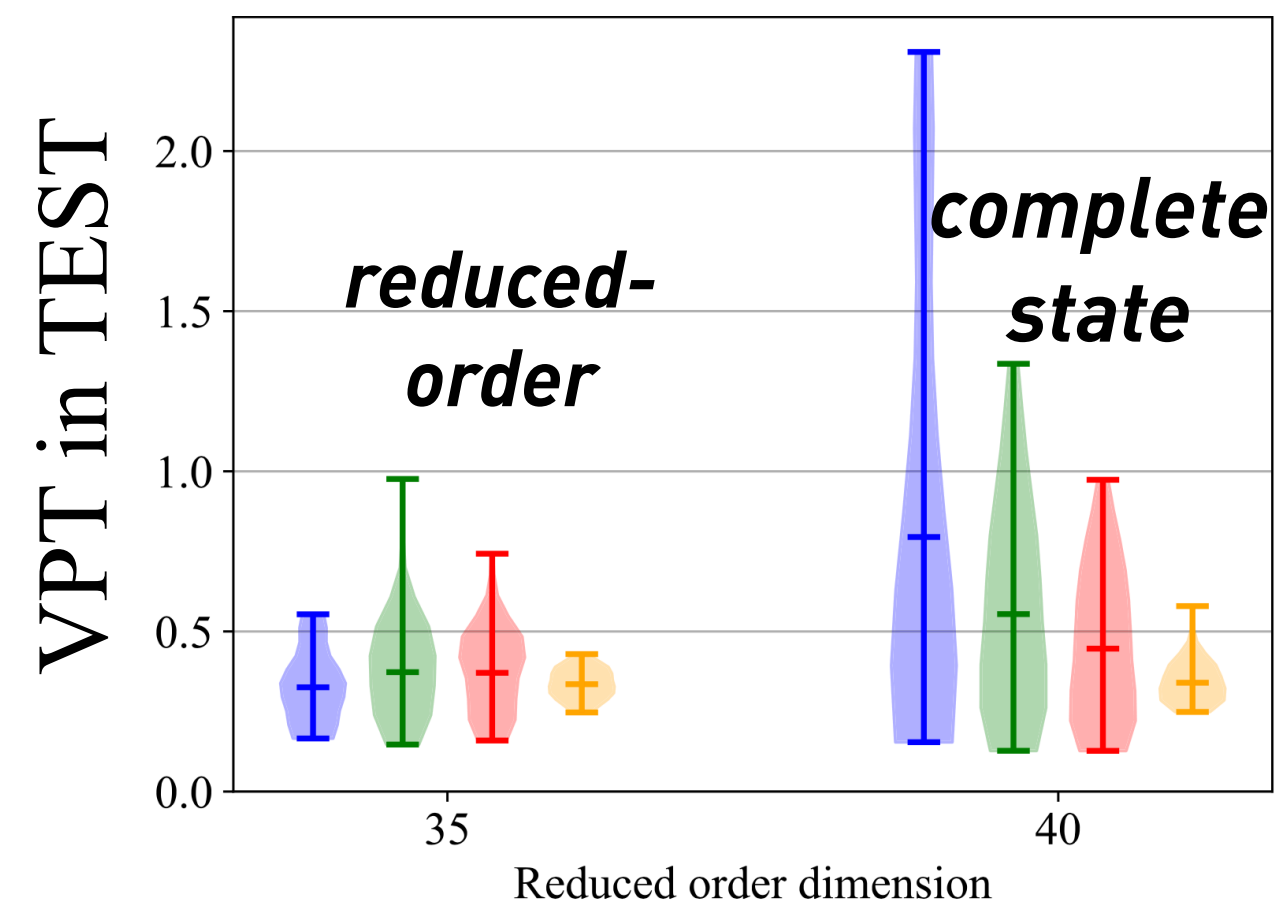
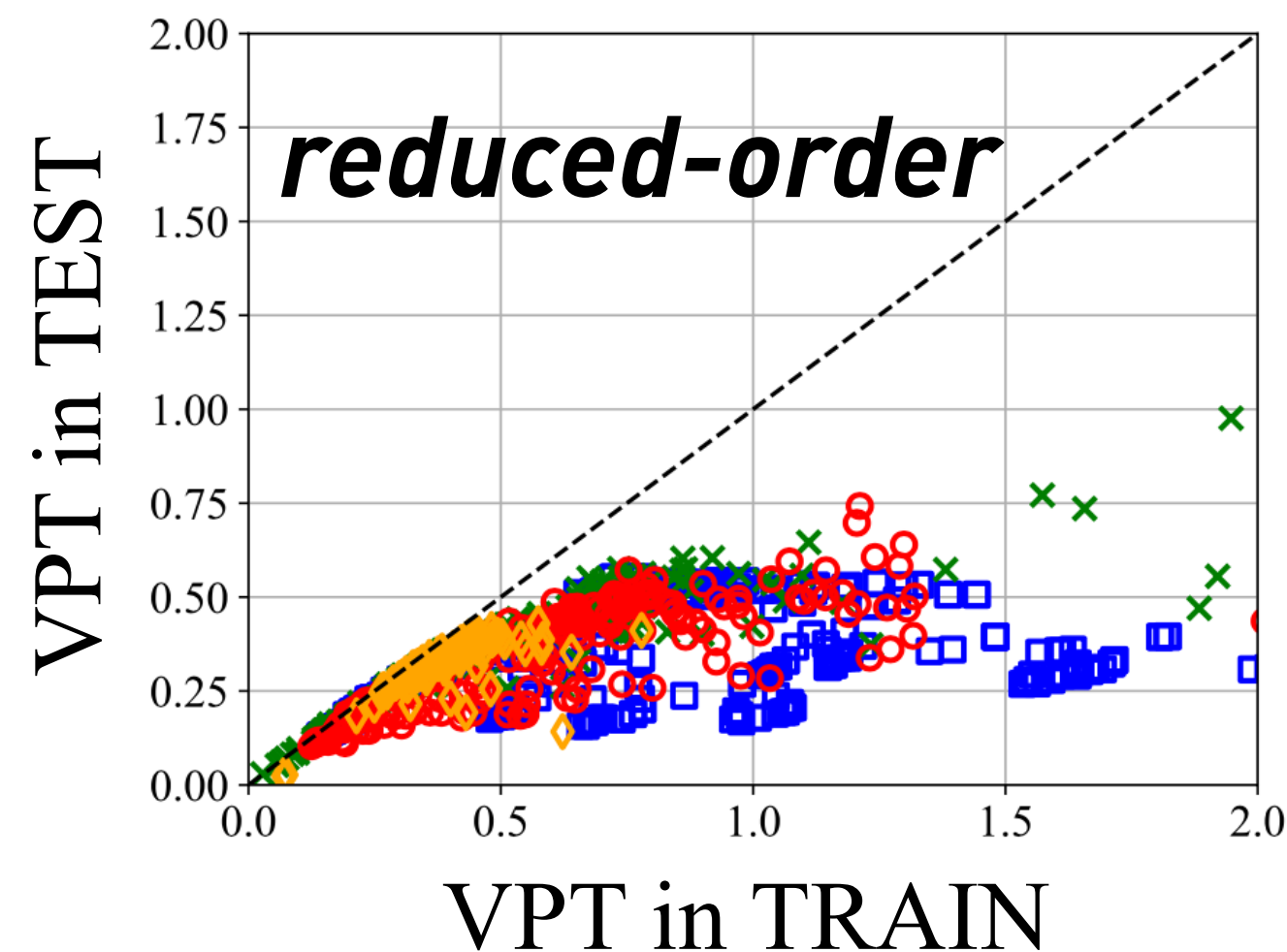
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- RC** superior in case of **complete (full) state** information (good generalization, cheaper to train)
- Gated architectures** superior in case of **reduced order state/observable** (more expensive to train)
- RC** has expressive power but lacks generalisation !
- Gated architectures** more robust against overfitting
- Regularisation procedures utilized in BPTT (zoneout, dropout) are effective



every marker is a trained model !

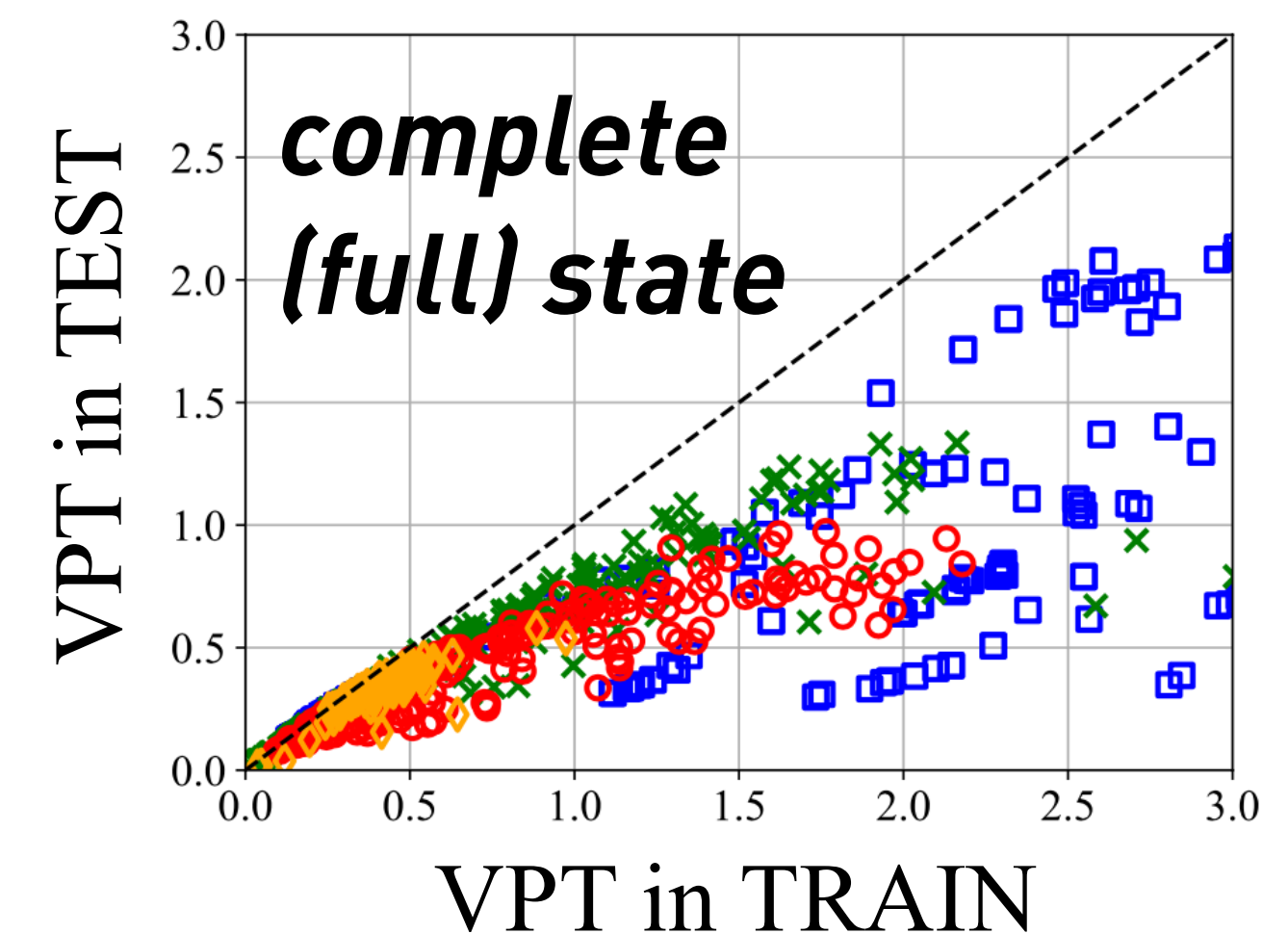
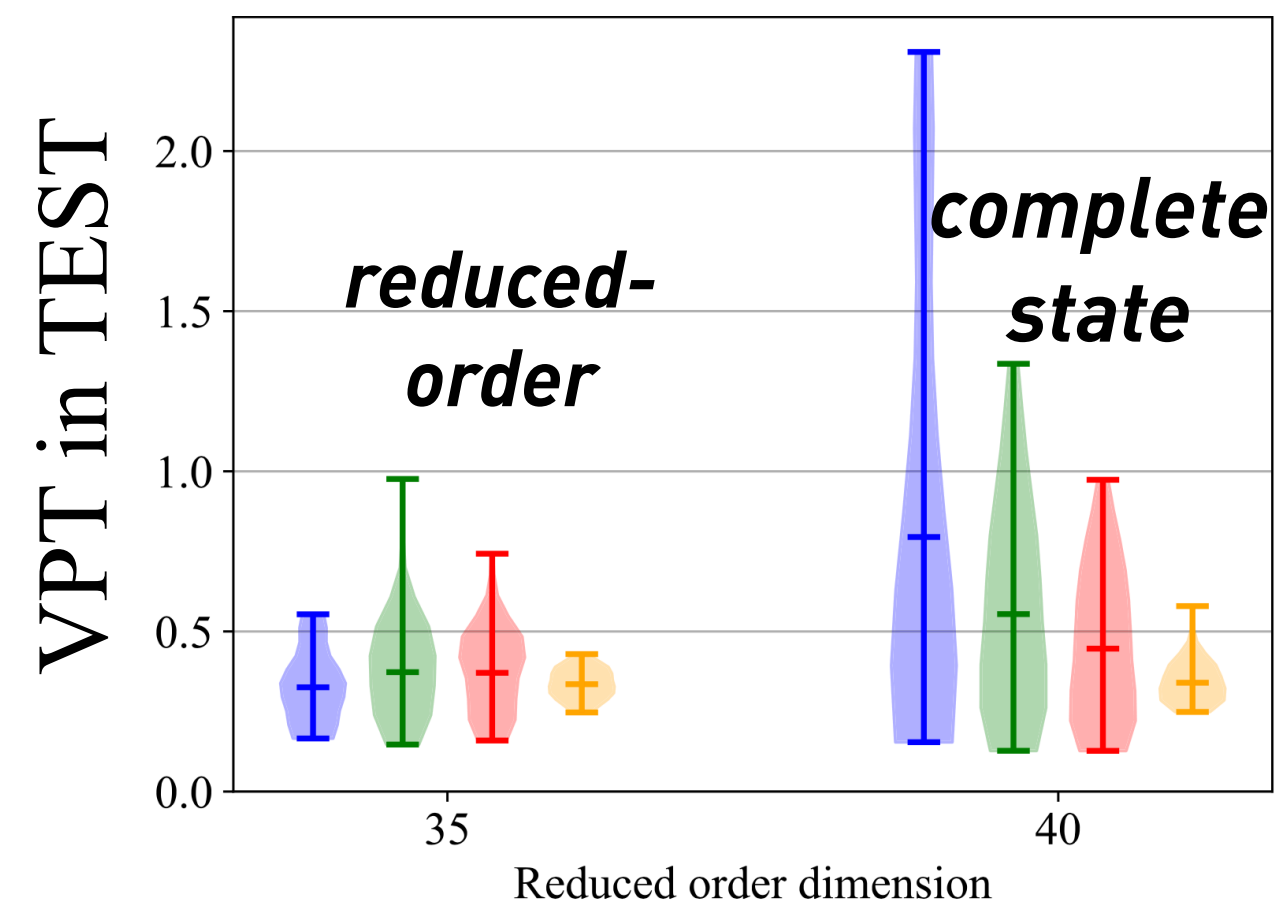
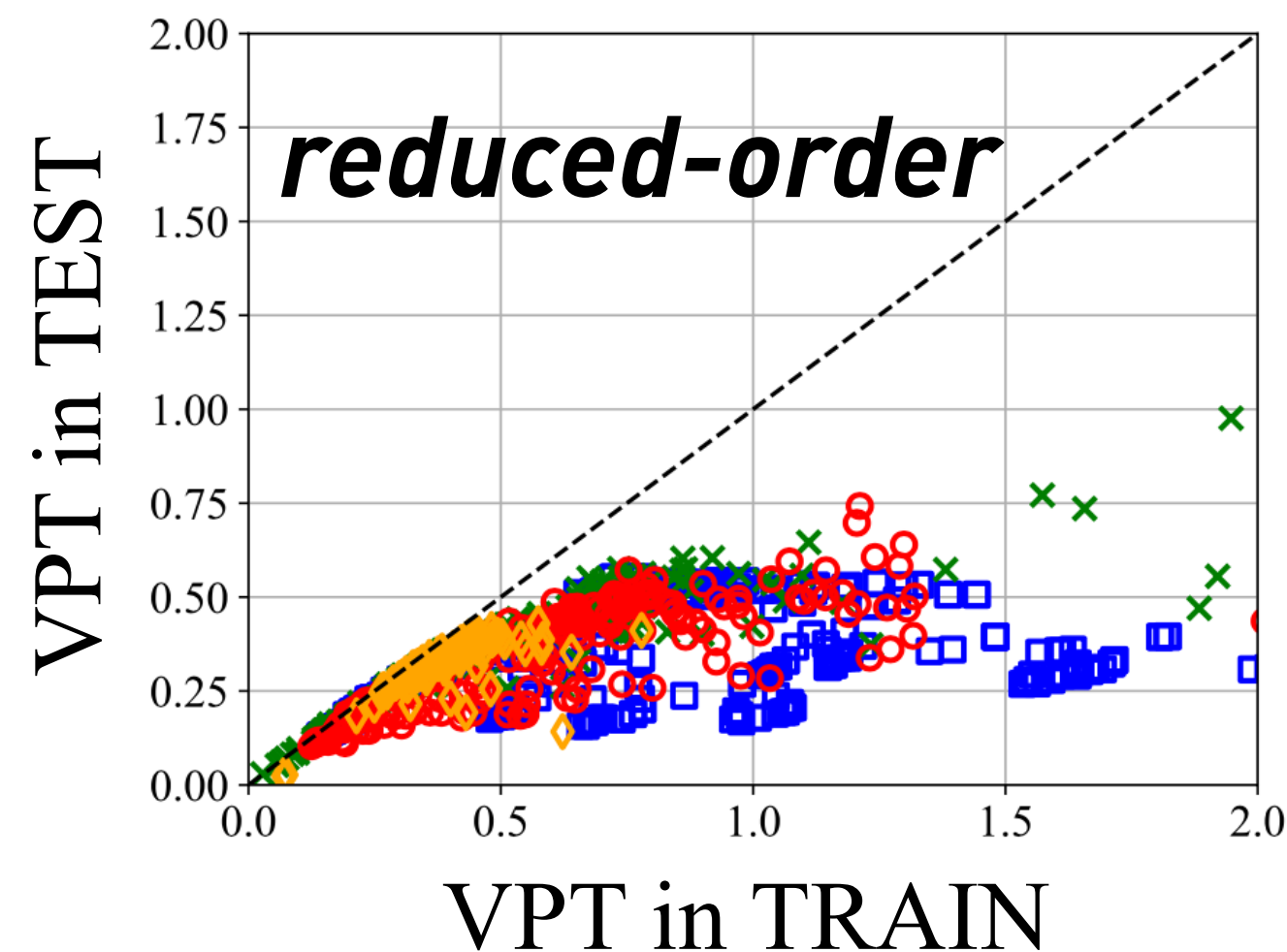
RC ■ (or □) ; GRU ✕ (or ✕) ; LSTM ● (or ○) ; Unit ◆ (or ◇) ; Ideal - - -



# Lorenz 96 - 35 / 40 mode observable

PR Vlachas , J Pathak , BR Hunt , TP Sapsis , M Girvan, E Ott and P Koumoutsakos, *Backpropagation algorithms and Reservoir Computing in Recurrent Neural Networks for the forecasting of complex spatiotemporal dynamics*, JNN, 2020

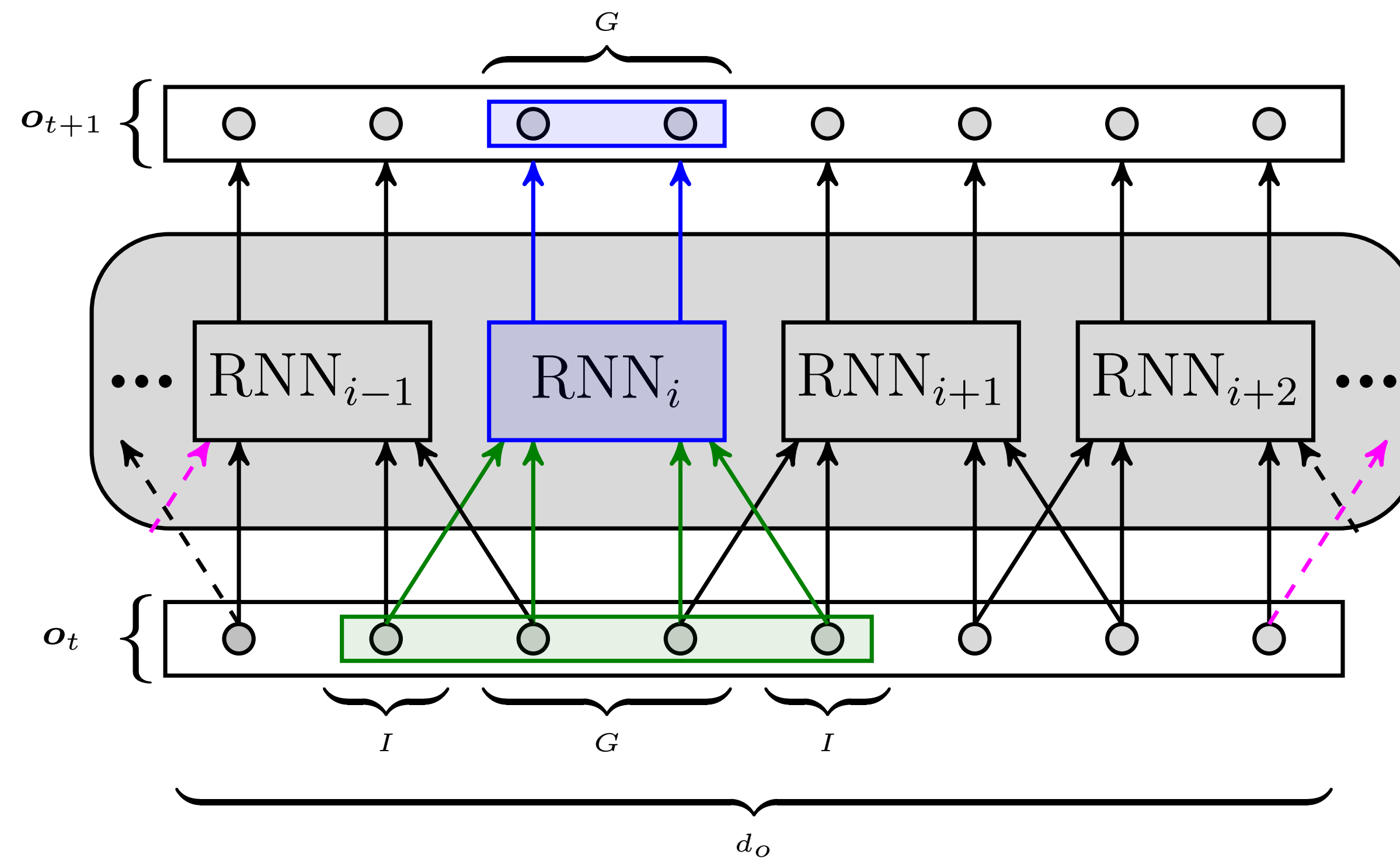
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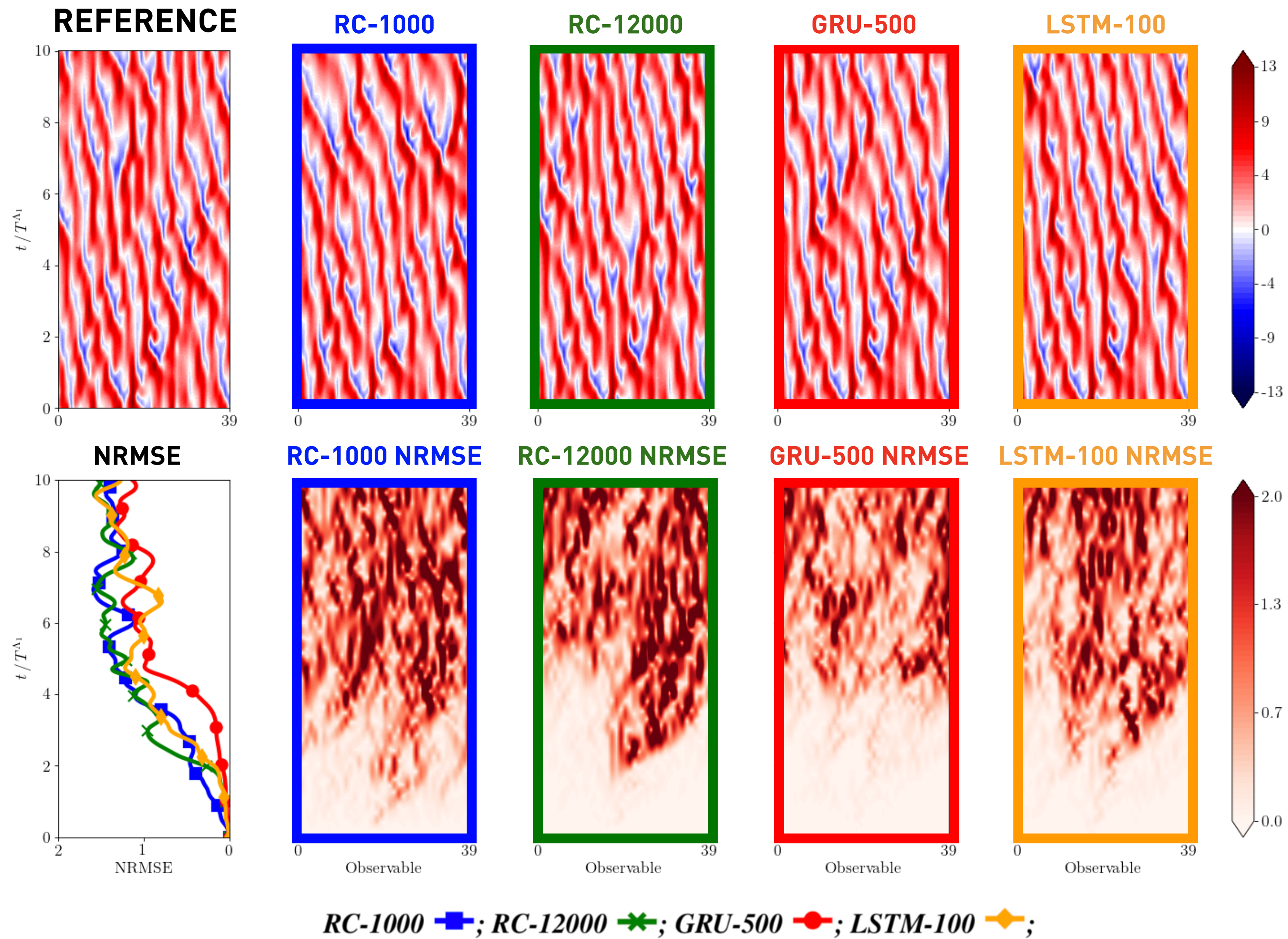


# Lorenz 96, $F = 8$ , full state information & parallelism

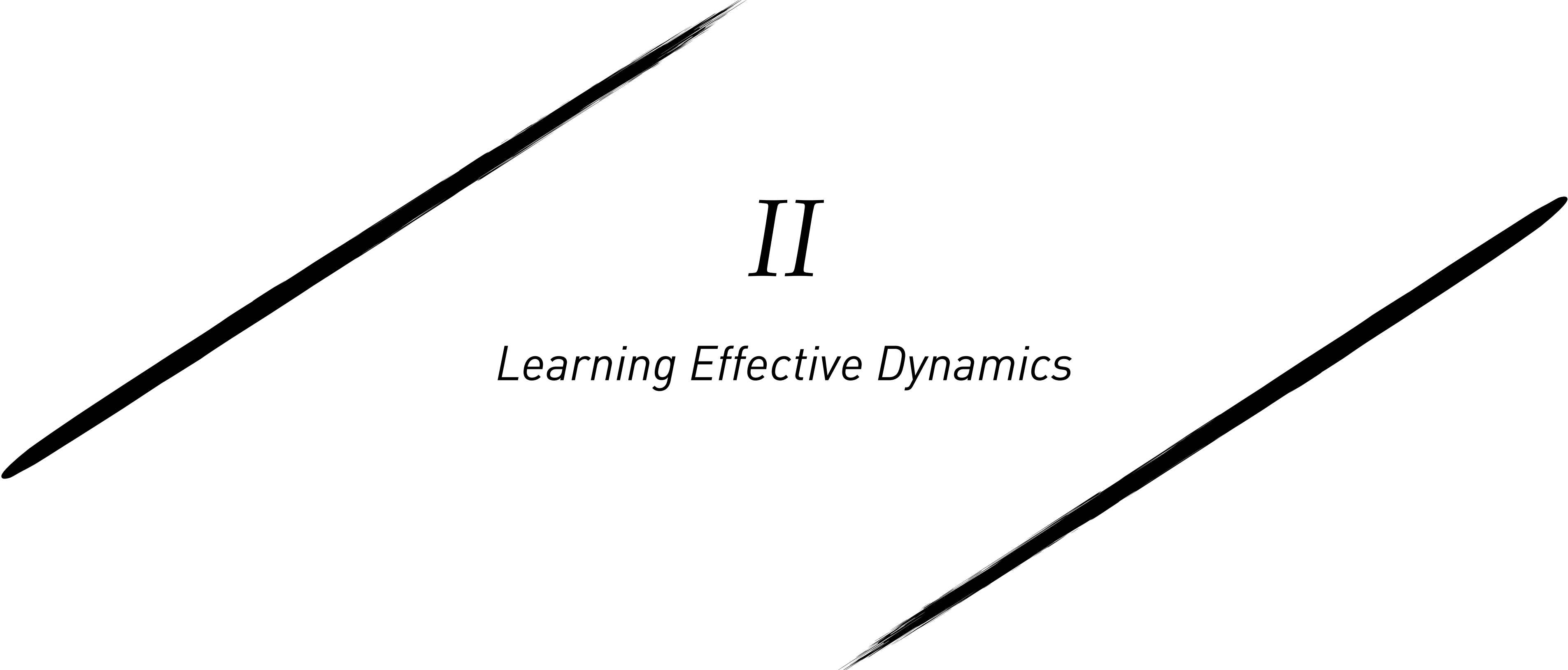




Lorenz 96,  $F = 8$ , full state information & parallelism







# *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



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

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- *Microscale simulations*: accurate **but** expensive to evaluate/not available



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

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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

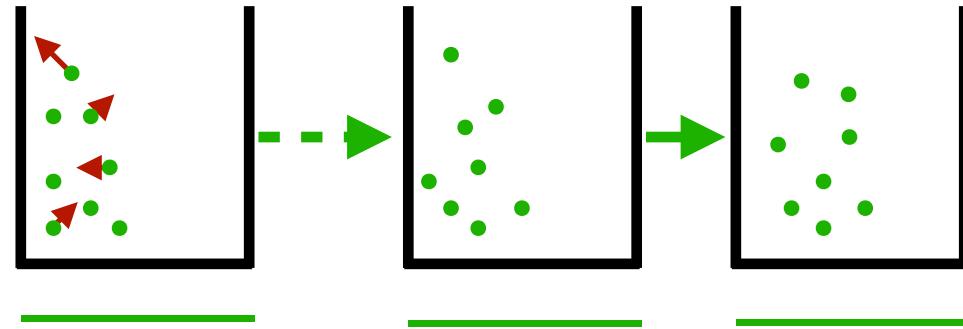
AND MANY MANY MORE ...



# *Equation Free Framework*



**$A_0$**  propagate  
(short times)  
micro scale

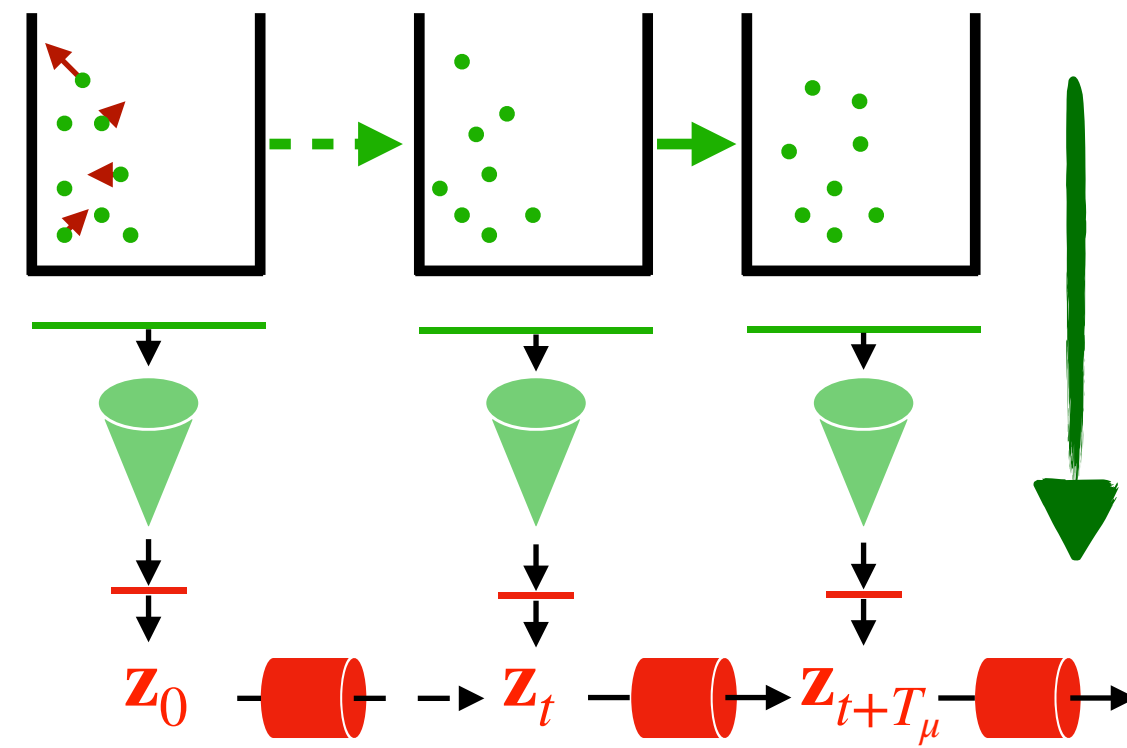


**A**

***Equation Free  
Framework***



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



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



**RESTRICTING /AVERAGING**

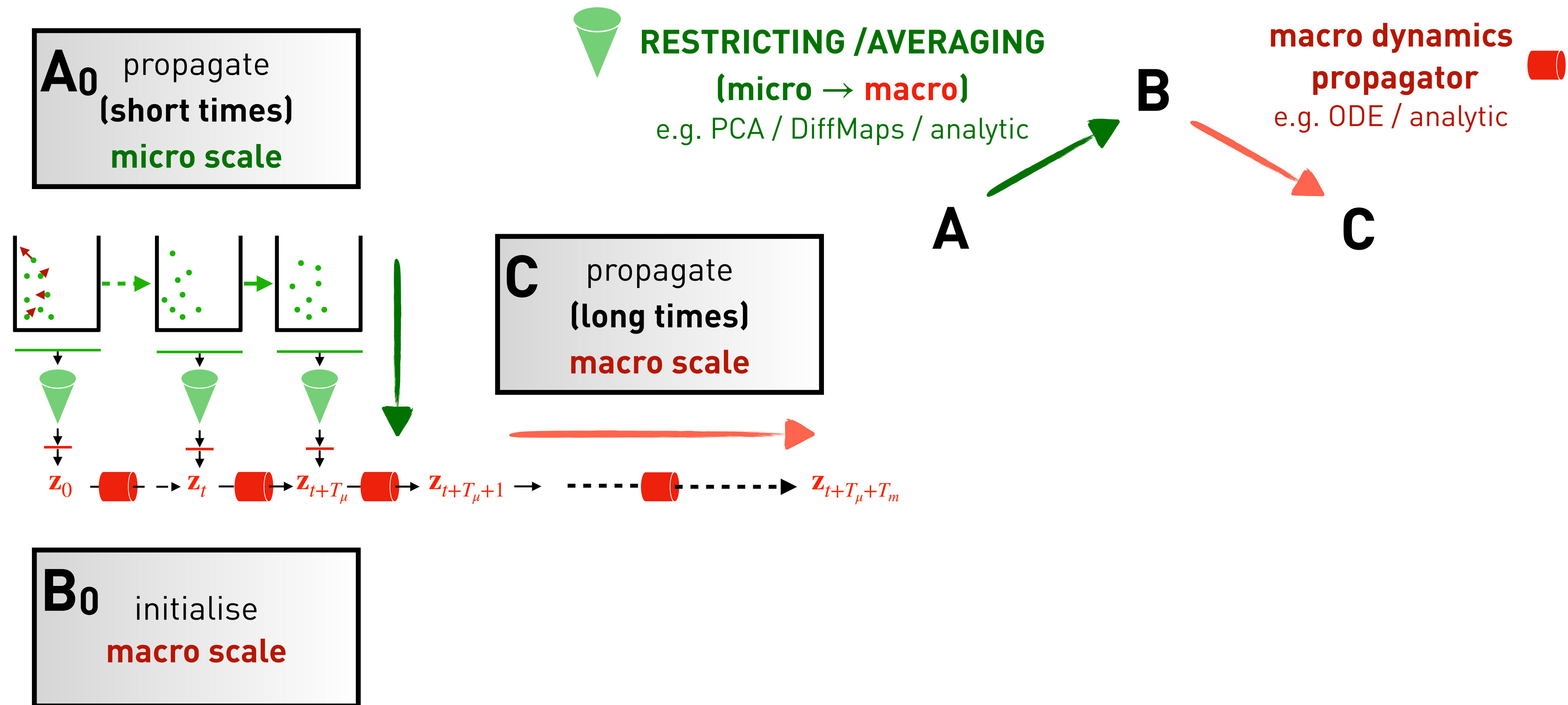
(micro → macro)

e.g. PCA / DiffMaps / analytic



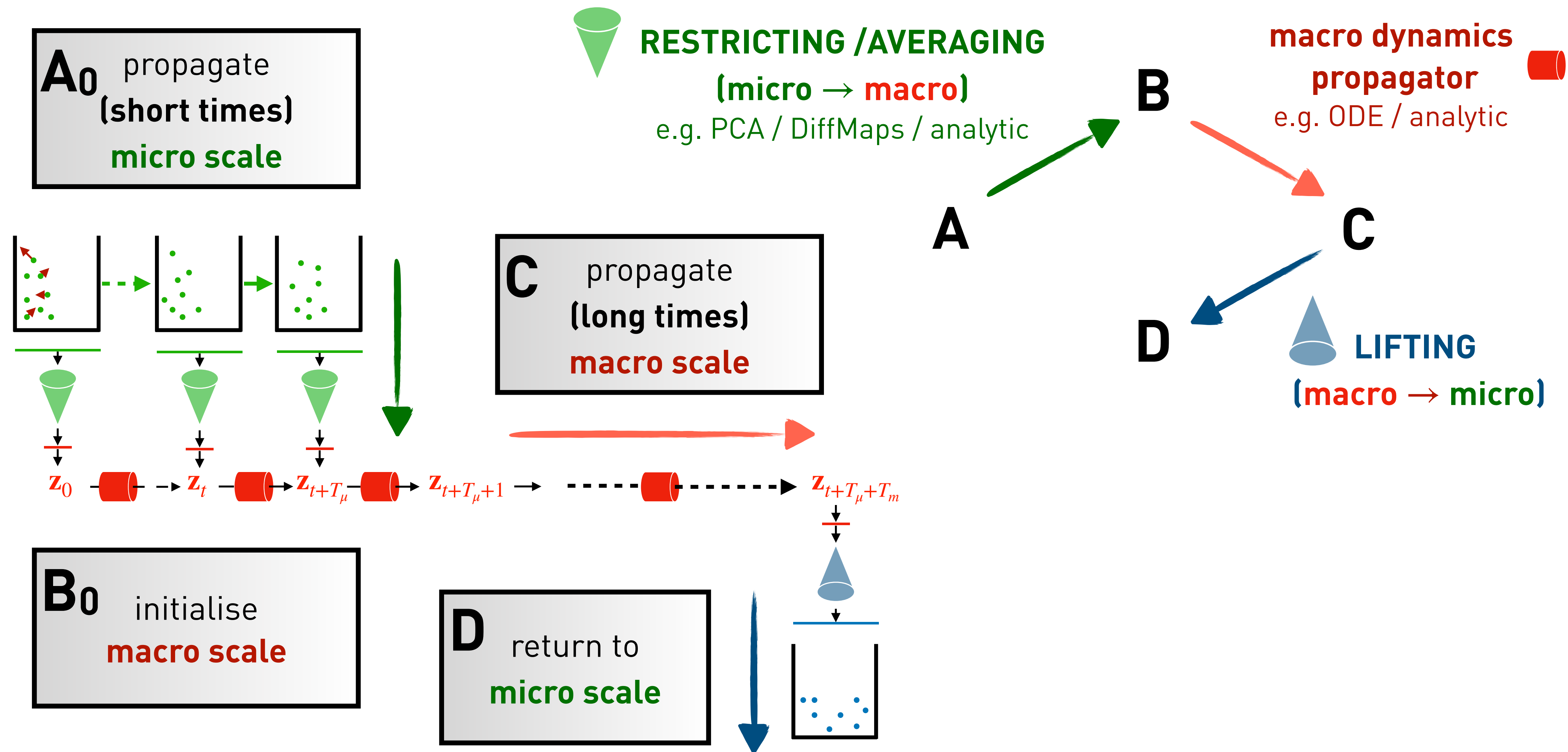
*Equation Free  
Framework*





# Equation Free Framework

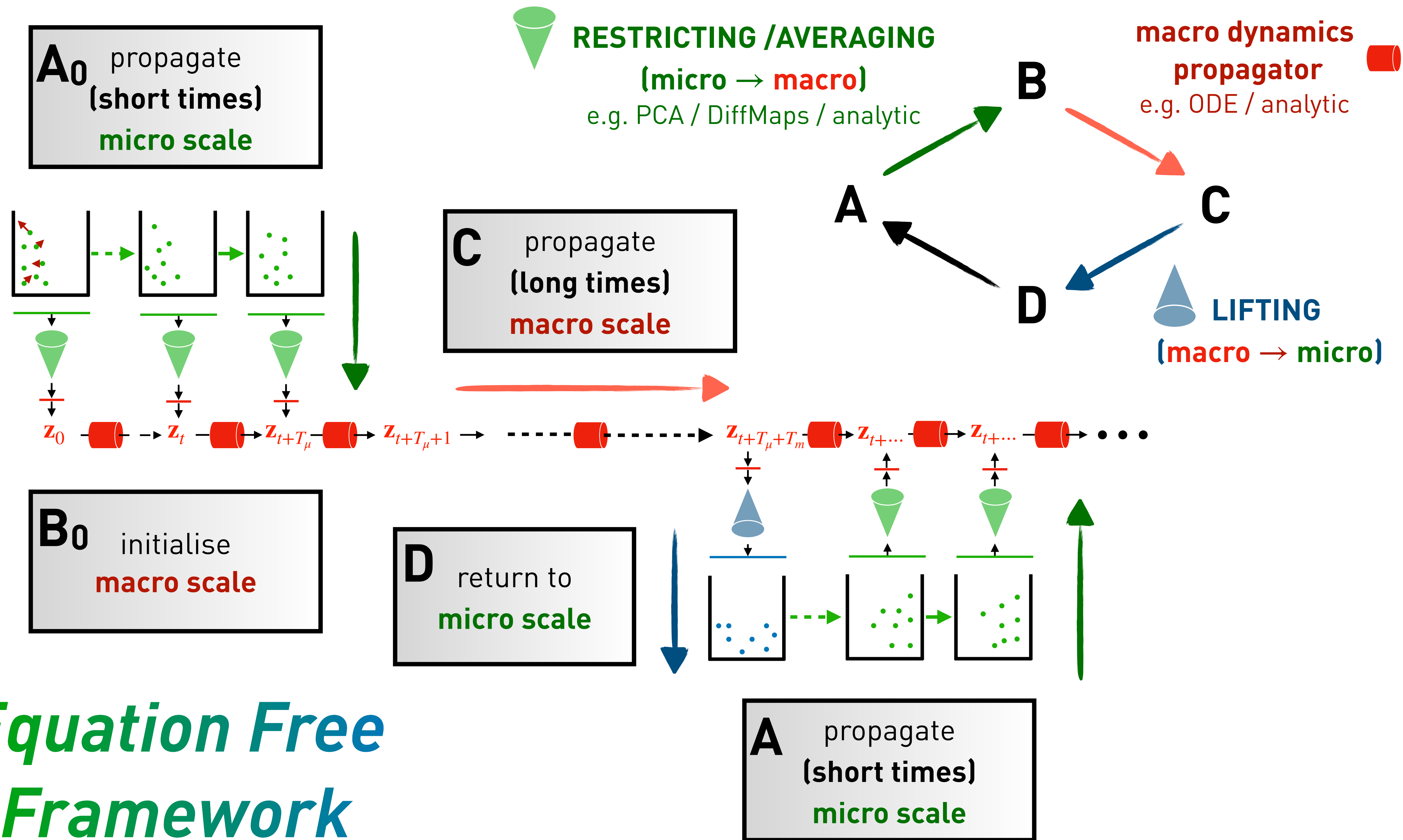




# Equation Free Framework

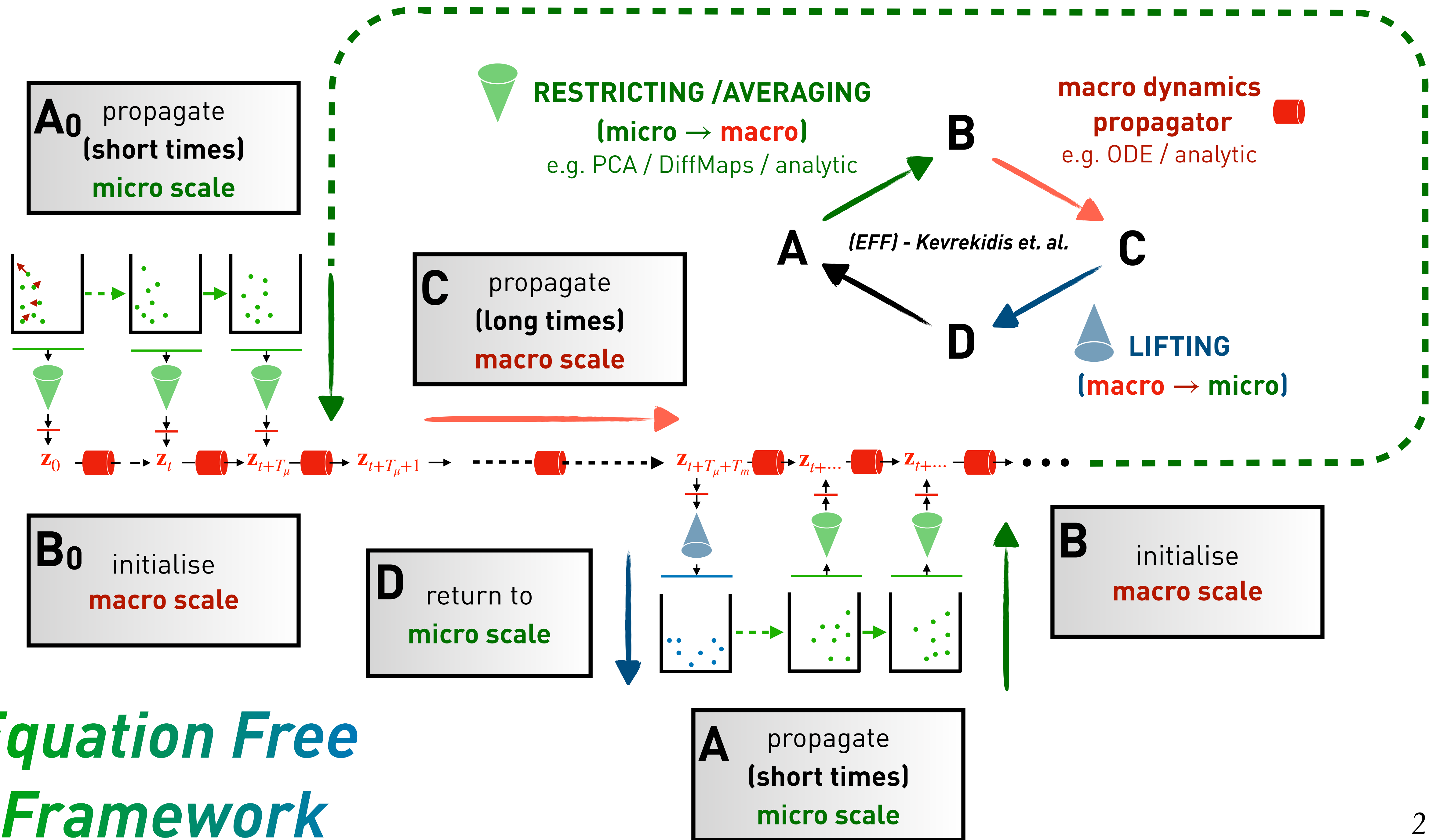


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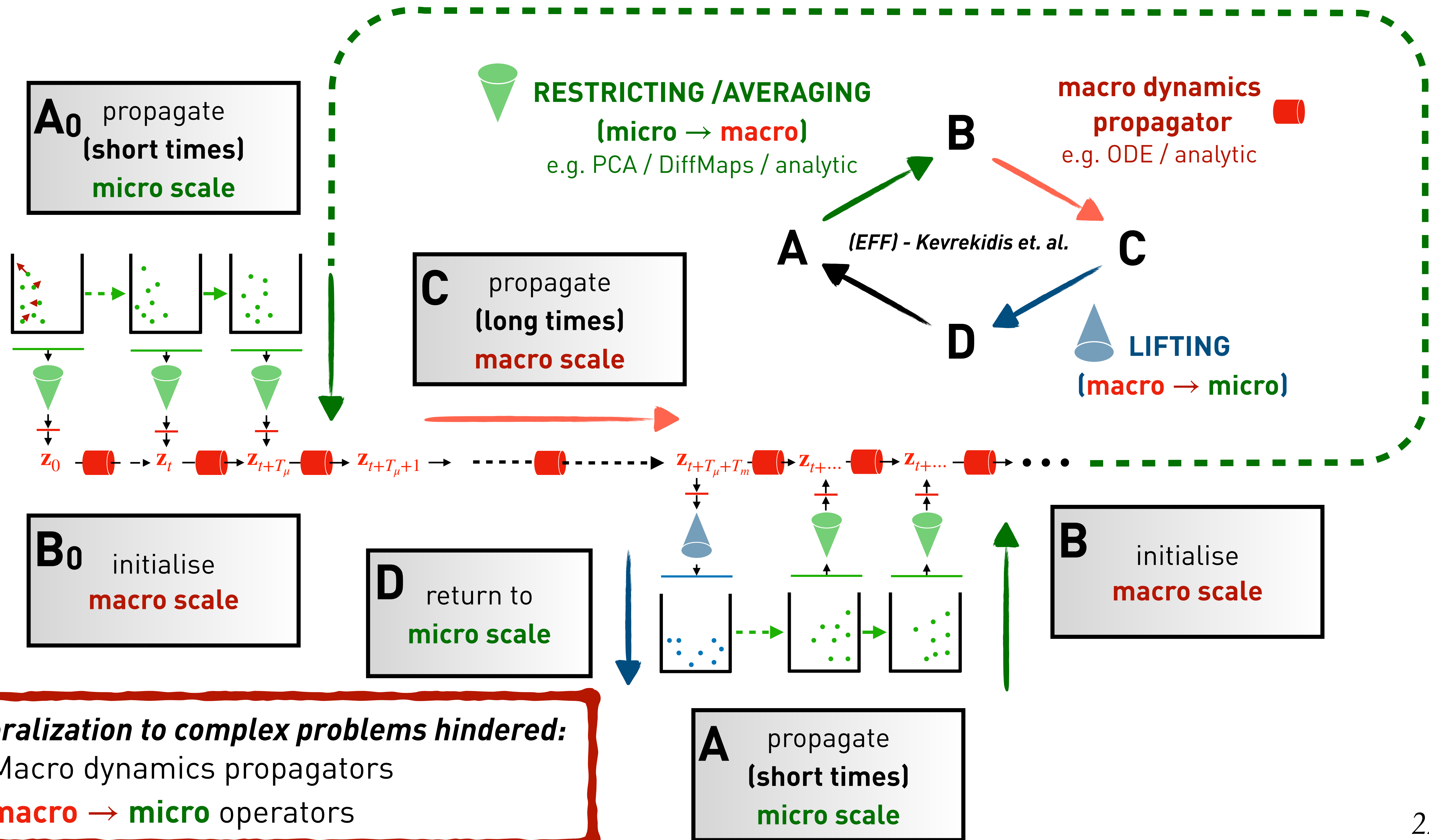




# Equation Free Framework









# Operators from Machine Learning

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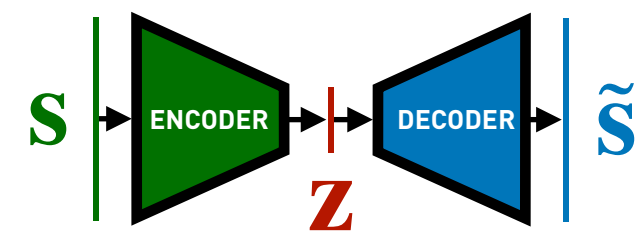


# Operators from Machine Learning

## (CONVOLUTIONAL) AUTOENCODERS

High dimensional  
state

Reconstruction



Low dimensional  
latent space

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

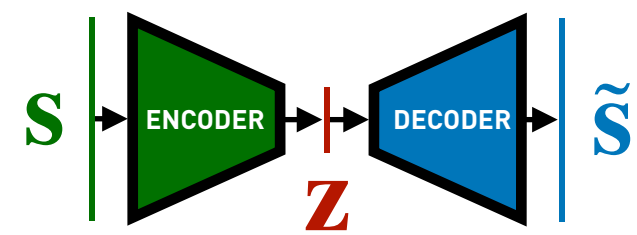


# Operators from Machine Learning

## (CONVOLUTIONAL) AUTOENCODERS

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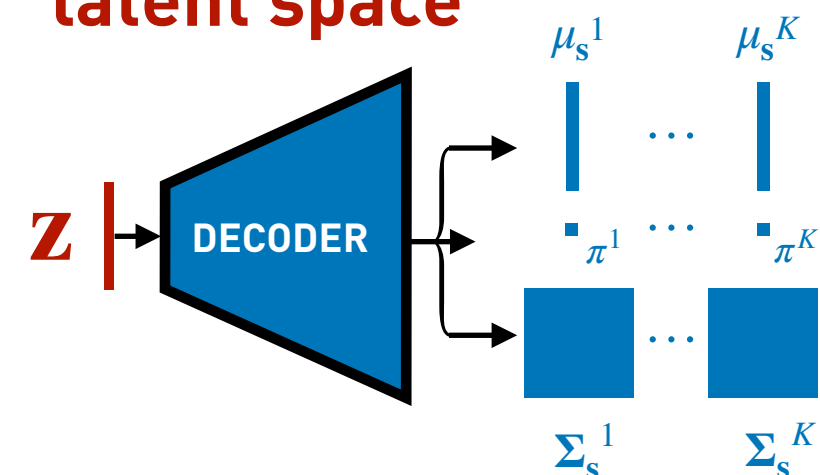


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## MIXTURE DENSITY NETWORKS

Low dimensional  
latent space



Parametrisation  
of  $p(\mathbf{s} | \mathbf{z})$

- 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**
- $$p(\mathbf{s} | \mathbf{z}) = \sum_{k=1}^K \pi_k \mathcal{N}(\mu_s^k, \Sigma_s^k)$$

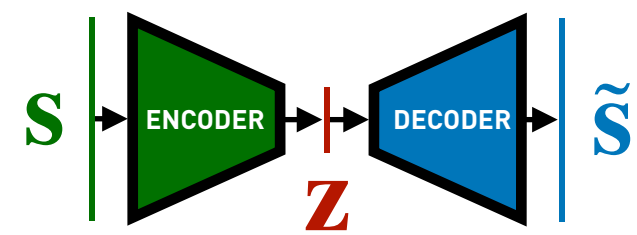


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High dimensional  
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Reconstruction

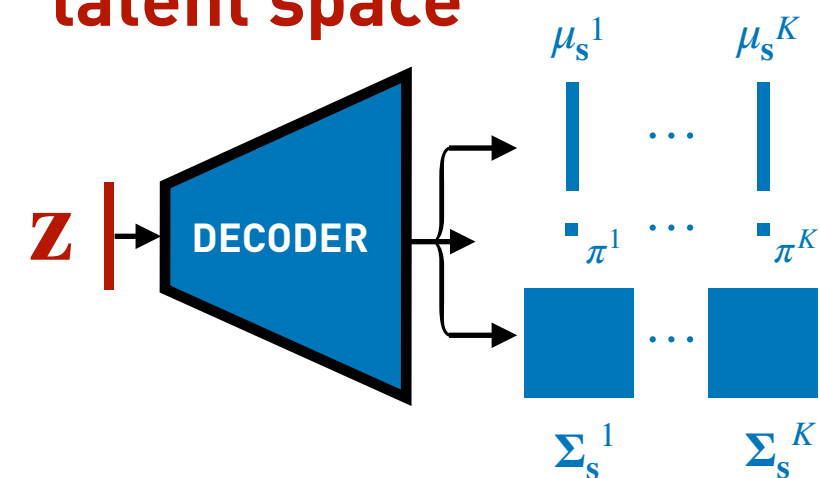


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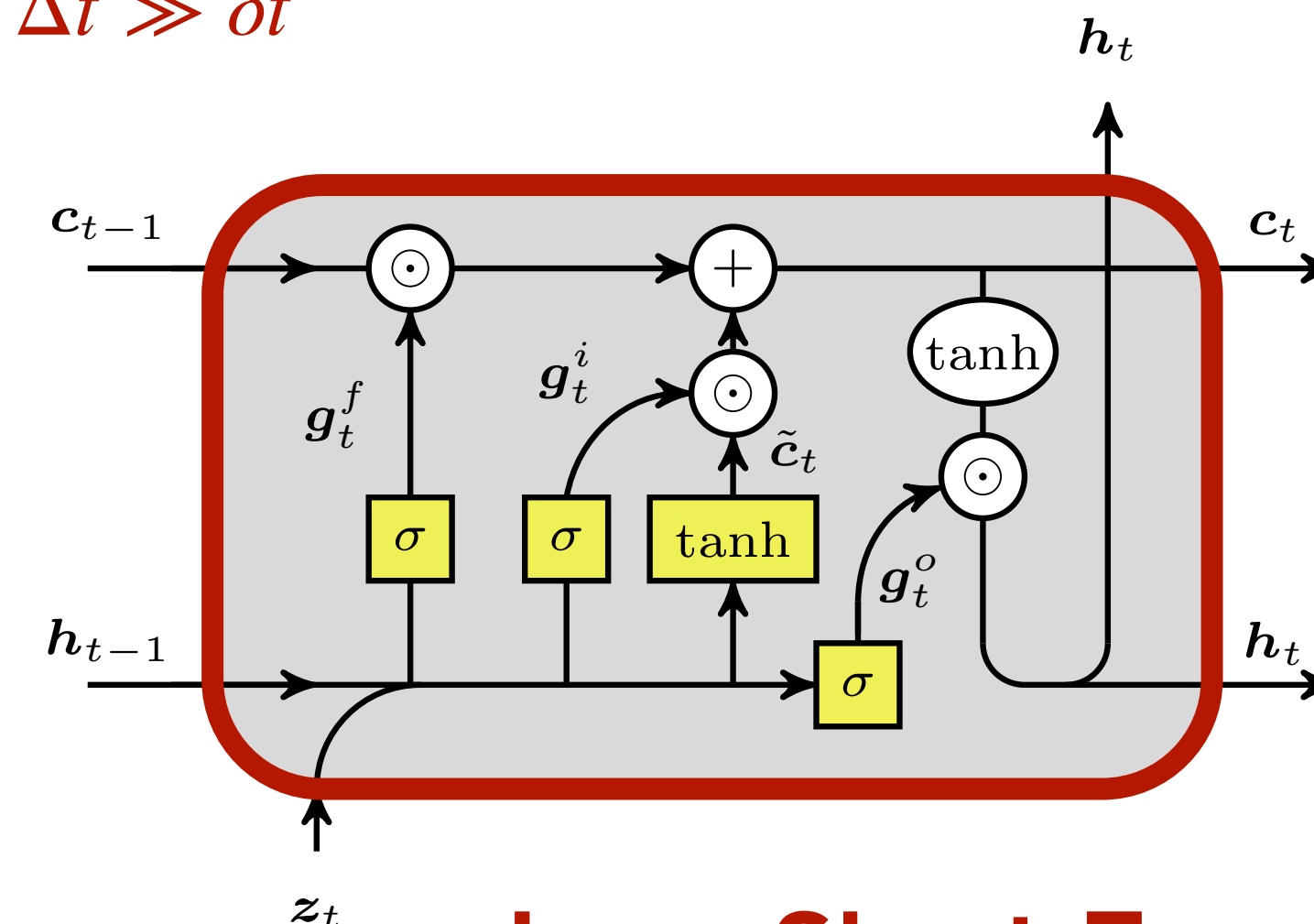
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- Non-linear non-Markovian dynamics  $z$  (**macro dynamics**)
- **Forecasting** using **RNNs**
- Tracking the **history** of the low order state  $z$  to model **non-Markovian** dynamics
- Forecasting  $z_{t+\Delta t}$  from short-term history
- $\Delta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

$\Delta t \gg \delta t$



**Long Short-Term Memory**

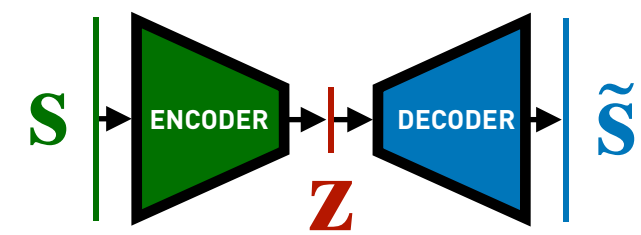


# Operators from Machine Learning

## (CONVOLUTIONAL) AUTOENCODERS

High dimensional  
state

Reconstruction

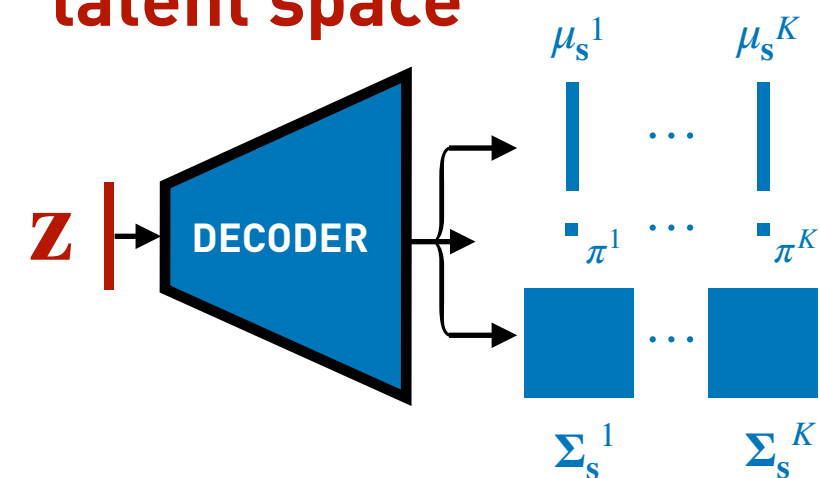


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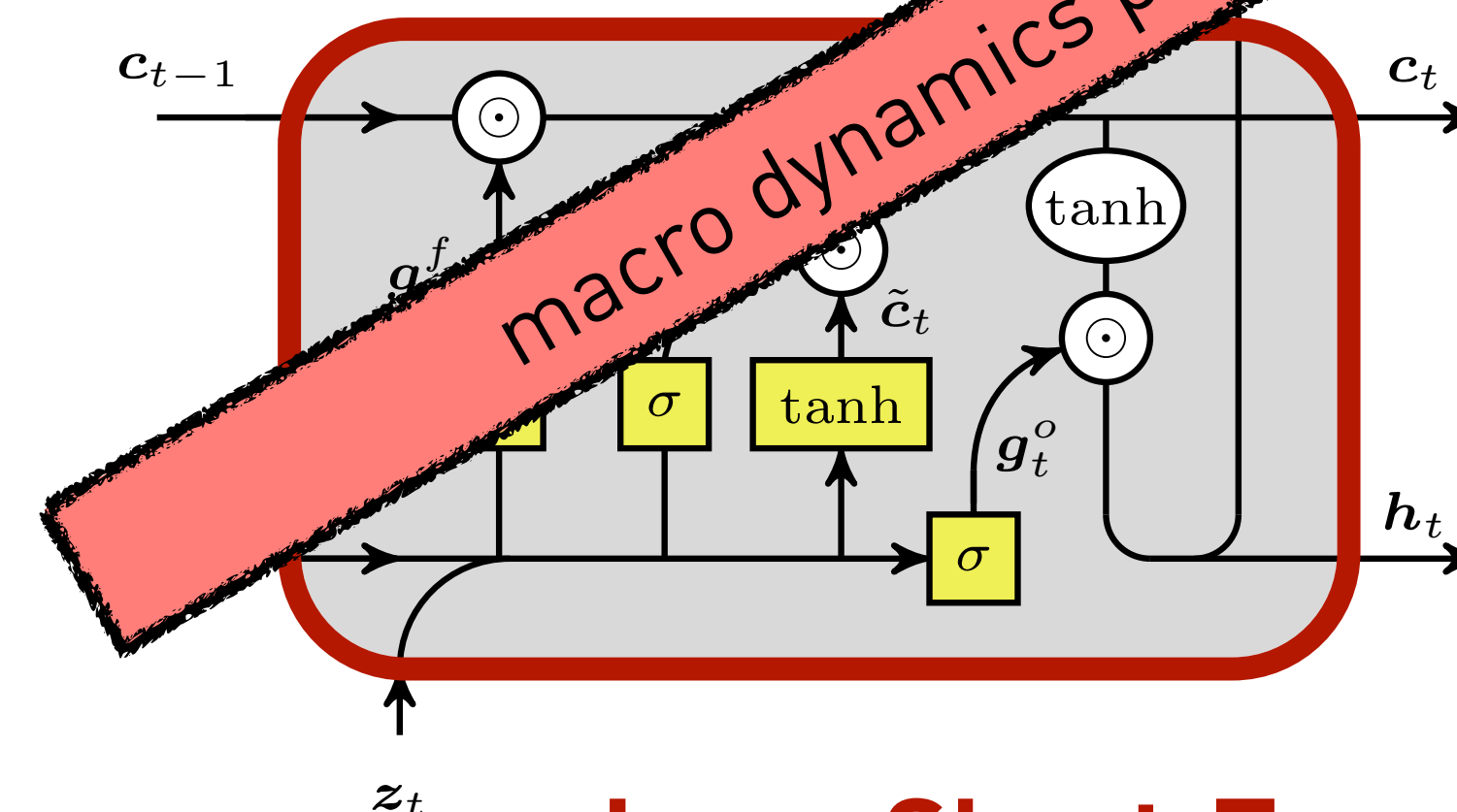


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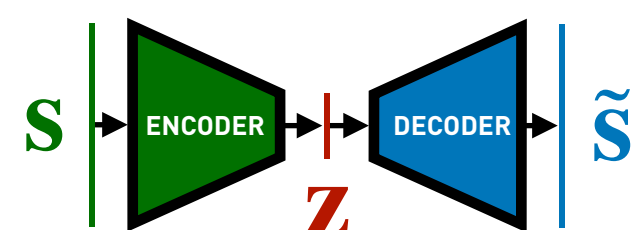


# Operators from Machine Learning

## (CONVOLUTIONAL) AUTOENCODERS

High dimensional state

Reconstruction



Low dimensional latent space

- Full high dimensional description of atoms / state / angles, bonds
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RESTRICTING/AVERAGING  
(micro  $\rightarrow$  macro)

## DENSITY NETWORKS

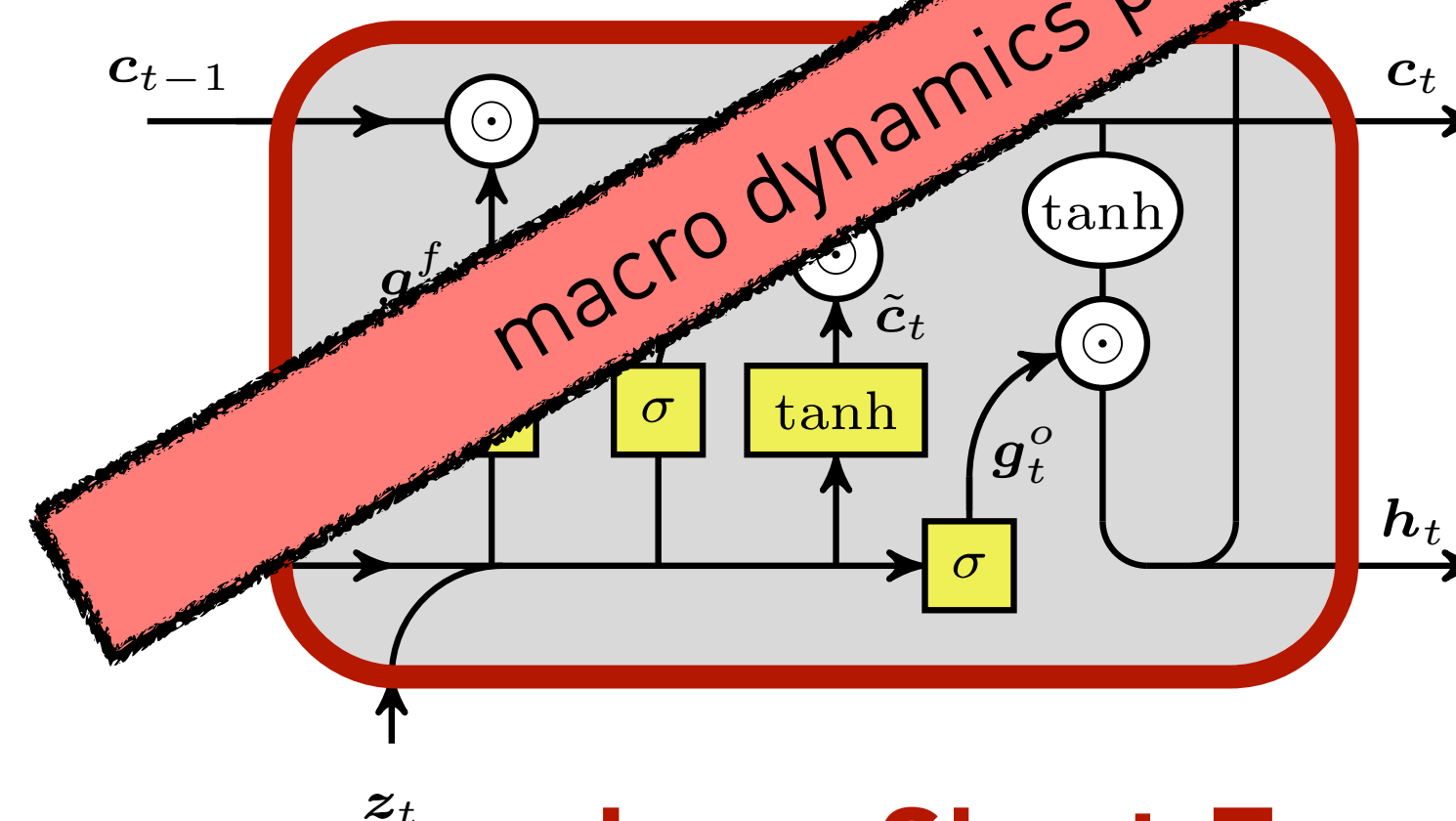
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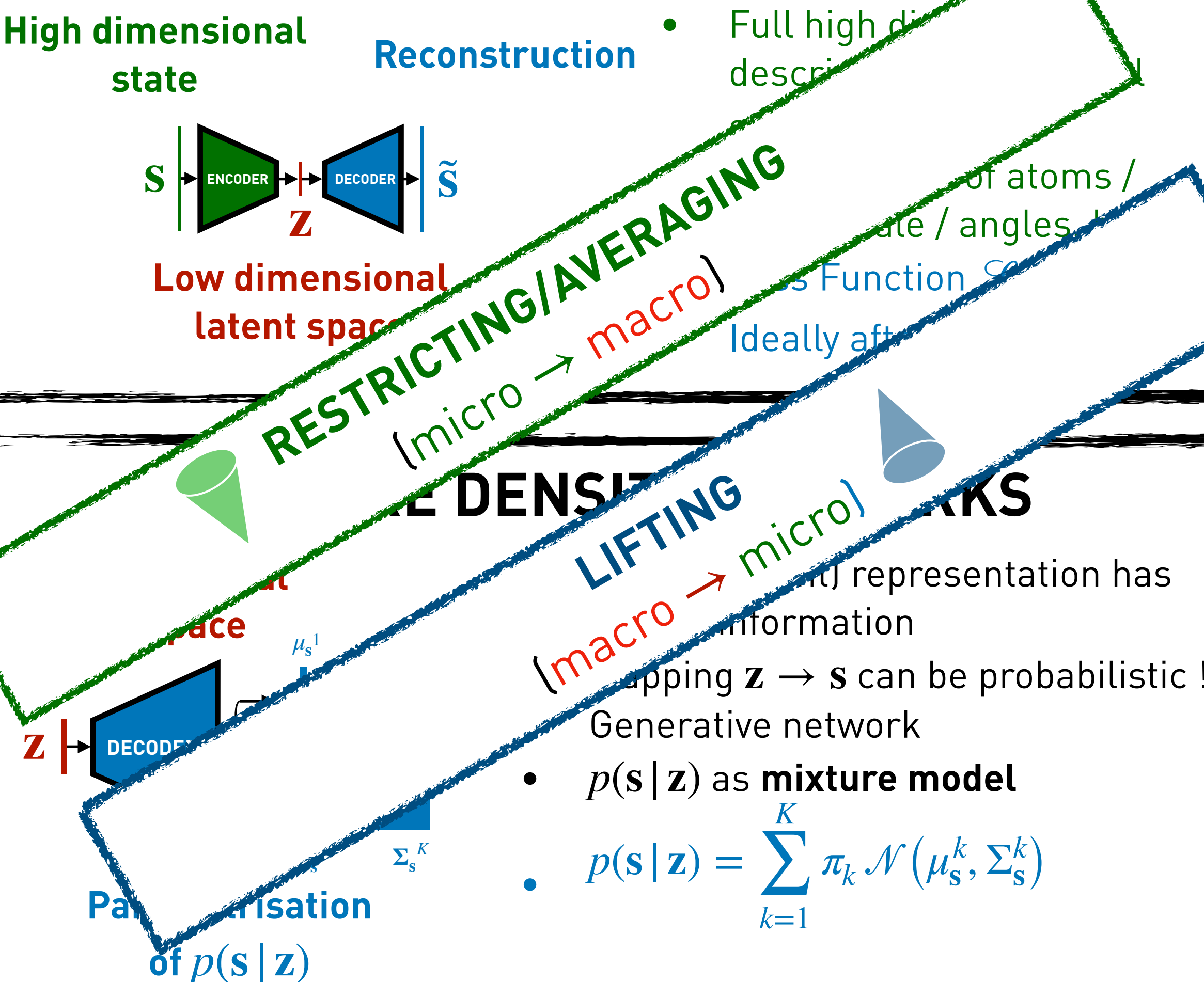


Long Short-Term Memory



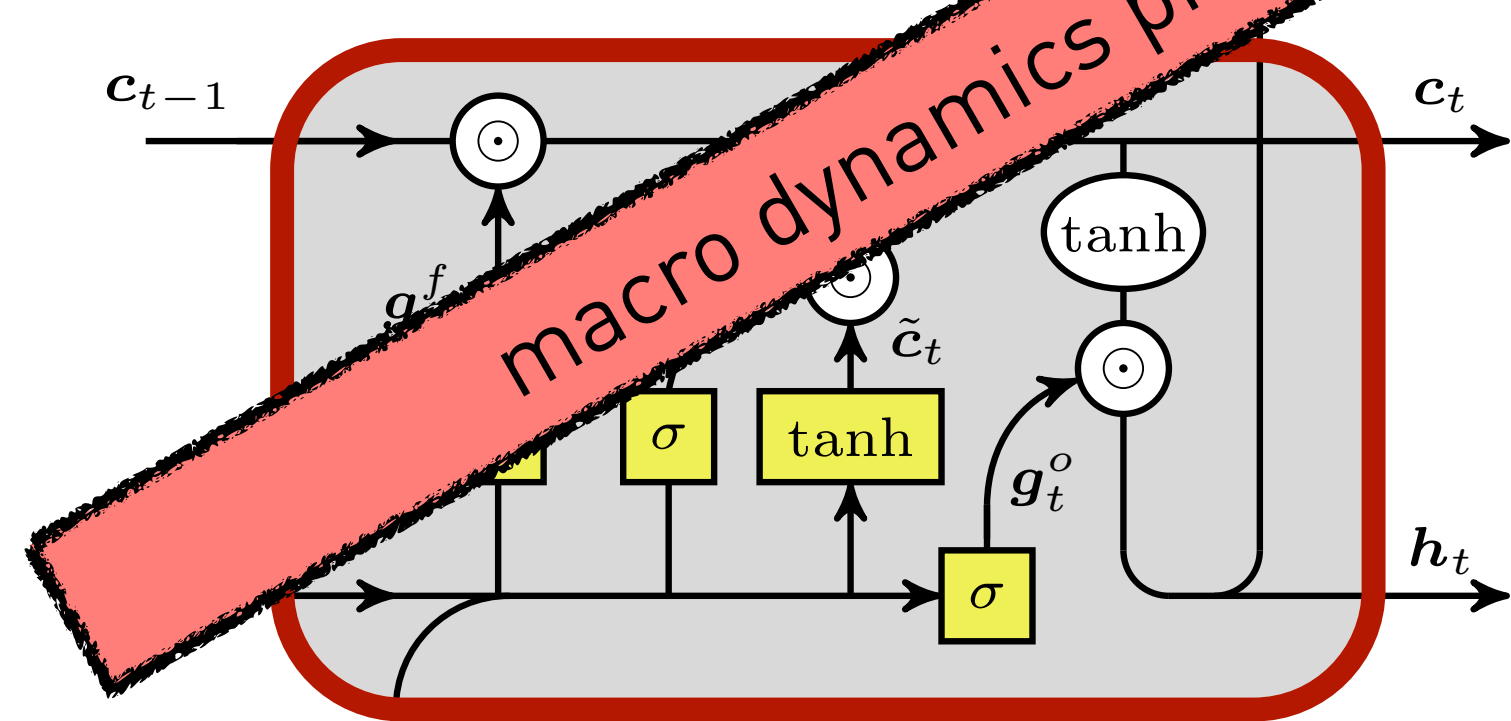
# Operators from Machine Learning

## (CONVOLUTIONAL) AUTOENCODERS



## RECURRENT NEURAL NETWORKS

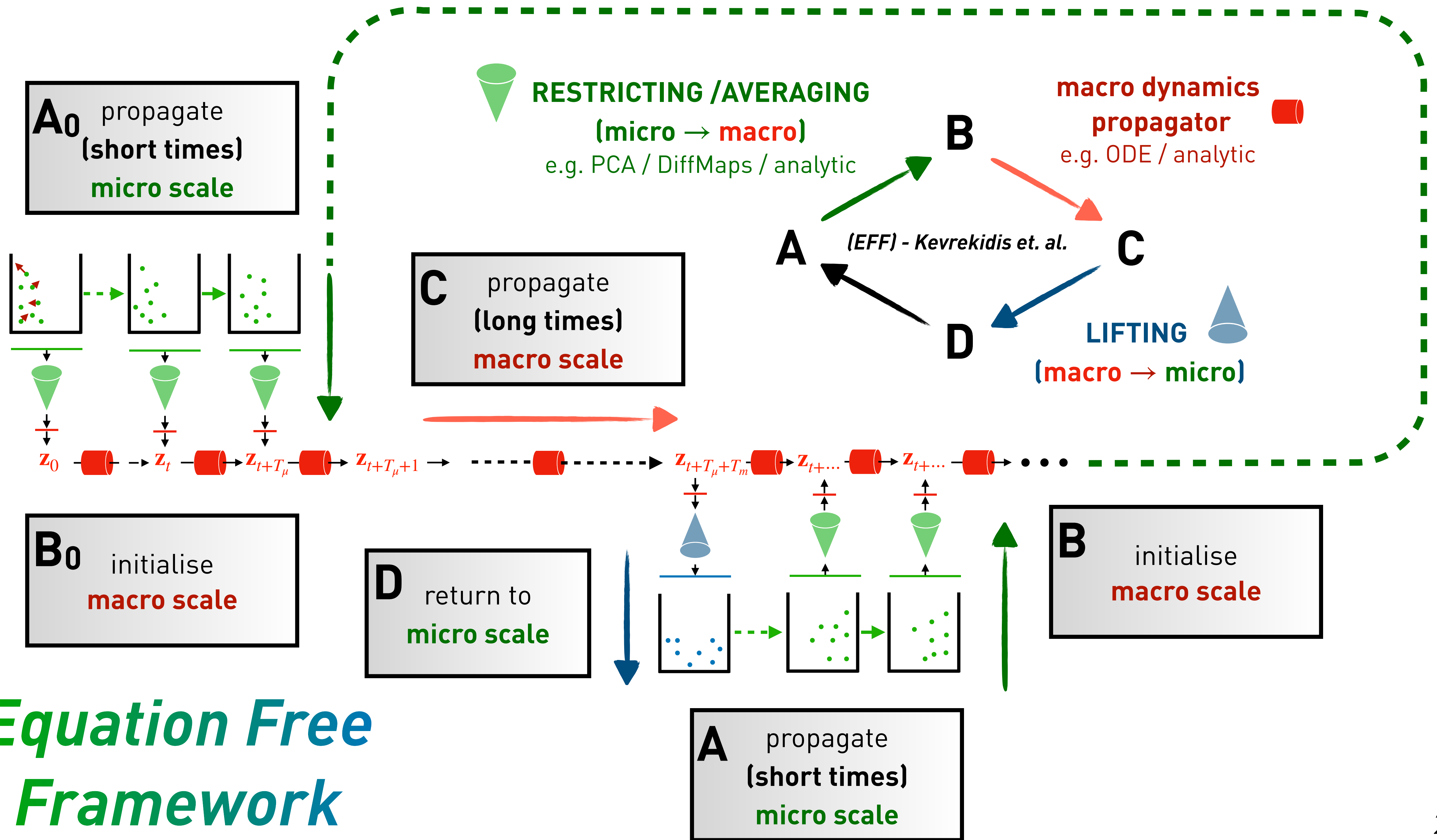
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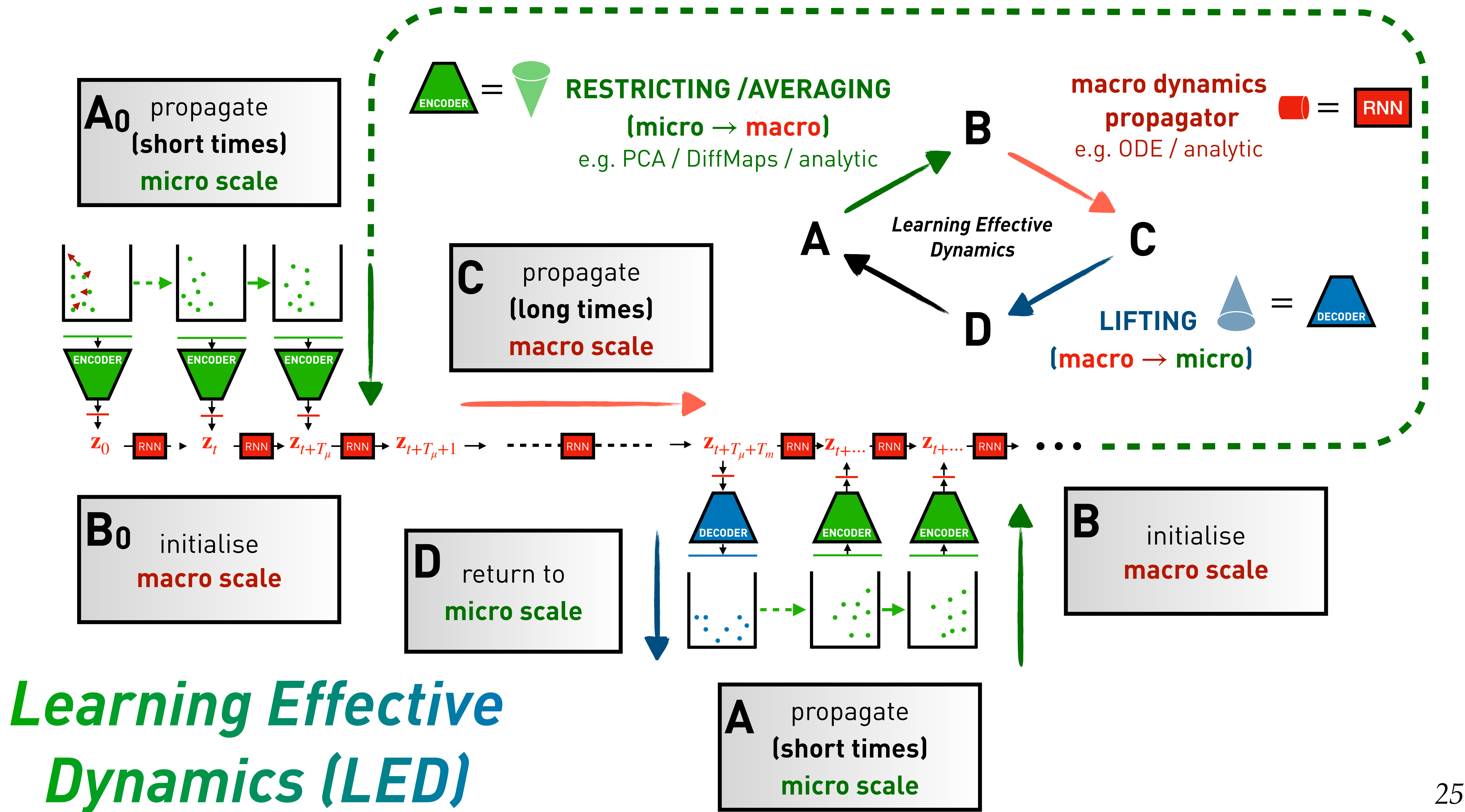
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# Equation Free Framework



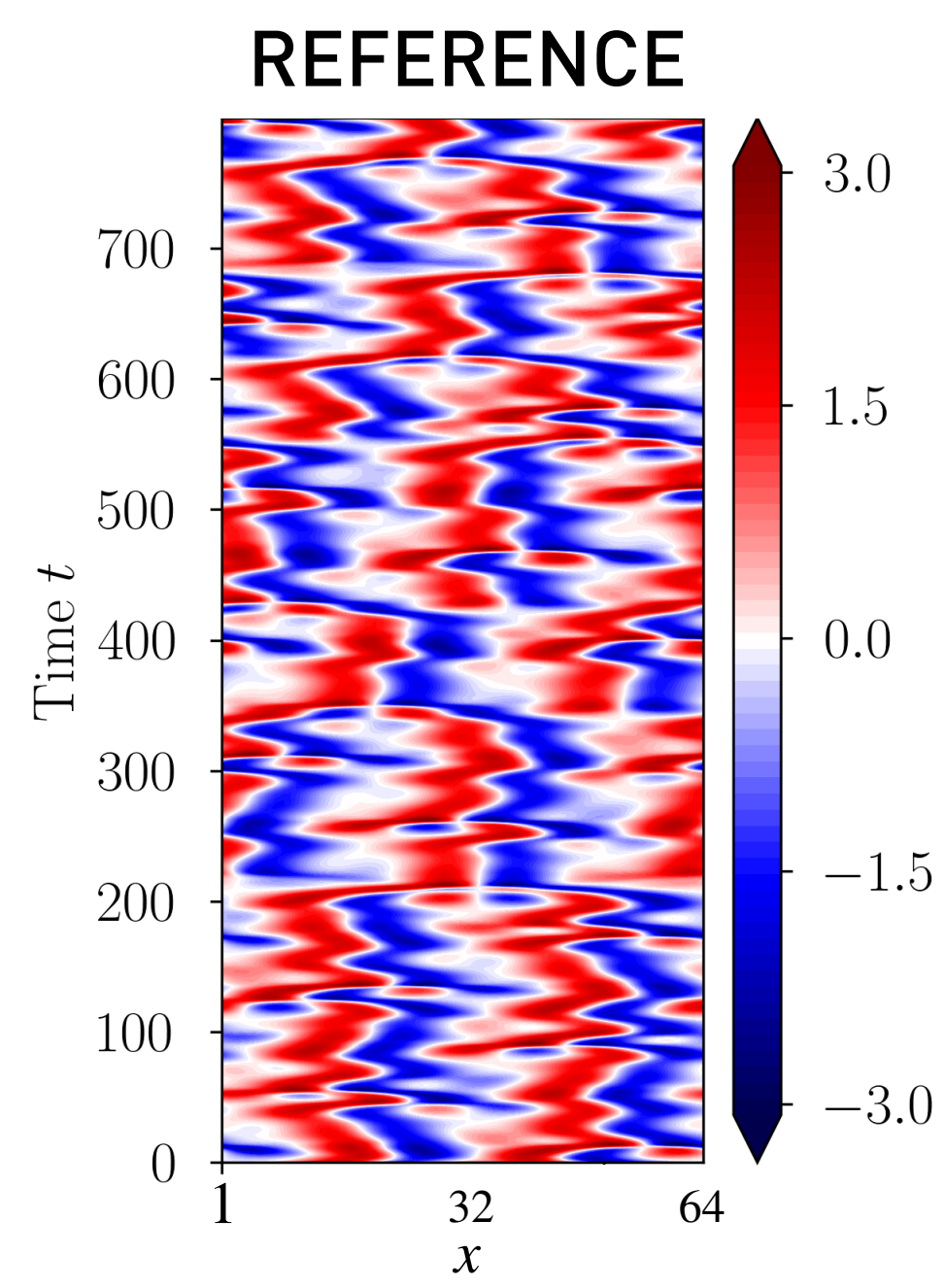






# Kuramoto-Sivashinsky ( $\tilde{L} \approx 3.5$ )

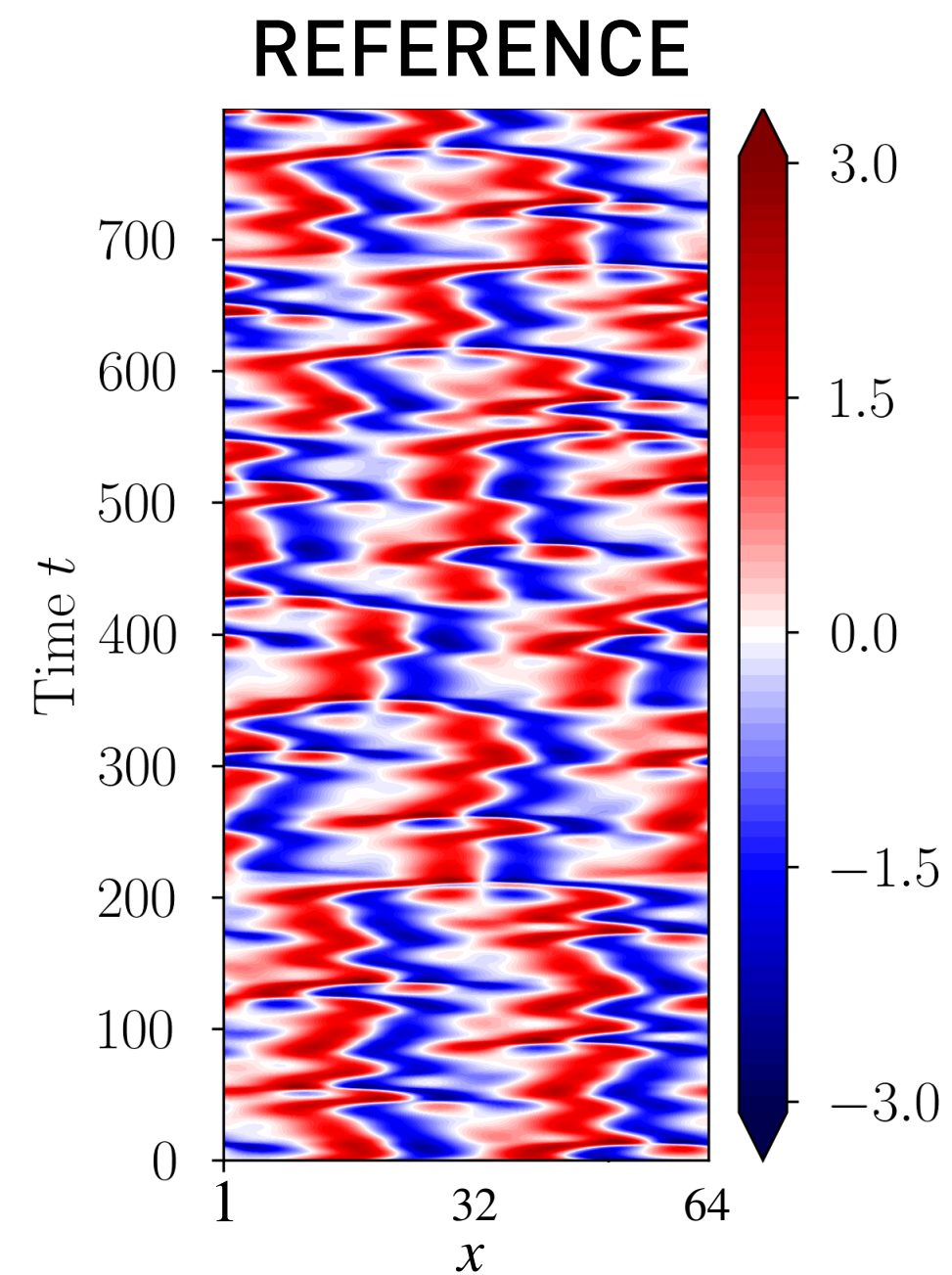
PR Vlachas, G Arampatzis, C Uhler, P Koumoutsakos,  
*Multiscale Simulations of Complex Systems*  
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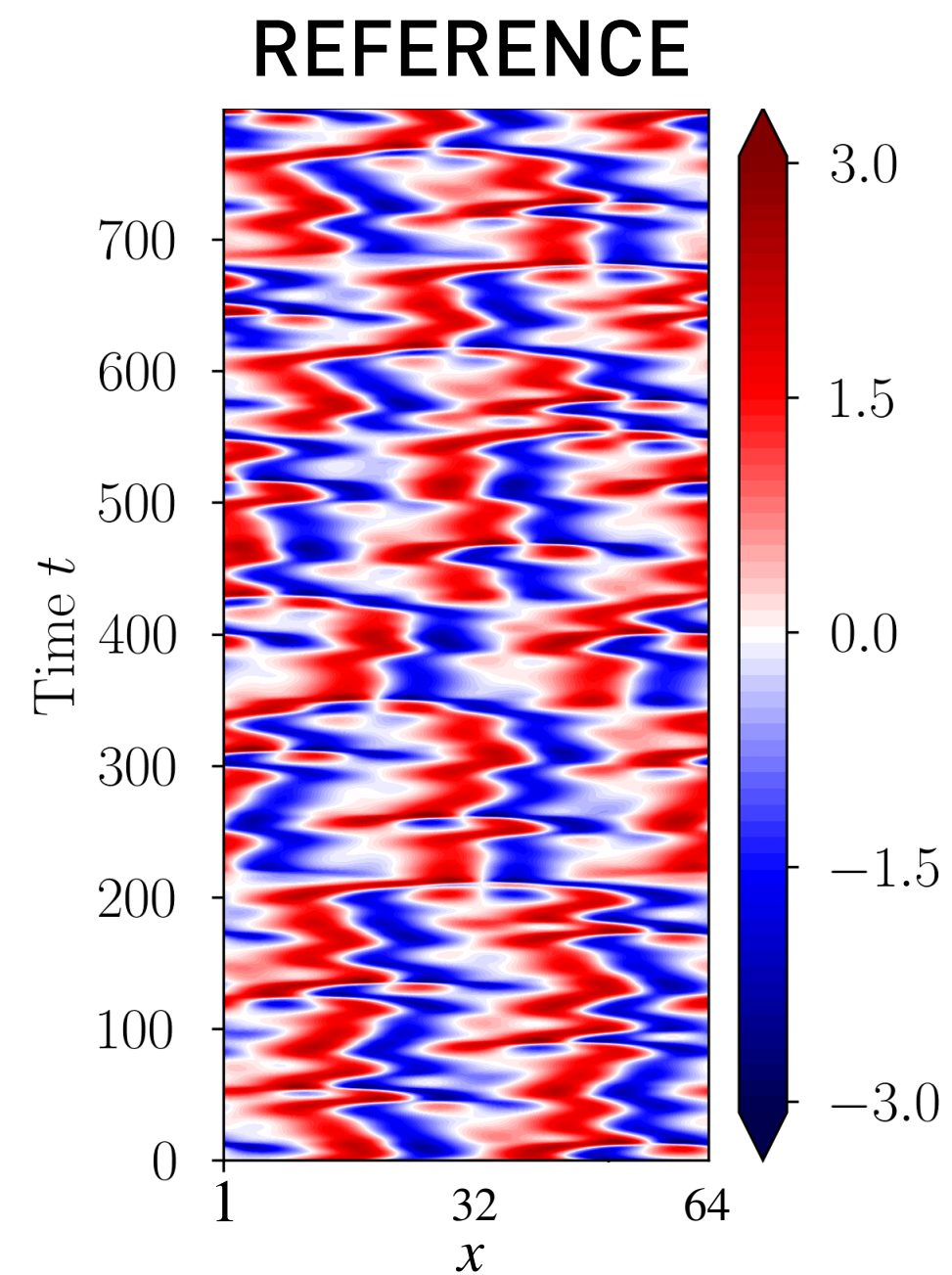
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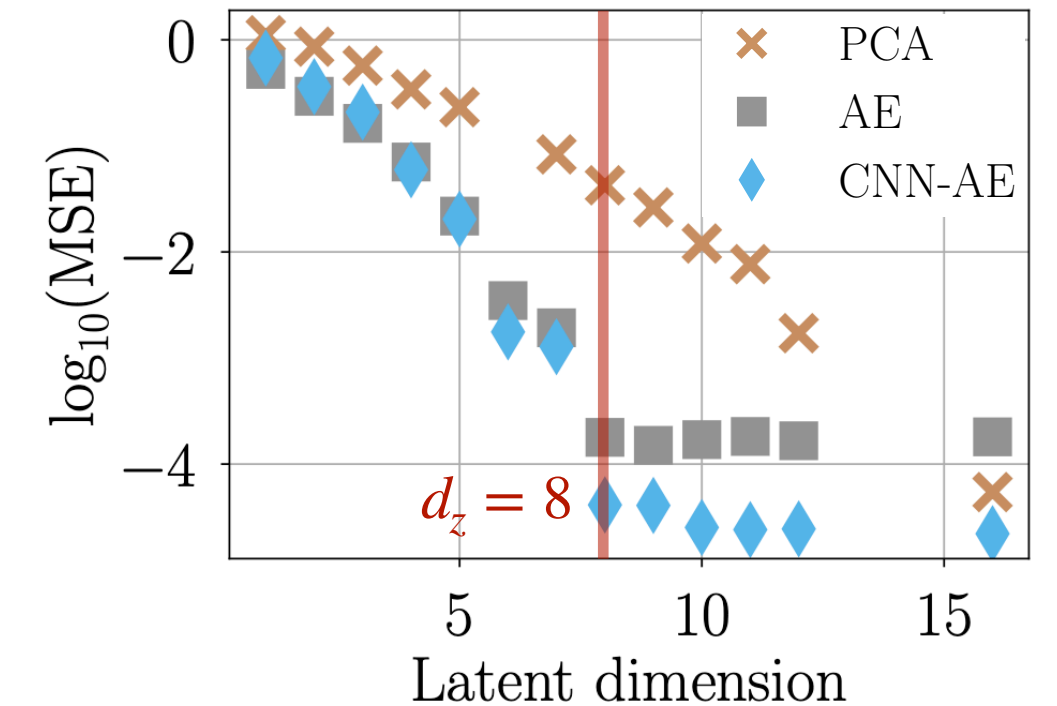
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**The AE error saturates after  $d_z = 8$**



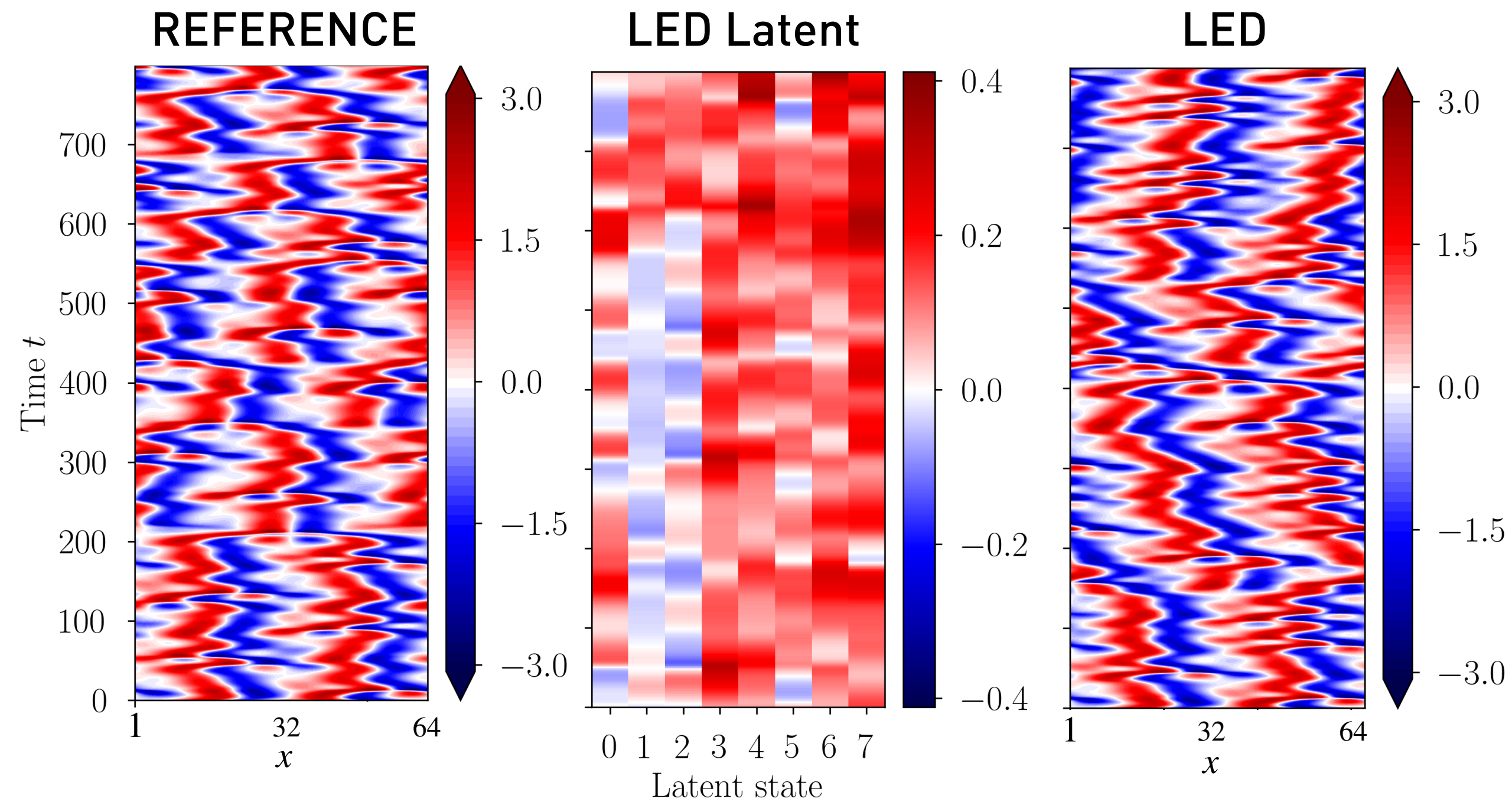
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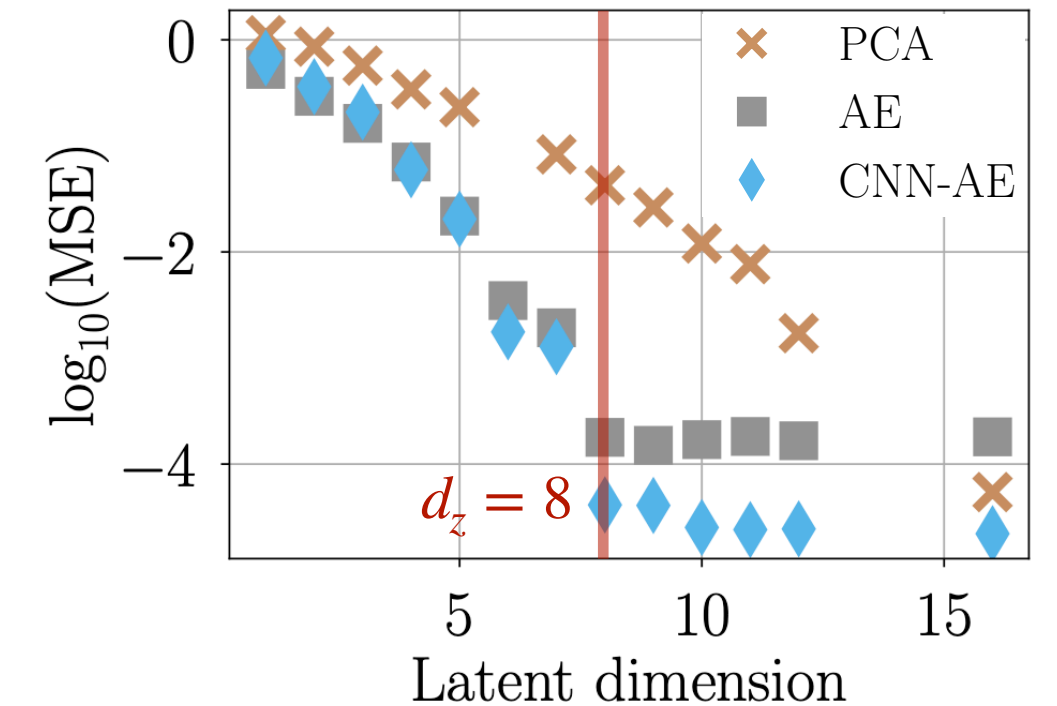
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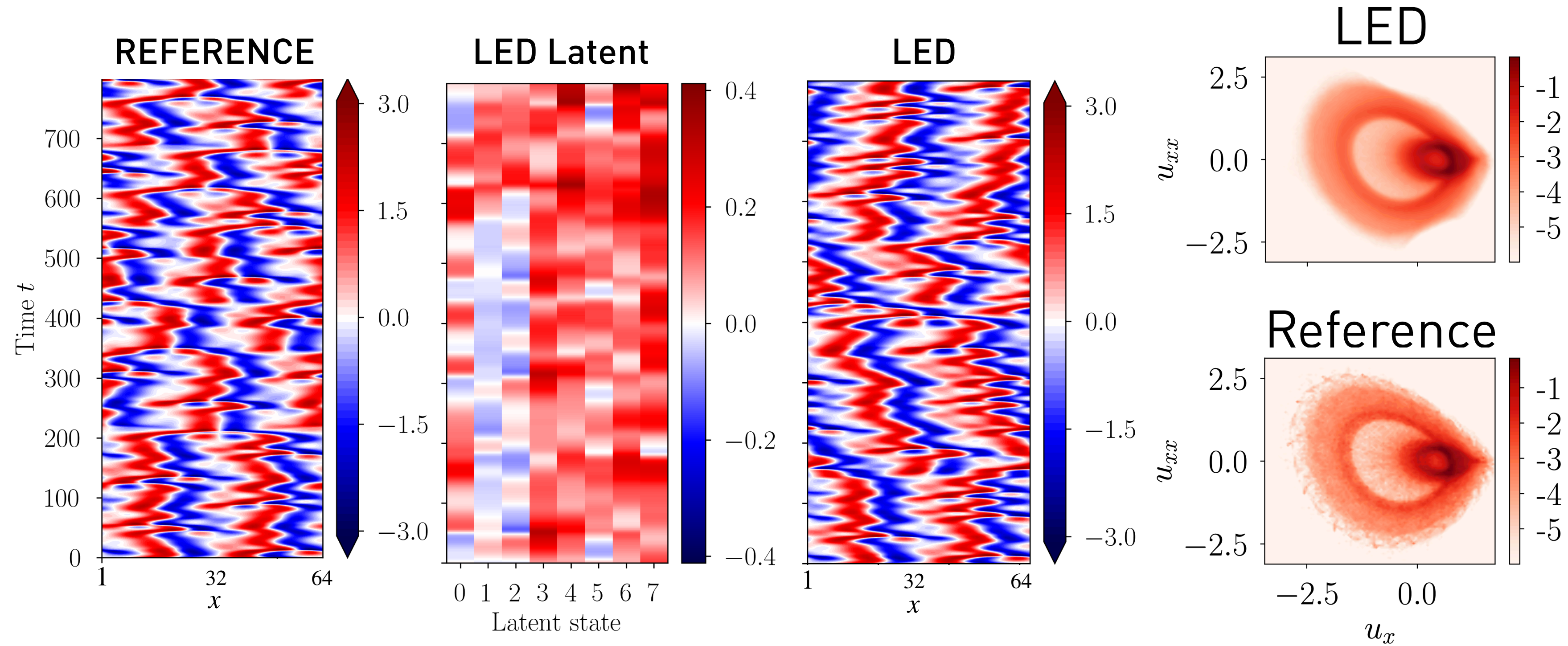
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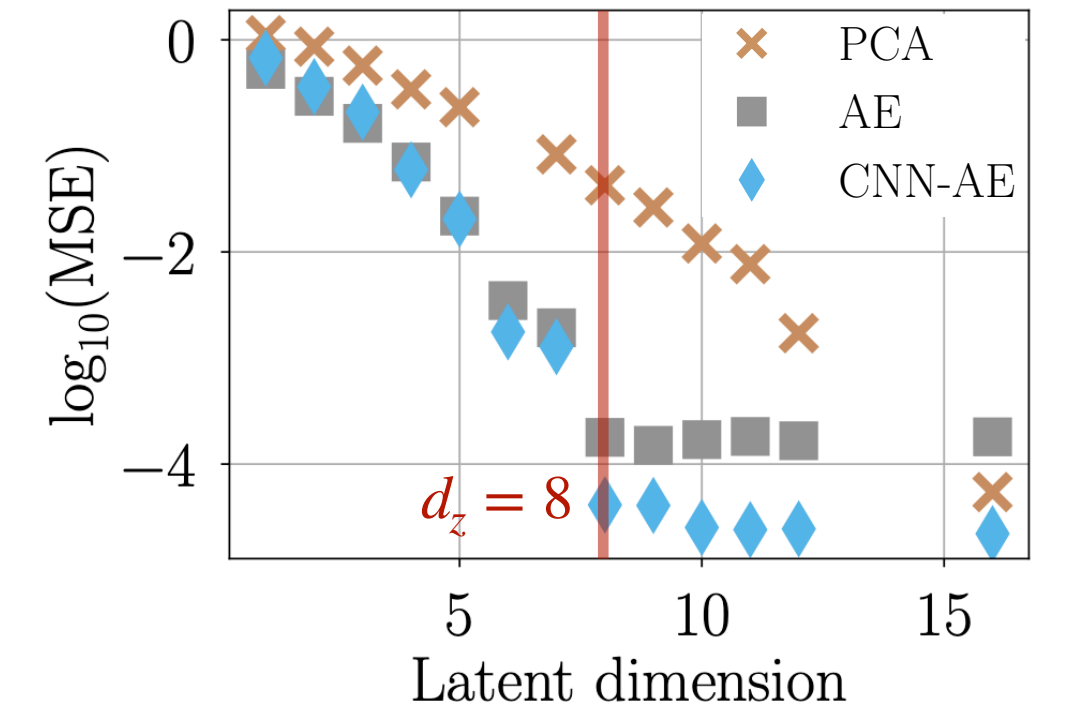
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- Reproducing the **statistics/long-term climate** accurately

The AE error saturates after  $d_z = 8$



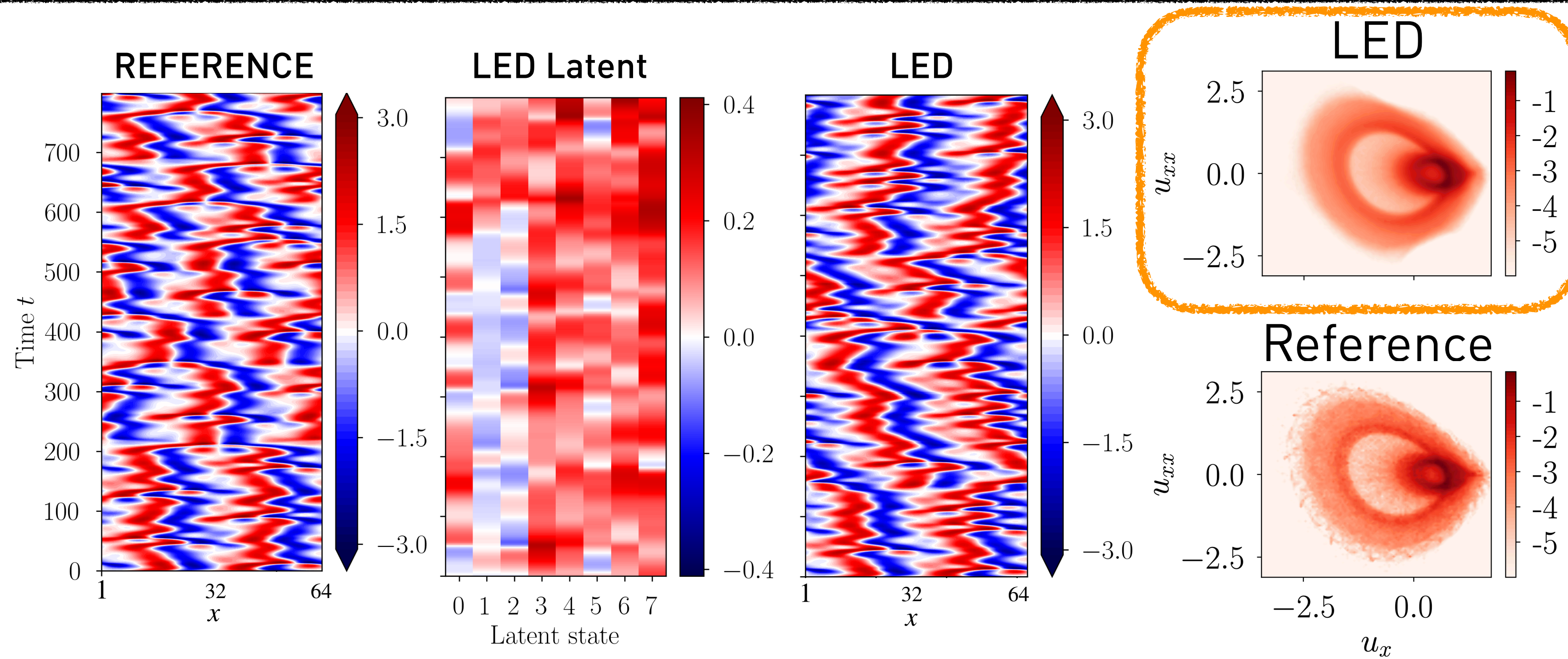
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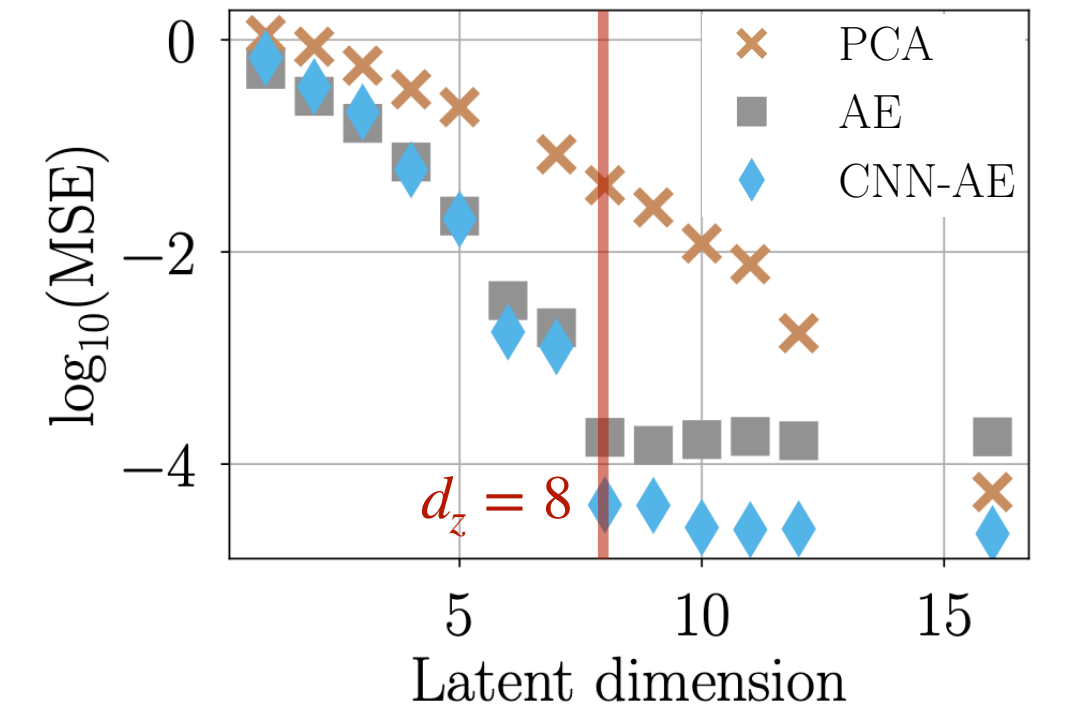
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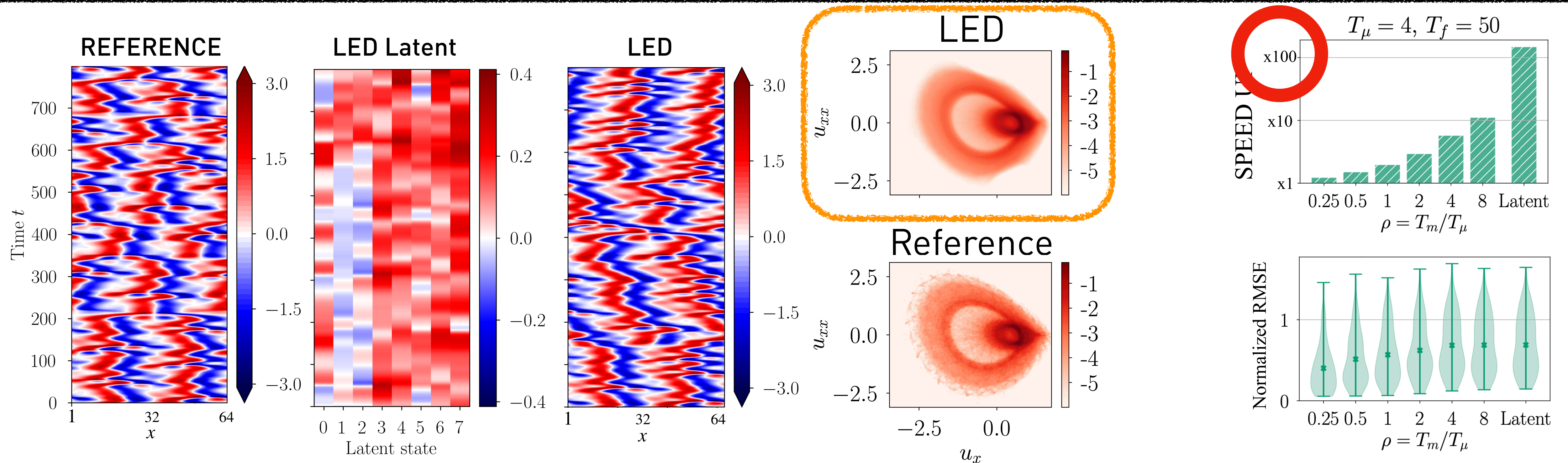
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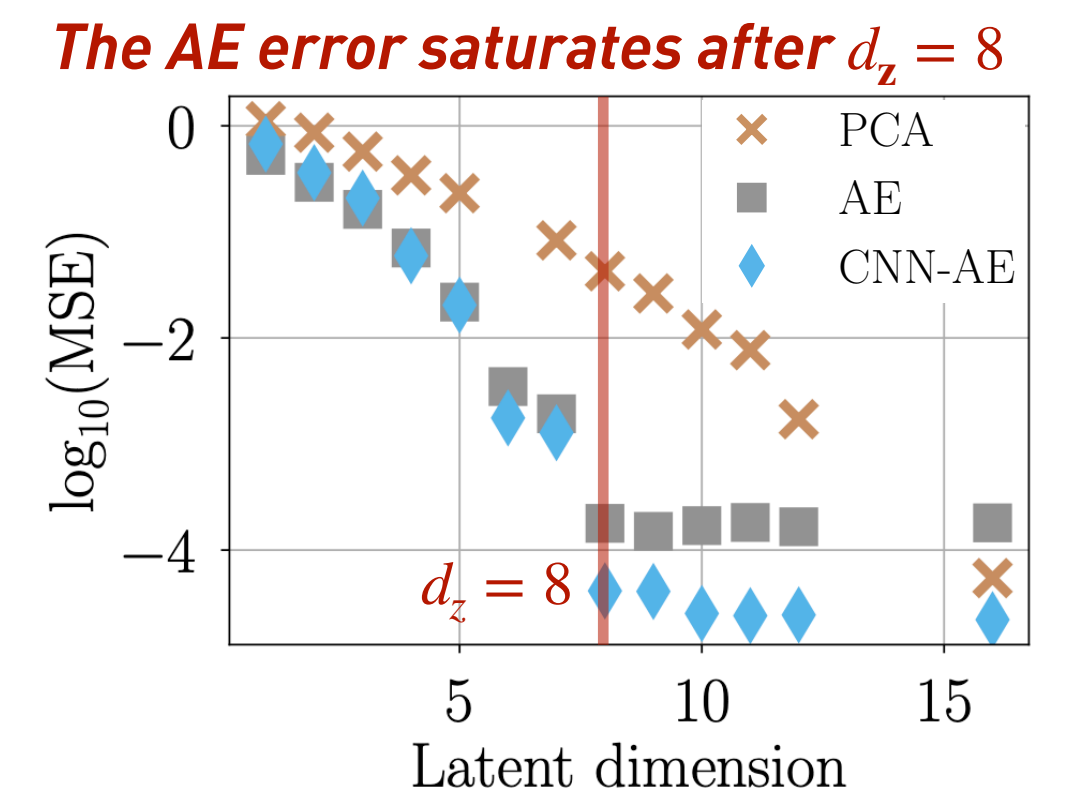


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- LED can identify and **reconstruct the dynamics** on an **8 dimensional** manifold
- Reproducing the **statistics/long-term climate** accurately
- **Two orders** of magnitude faster compared to the stiff ODE solver used



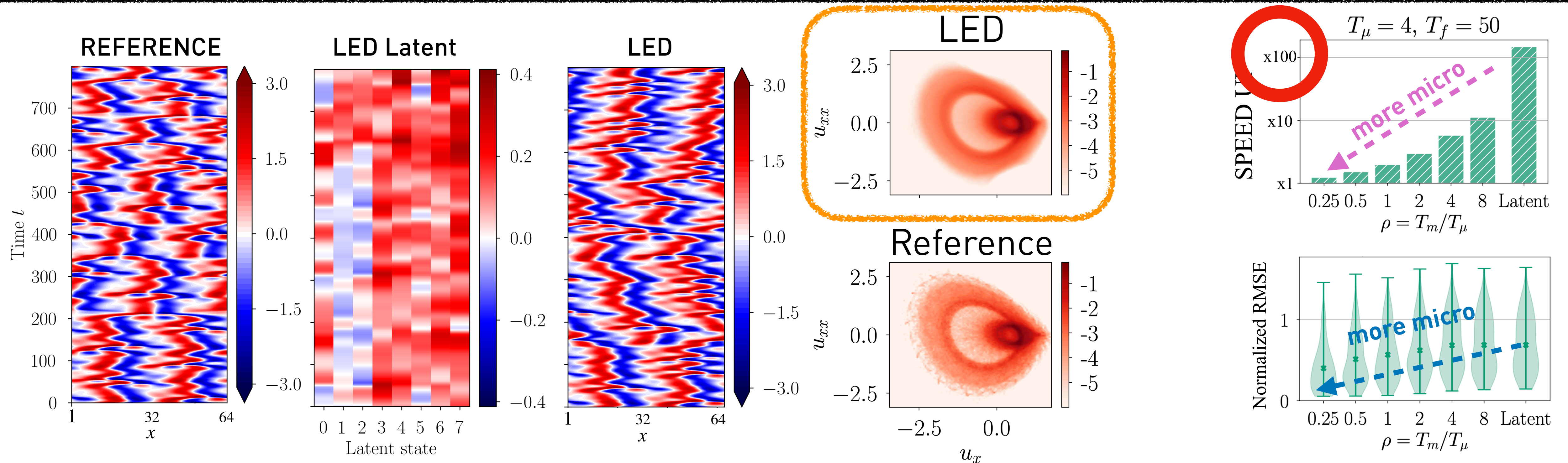
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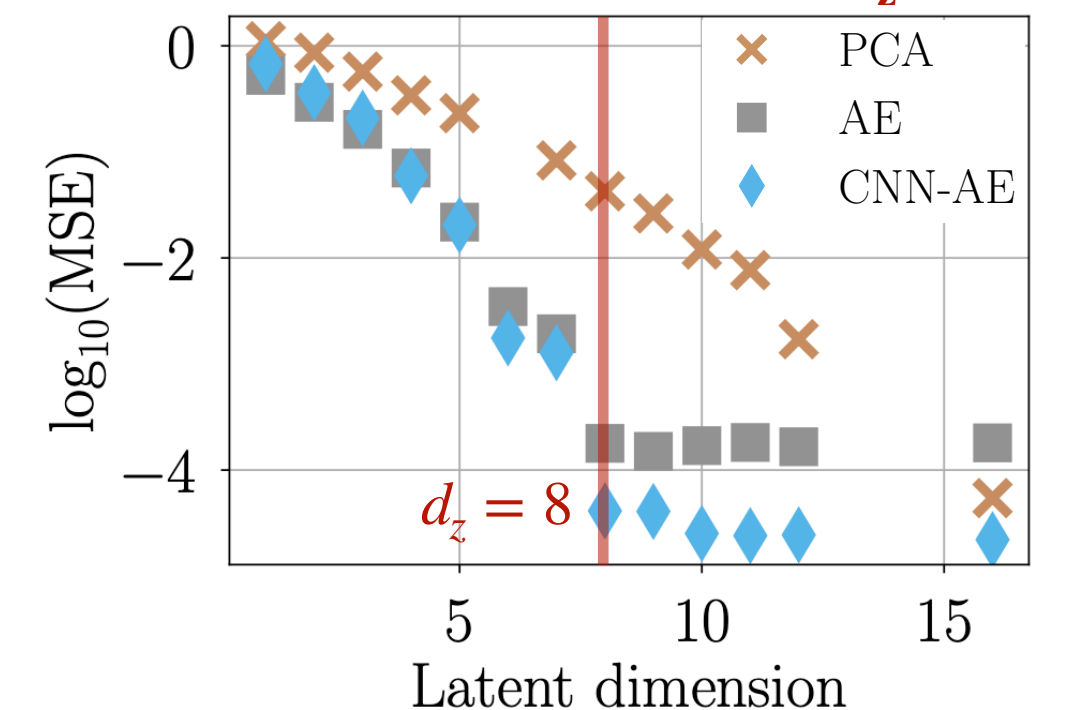
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- Reproducing the **statistics/long-term climate** accurately
- **Two orders** of magnitude faster compared to the stiff ODE solver used
- LED: Control the tradeoff between **approximation error** and **speed-up**

**The AE error saturates after  $d_z = 8$**



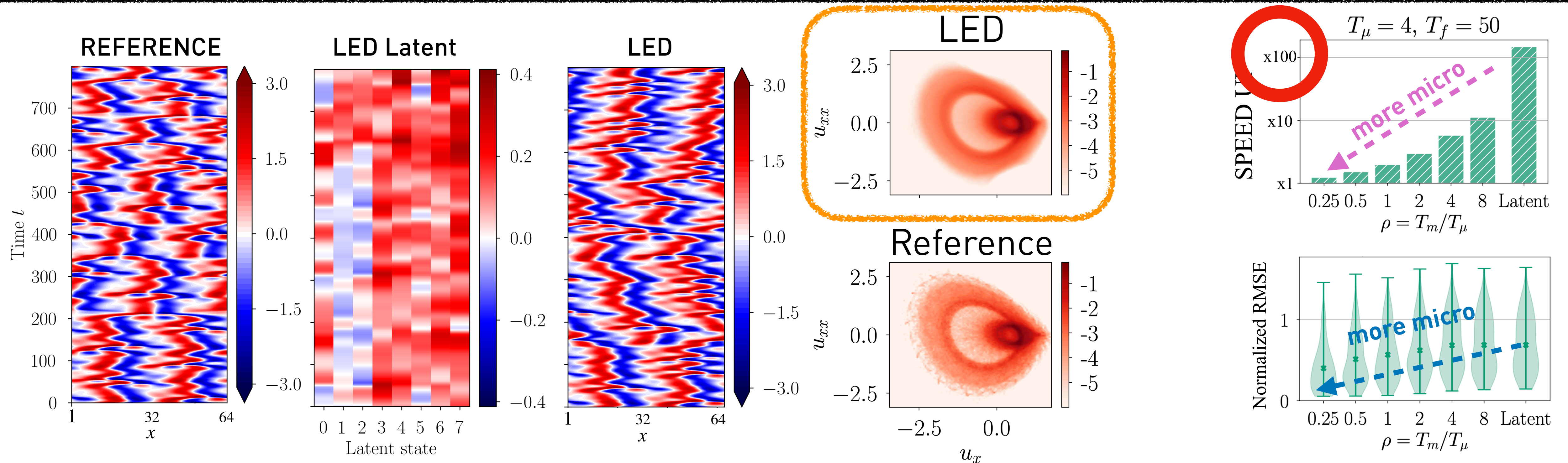
[1] Robinson, J. C. "Inertial manifolds for the kuramoto-sivashinsky equation." *Physics Letters A* **184**, 190–193 (1994).

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

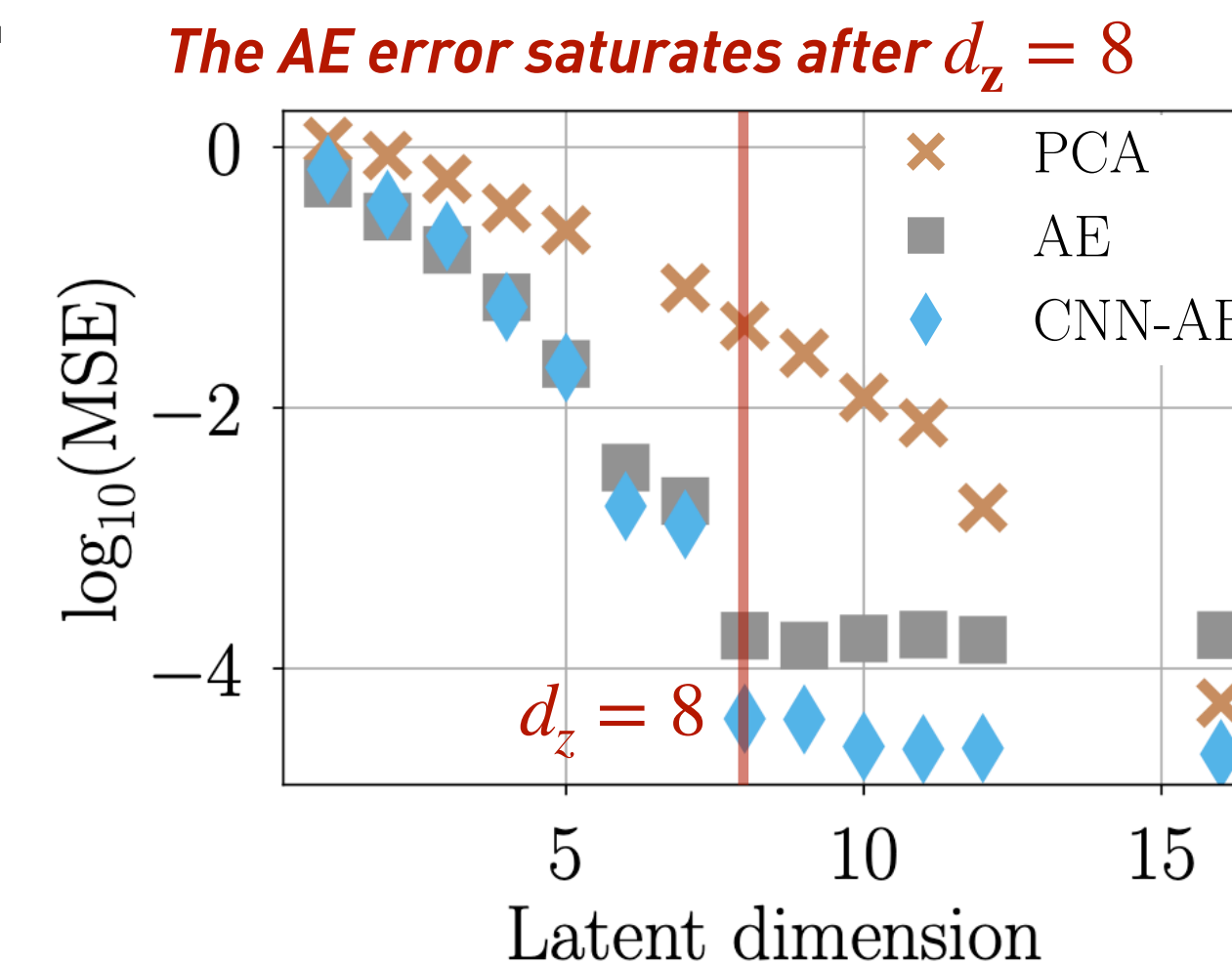


# Kuramoto-Sivashinsky ( $\tilde{L} \approx 3.5$ )

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



- For  $L = 22$ ,  $\nu = 1$ , and periodic boundaries **effective dynamics lie on an 8 dimensional manifold [1, 2]** but learning a **propagator** of these dynamics is difficult
- LED can identify and **reconstruct the dynamics** on an **8 dimensional** manifold
- Reproducing the **statistics/long-term climate** accurately
- **Two orders** of magnitude faster compared to the stiff ODE solver used
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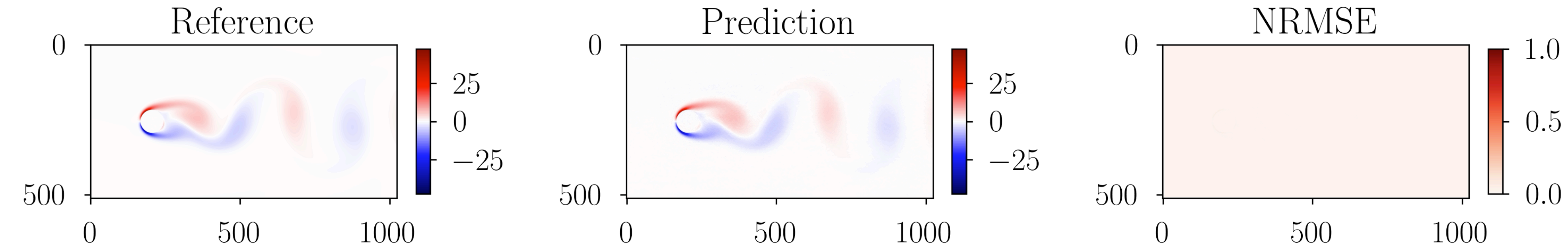
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# Cylinder at $Re = 100$ - (LED $d_z = 4$ )

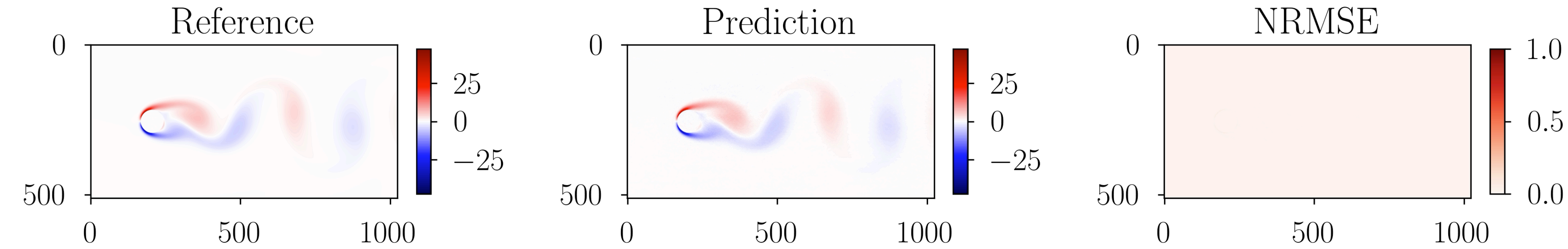
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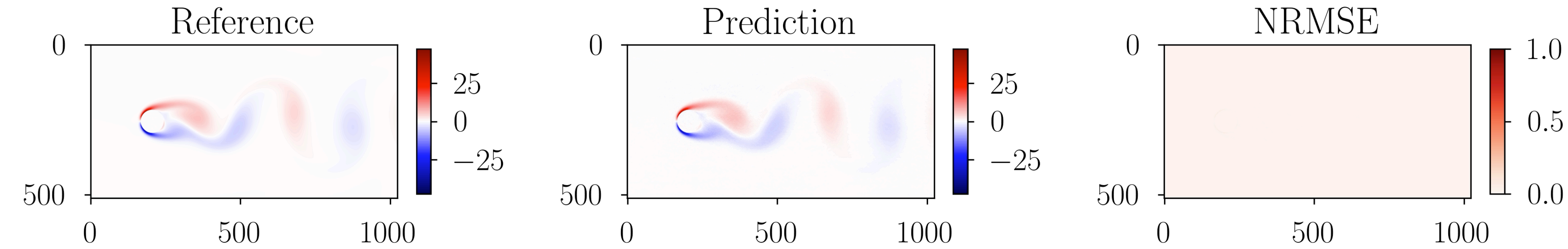


- Micro solver: Finite Differences (CubimUP2D) employing 12 cores



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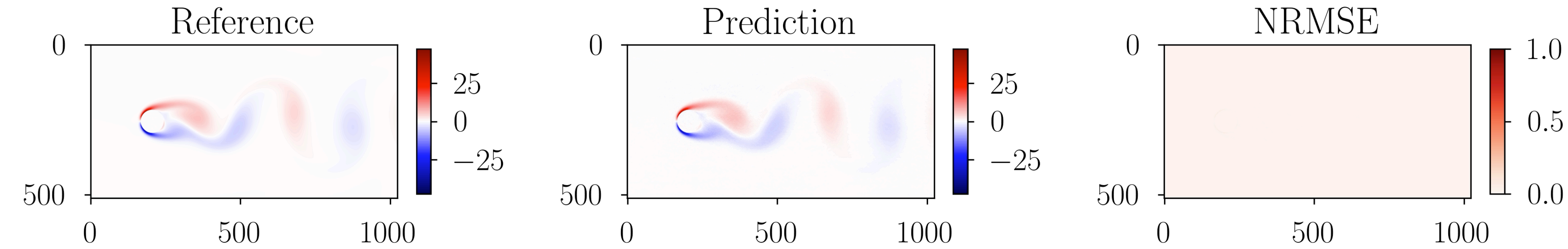


- Micro solver: Finite Differences (CubimUP2D) employing 12 cores
- State: velocity in x- and y- direction, pressure, and **vorticity**  $\mathbf{s}_t \in \mathbb{R}^{4 \times 512 \times 1024}$



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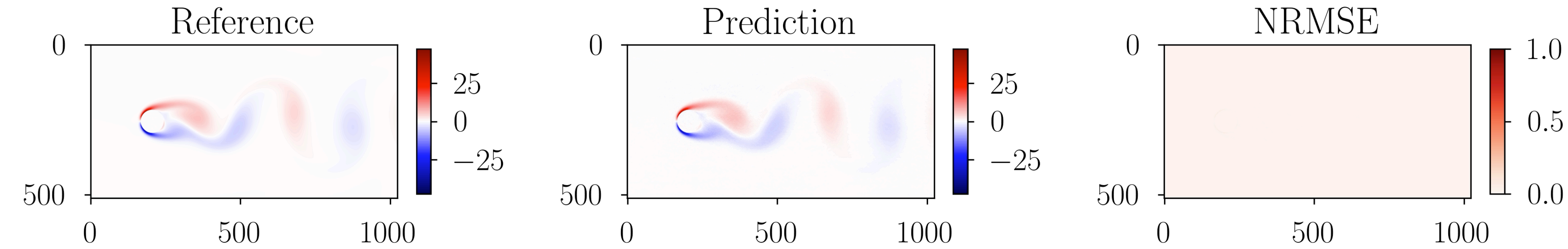
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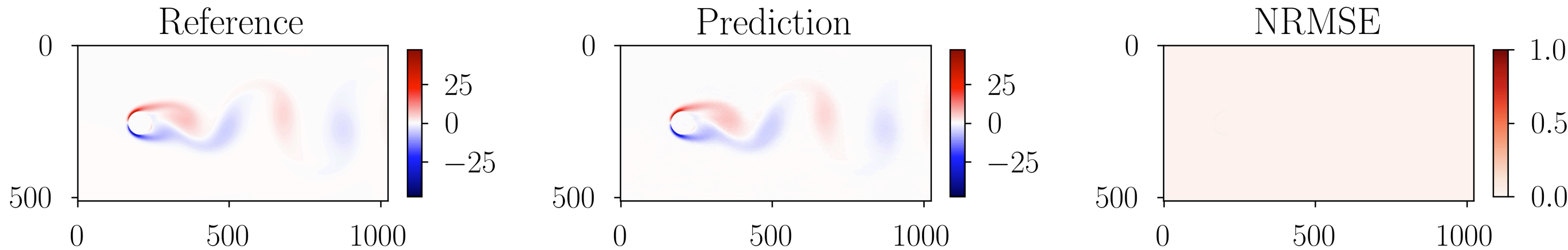
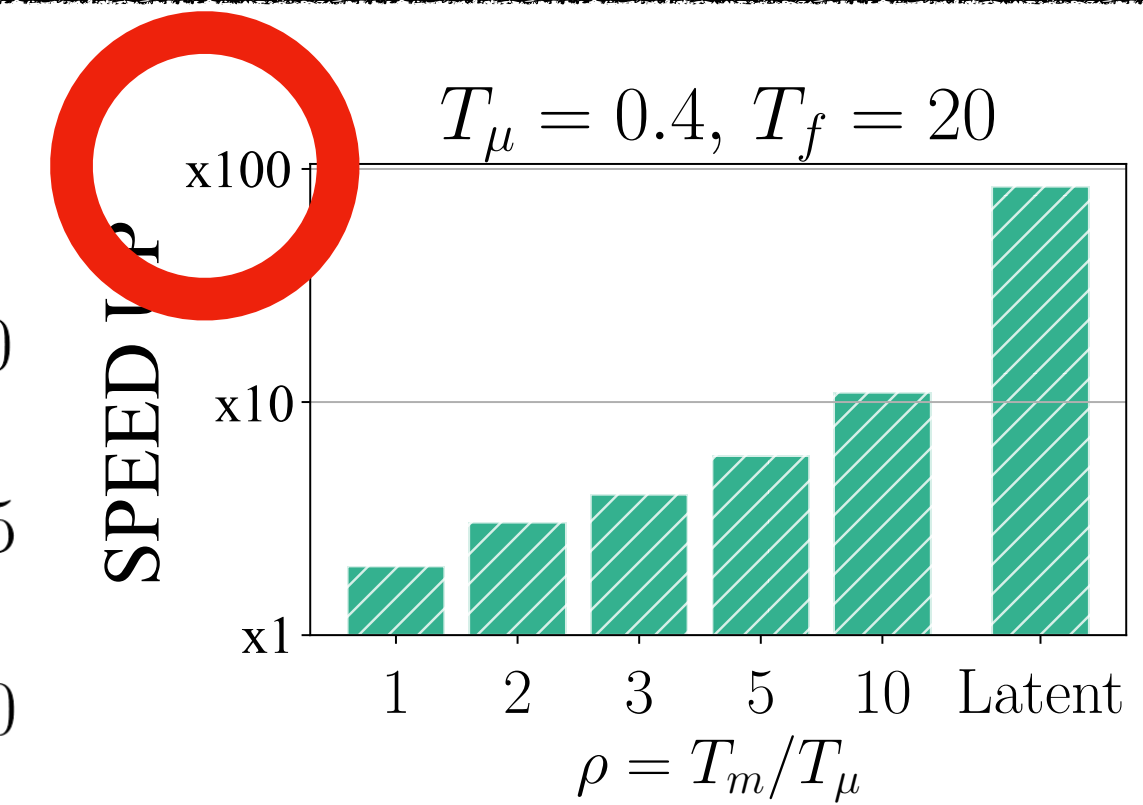
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- LED captures **long-term evolution** of velocity and pressure fields (low NRMSE)



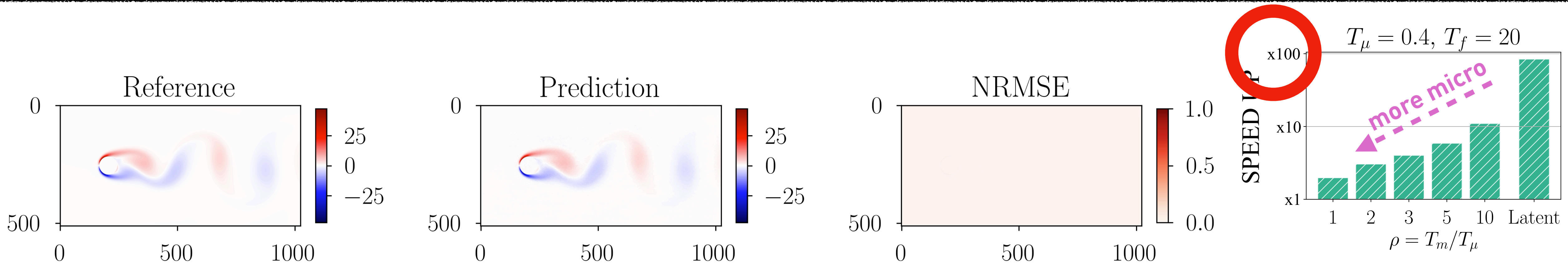
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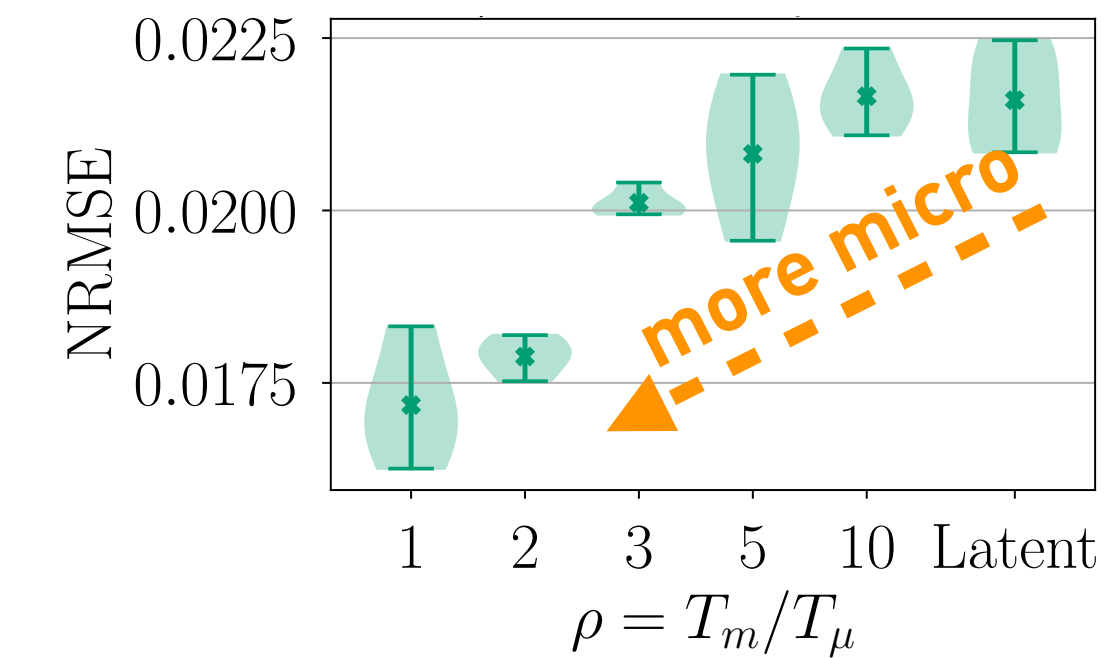
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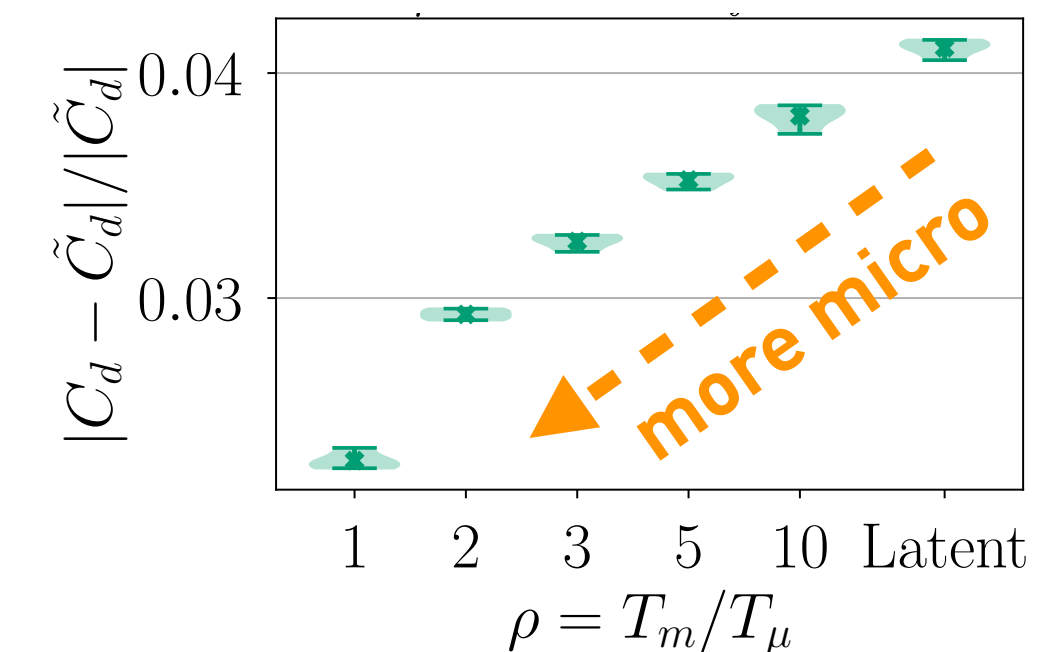
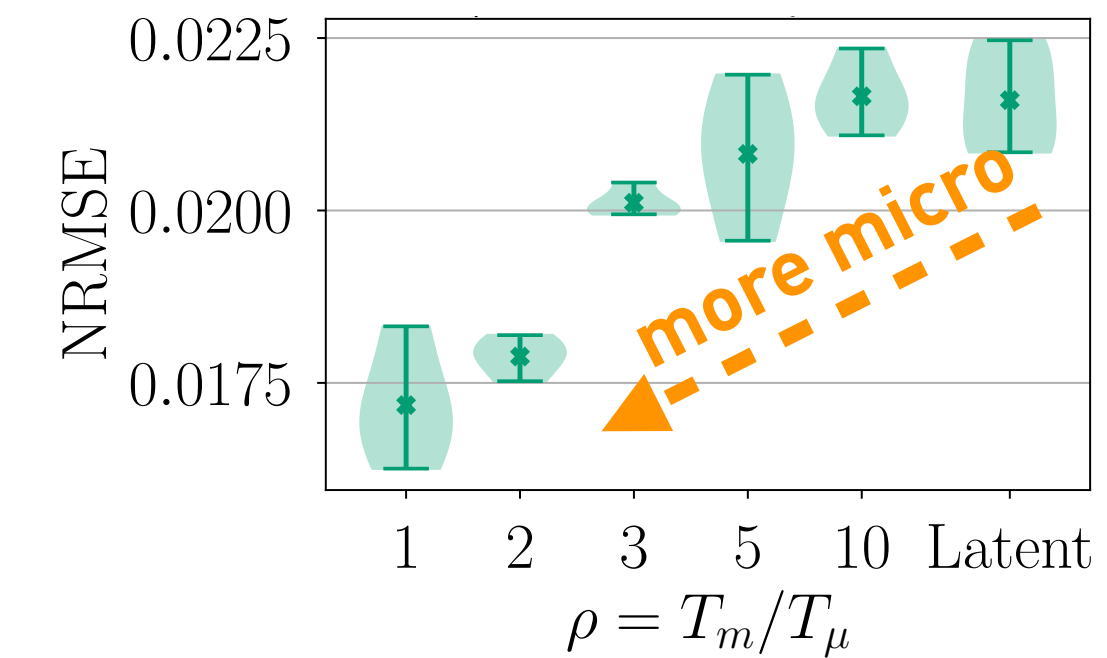
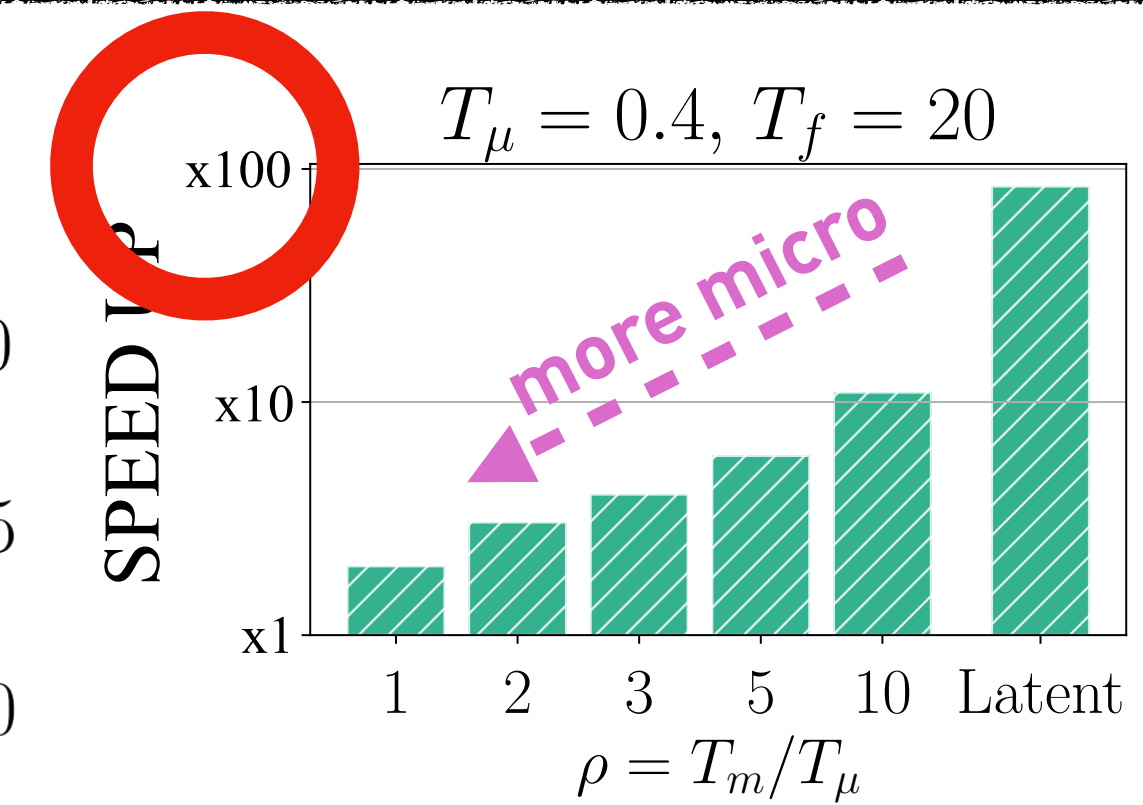
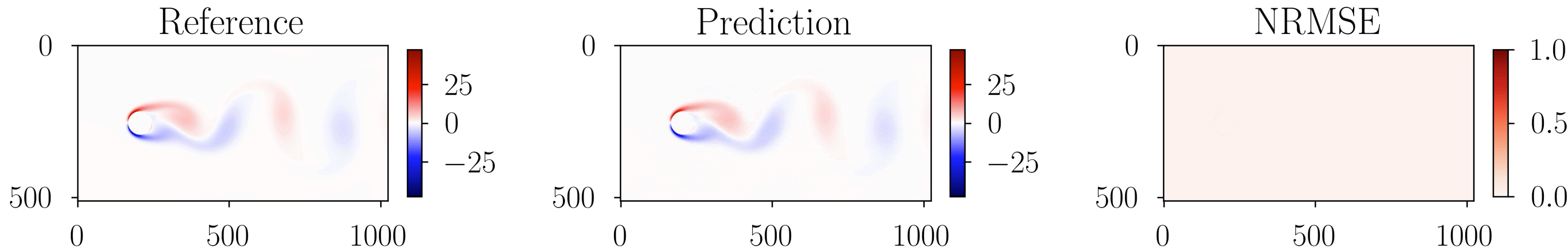


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# Cylinder at $Re = 100$ - (LED $d_z = 4$ )

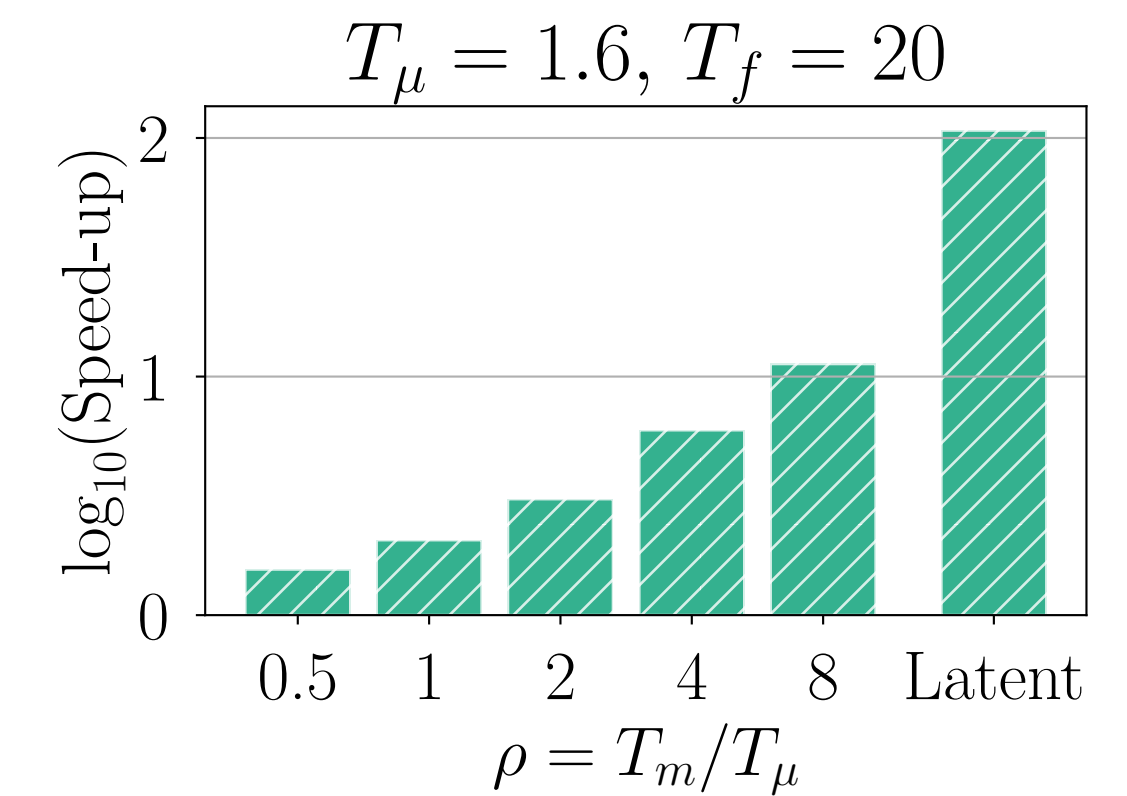
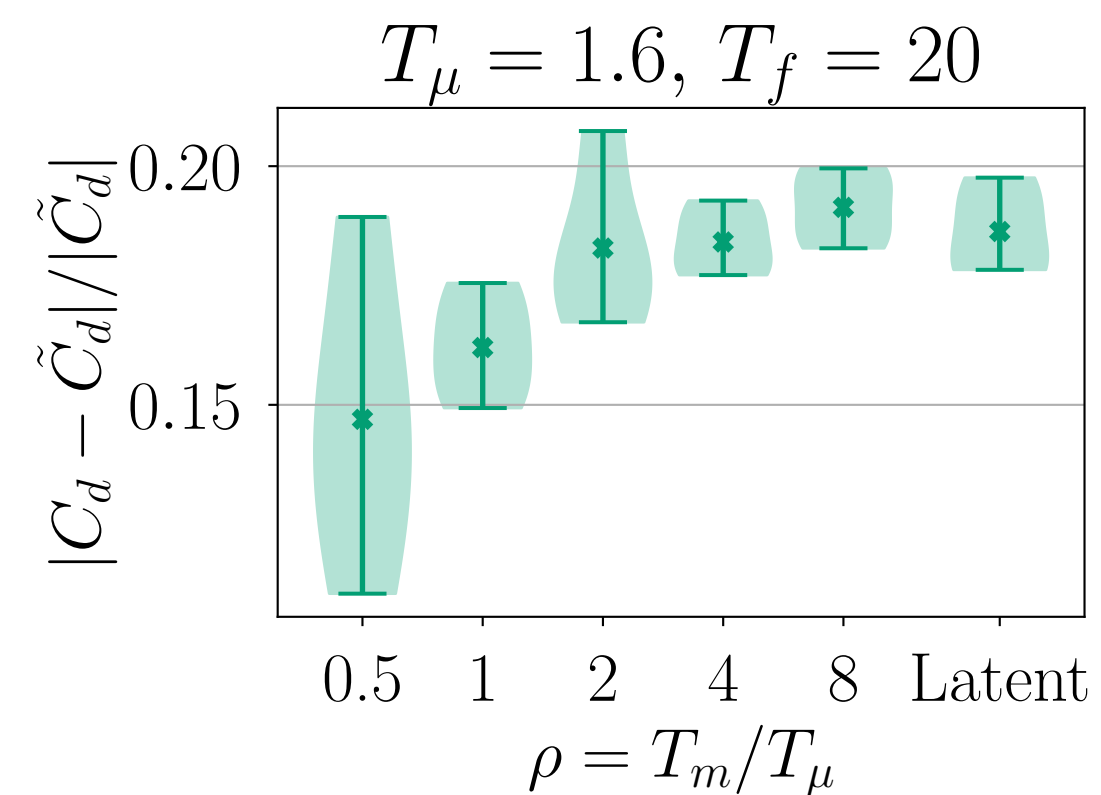
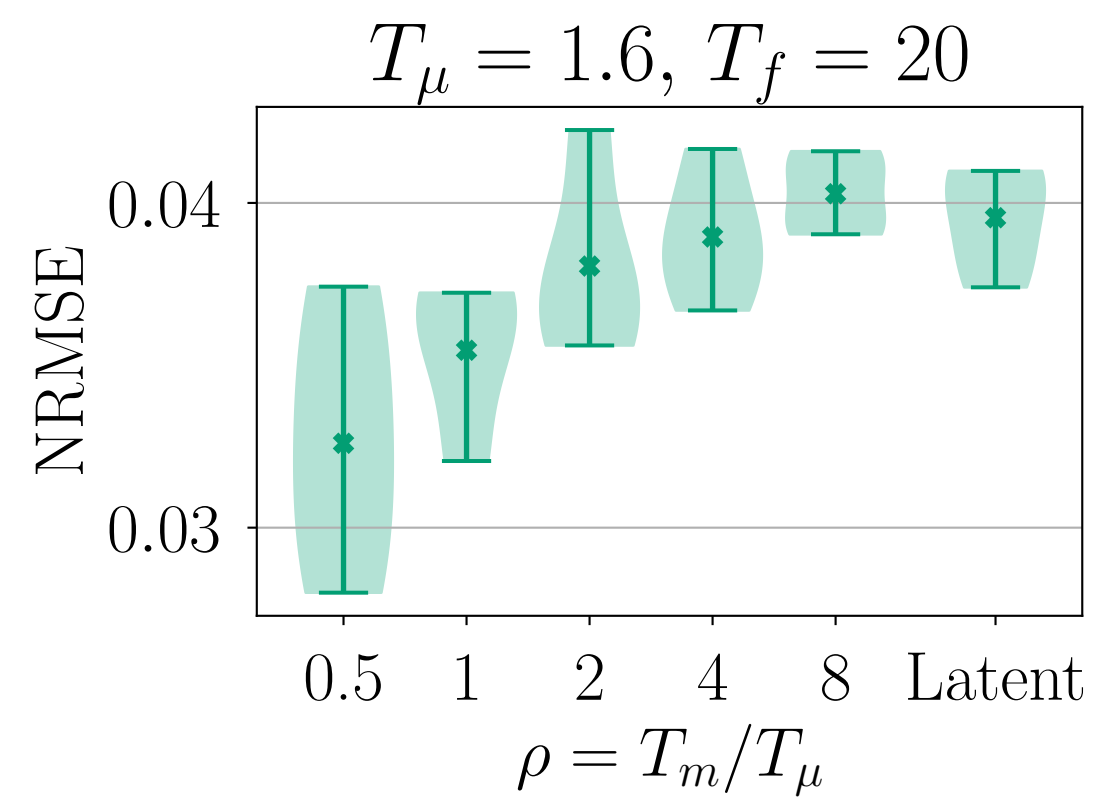
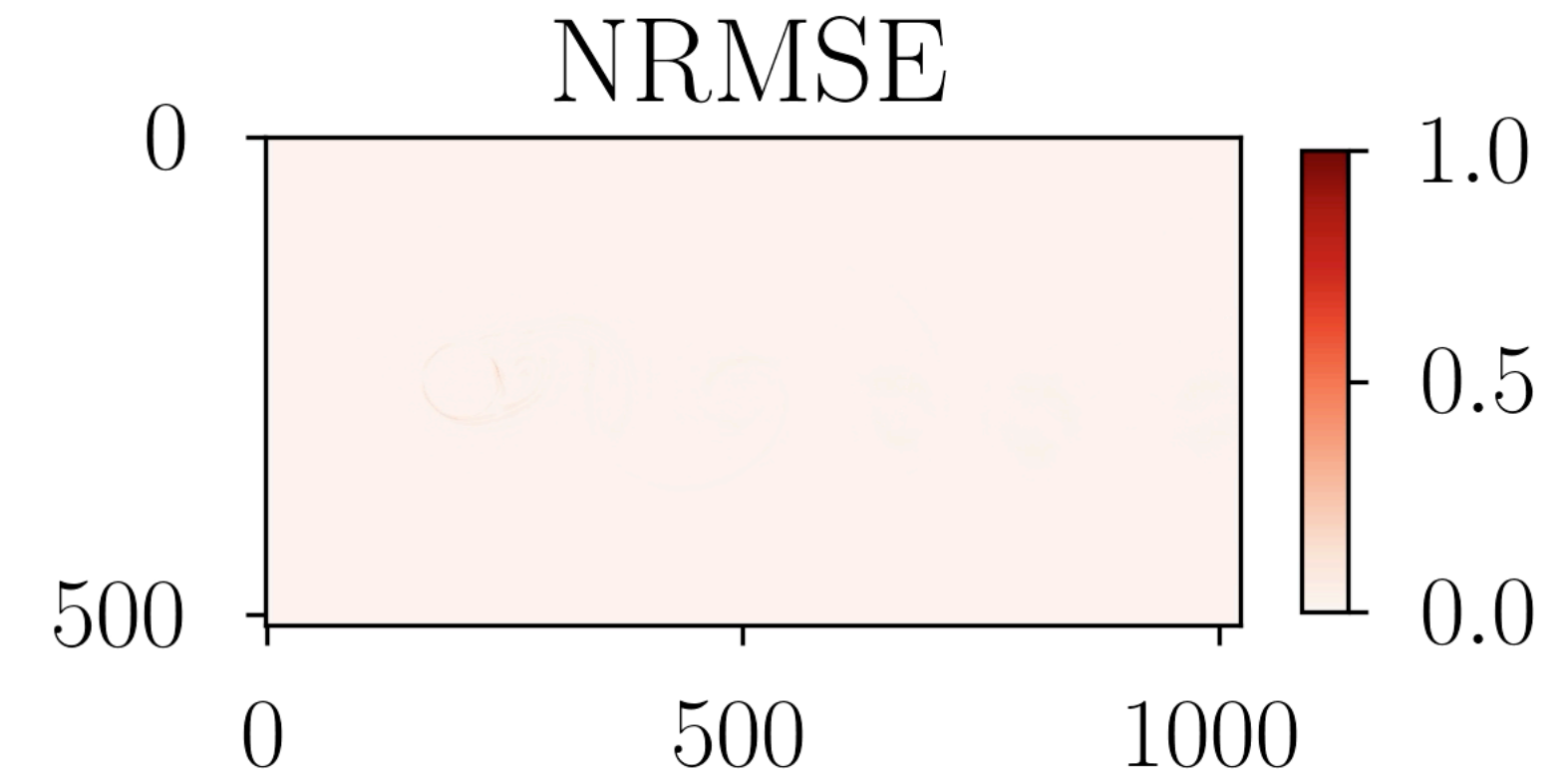
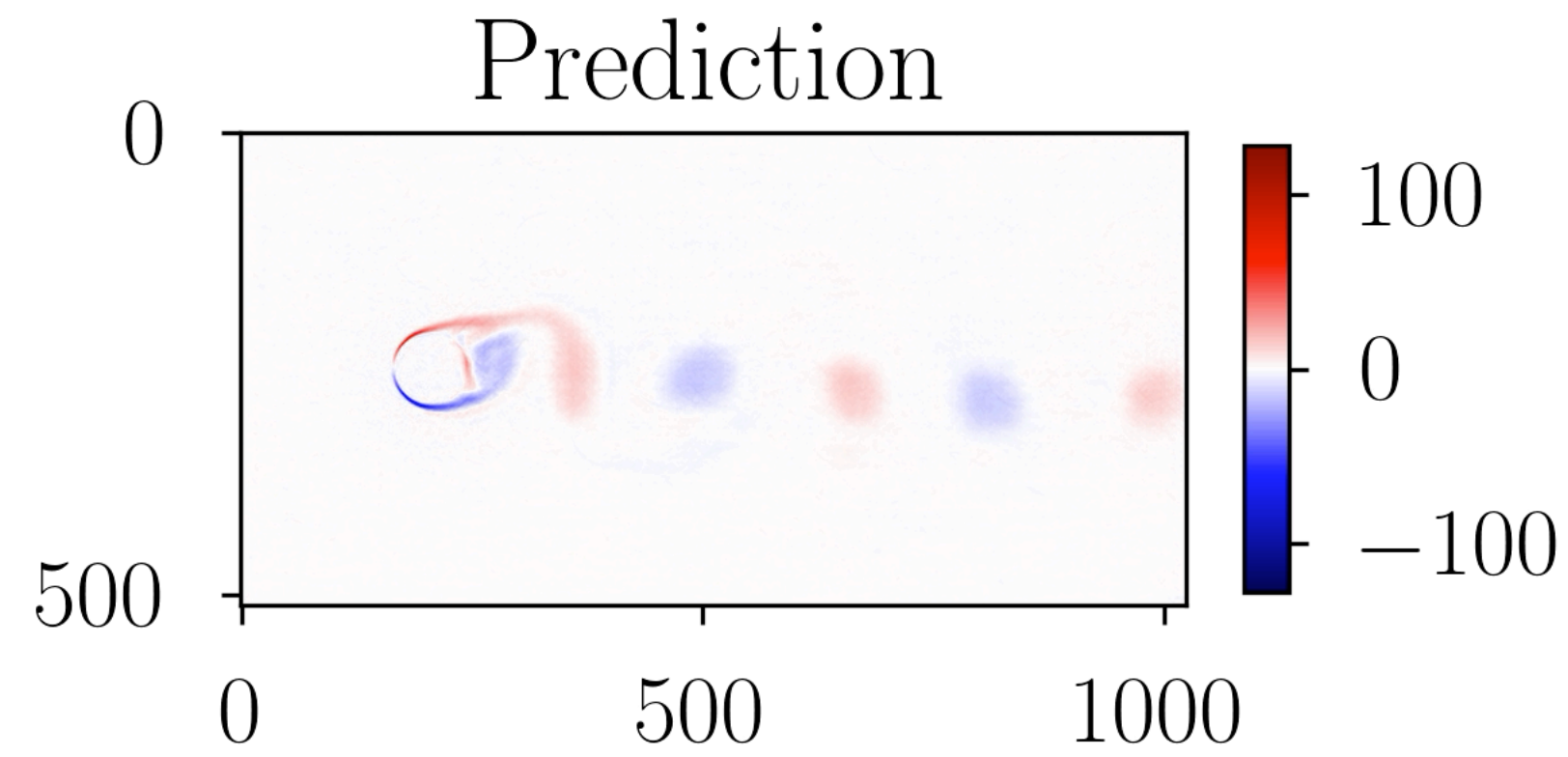
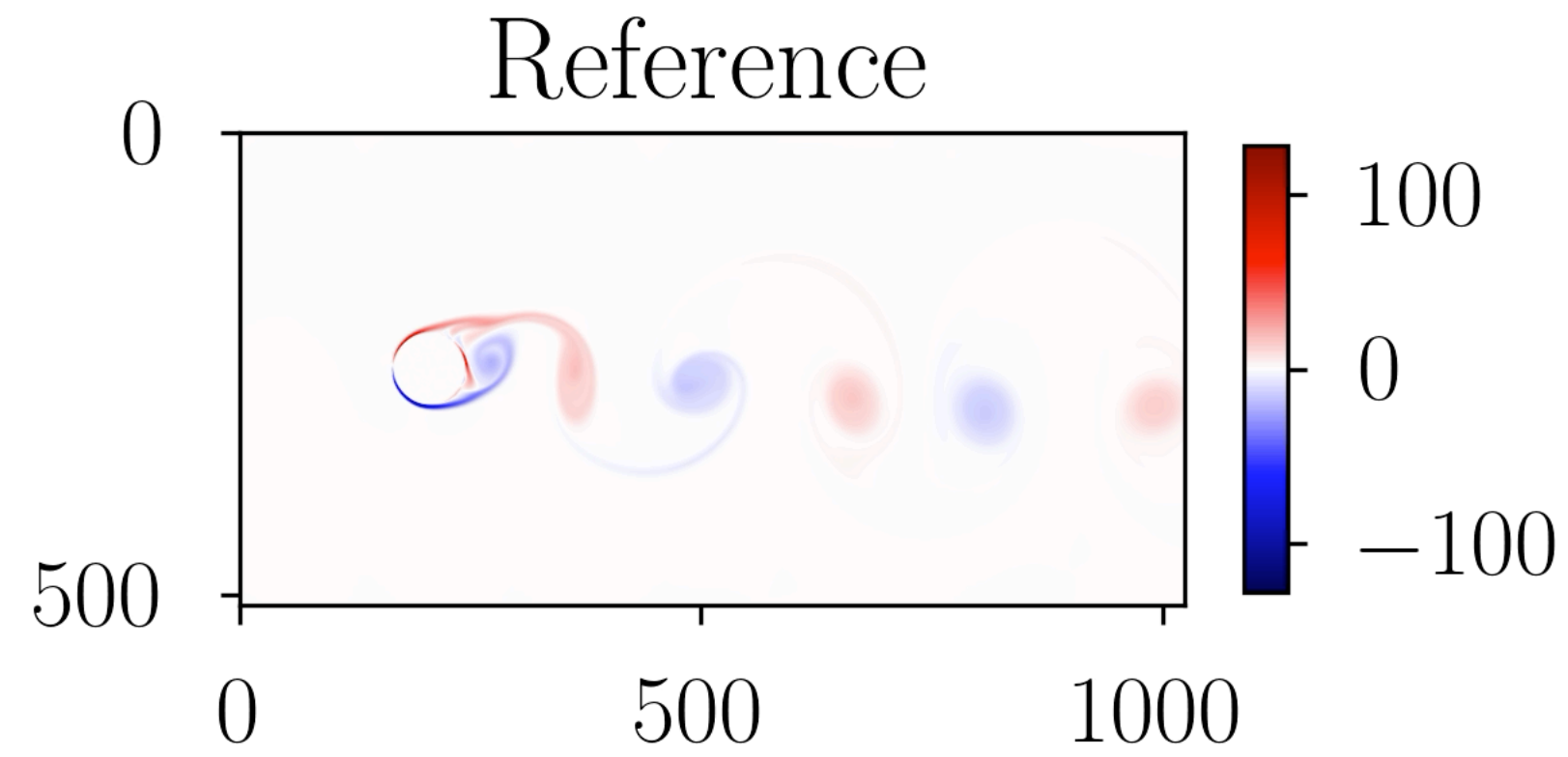


- Micro solver: Finite Differences (CubimUP2D) employing 12 cores
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- LED with latent dimension of  $d_z = 4, \Delta t = 0.2$
- LED captures **long-term evolution** of velocity and pressure fields (low NRMSE)
- LED is up to **two orders of magnitude** faster than CubismUP2D
- Multiscale LED **reduces the approximation error** at the cost of **reduced speed-up**
- Recovers drag coefficient with  $\approx 2 - 4\%$  error



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

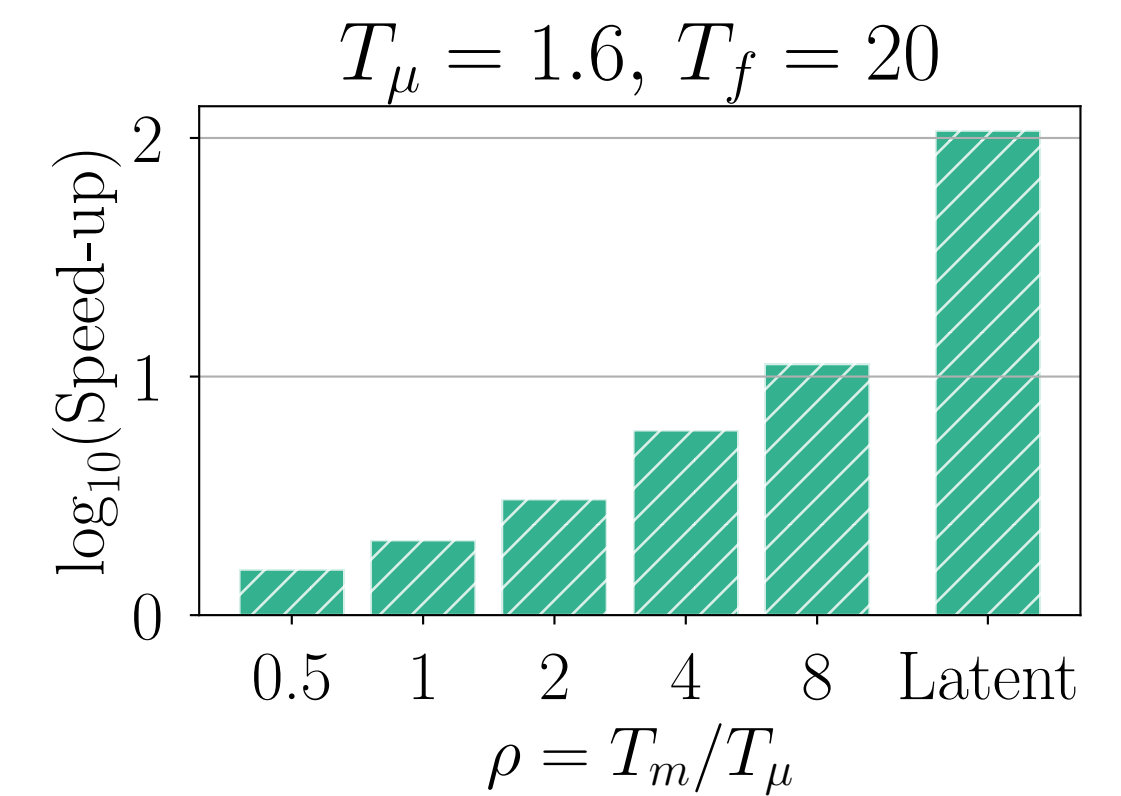
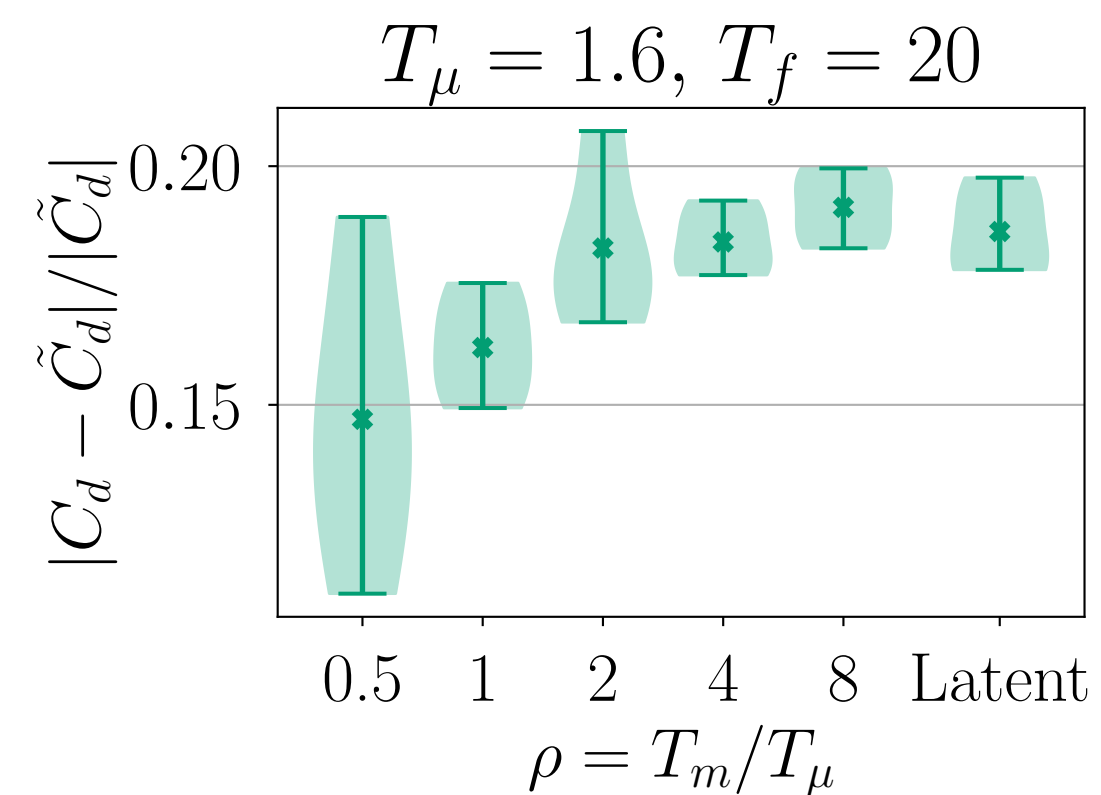
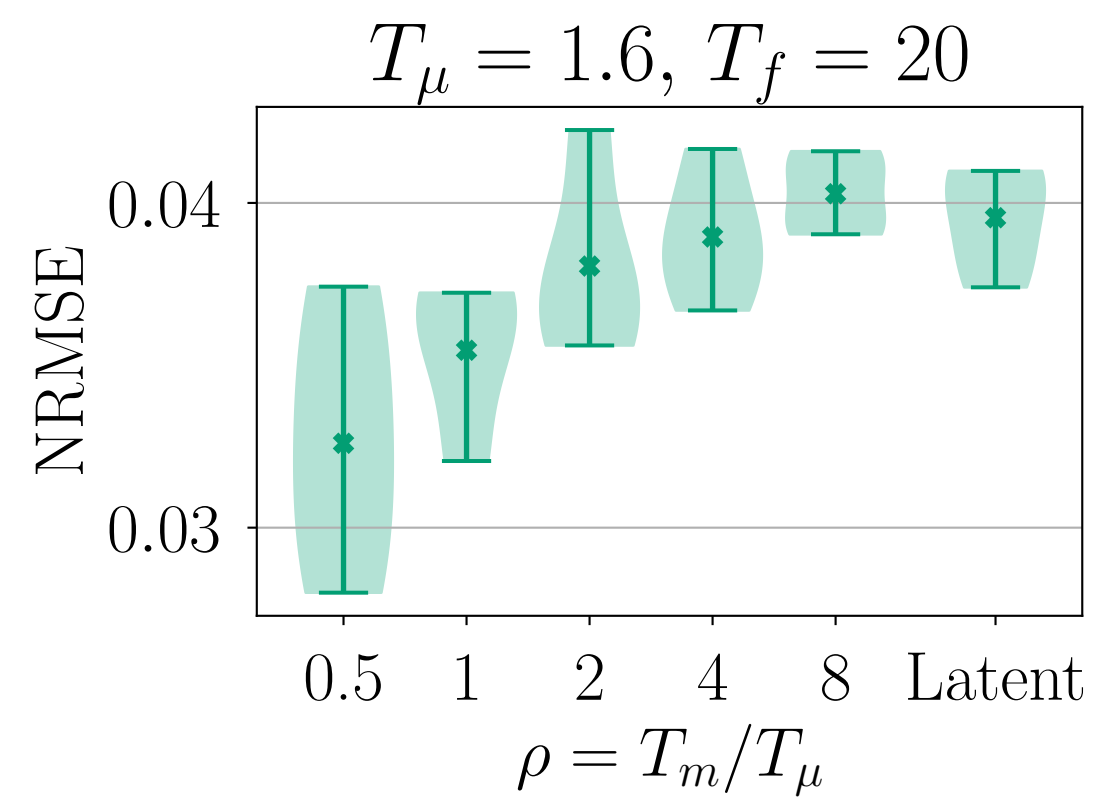
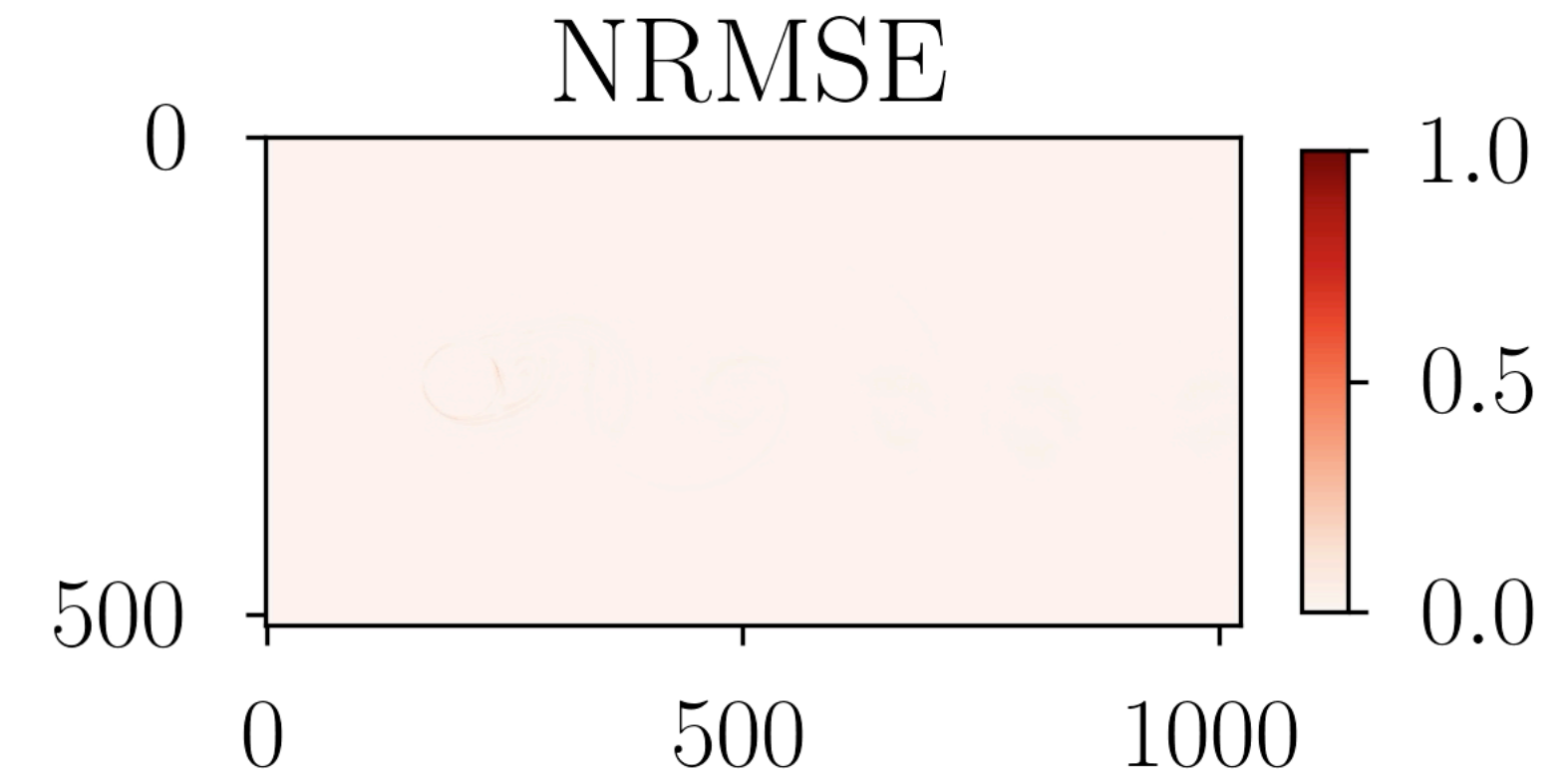
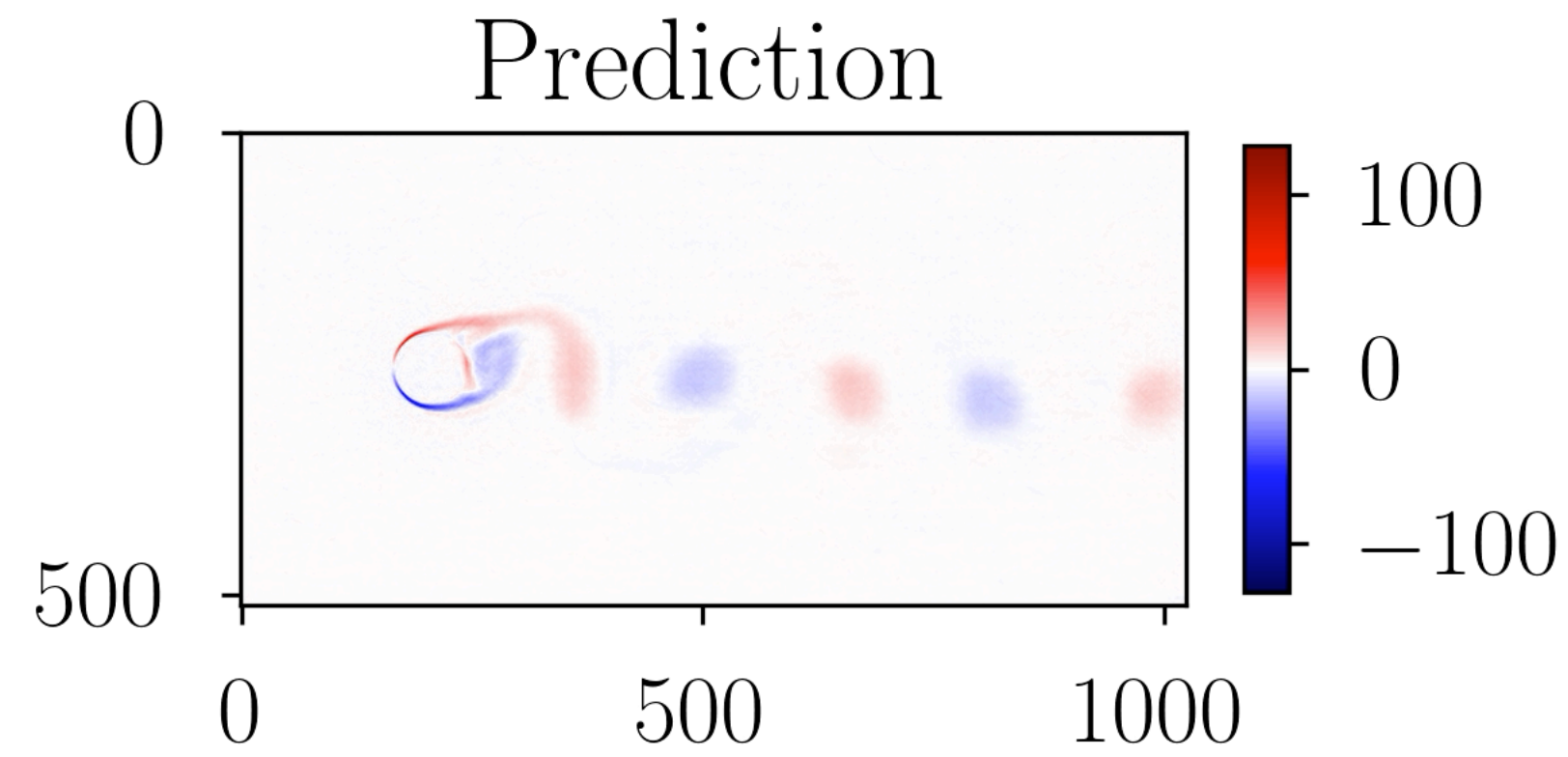
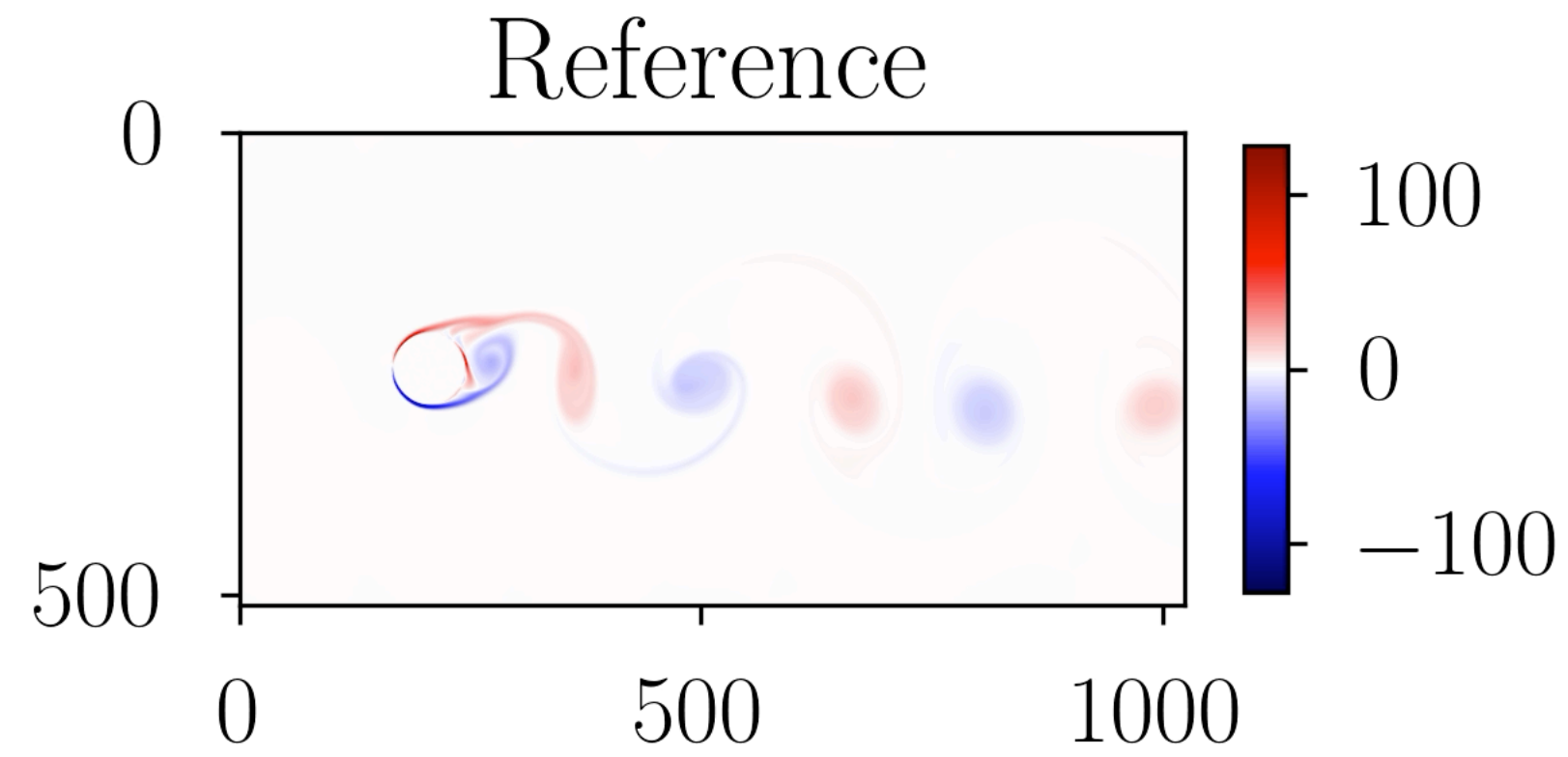
PR Vlachas, G Arampatzis, C Uhler, P Koumoutsakos,  
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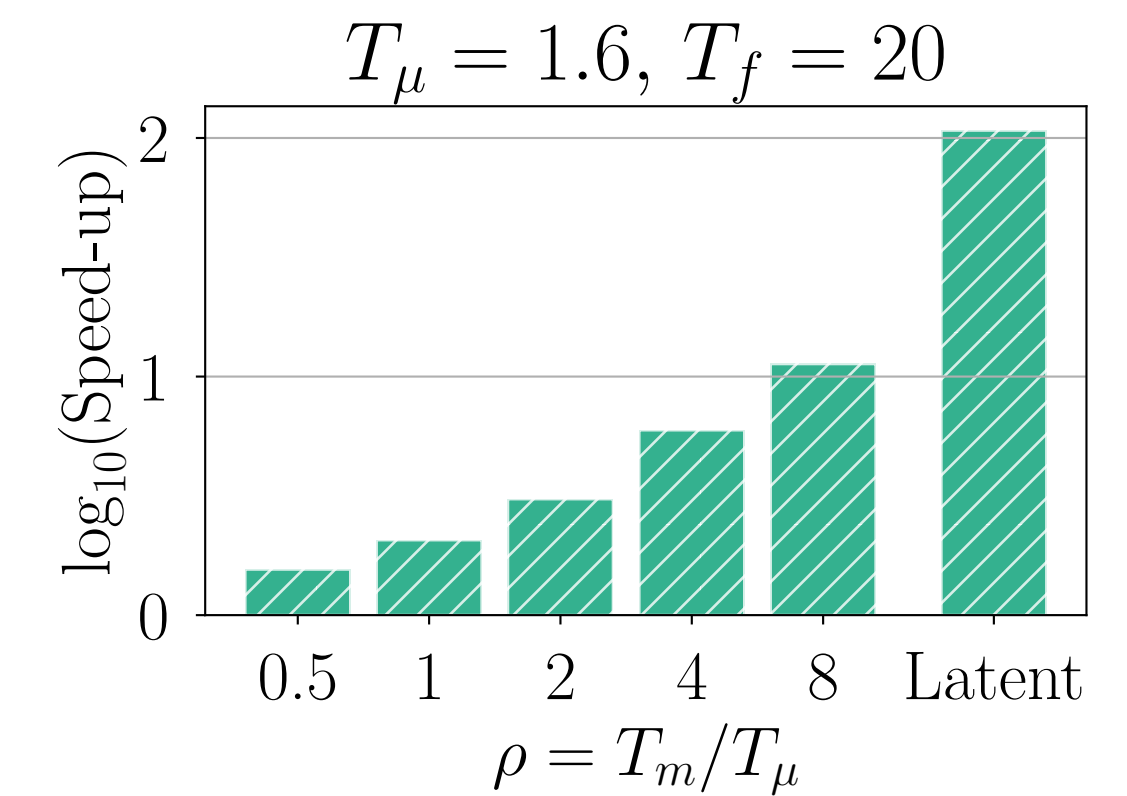
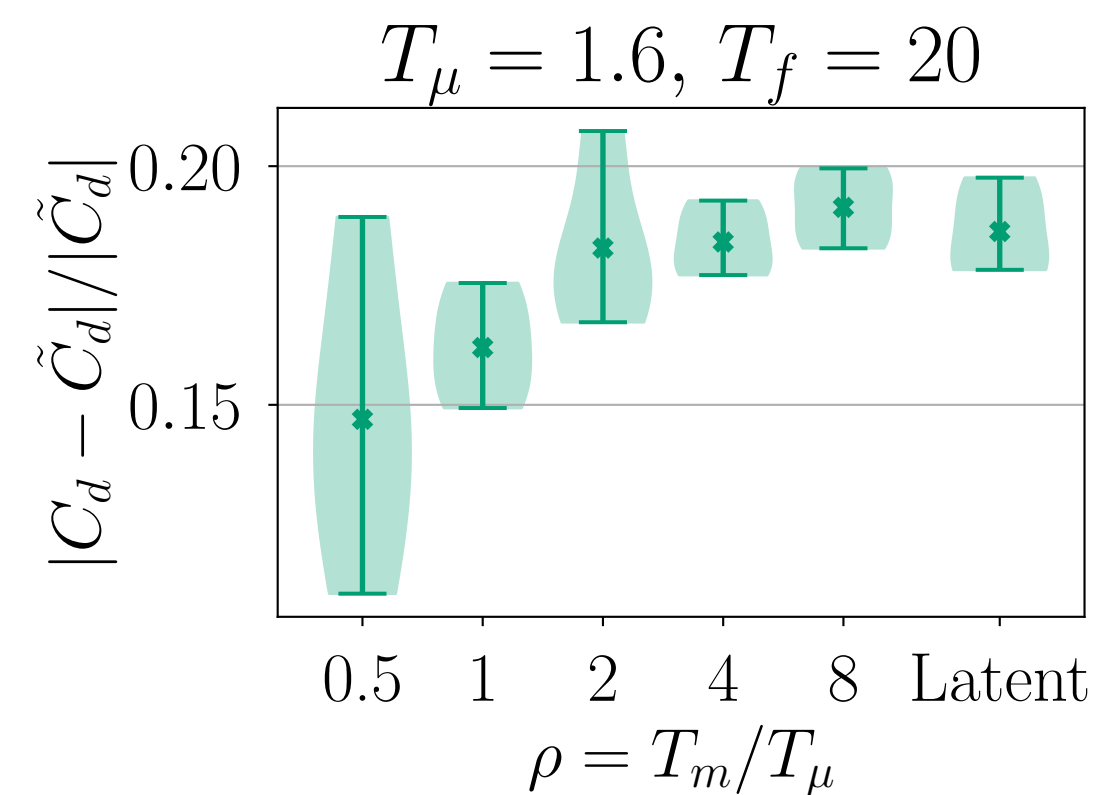
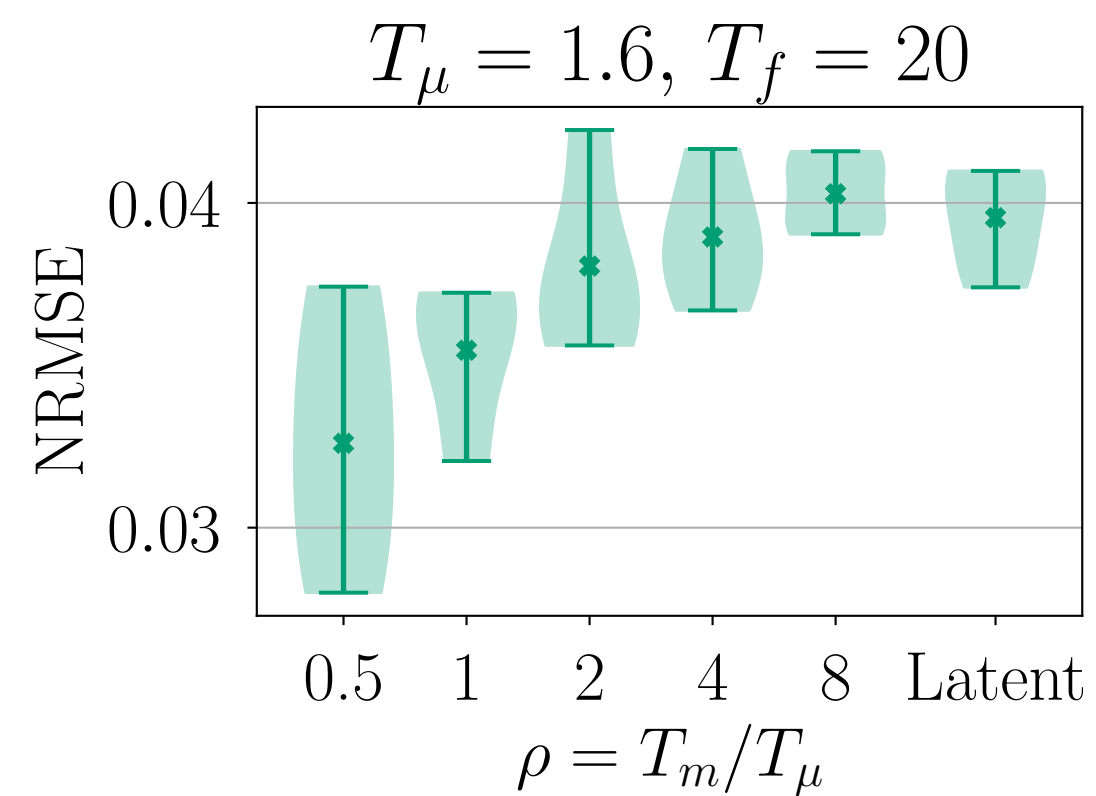
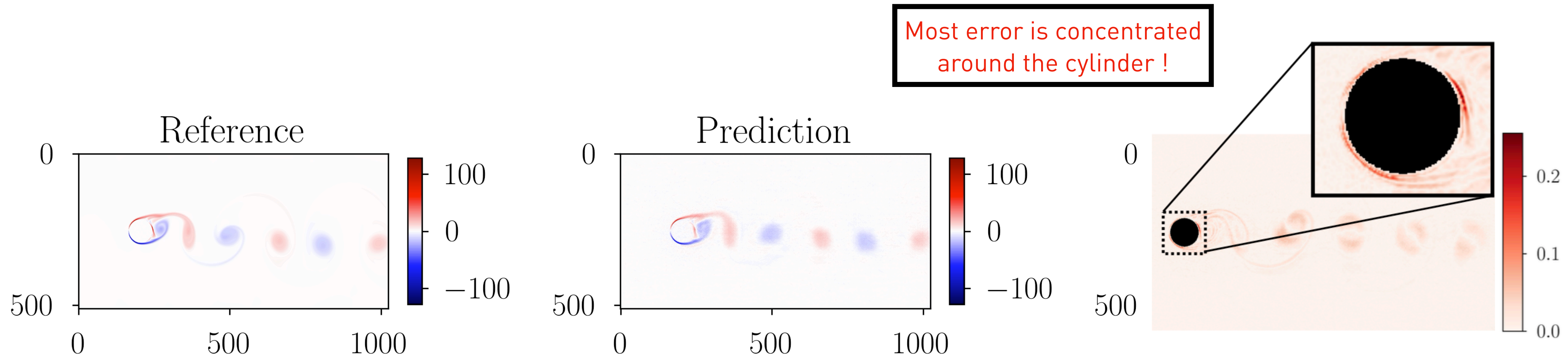
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# Comparisons of Latent Propagators

PR Vlachas, G Arampatzis, C Uhler, P Koumoutsakos,  
*Multiscale Simulations of Complex Systems  
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Mean normalised absolute difference:

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

$$\text{MNAD} = \frac{1}{N_T} \sum_{j=1}^{N_T} \text{NAD}(t_j)$$

**SINDy**

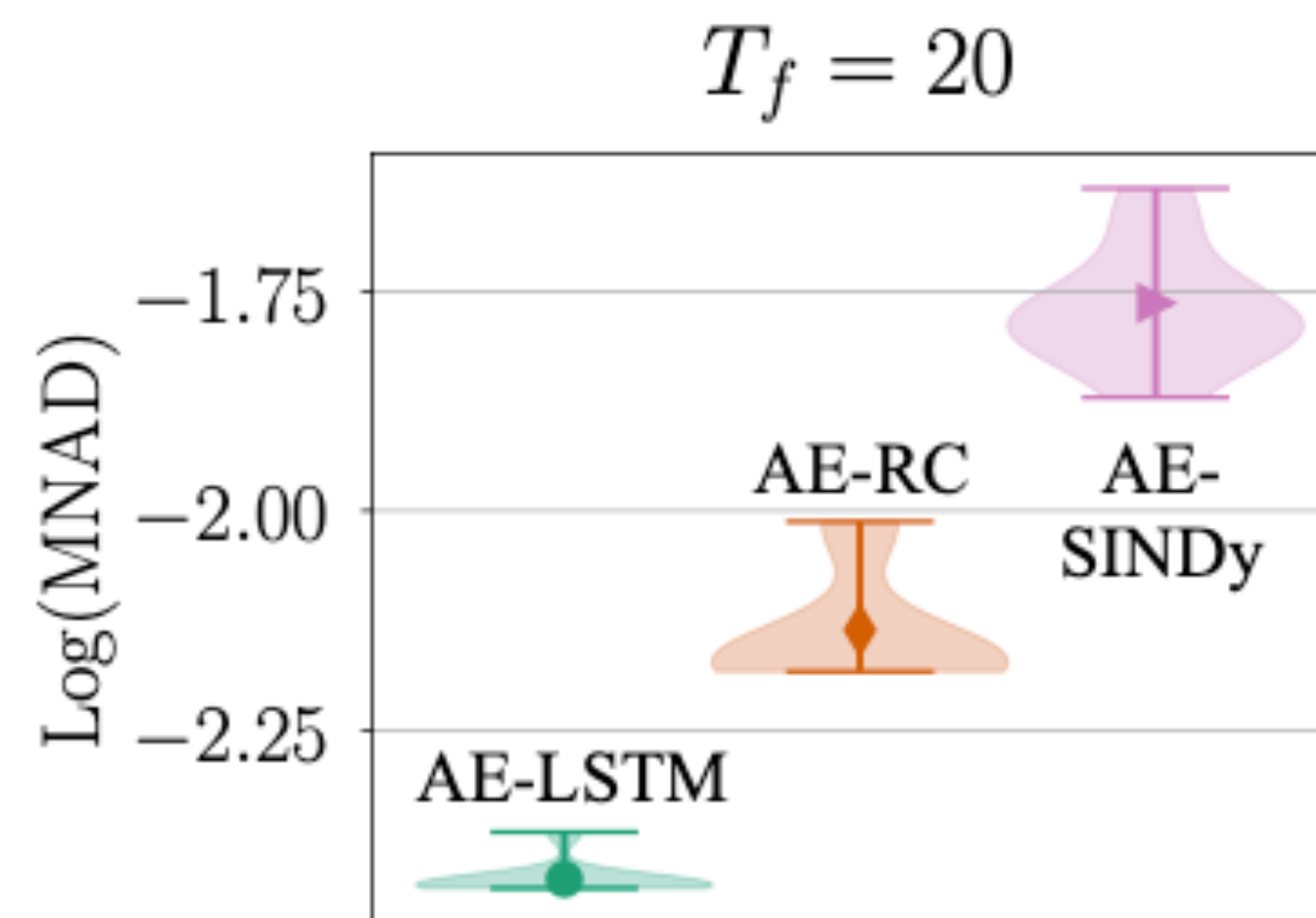
SL Brunton, JL Proctor, JN Kutz,  
*Discovering governing equations from  
data by sparse identification of  
nonlinear dynamical systems,*  
PNAS (2016)

**RC**

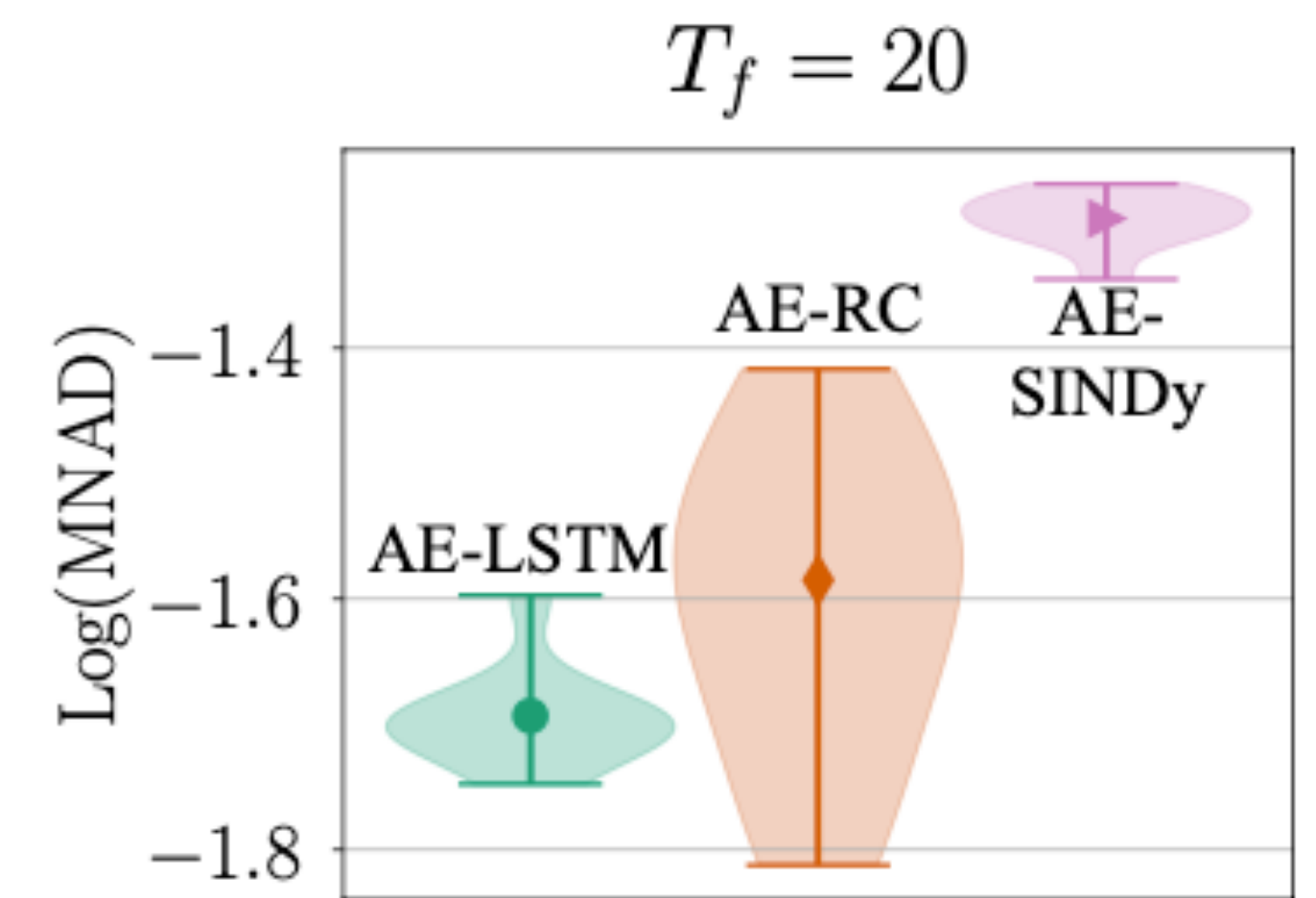
J Pathak, B Hunt, M Girvan, Z  
Lu, E Ott, *Model-free prediction of  
large spatiotemporally chaotic  
systems from data: A reservoir  
computing approach,*  
Physical review letters, 2018

**LSTM**

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



$Re = 100$



$Re = 1000$





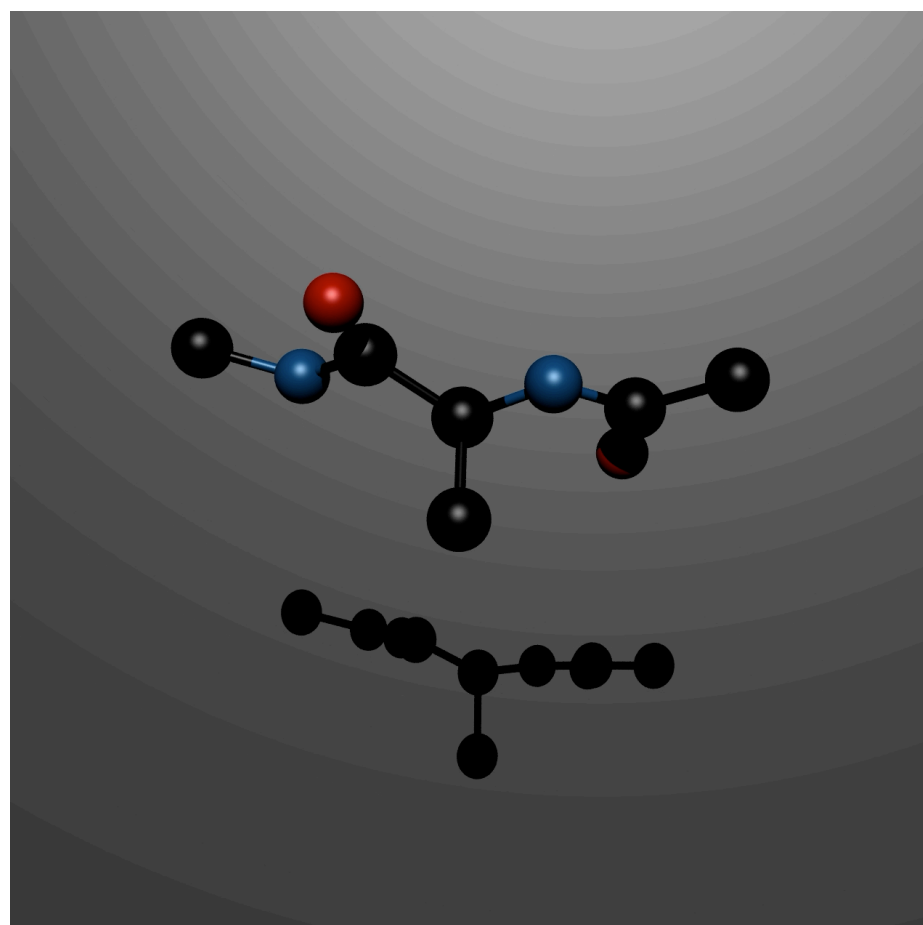
# *III*

*Learning Effective Dynamics for  
Molecular Systems*



# Alanine Dipeptide

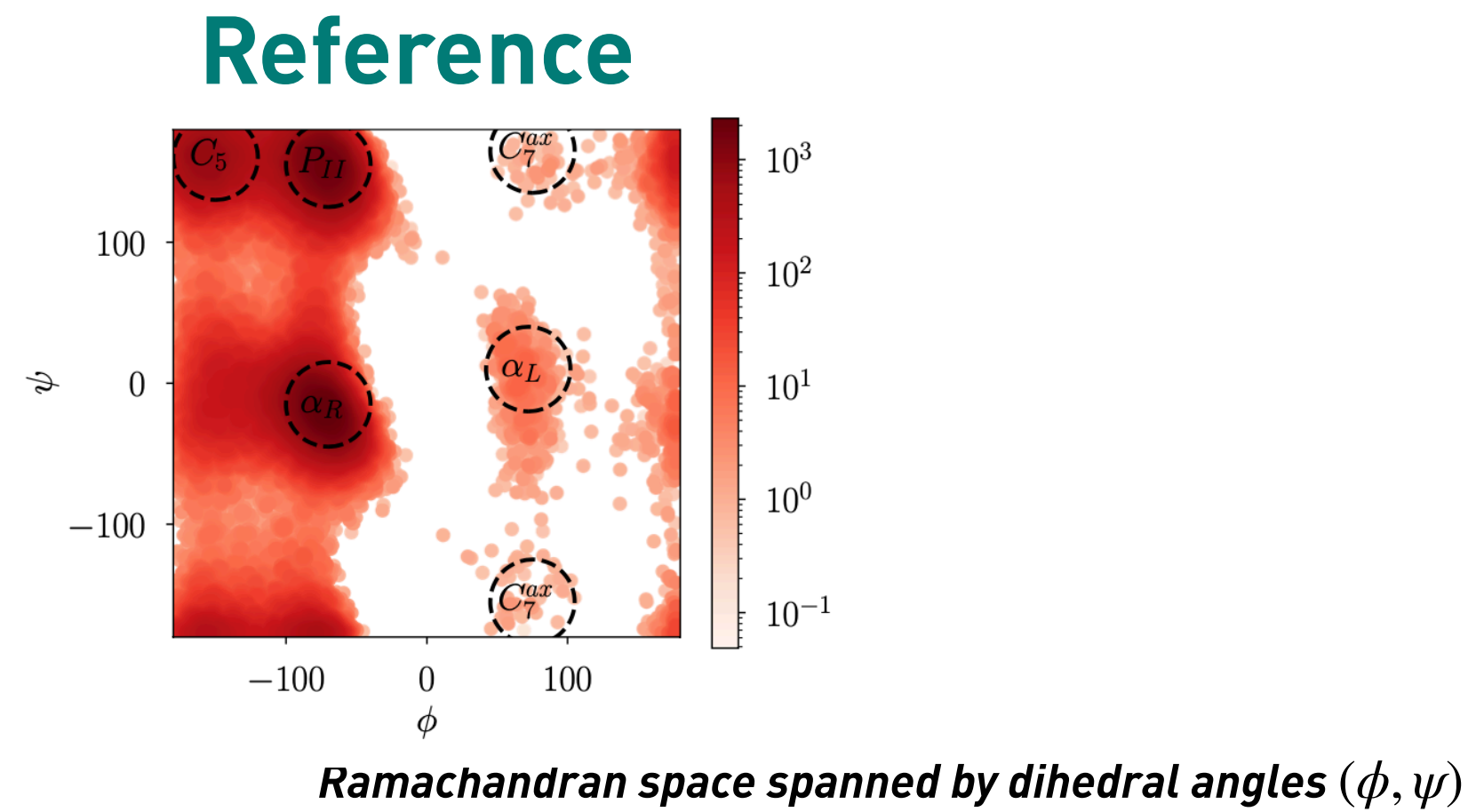
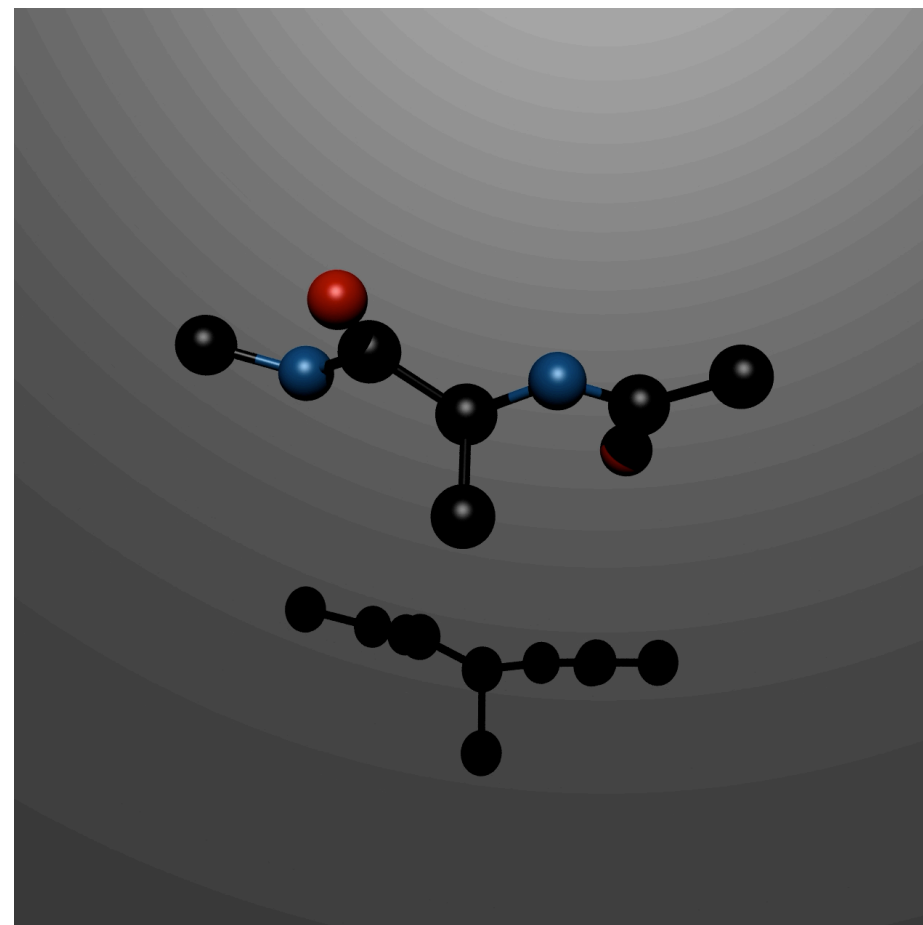
PR Vlachas, J Zavadlav, M Praprotnik, P Koumoutsakos,  
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**Journal of Chemical Theory & Computation, 2021**





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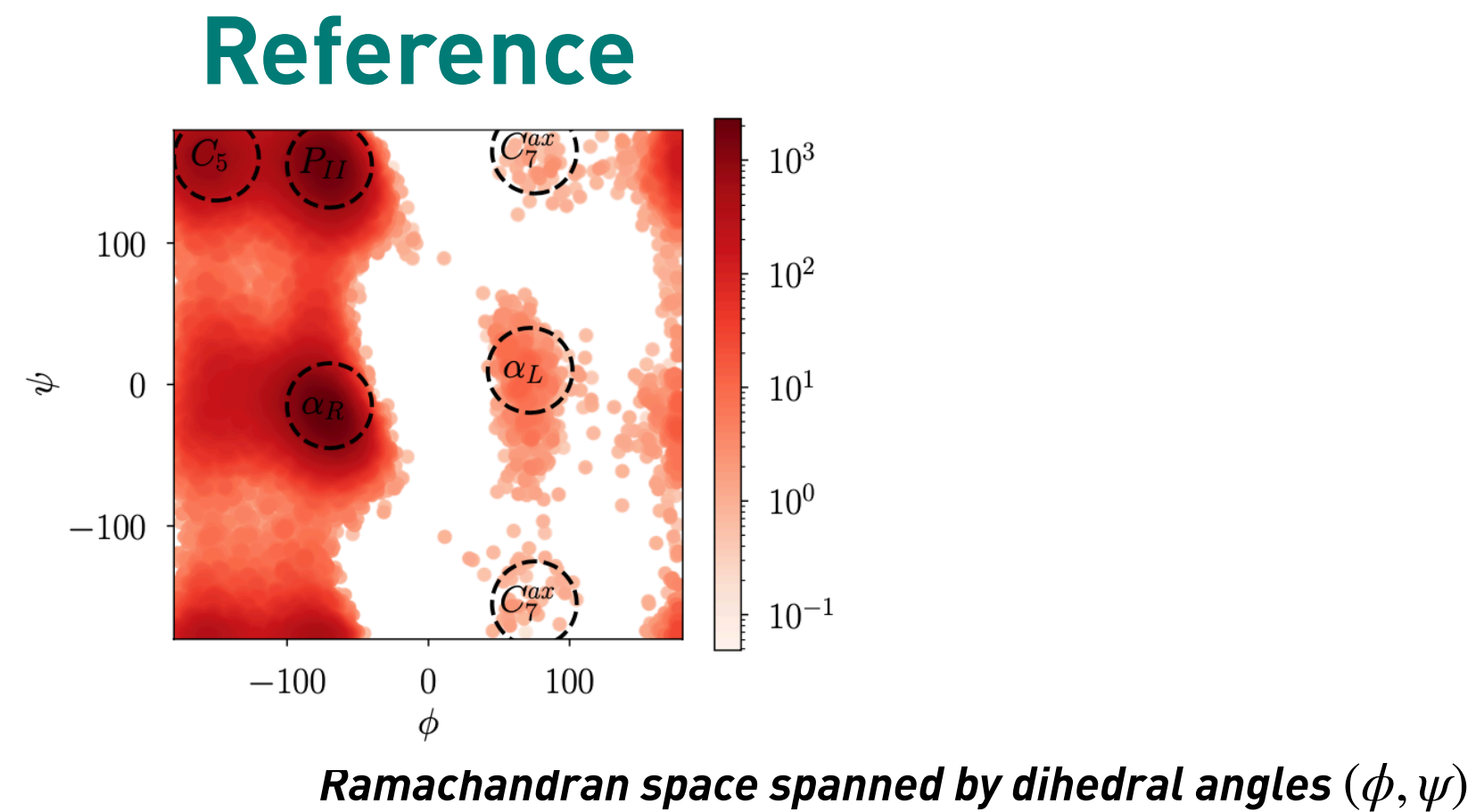
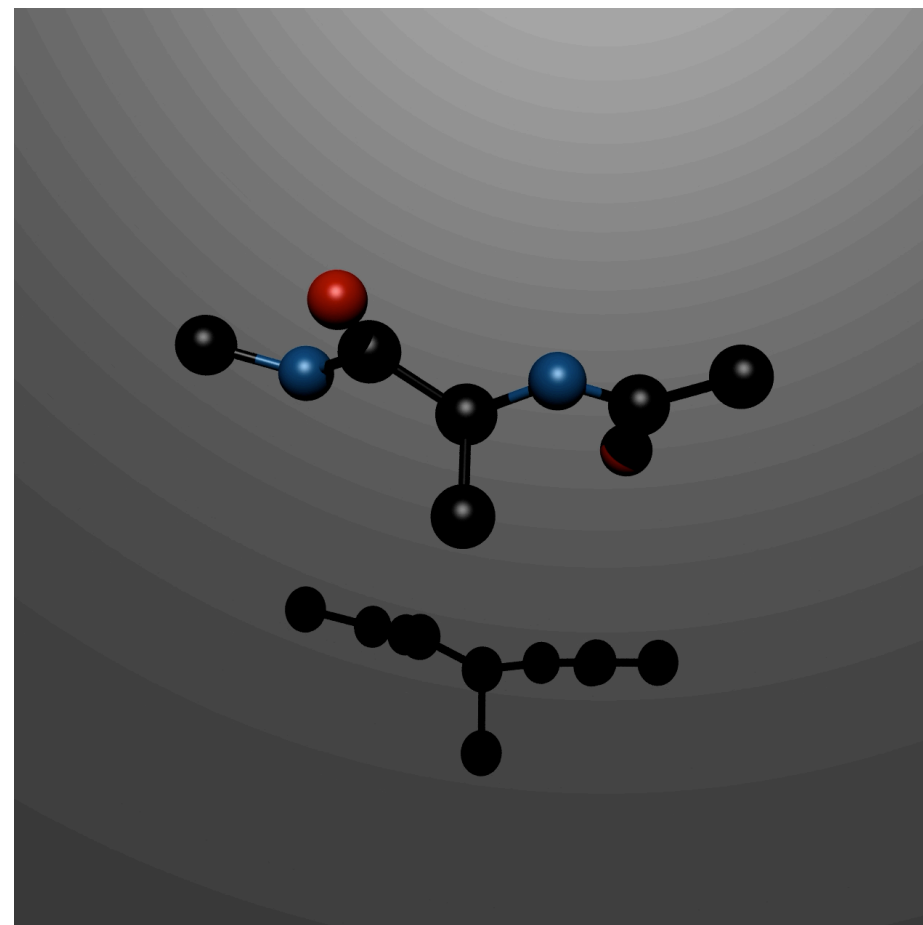


- Alanine dipeptide dynamics in water solved with Molecular Dynamics (MD solver)



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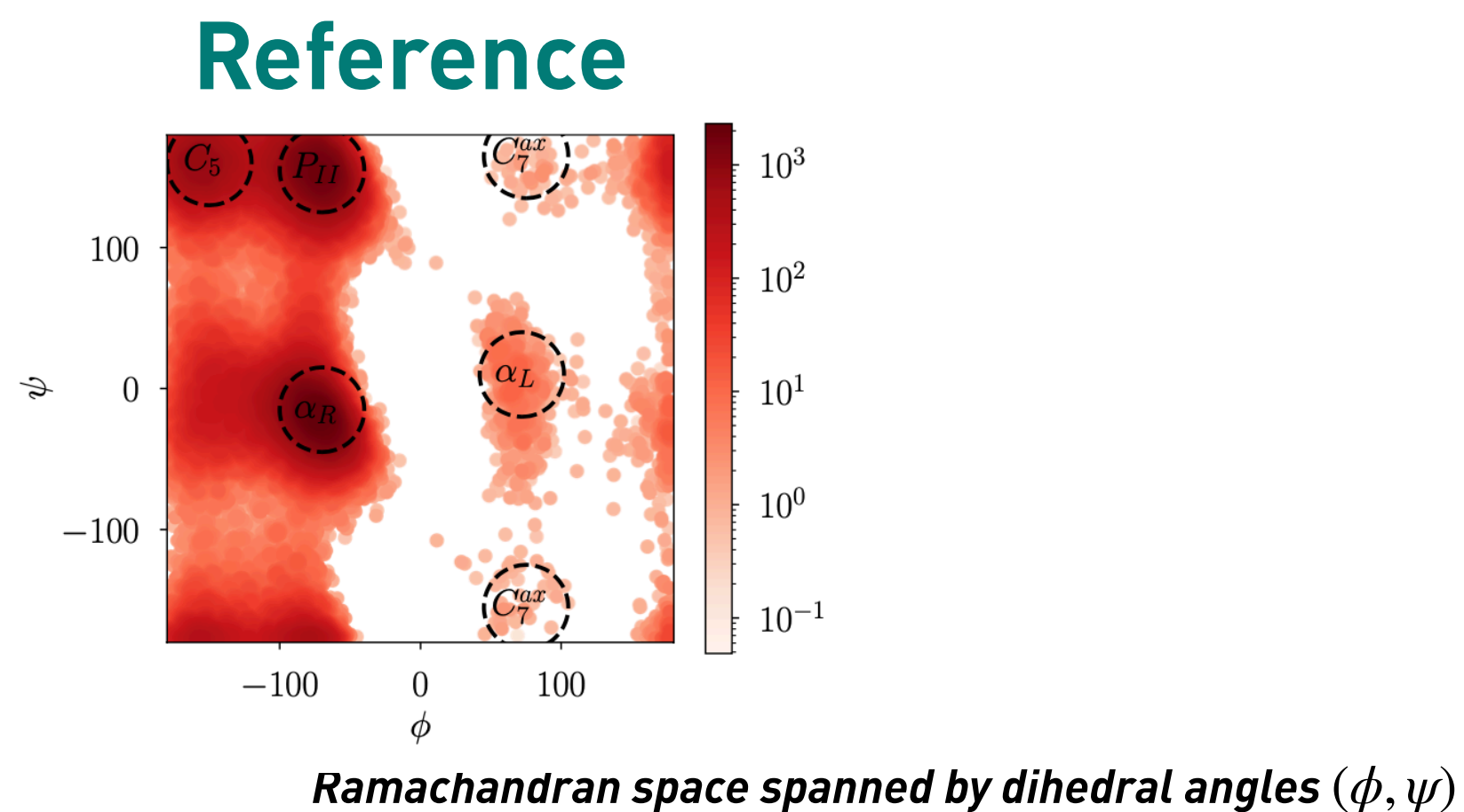
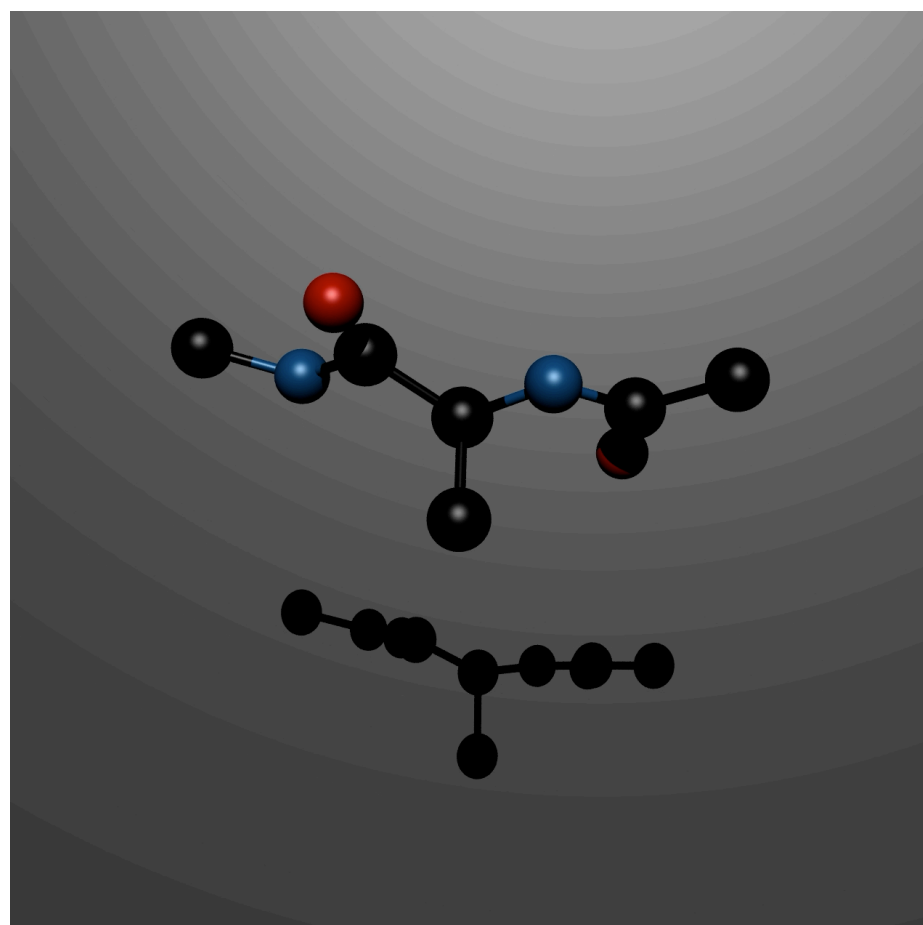


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- Stochastic transitions between **5 meta-stable states**  $\{P_{II}, C_5, \alpha_R, \alpha_L, C_7^{ax}\}$



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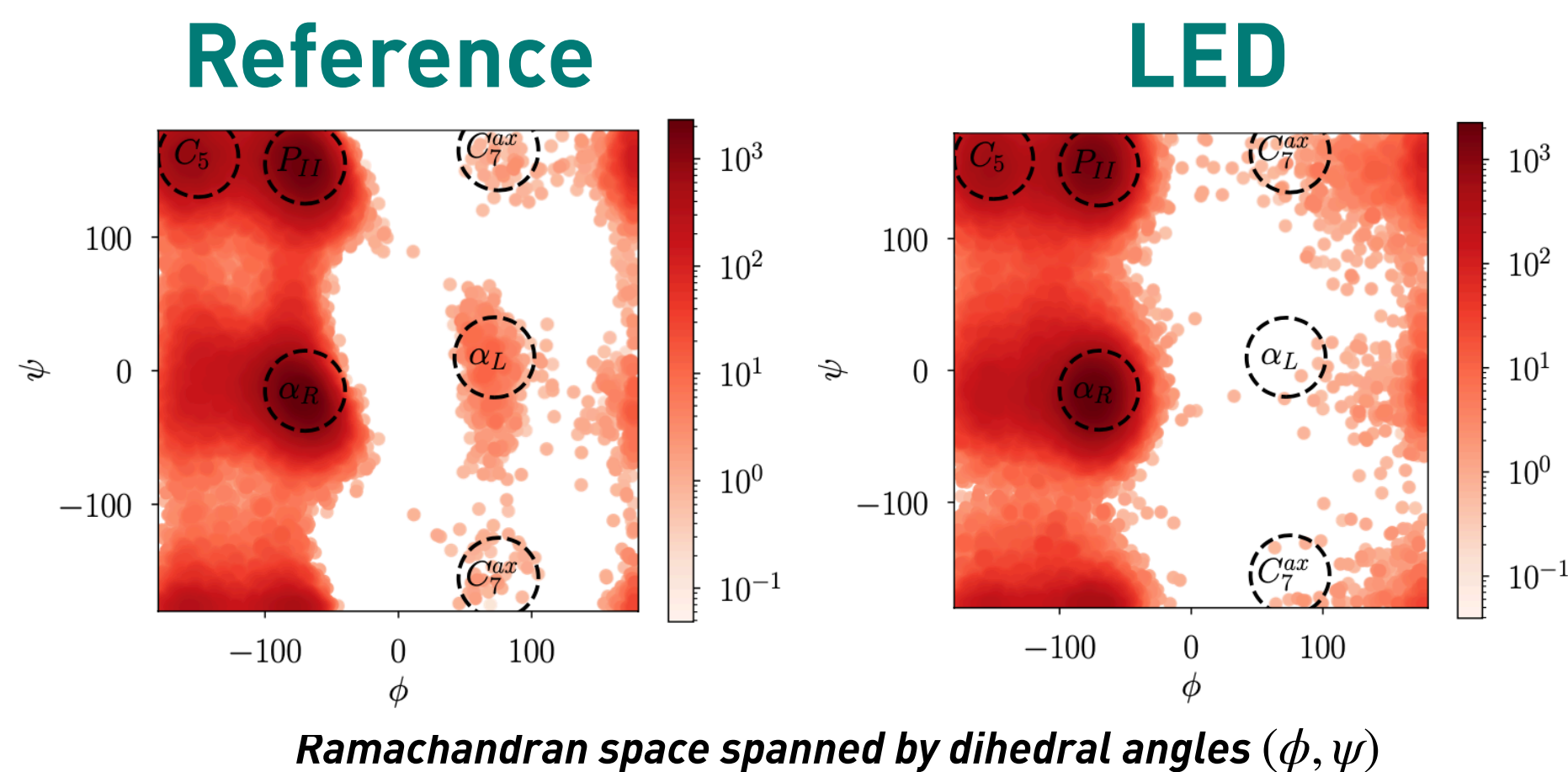
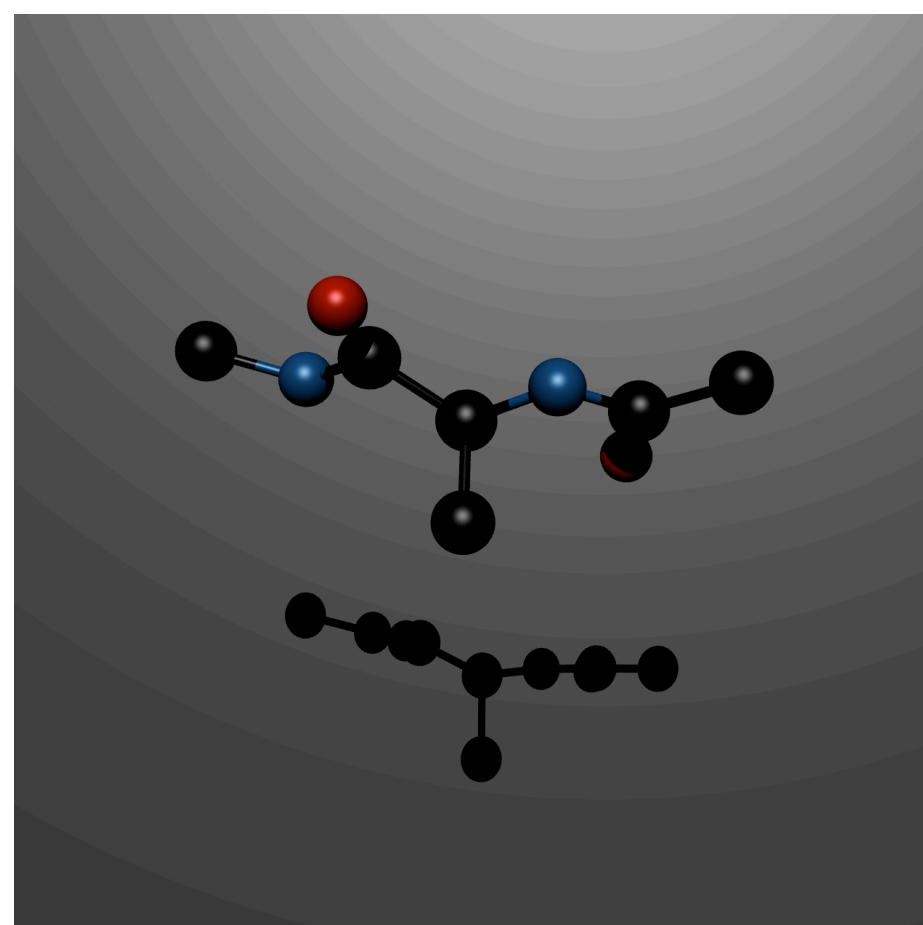


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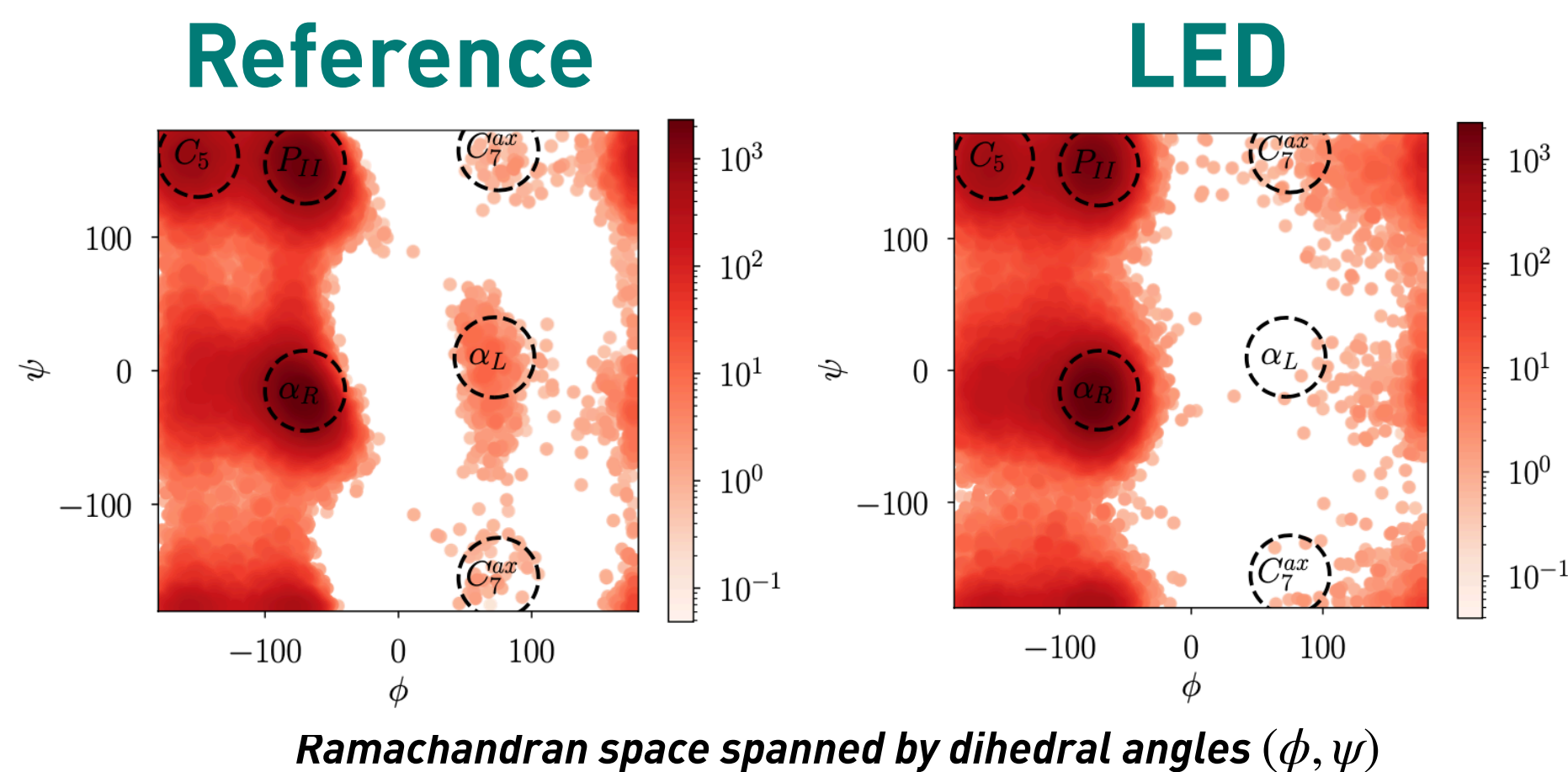
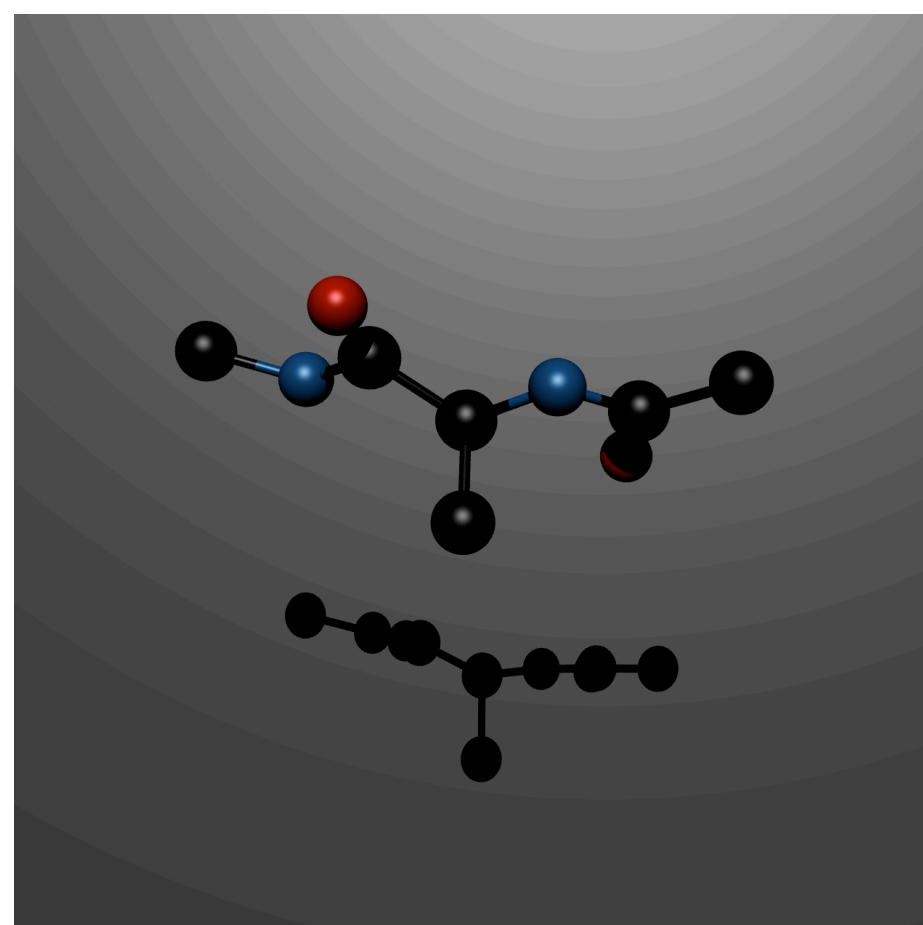


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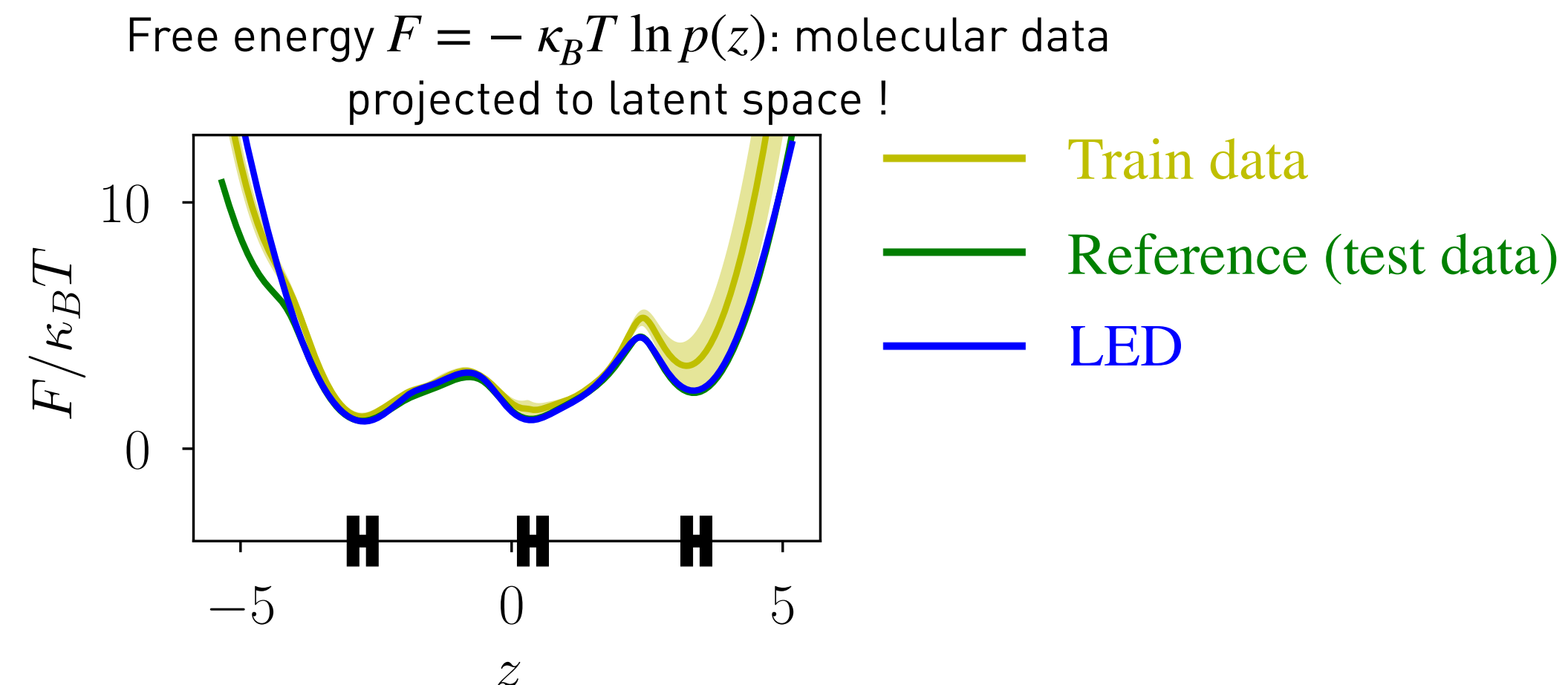
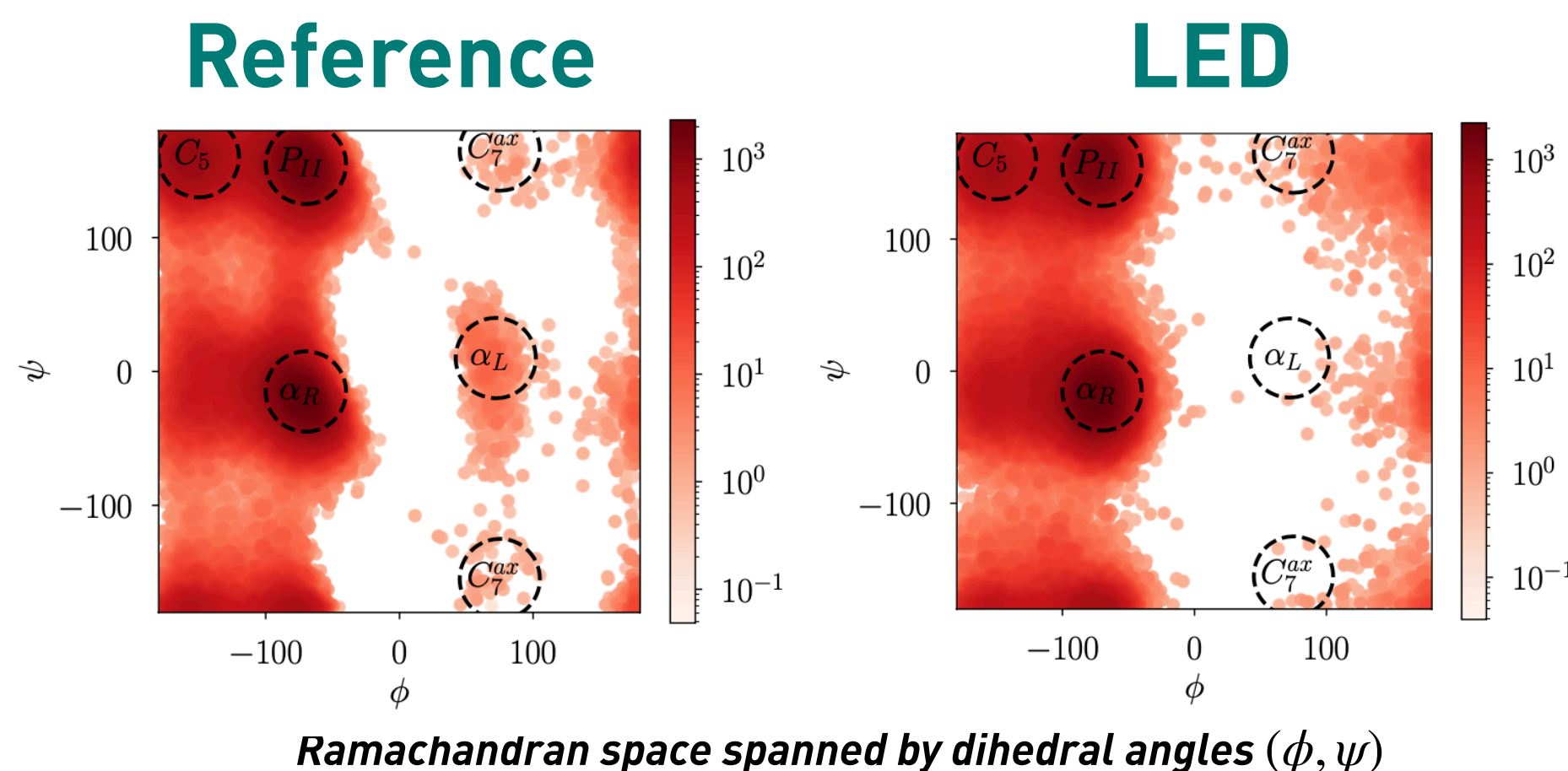
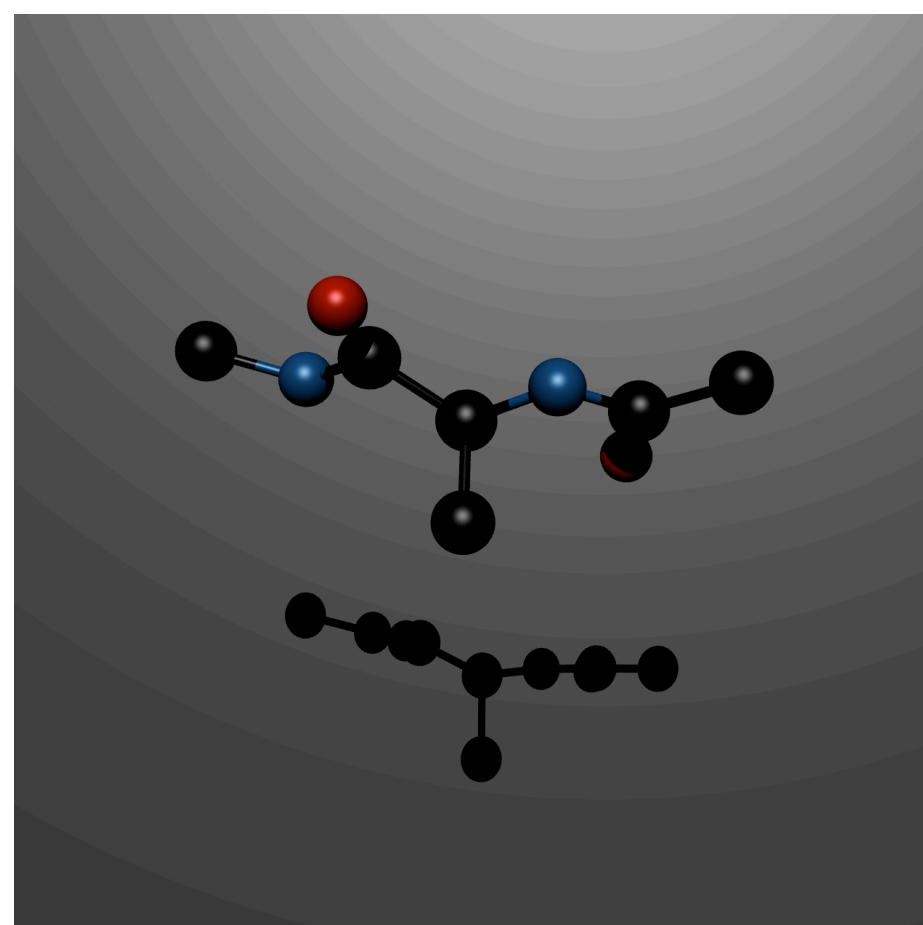


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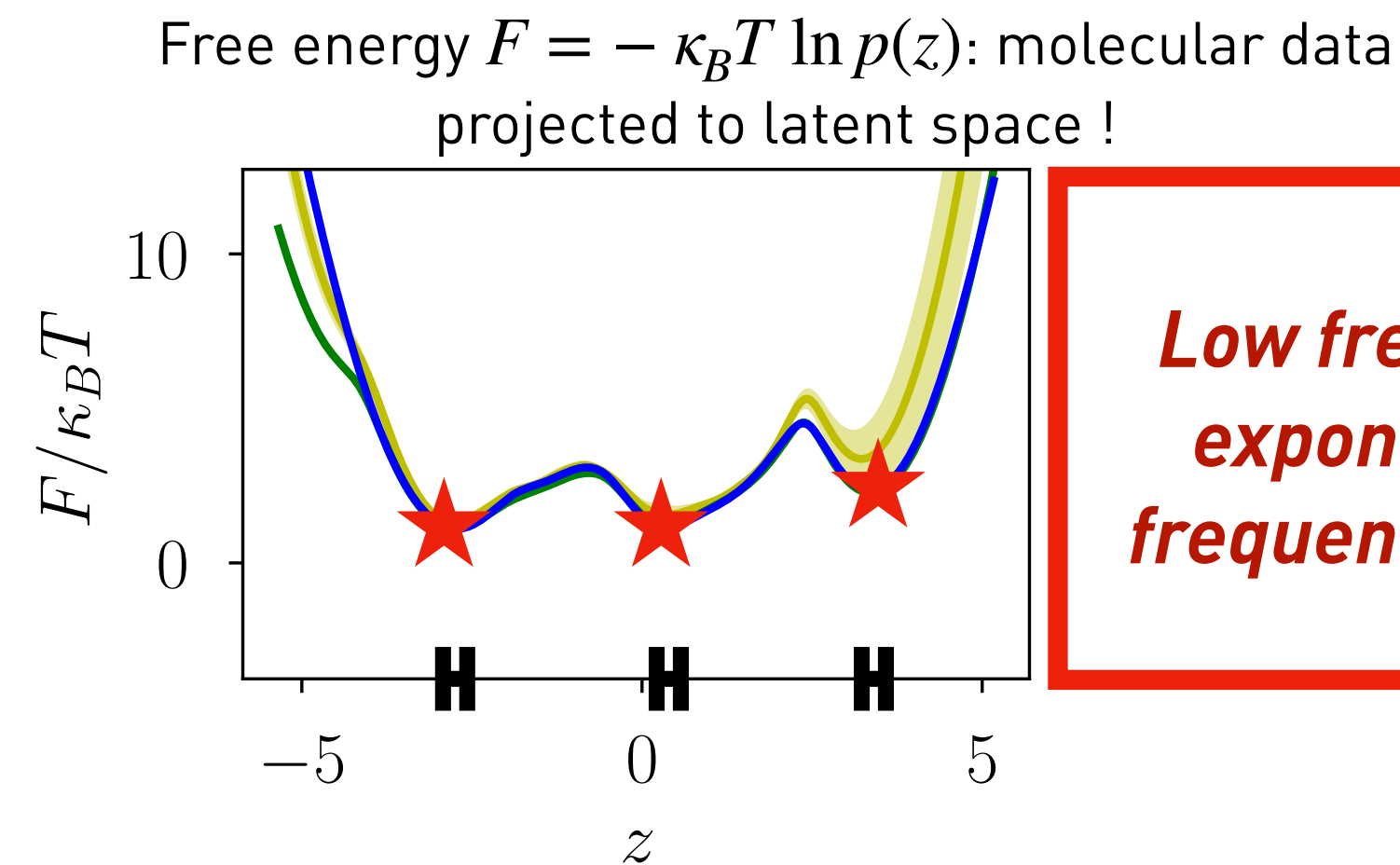
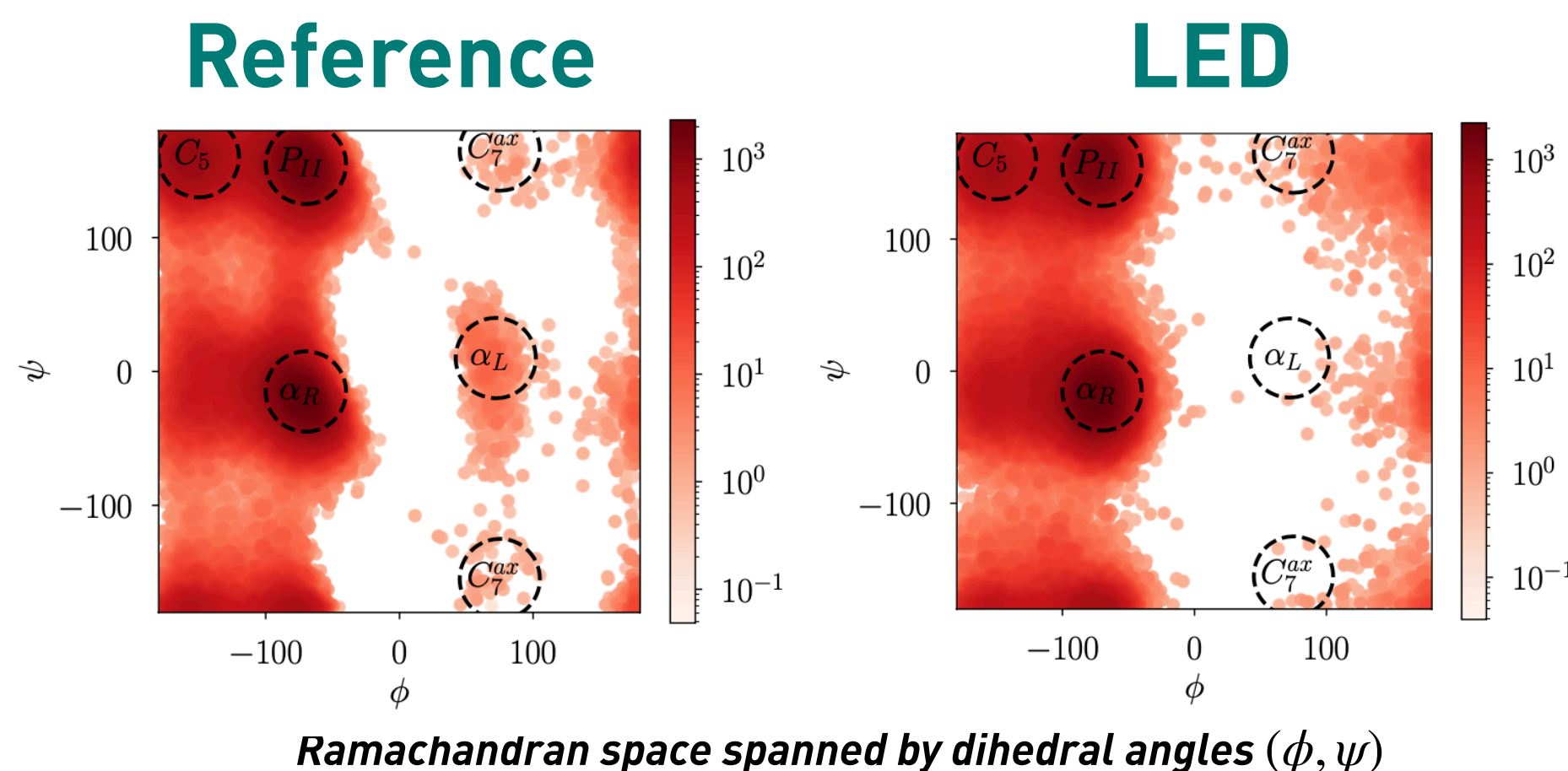
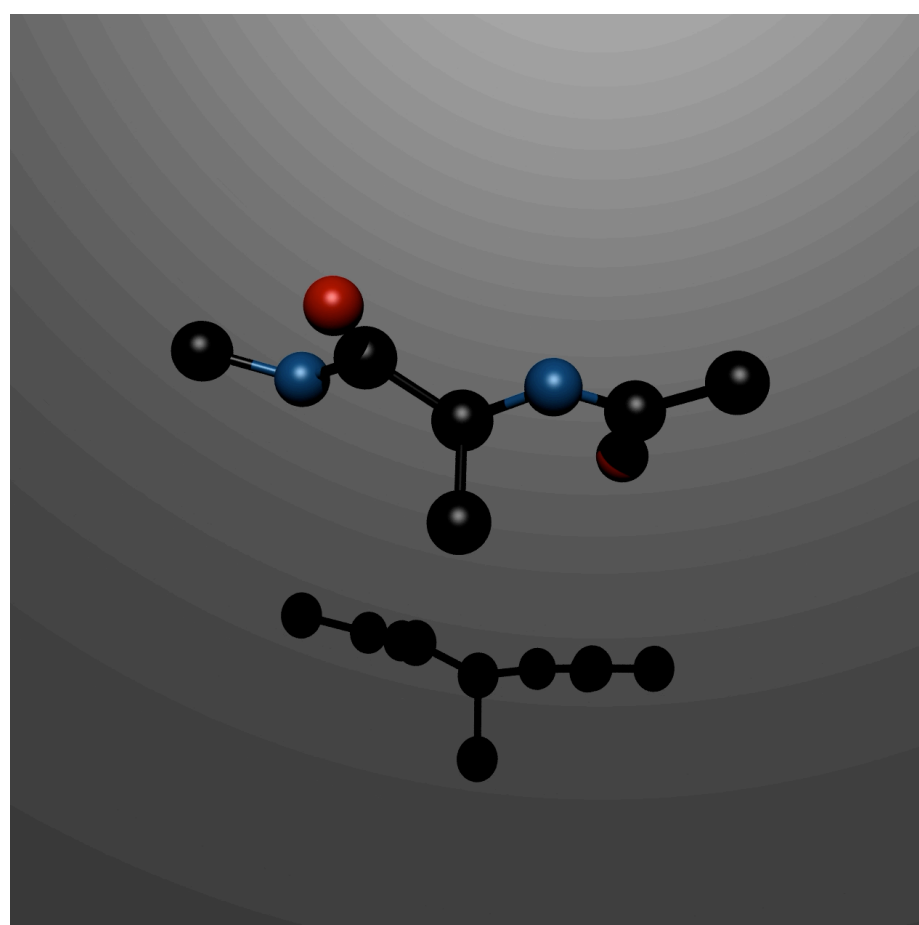


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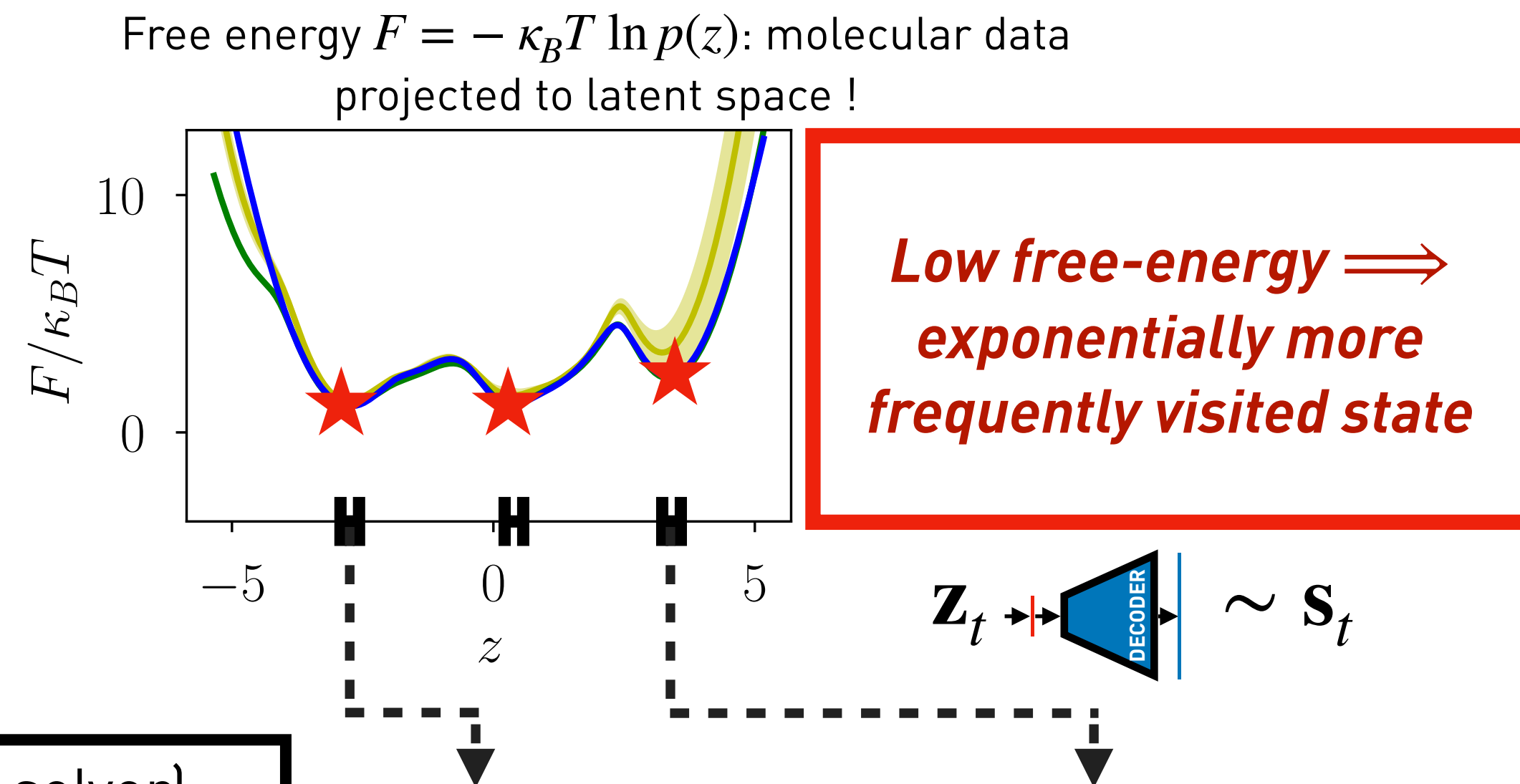
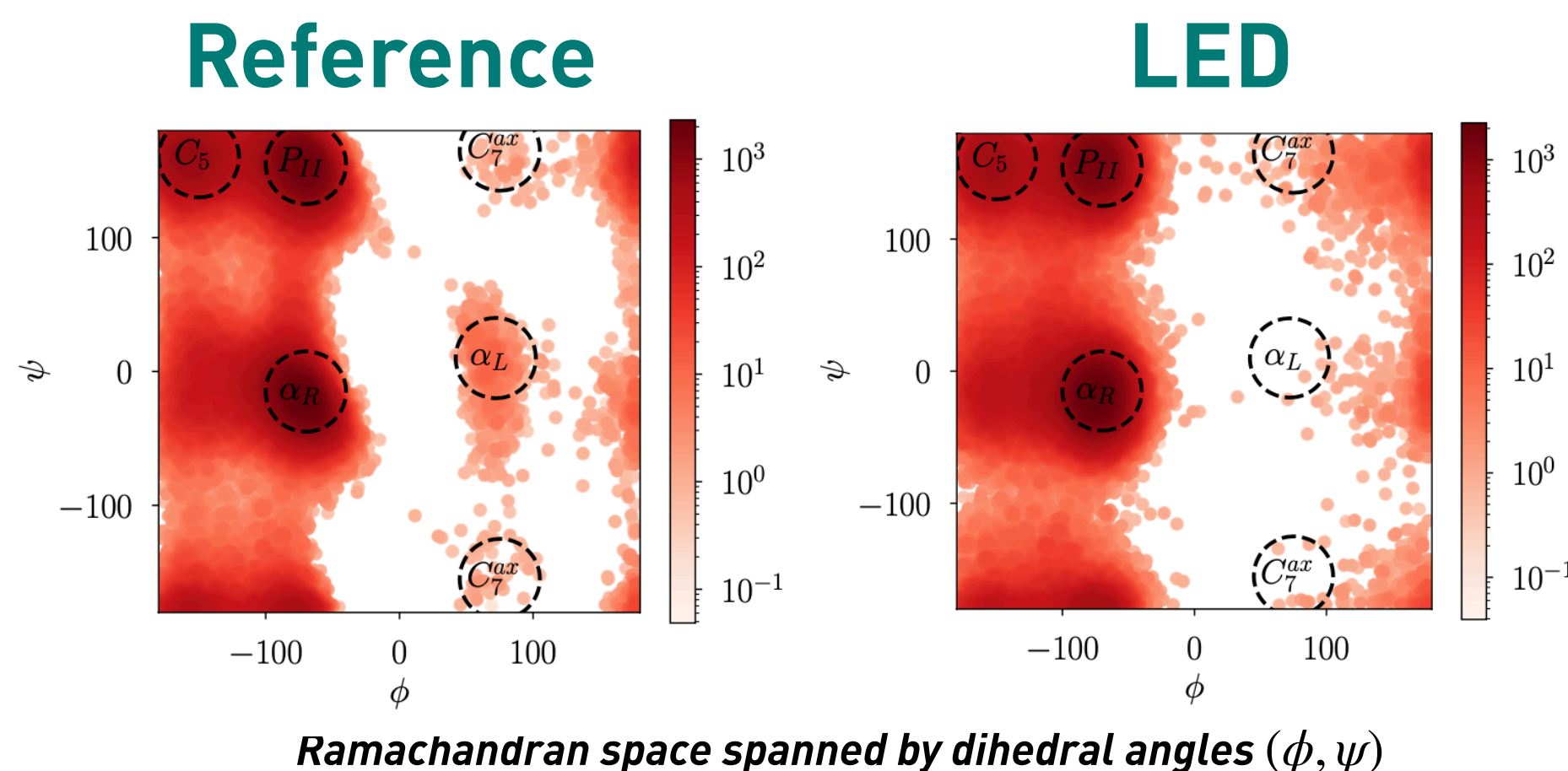
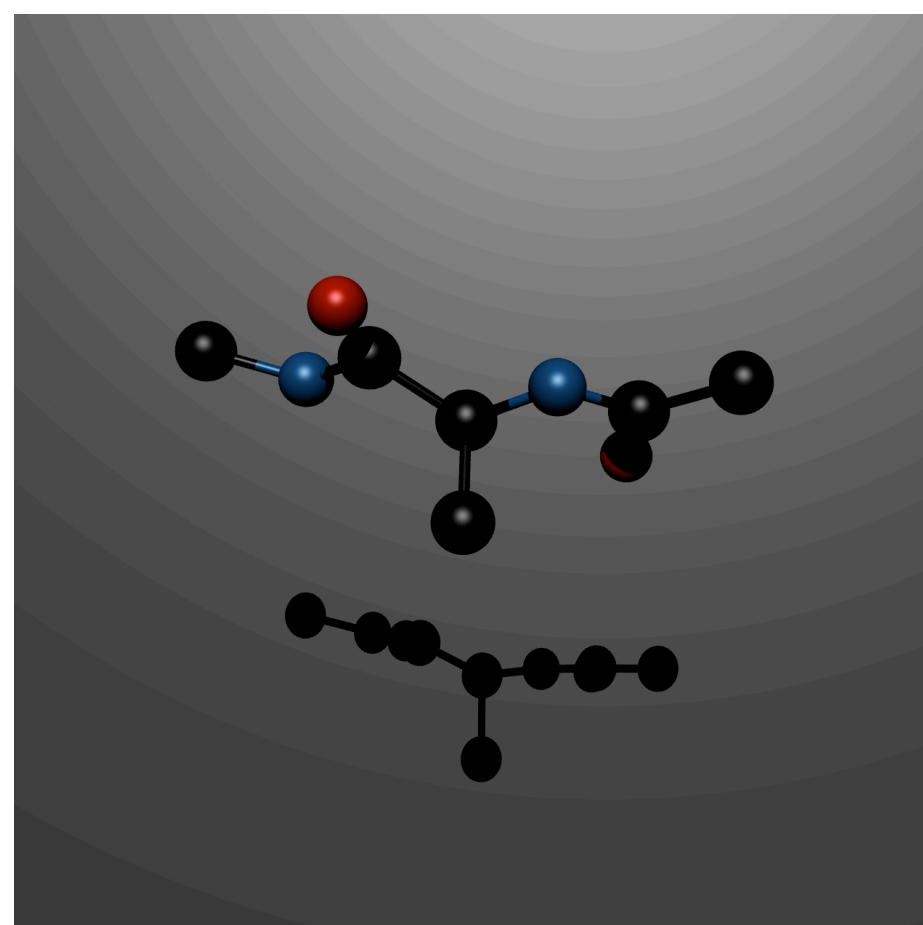
**Low free-energy  $\Rightarrow$   
 exponentially more  
 frequently visited state**

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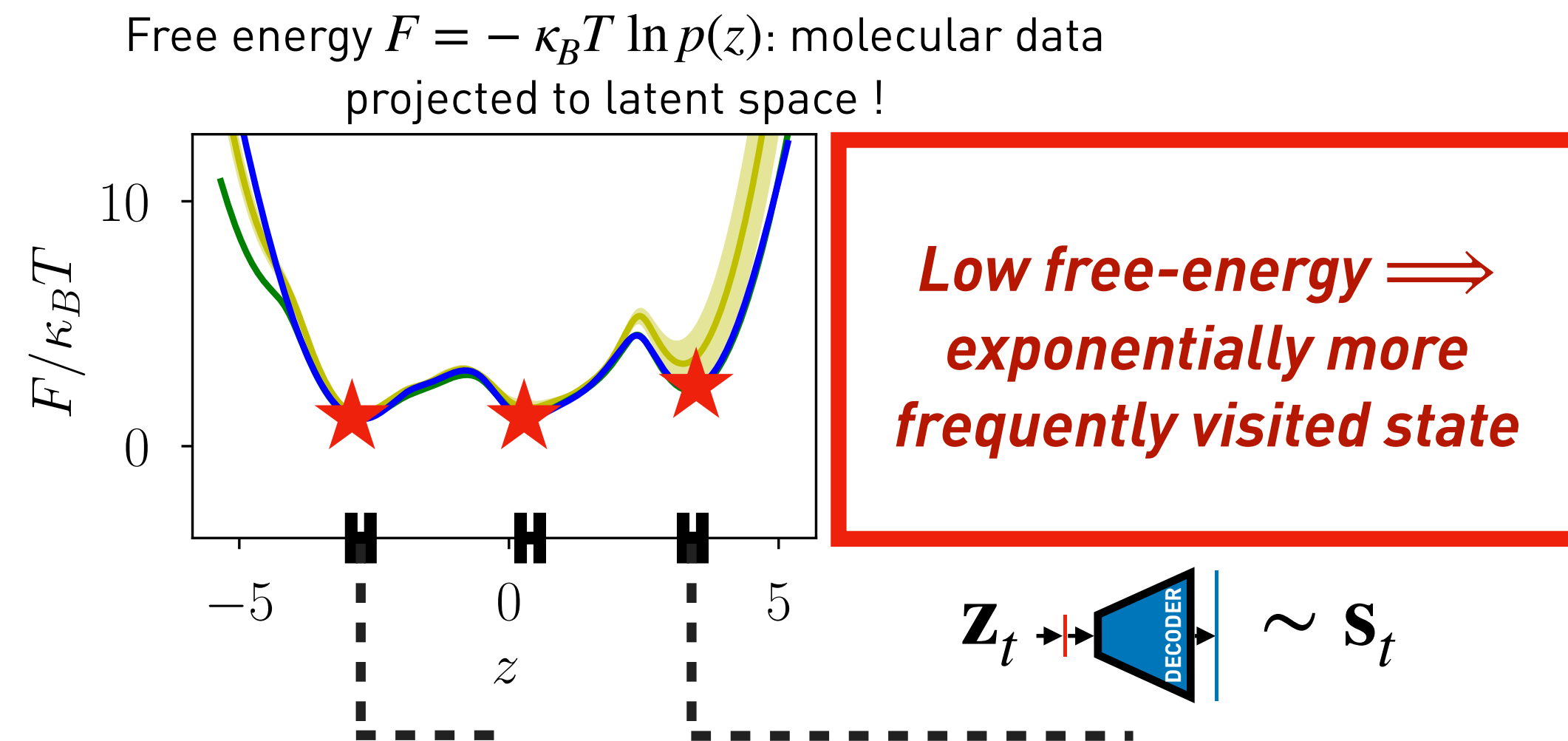
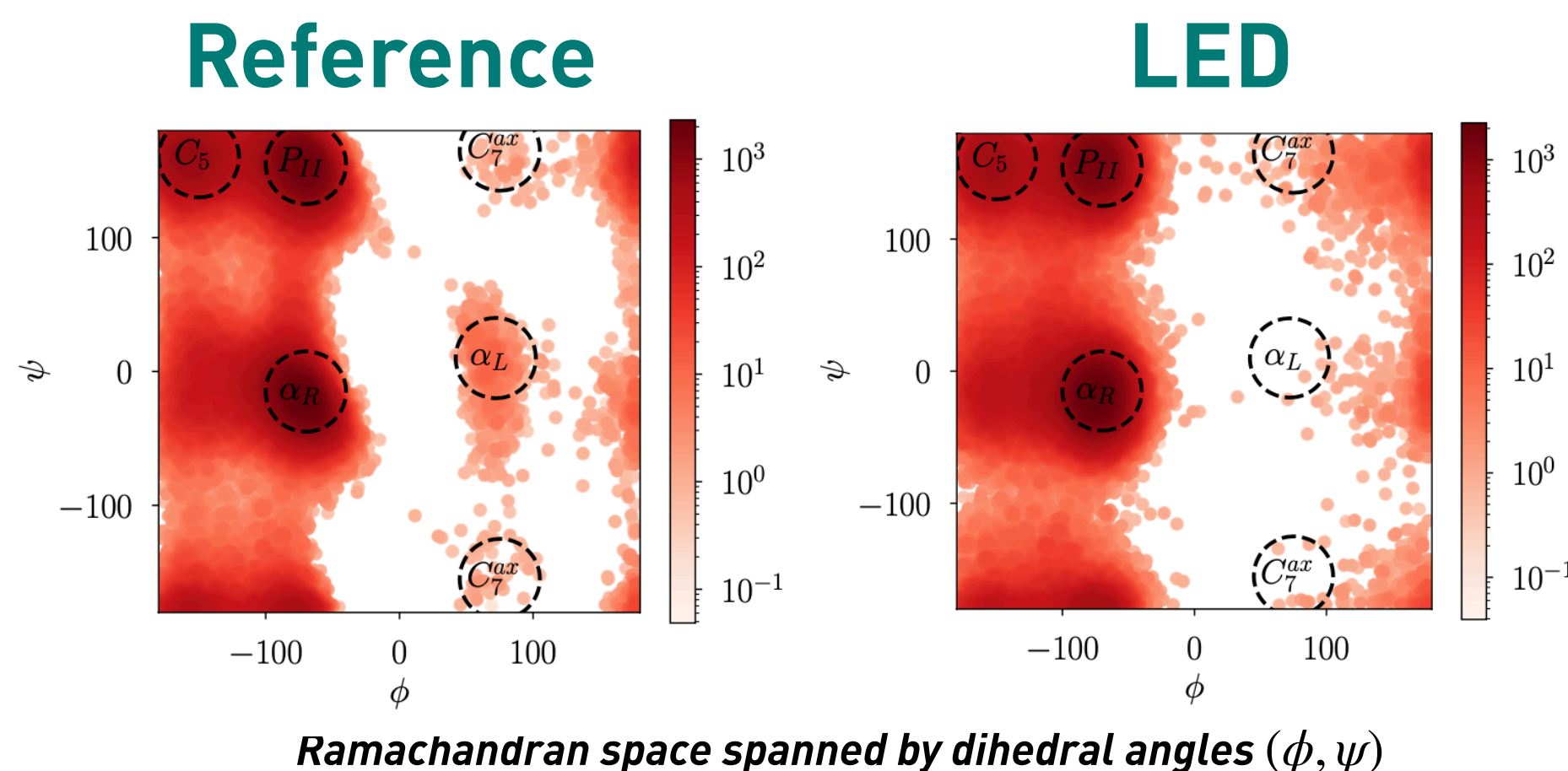
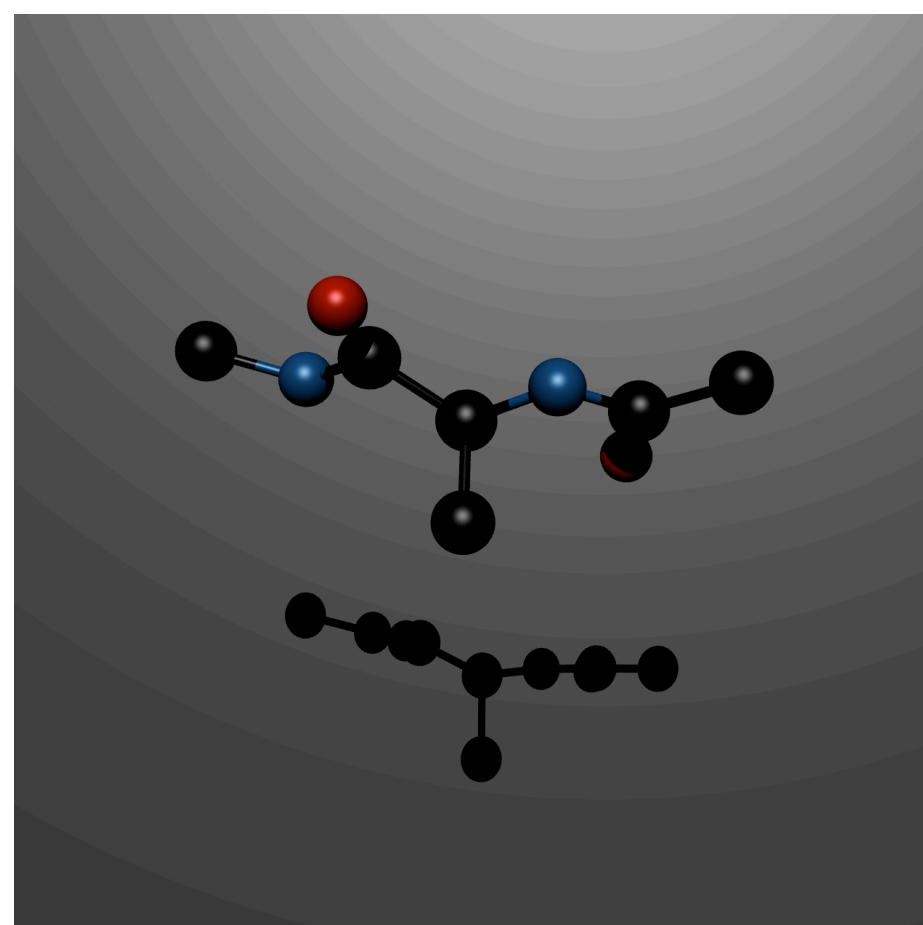


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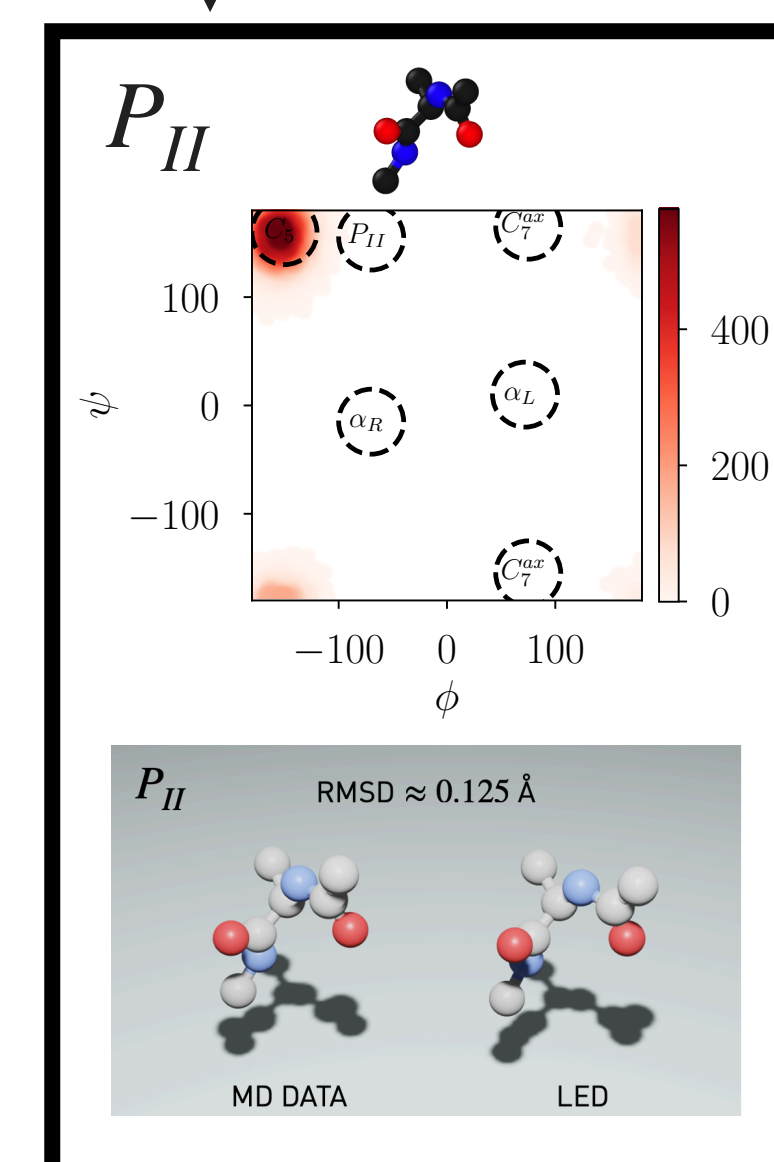
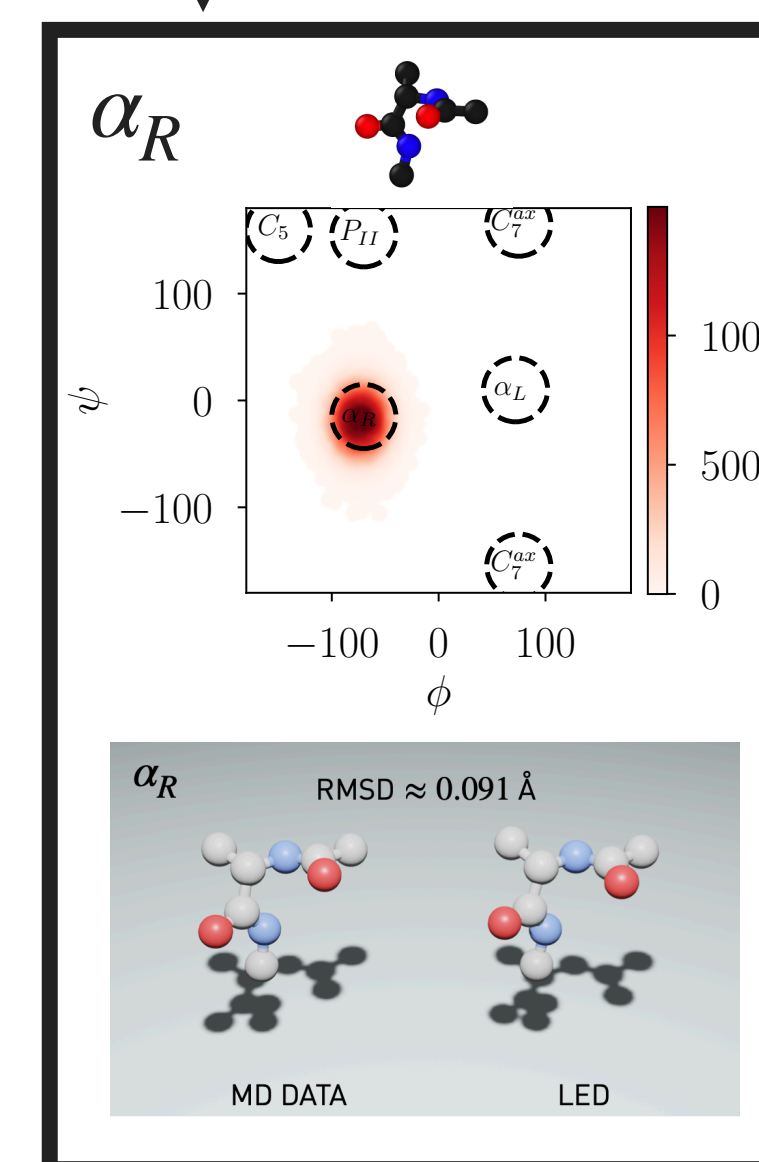


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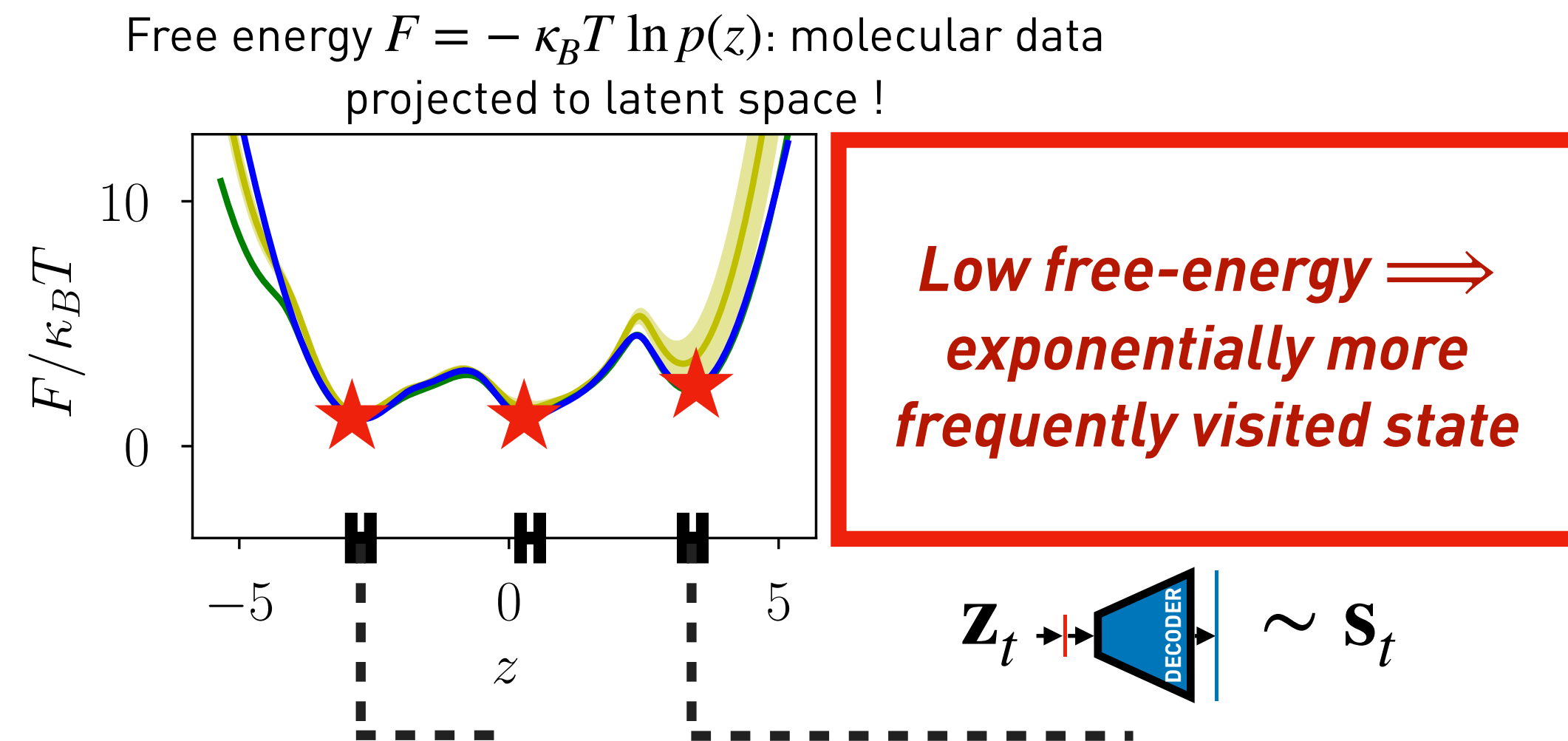
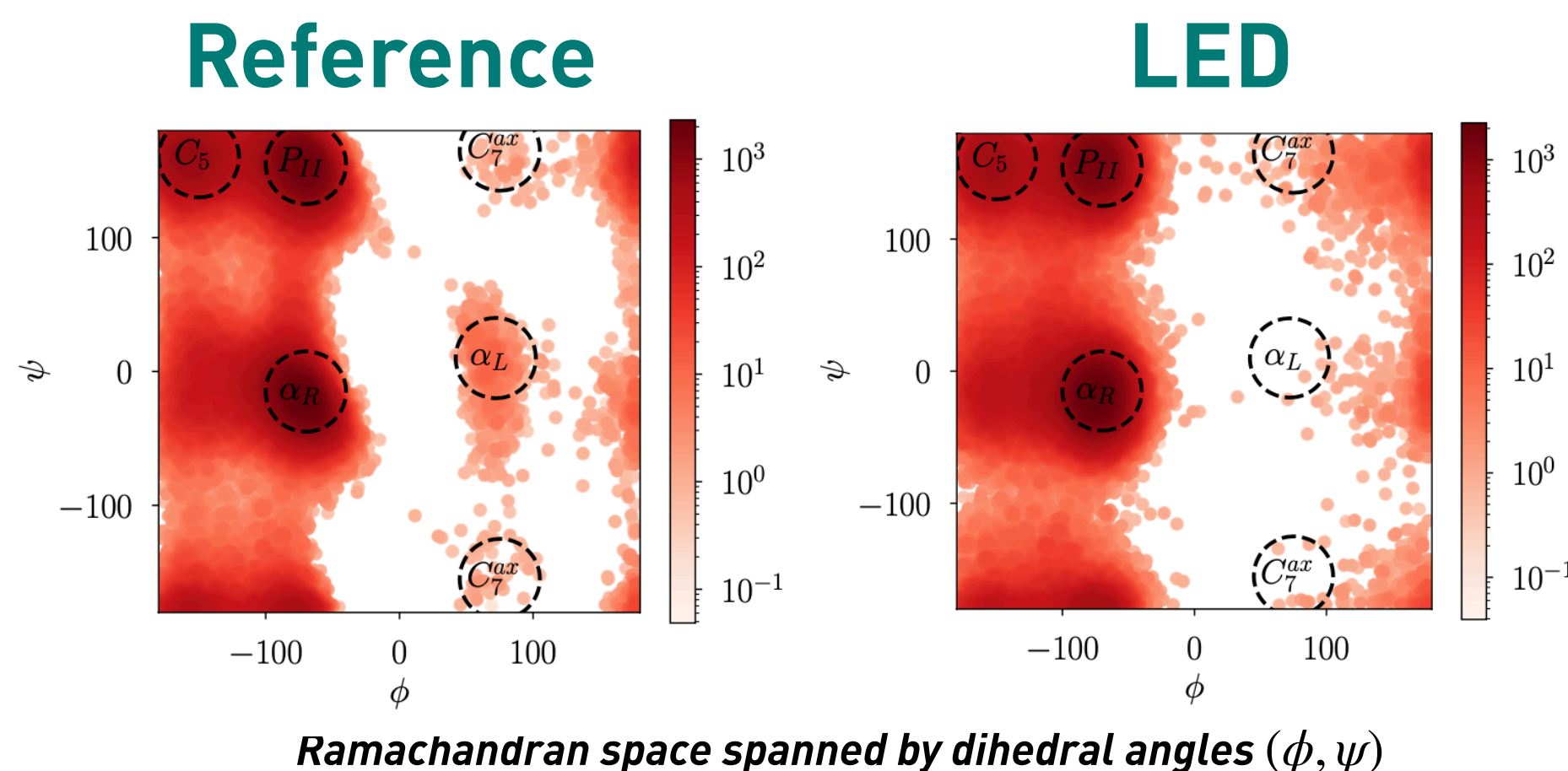
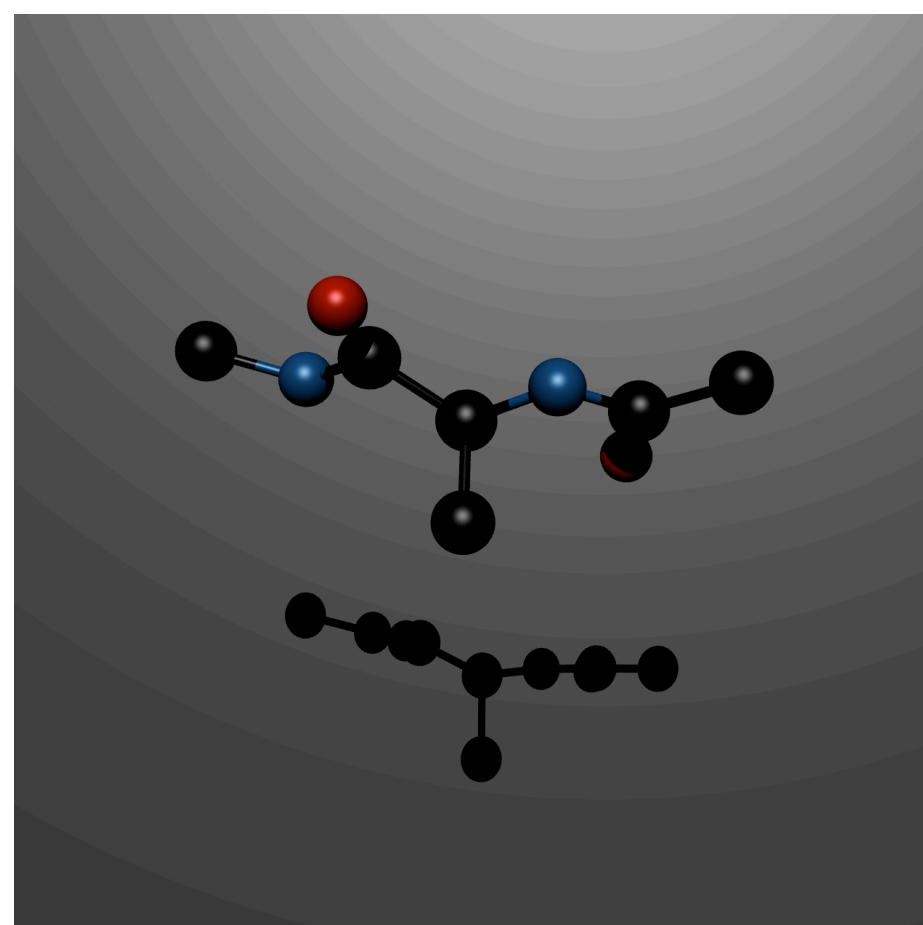
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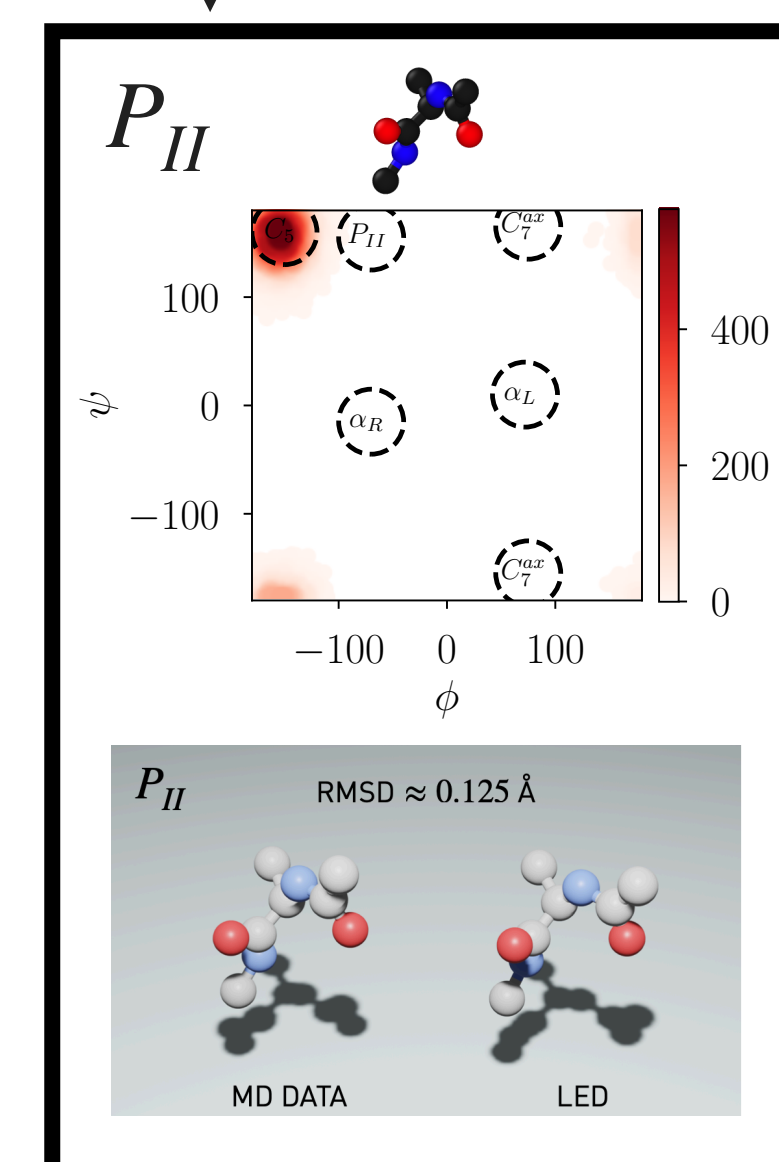
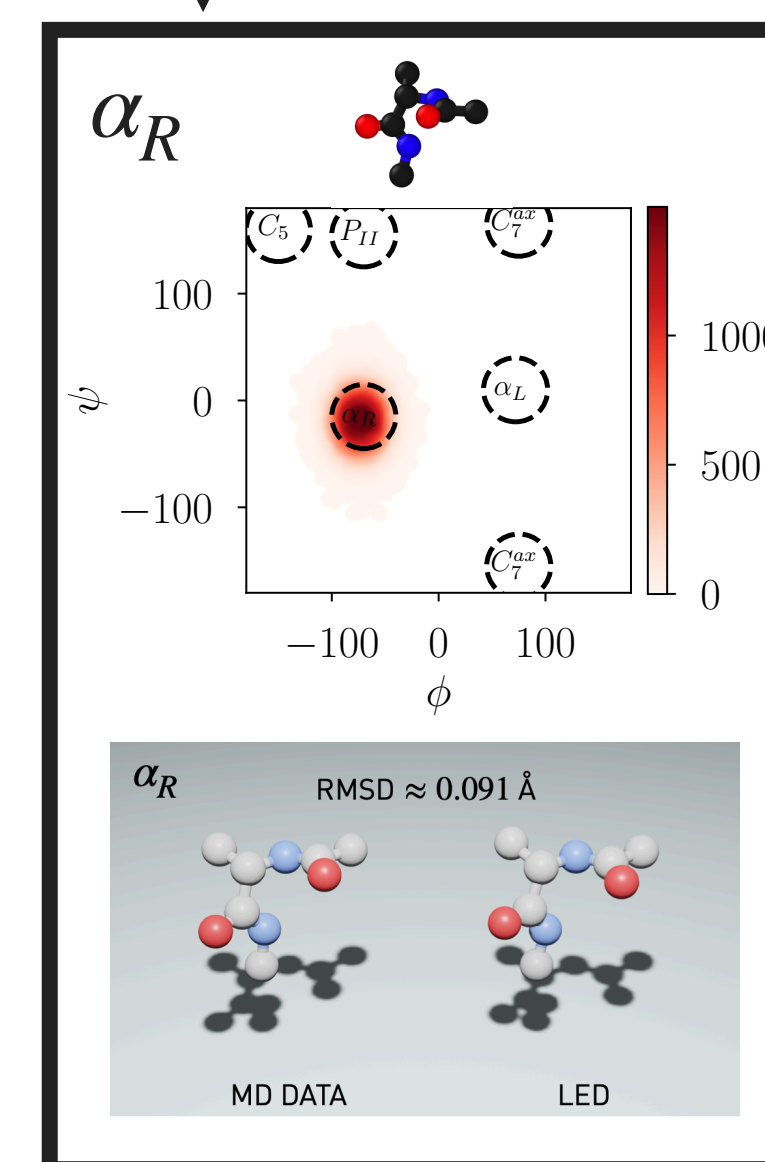


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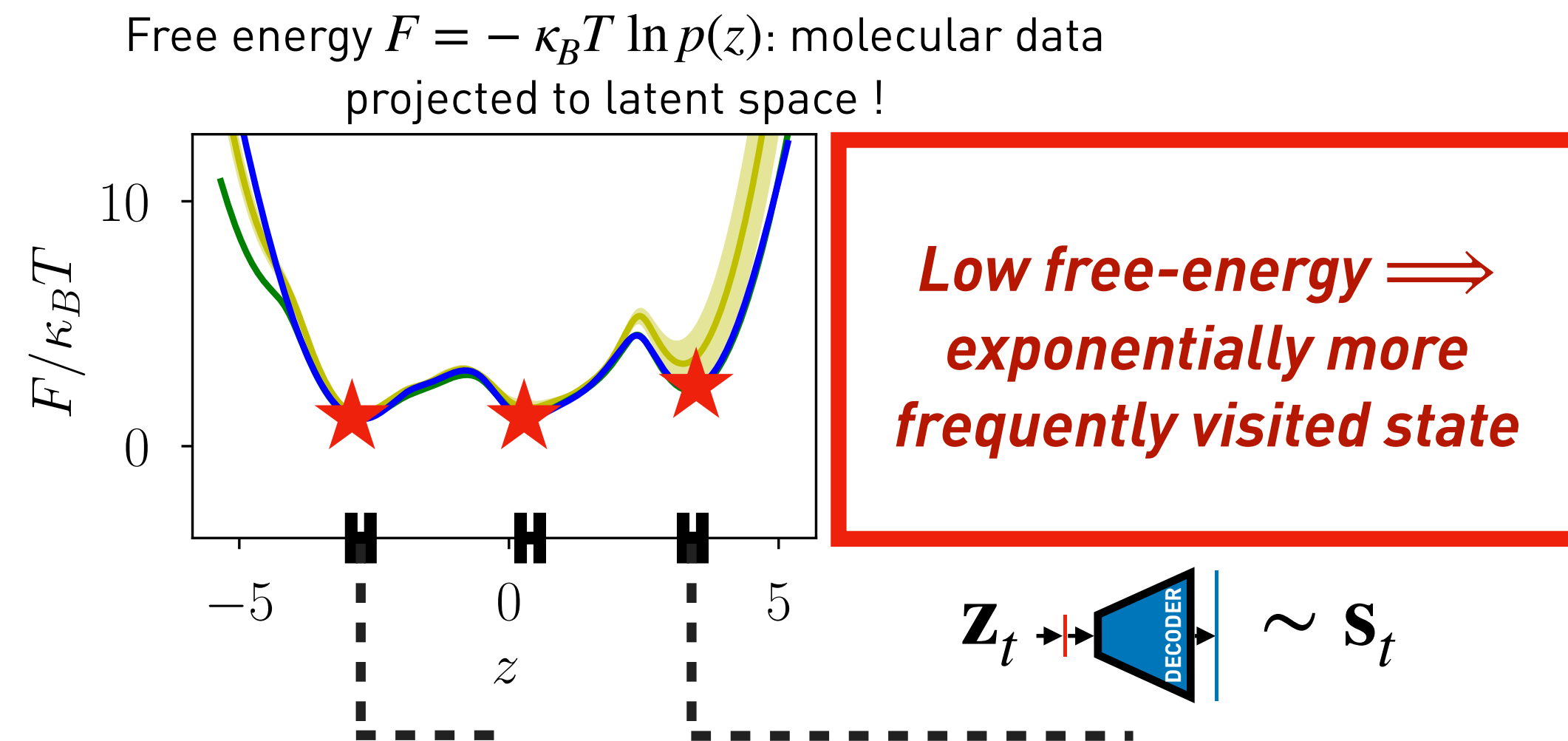
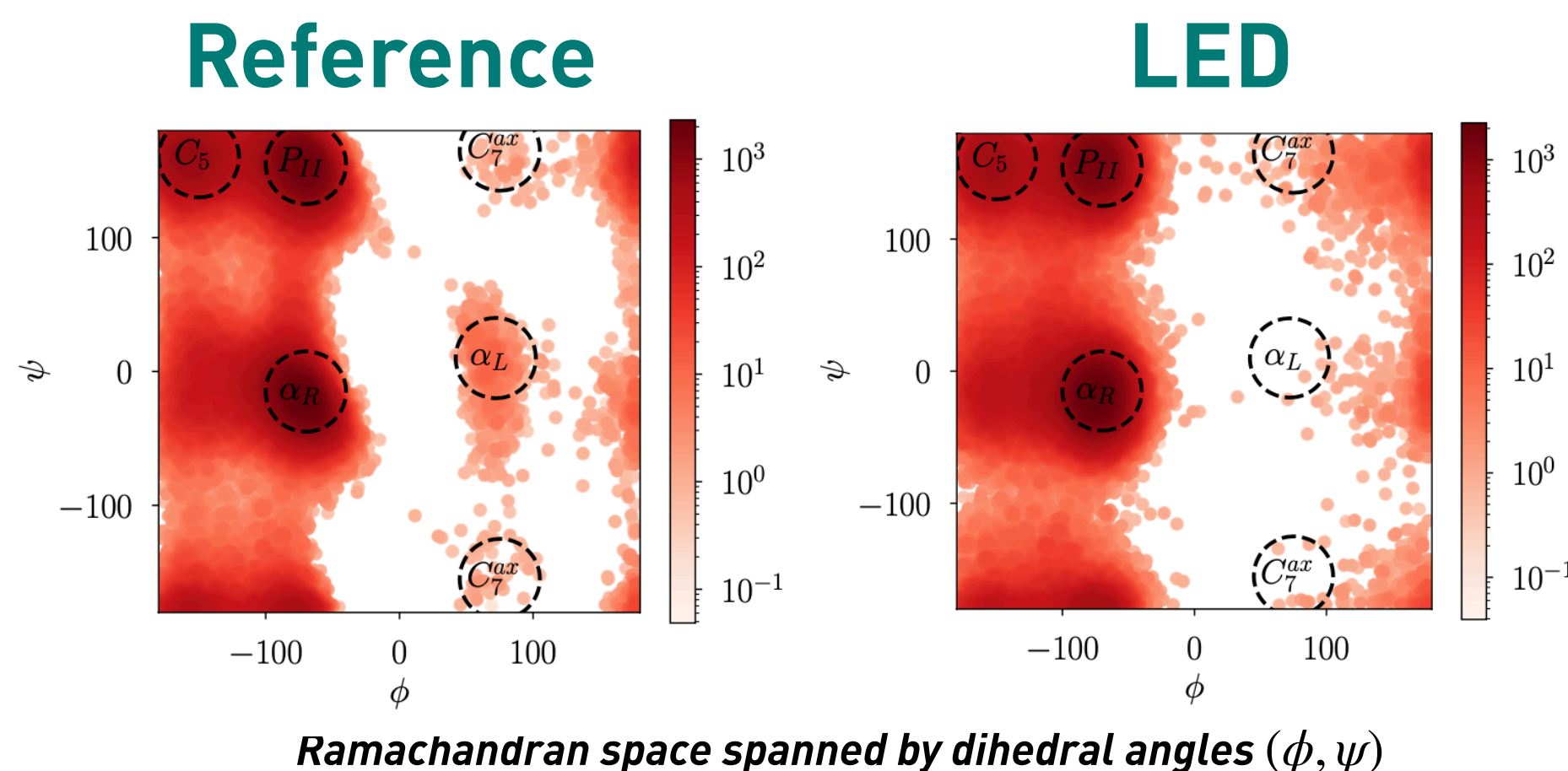
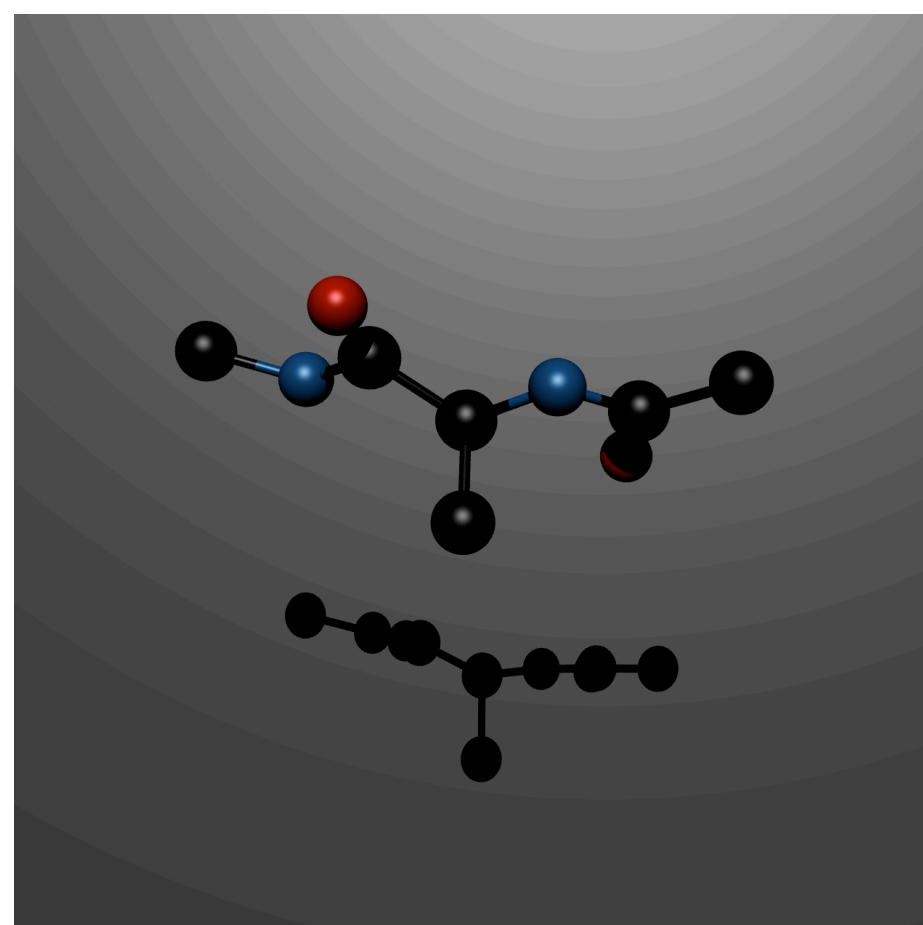
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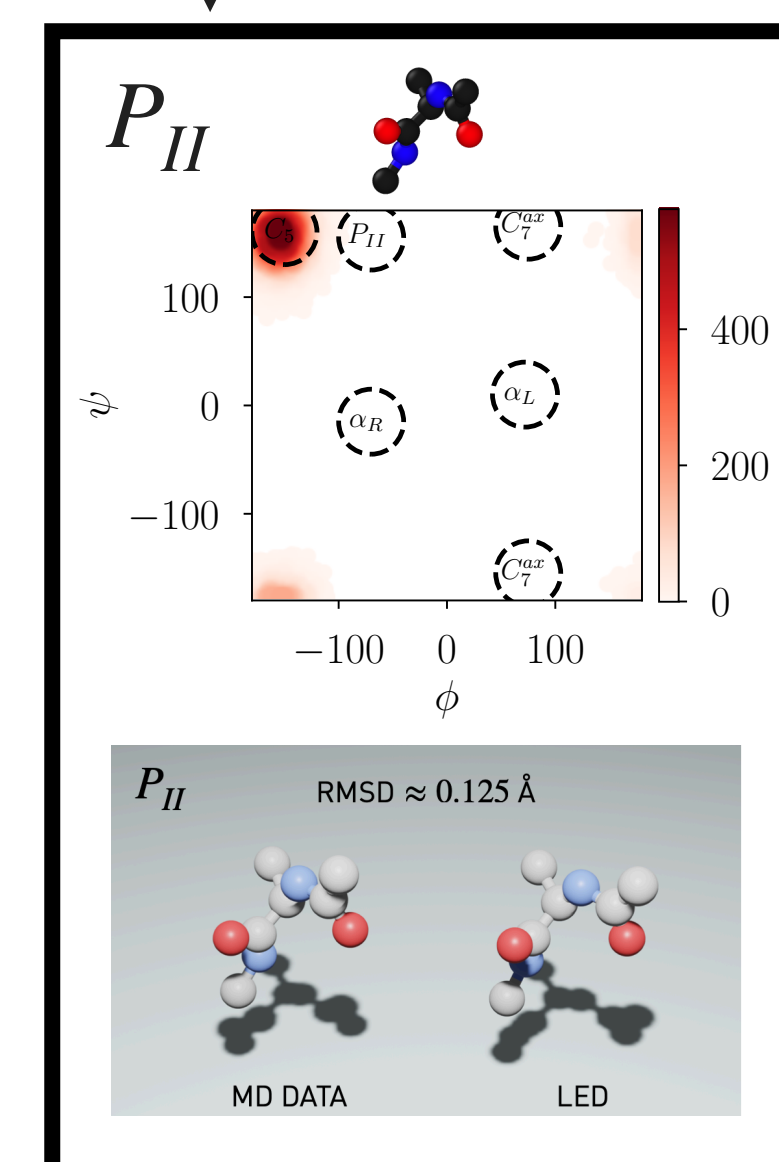
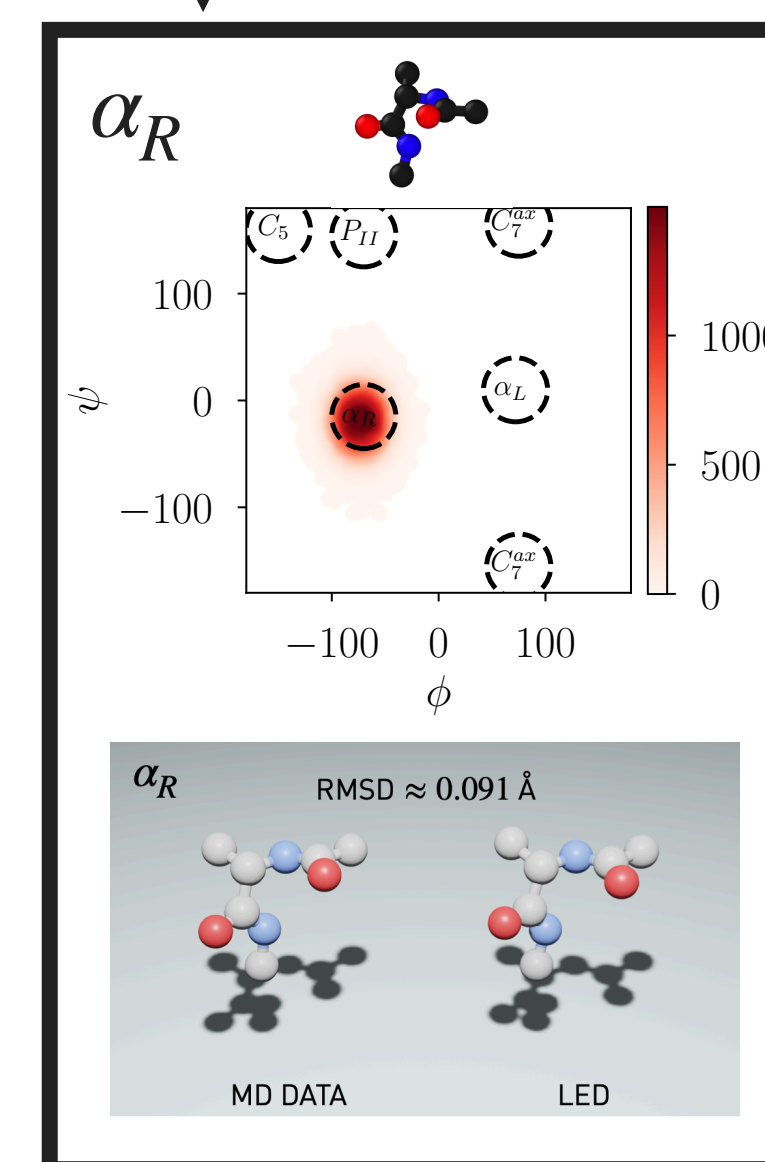


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# Avenues for Future Research

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*Ivica Kičić*

*George Arampatzis*

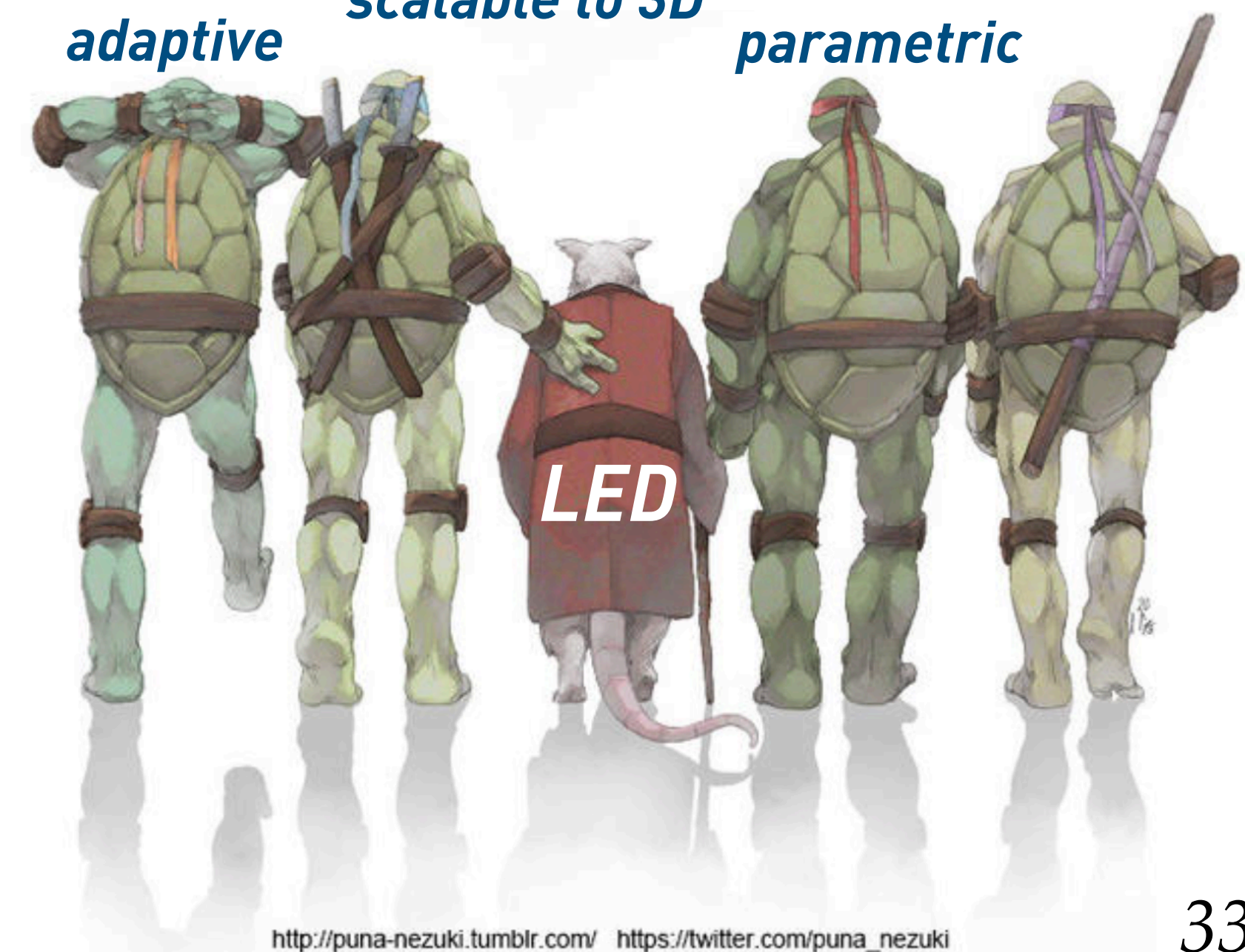
**AdaLED**

*uncertainty  
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*scalable to 3D*

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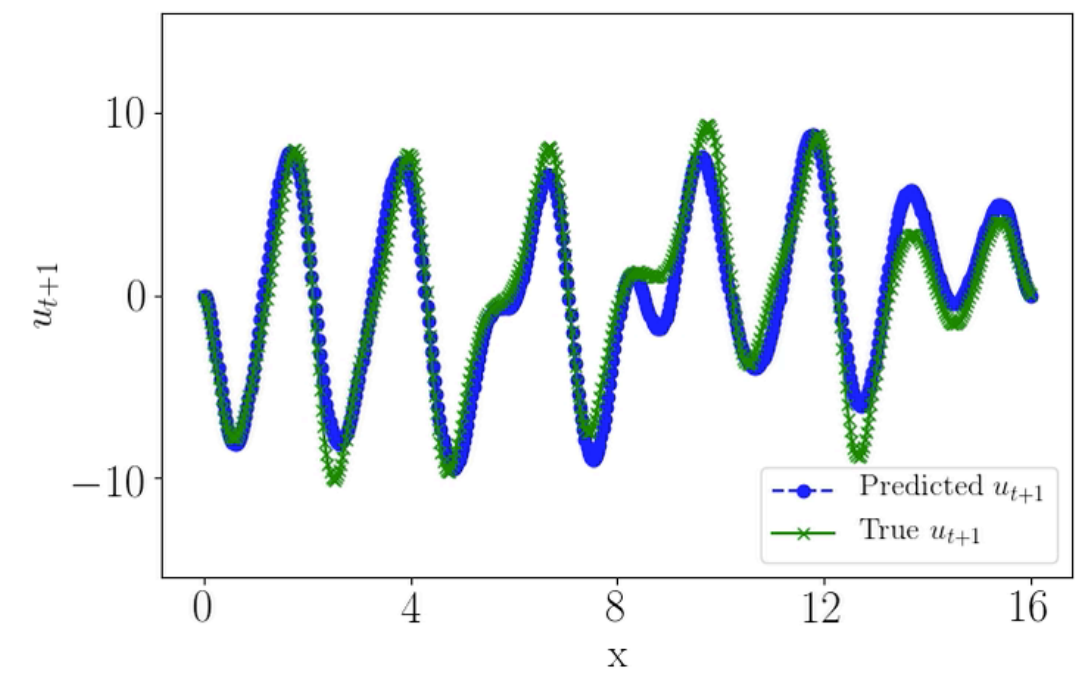
*parametric*









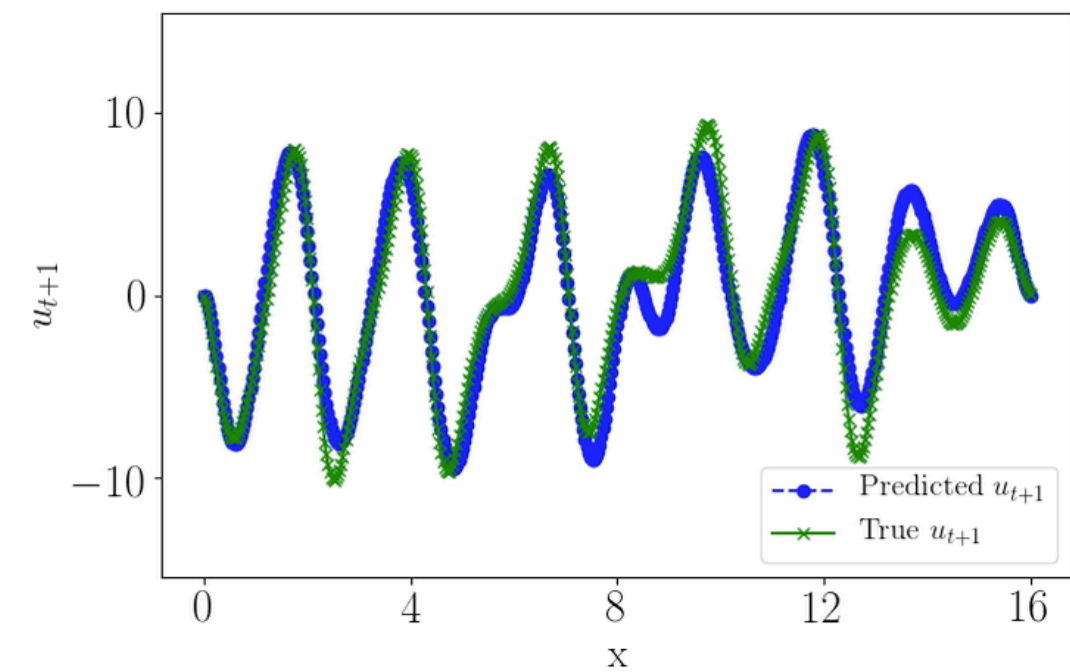


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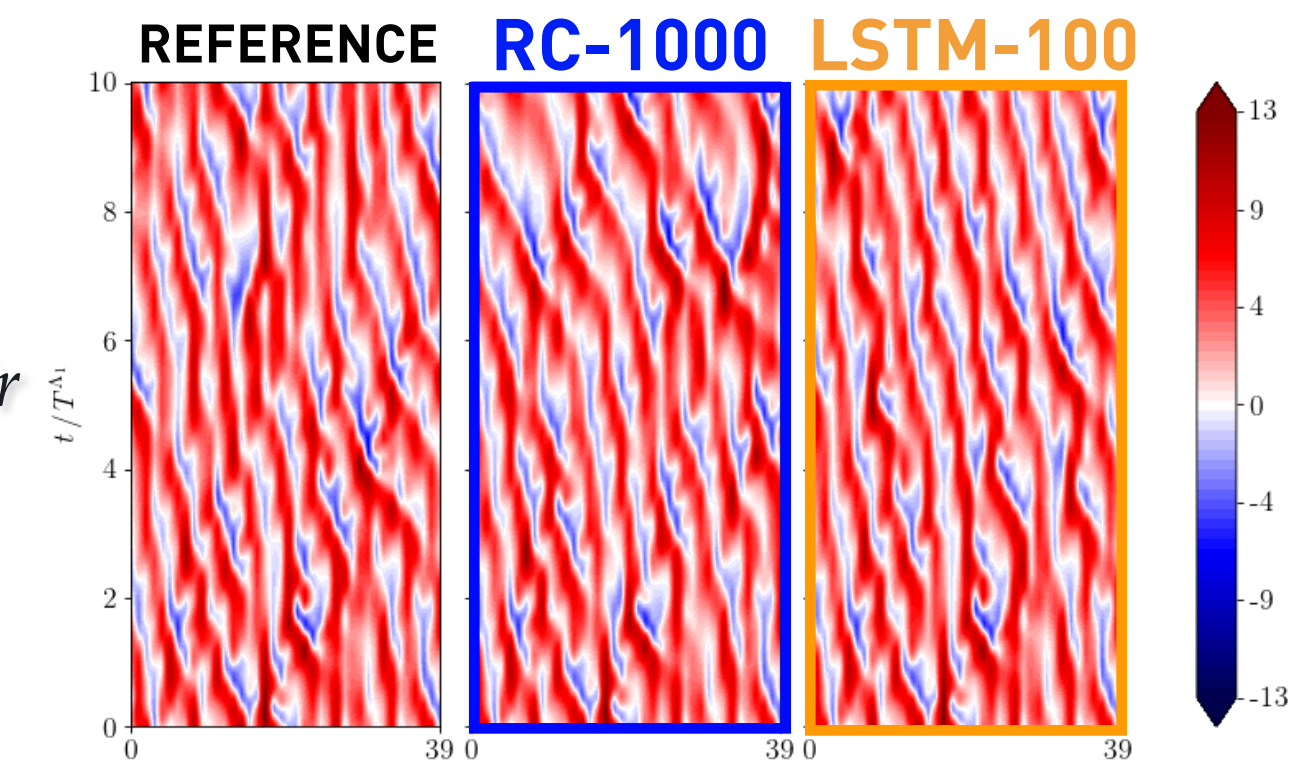


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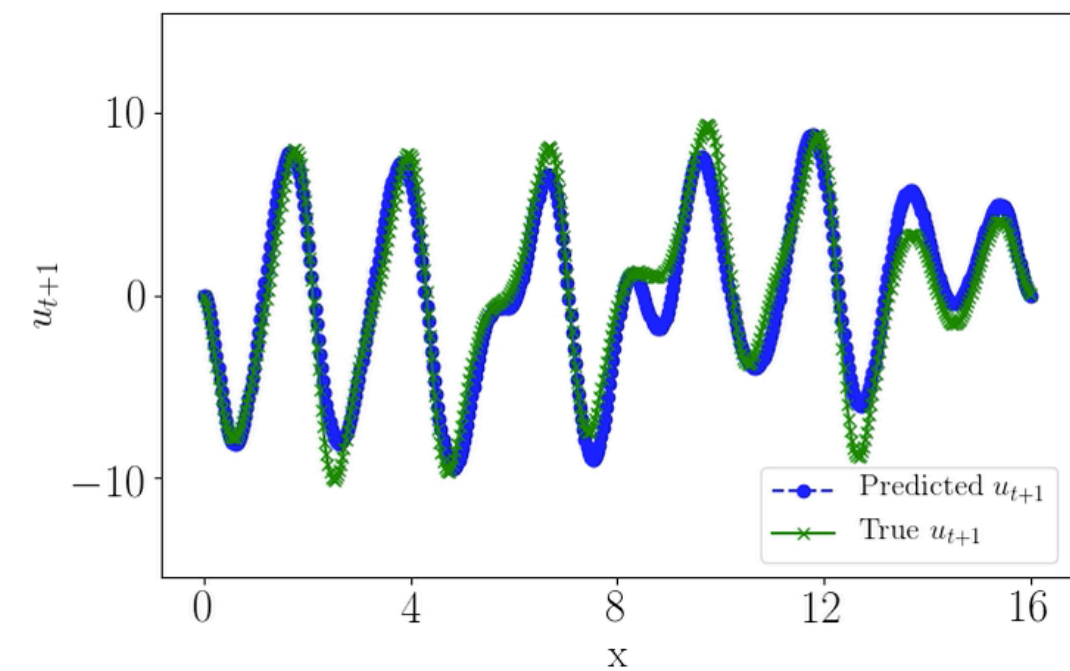
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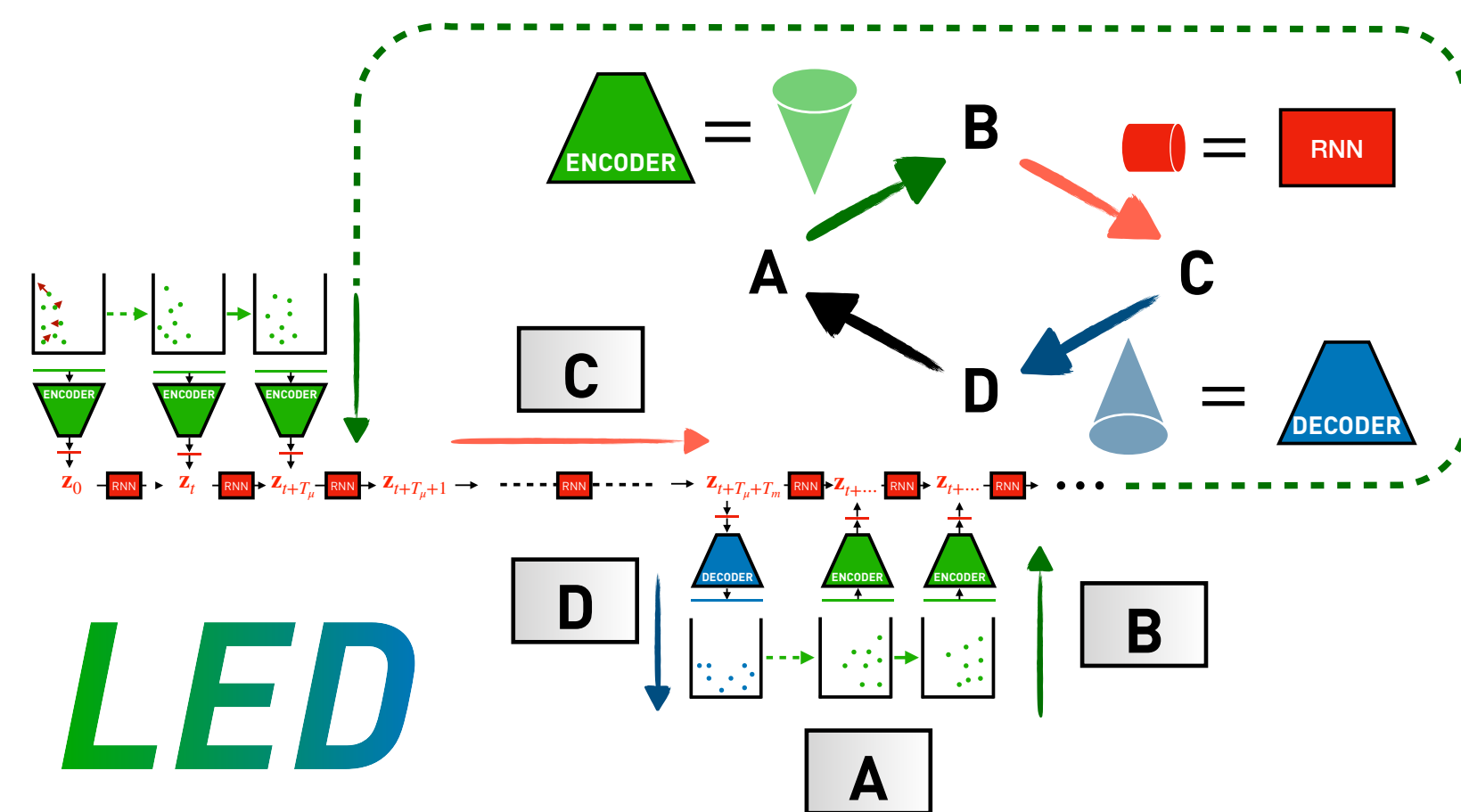
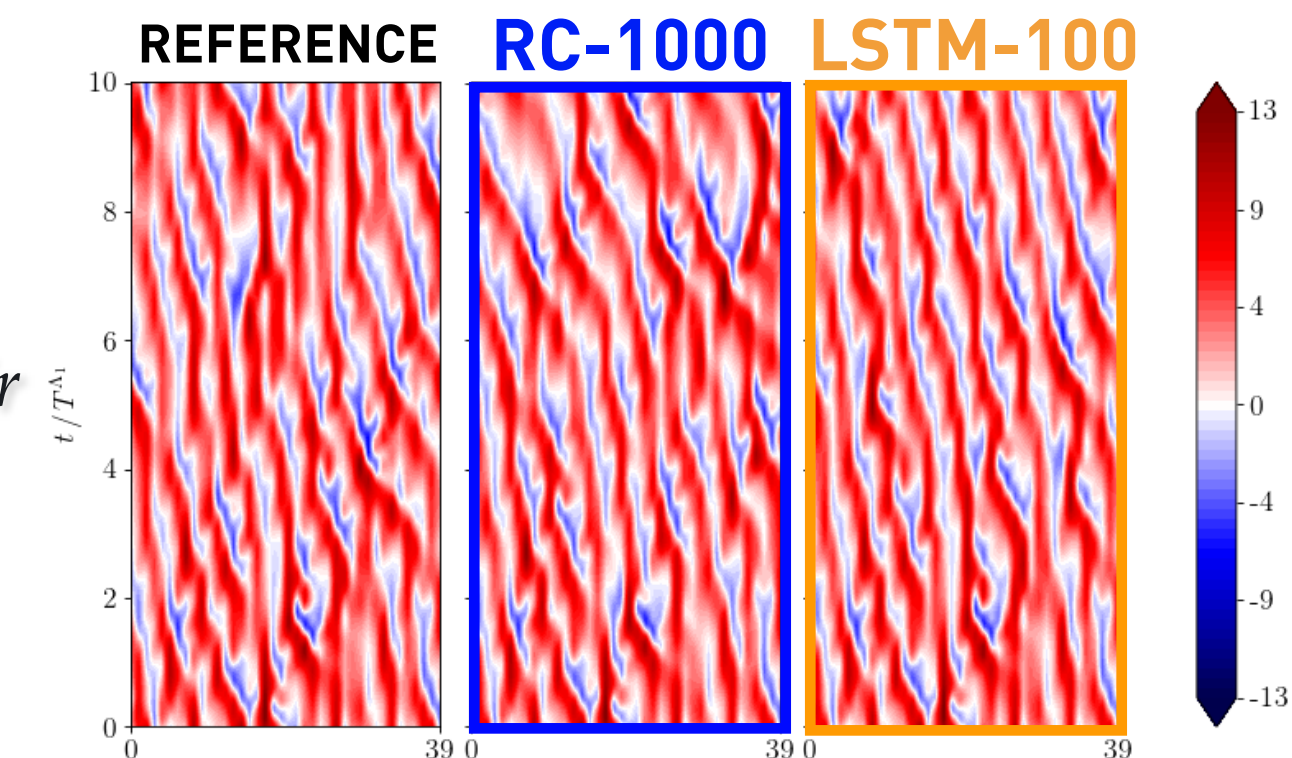


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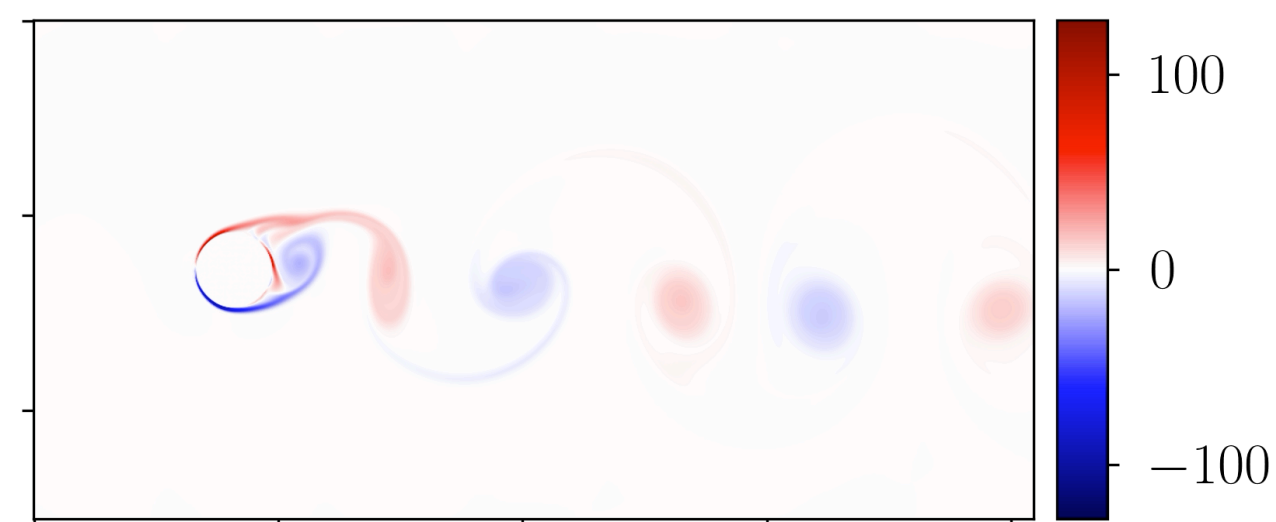
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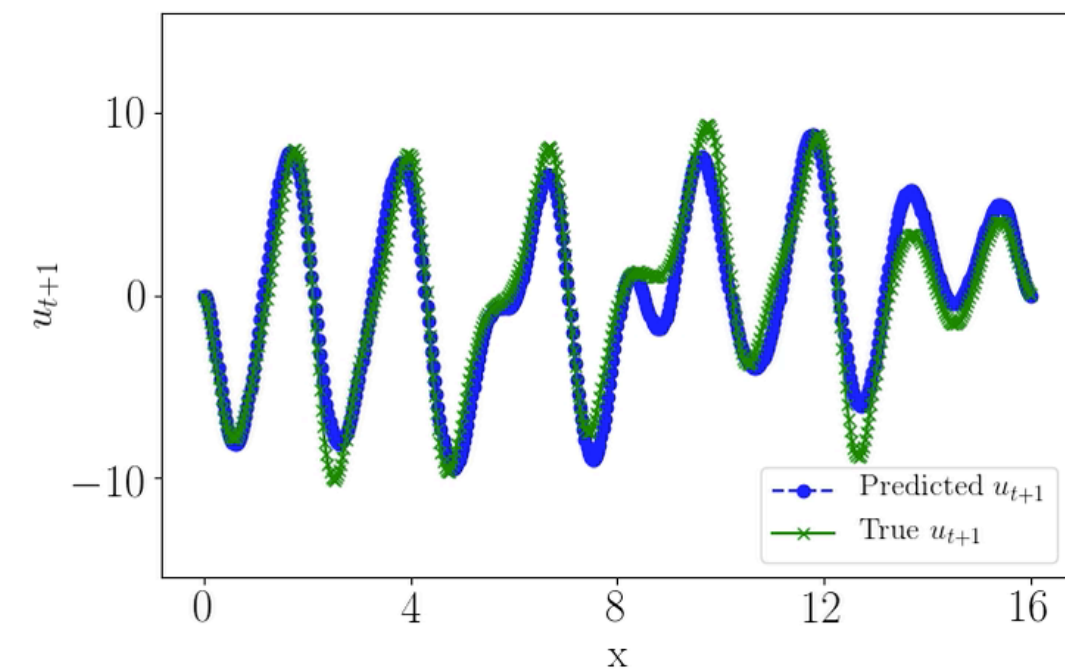
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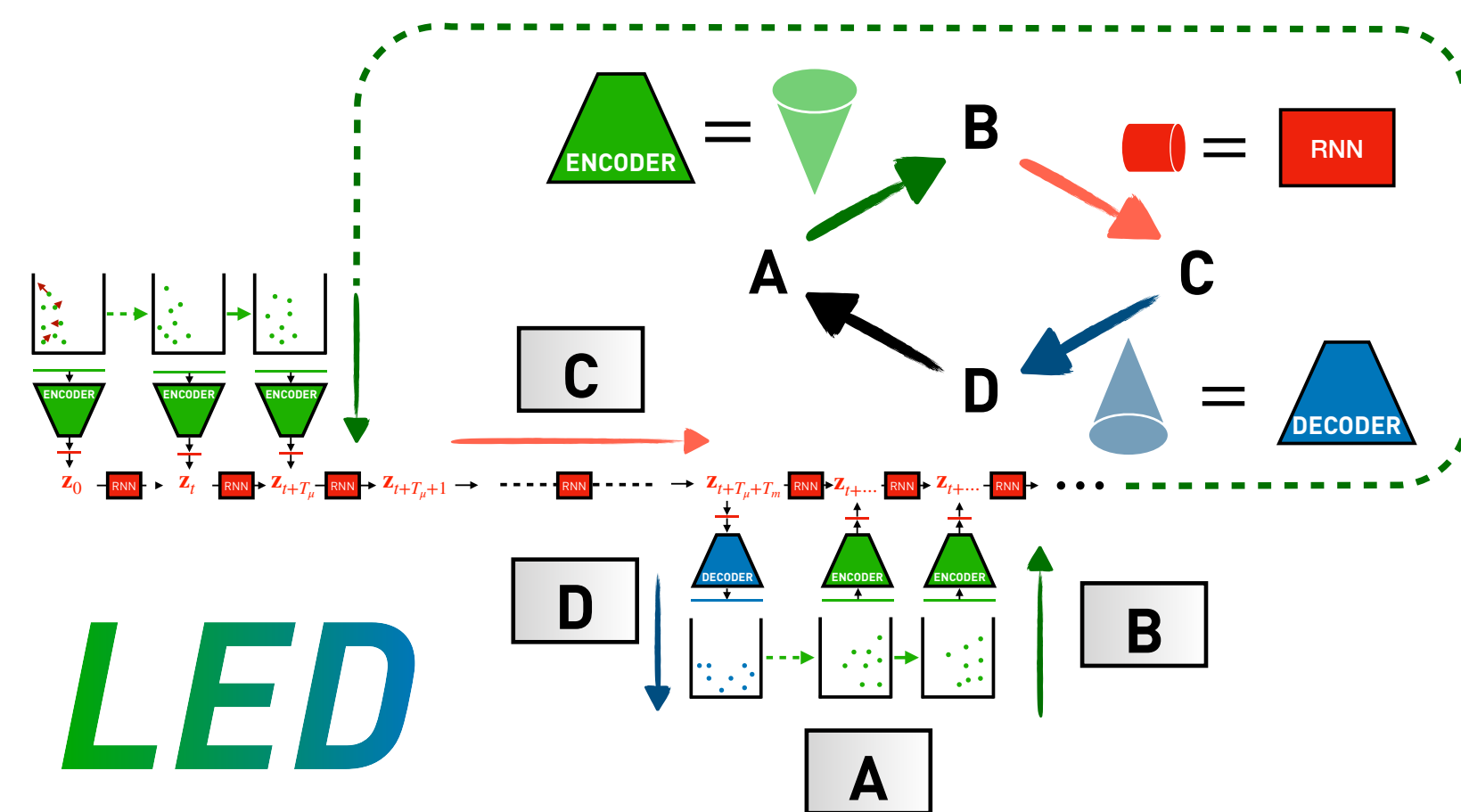
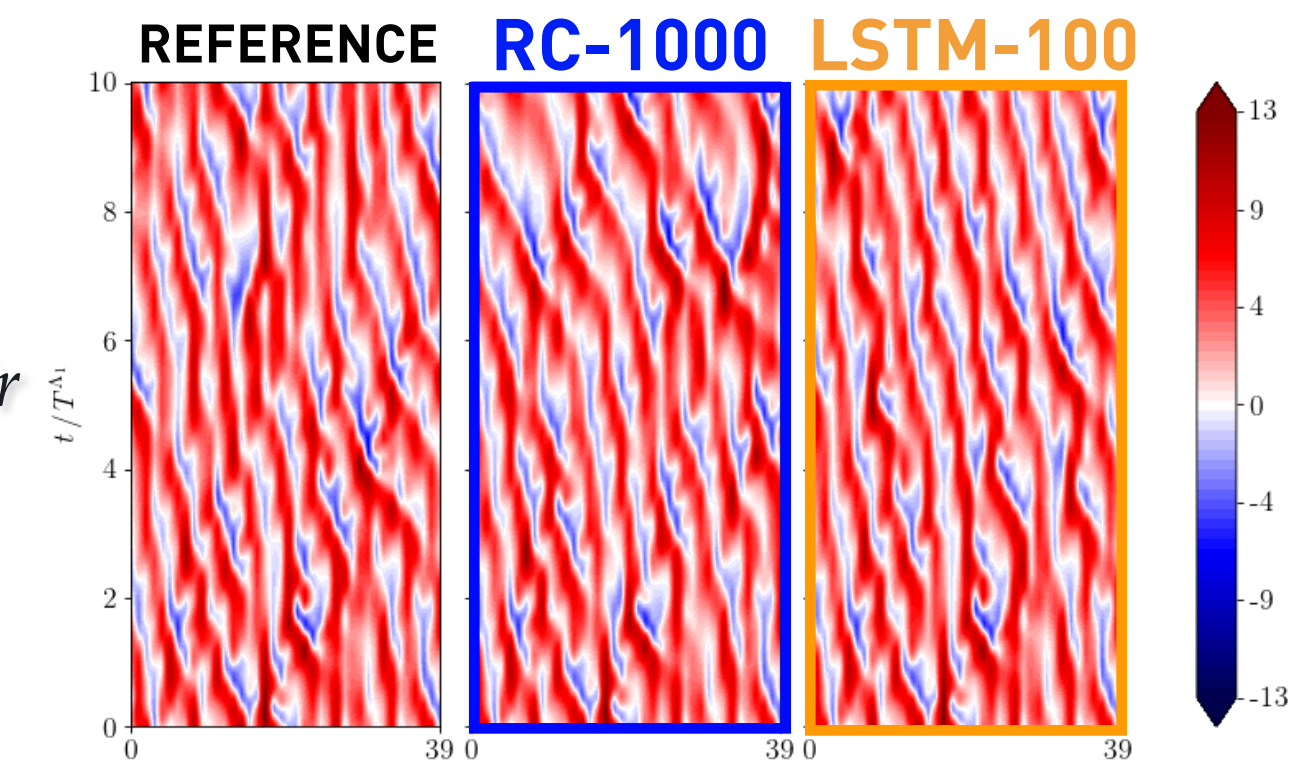


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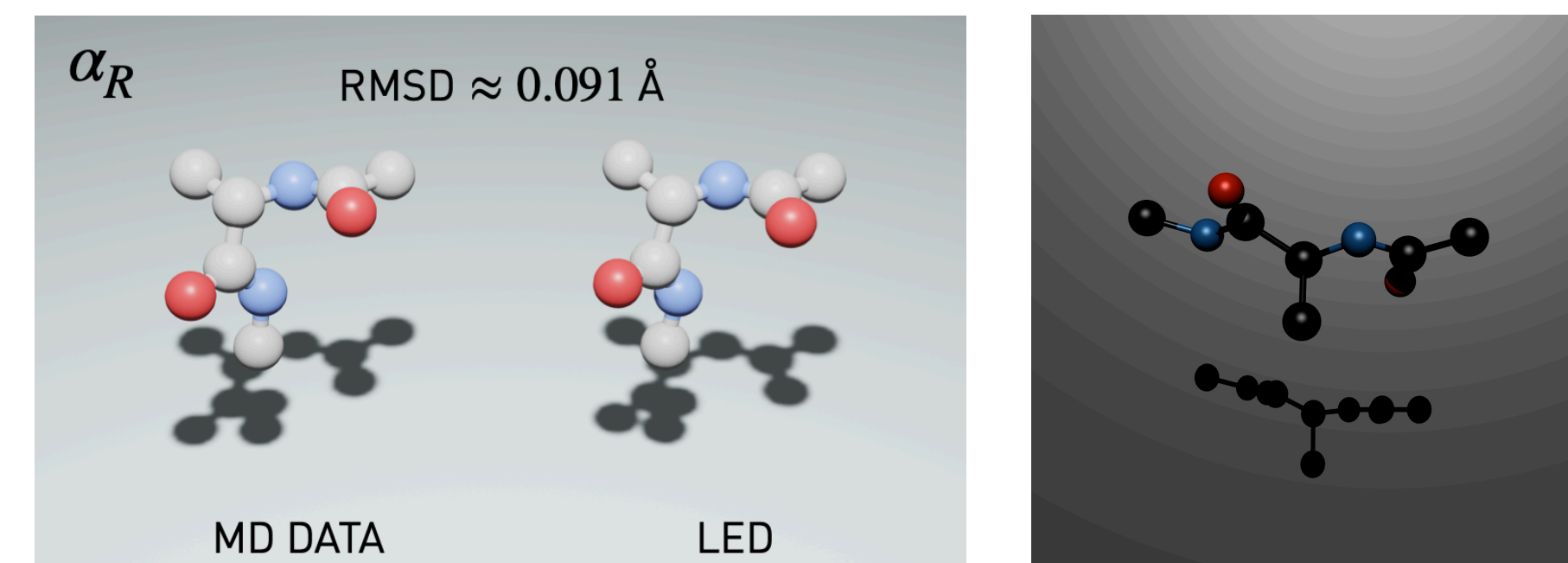
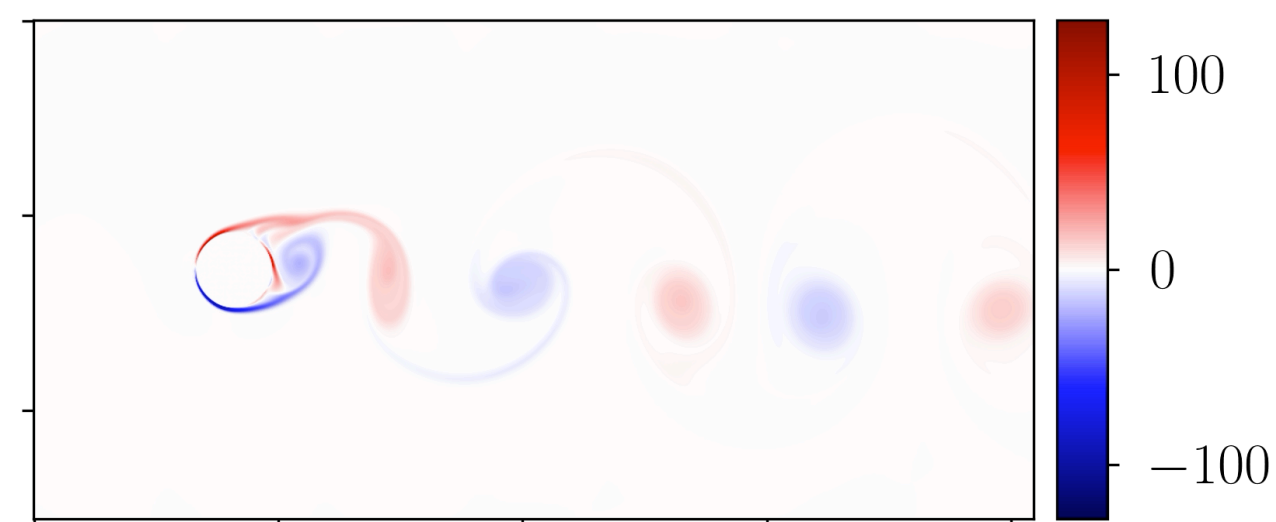
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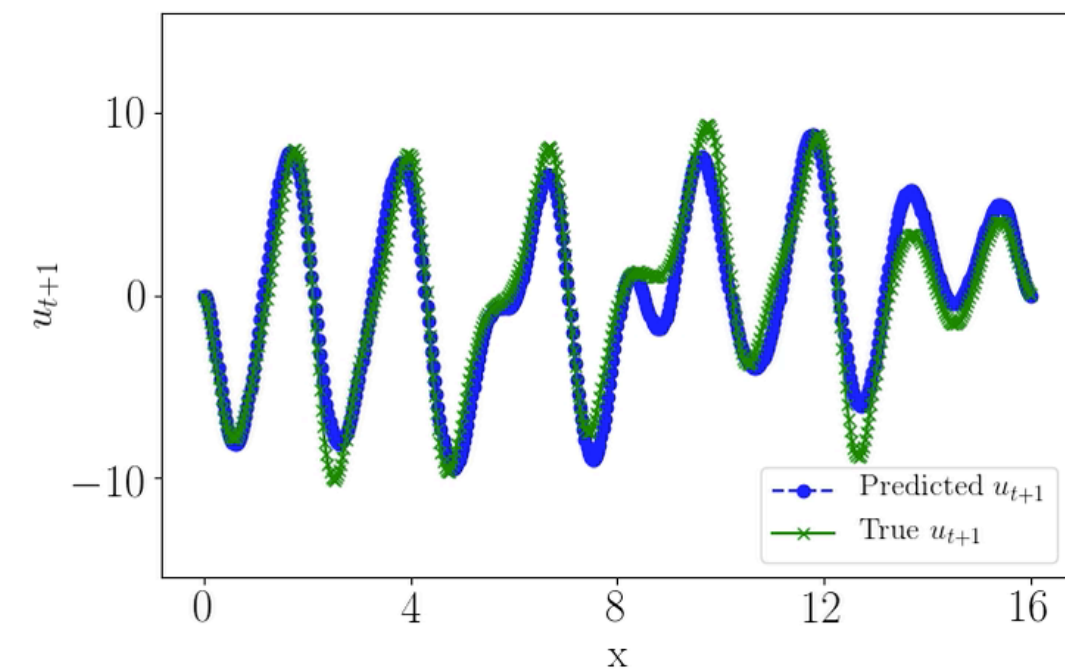


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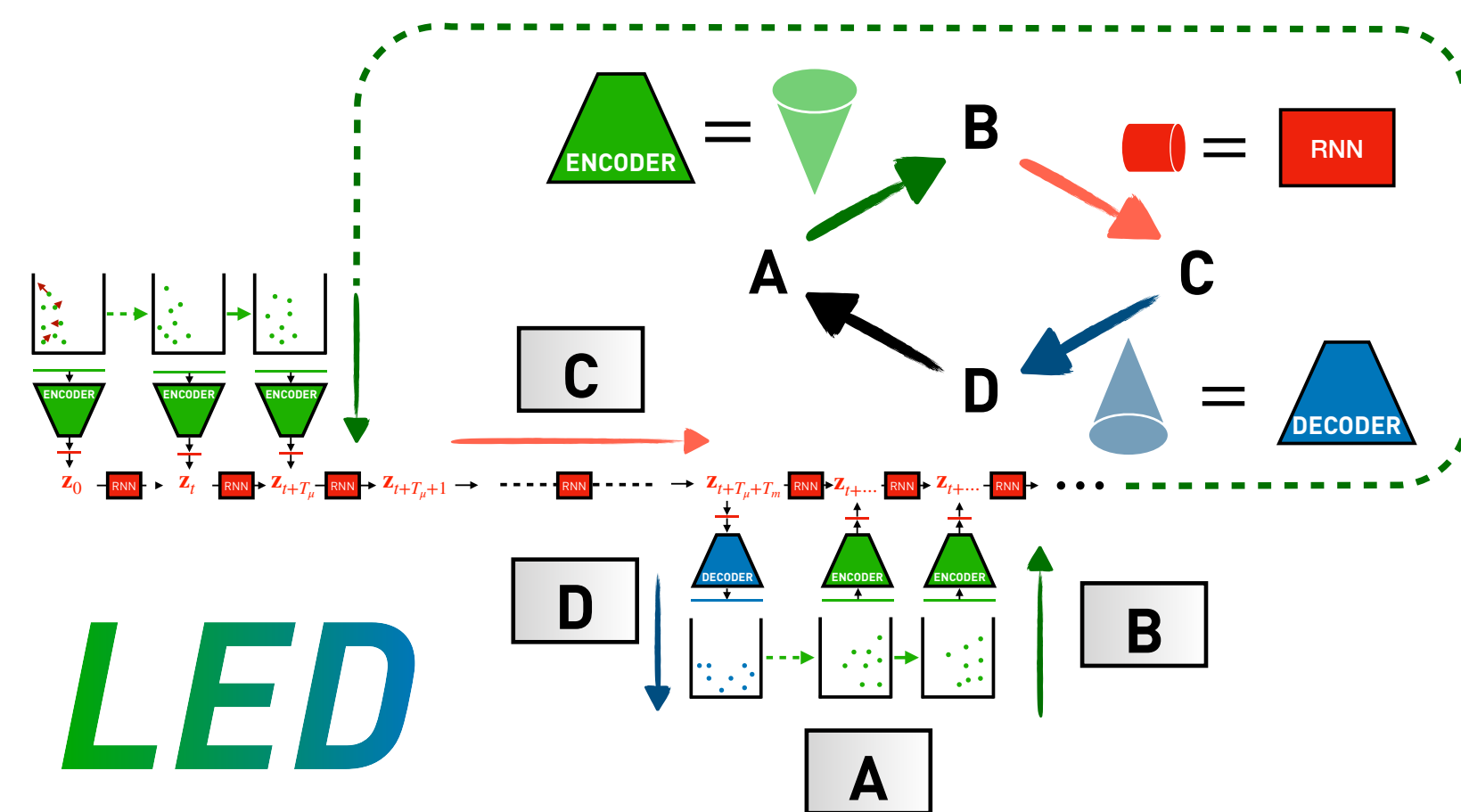
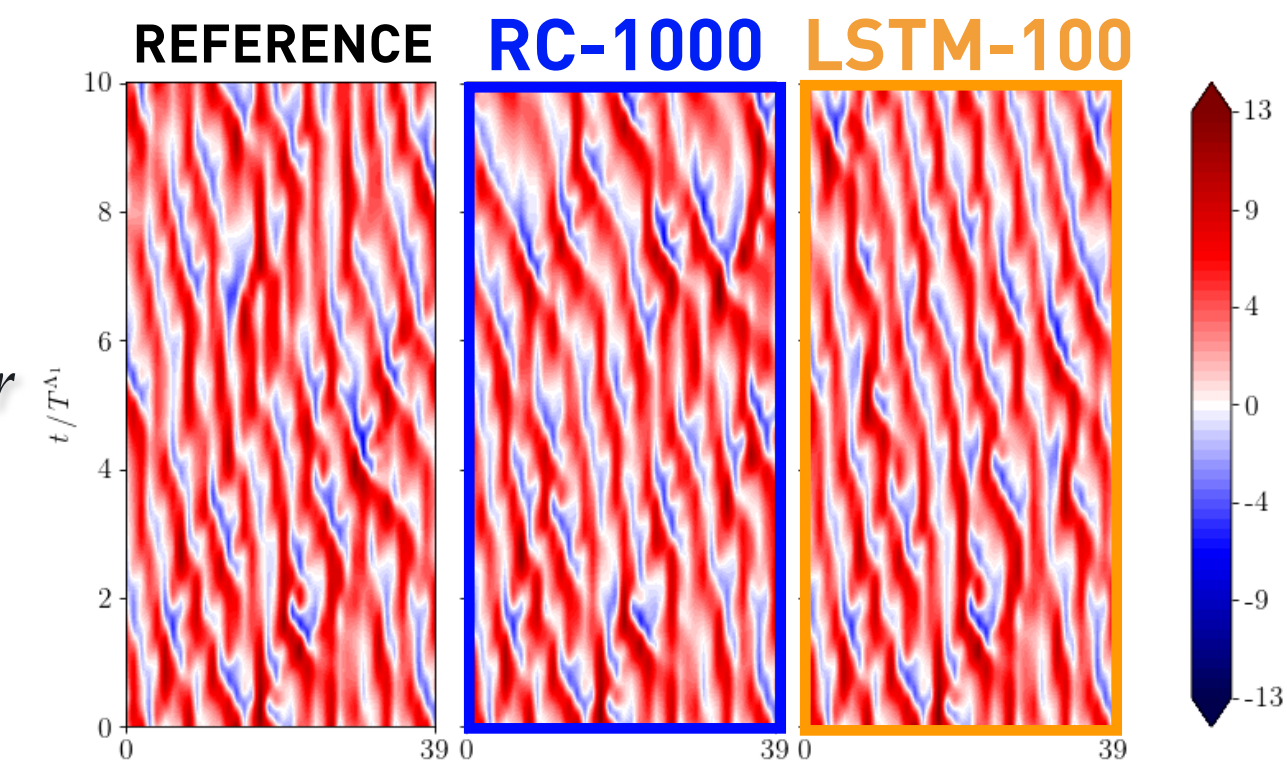


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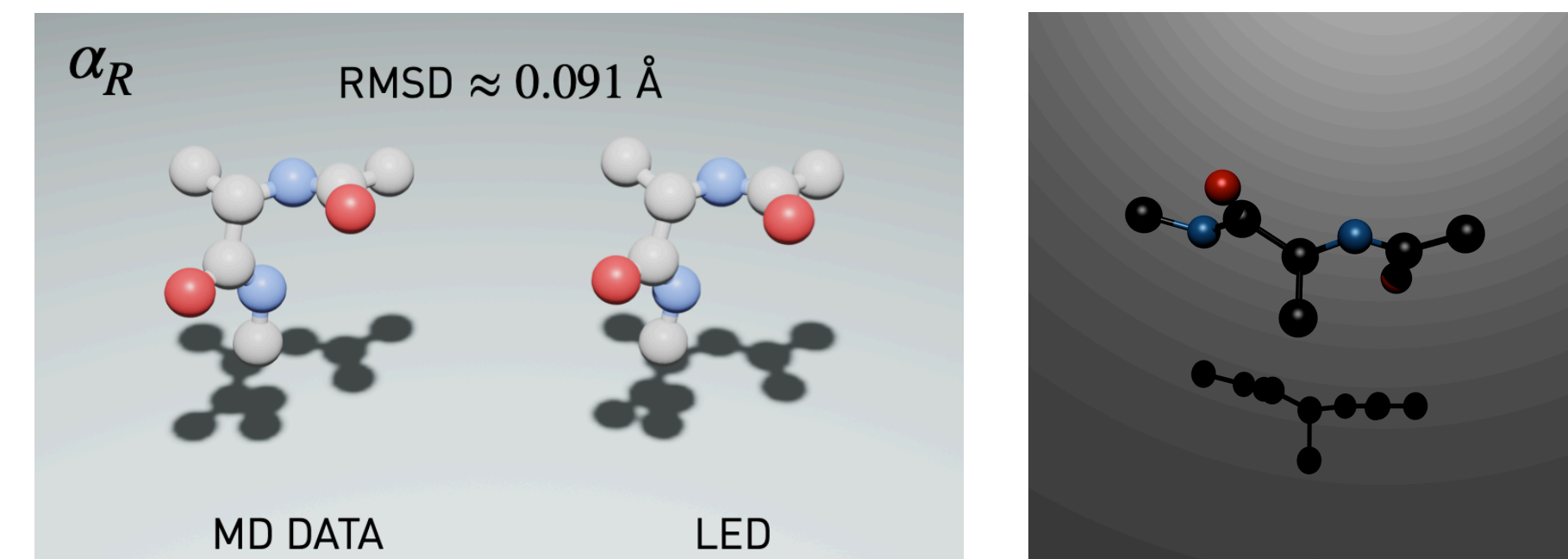
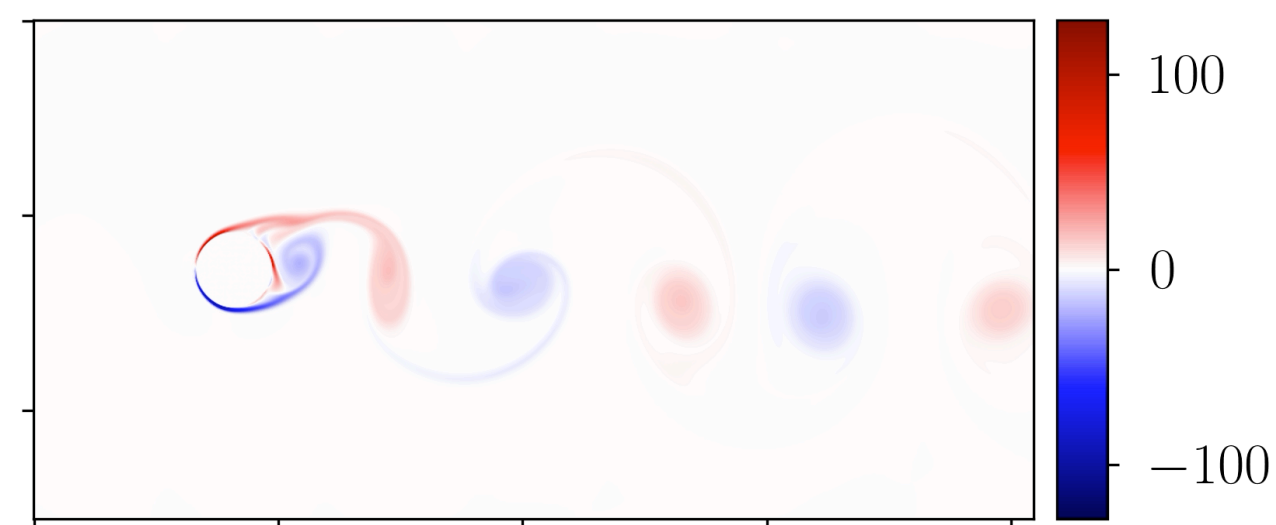
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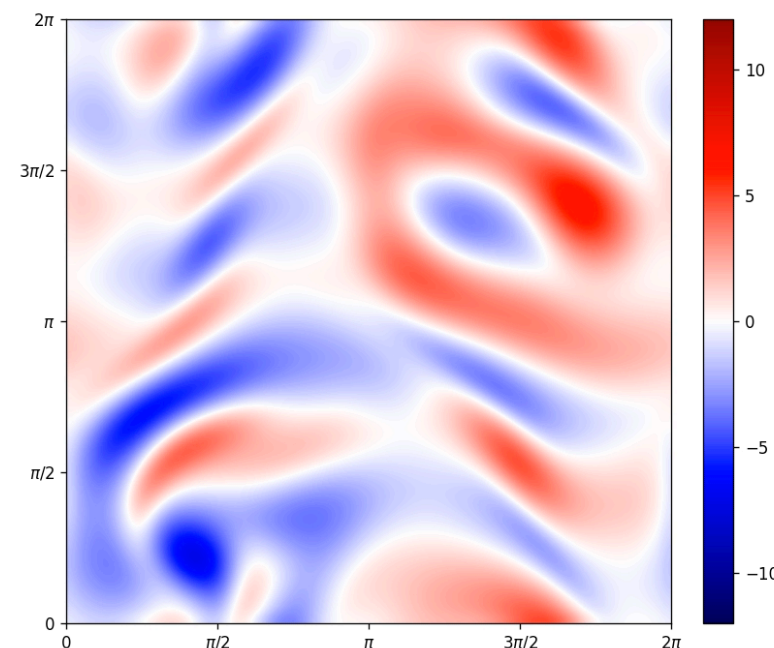
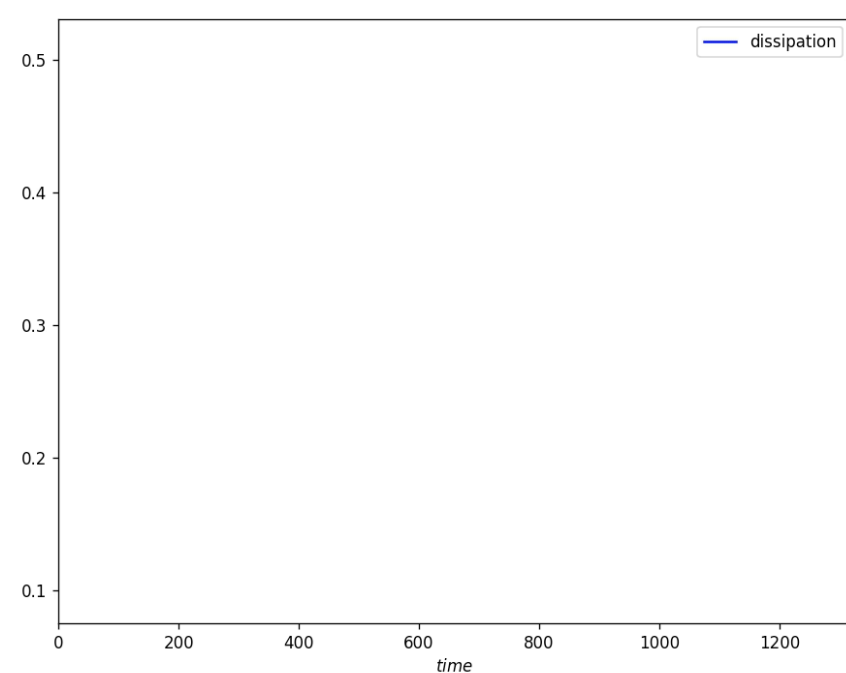
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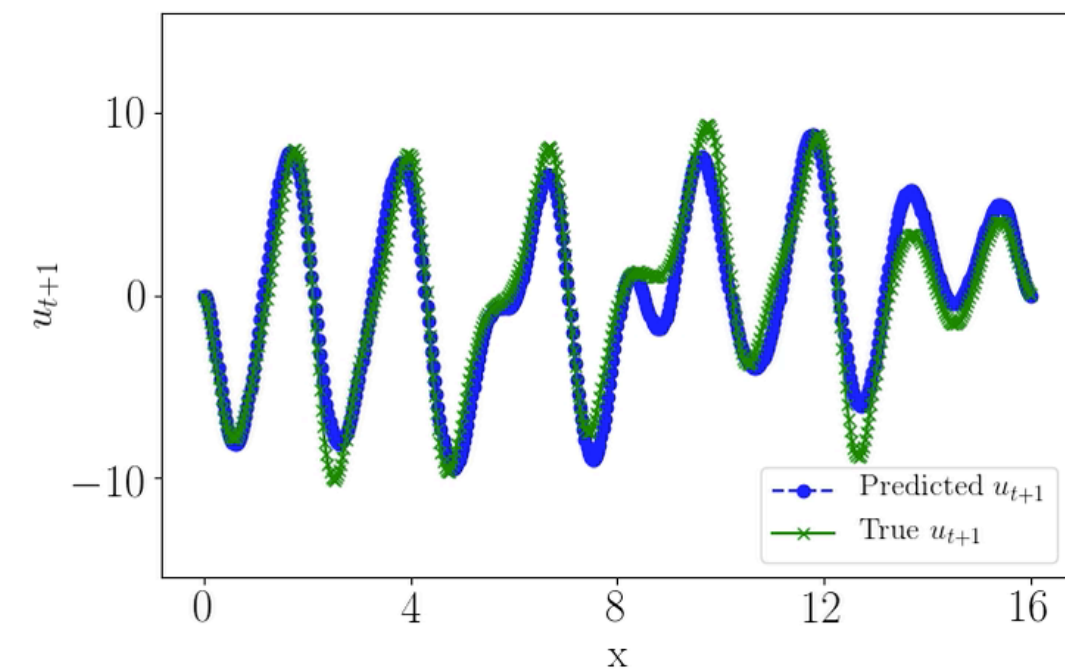
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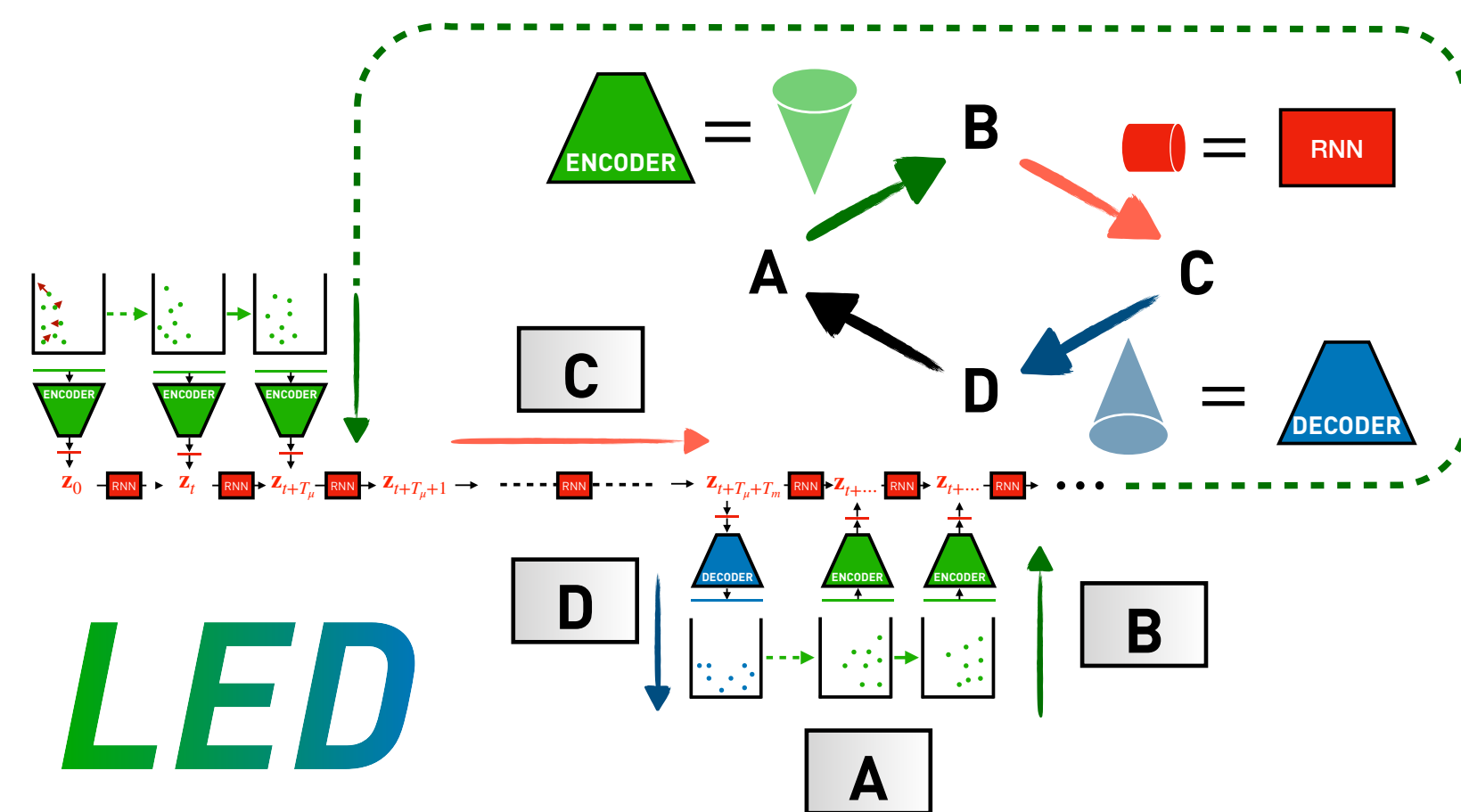
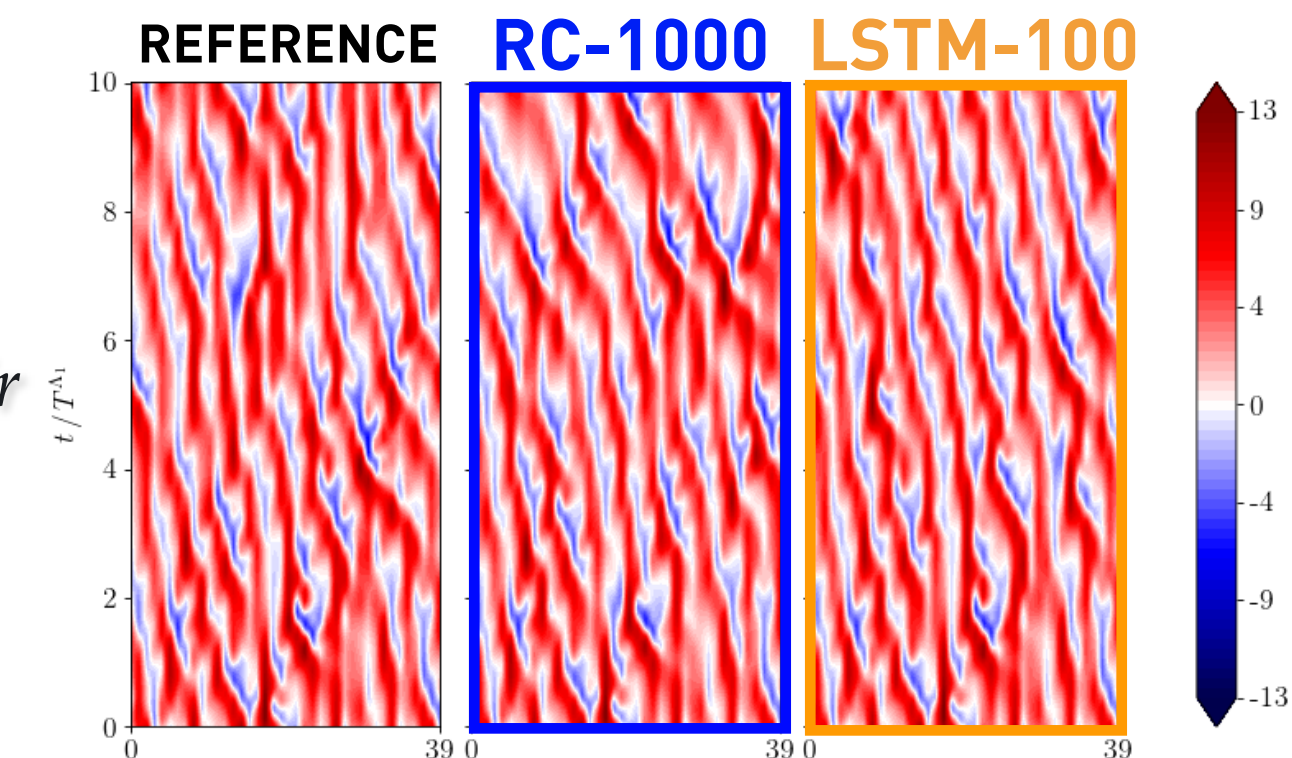


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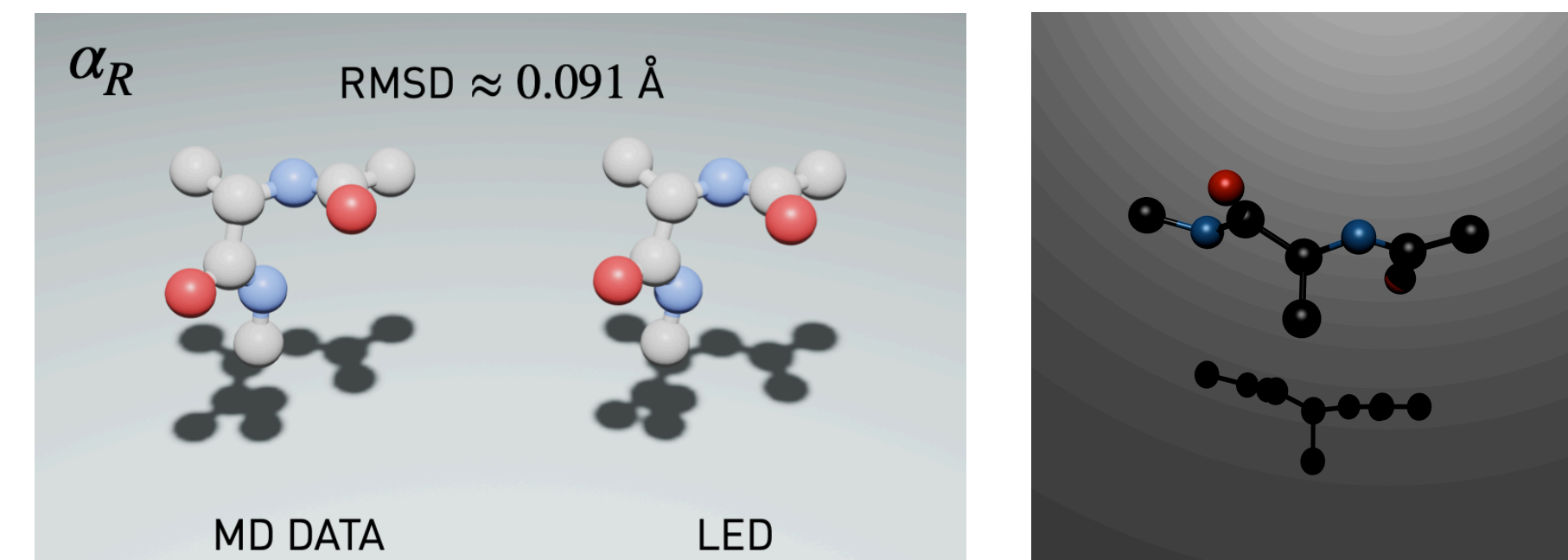
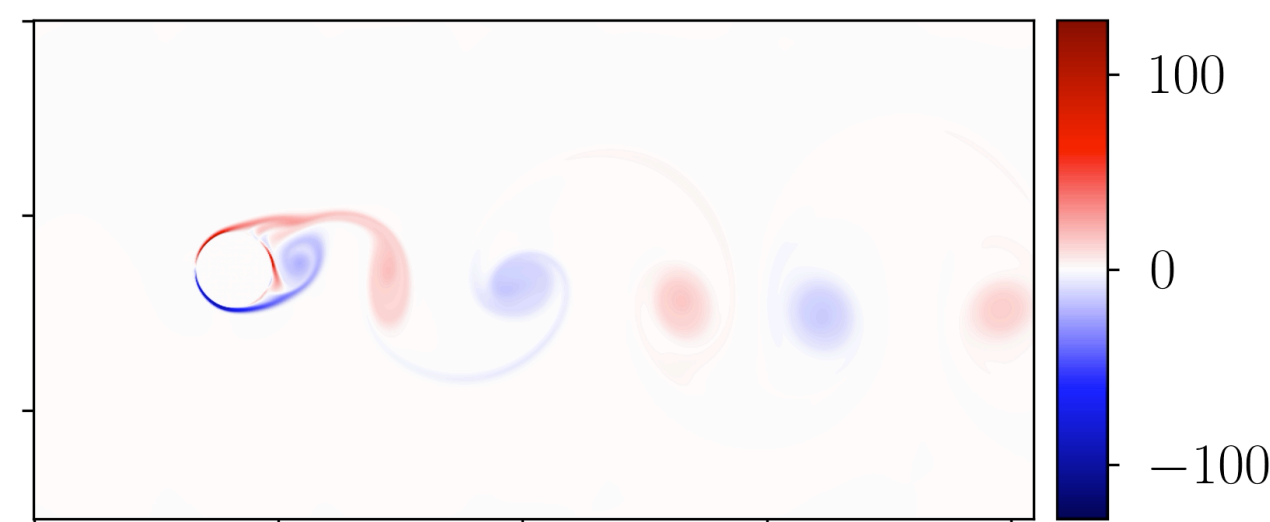
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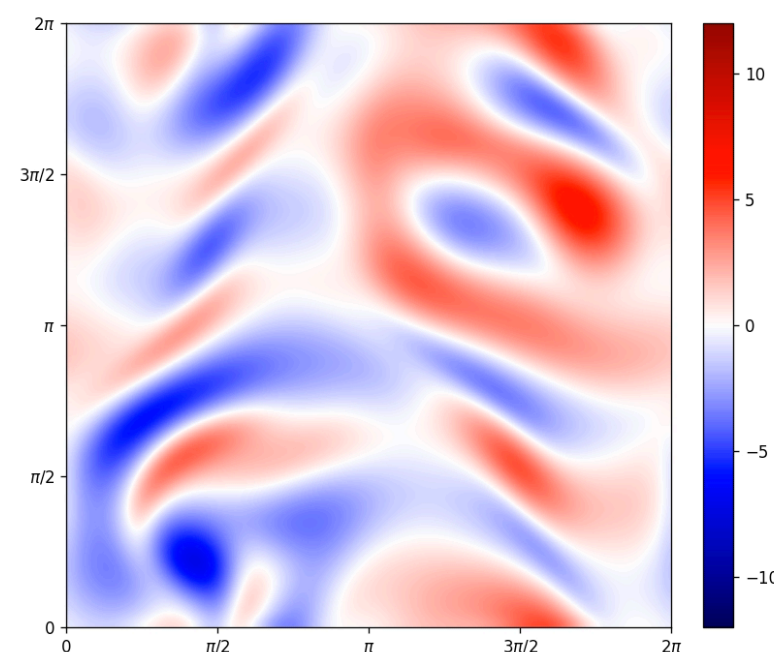
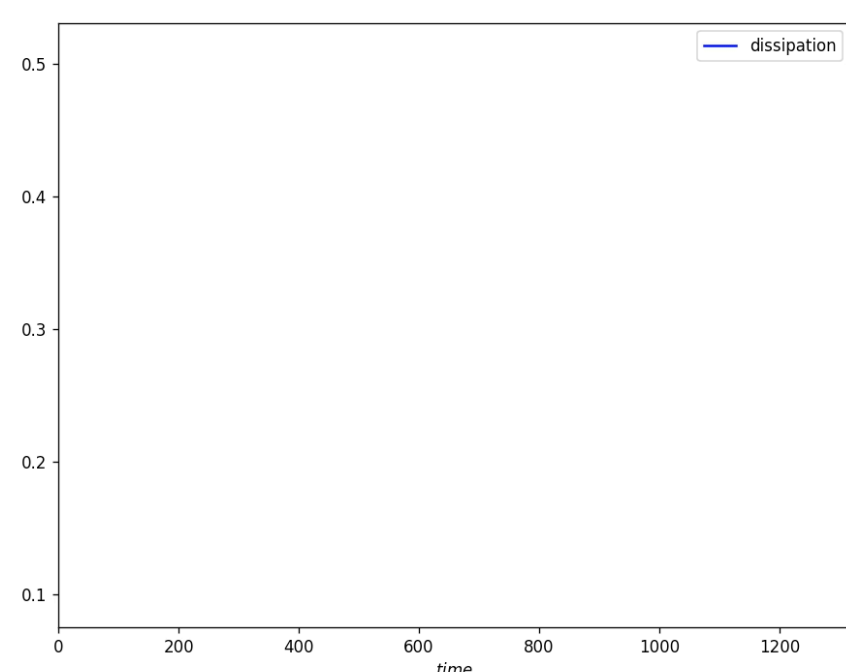
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