ETH zürich

Third Symposium on Machine Learning and Dynamical Systems
September 27, 2022

Learning and Forecasting the Effective Dynamics of Complex Systems across Scales

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AI2C Technologies, CSE-Lab ETH Zurich

Motivation

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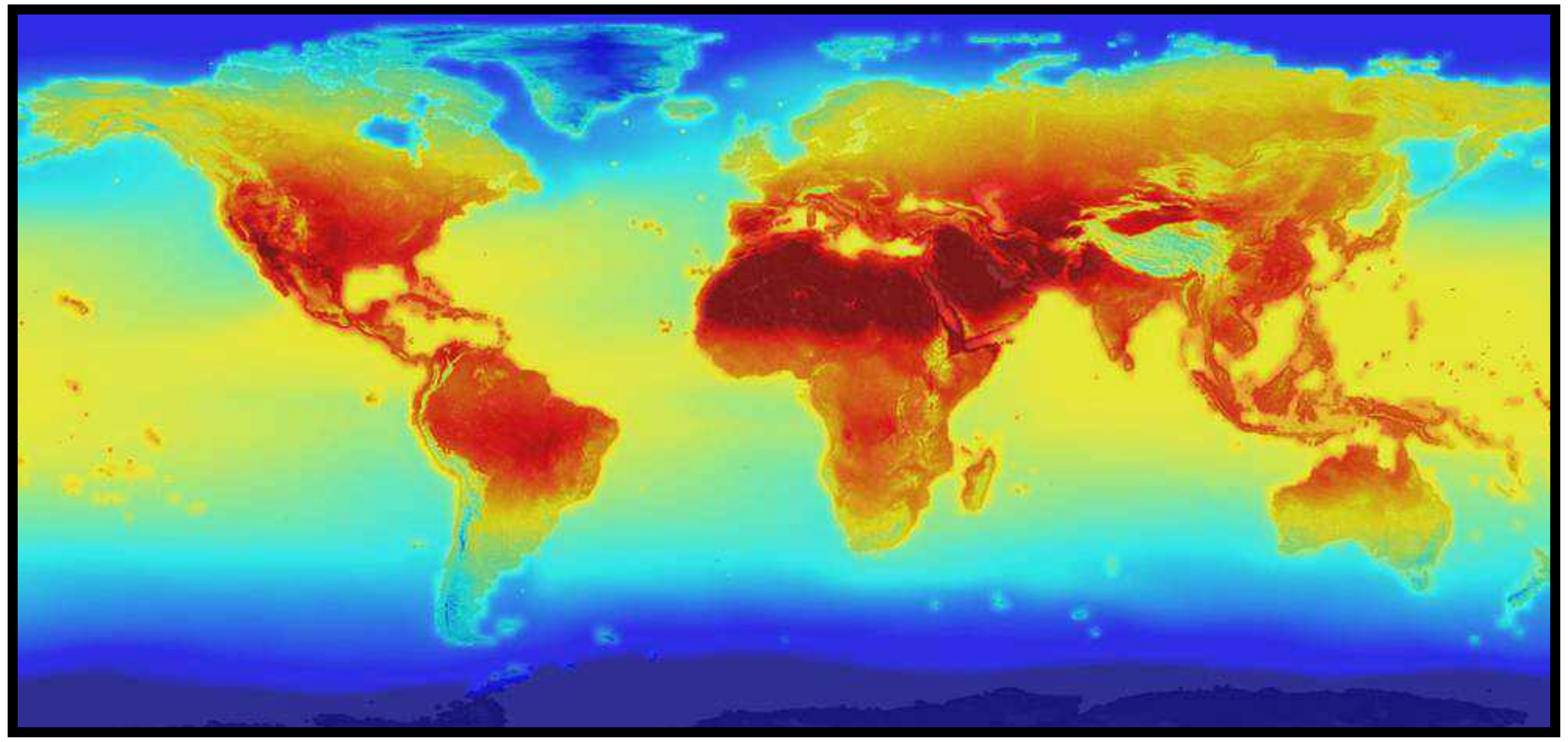

Climate

- Complex multiscale systems
  (deterministic, stochastic, chaotic)

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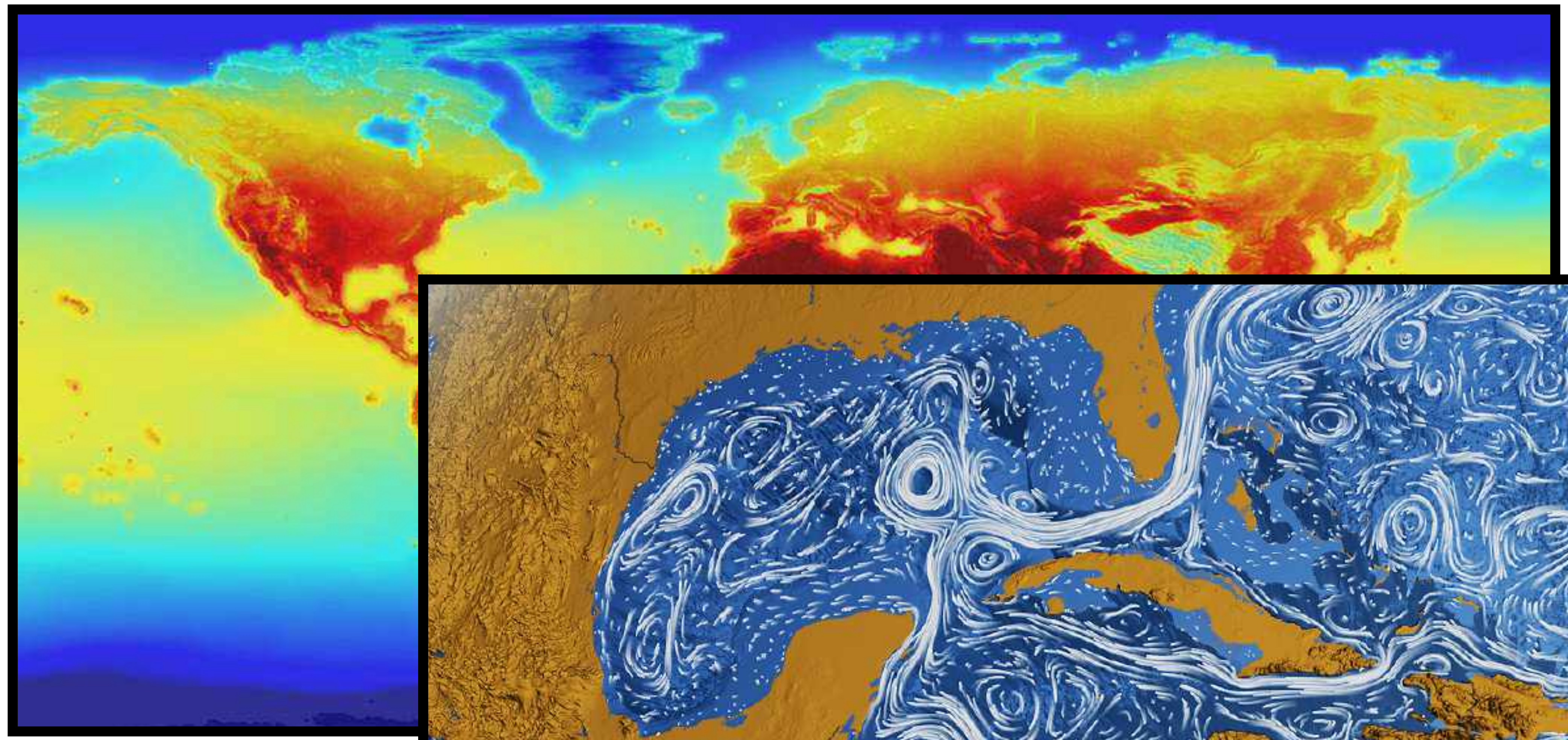

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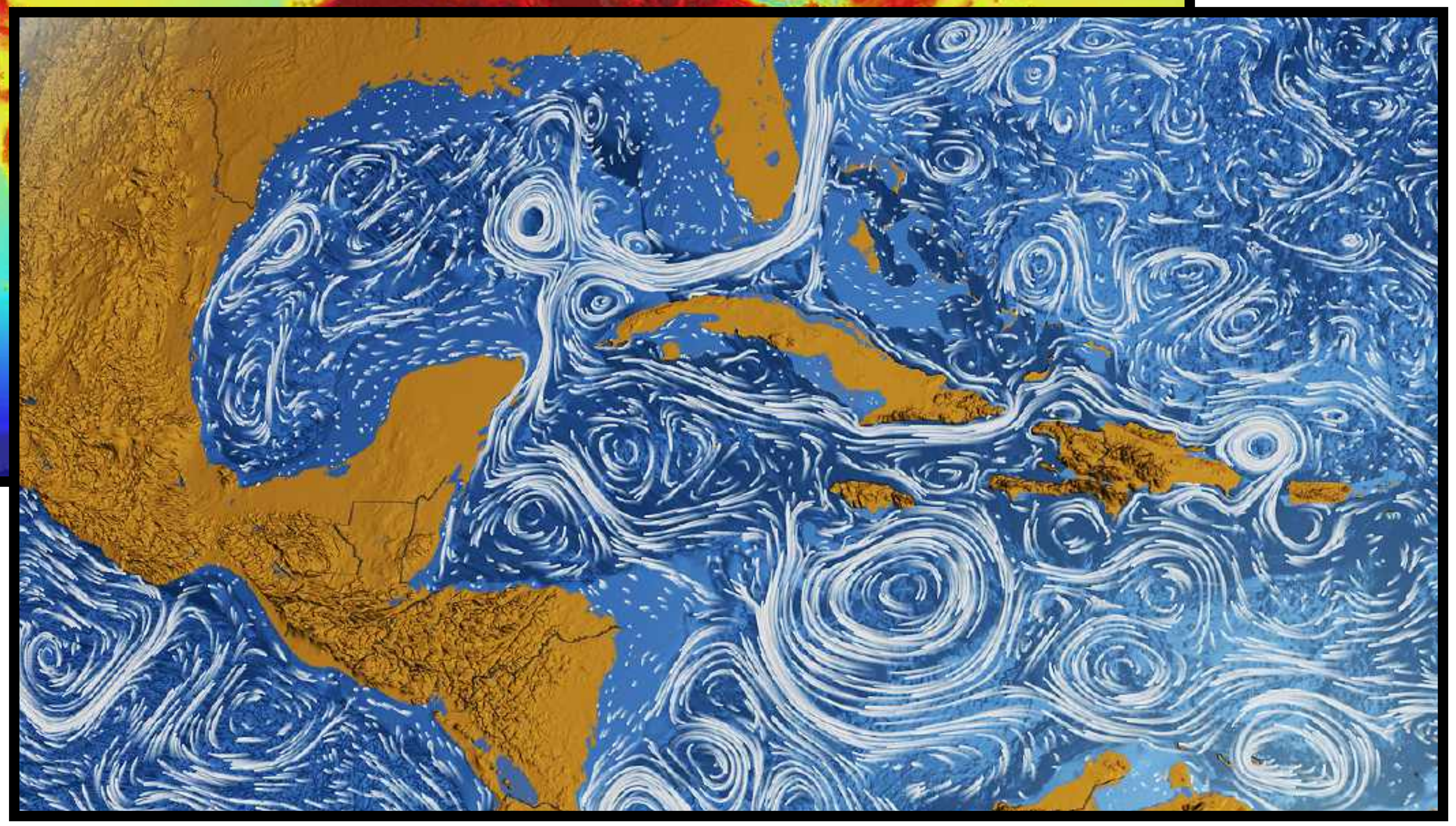

Ocean currents

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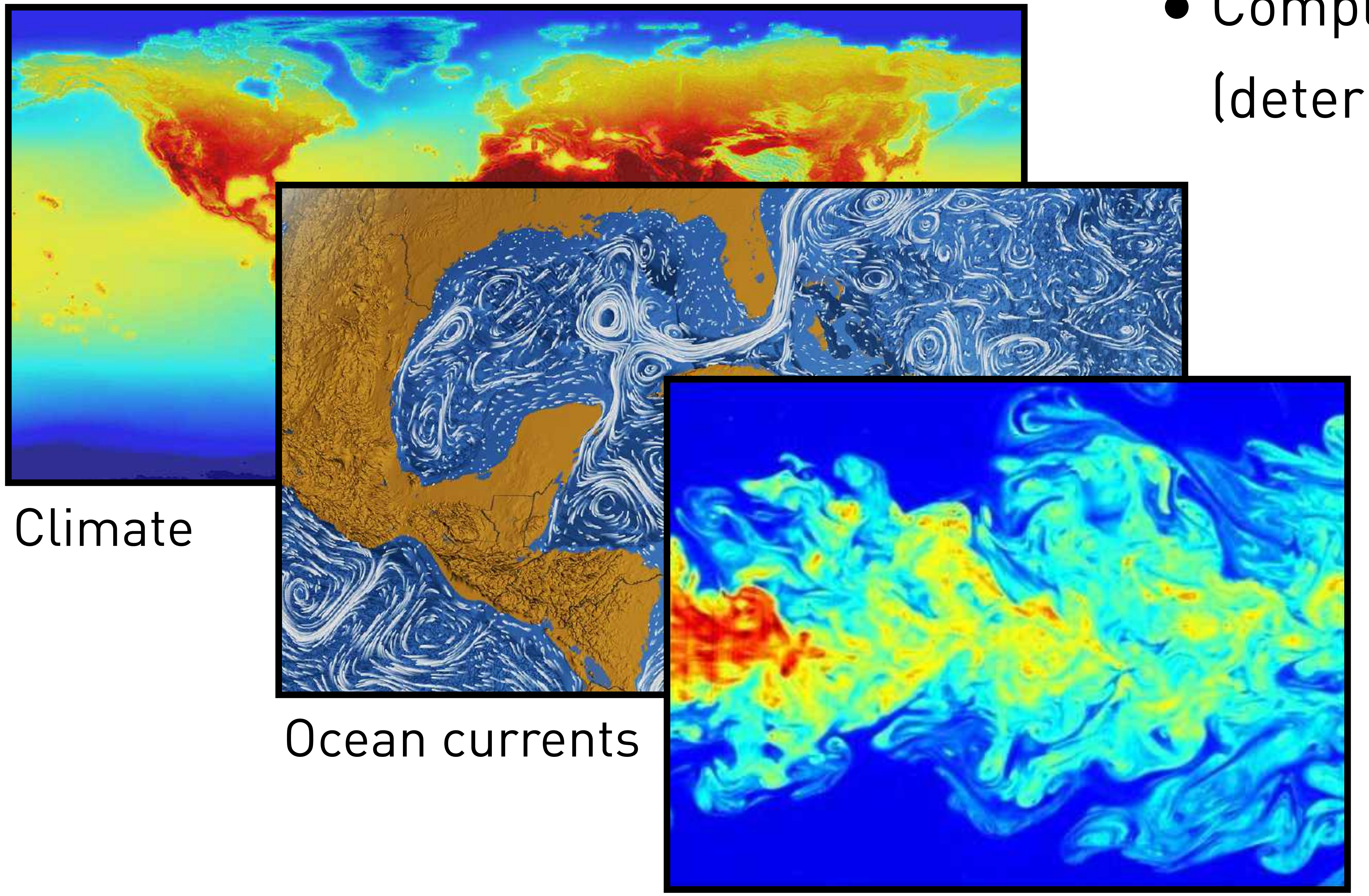

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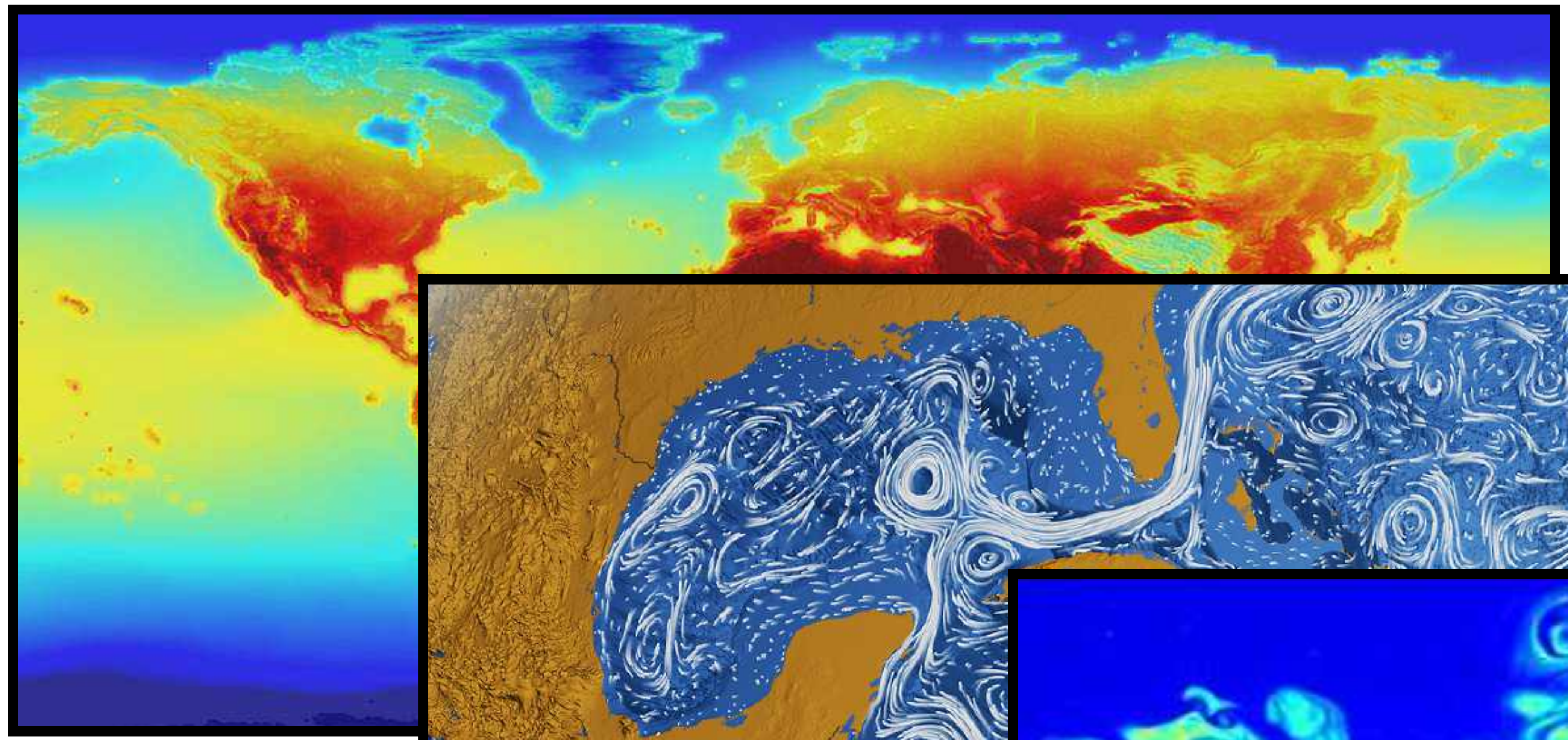

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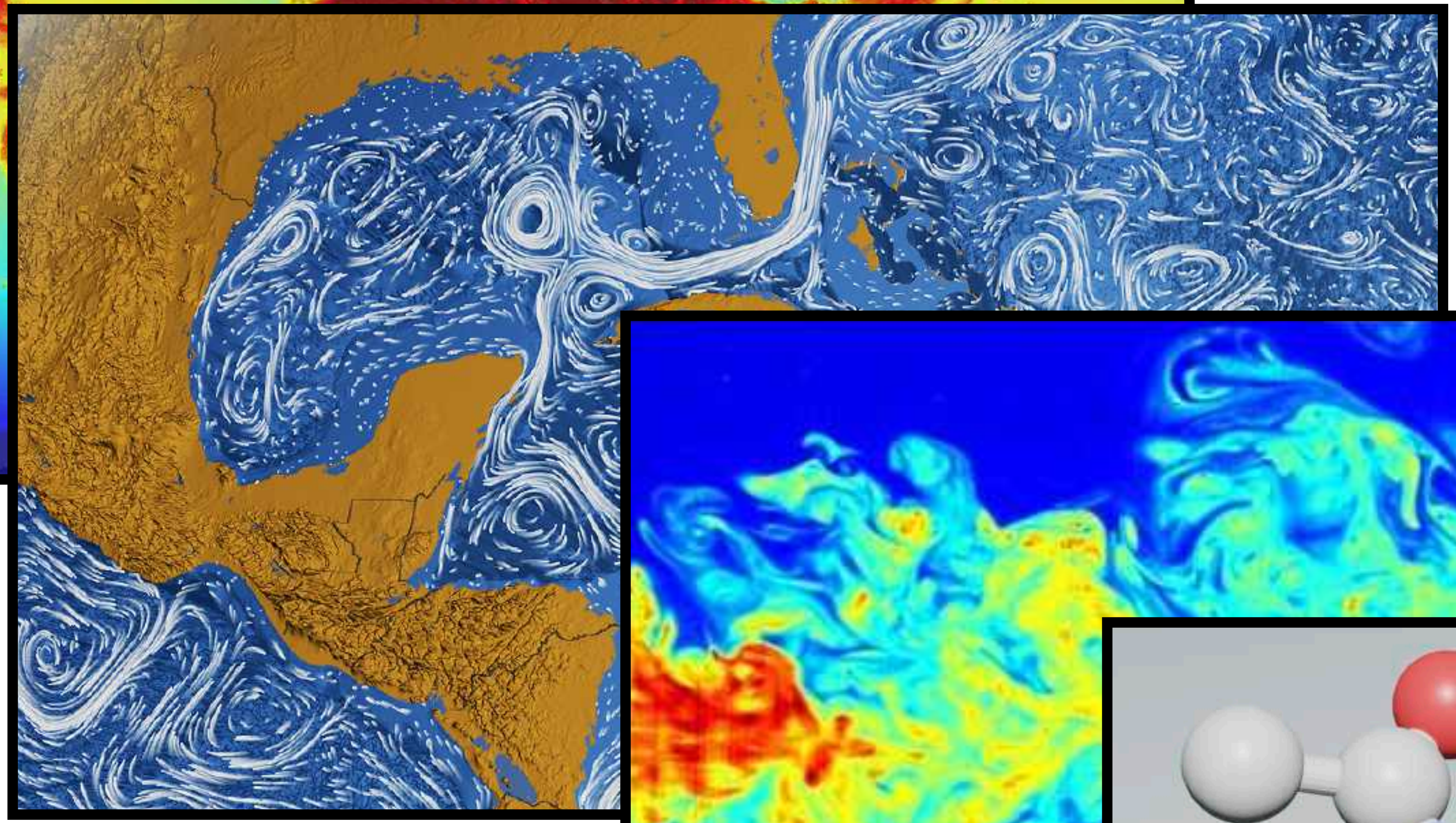

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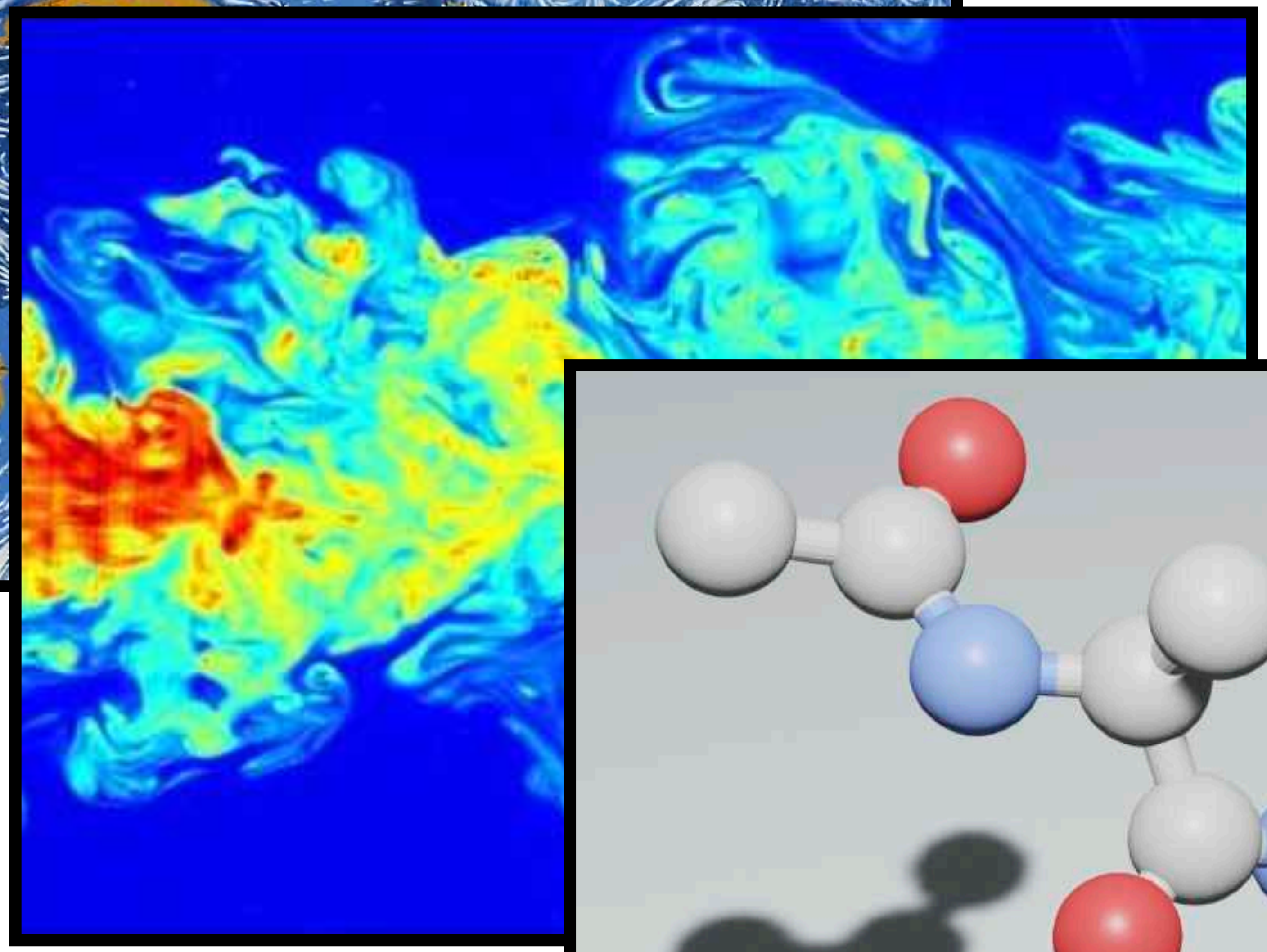

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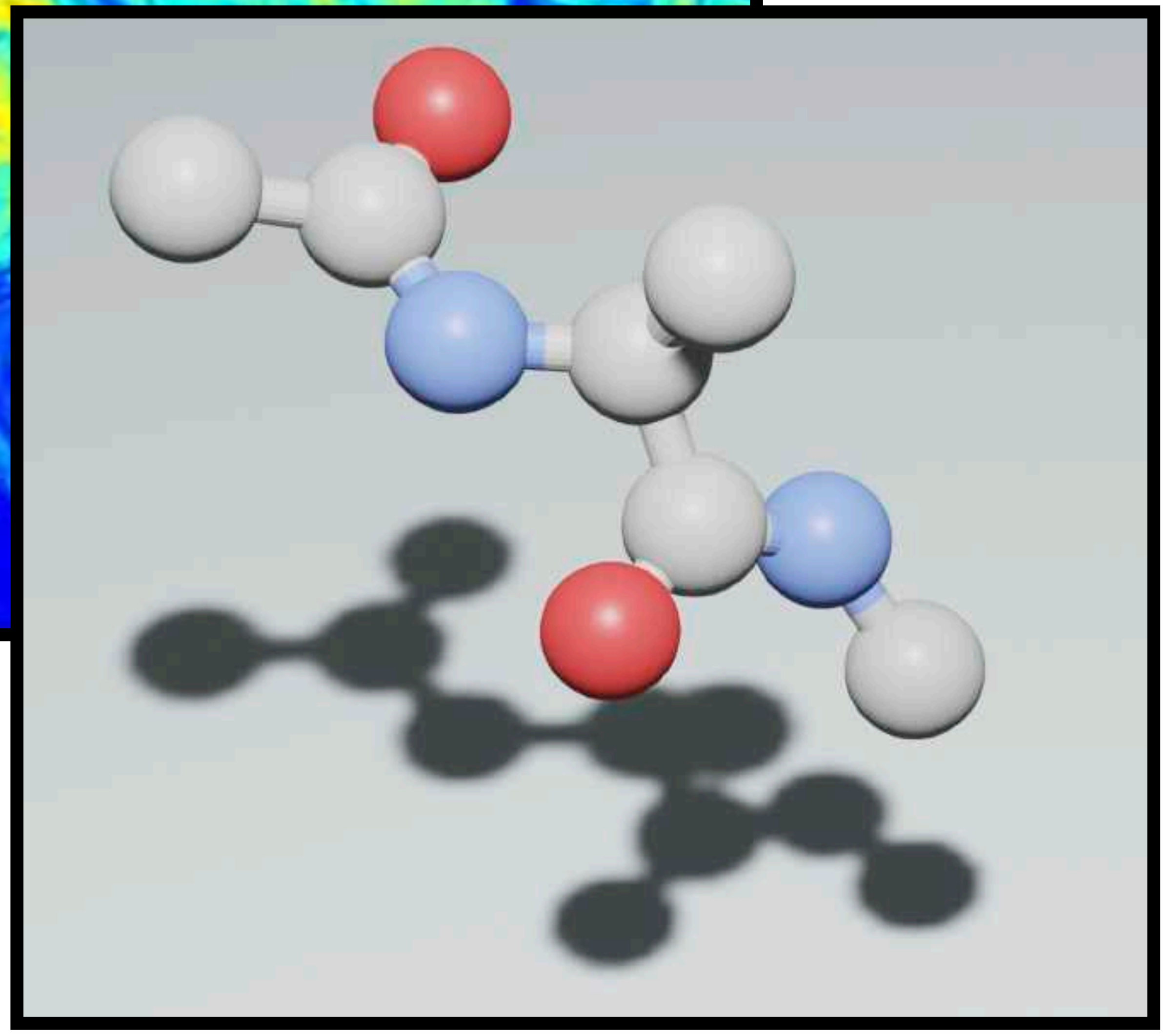

Proteins

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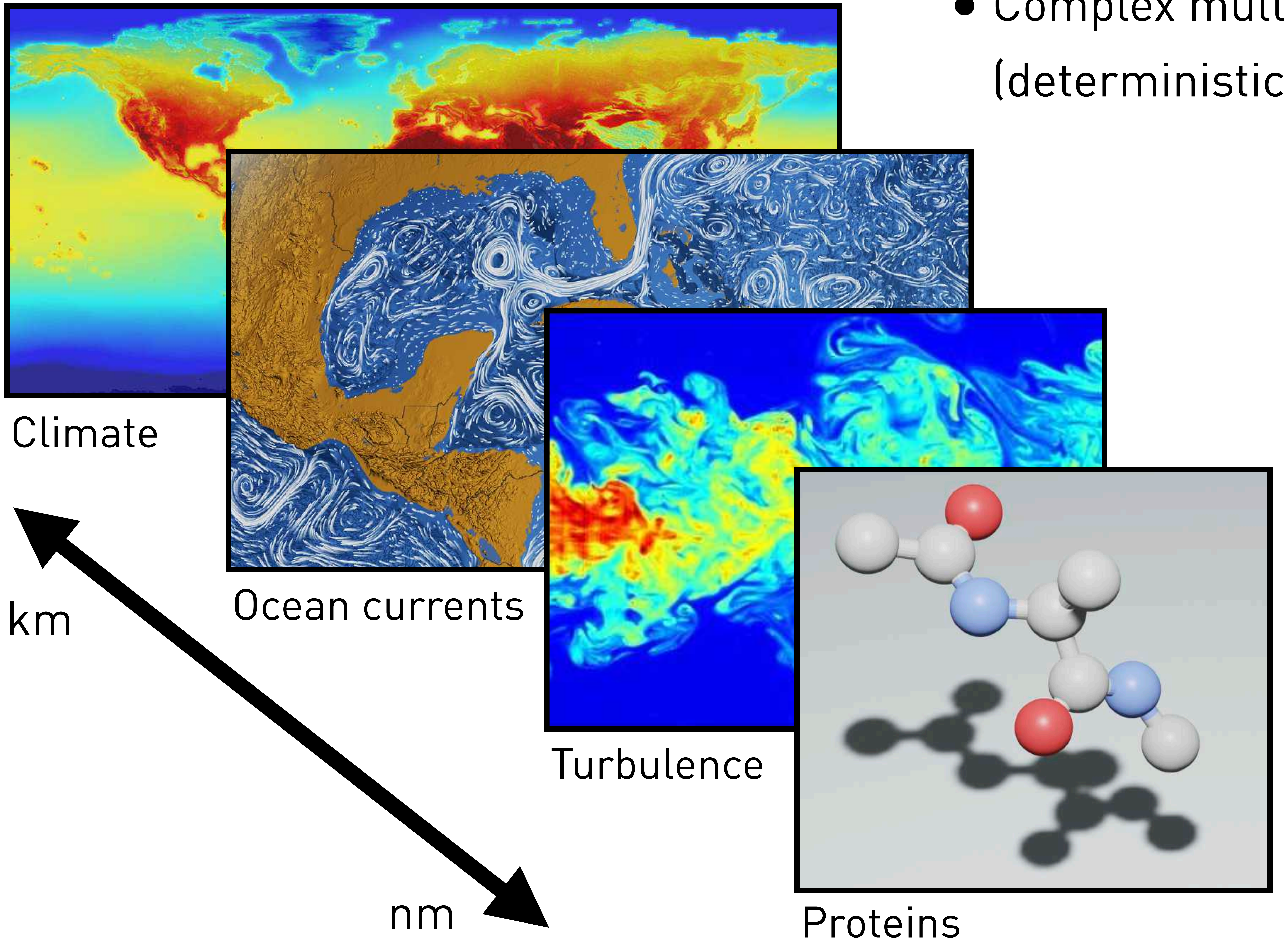

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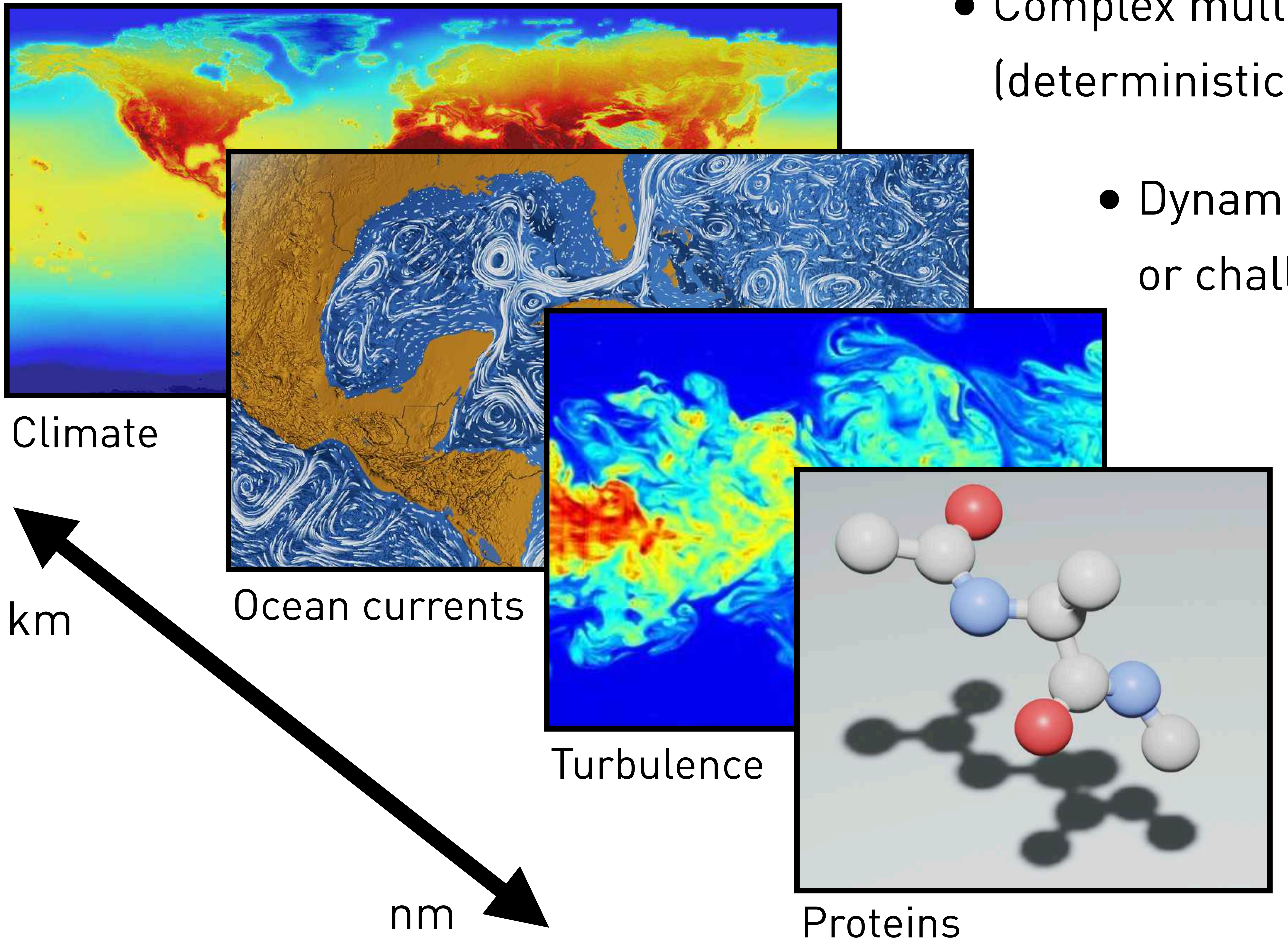

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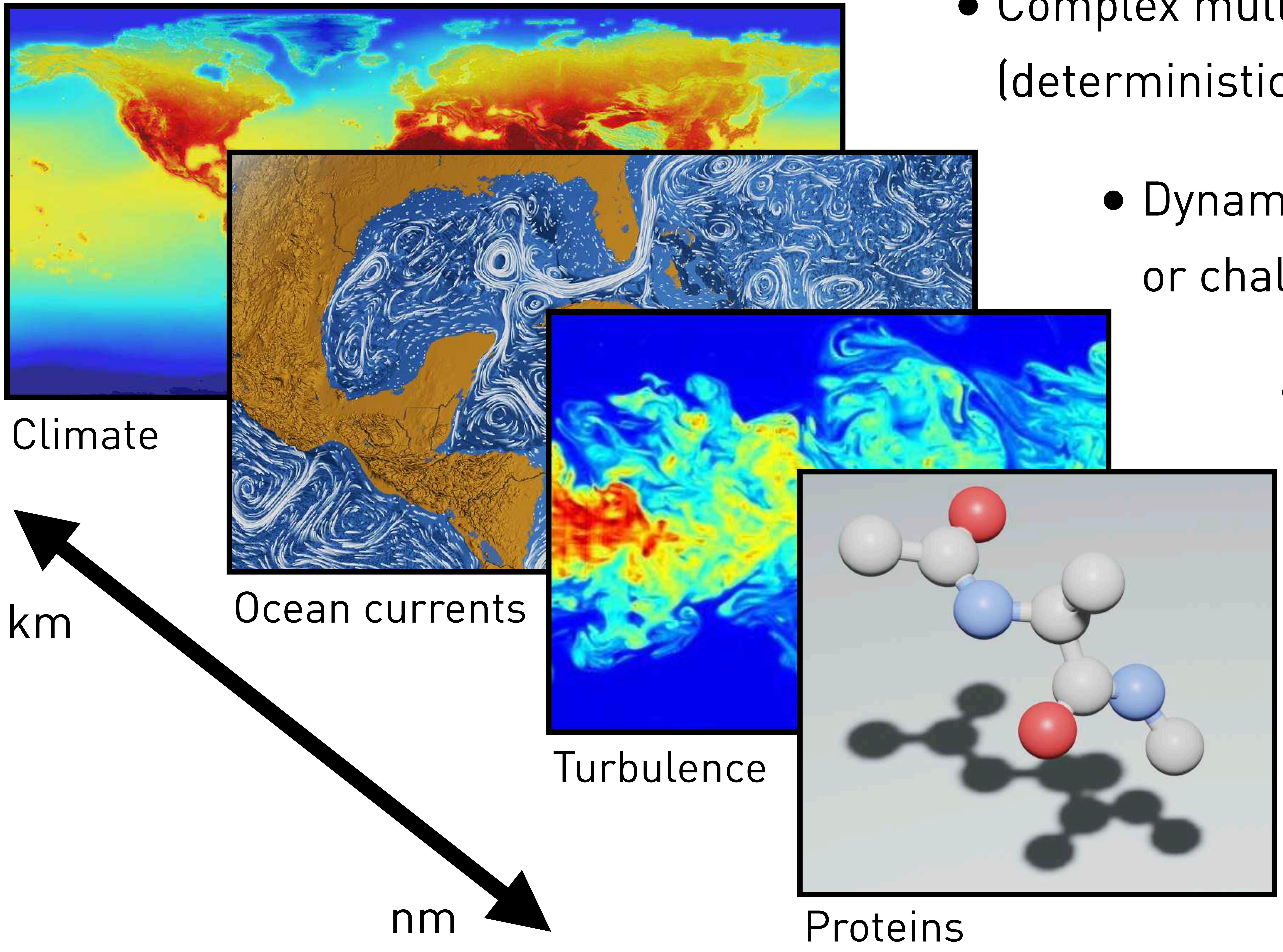

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    - Can we design fast (multiscale) methods that reproduce system dynamics?

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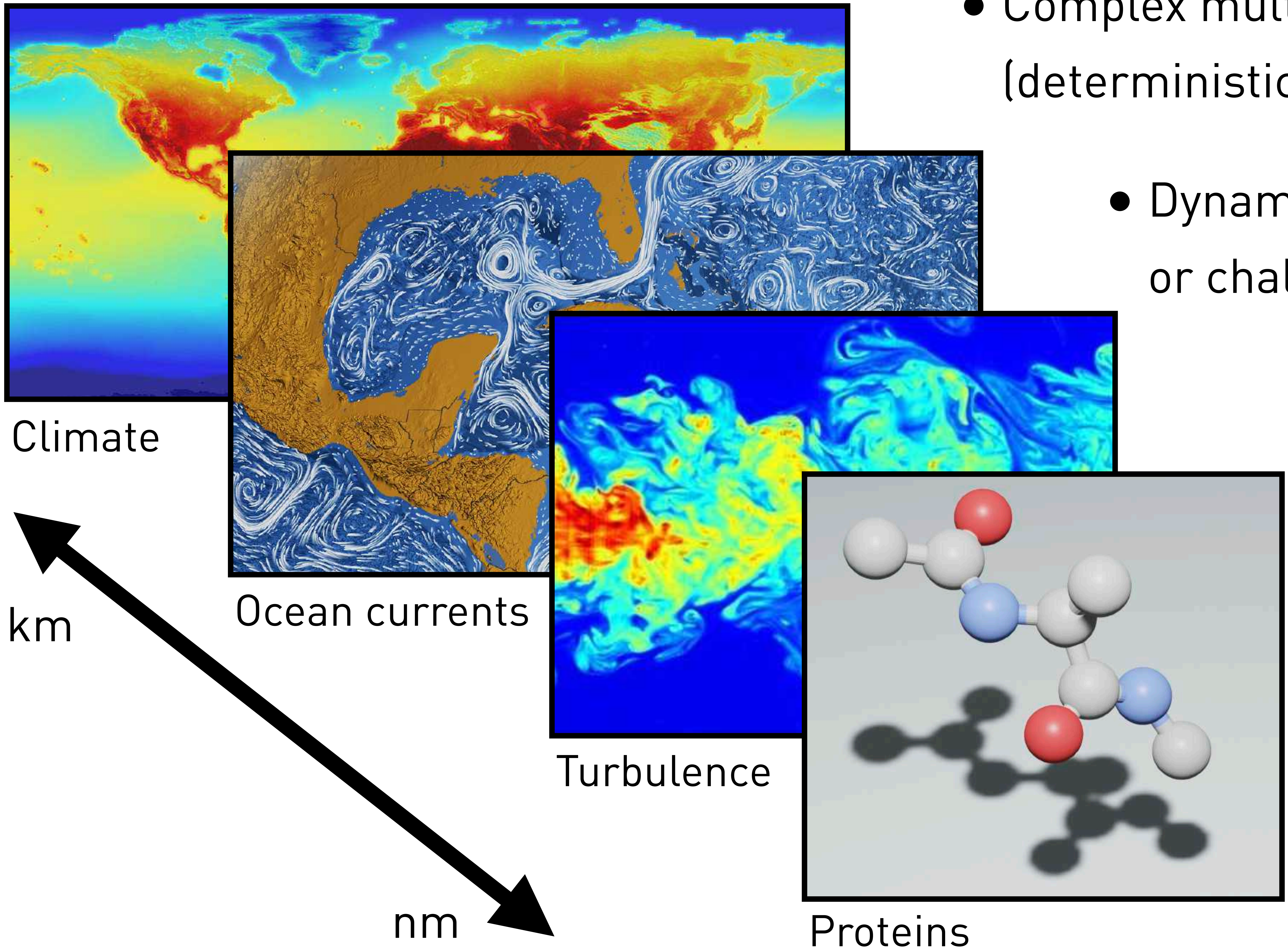

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            - Examples:
              LES/RANS
              Surrogate models / DMD
              Coarse graining models of molecular systems

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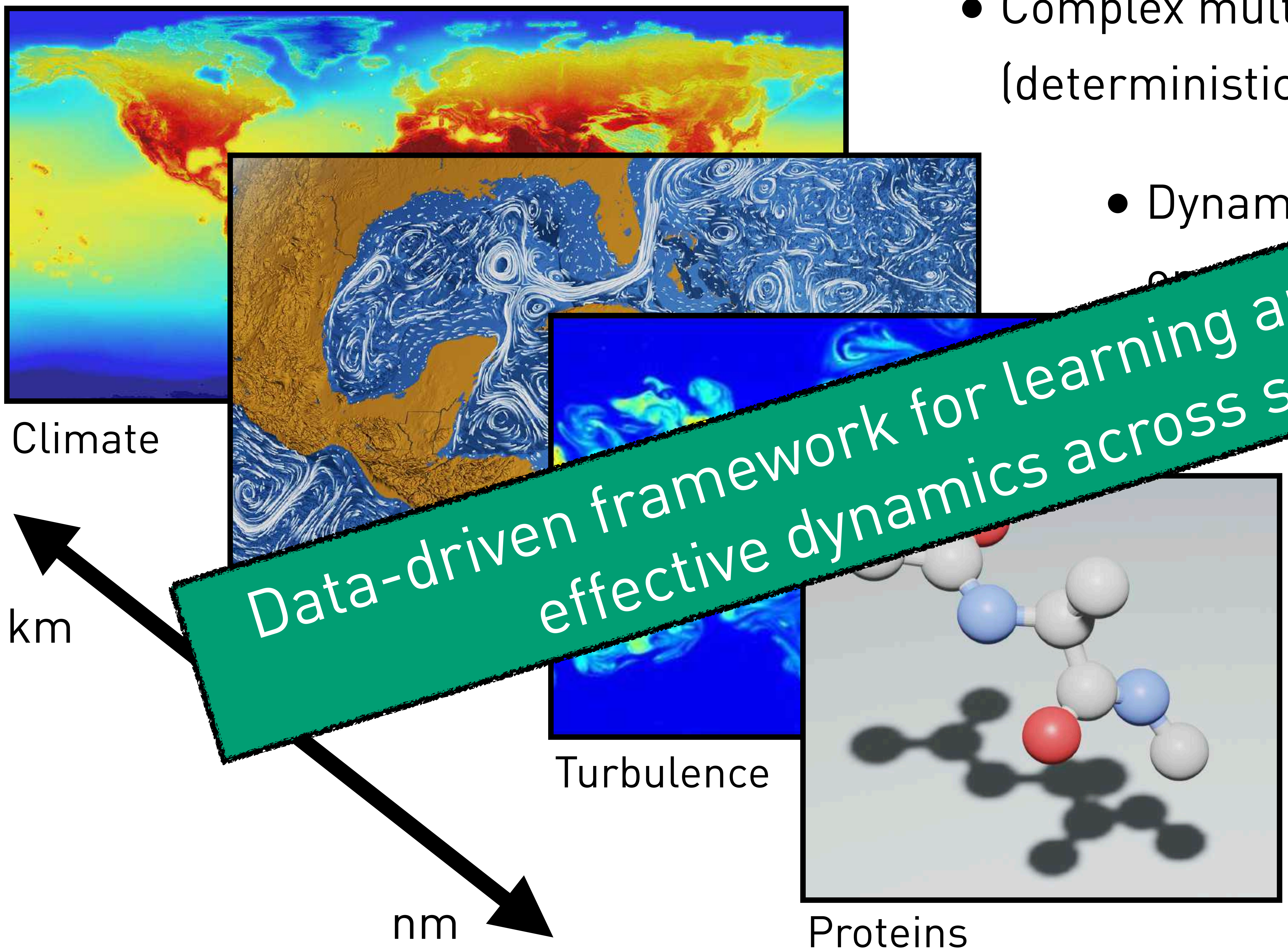

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Data-driven framework for learning and forecasting effective dynamics across scales

I

Forecasting Complex Dynamics with Recurrent Neural Networks

Recurrent Neural Networks (RNNs)

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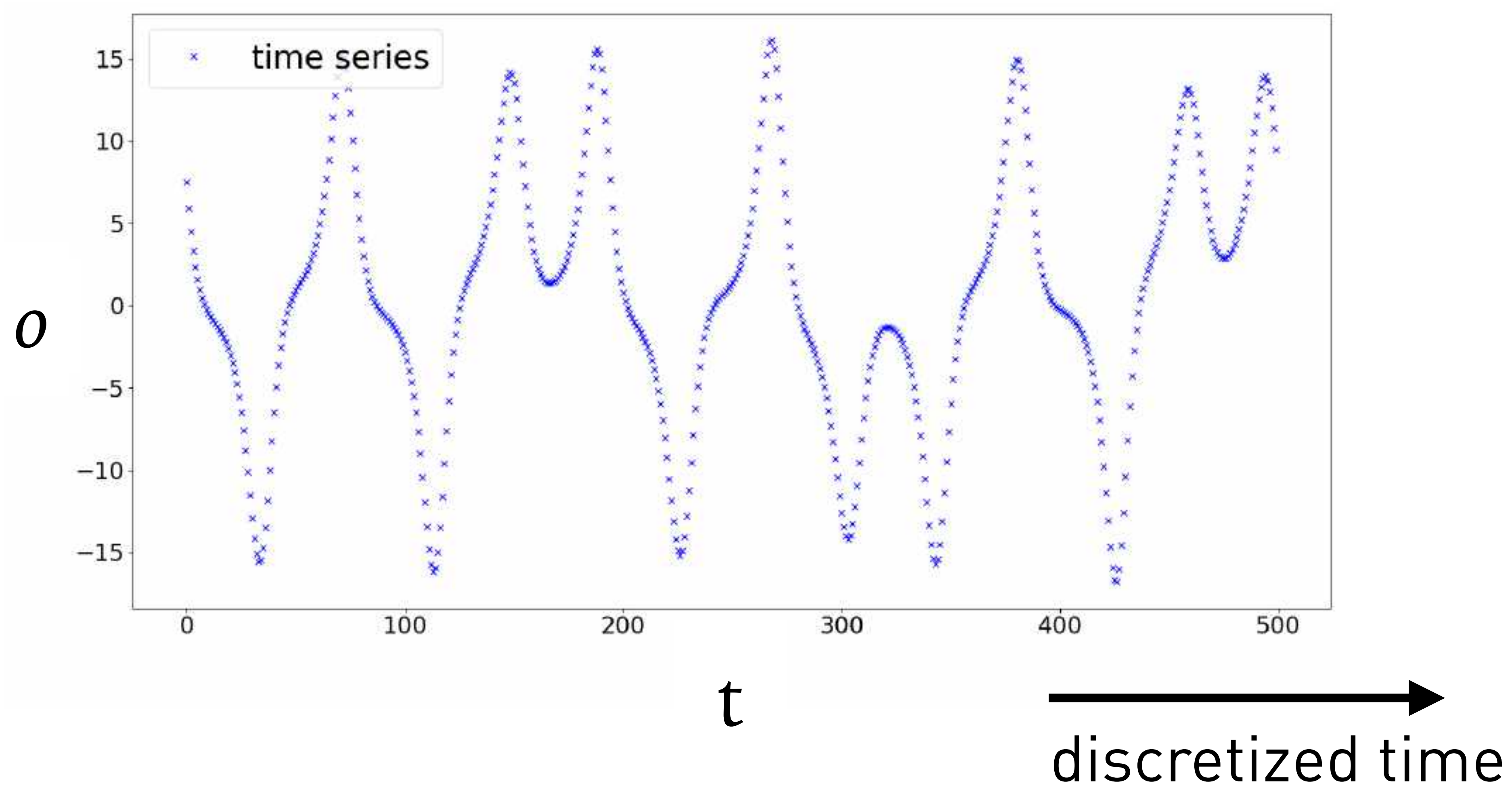

Data from trajectories

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

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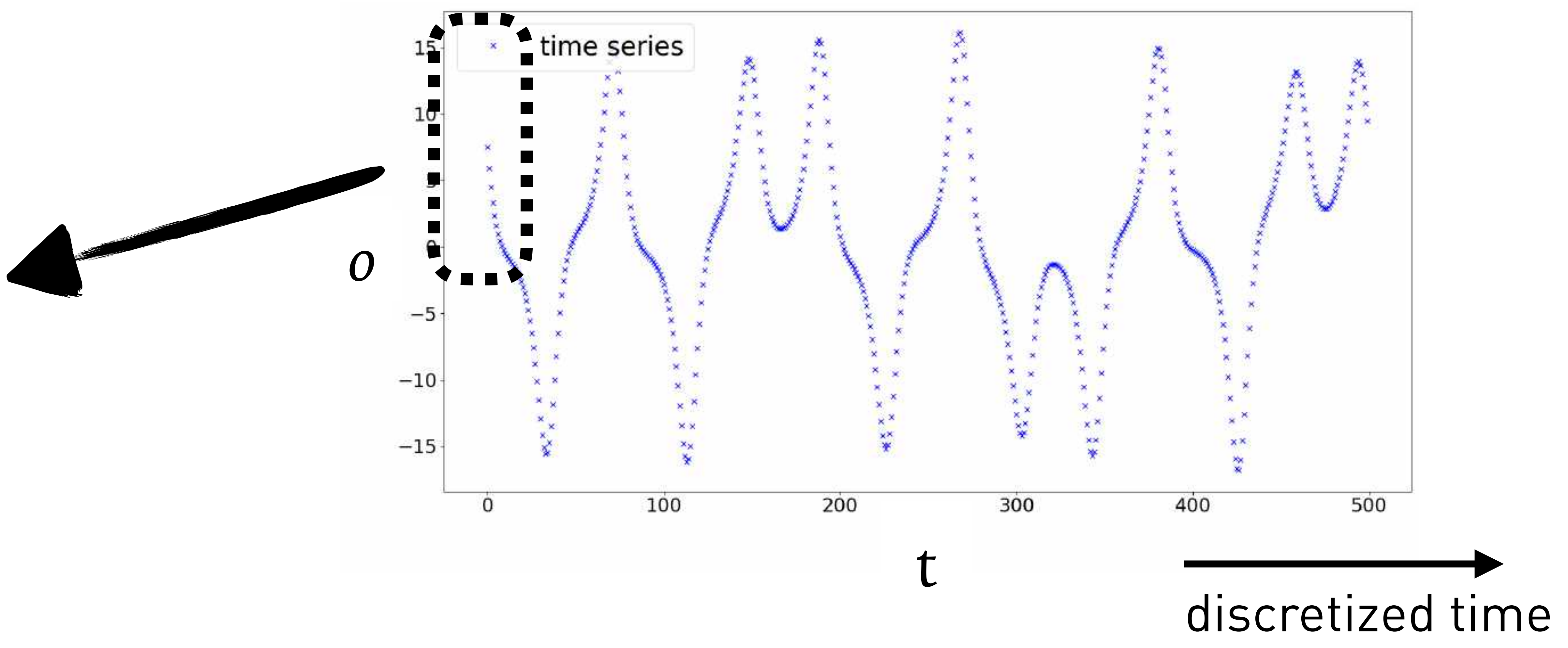

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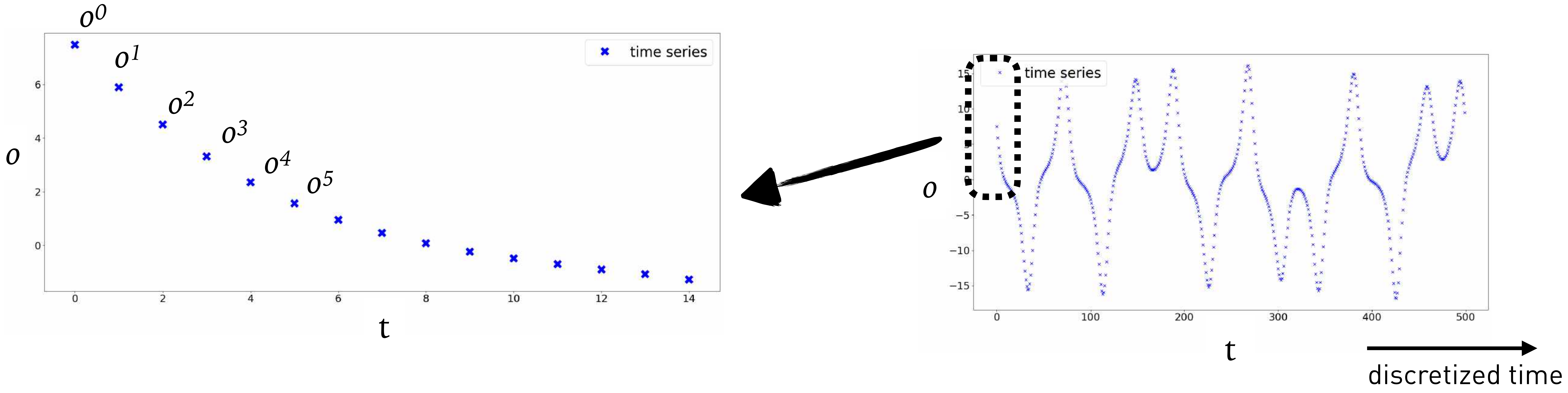

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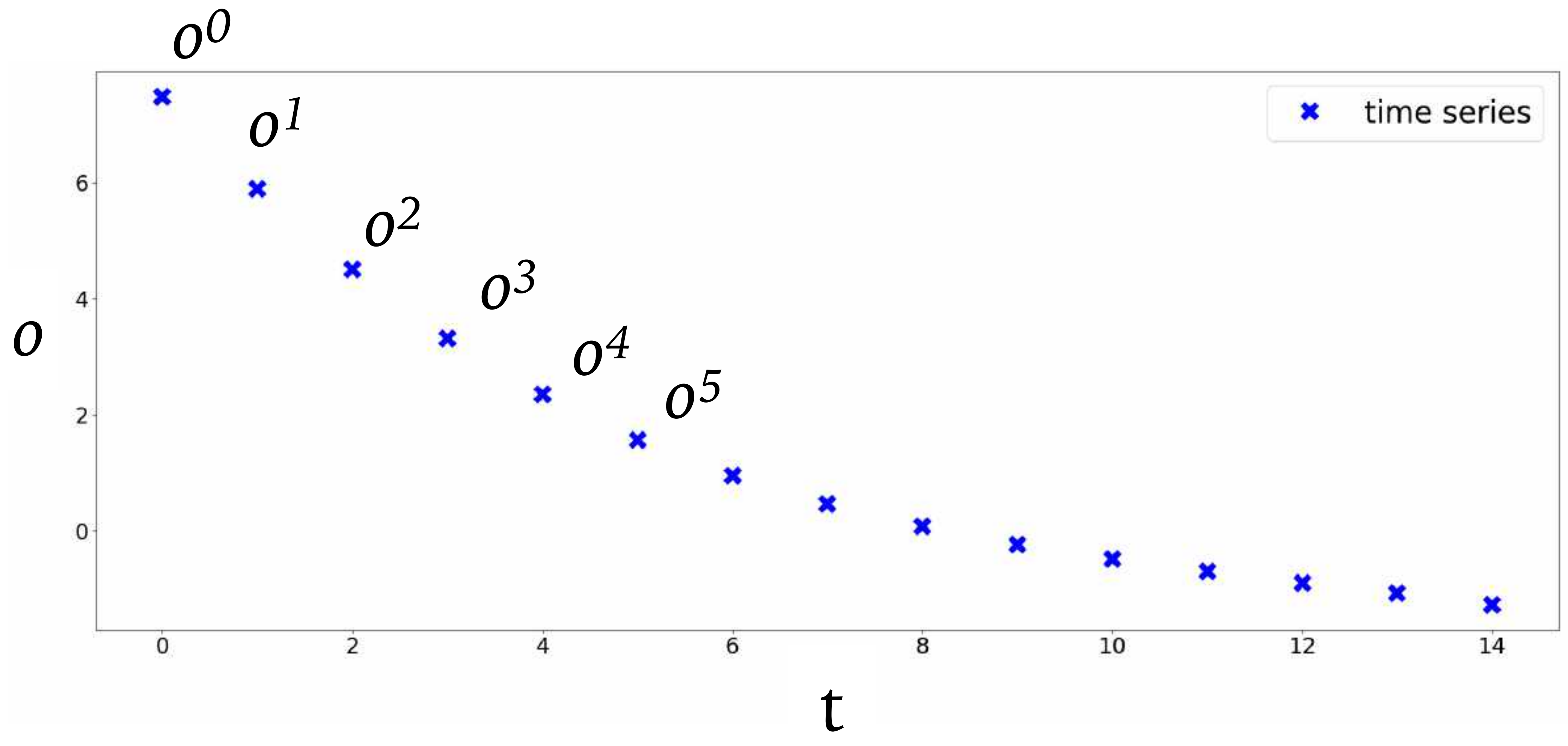

Model $o^{t+1} = o^t + \Delta t\, \dot{o}^t$

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

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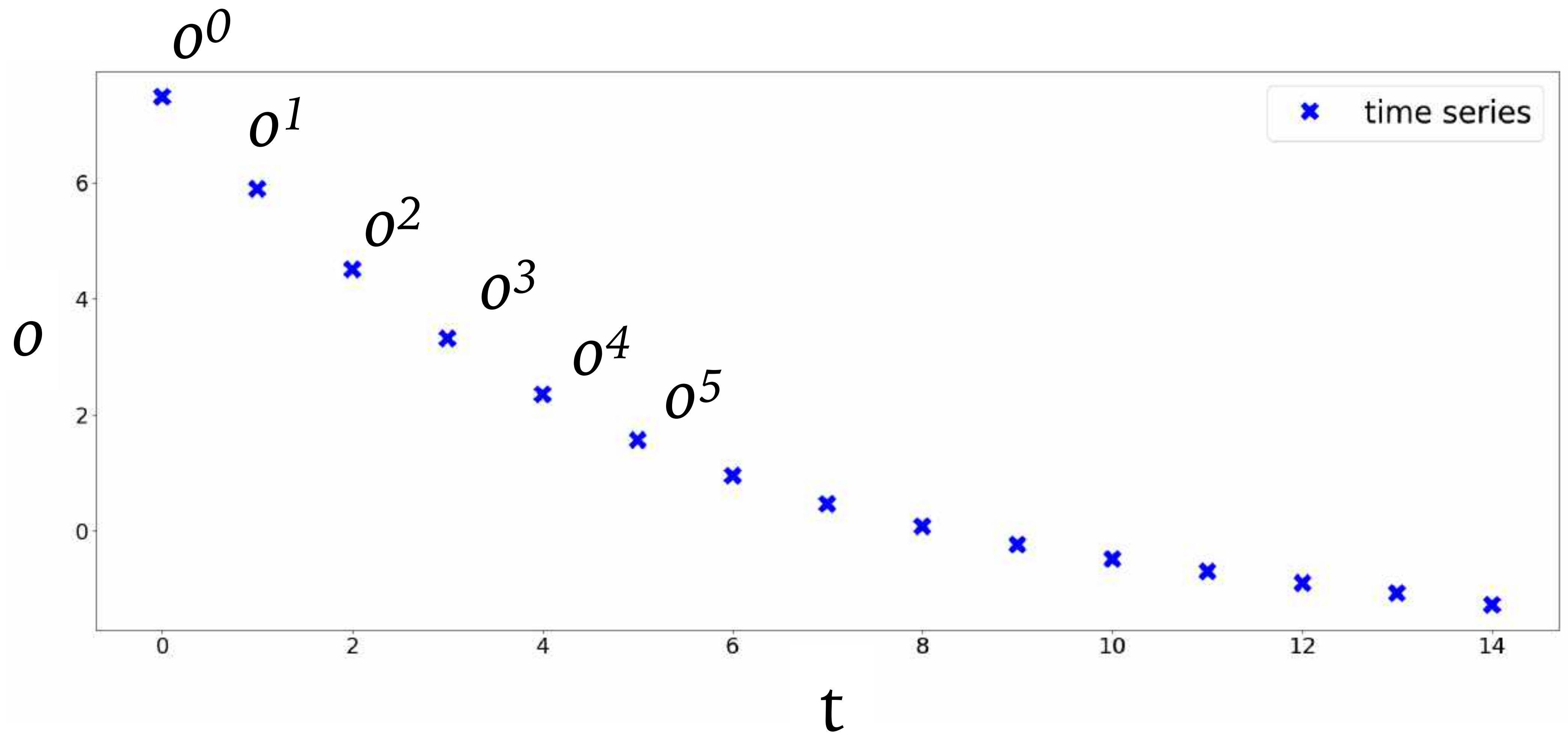

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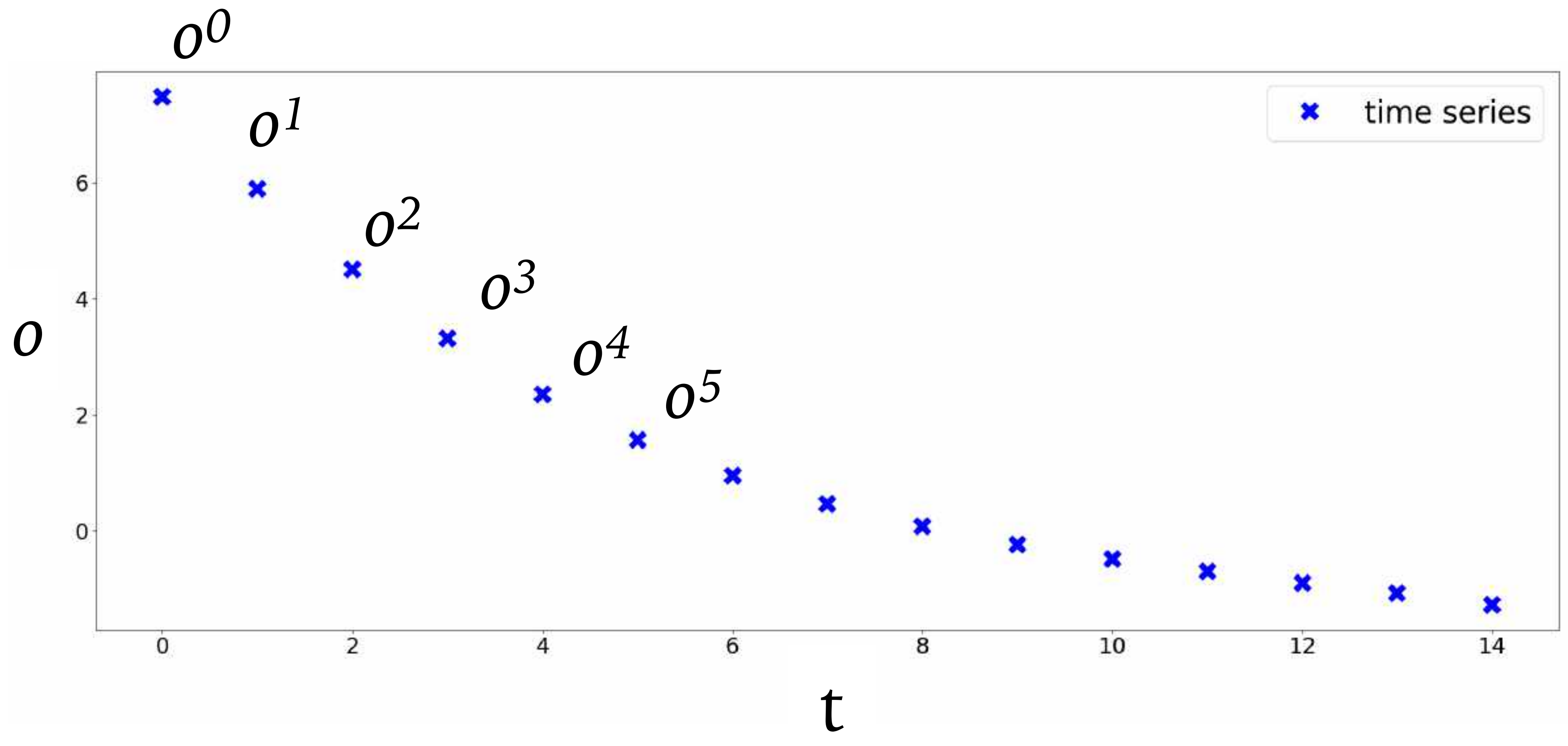

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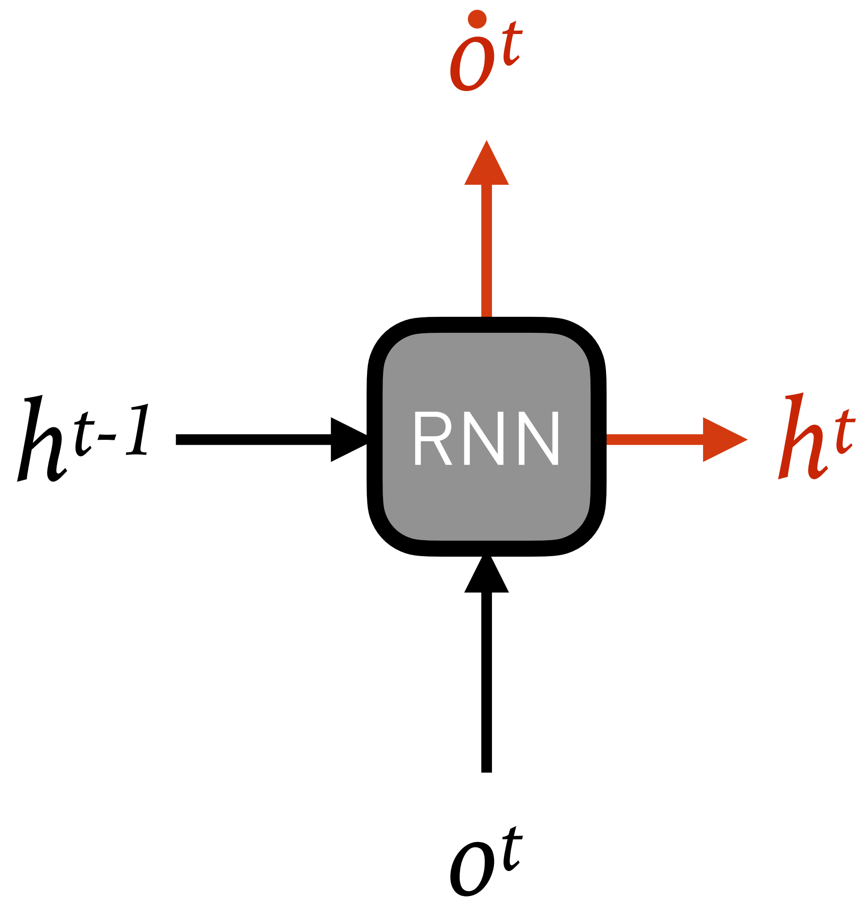

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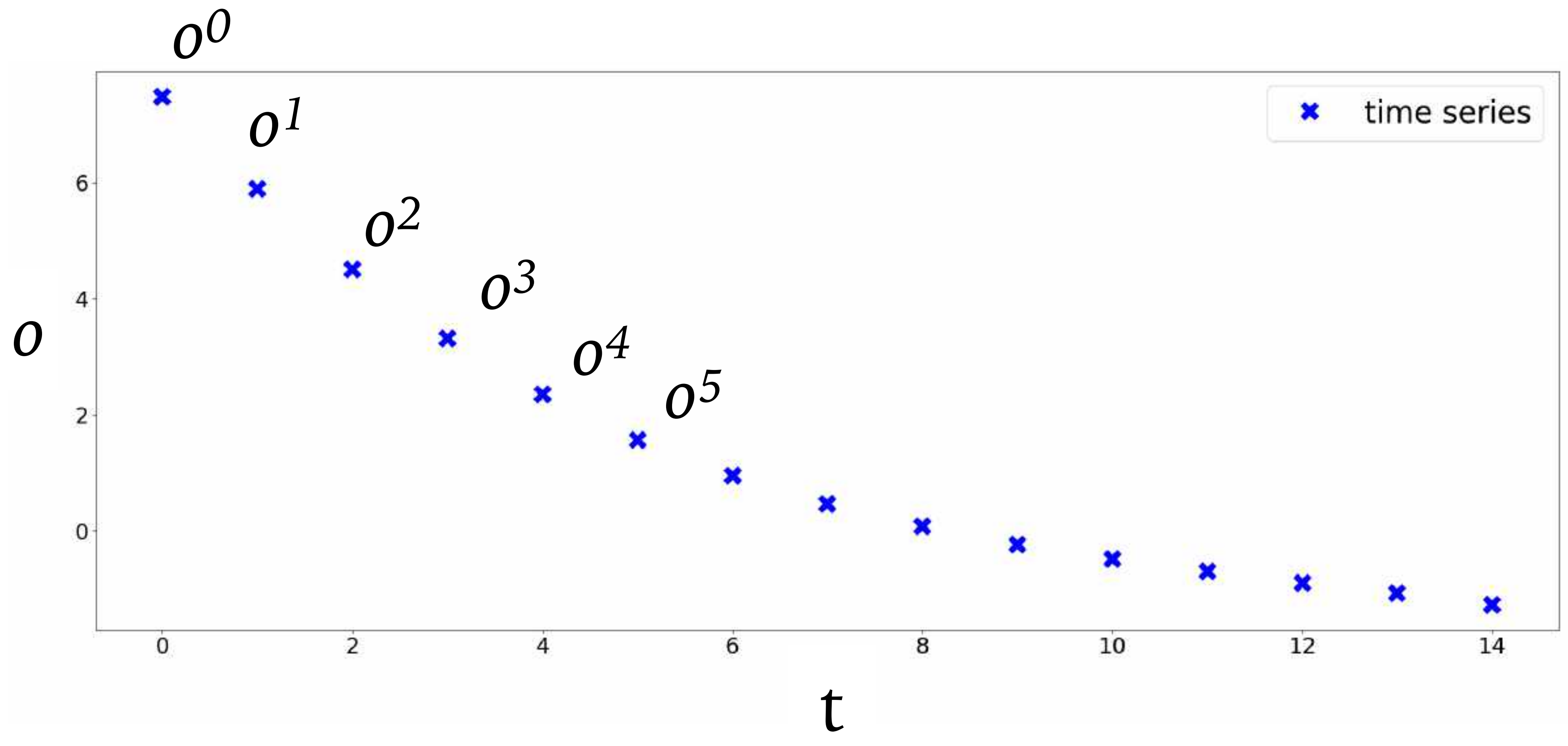

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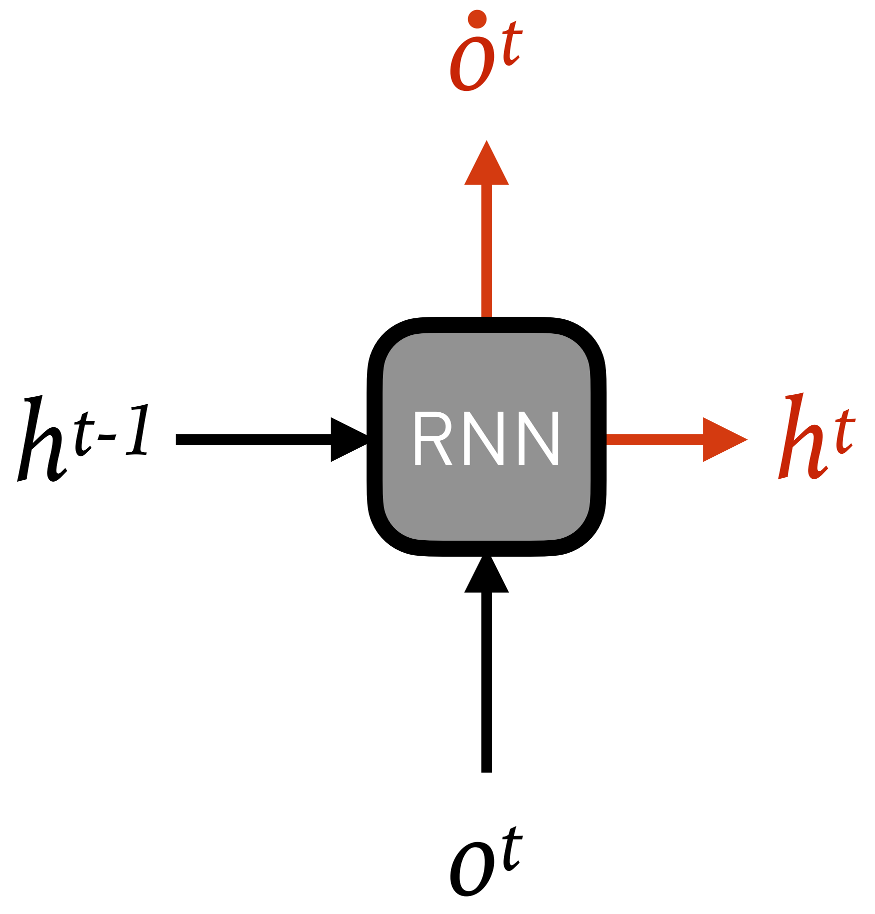

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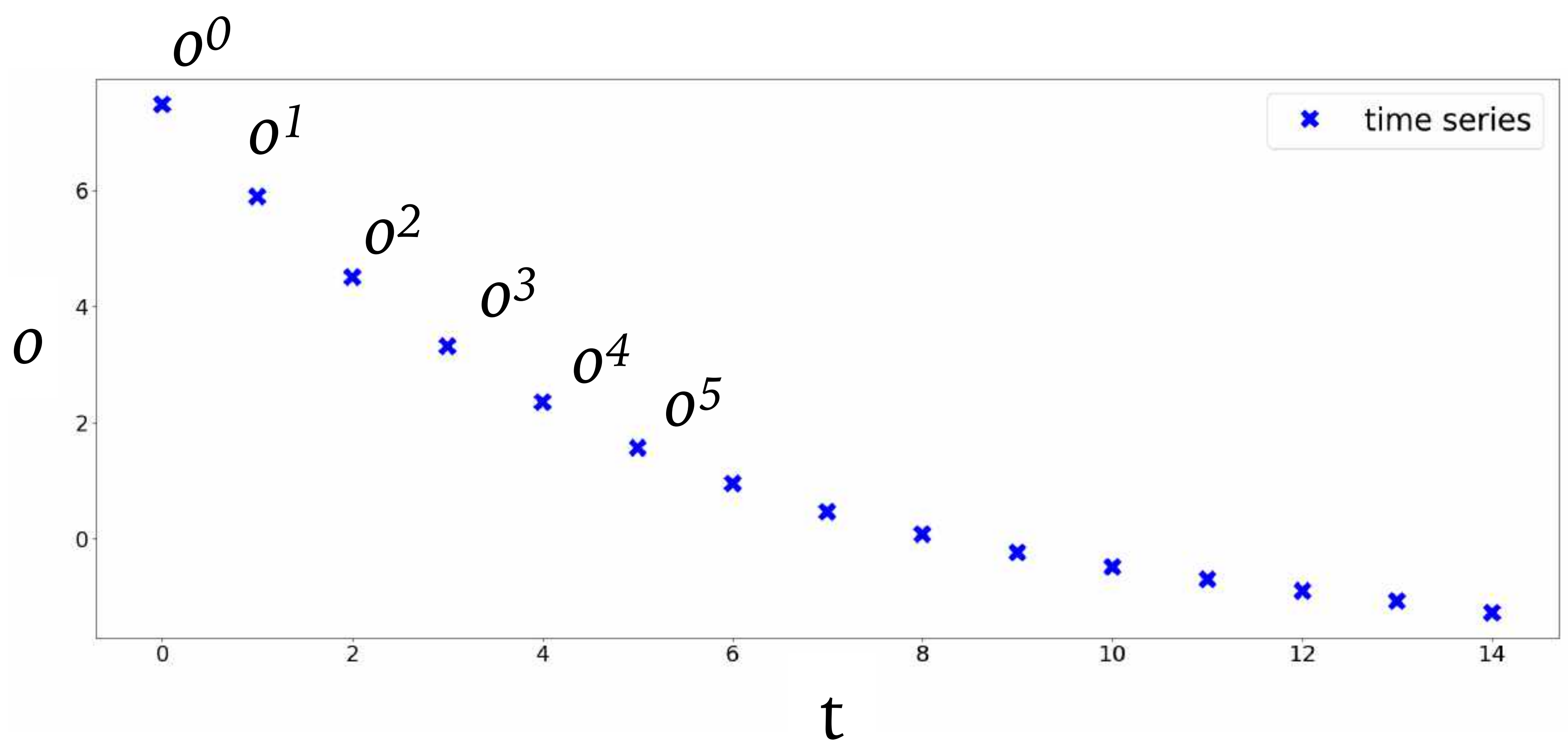

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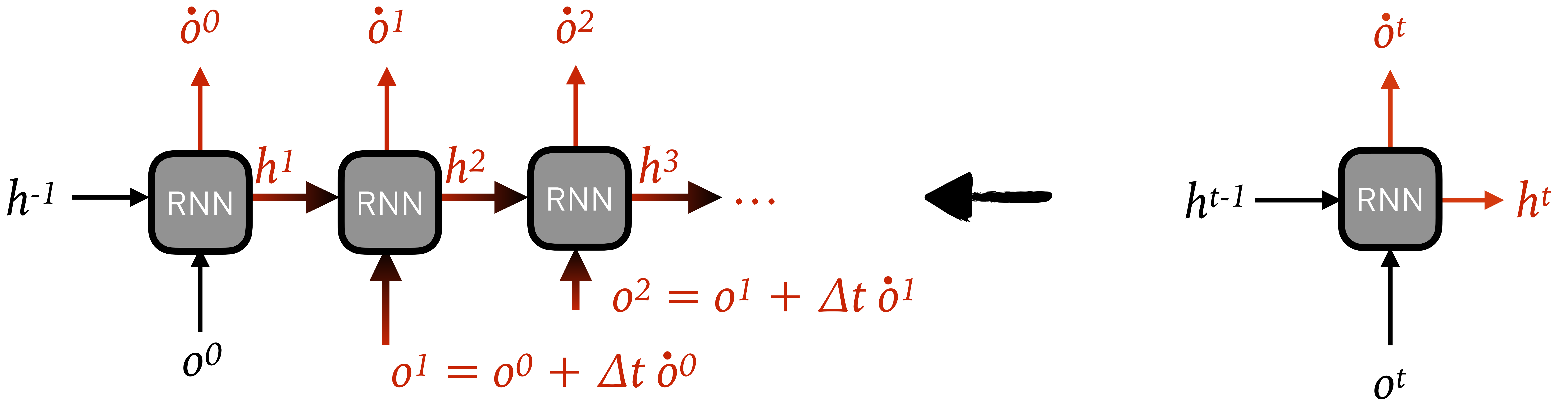

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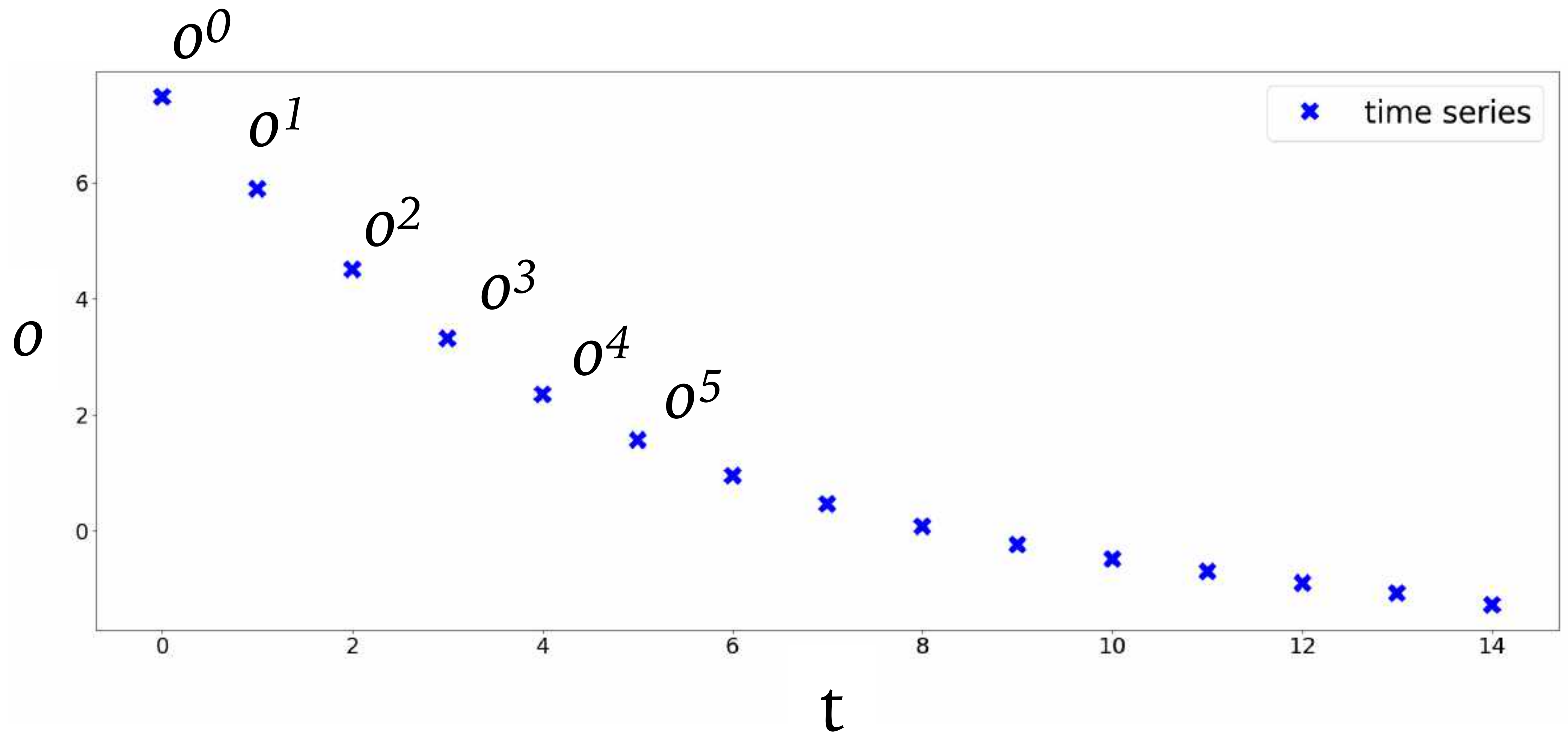

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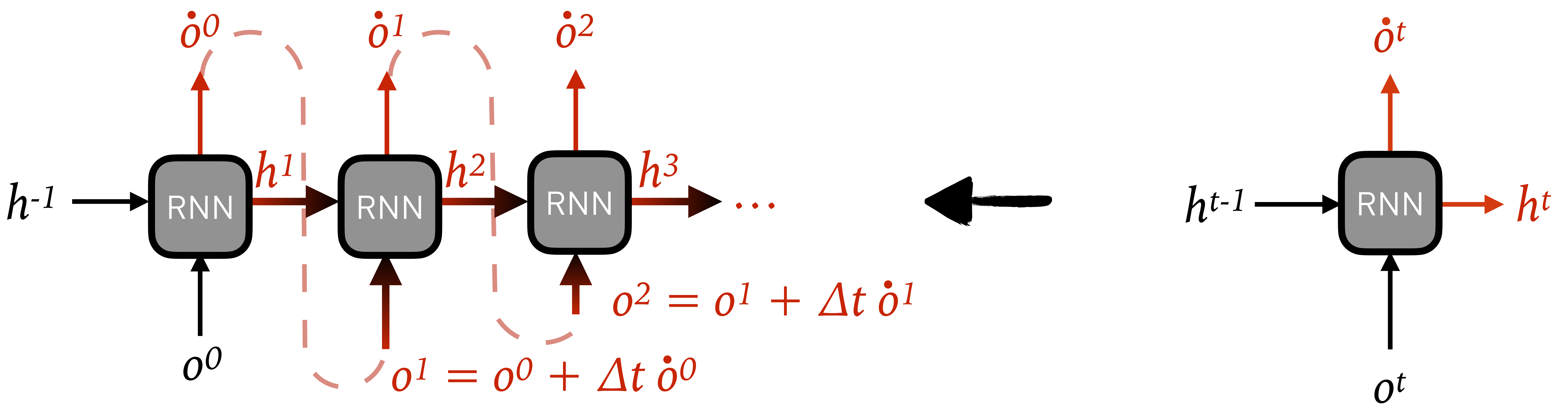
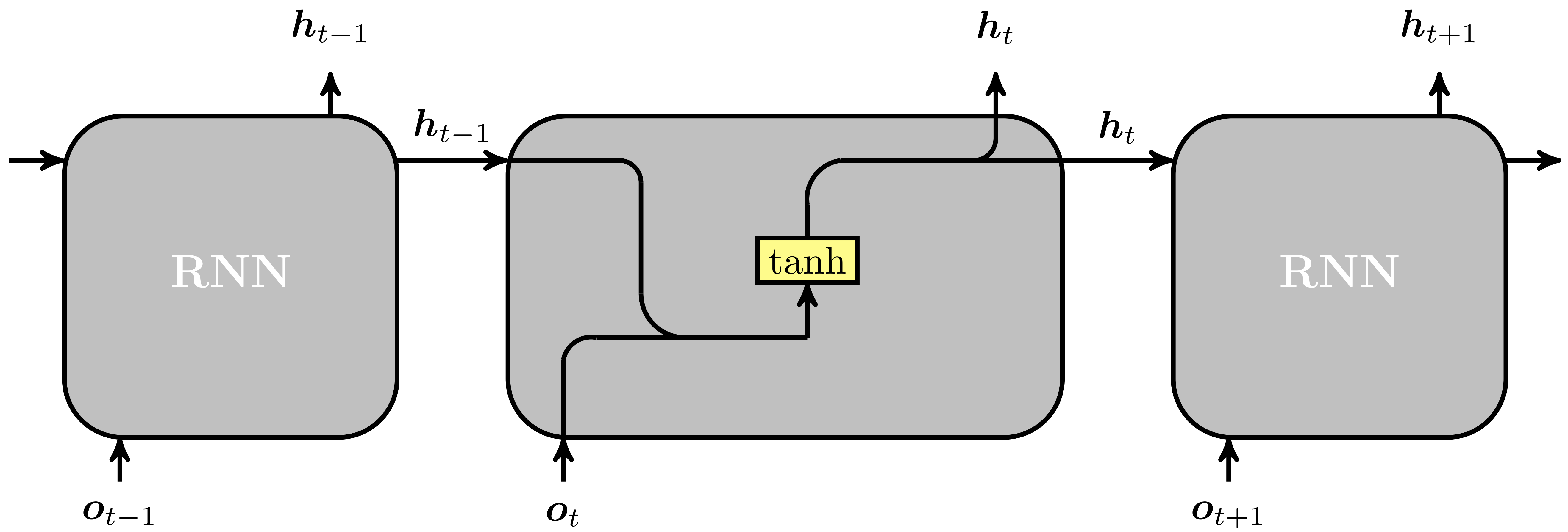


Elman RNN (1990)



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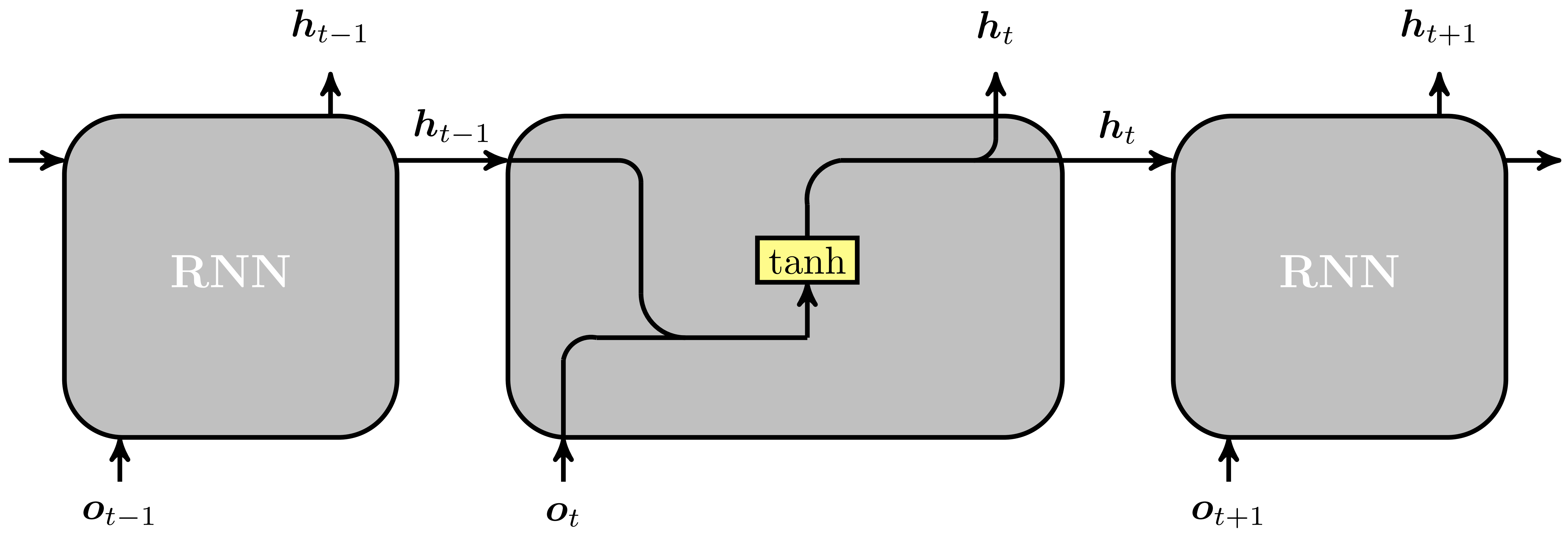

Hidden-to-hidden mapping

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

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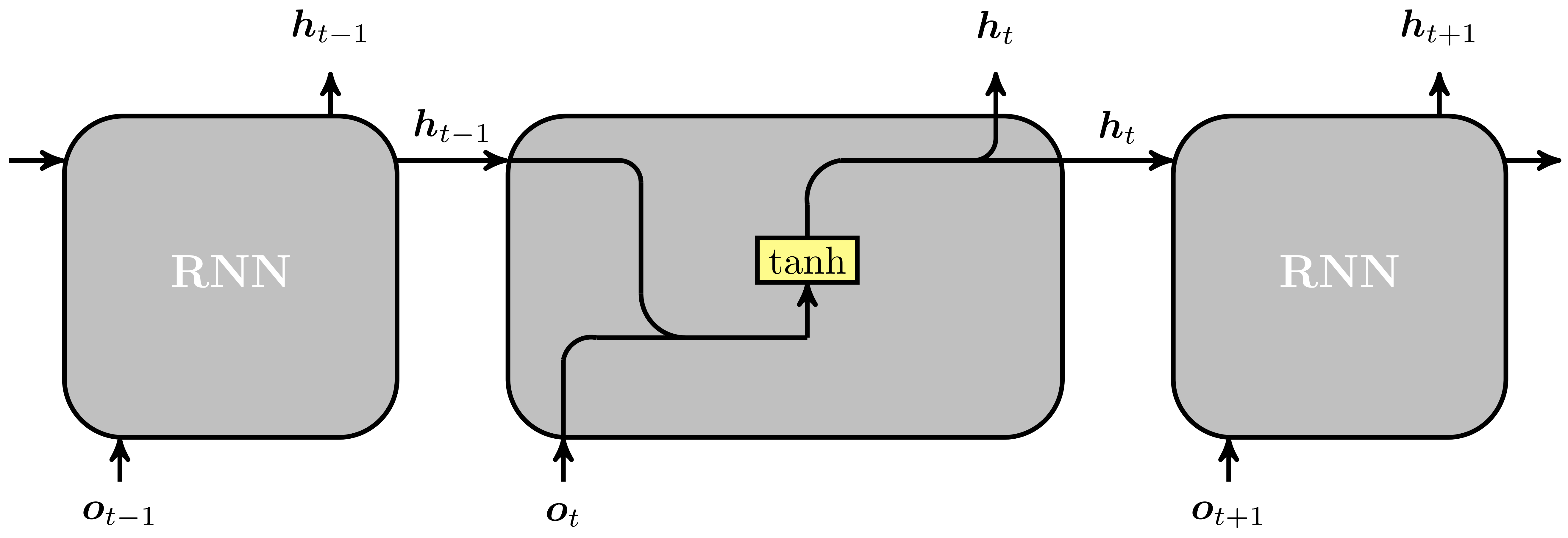

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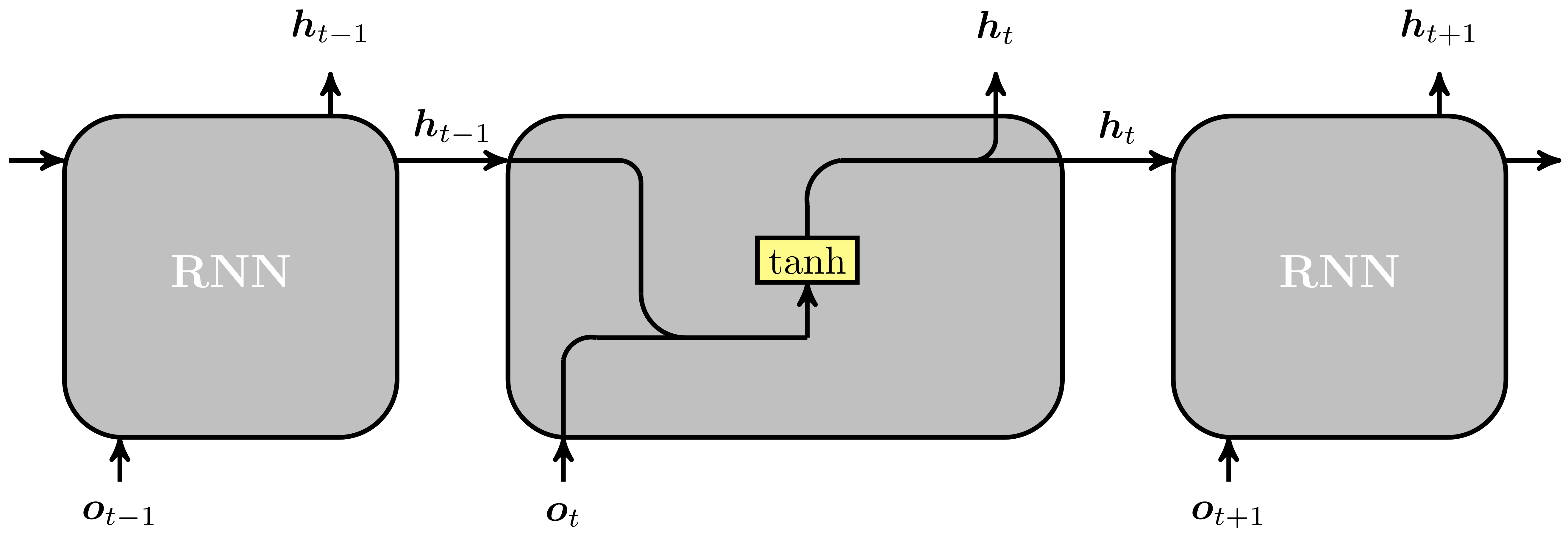

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Parameters (WEIGHTS) to be learned:

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

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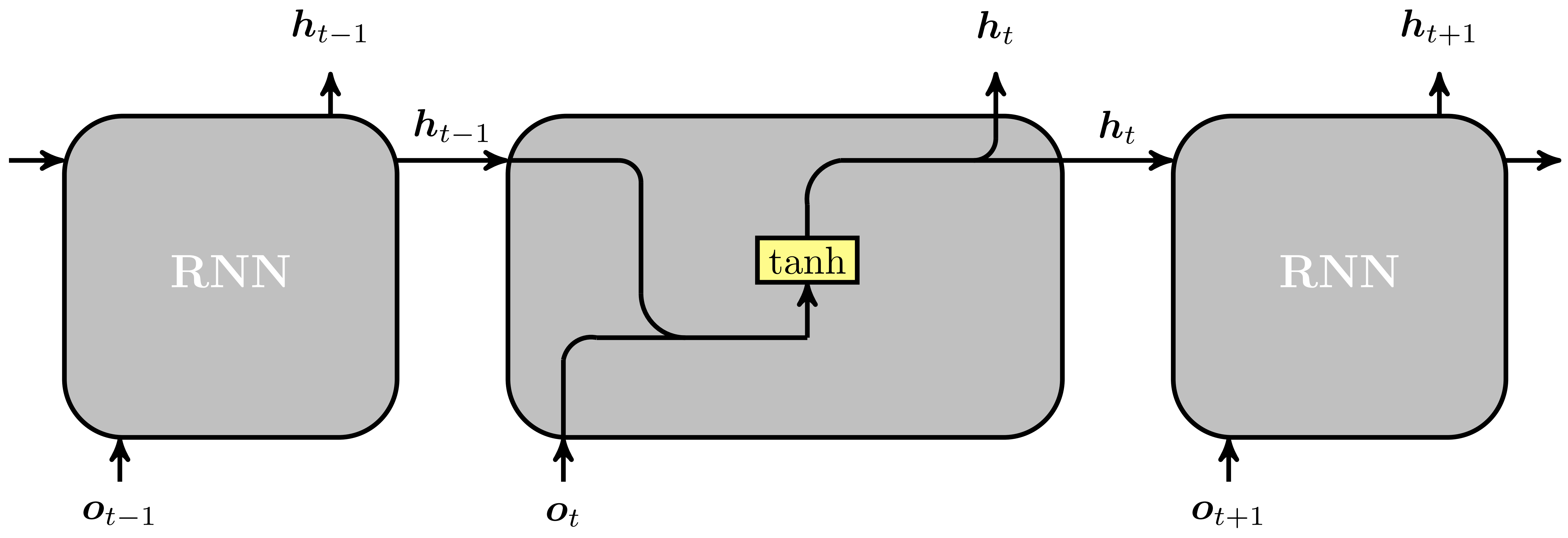

Training this network (fitting the WEIGHTS to data) is difficult.
(vanishing gradients problem)

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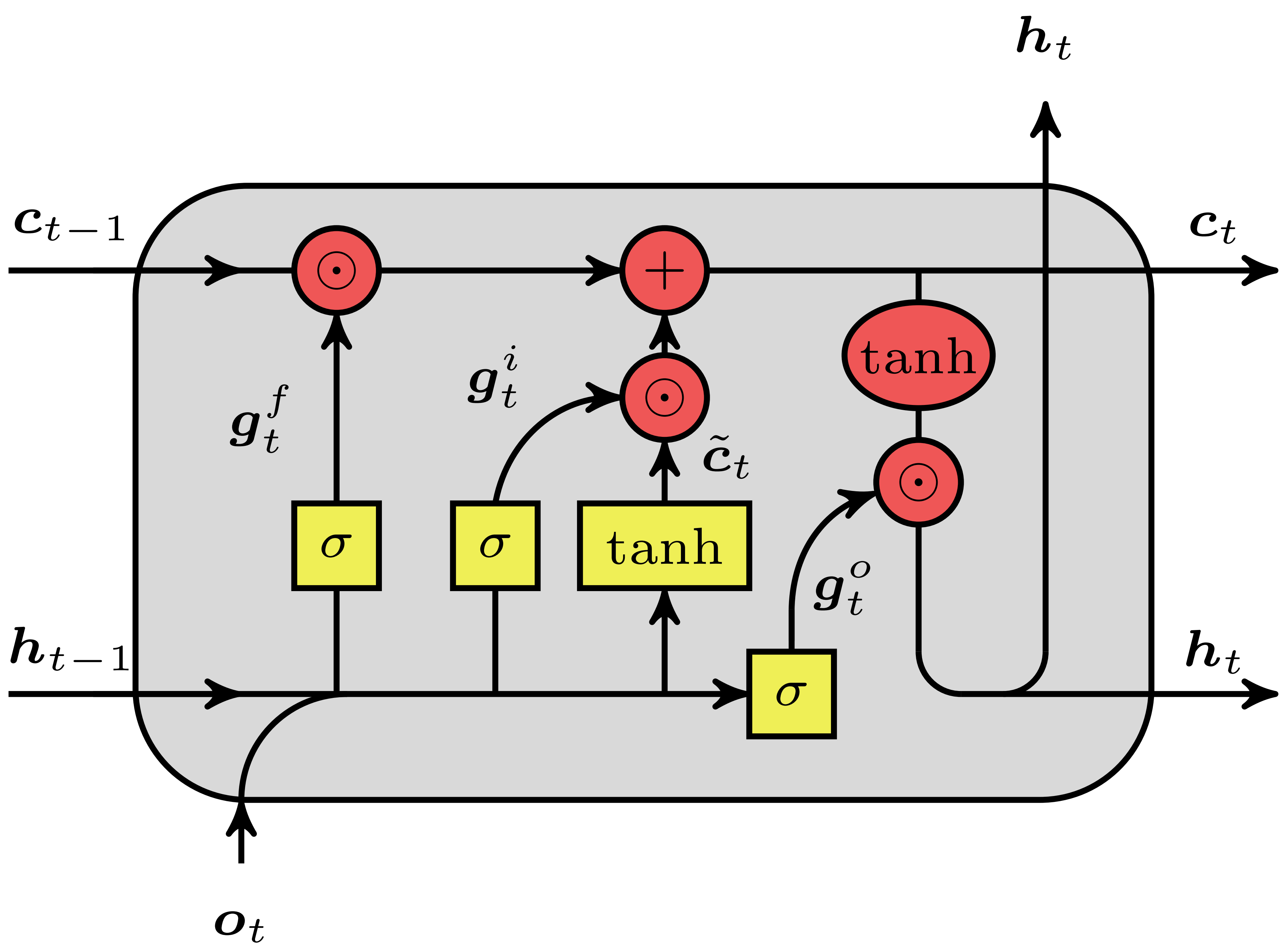
Long Short-Term Memory (LSTM) S. Hochreiter and J. Schmidhuber (1997)



Long Short-Term Memory Cell

Kuramoto-Sivashinsky

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

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

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

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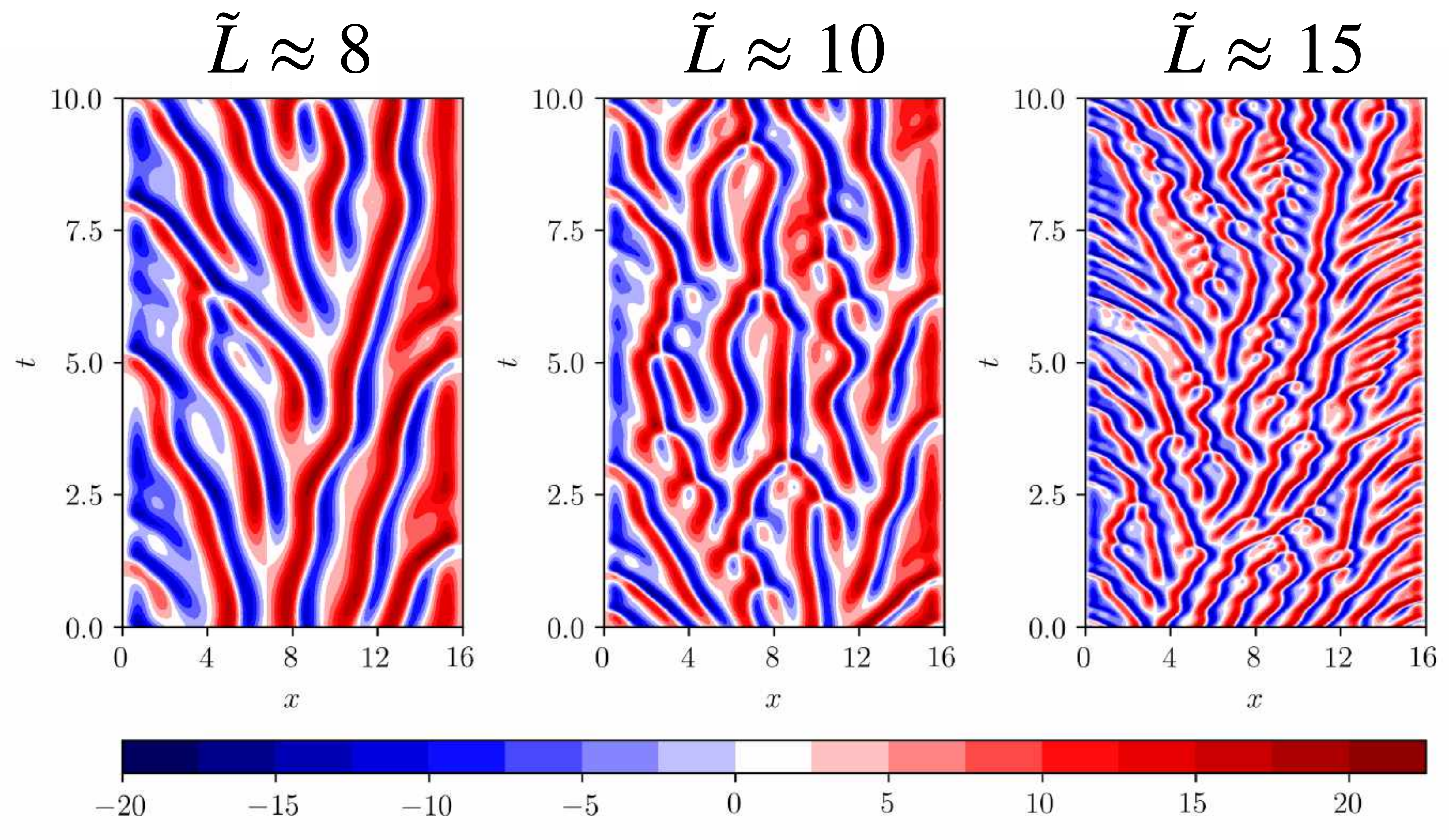

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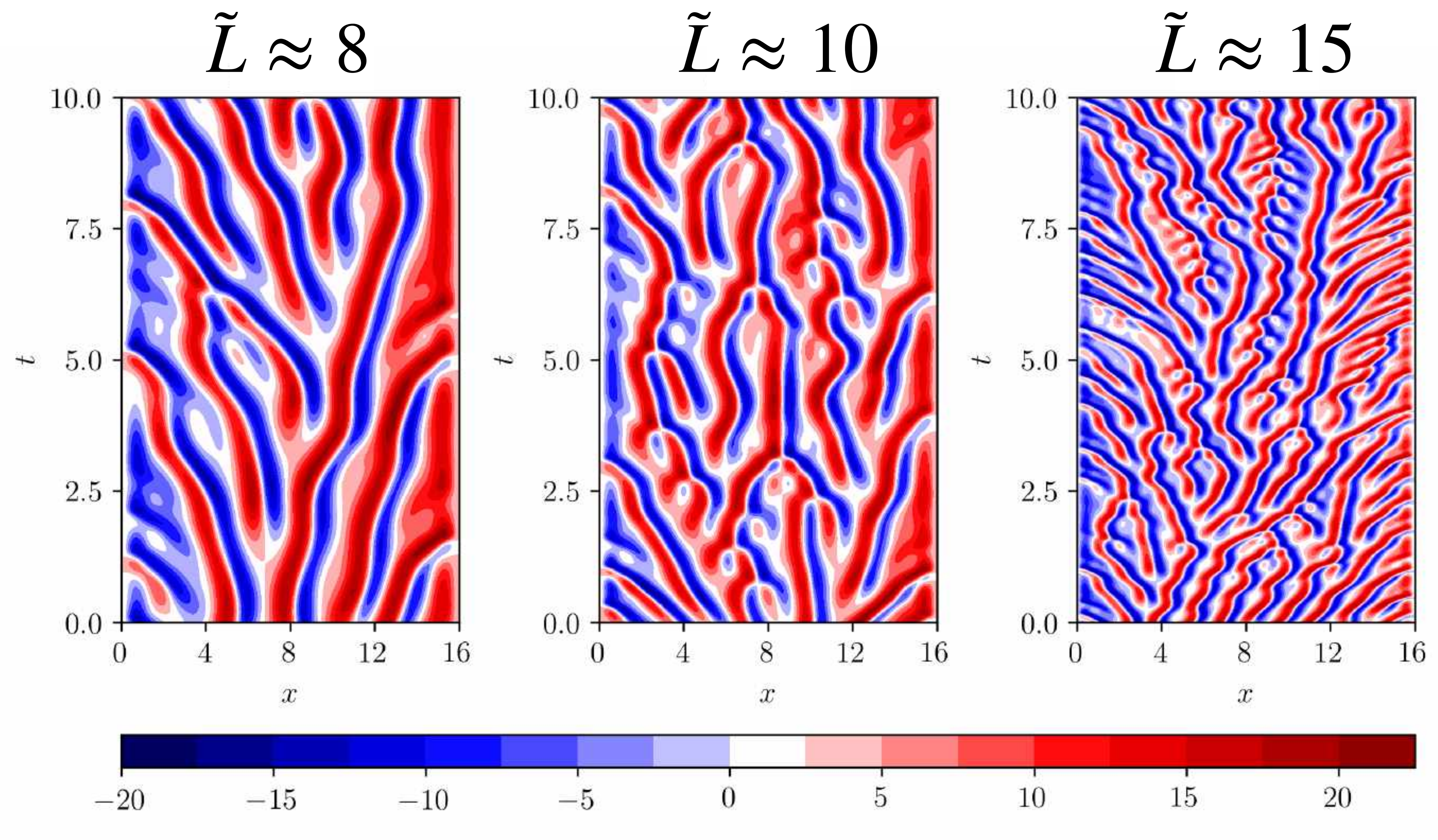

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Discretization with $d_u = 512$ gridpoints

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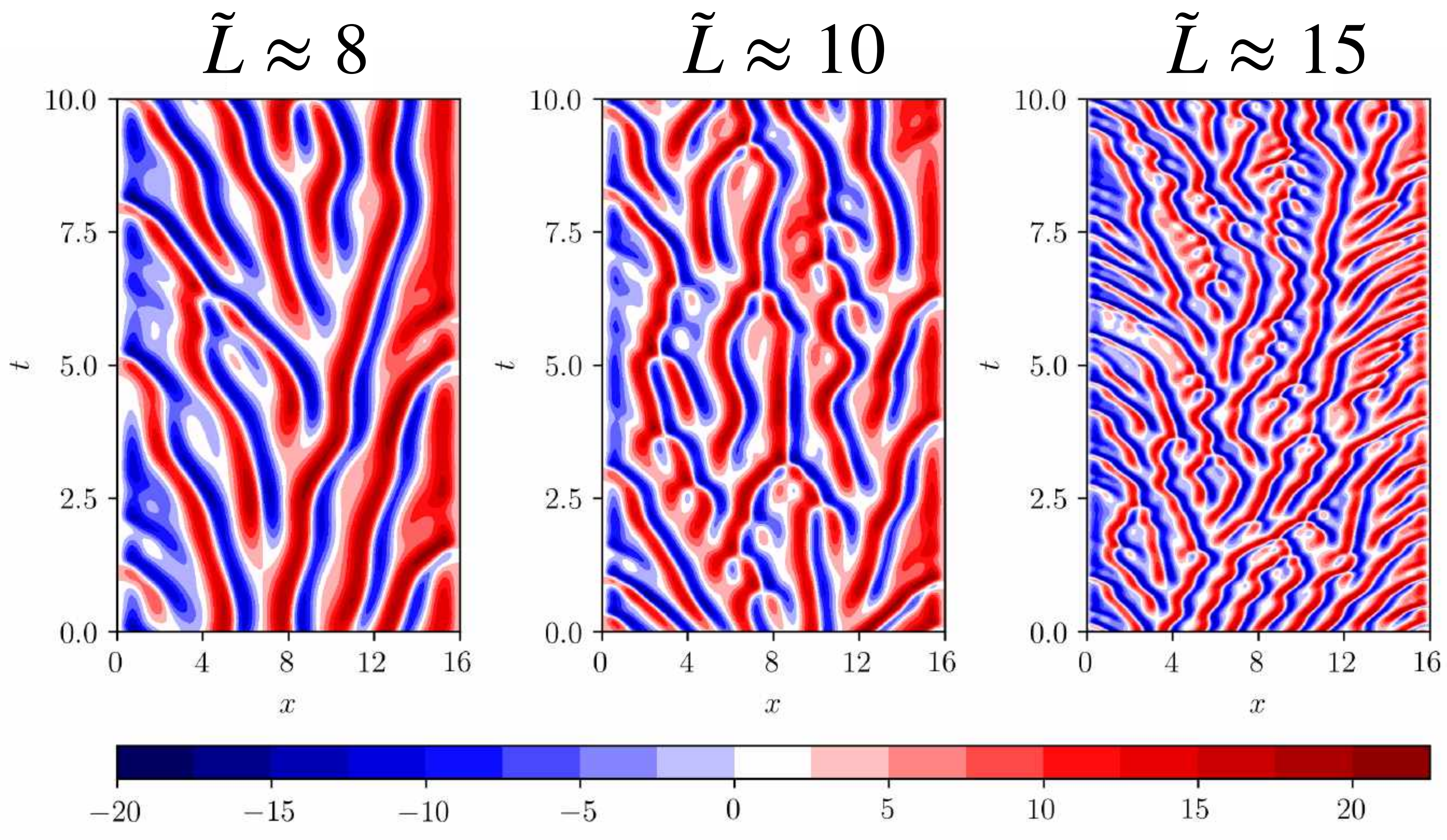

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$$\frac{du_i}{dt} = -\nu \frac{u_{i-2} - 4u_{i-1} + 6u_i - 4u_{i+1} + u_{i+2}}{\Delta x^4} - \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} - \frac{u_{i+1}^2 - u_{i-1}^2}{4\Delta x}$$

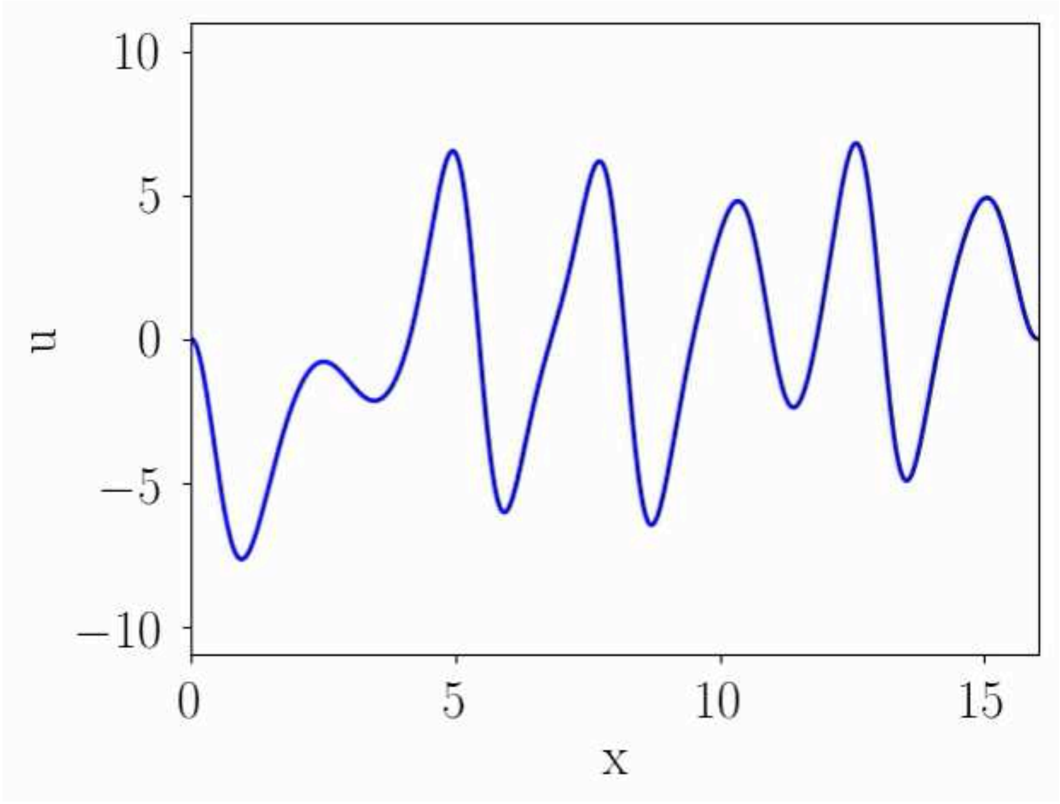
Integration with $dt = 0.02$ up to $T = 10^4$
(after discarding initial transients)
500.000 **samples**

Constructing the observable - training data

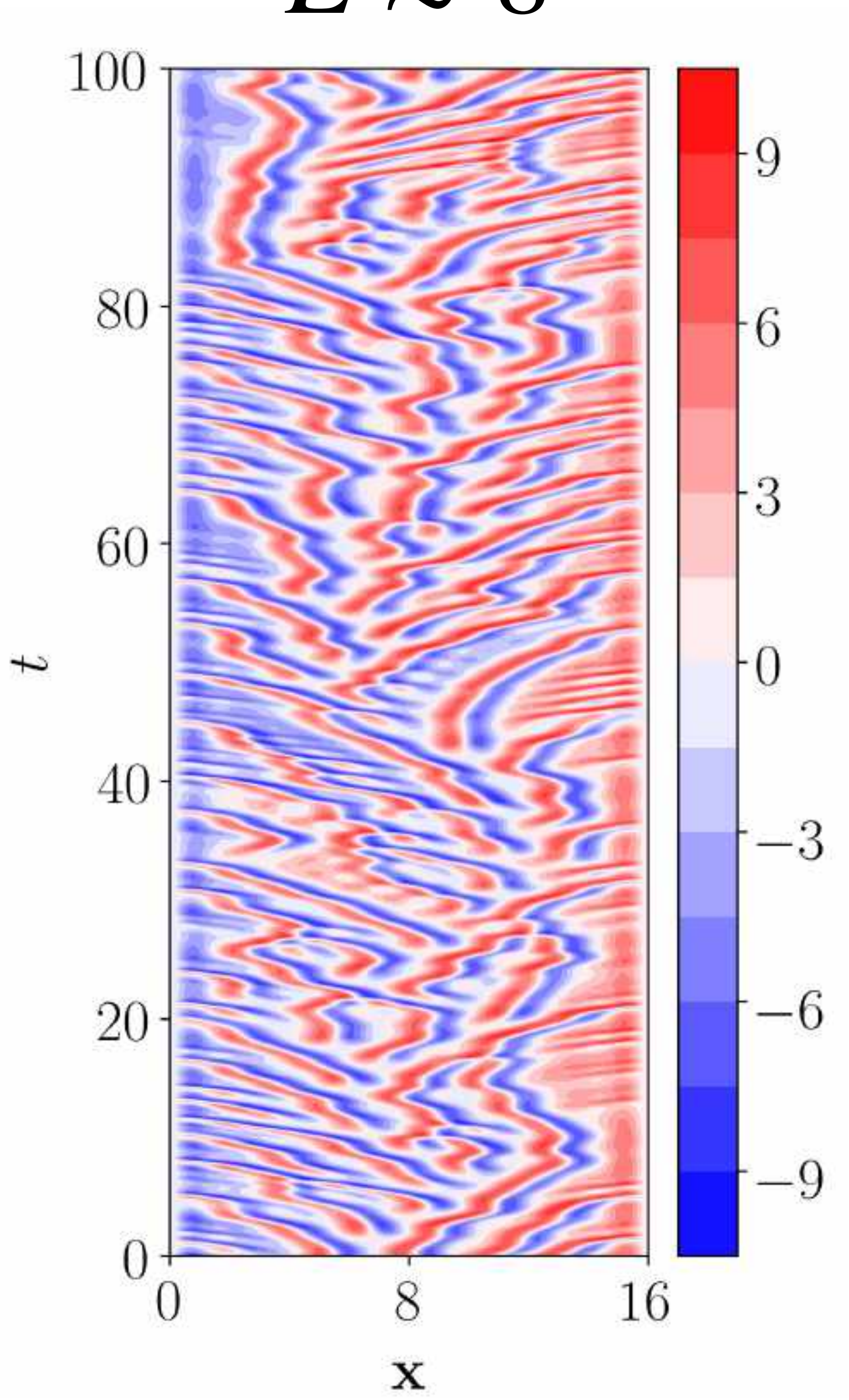
High dimensional

High dimensional simulation data

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



$\tilde{L} \approx 8$



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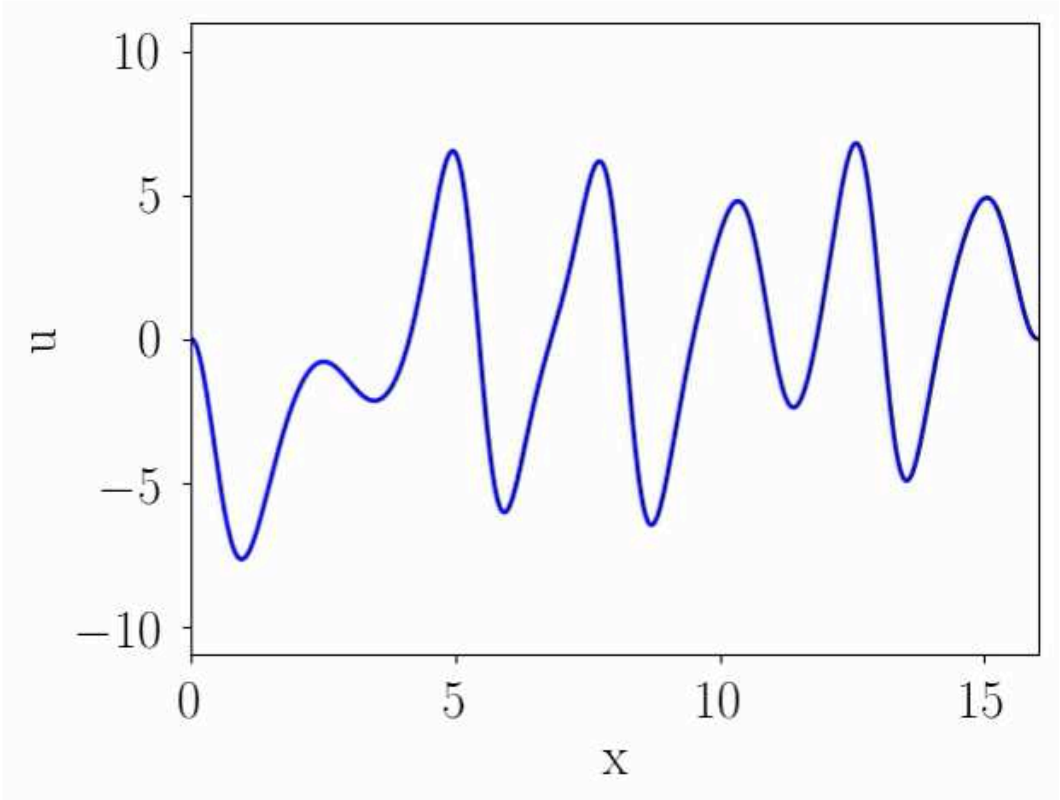

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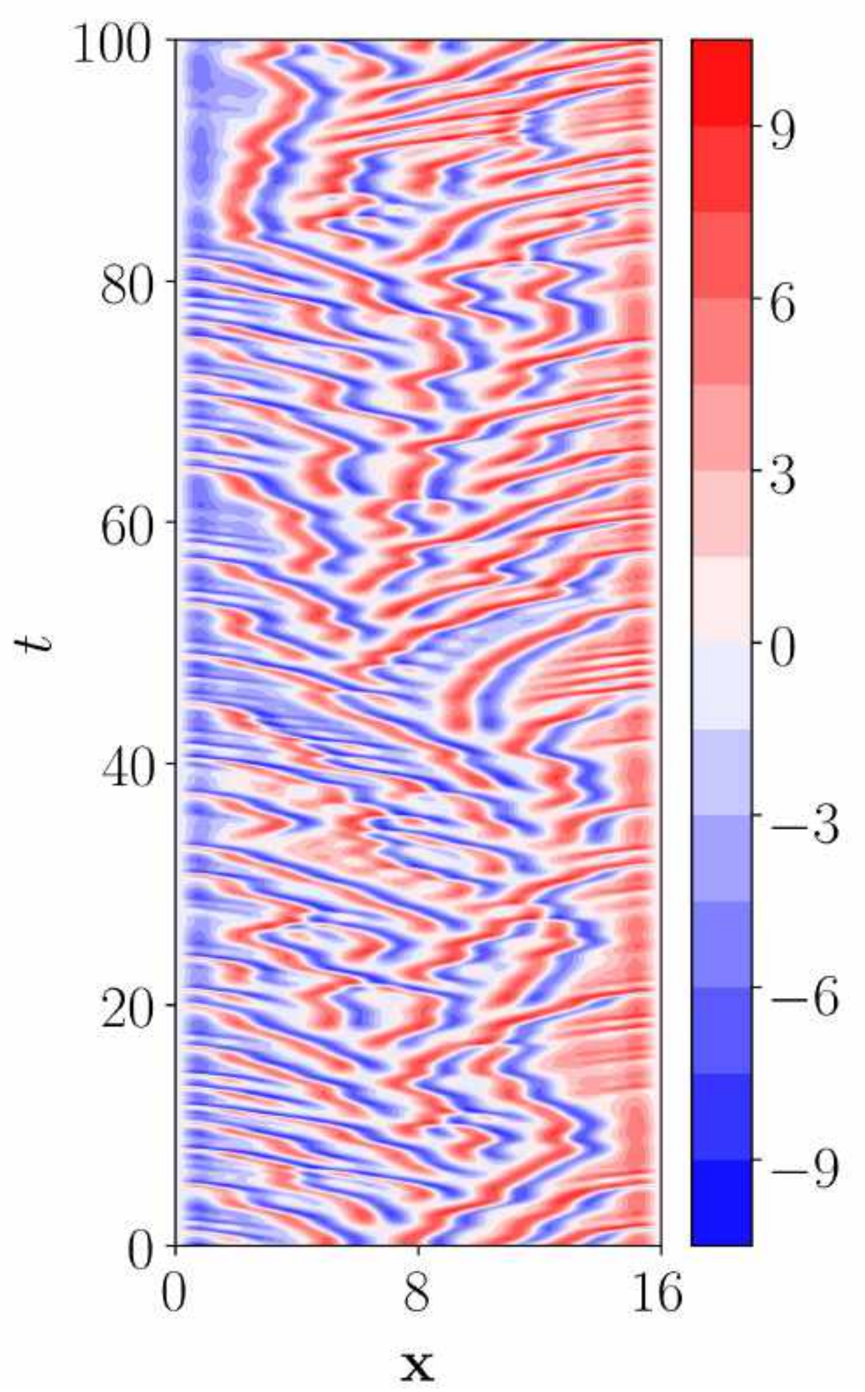

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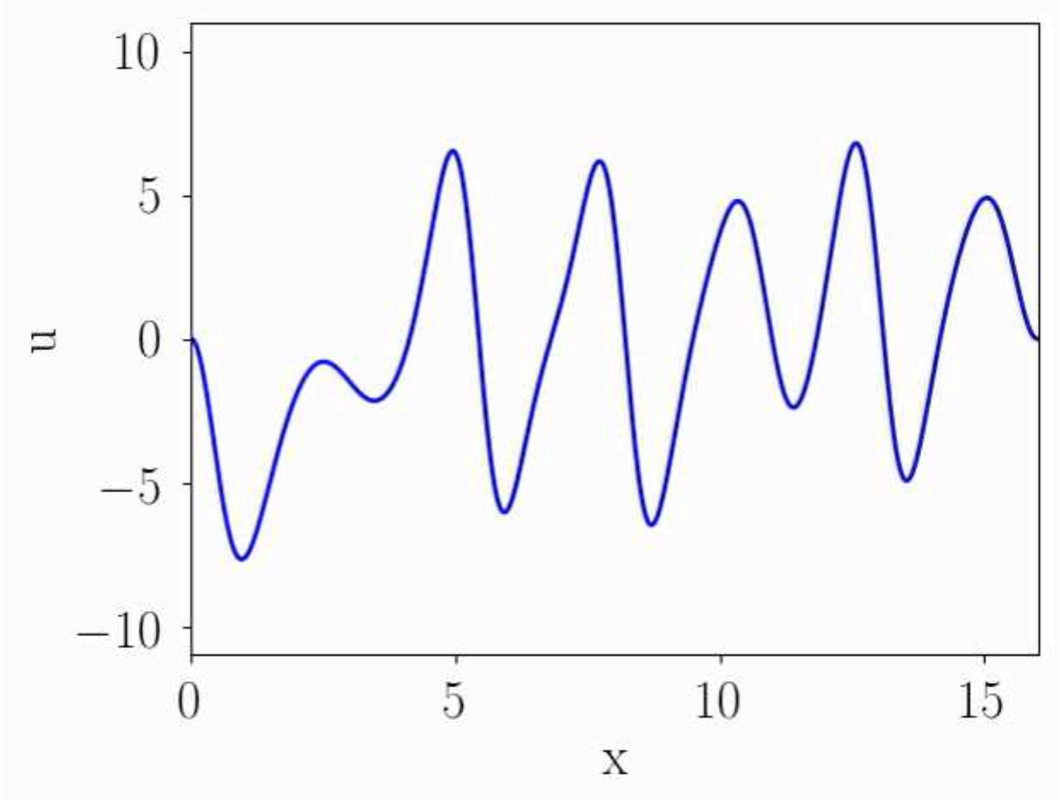

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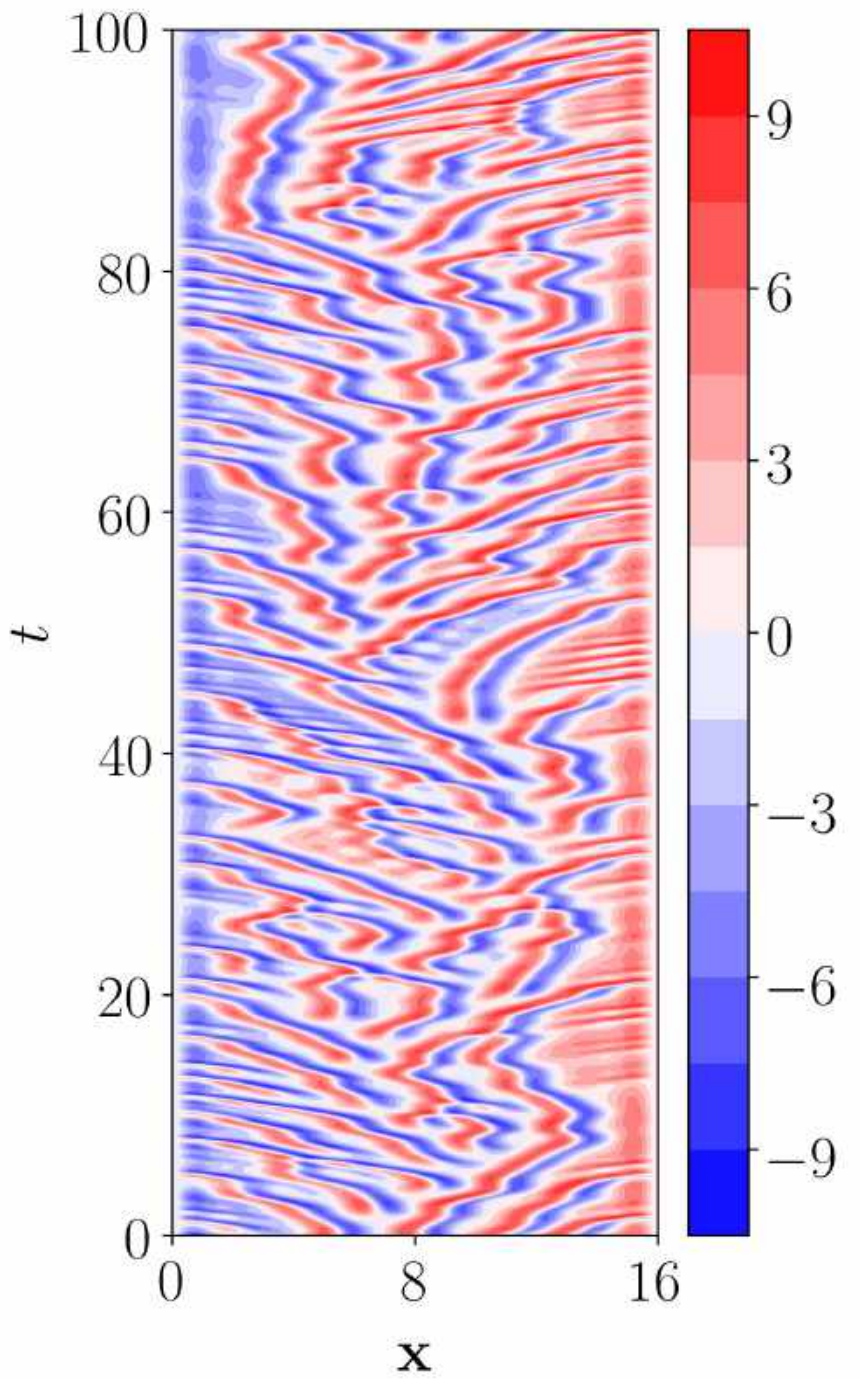
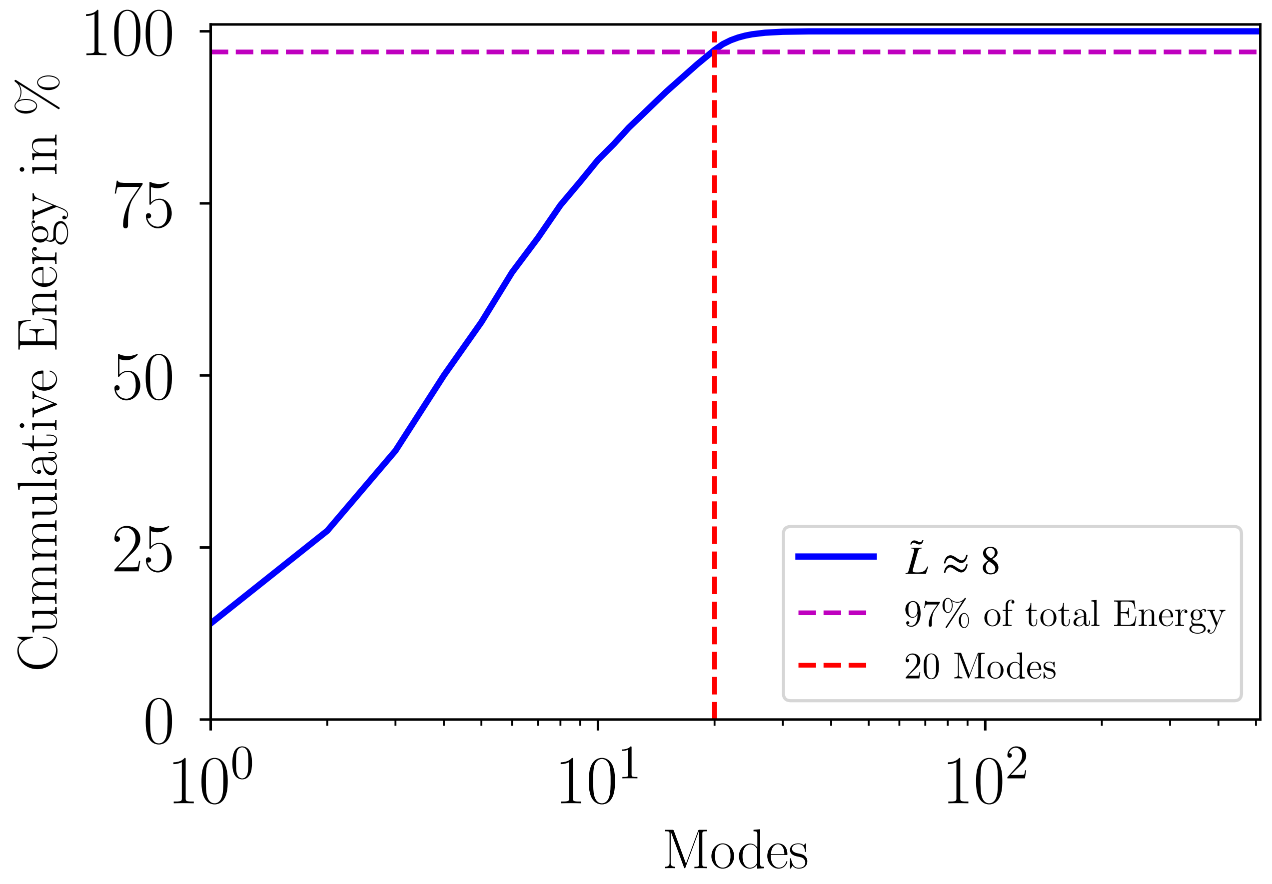


SVD / PCA

Singular Value Decomposition



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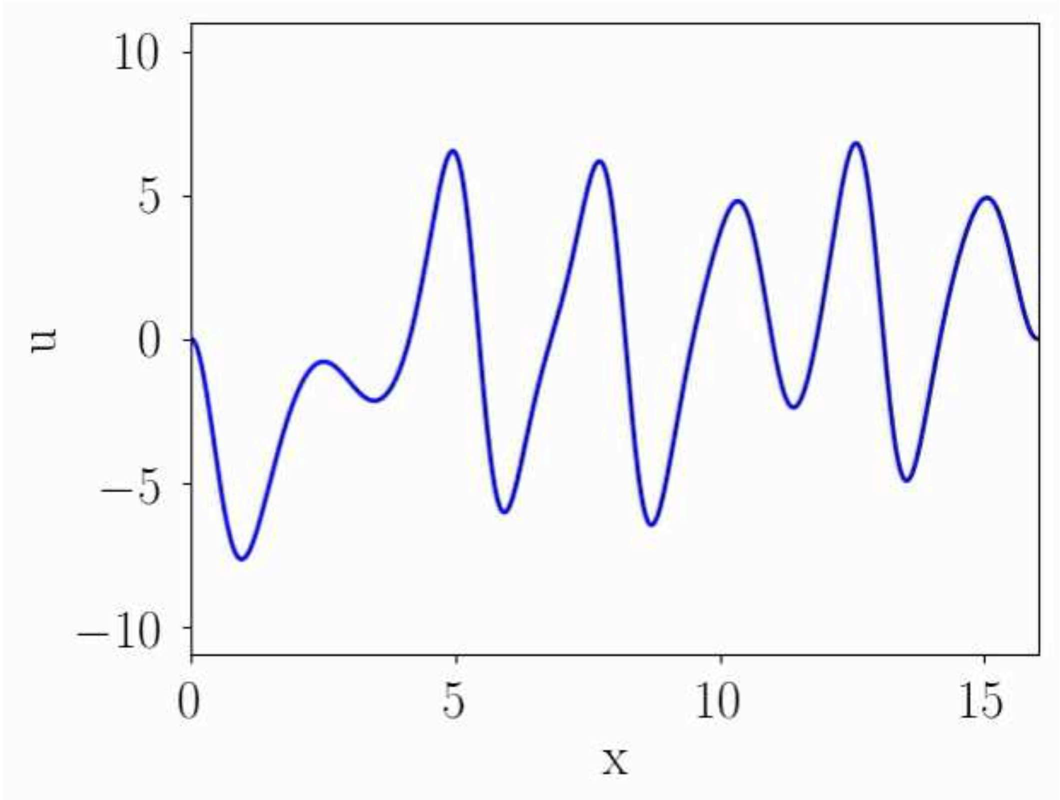

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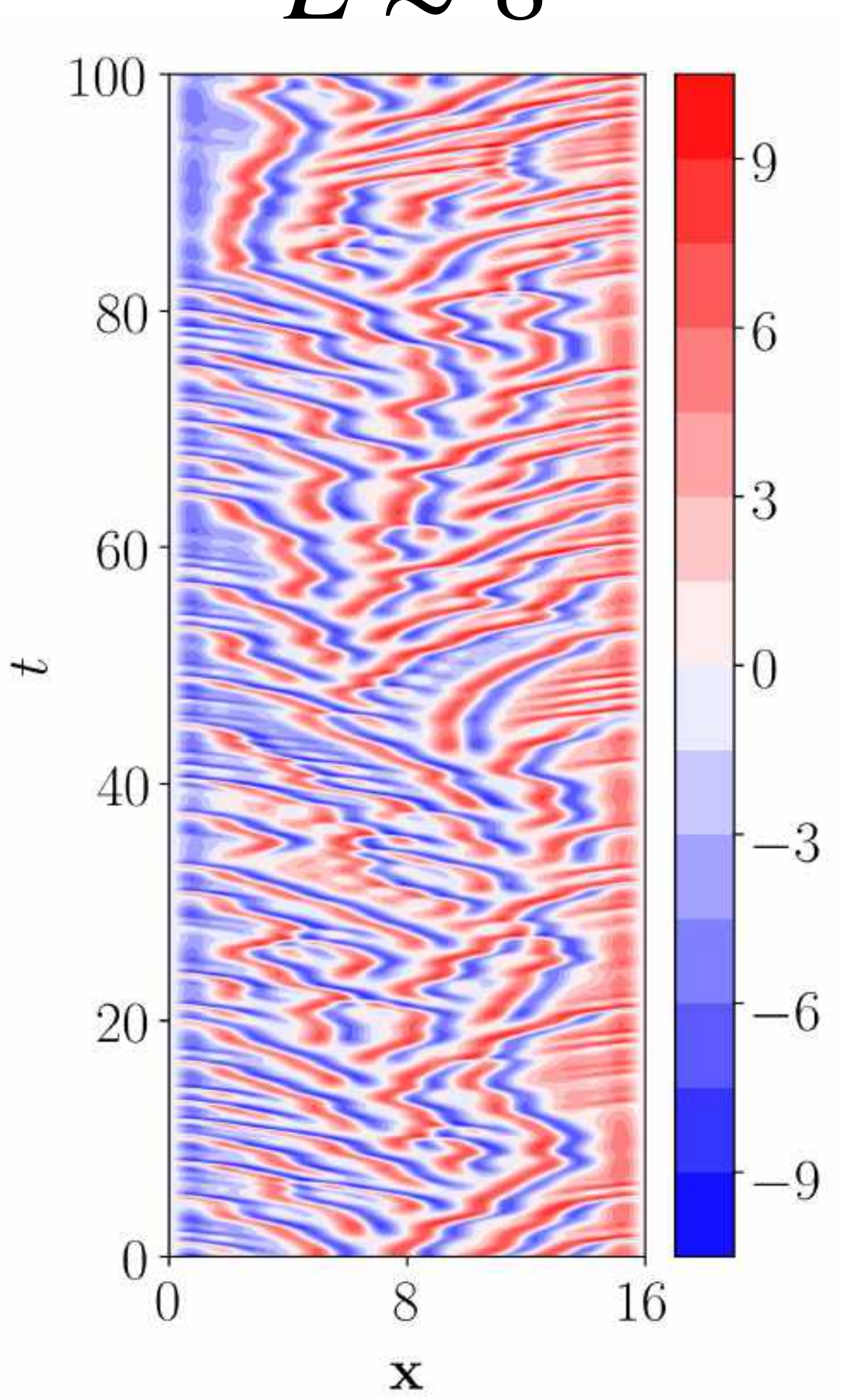
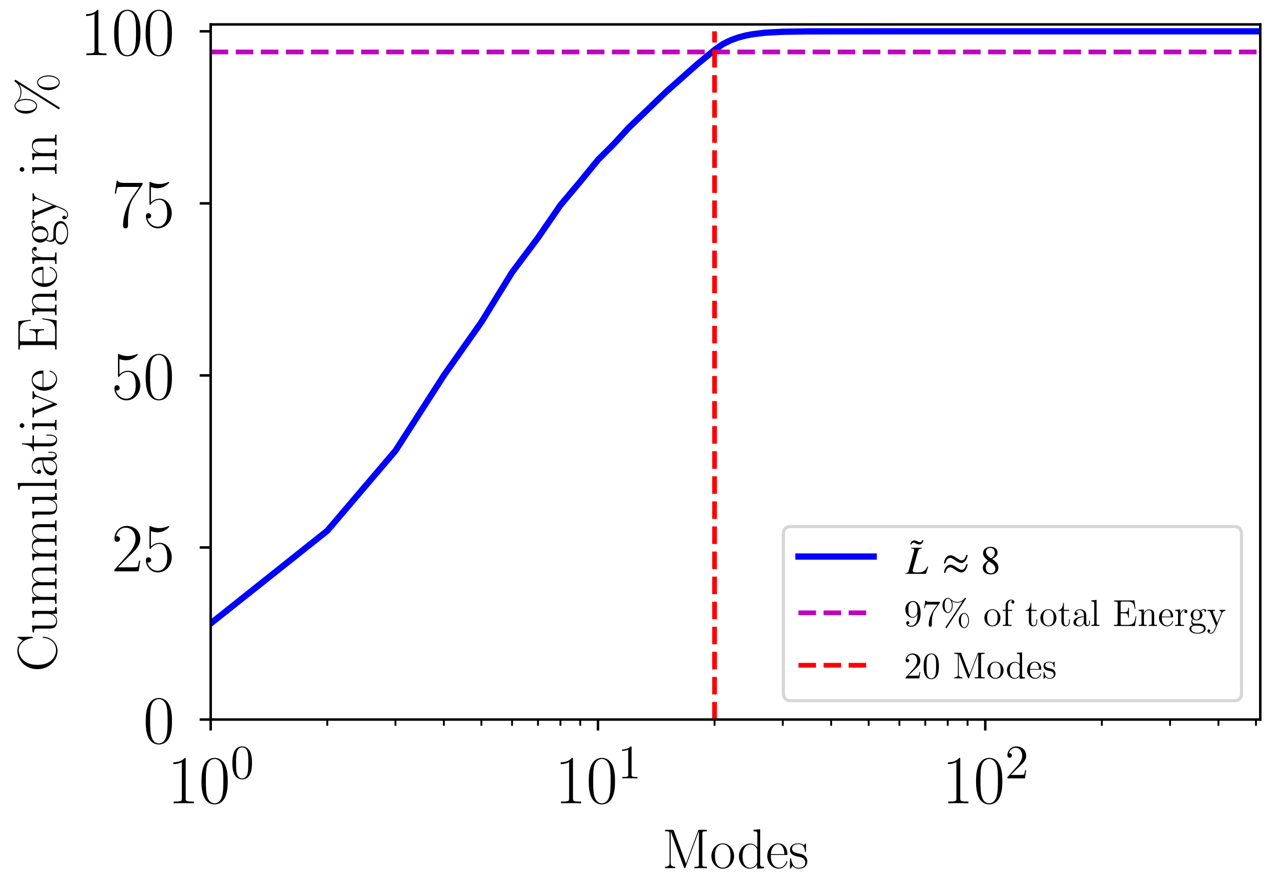


SVD / PCA

Singular Value Decomposition

Throw away modes with low energy



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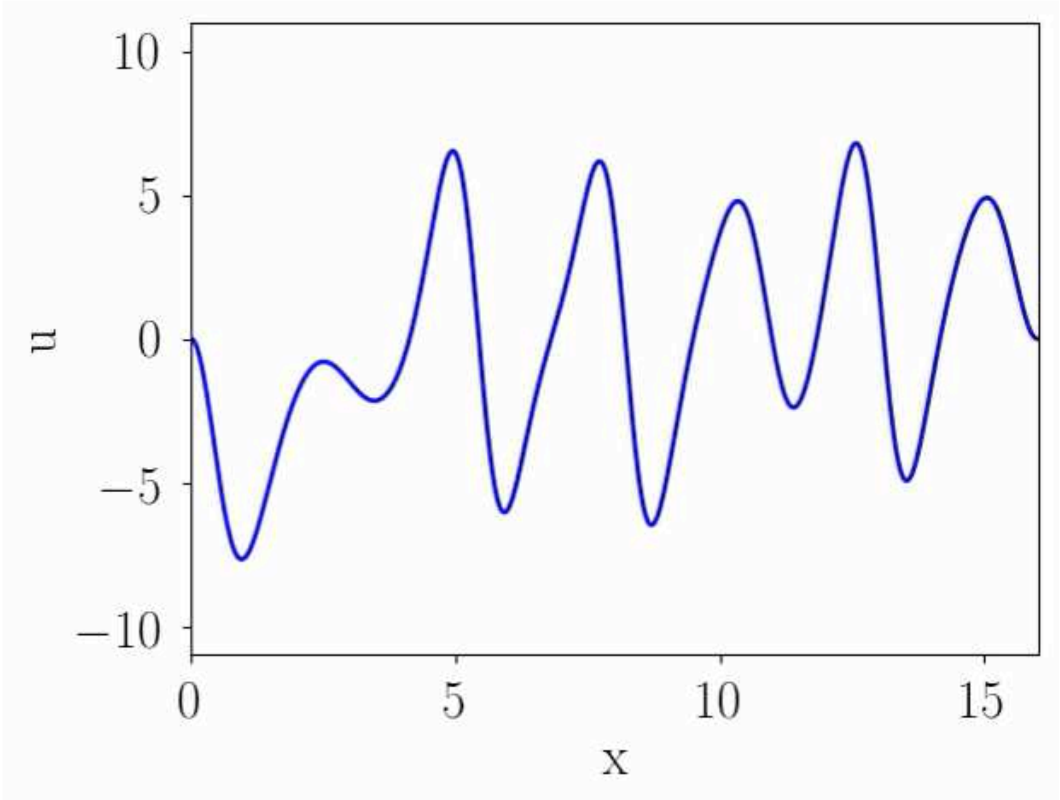

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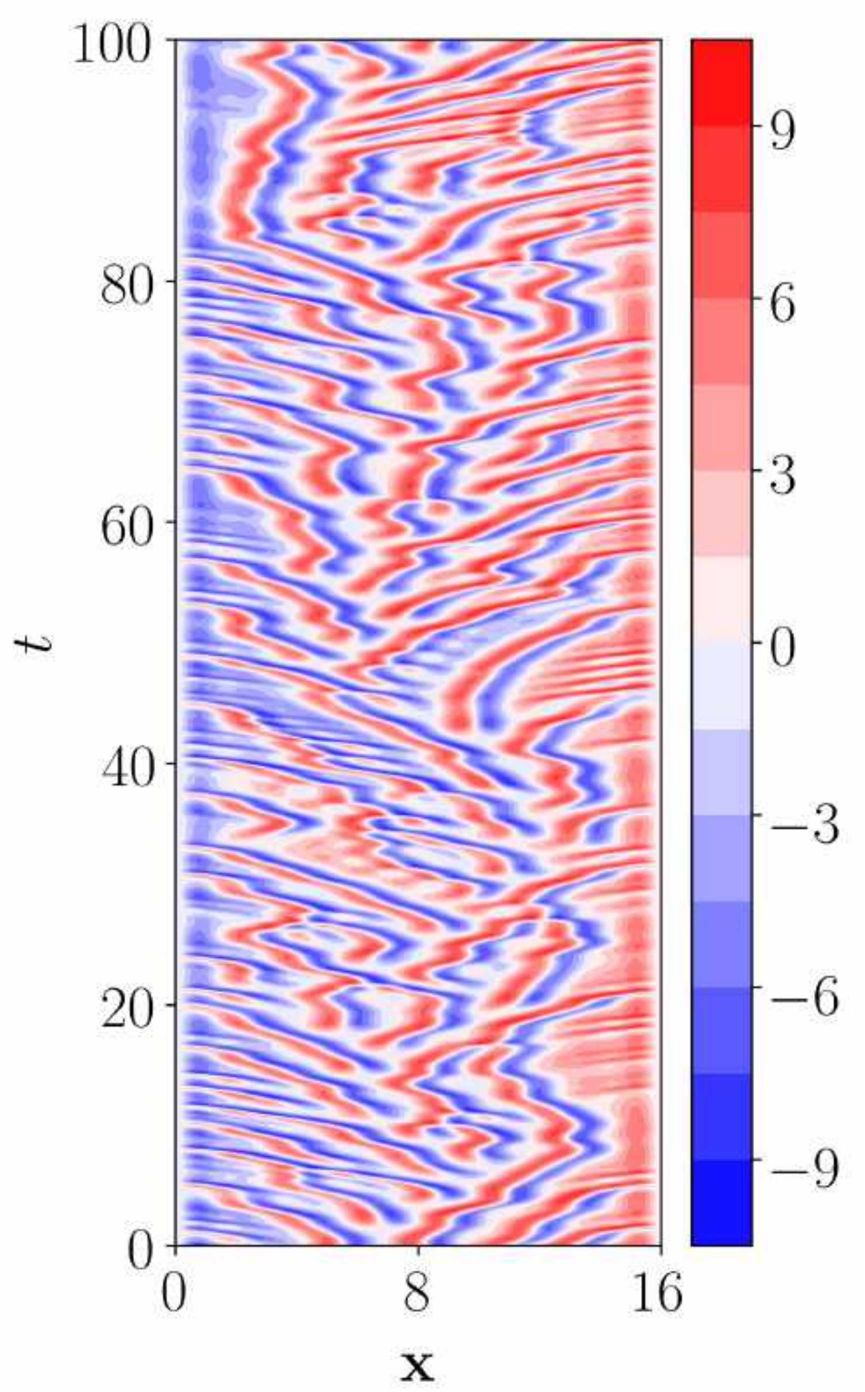

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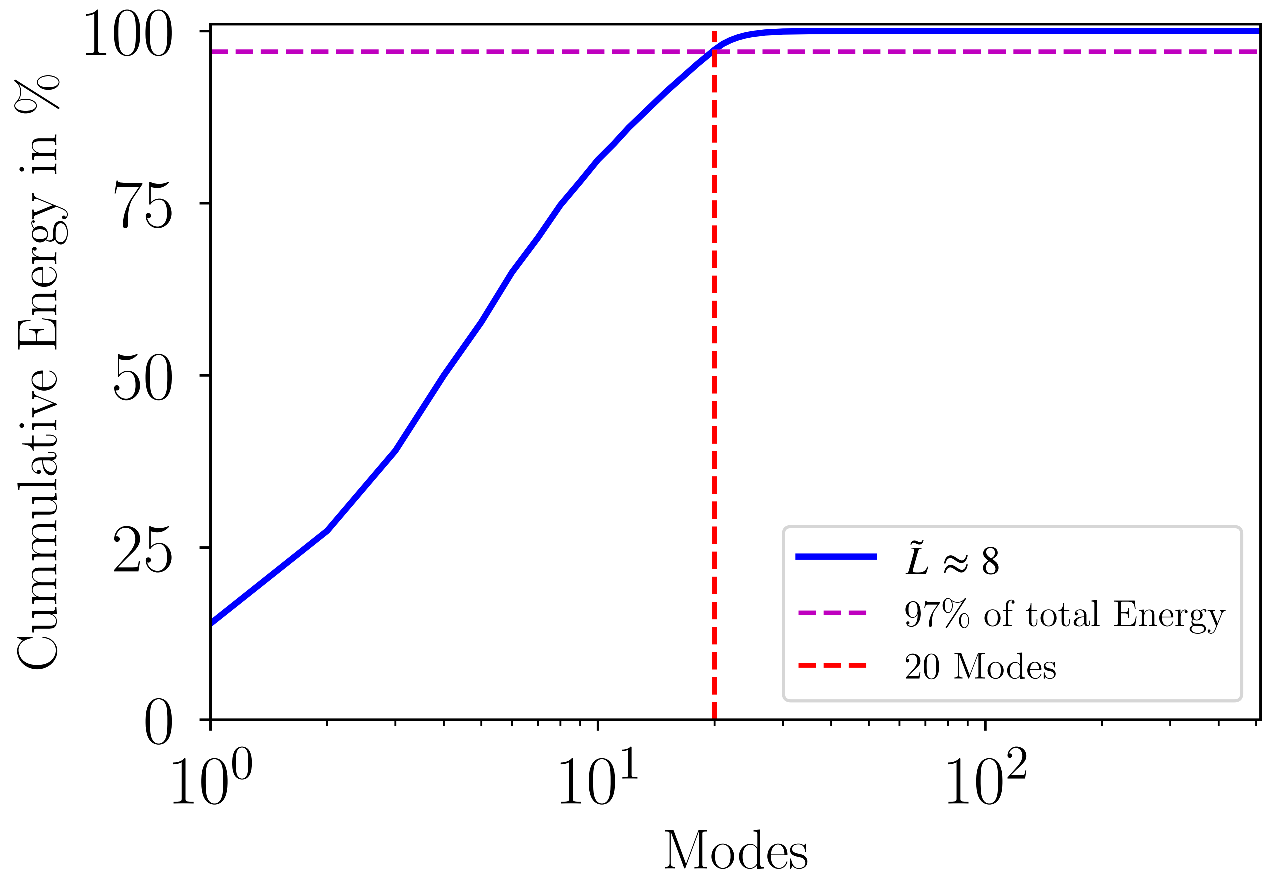

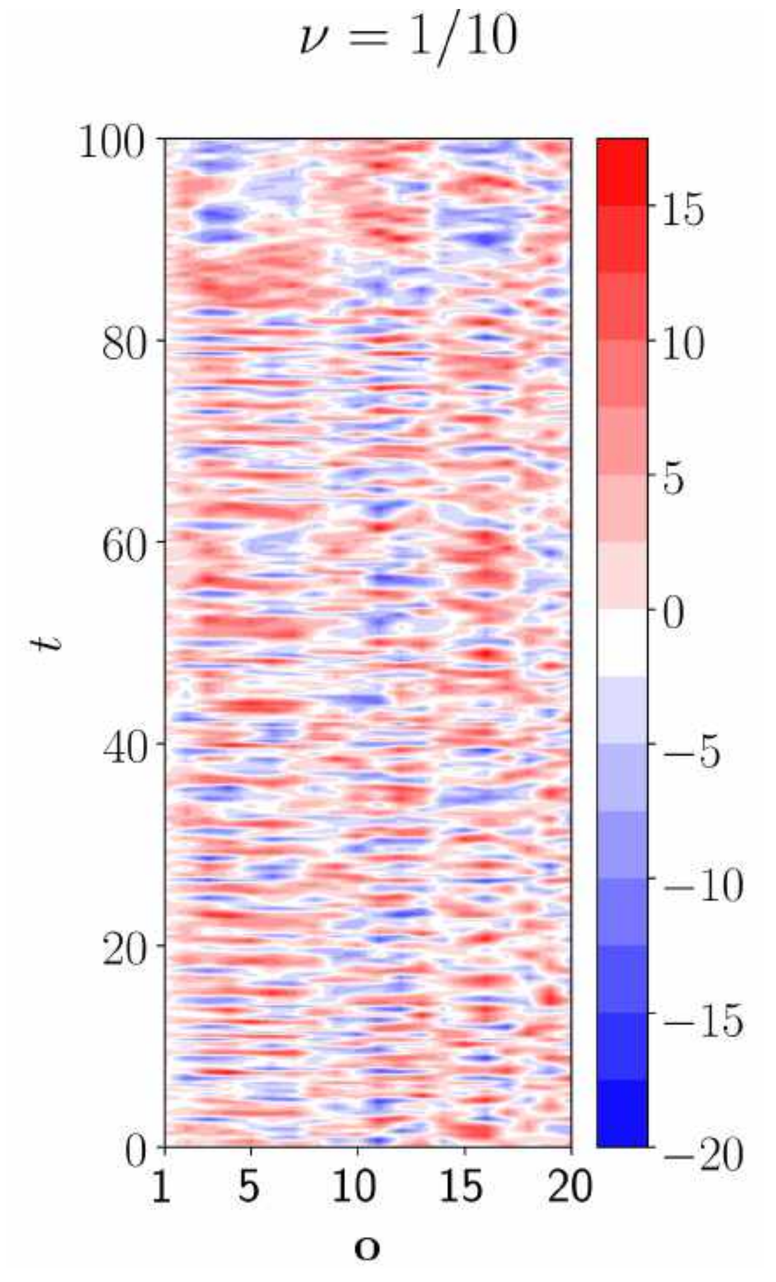

20 Modes (observable)

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

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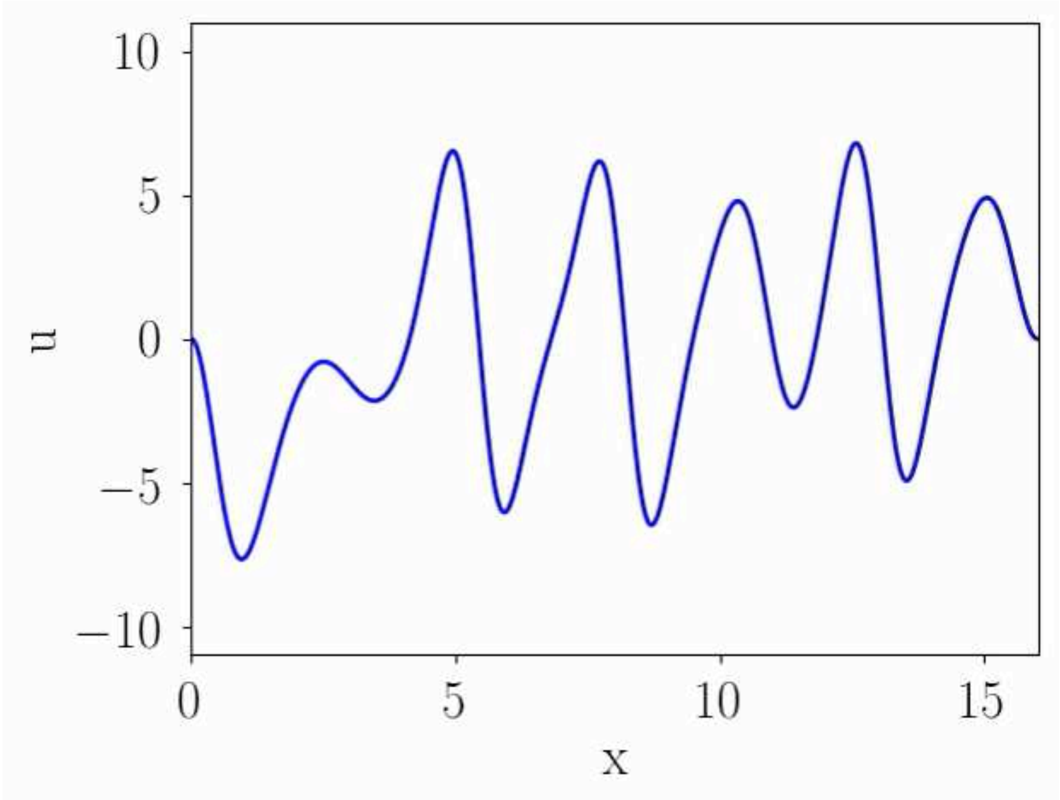
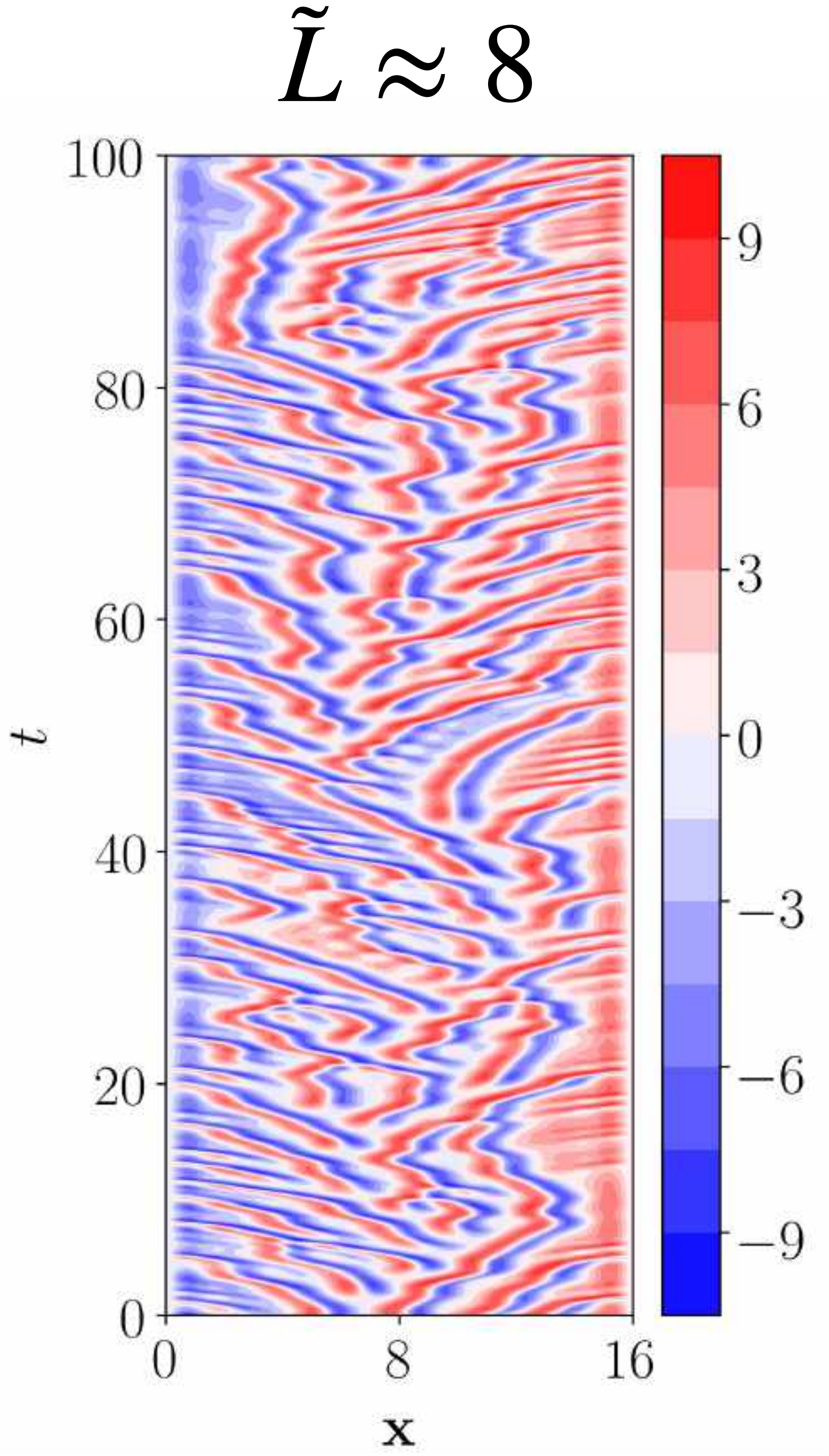
- $u_t \in \mathbb{R}^{512}$

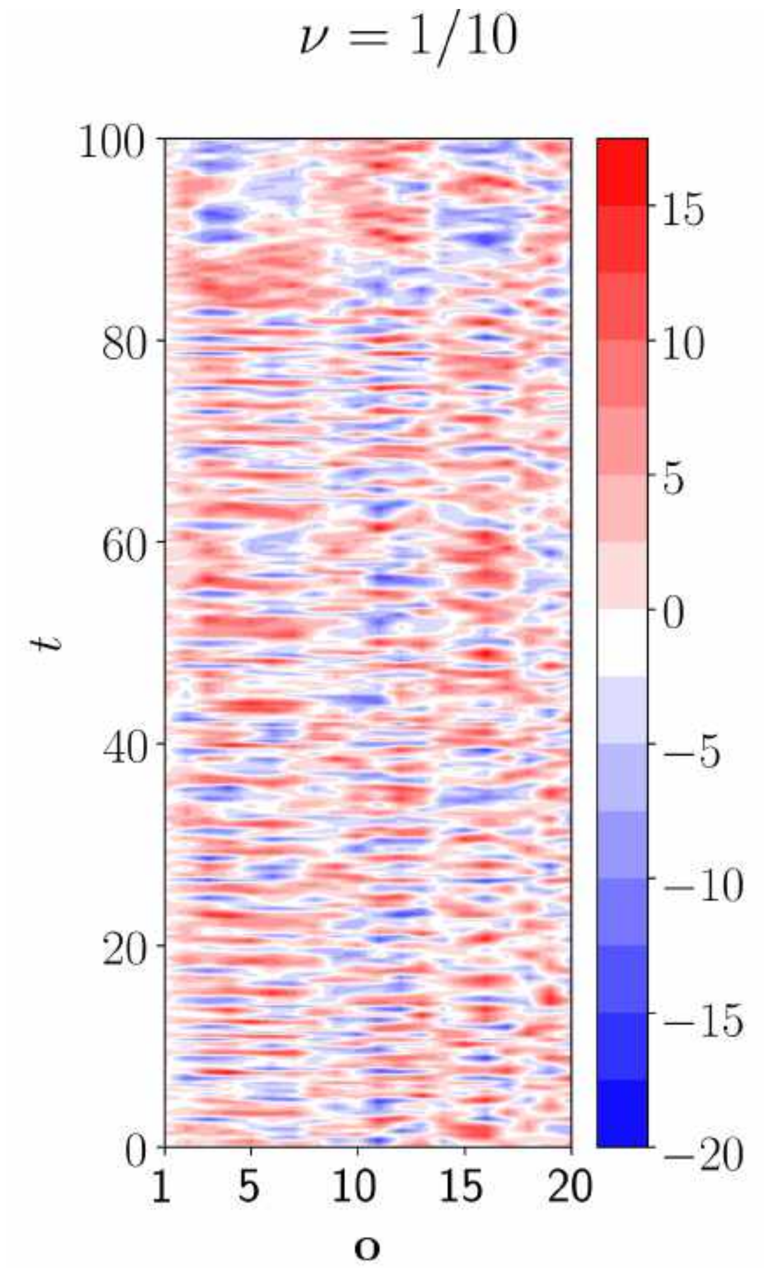




SVD / PCA

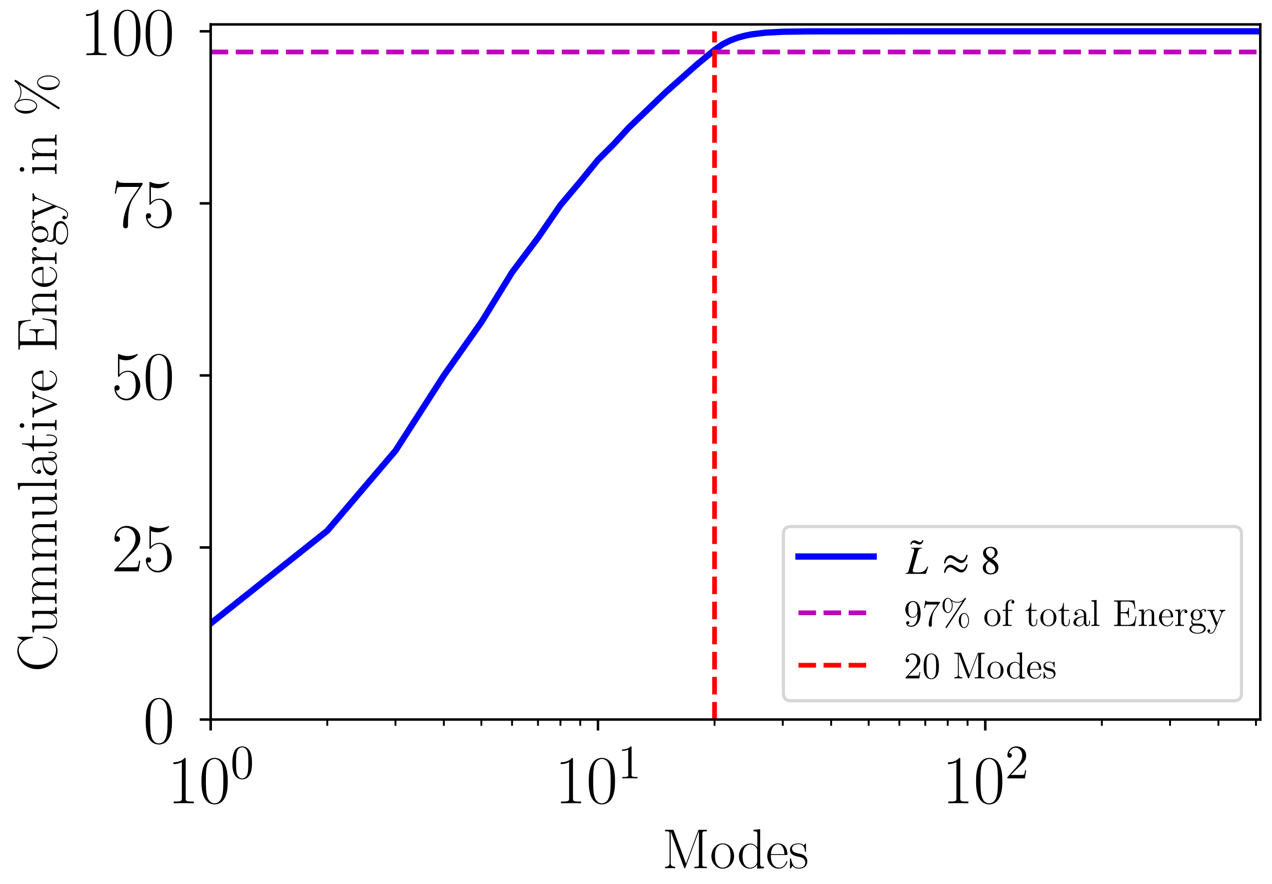
Singular Value Decomposition

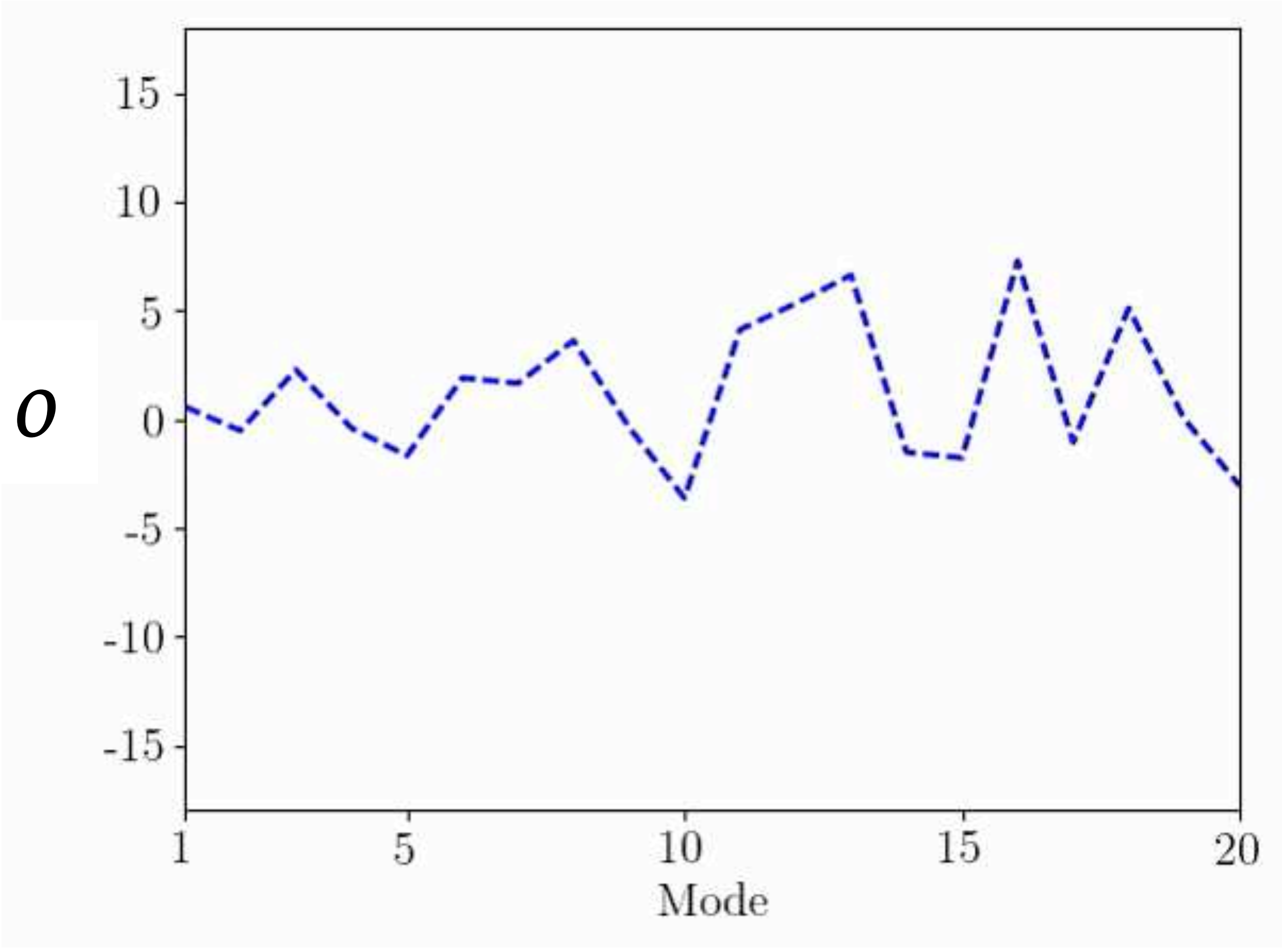
Throw away modes with low energy



20 Modes (observable)

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





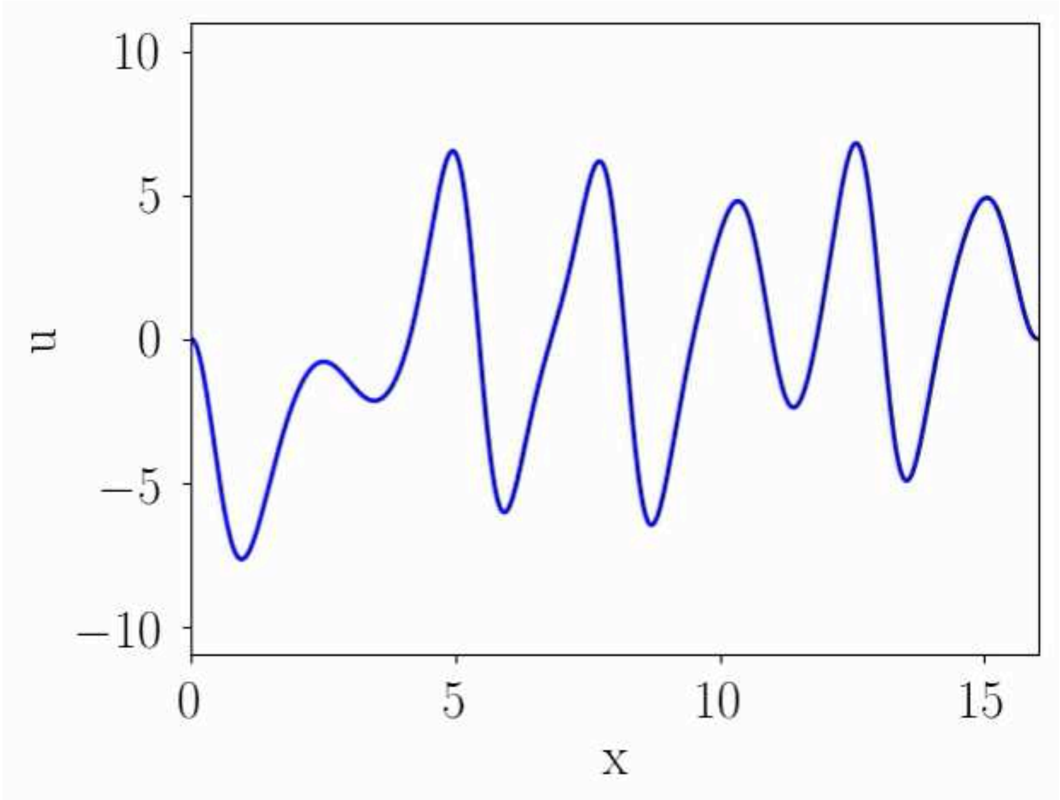
*Low dimensional **reduced-order** state (most energetic modes)*

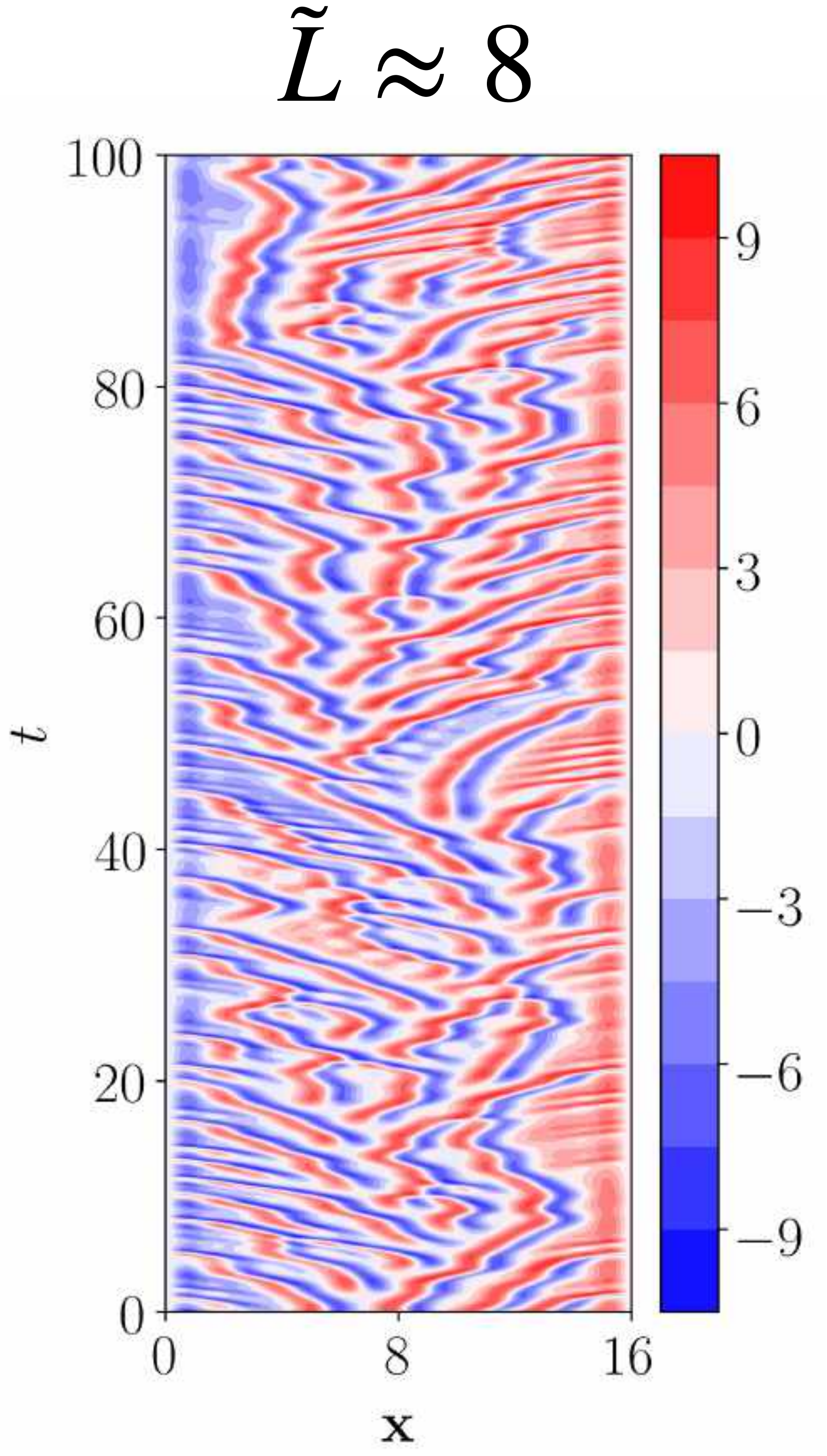
Constructing the observable - training data

High dimensional

High dimensional simulation data

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

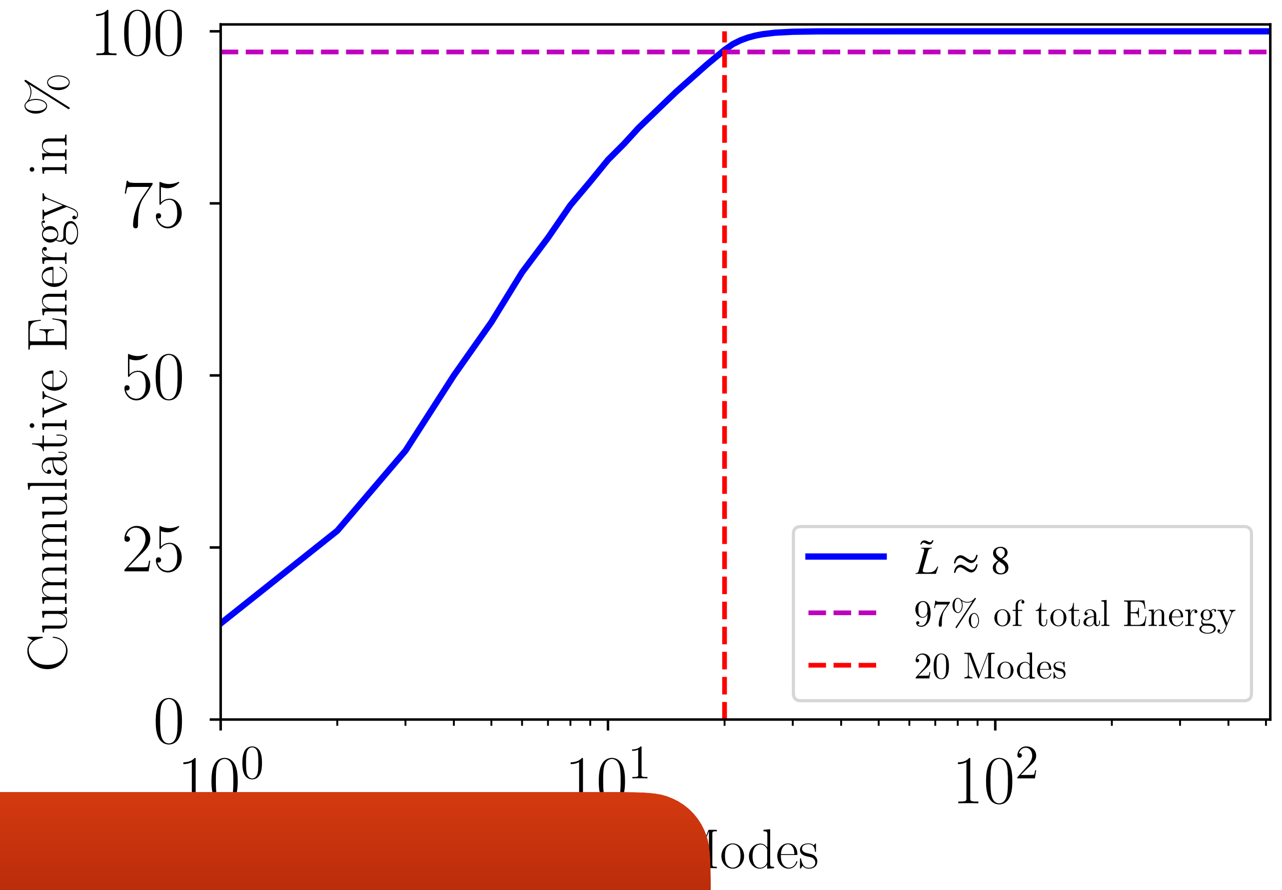


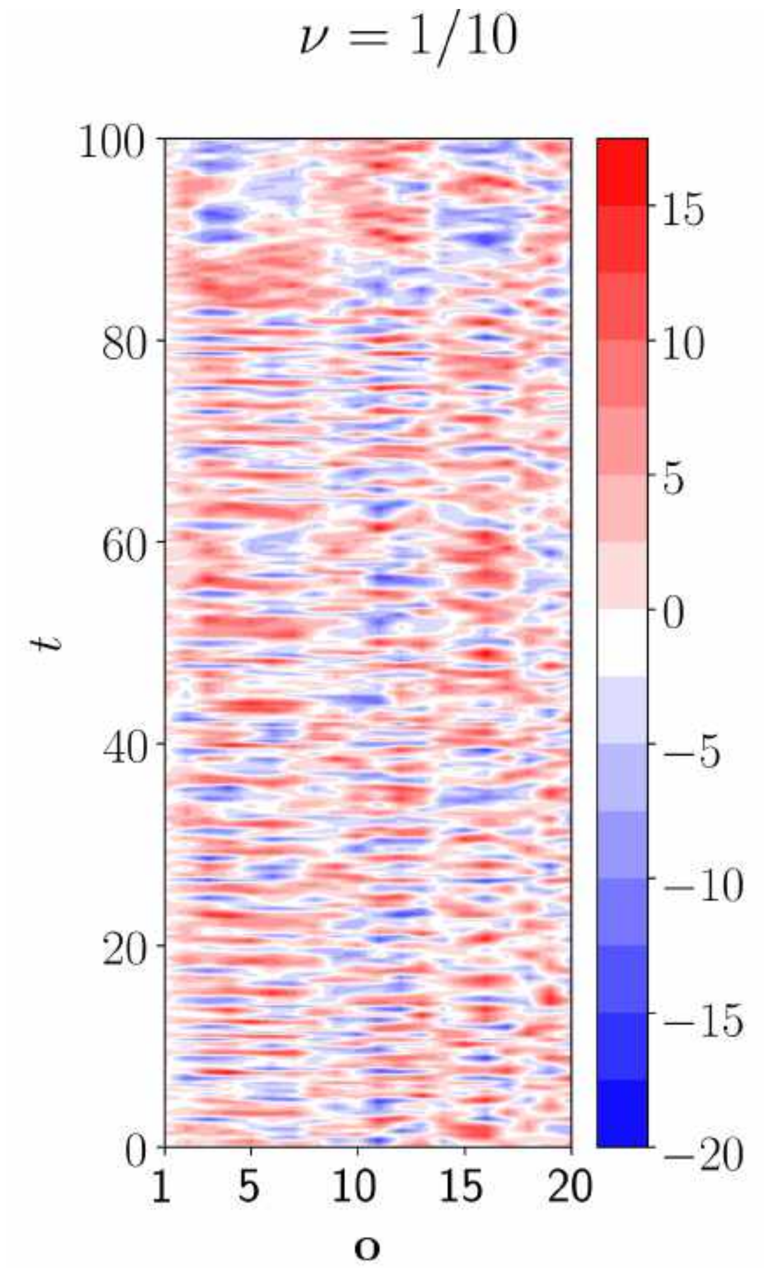


SVD / PCA

Singular Value Decomposition

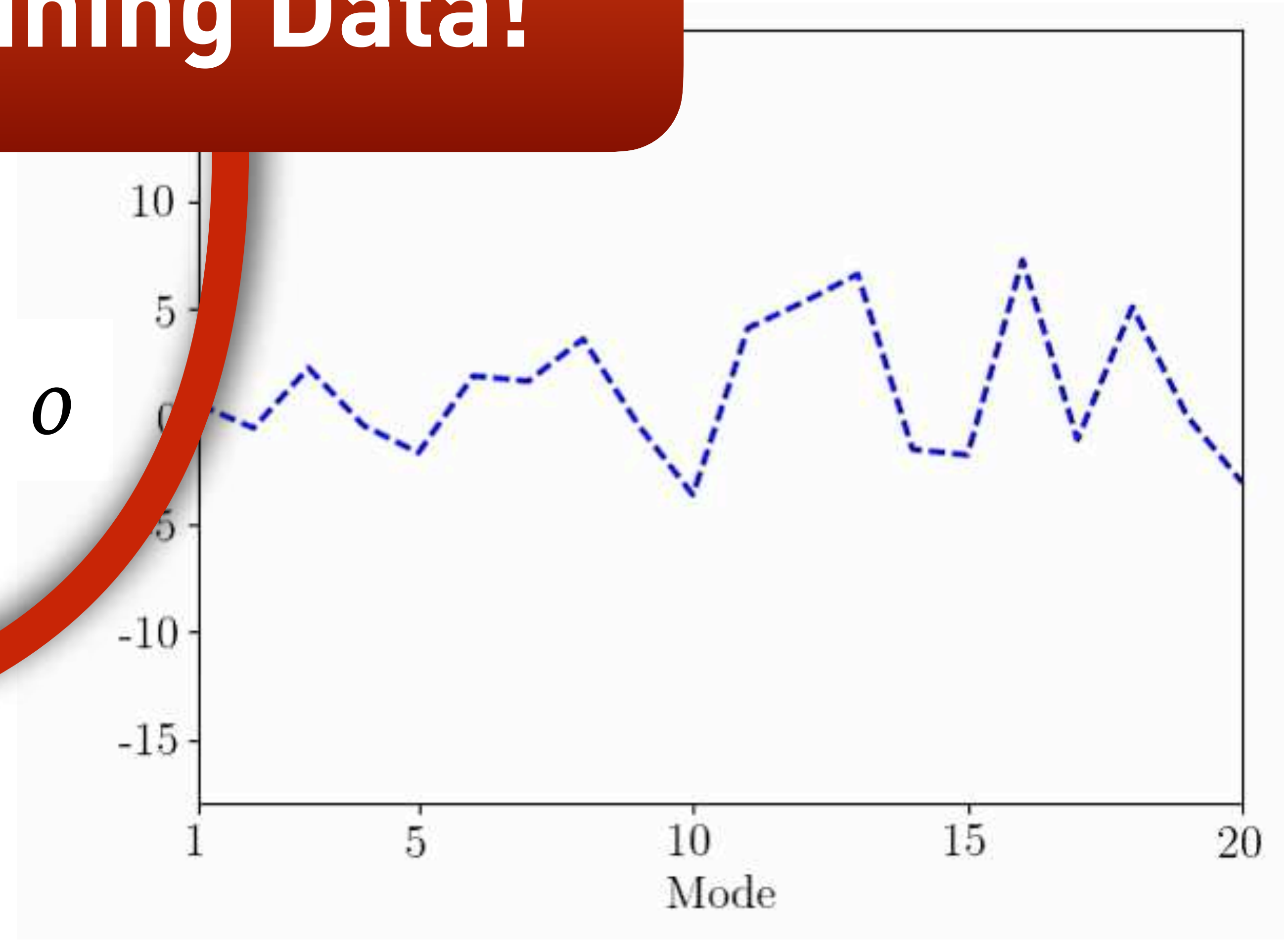
Throw away modes with low energy





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

Training Data!



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

Forecasting on UNSEEN data - Iterative prediction in practice

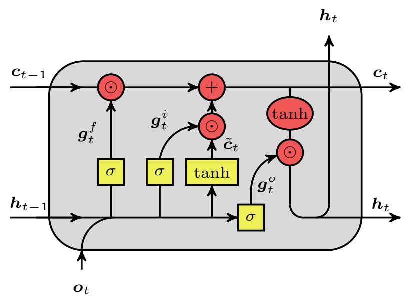
Forecasting on UNSEEN data - Iterative prediction in practice

data

Forecasting on UNSEEN data - Iterative prediction in practice

data

&

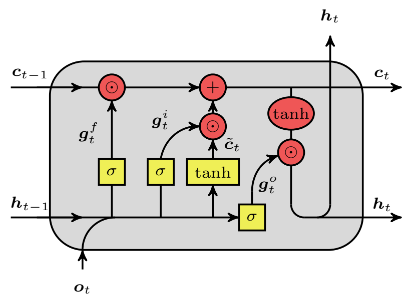


model

Forecasting on UNSEEN data - Iterative prediction in practice

data

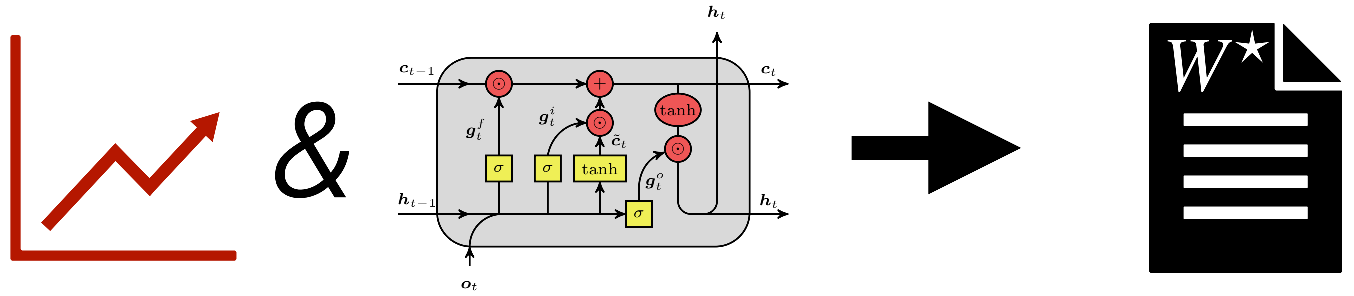
&



model

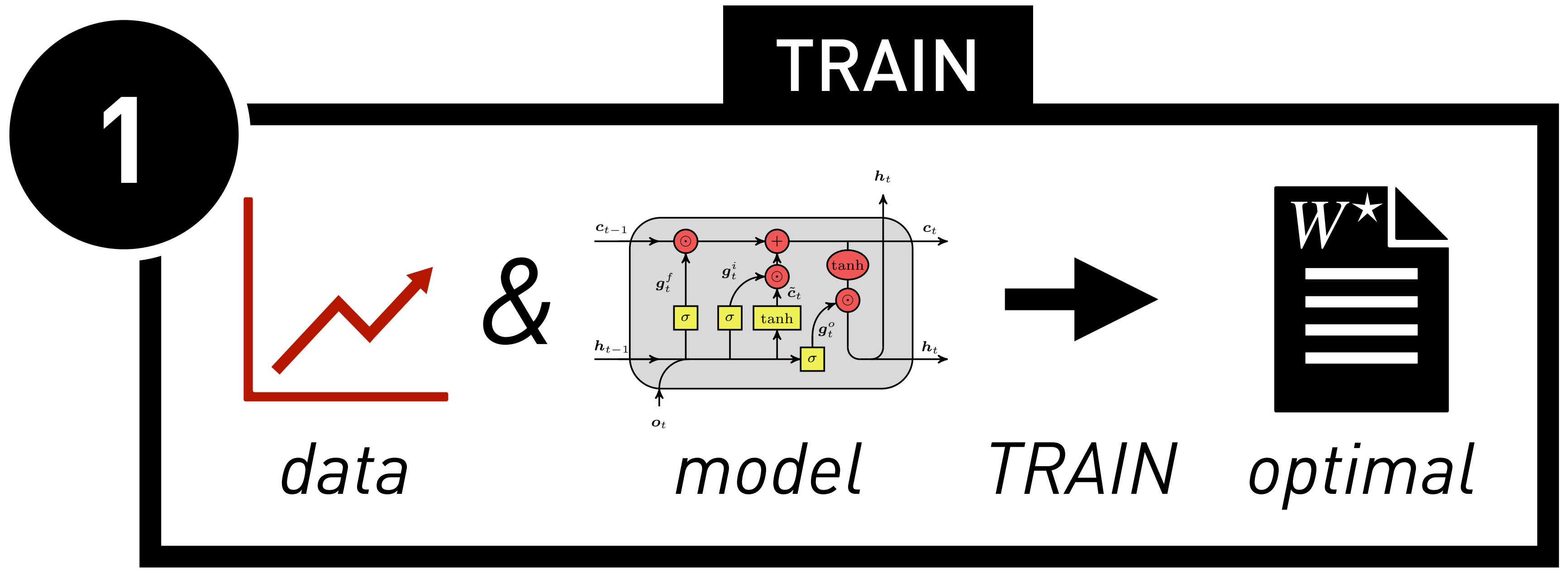
TRAIN

Forecasting on UNSEEN data - Iterative prediction in practice



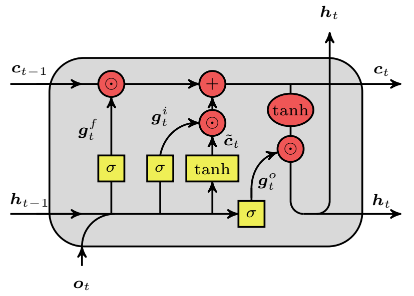
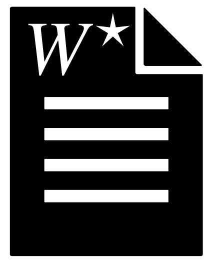
data *model* *TRAIN* *optimal*

Forecasting on UNSEEN data - Iterative prediction in practice



Forecasting on UNSEEN data - Iterative prediction in practice

1 **TRAIN**


&

→


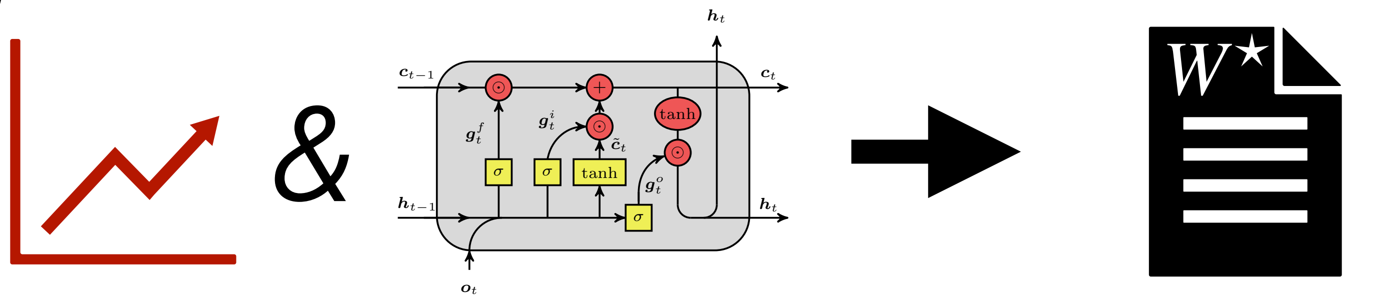
data *model* *TRAIN* *optimal*

2 **TEST**

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

Forecasting on UNSEEN data - Iterative prediction in practice

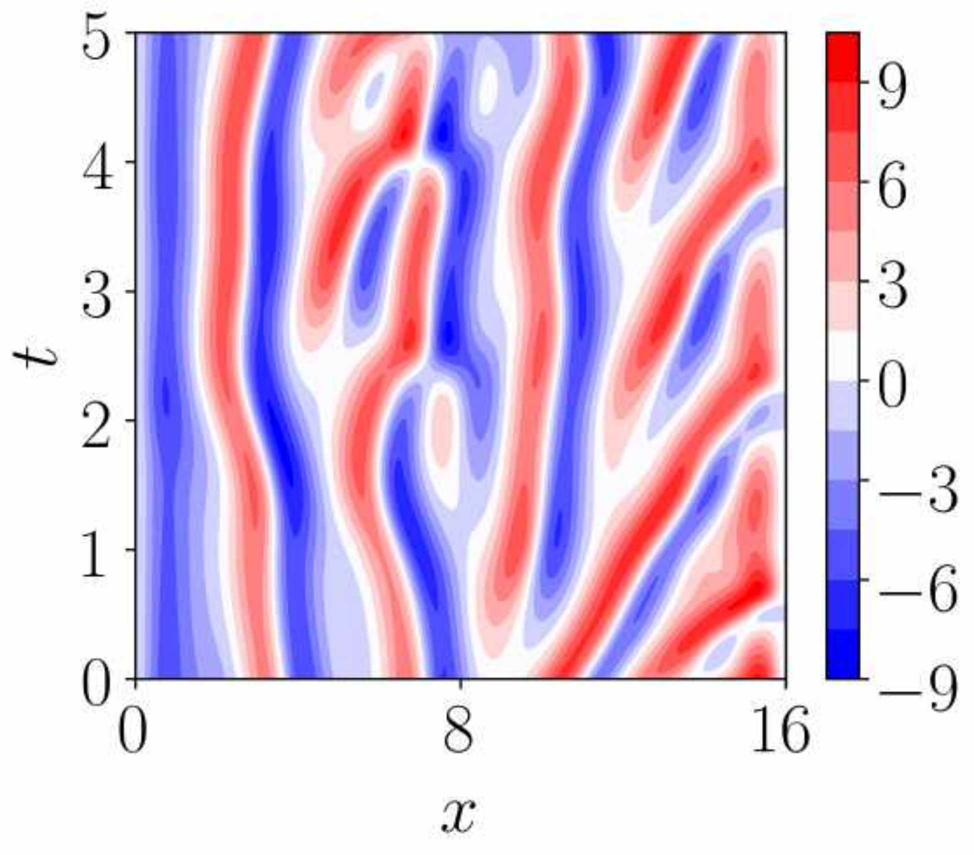
1 TRAIN



2 TEST

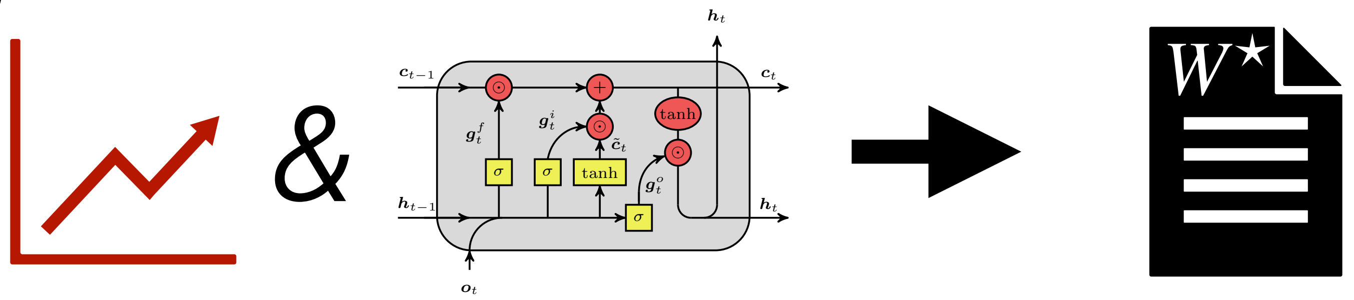
How to predict the dynamics of TEST (unseen) data?

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



Forecasting on UNSEEN data - Iterative prediction in practice

1 **TRAIN**

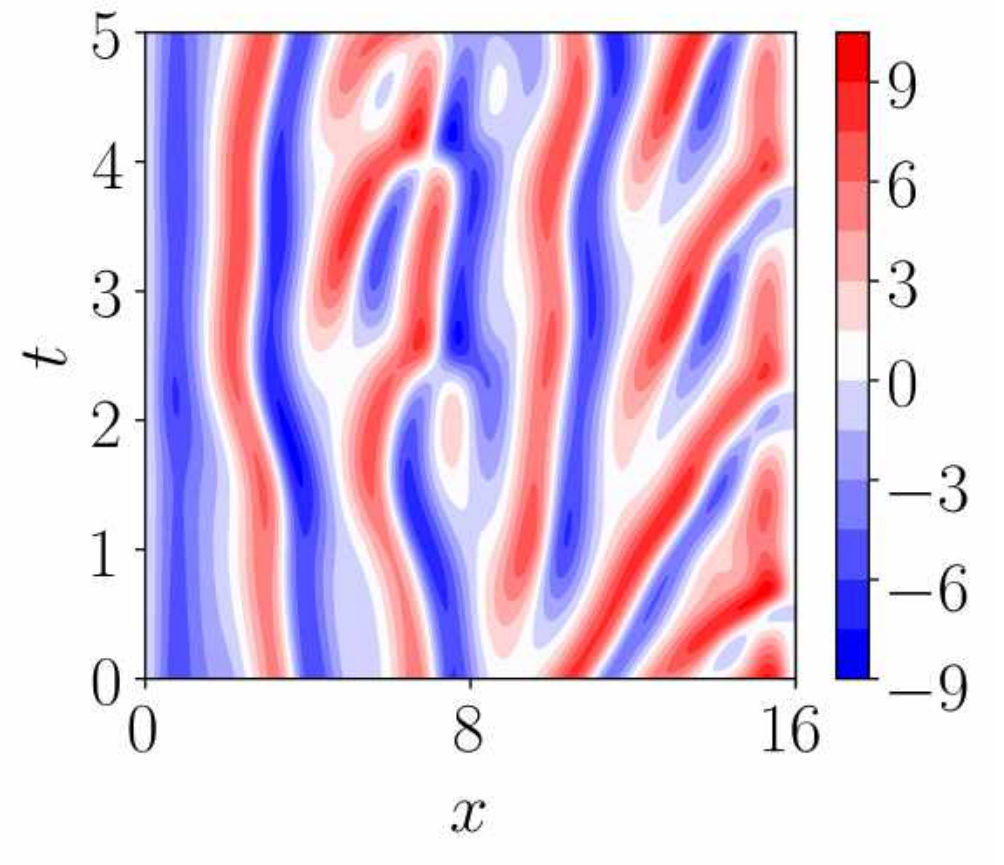


data *model* *TRAIN* *optimal*

2 **TEST**

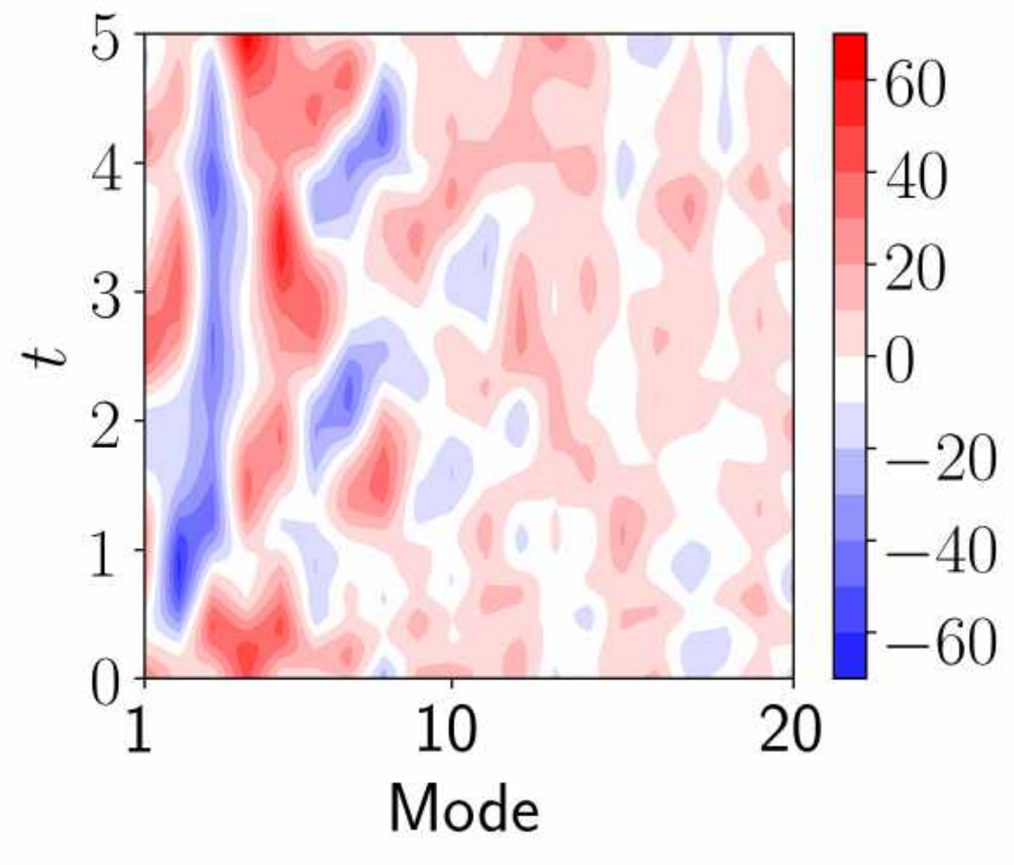
How to predict the dynamics of TEST (unseen) data?

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



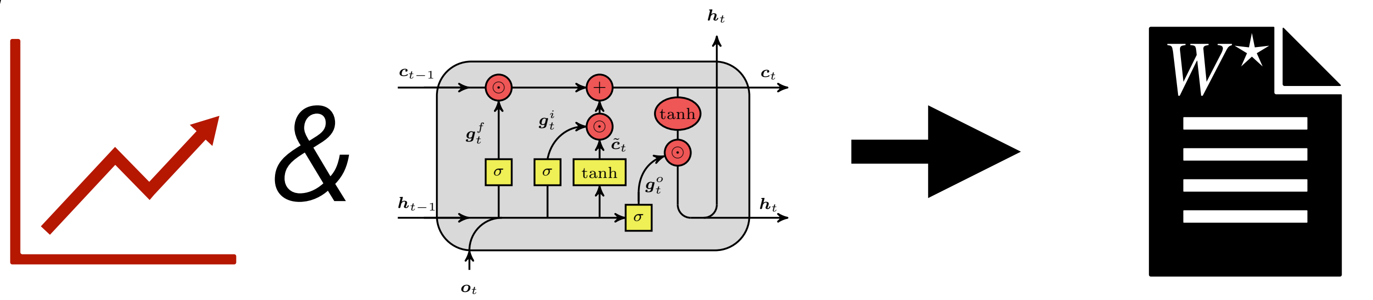
SVD

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



Forecasting on UNSEEN data - Iterative prediction in practice

1 TRAIN



data *model* *TRAIN* *optimal*

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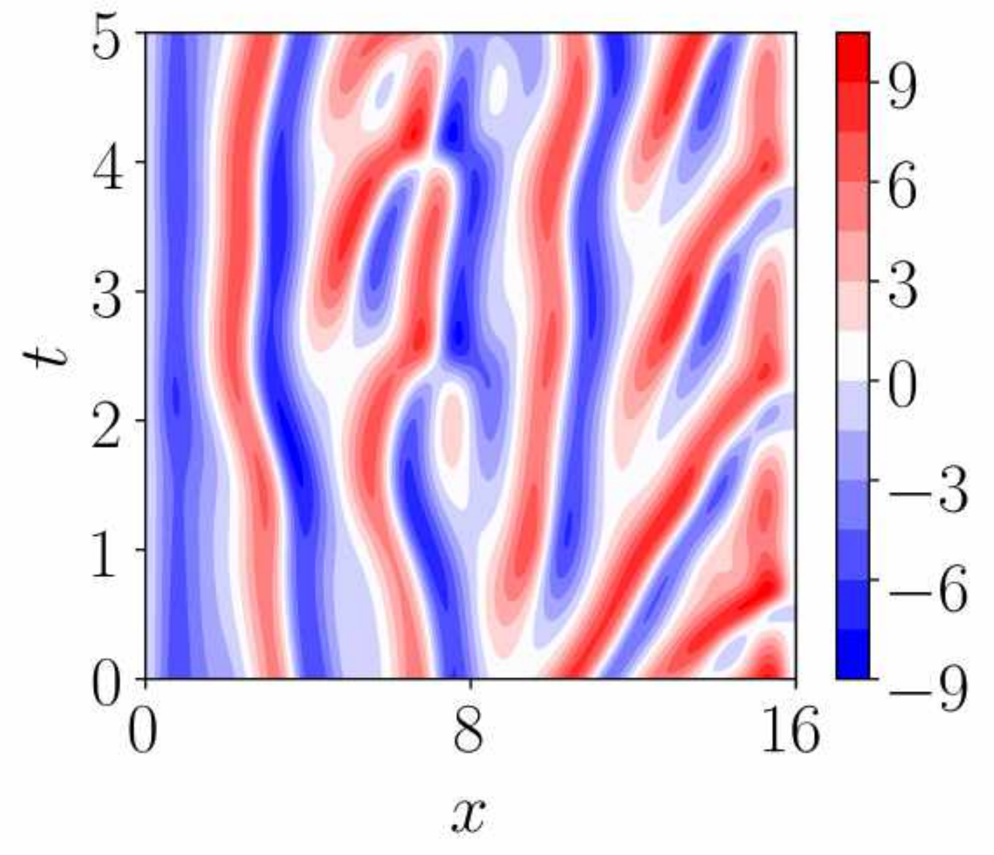
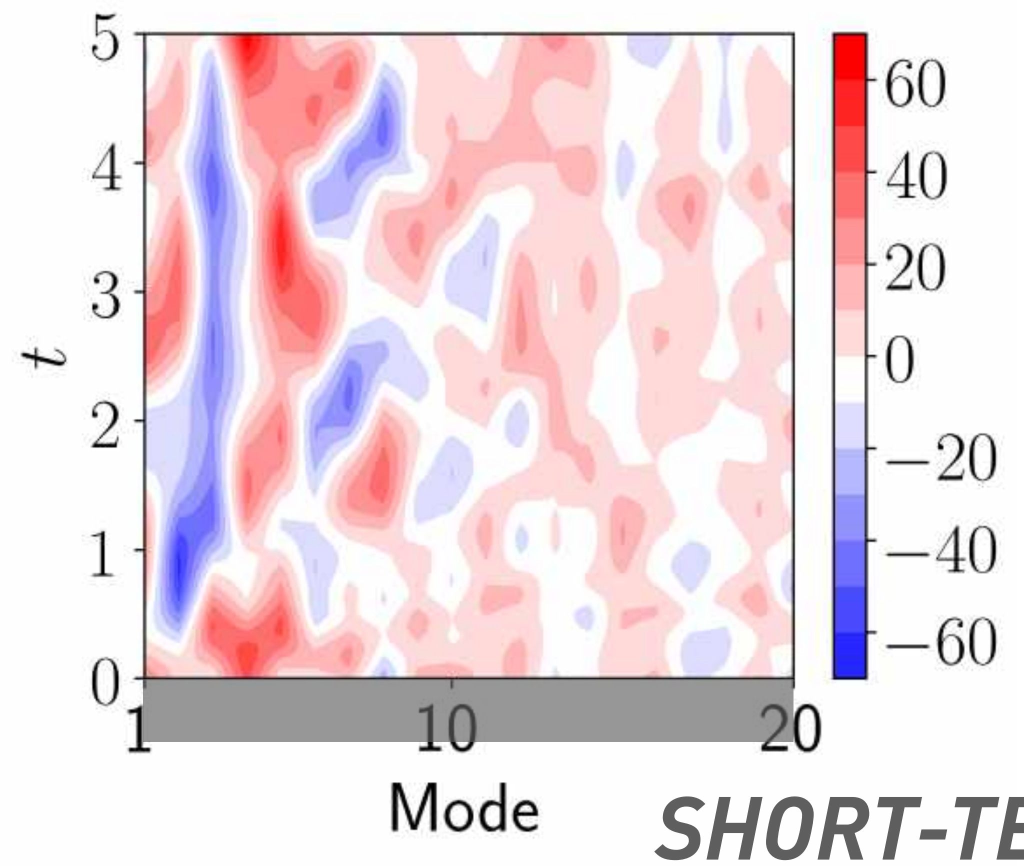
How to predict the dynamics of TEST (unseen) data?

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



SVD

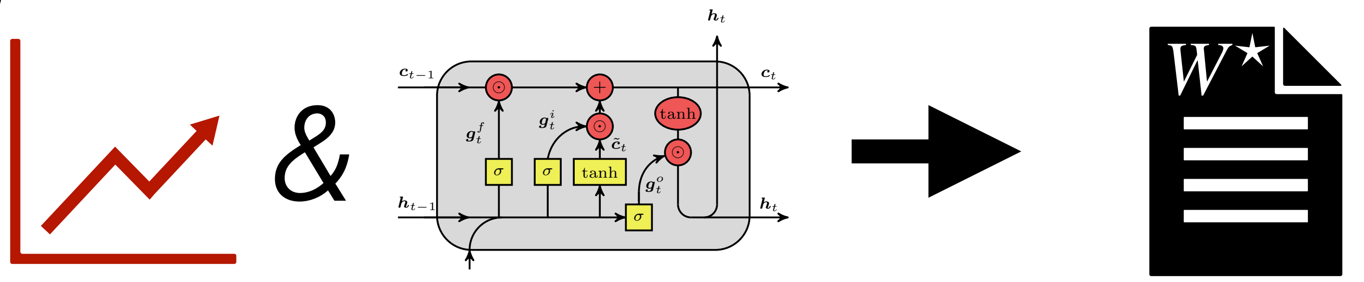
SVD Mode dynamics (reference)



SHORT-TERM HISTORY (known)

Forecasting on UNSEEN data - Iterative prediction in practice

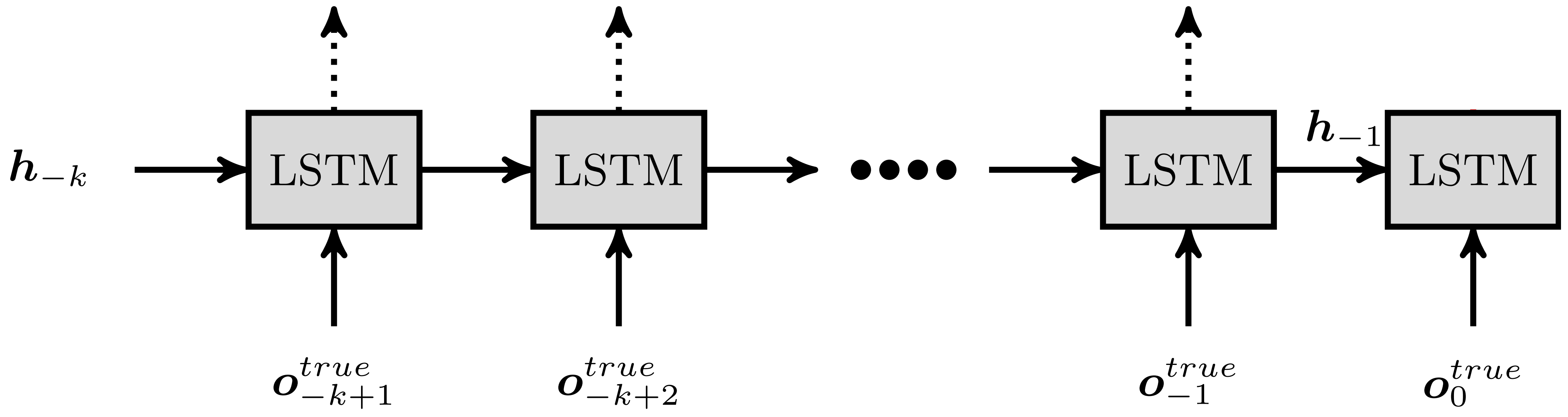
1 TRAIN



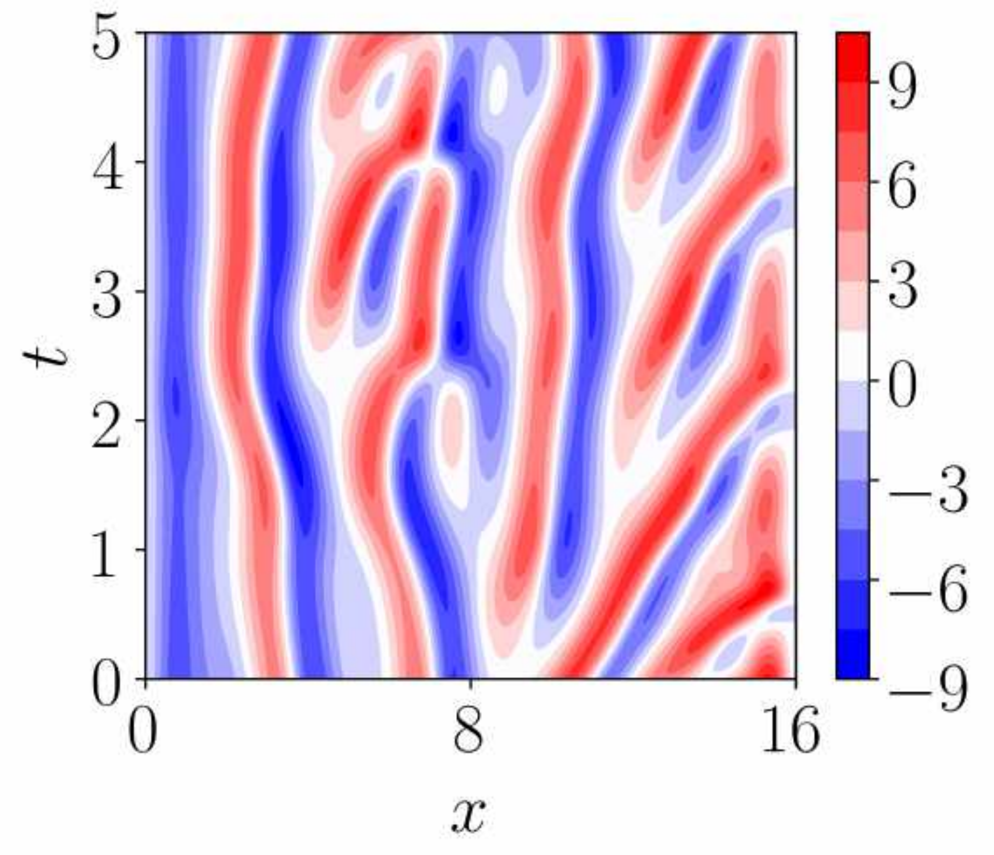
data & *model* *TRAIN* *optimal*

2 TEST

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

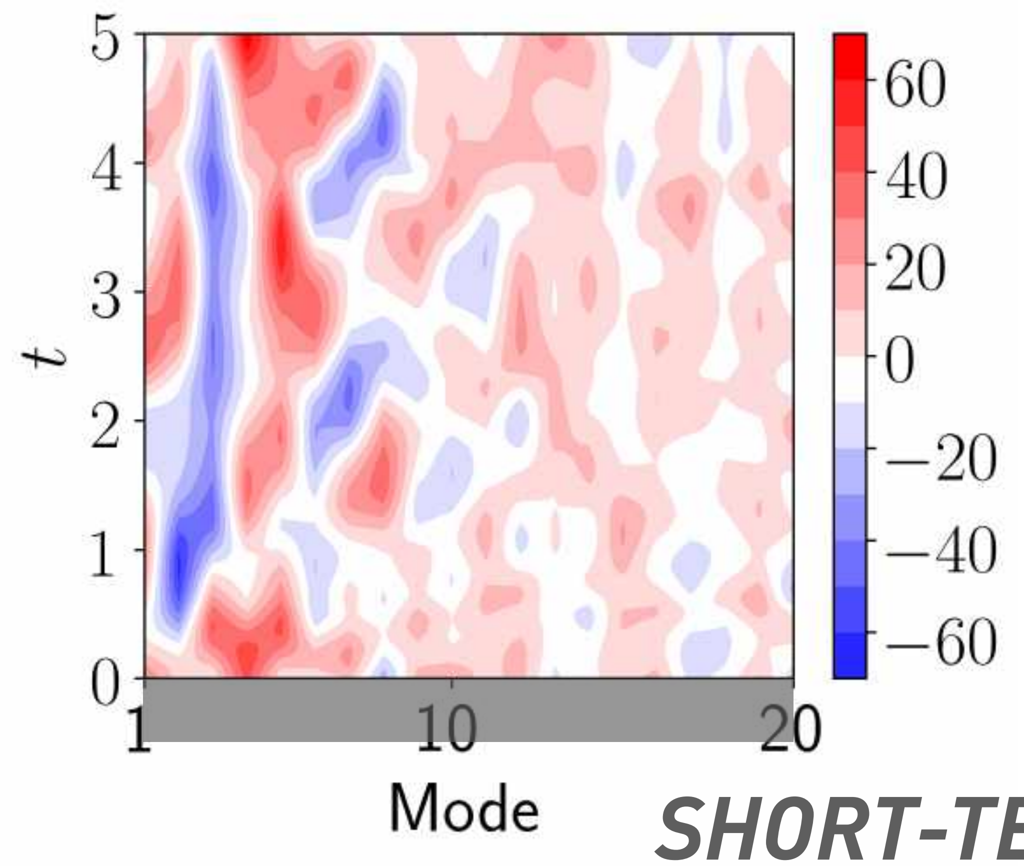


TEST: *UNKNOWN* *state dynamics (reference)*



SVD

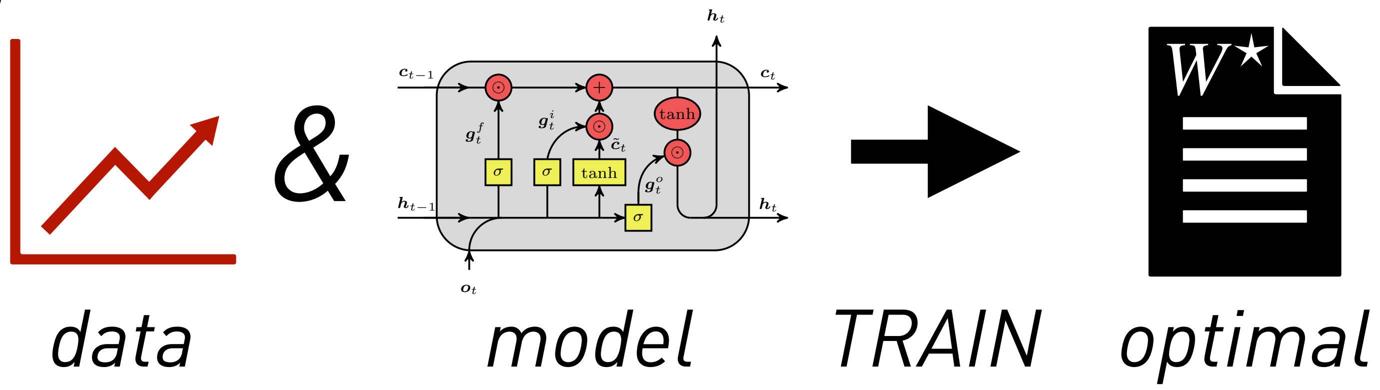
SVD Mode dynamics (reference)



SHORT-TERM HISTORY (known)

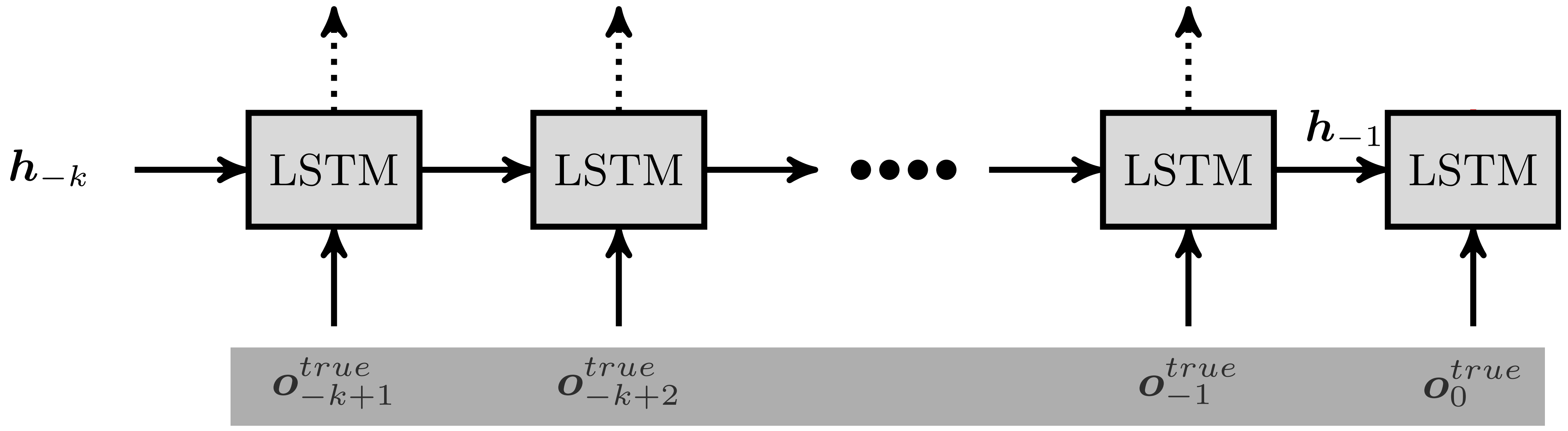
Forecasting on UNSEEN data - Iterative prediction in practice

1 TRAIN



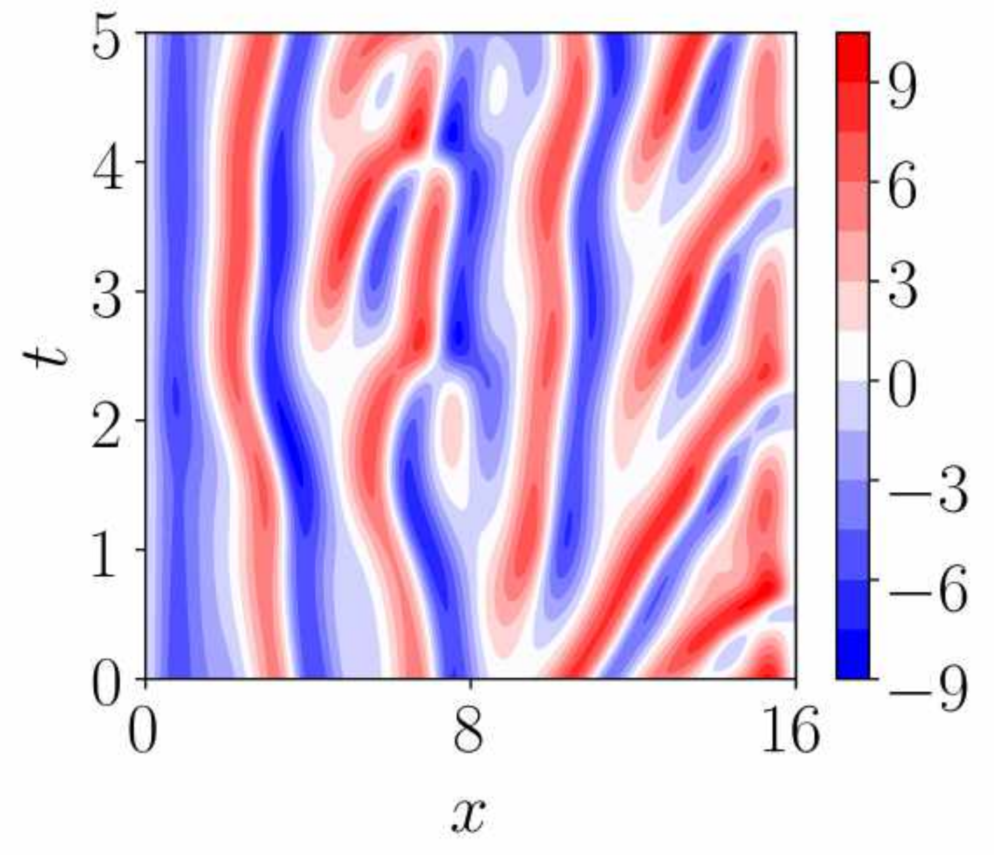
2 TEST

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



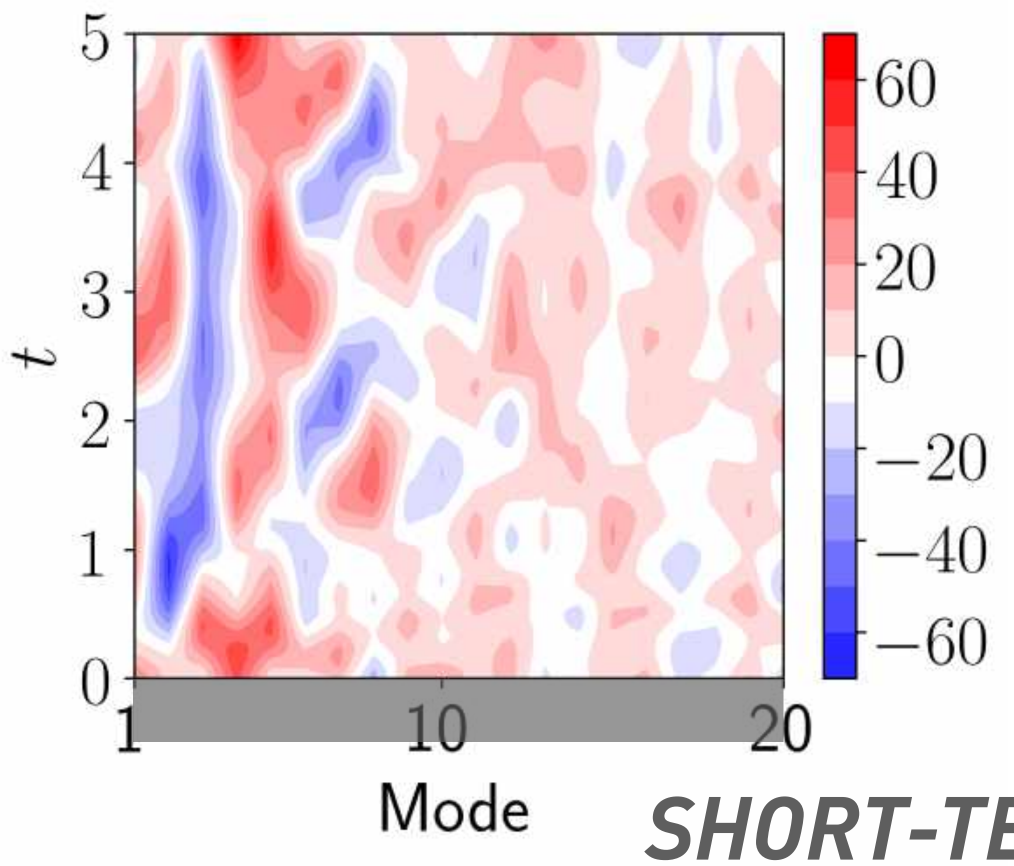
SHORT-TERM HISTORY (known)

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



SVD

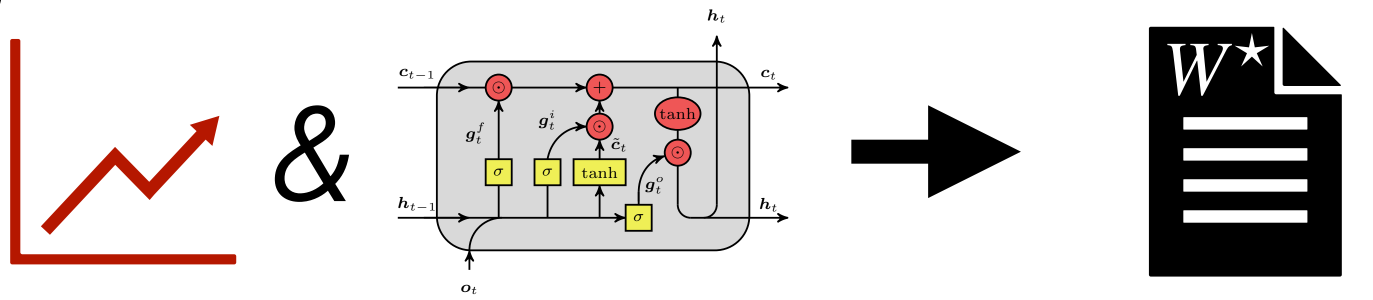
SVD Mode dynamics (reference)



SHORT-TERM HISTORY (known)

Forecasting on UNSEEN data - Iterative prediction in practice

1 **TRAIN**



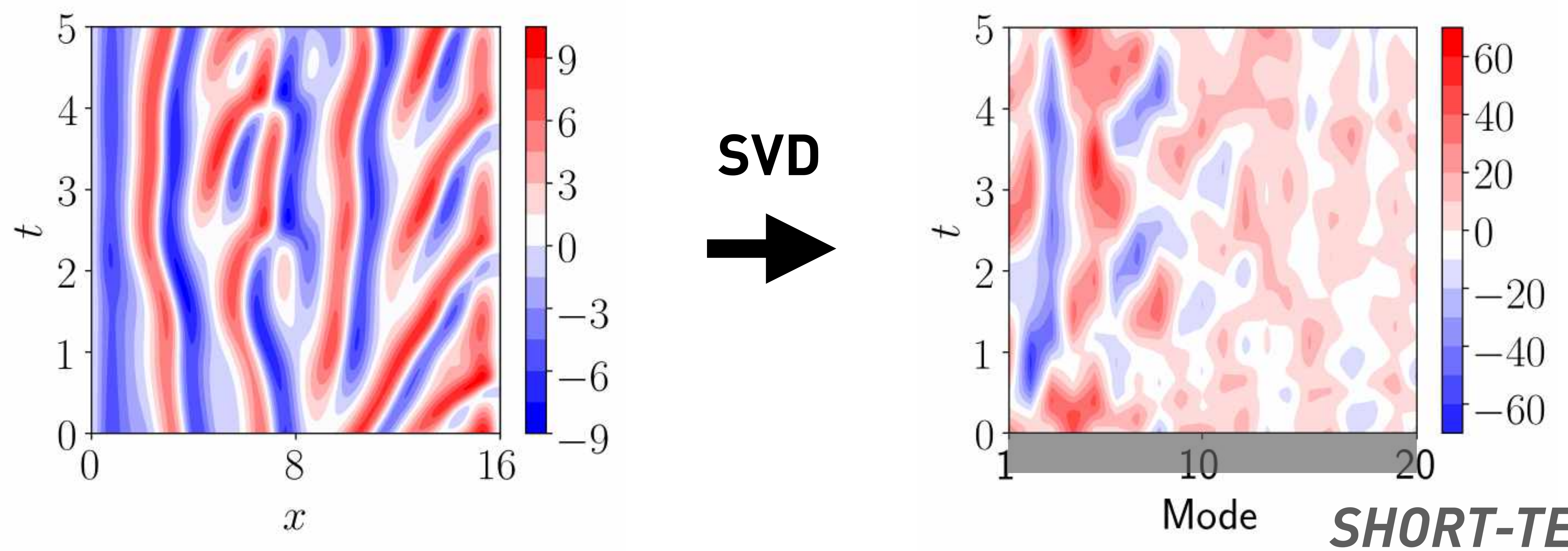
data & *model* → *TRAIN* *optimal*

2 **TEST**

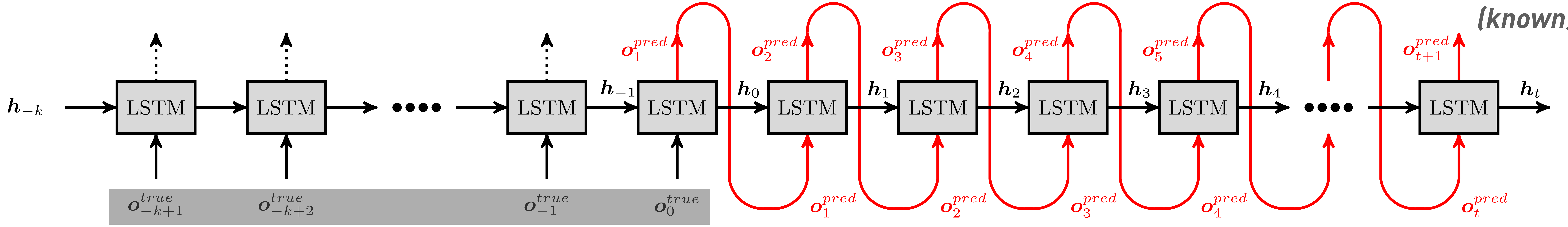
How to predict the dynamics of TEST (unseen) data?

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

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



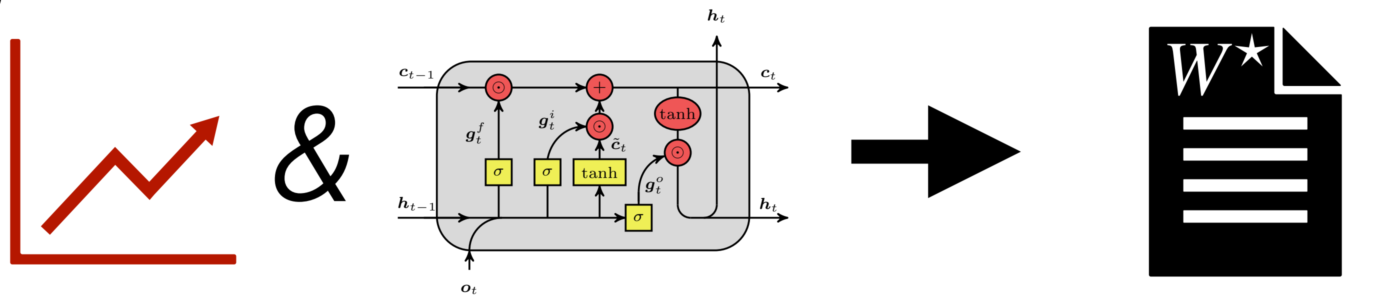
SHORT-TERM HISTORY (known)



SHORT-TERM HISTORY (known)

Forecasting on UNSEEN data - Iterative prediction in practice

1 TRAIN



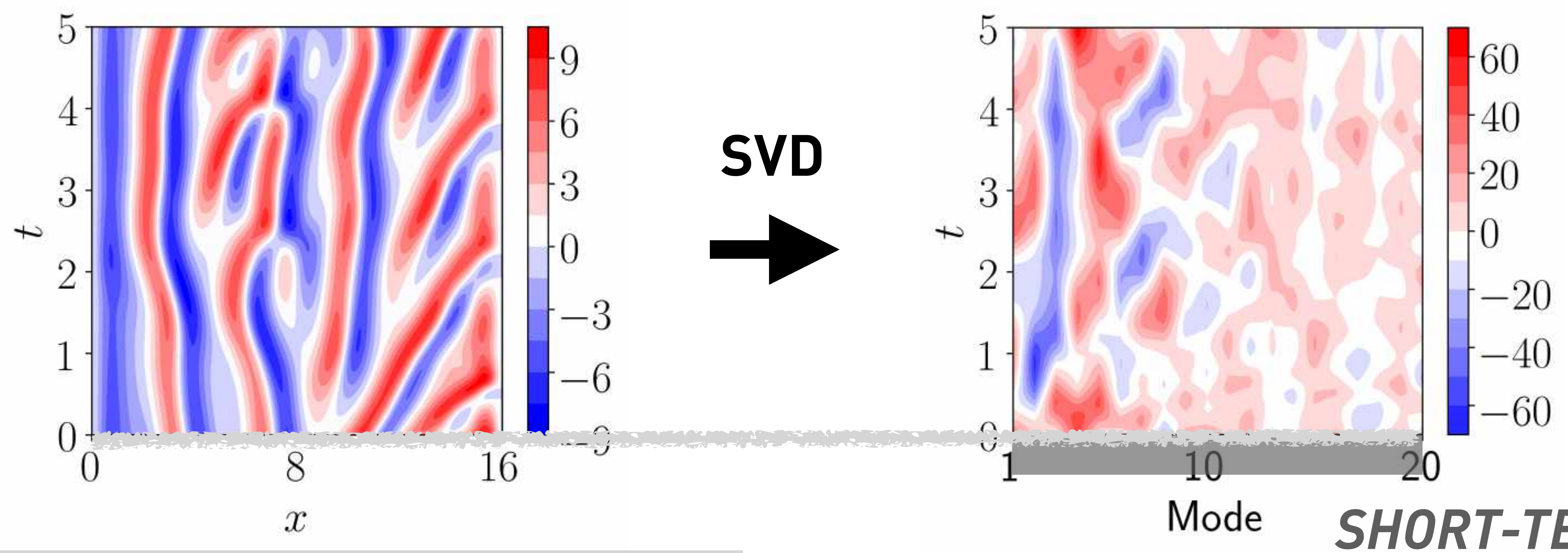
2 TEST

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

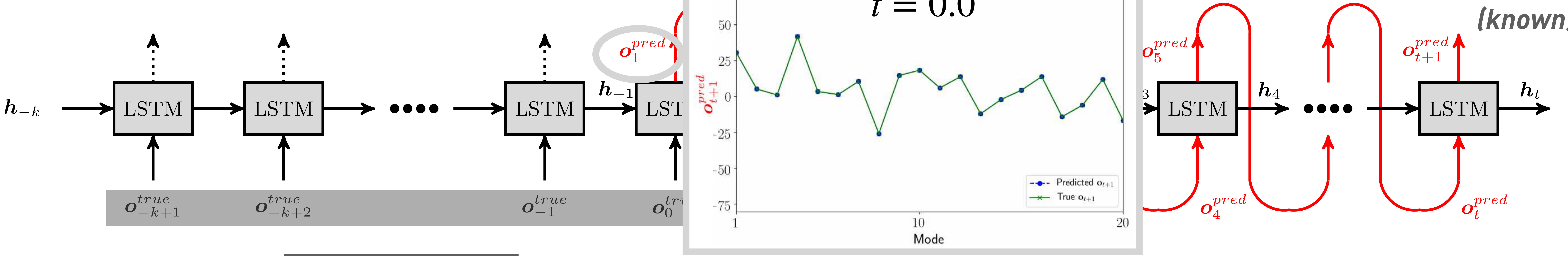
TEST: *UNKNOWN* state dynamics (reference)

SVD

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



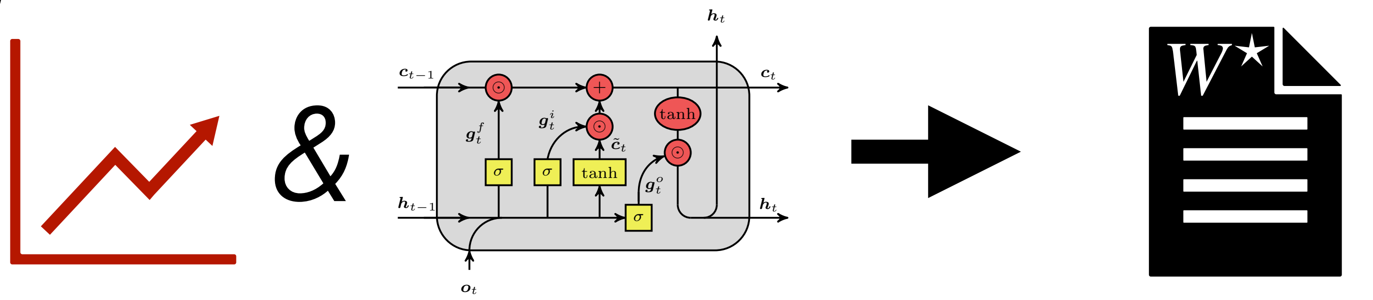
SHORT-TERM HISTORY (known)



SHORT-TERM HISTORY (known)

Forecasting on UNSEEN data - Iterative prediction in practice

1 **TRAIN**



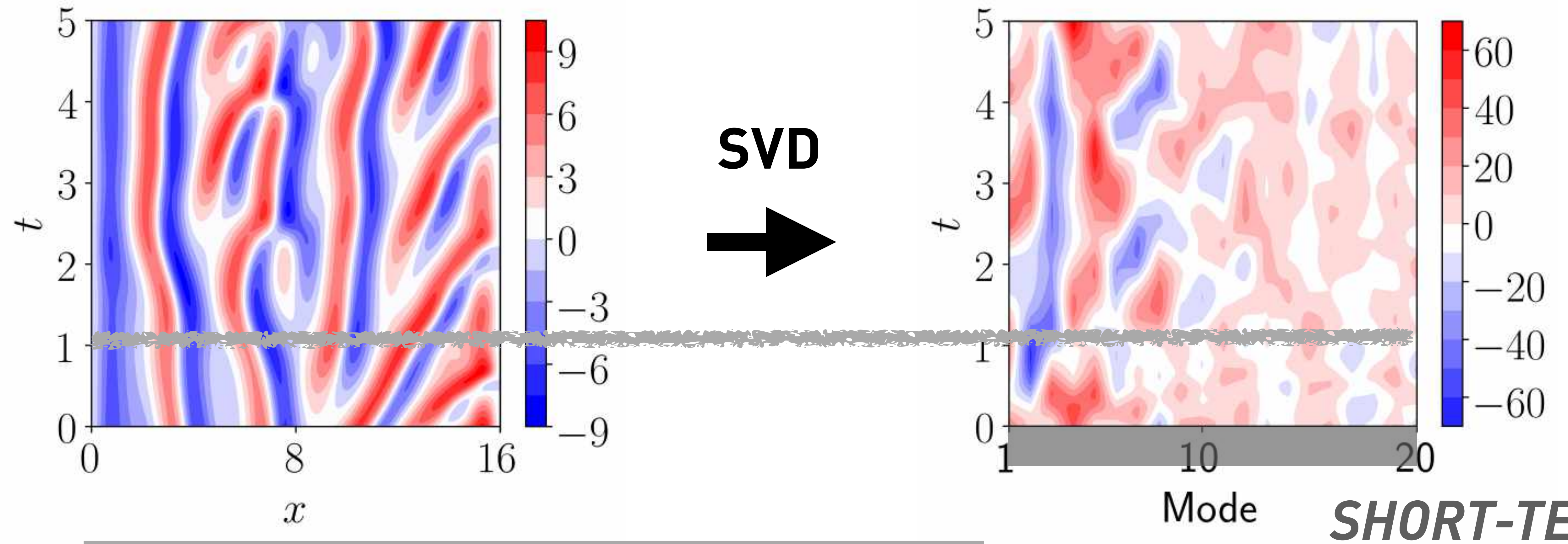
data *model* *TRAIN* *optimal*

2 **TEST**

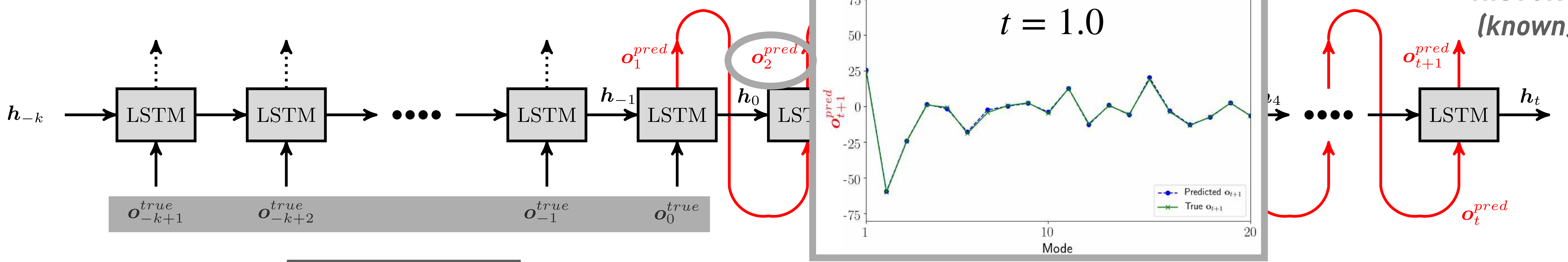
How to predict the dynamics of TEST (unseen) data?

TEST: *UNKNOWN* state dynamics (reference)

SVD Mode dynamics (reference)



SHORT-TERM HISTORY (known)

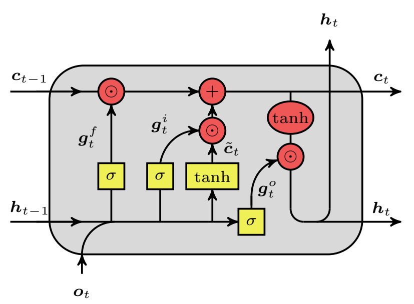


SHORT-TERM HISTORY (known)

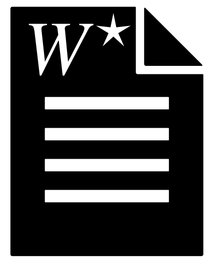
Forecasting on UNSEEN data - Iterative prediction in practice

1 **TRAIN**

&



→ *TRAIN*

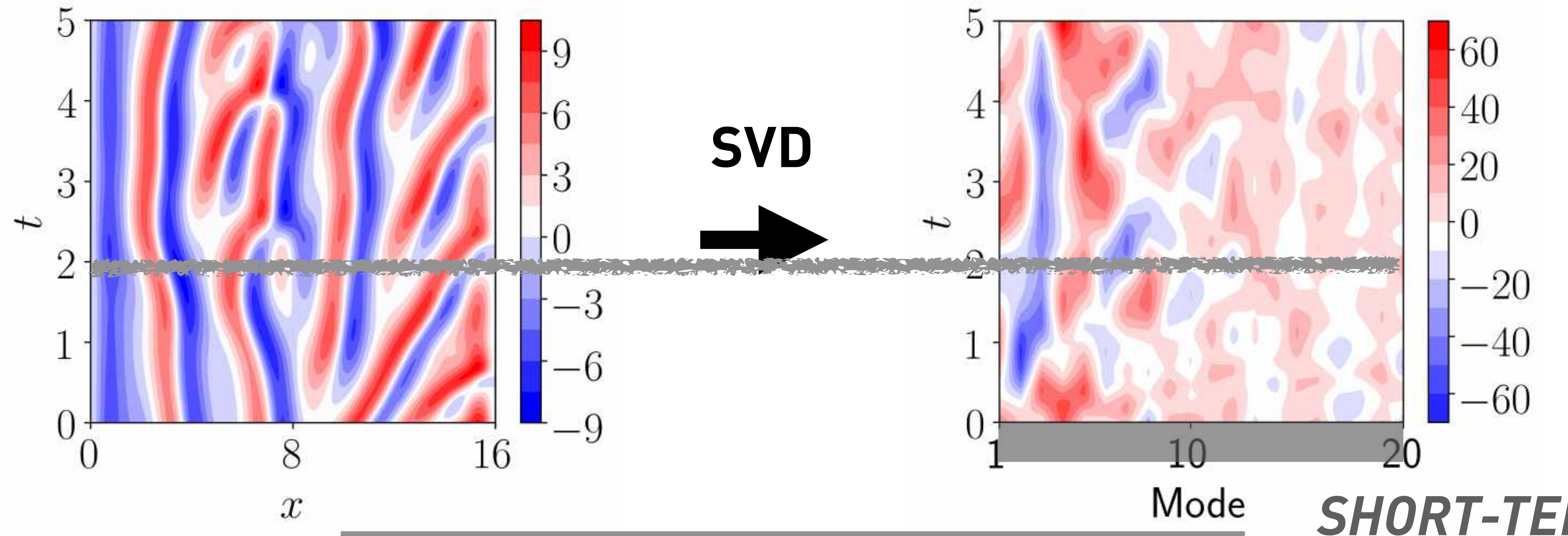


2 **TEST**

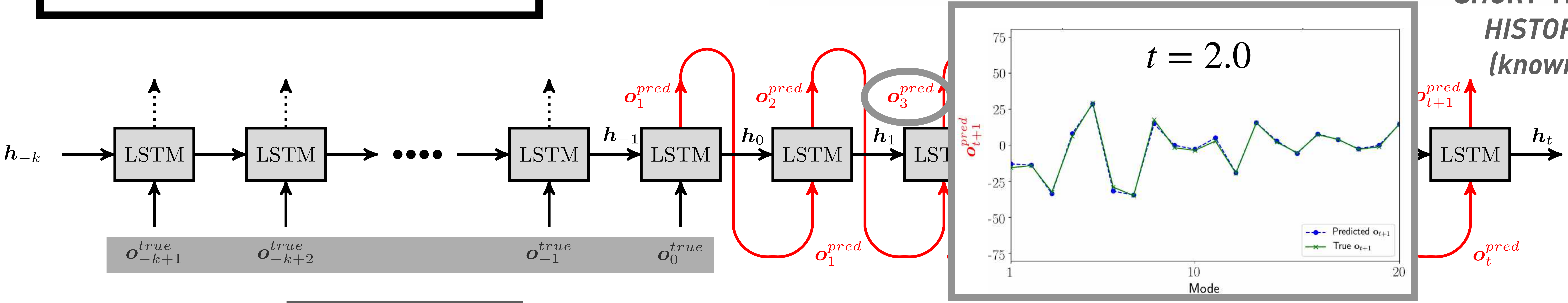
How to predict the dynamics of TEST (unseen) data?

TEST: *UNKNOWN* state dynamics (reference)

SVD Mode dynamics (reference)



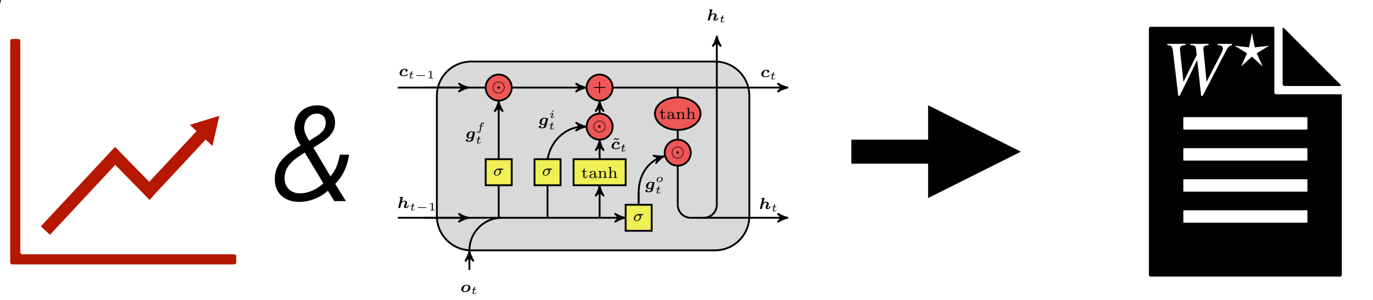
SHORT-TERM HISTORY (known)



SHORT-TERM HISTORY (known)

Forecasting on UNSEEN data - Iterative prediction in practice

1 **TRAIN**



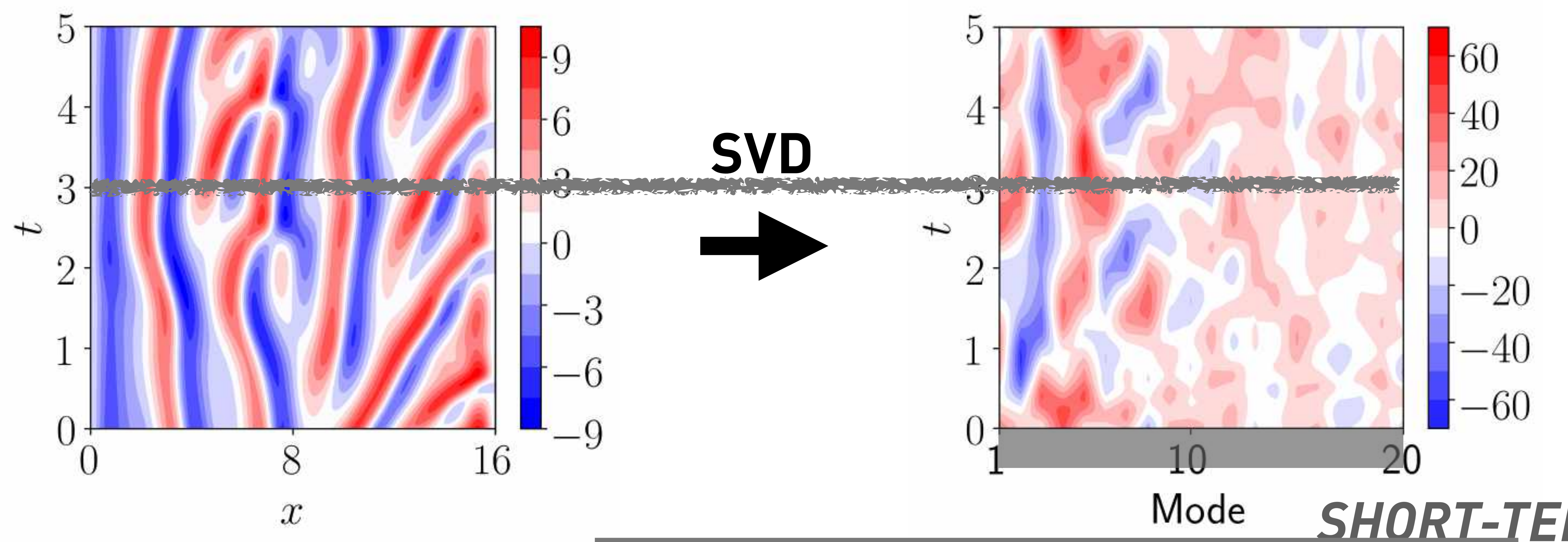
data *model* *TRAIN* *optimal*

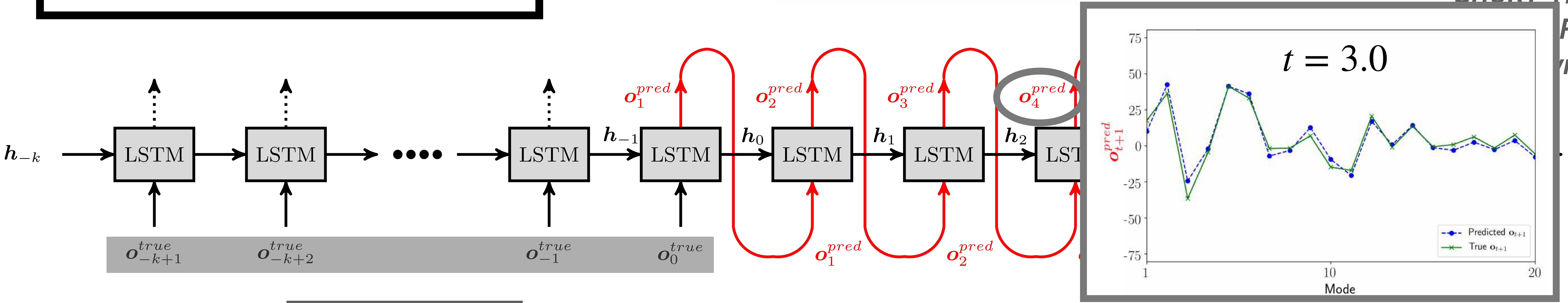
2 **TEST**

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

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

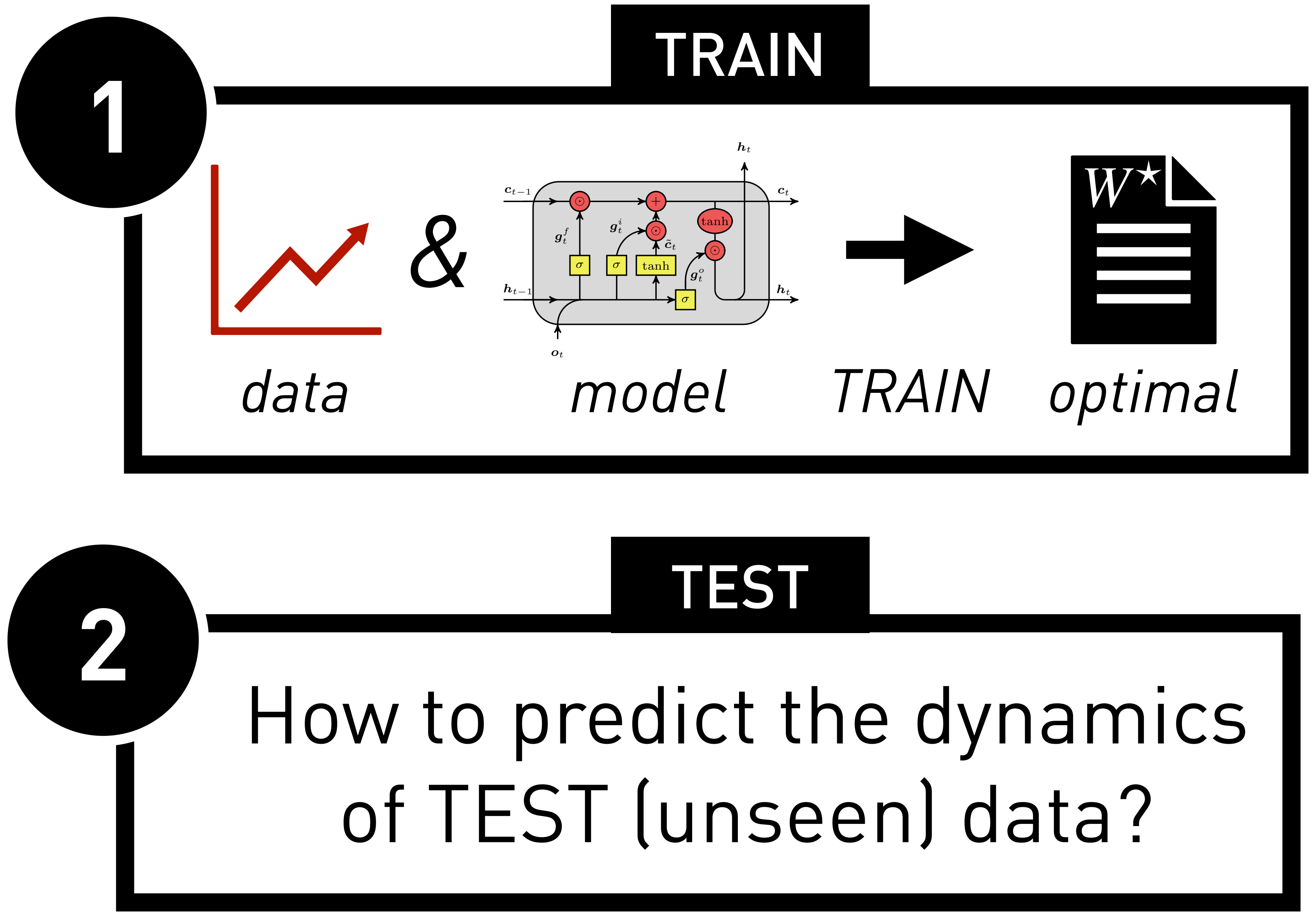
***SVD Mode* dynamics (reference)**

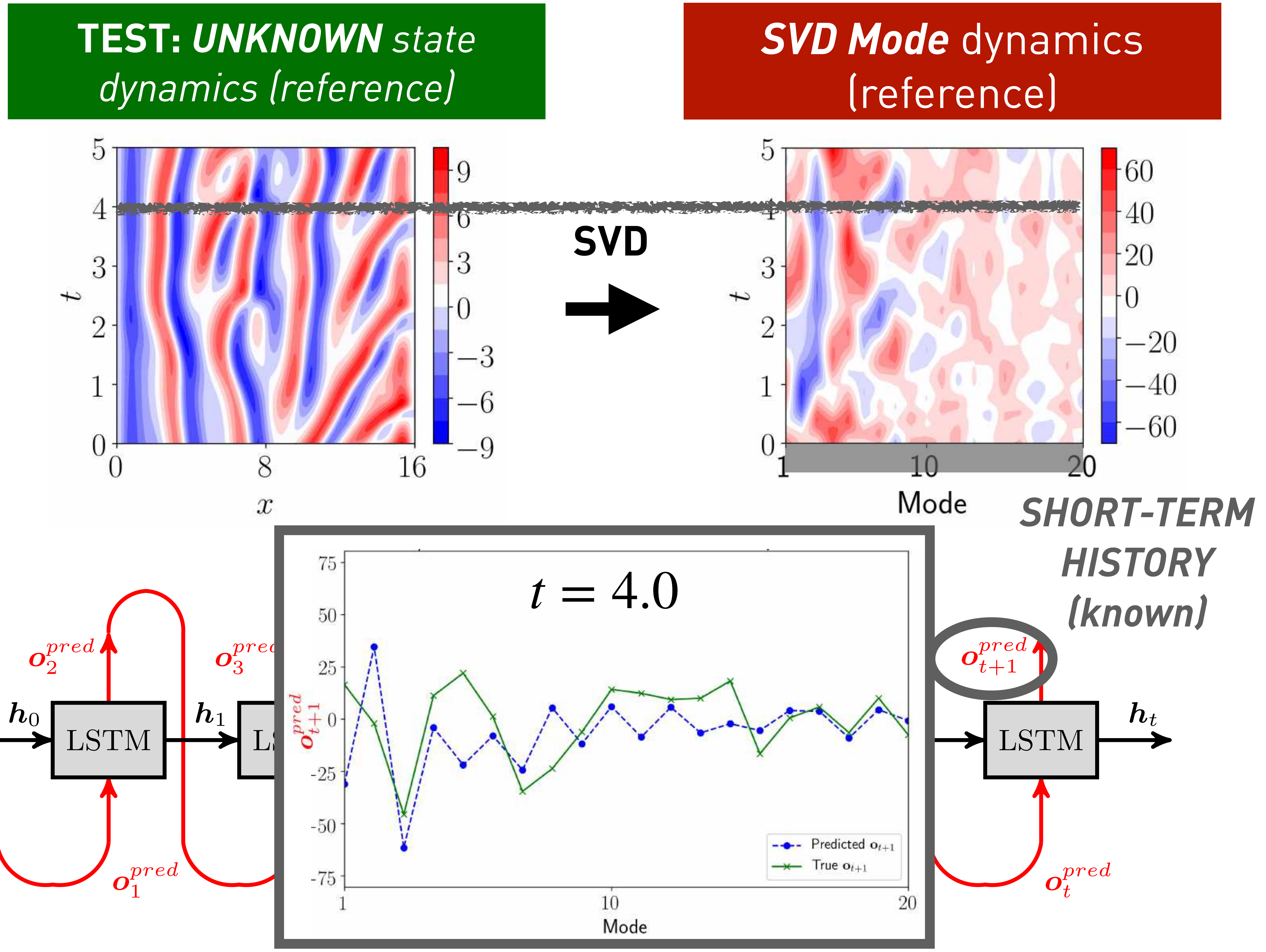


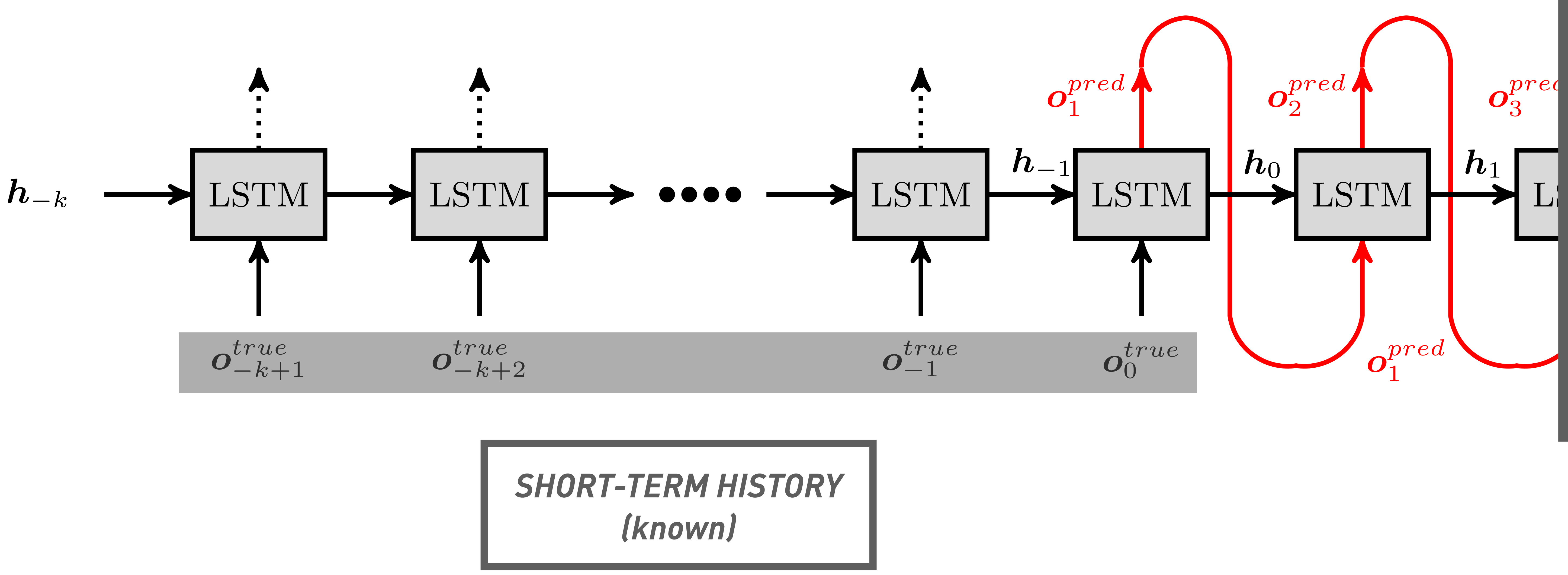


SHORT-TERM HISTORY (known)

Forecasting on UNSEEN data - Iterative prediction in practice

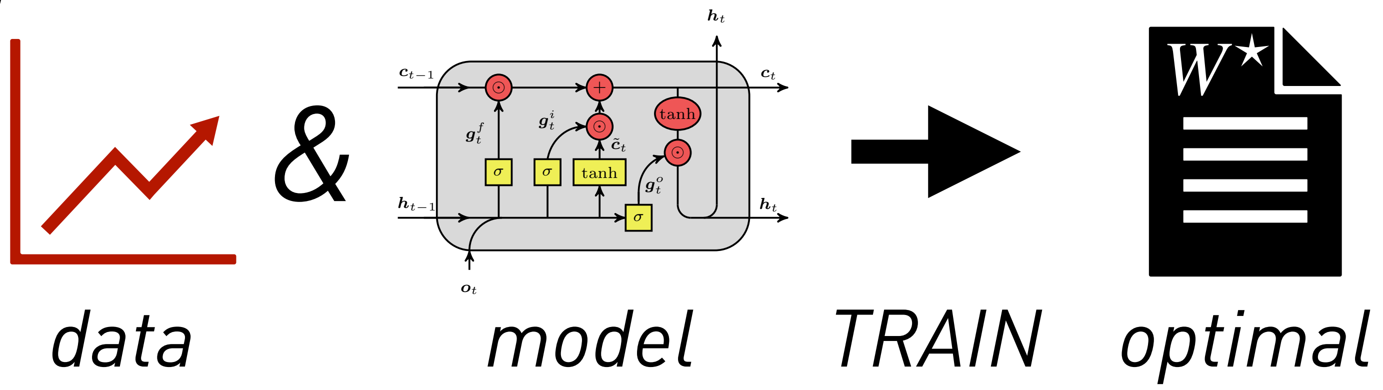






Forecasting on UNSEEN data - Iterative prediction in practice

1 TRAIN

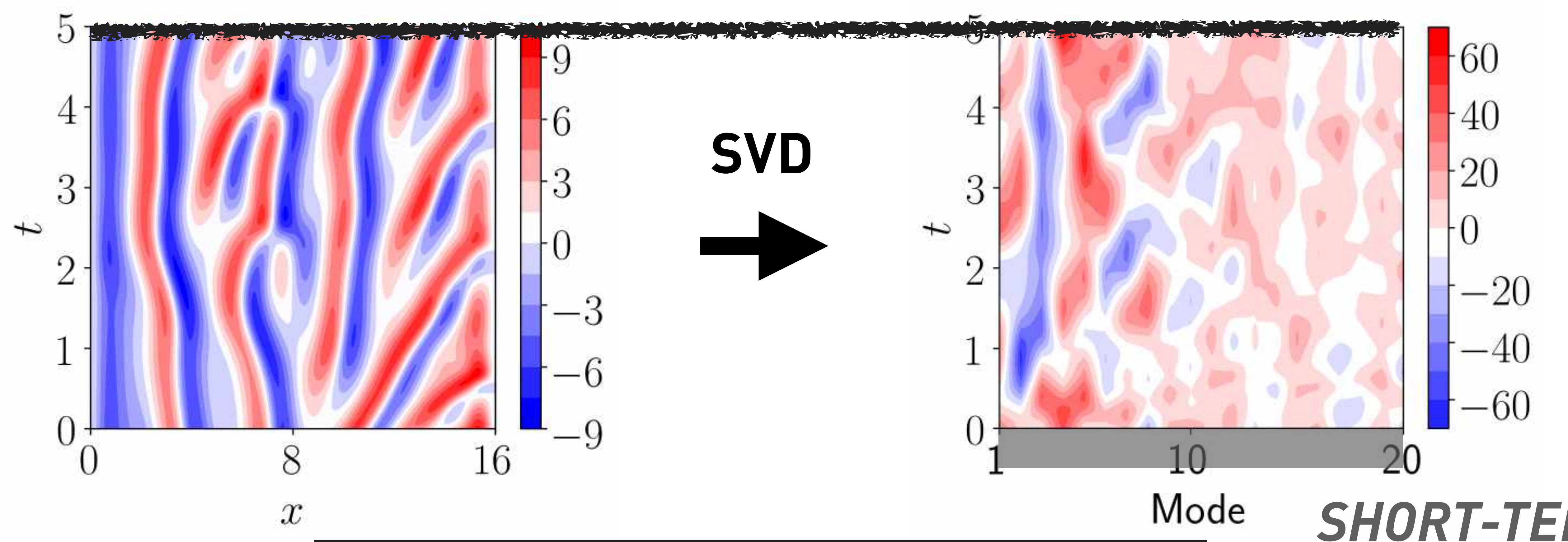


2 TEST

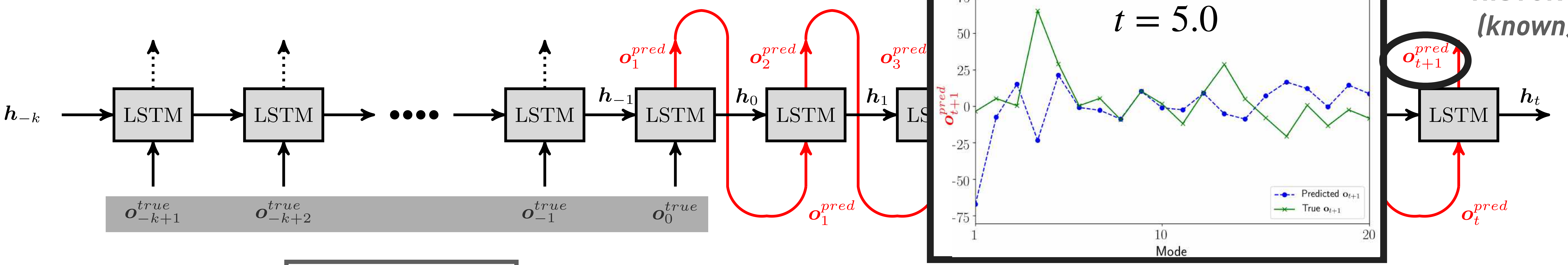
How to predict the dynamics of TEST (unseen) data?

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

SVD Mode dynamics (reference)



SHORT-TERM HISTORY (known)



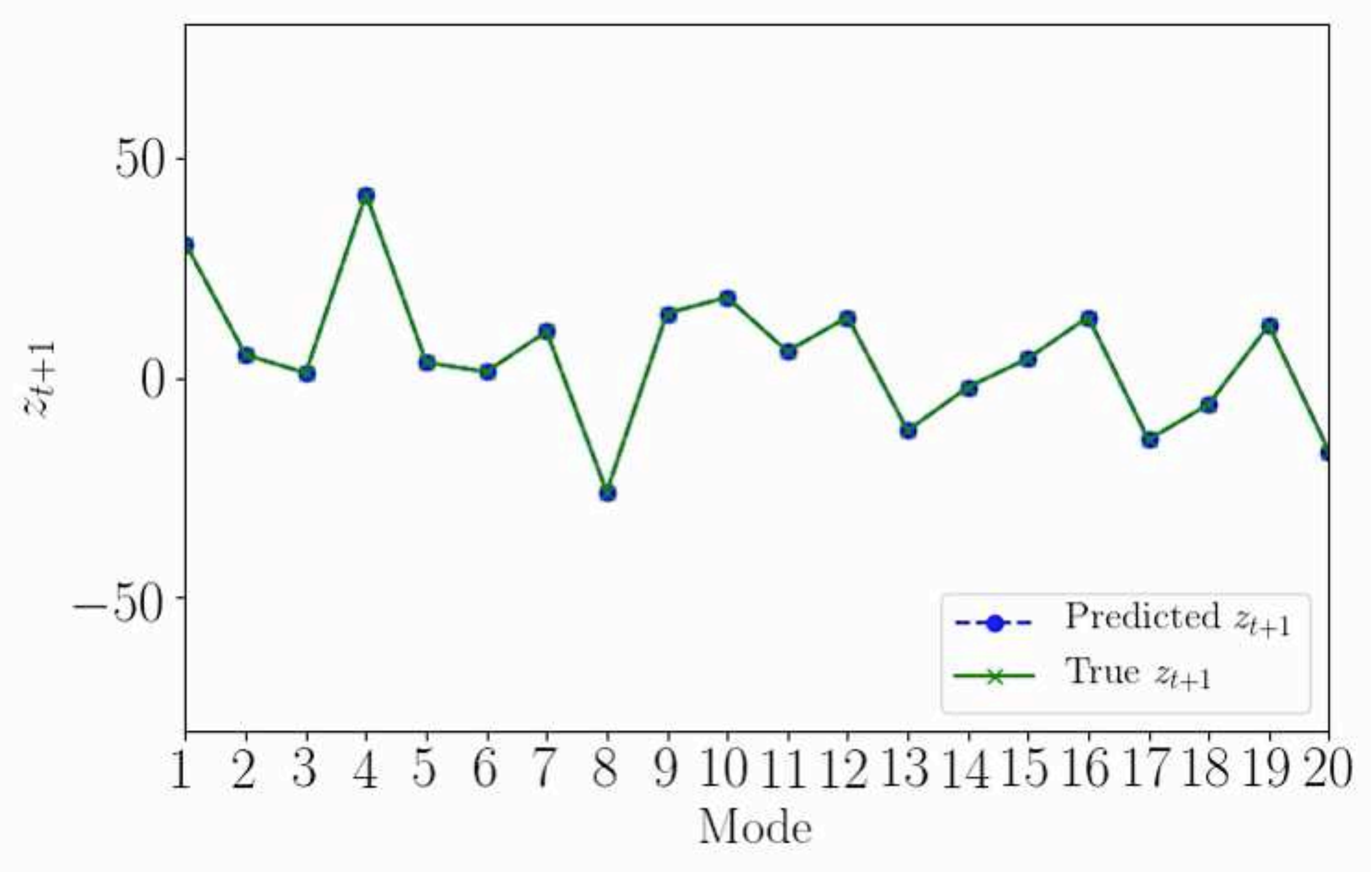
SHORT-TERM HISTORY (known)

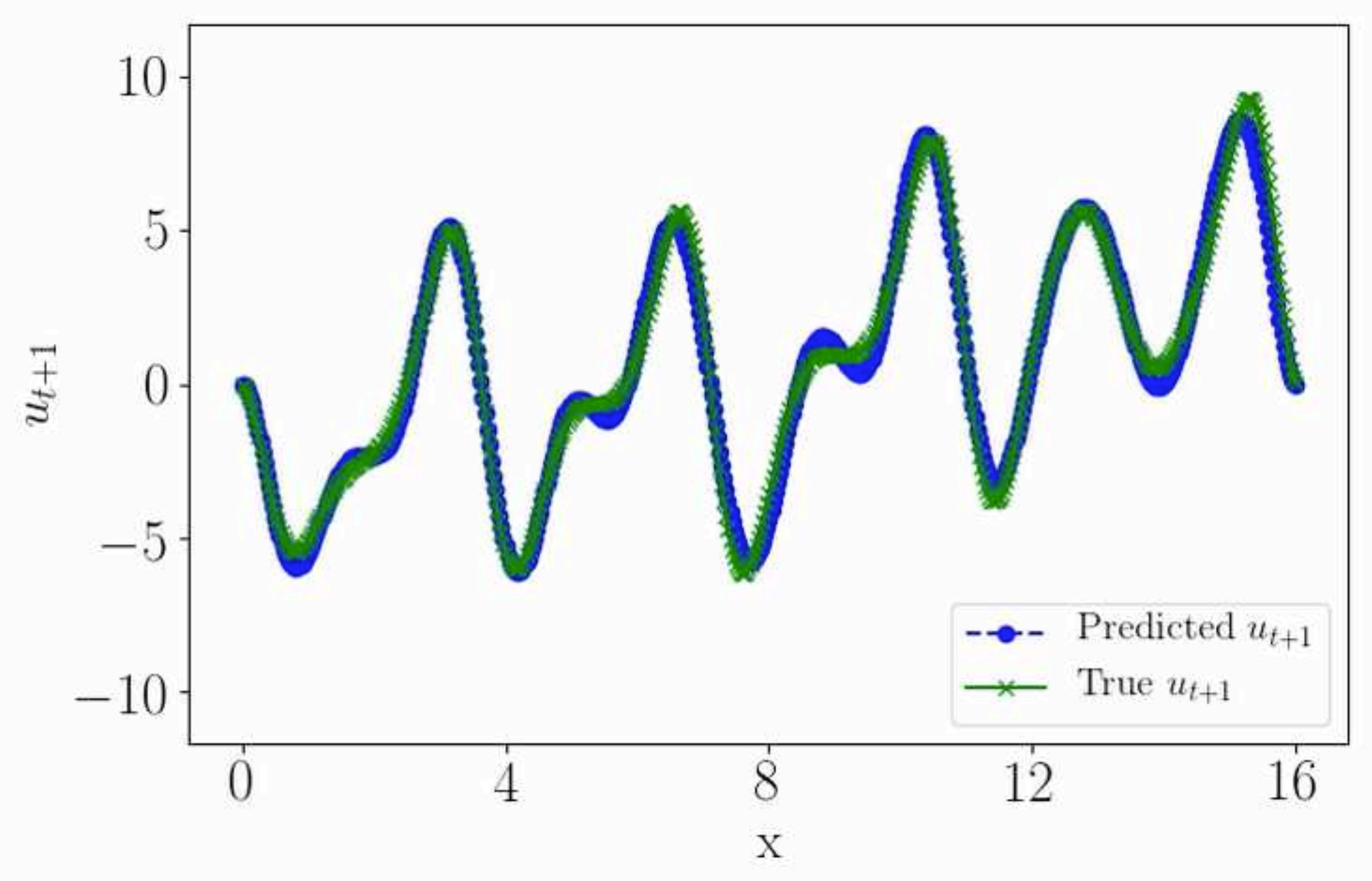
Accumulation of prediction error

prediction in **reduced** space

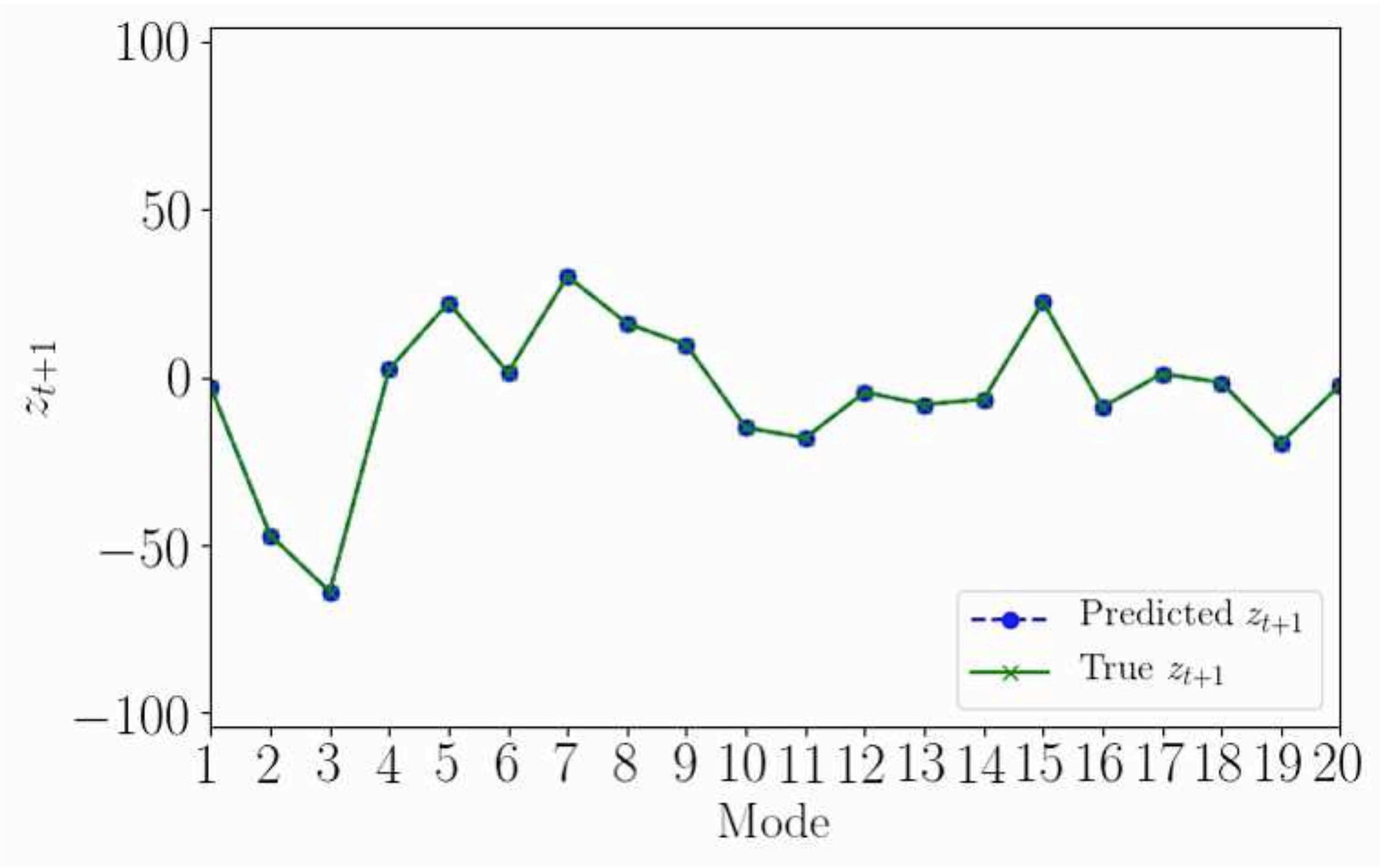
expanded in **high-dimensional** space

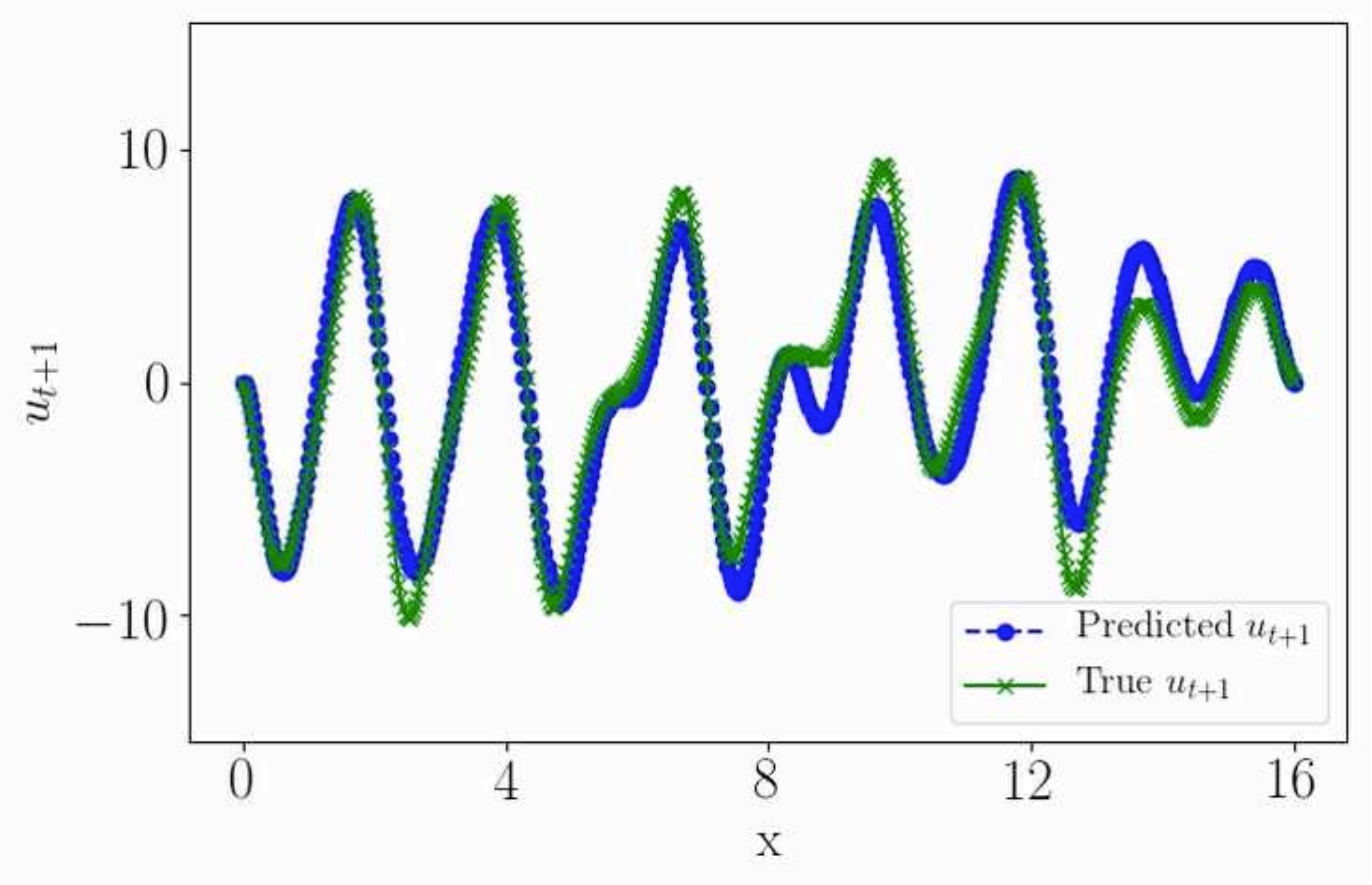
$\tilde{L} \approx 8$





$\tilde{L} \approx 10$





Accumulation of prediction error

prediction in **reduced** space

expanded in **high-dimensional** space

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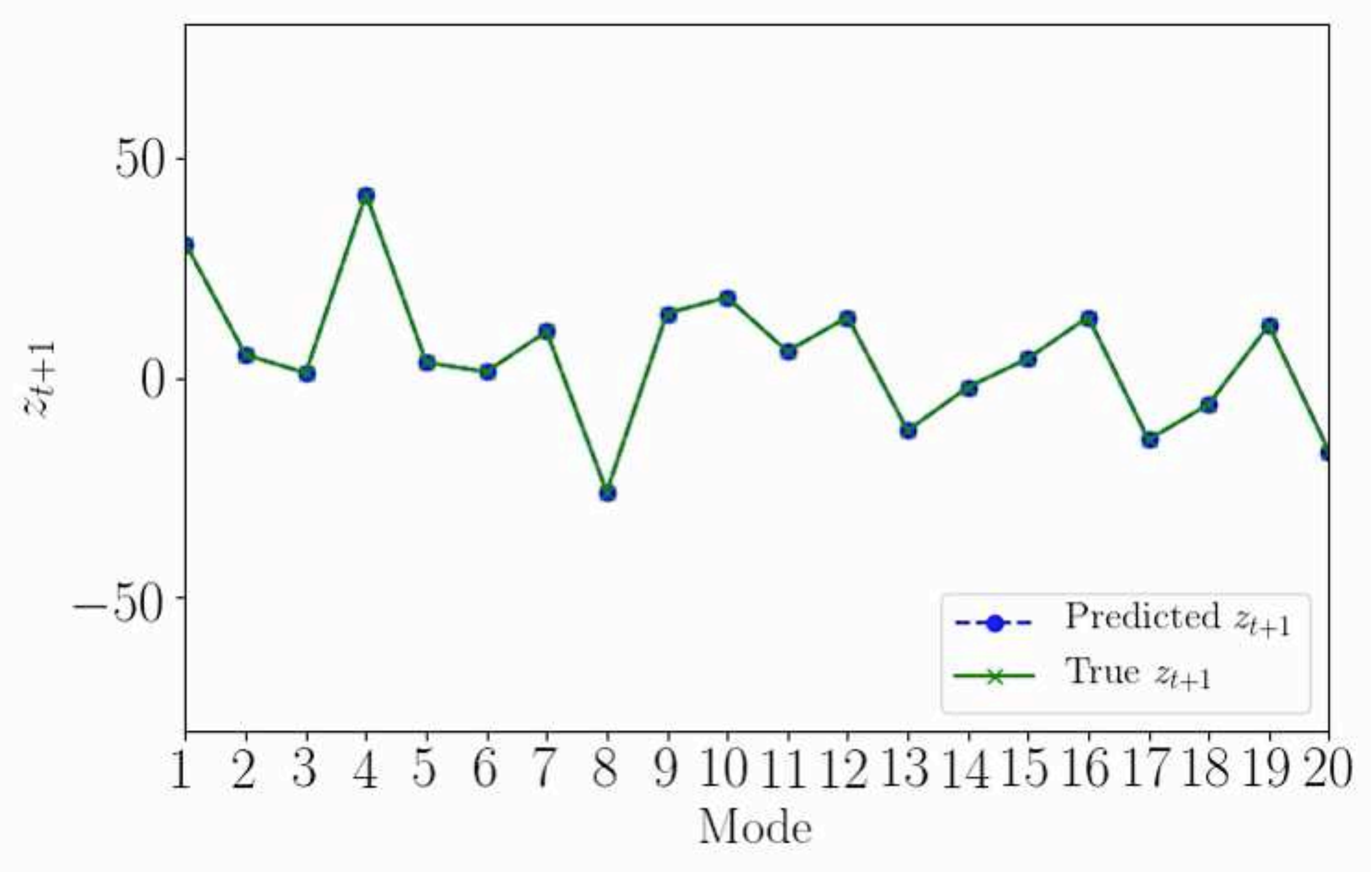

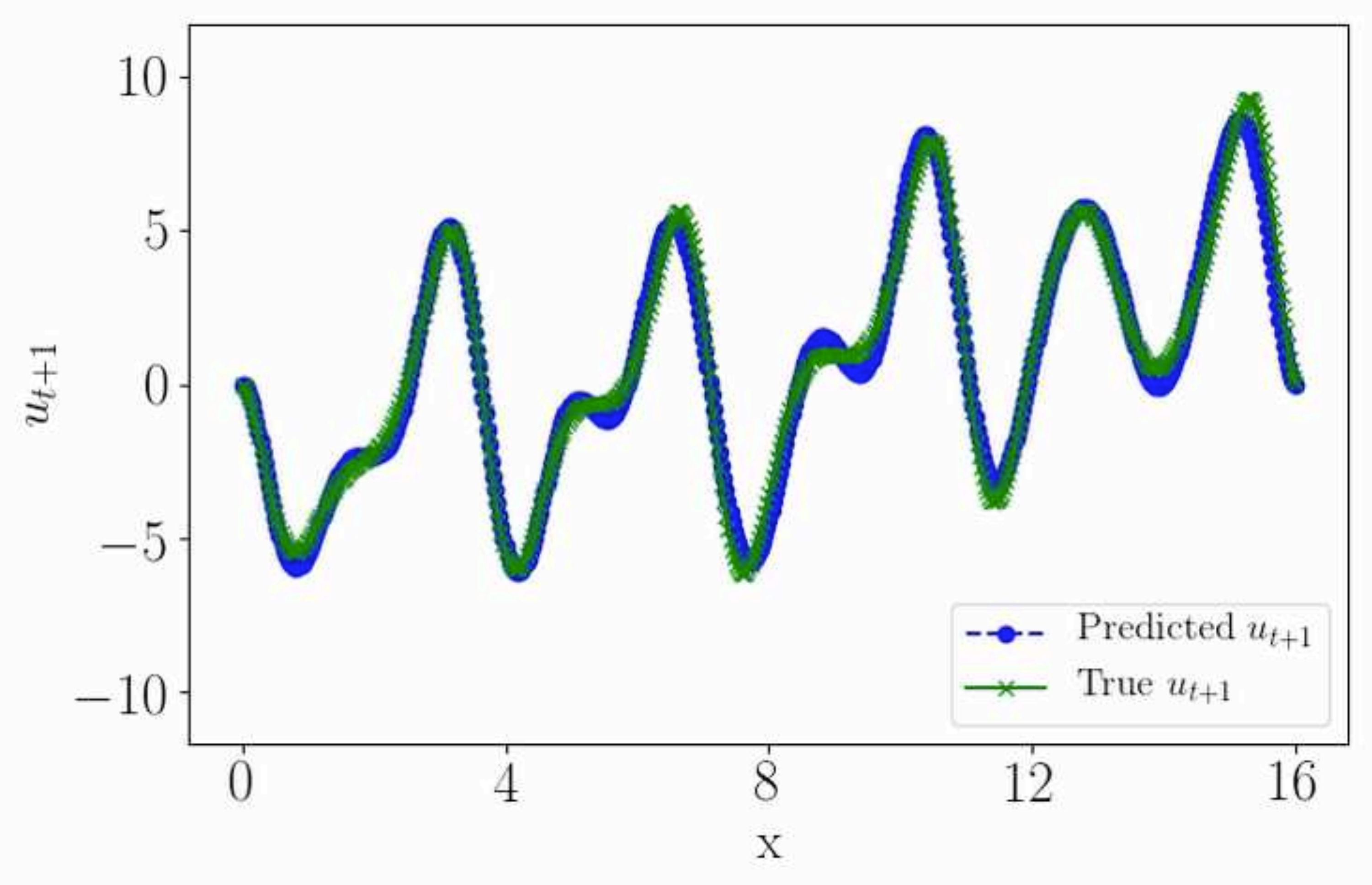

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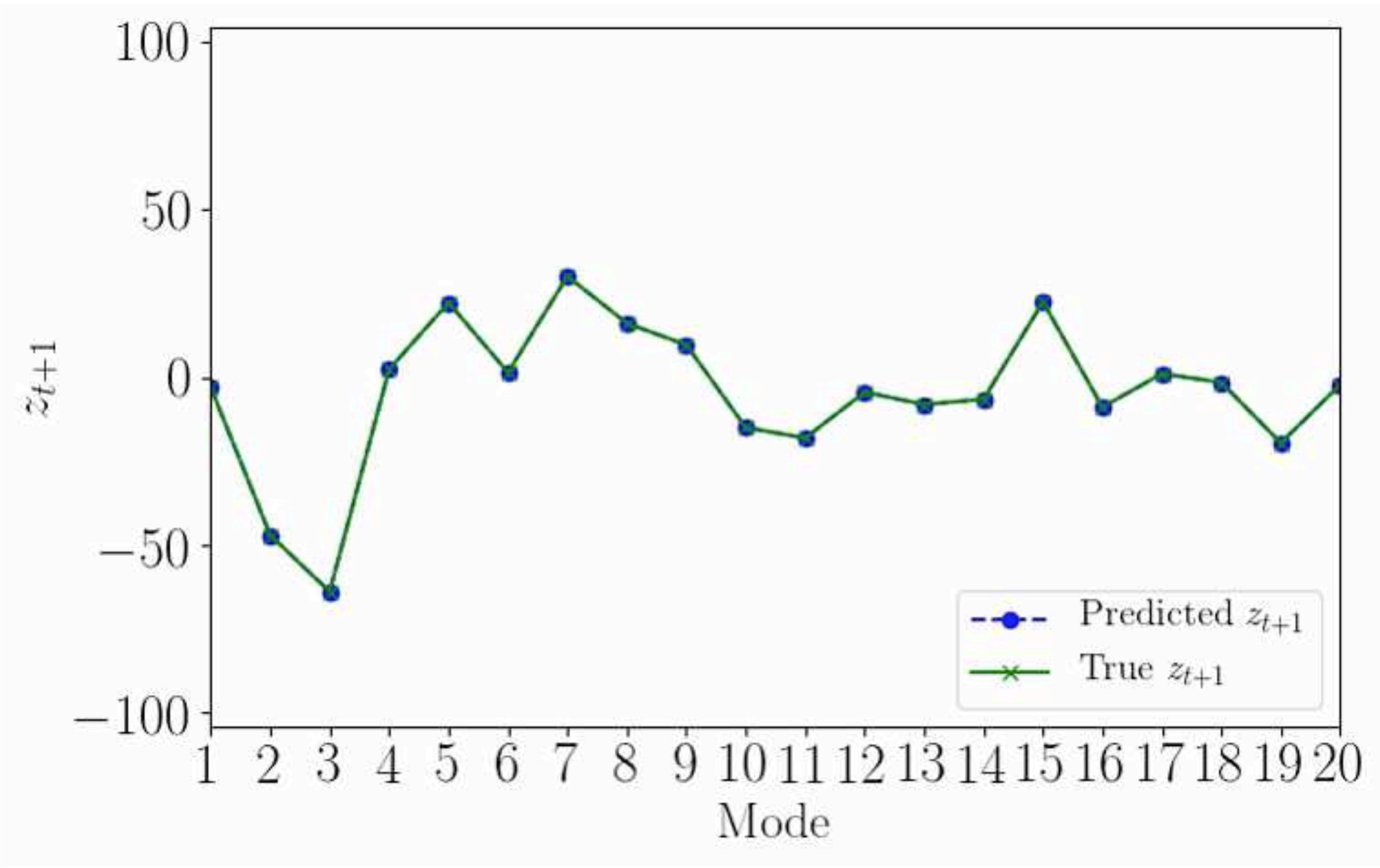

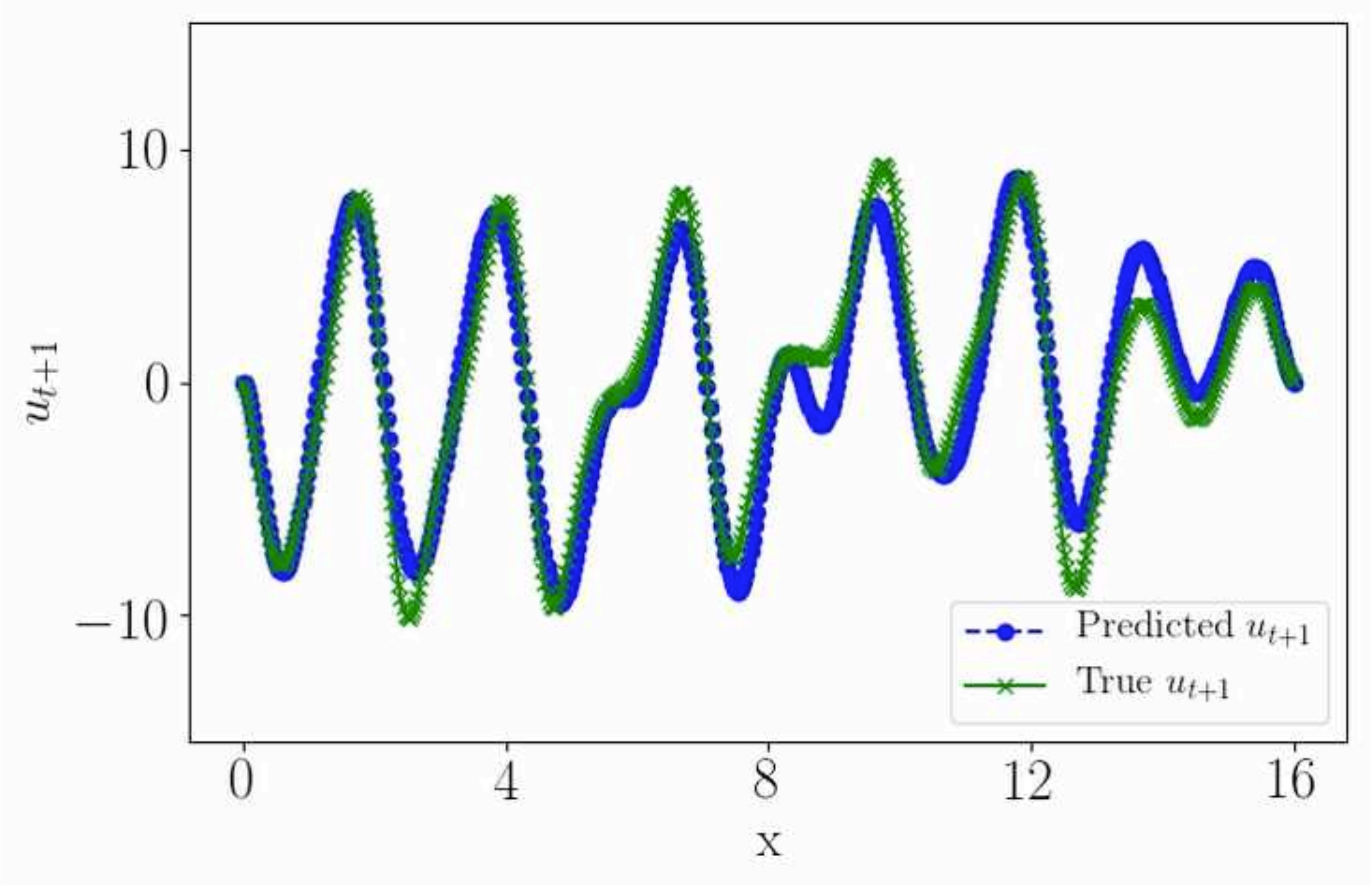

Challenges

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
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- Dynamics underrepresented in training data
- Scarce data in attractor boundaries

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- Scarce data in attractor boundaries
- Under-resolved high dimensional dynamics

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Hybrid LSTM - MSM

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

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

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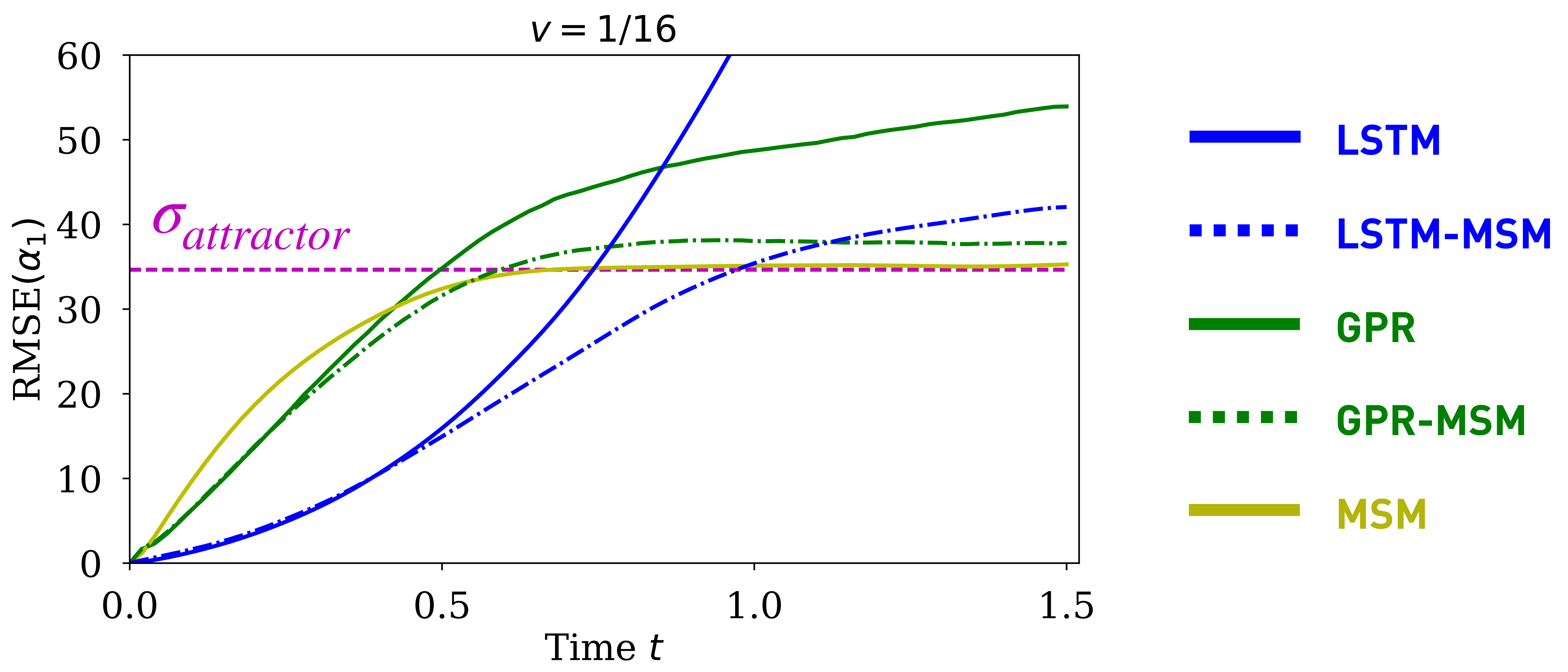
Results on KS - *Comparison with Gaussian Process Regression (GPR)*

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

Root mean square error:

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



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

PR Vlachas, W Byeon, Z Wan, T Sapsis, P Koumoutsakos, *Data-driven forecasting of high-dimensional chaotic systems with long short-term memory networks,* **Proc. Roy. Soc. A , 2018**

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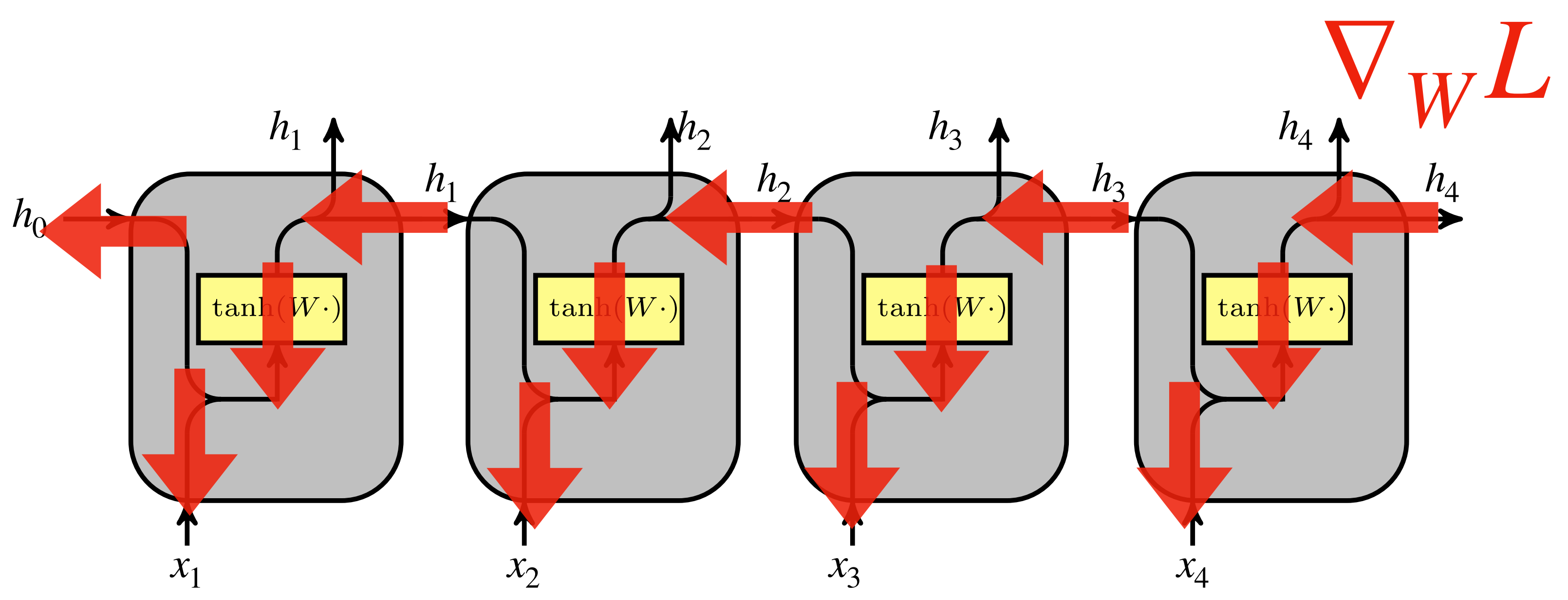

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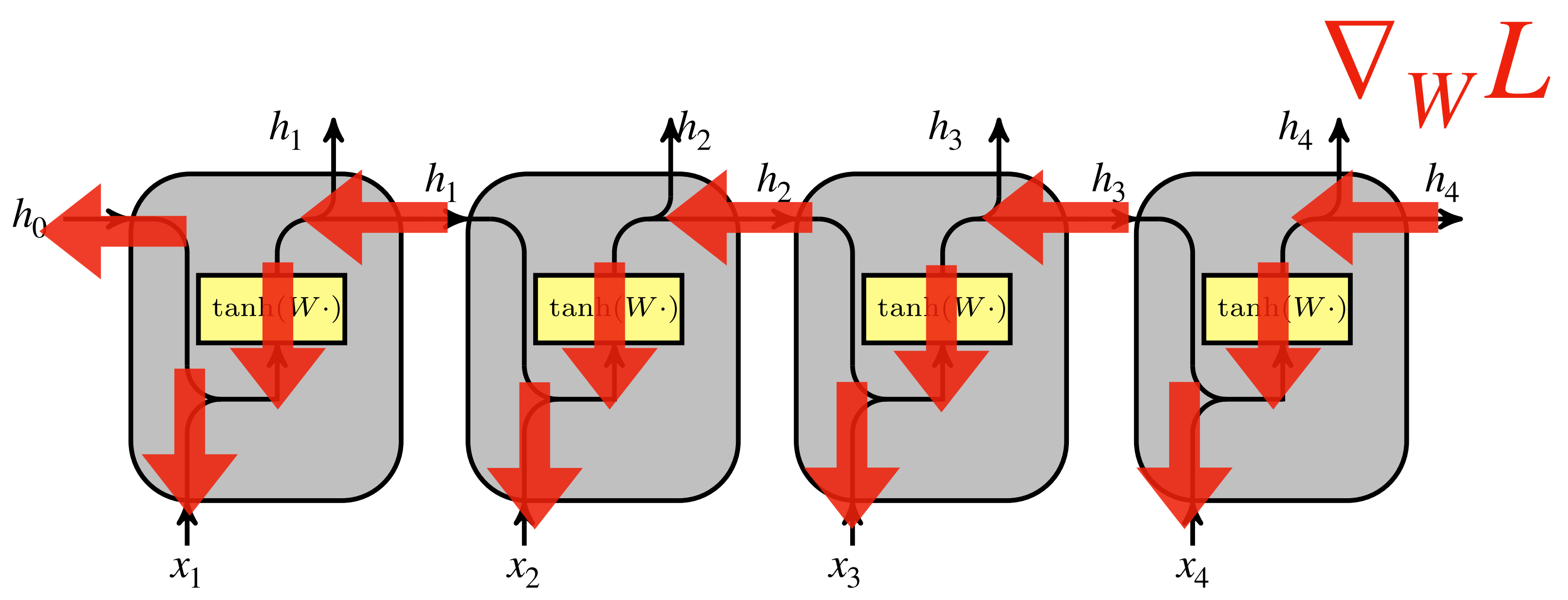

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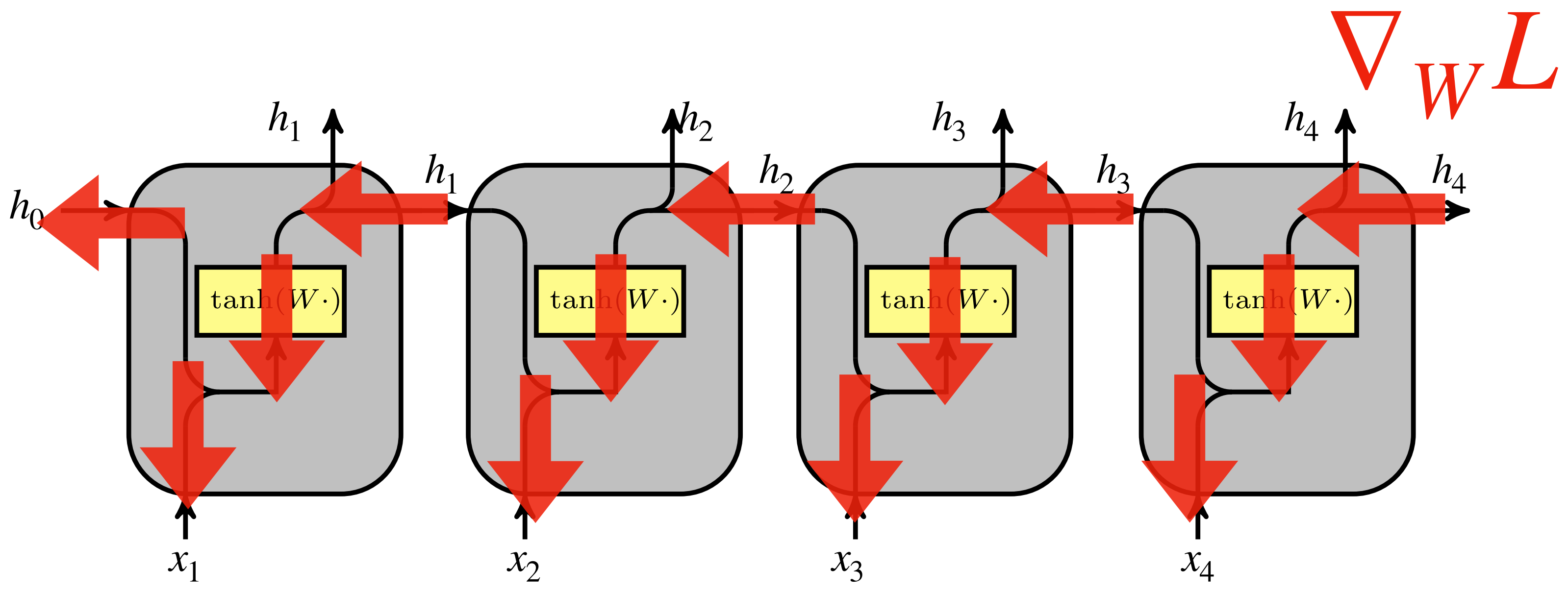
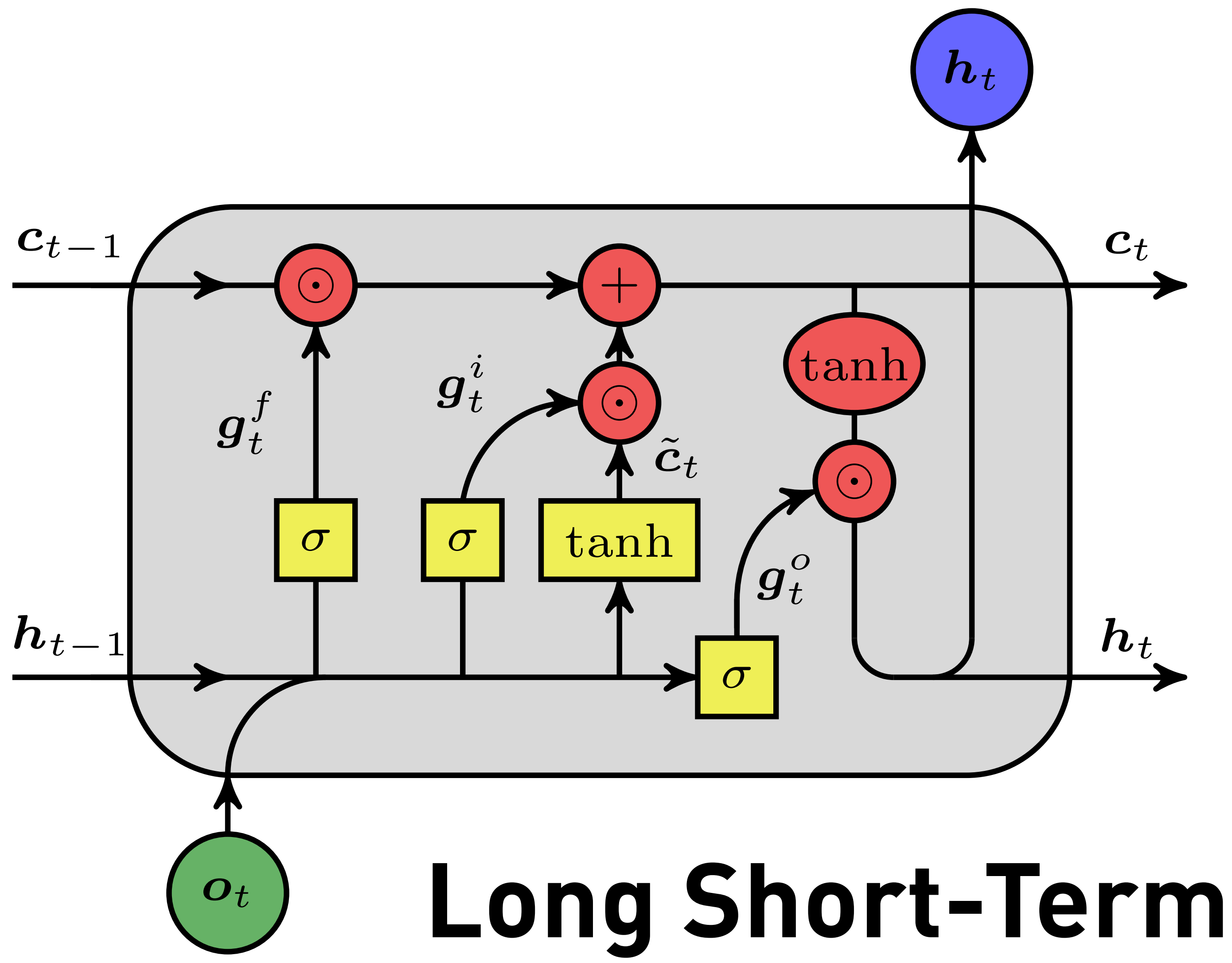


Mitigation? Sophisticated architectures



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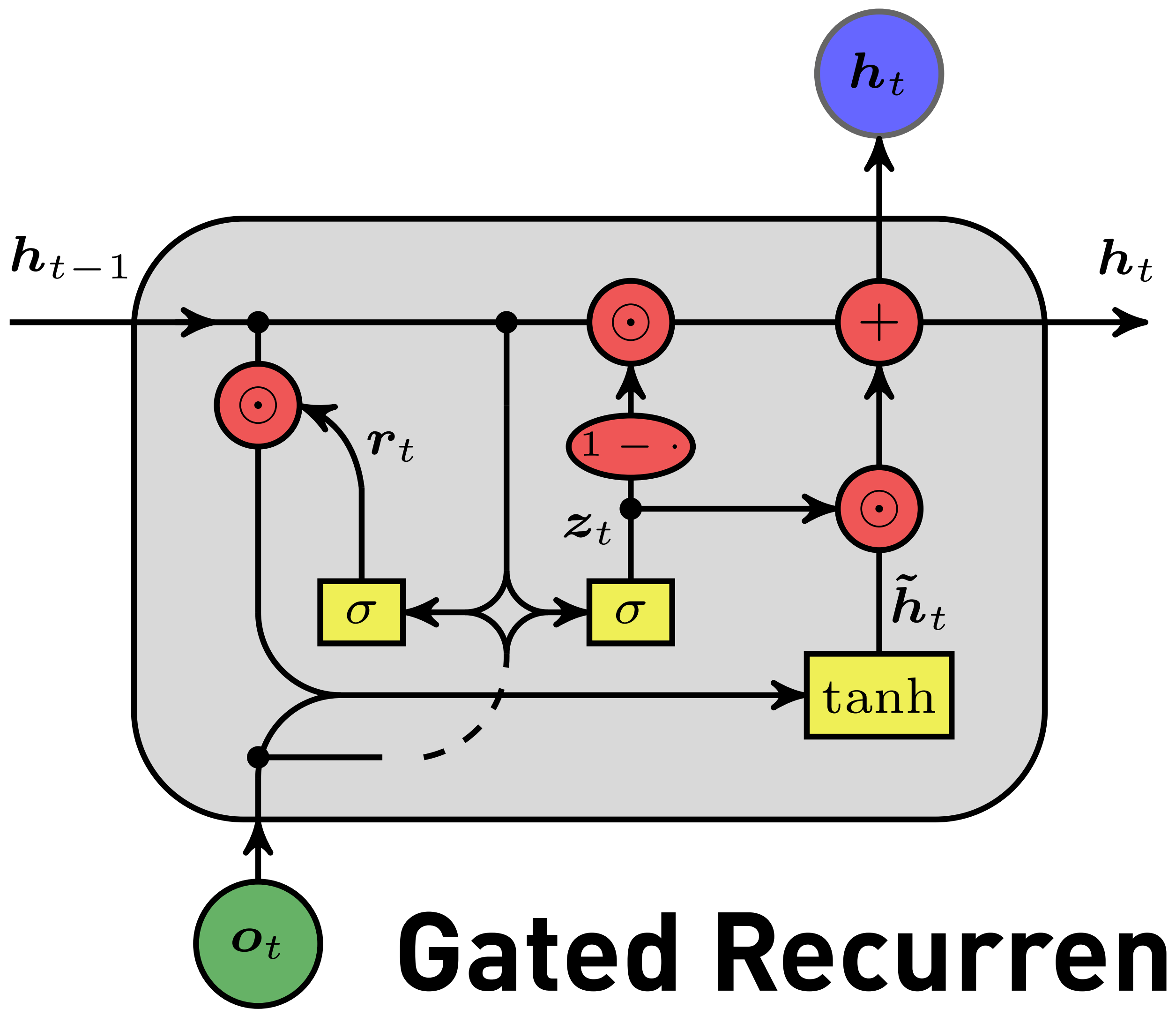

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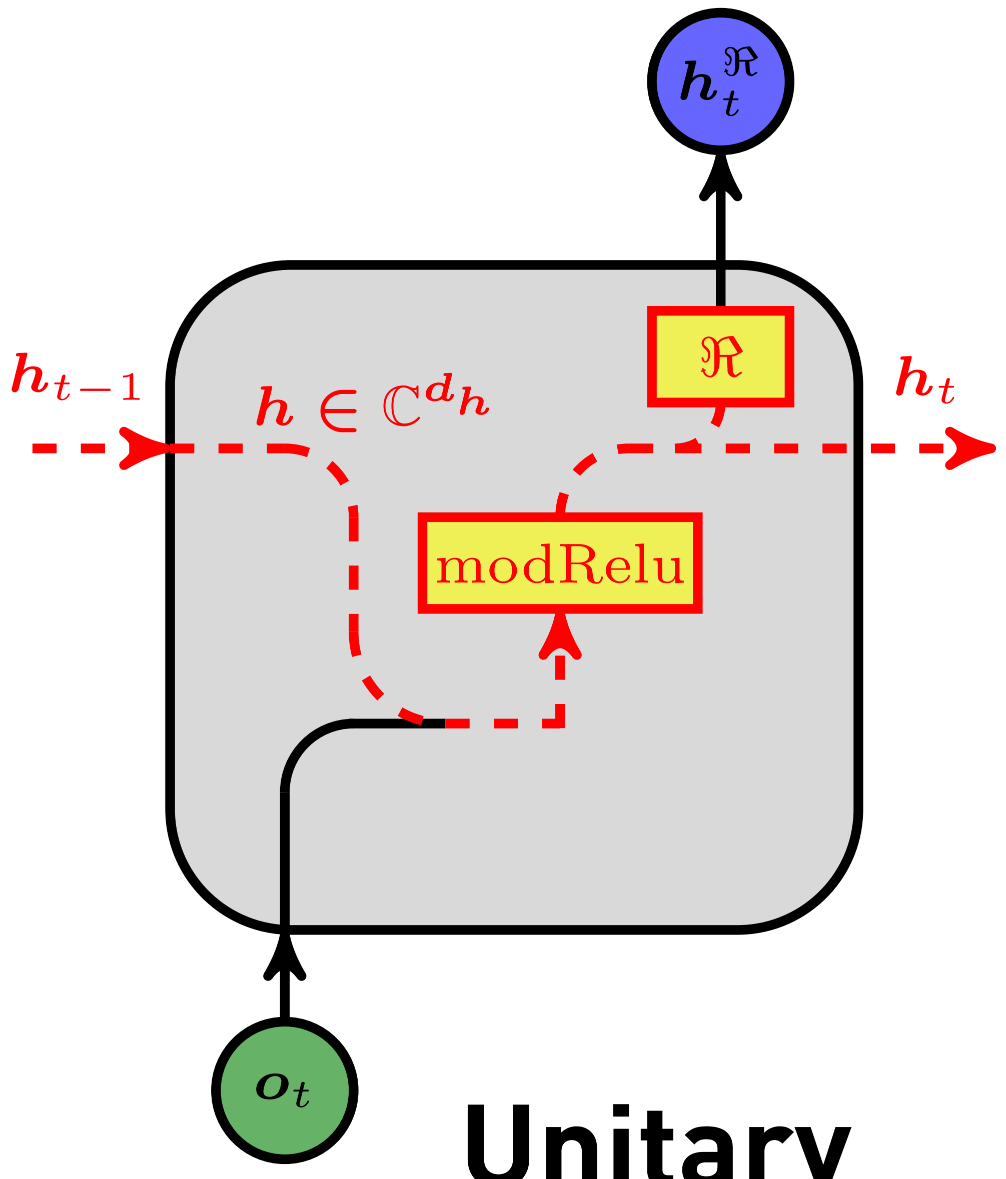

Unitary

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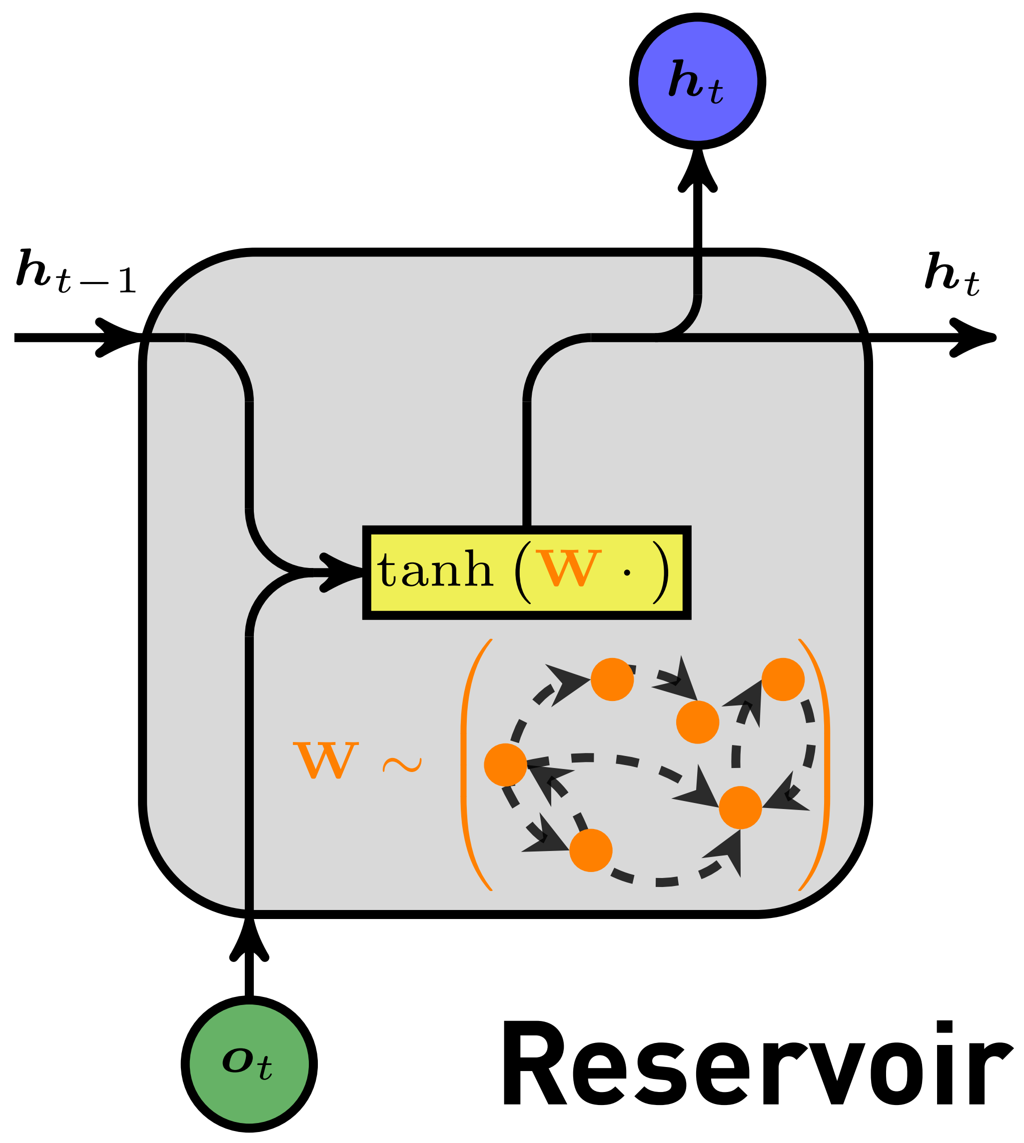

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- Pathak, Ott, et. al. (2017, 2018)
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- **Random** ***sparse*** recurrent weight matrix with ***spectral radius smaller than one***
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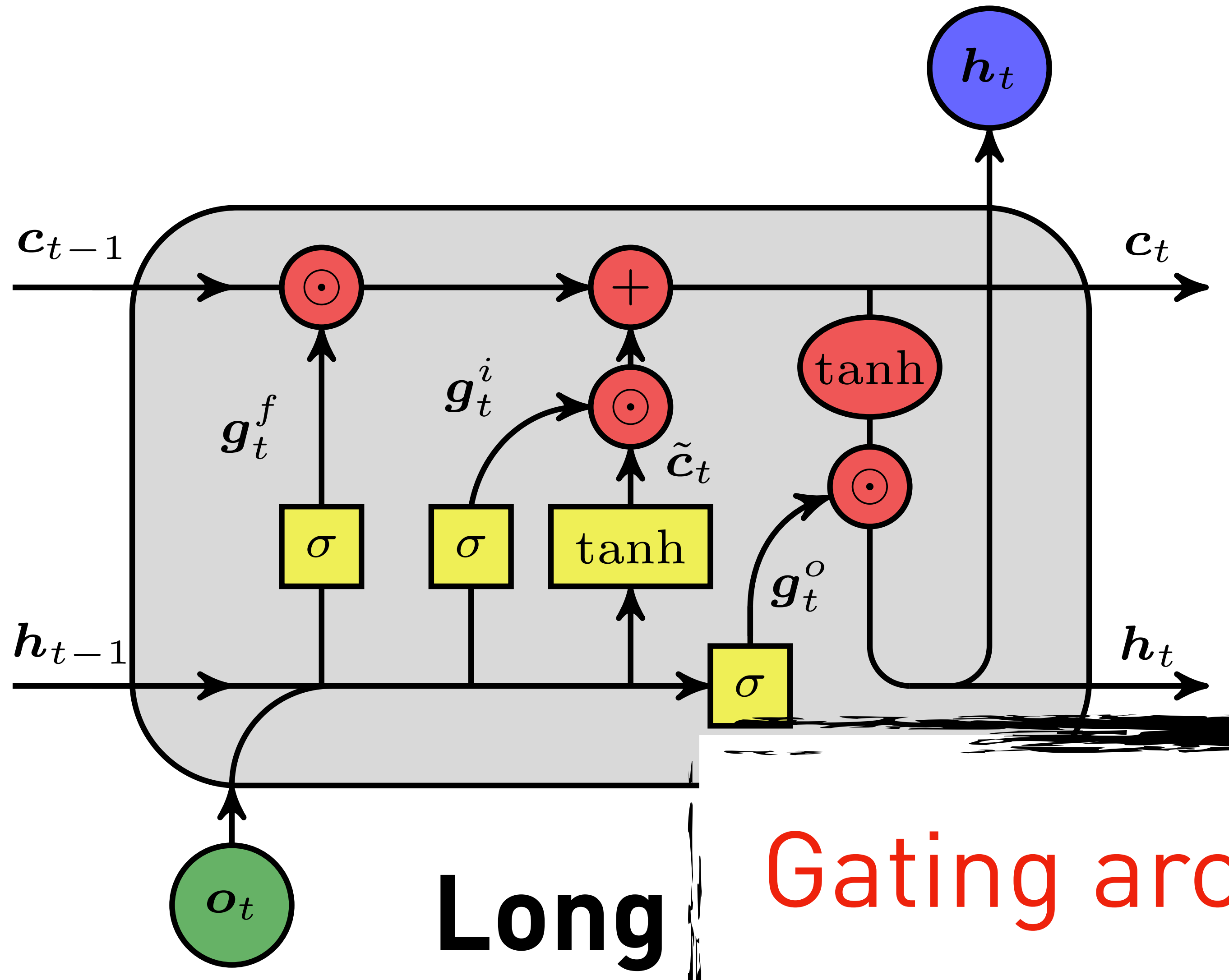

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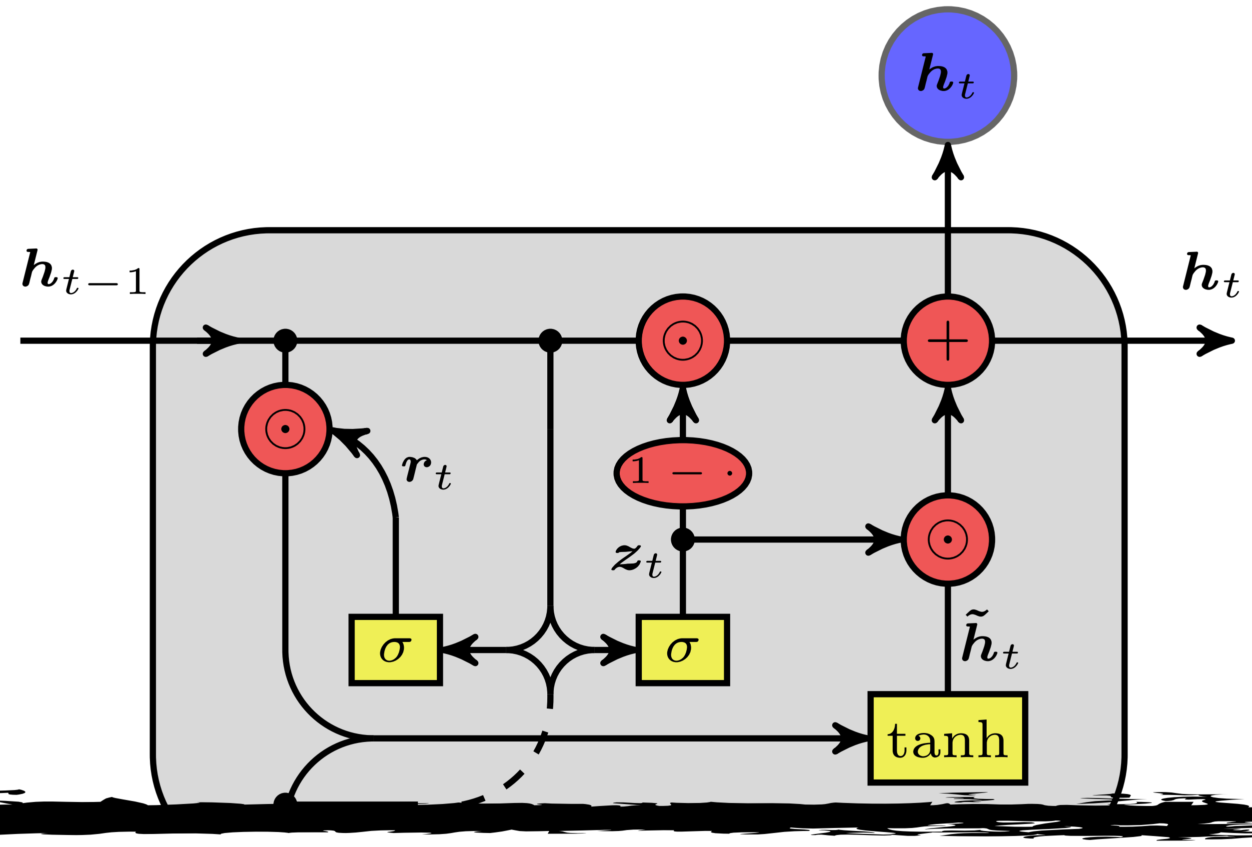

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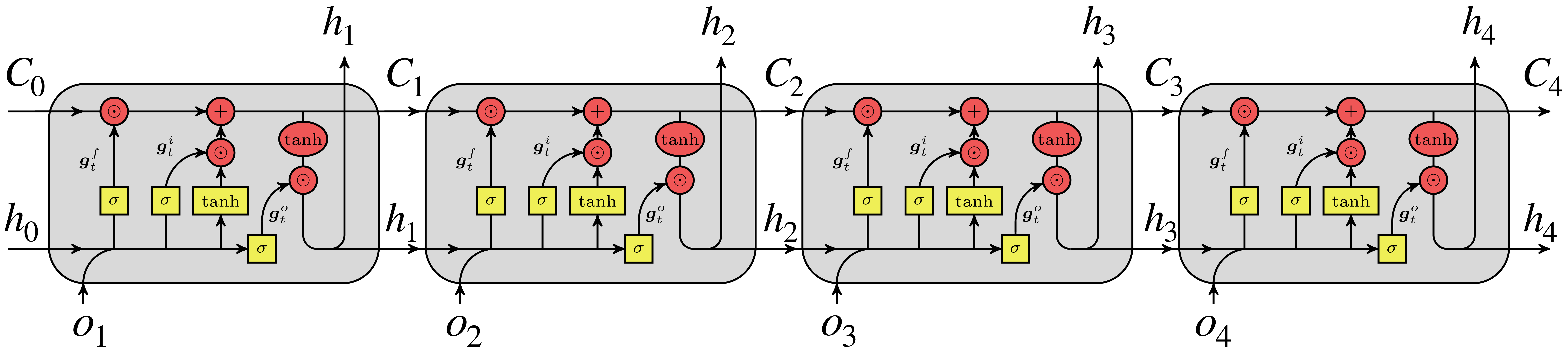

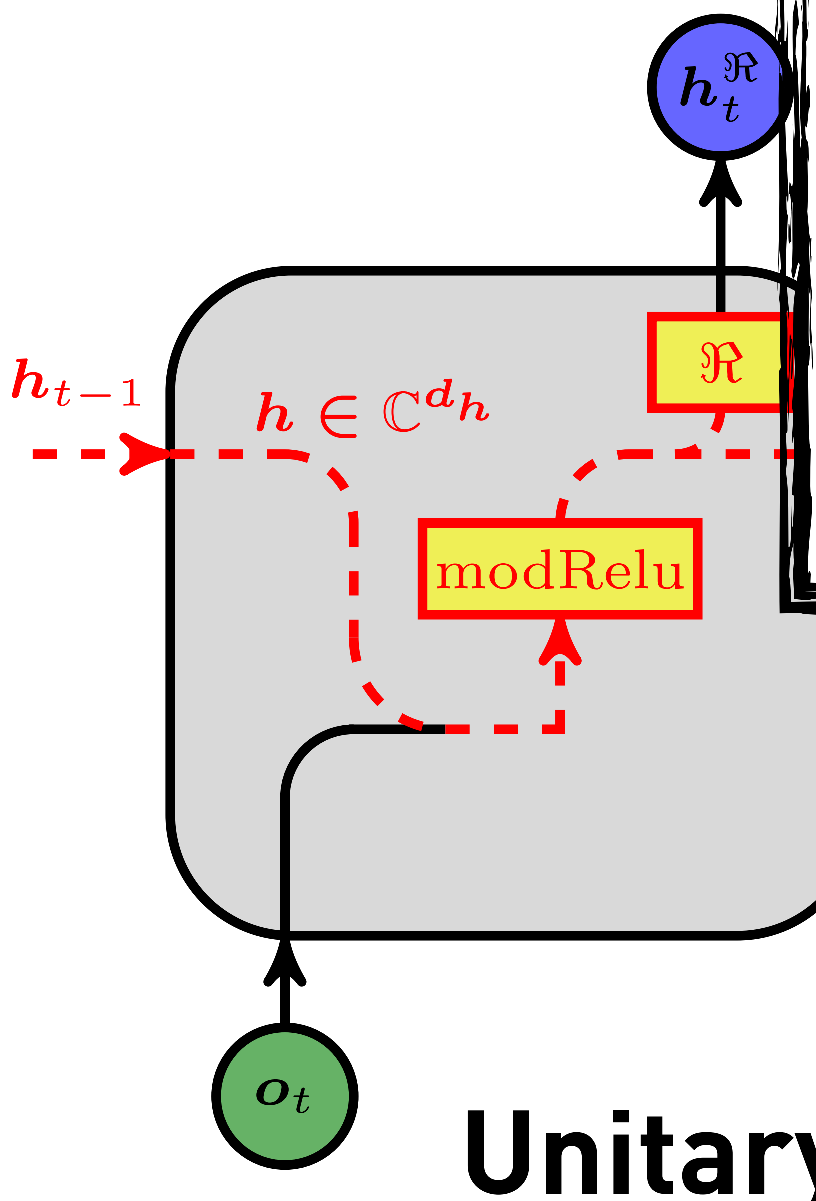

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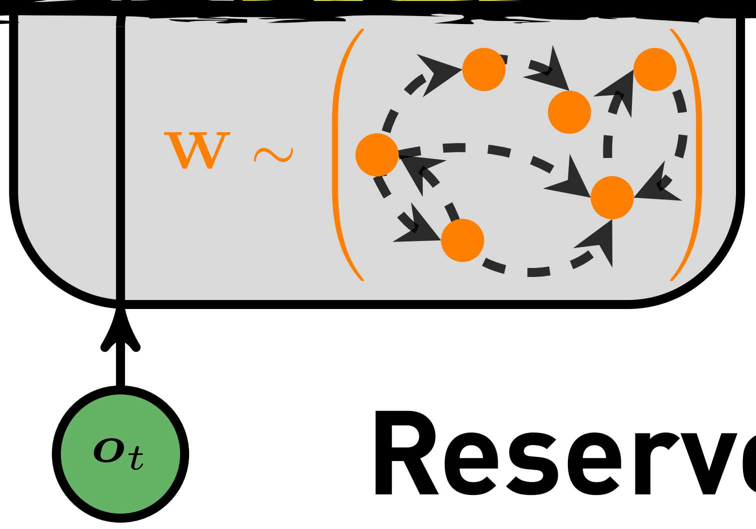

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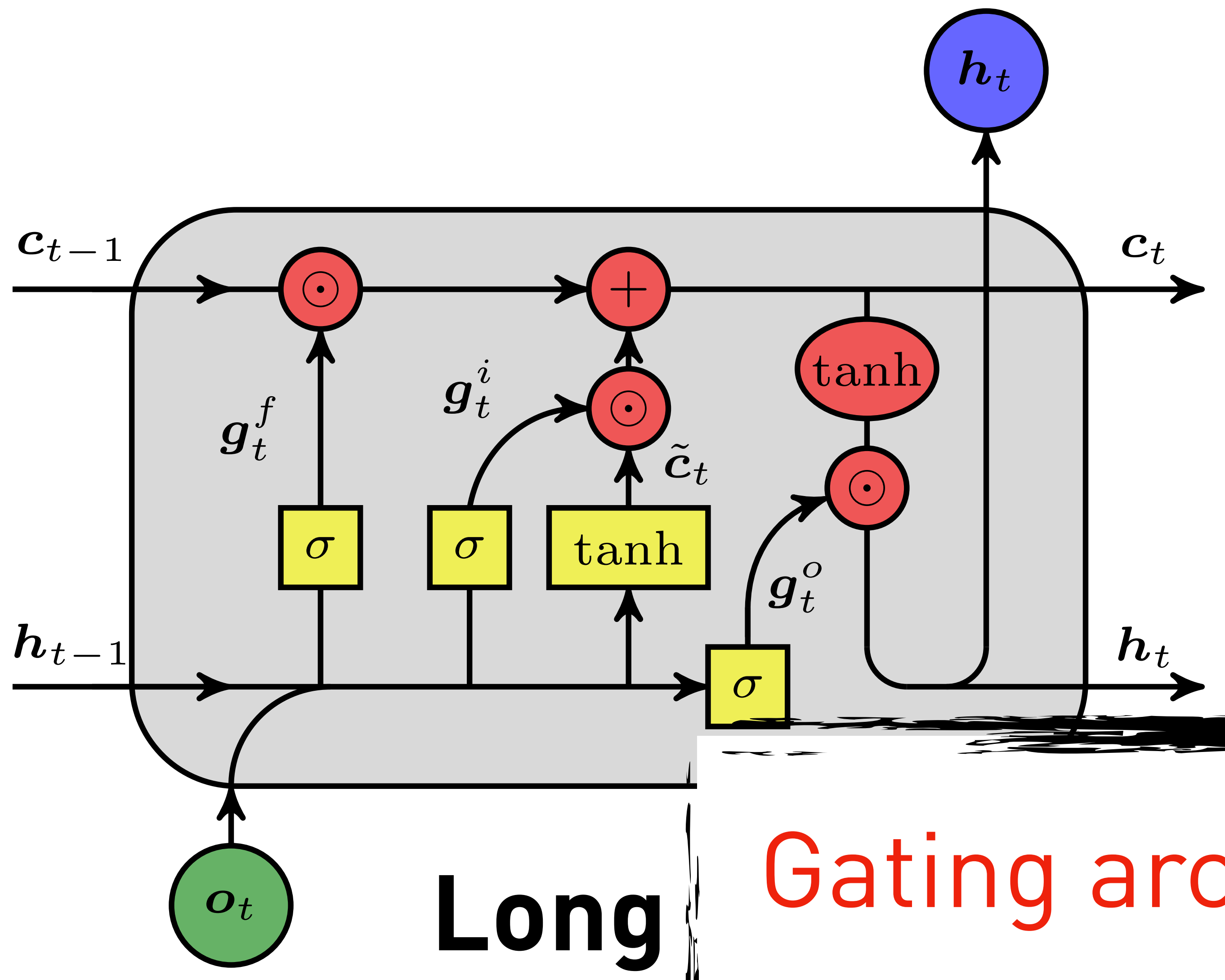

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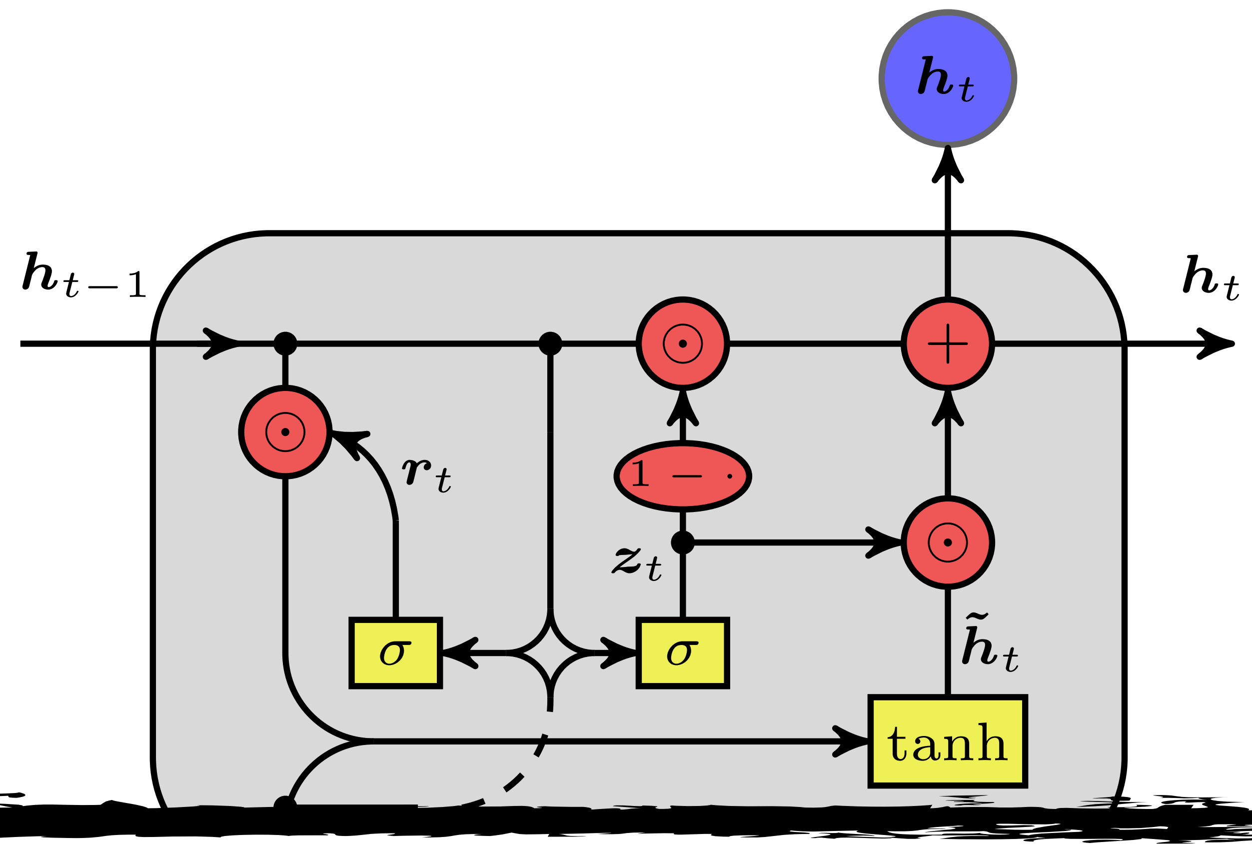

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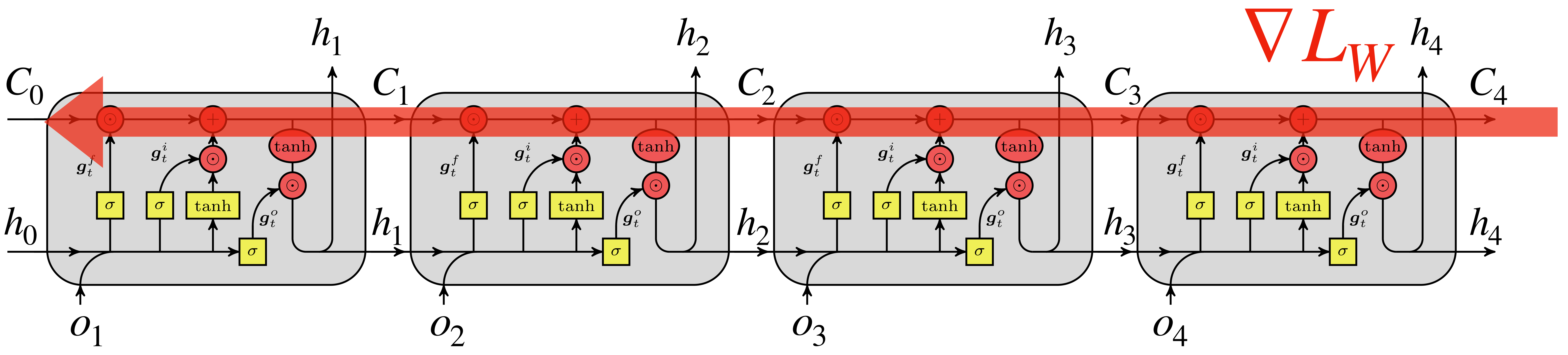

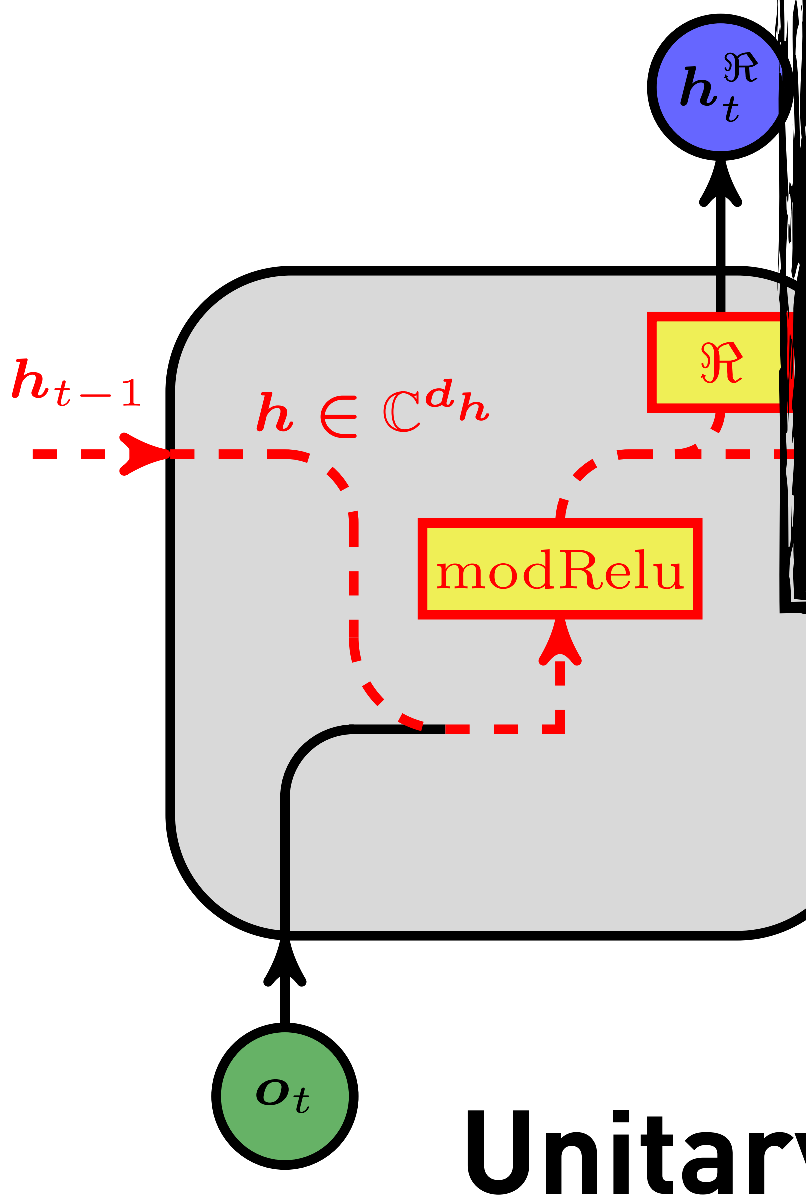

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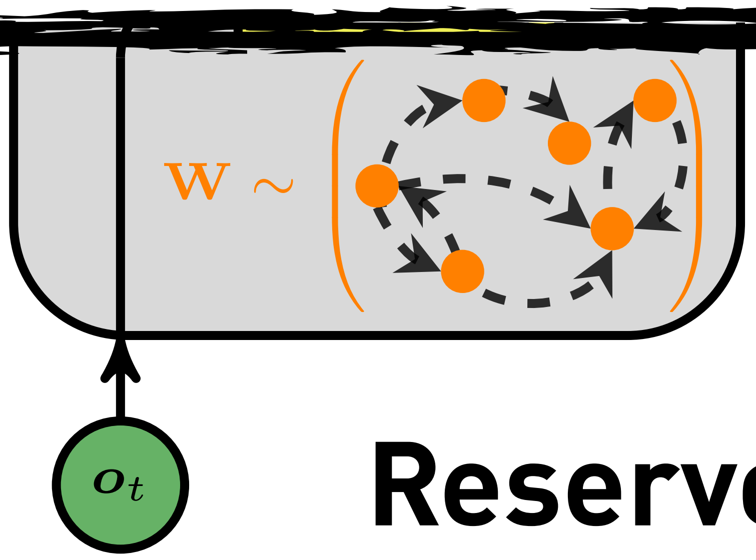

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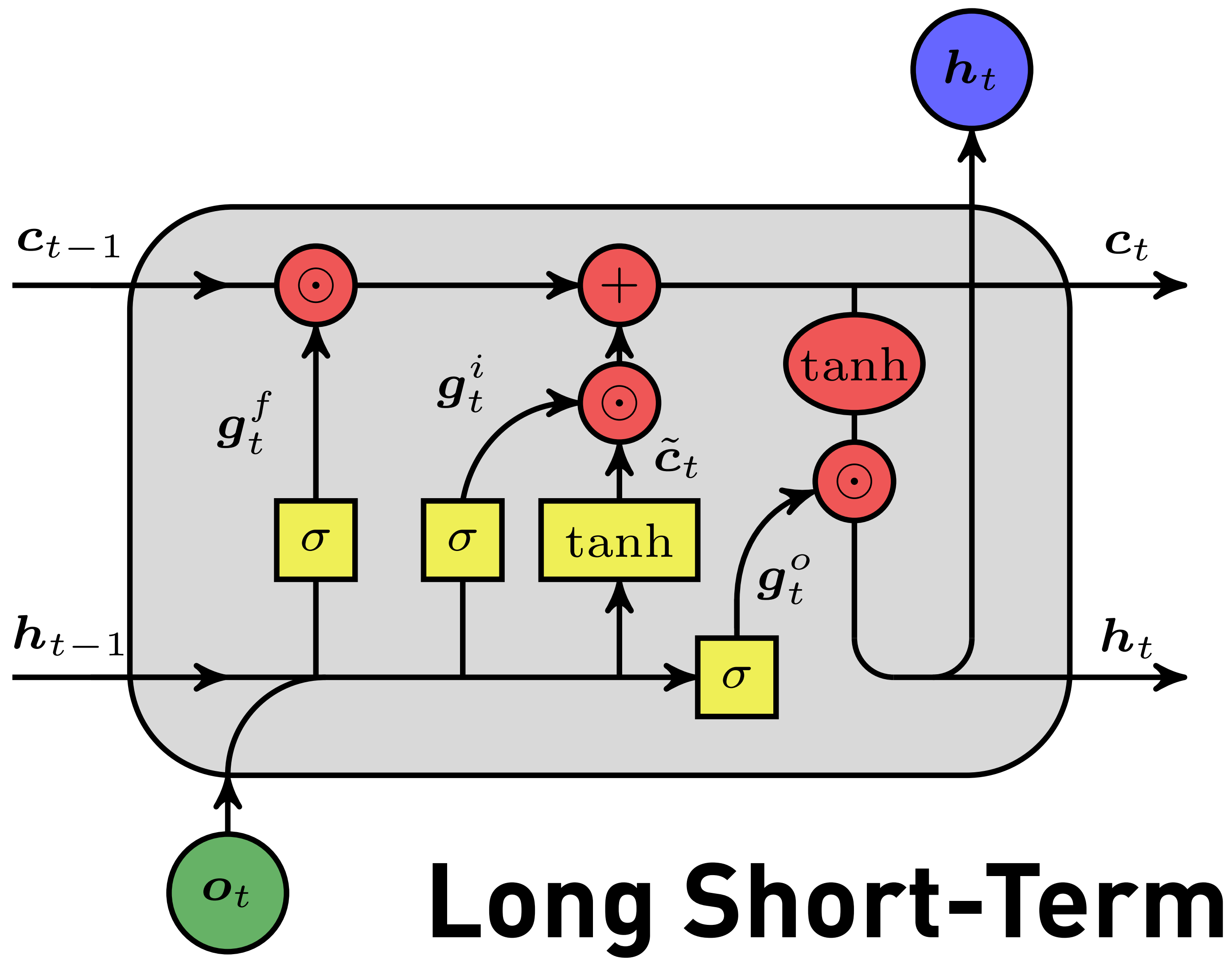

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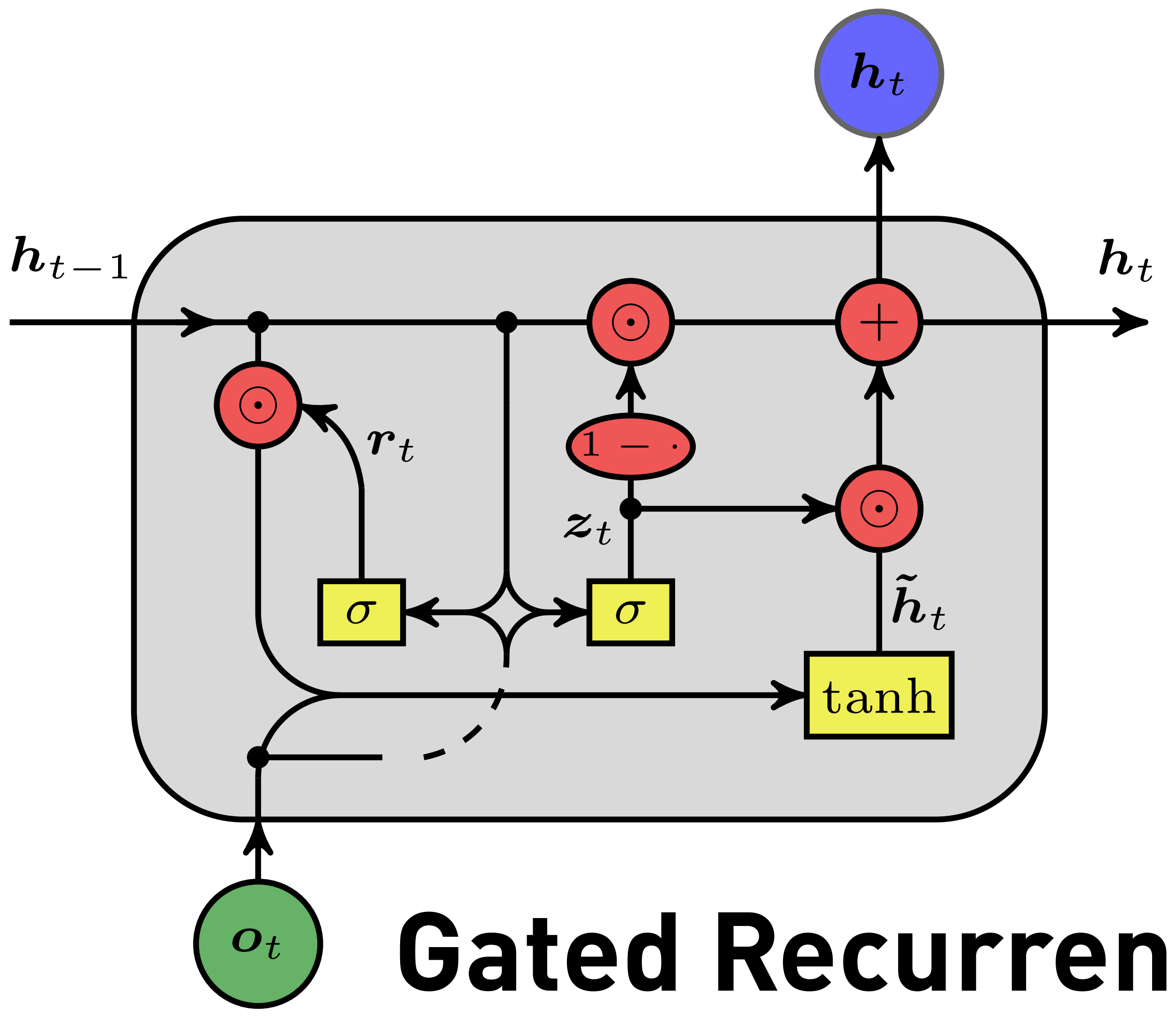

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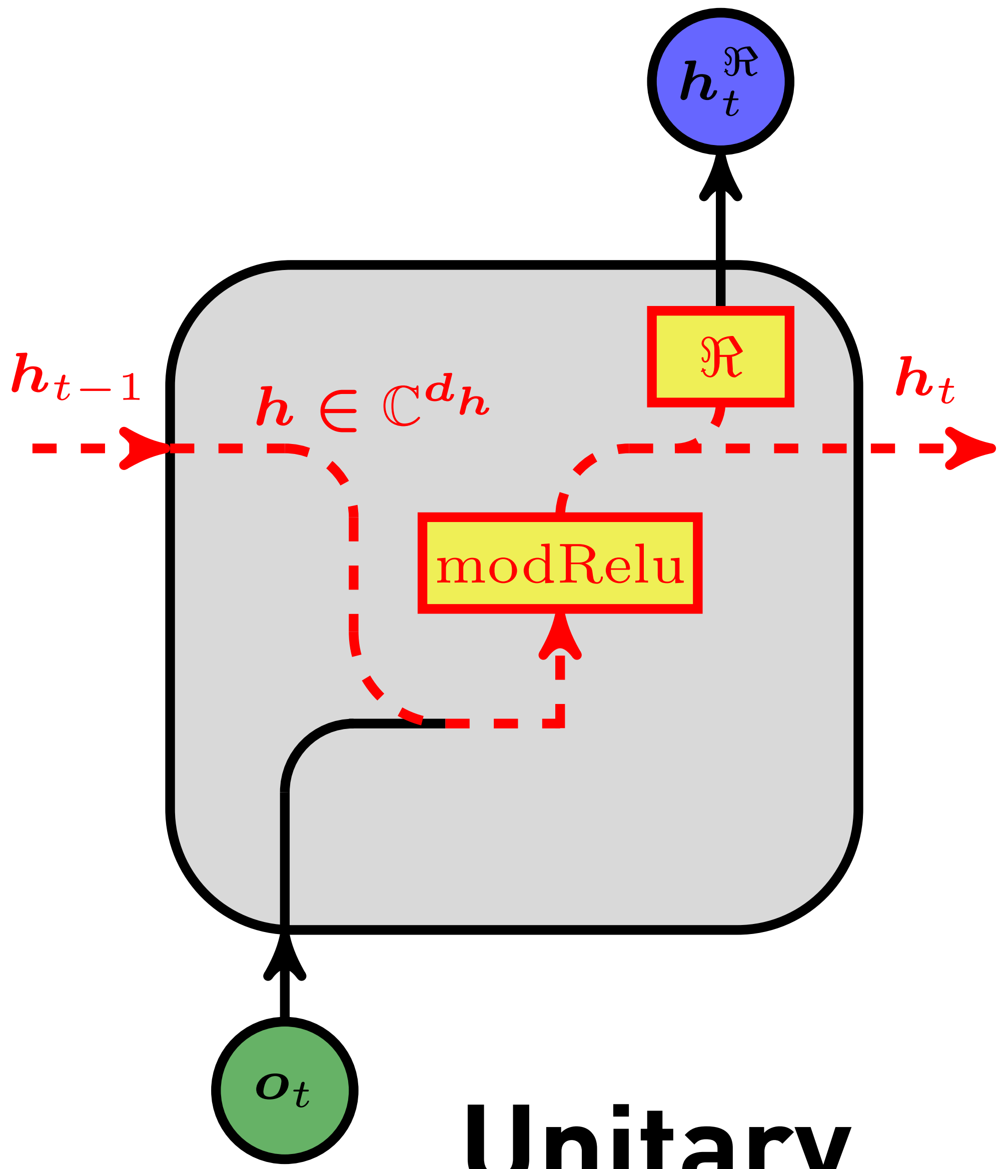

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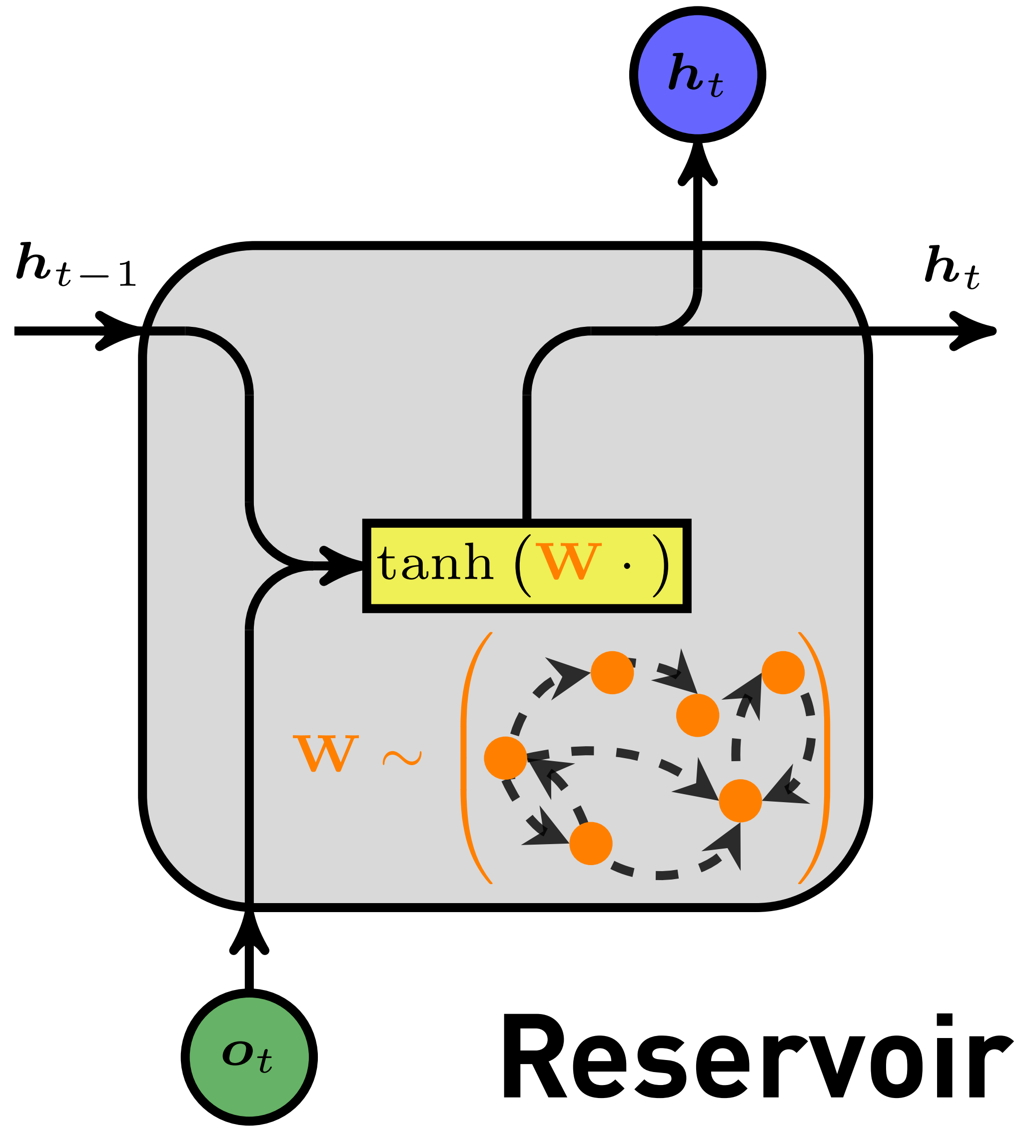

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Lorenz 96 - 35 / 40 mode observable

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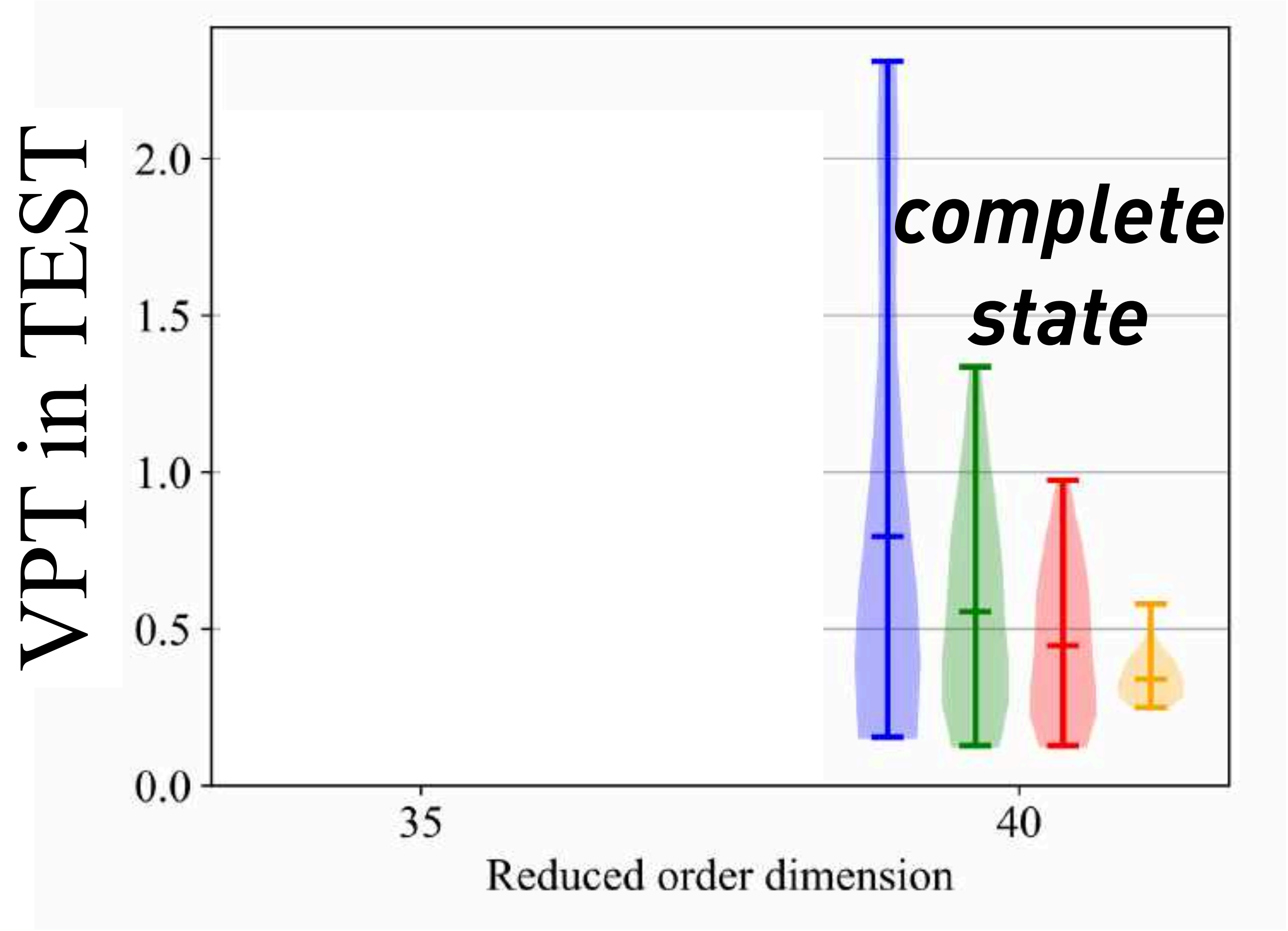

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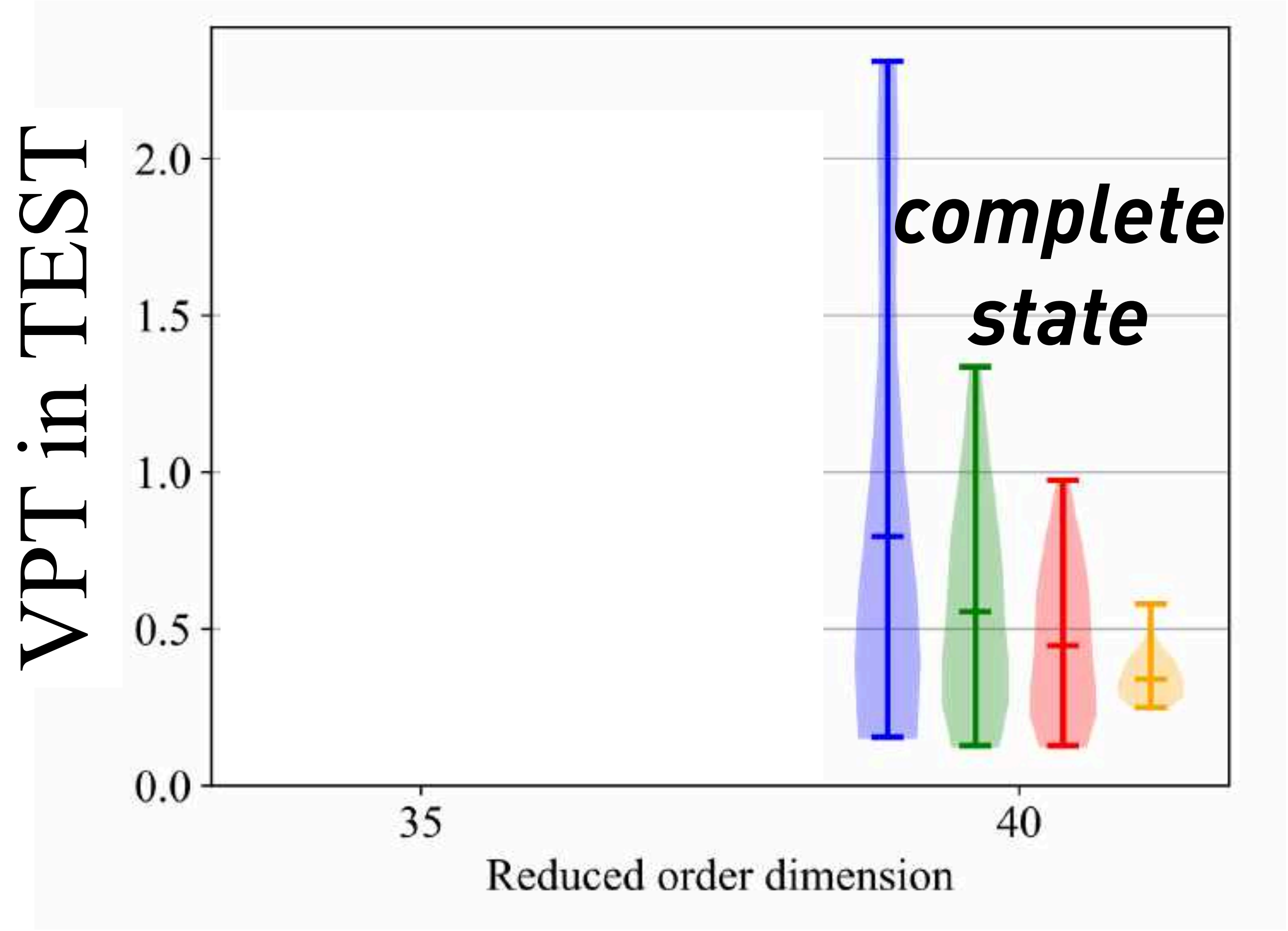

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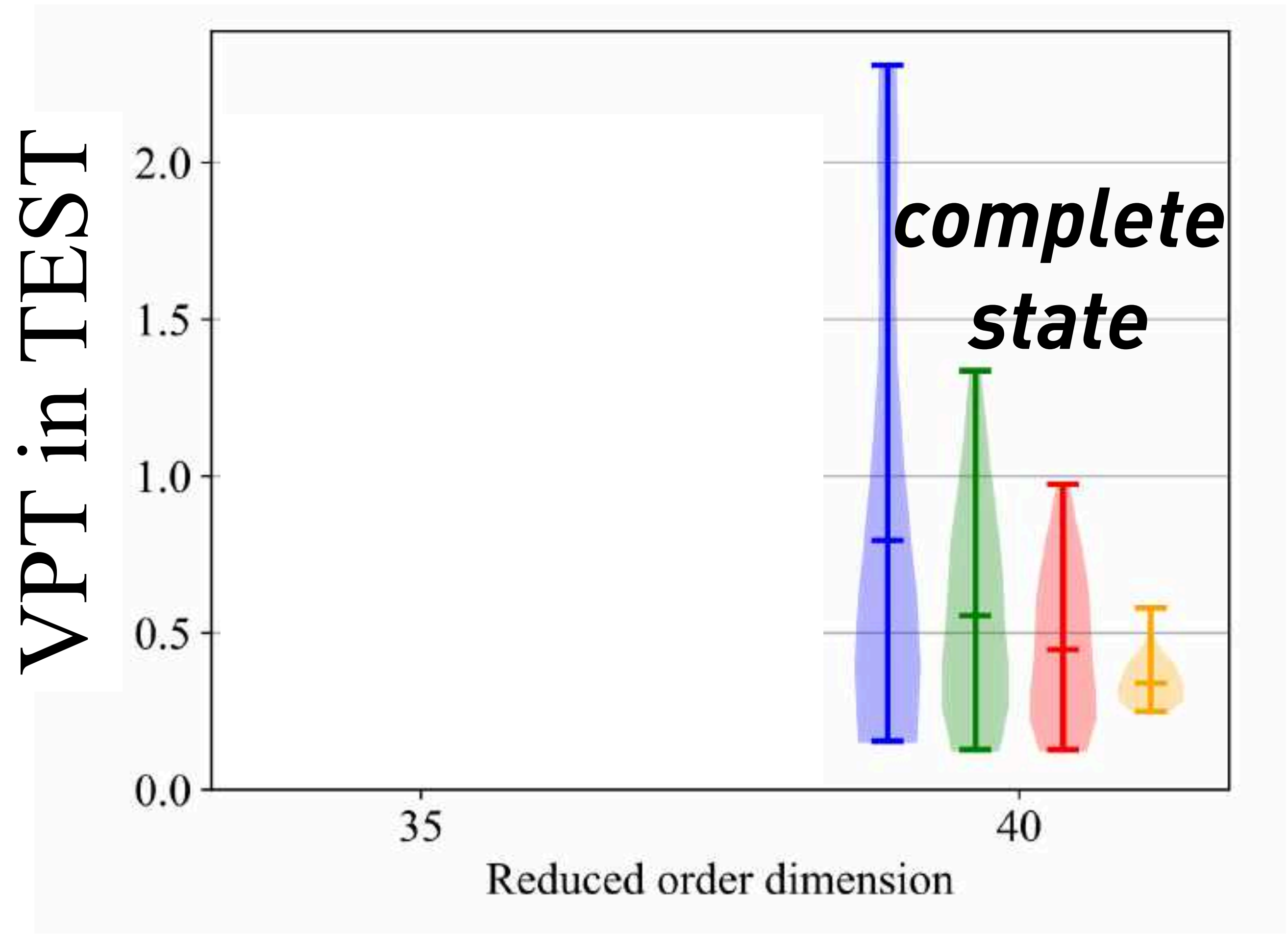

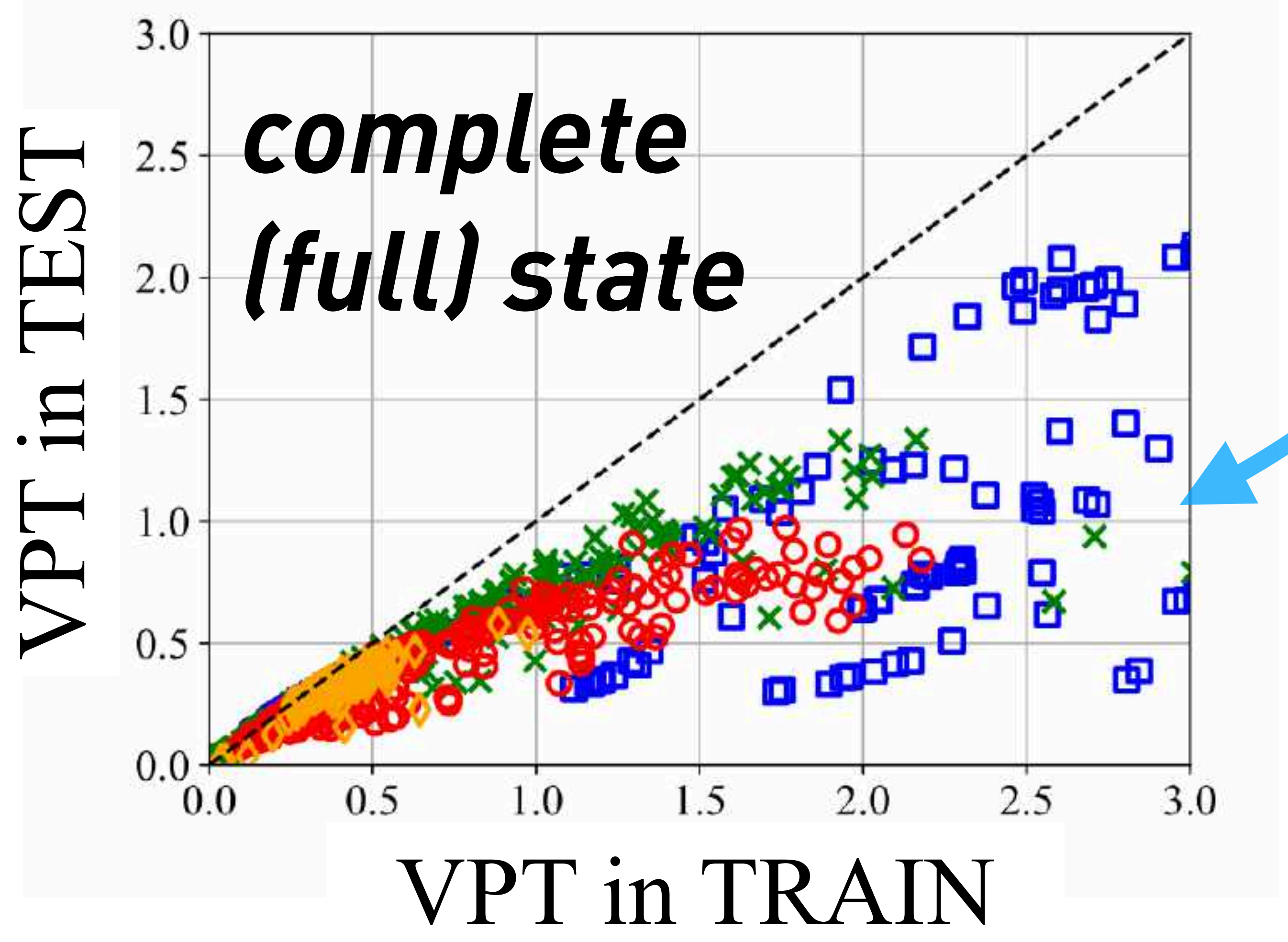

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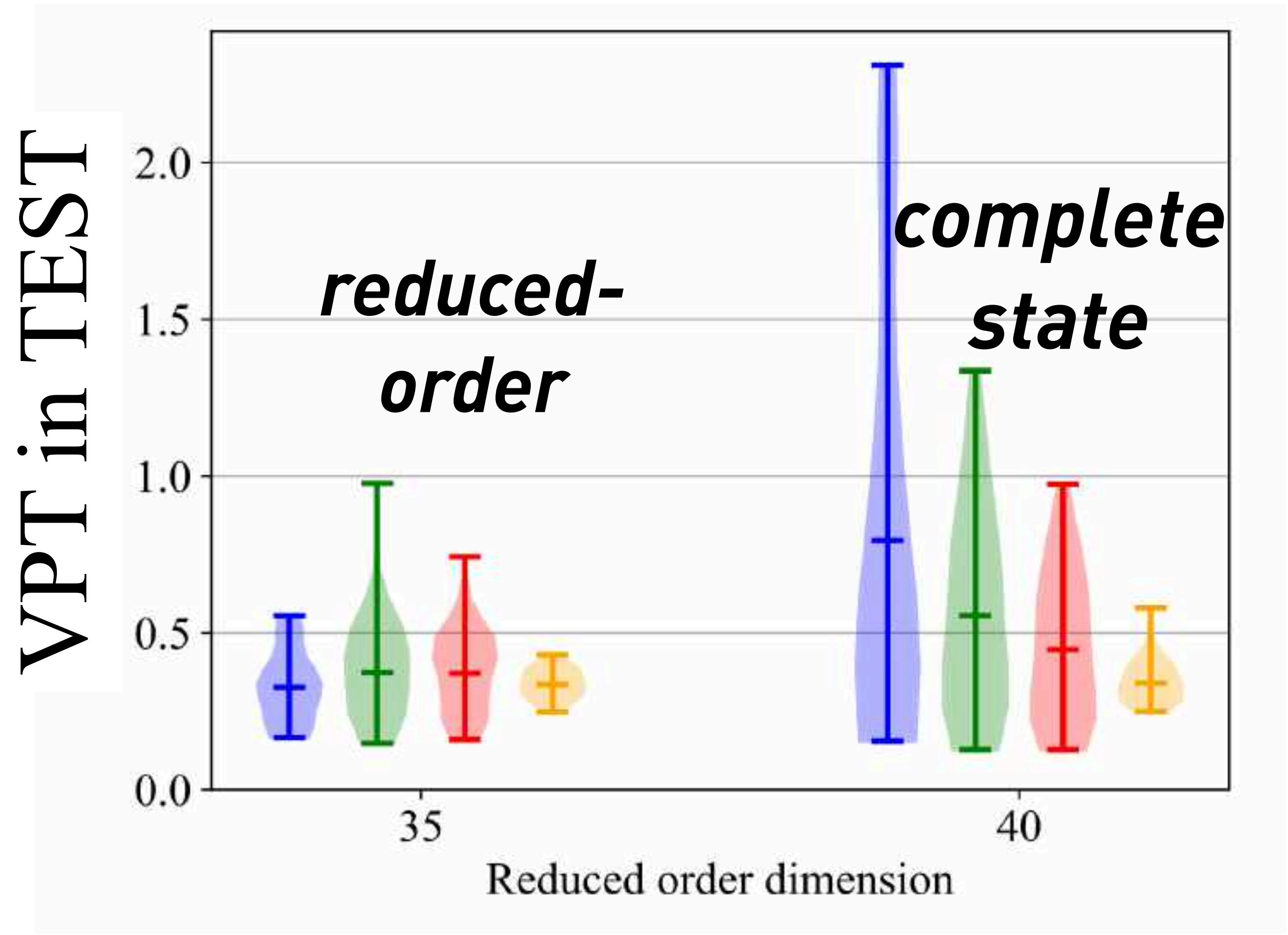

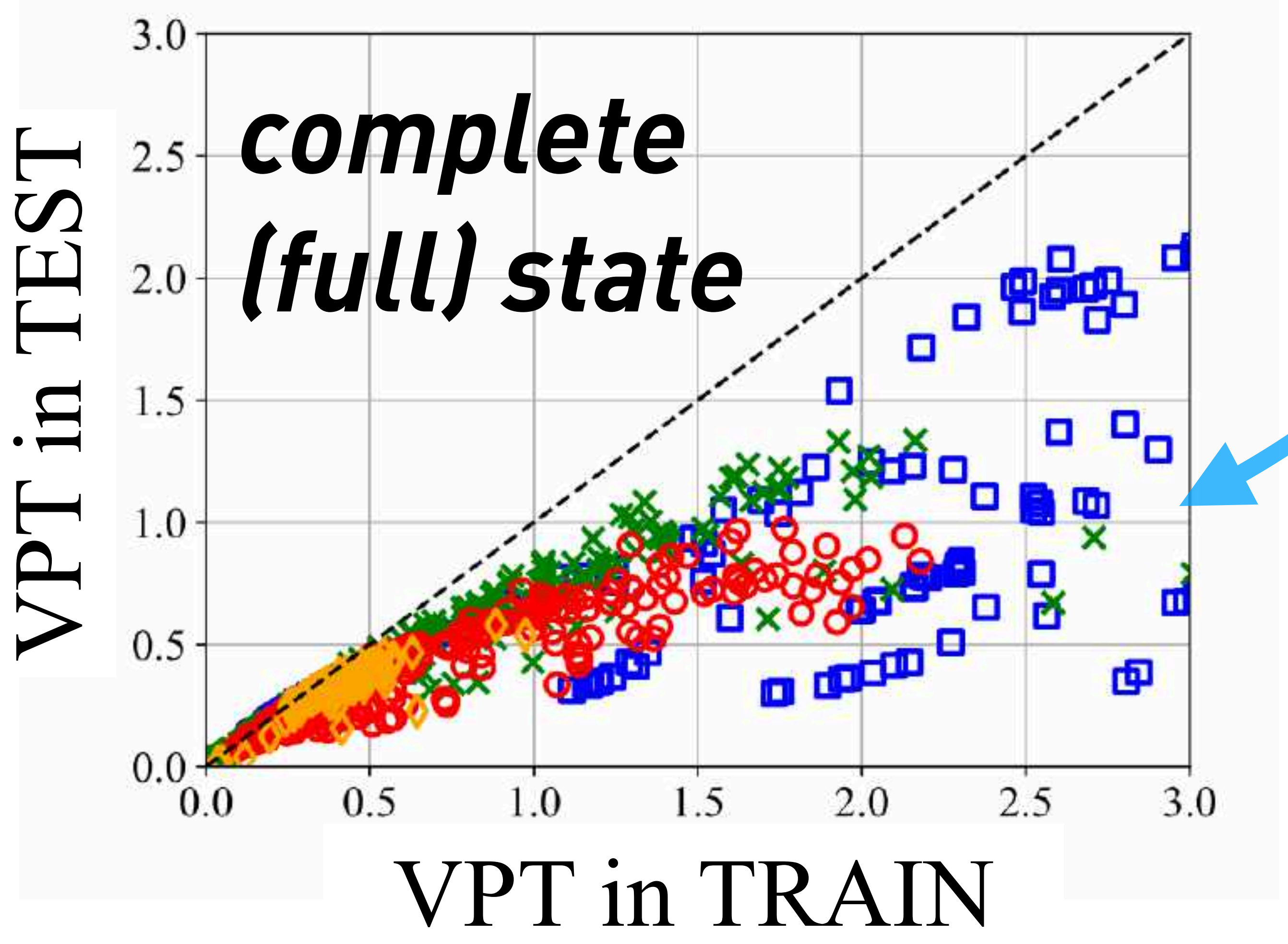

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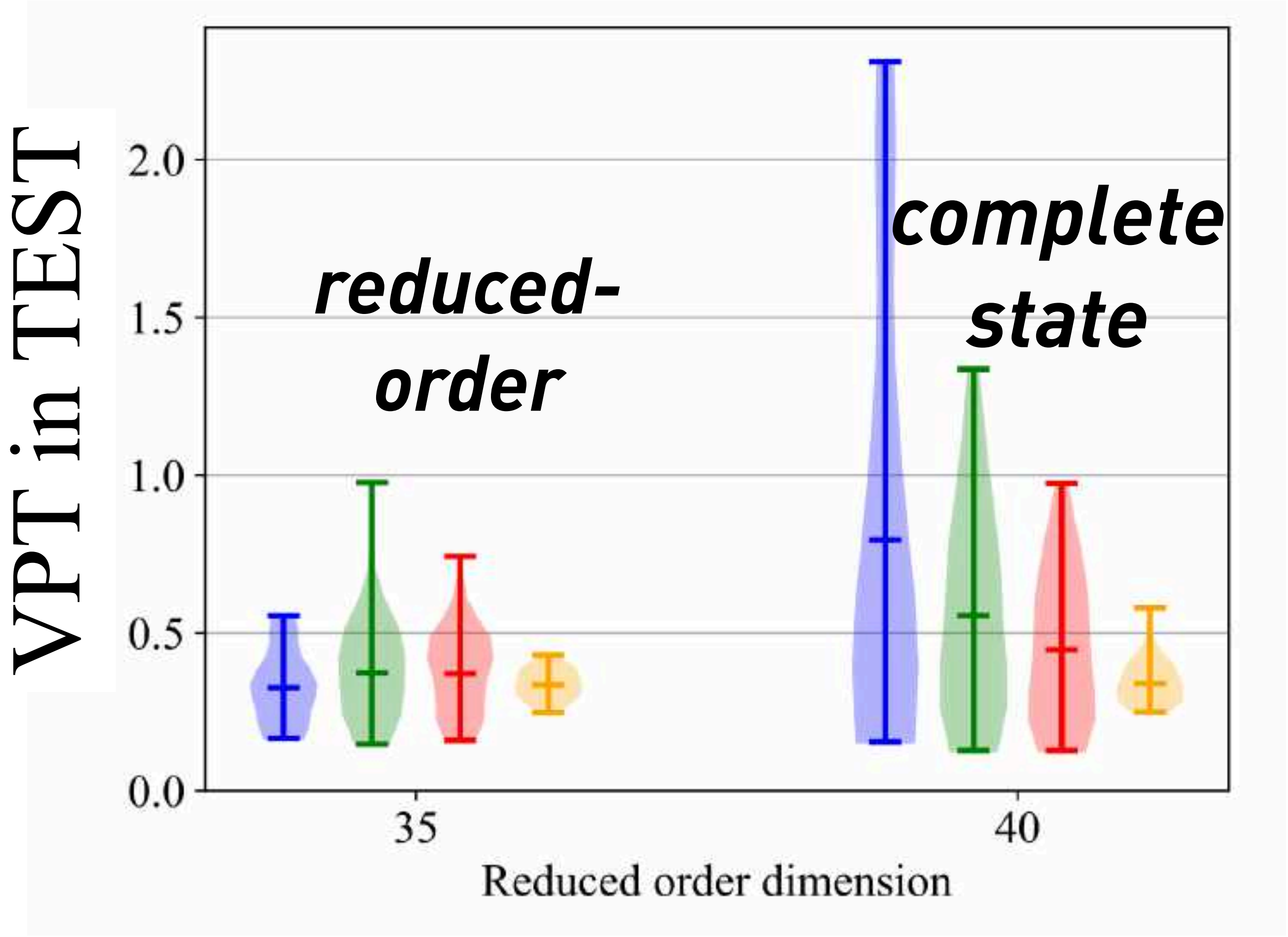

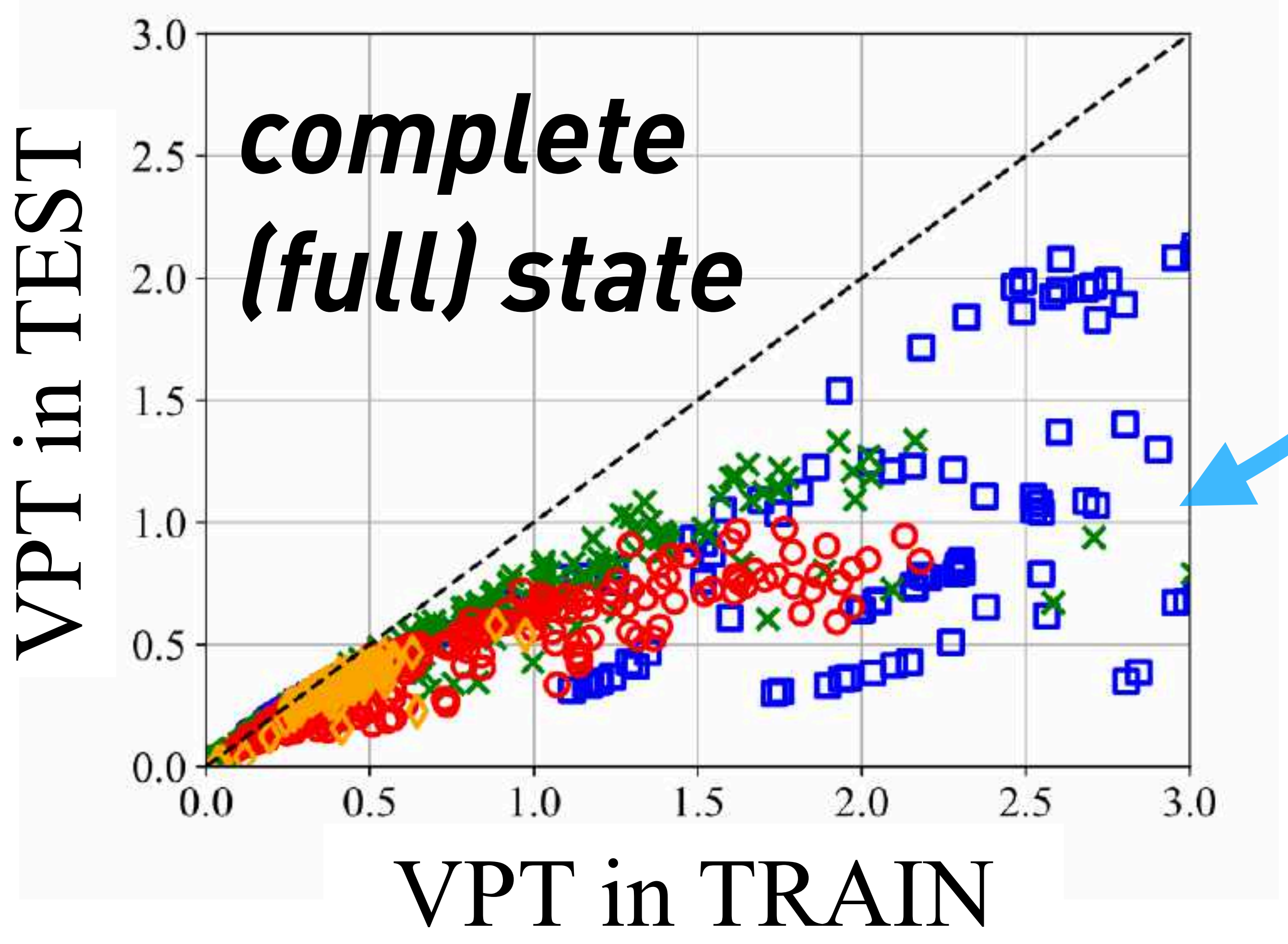

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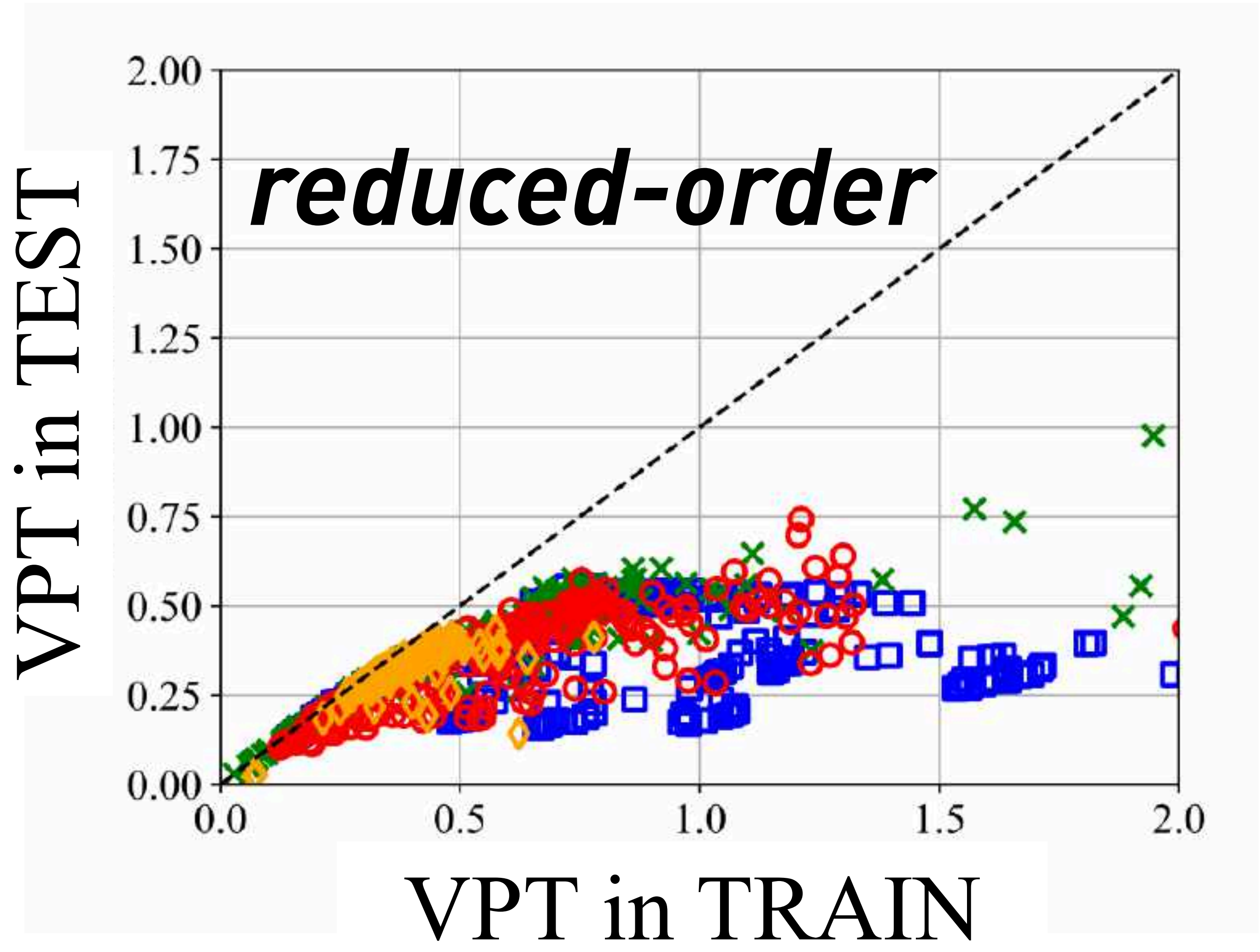

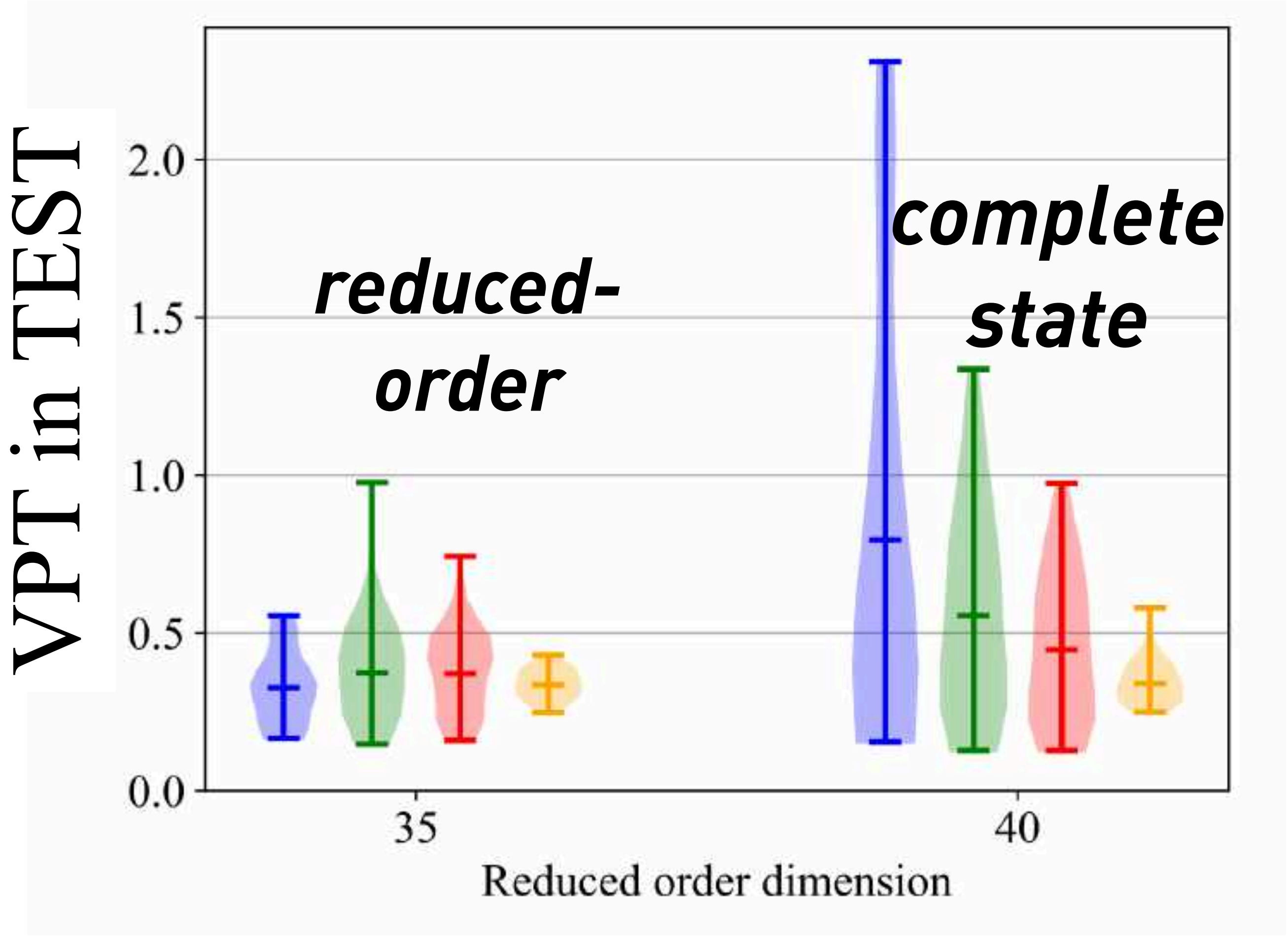

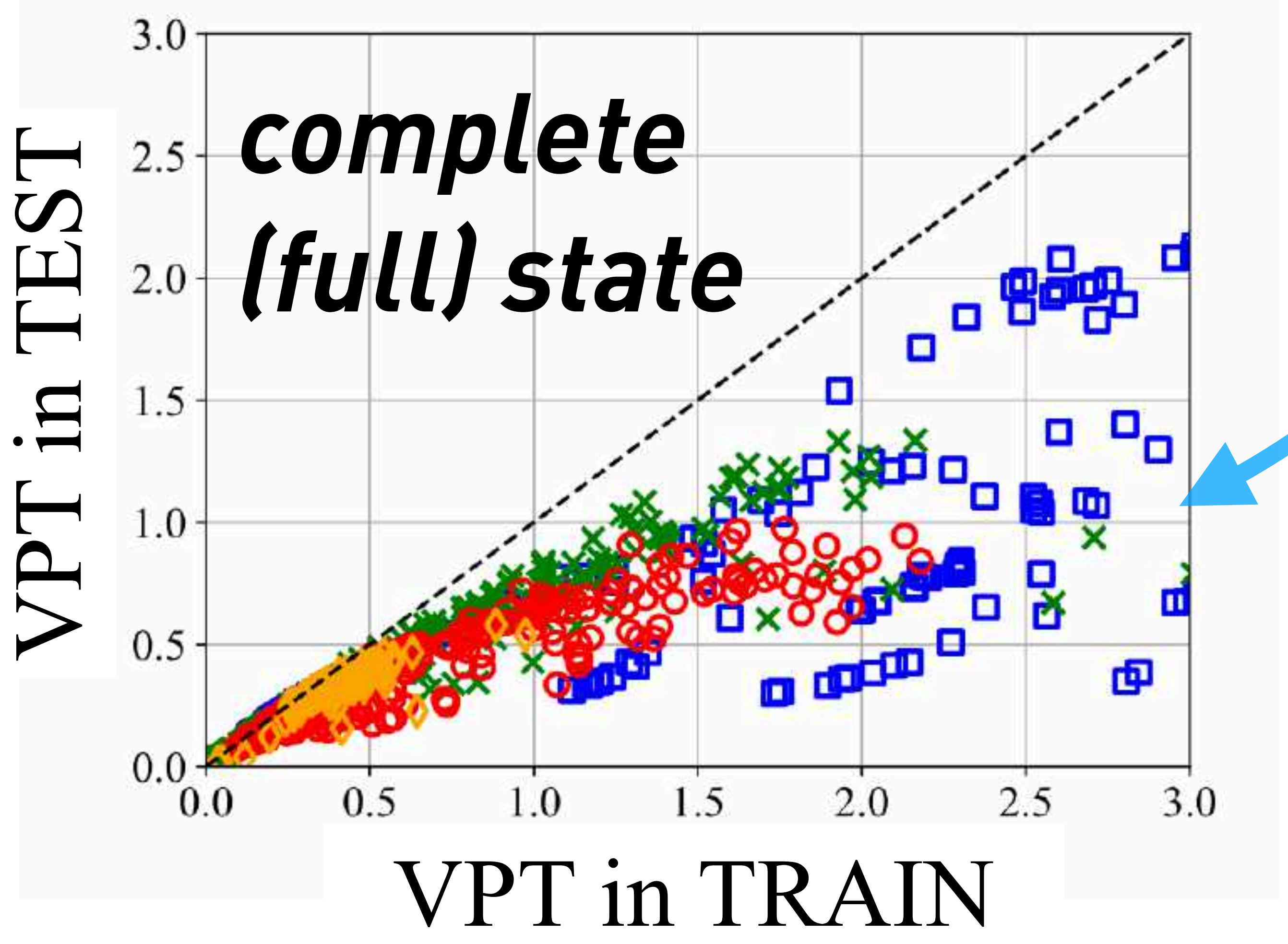

RC (or □) ; GRU (or ✕) ; LSTM (or ○) ; Unit (or ◇) ; Ideal ;

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**

- Valid prediction time $\text{VPT} = \frac{1}{T_{\Lambda_1}} \underset{t_f}{\text{argmax}} \{t_f \mid \text{NRMSE}(\mathbf{o}_t) < \epsilon, \forall t \leq t_f\}$, $\epsilon = 0.5$ here (the higher, the better)
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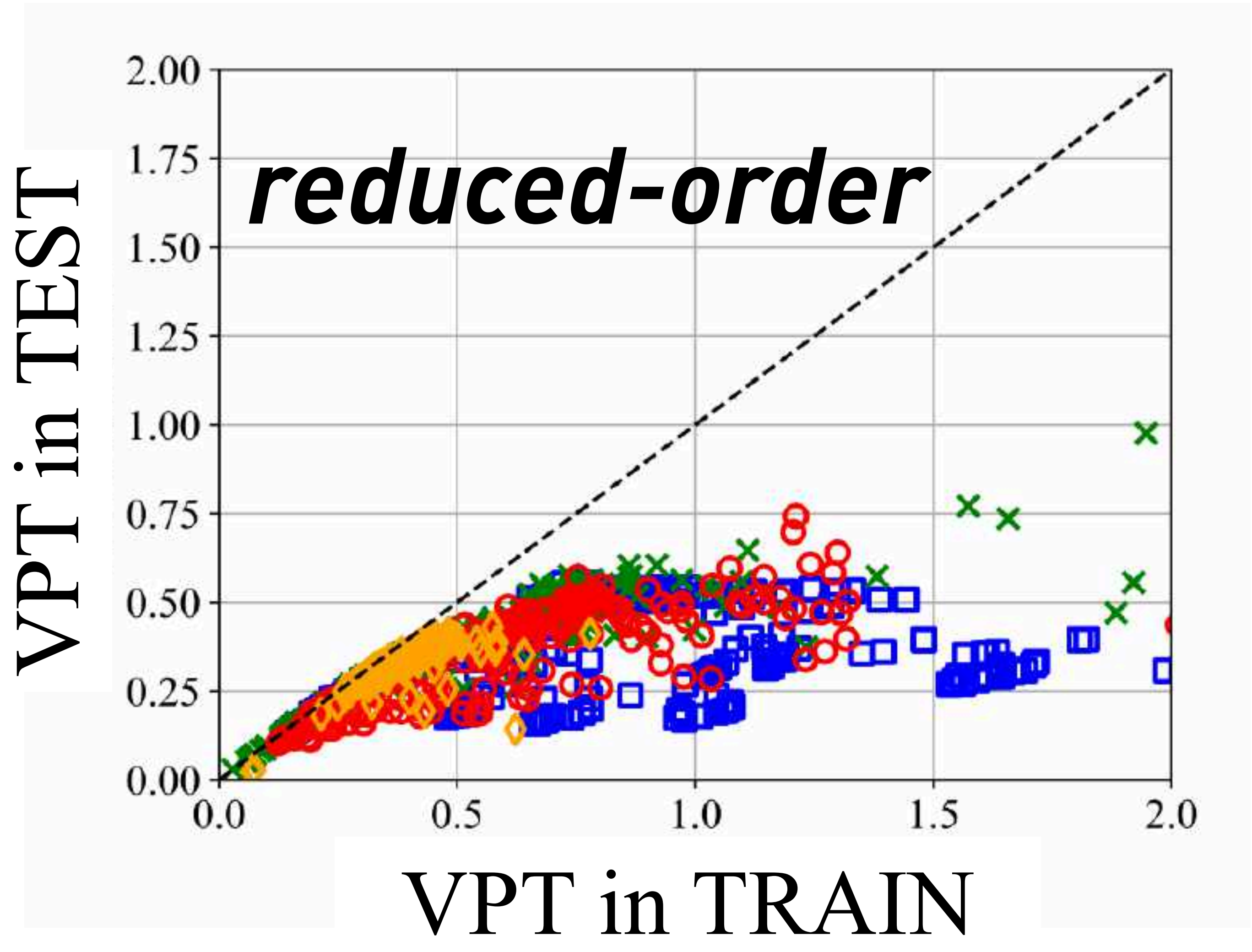
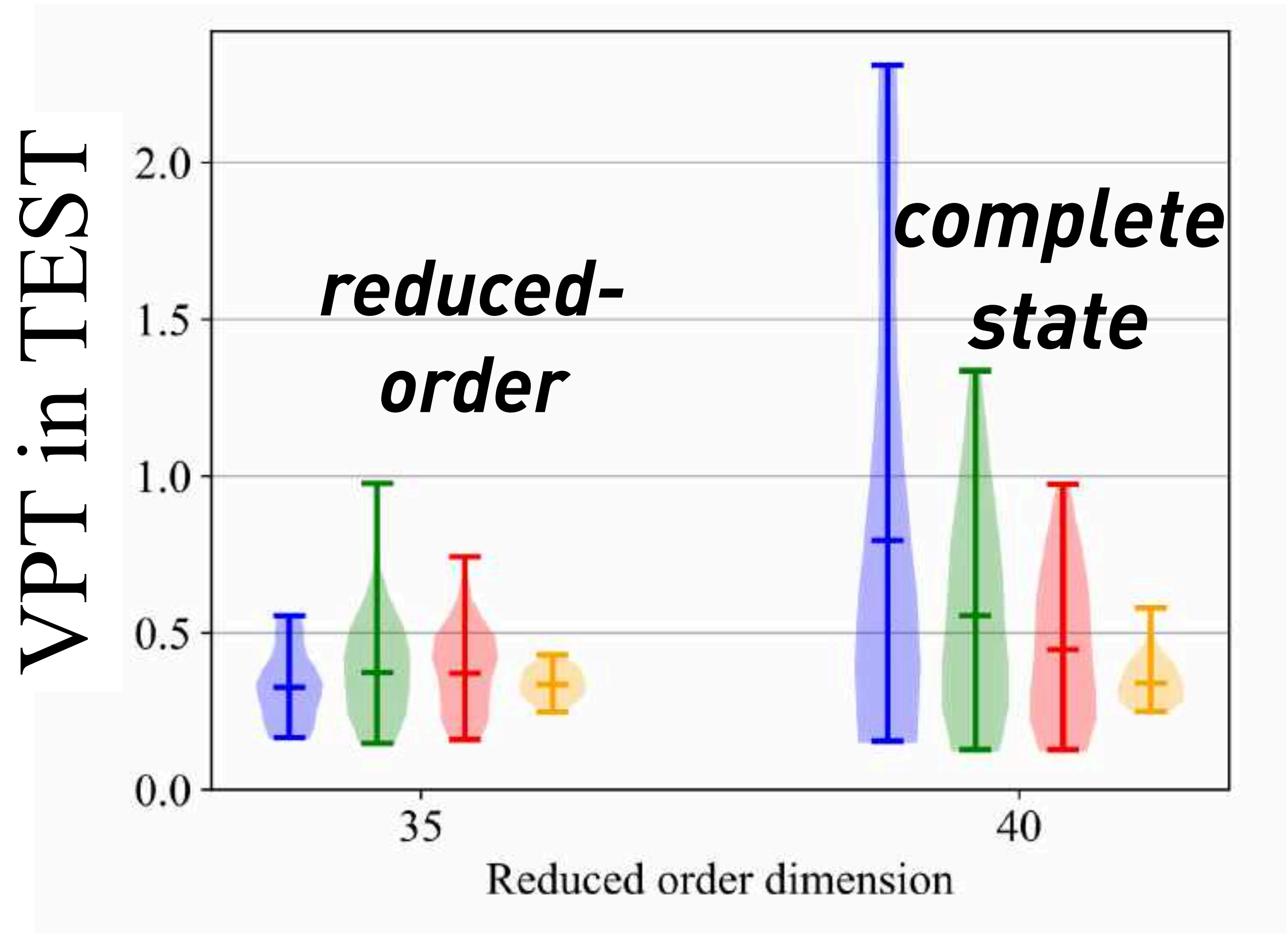
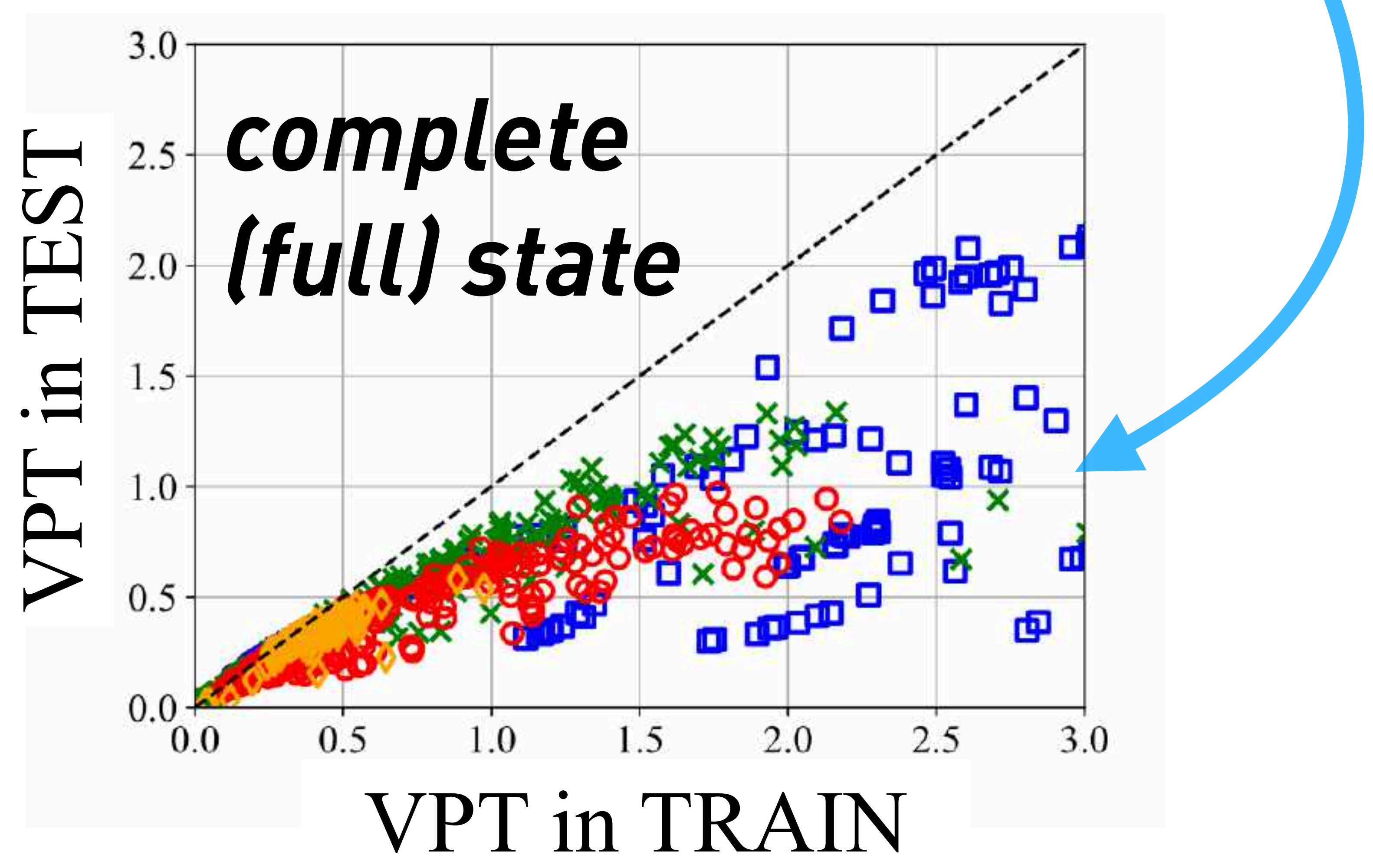
every marker is a trained model !







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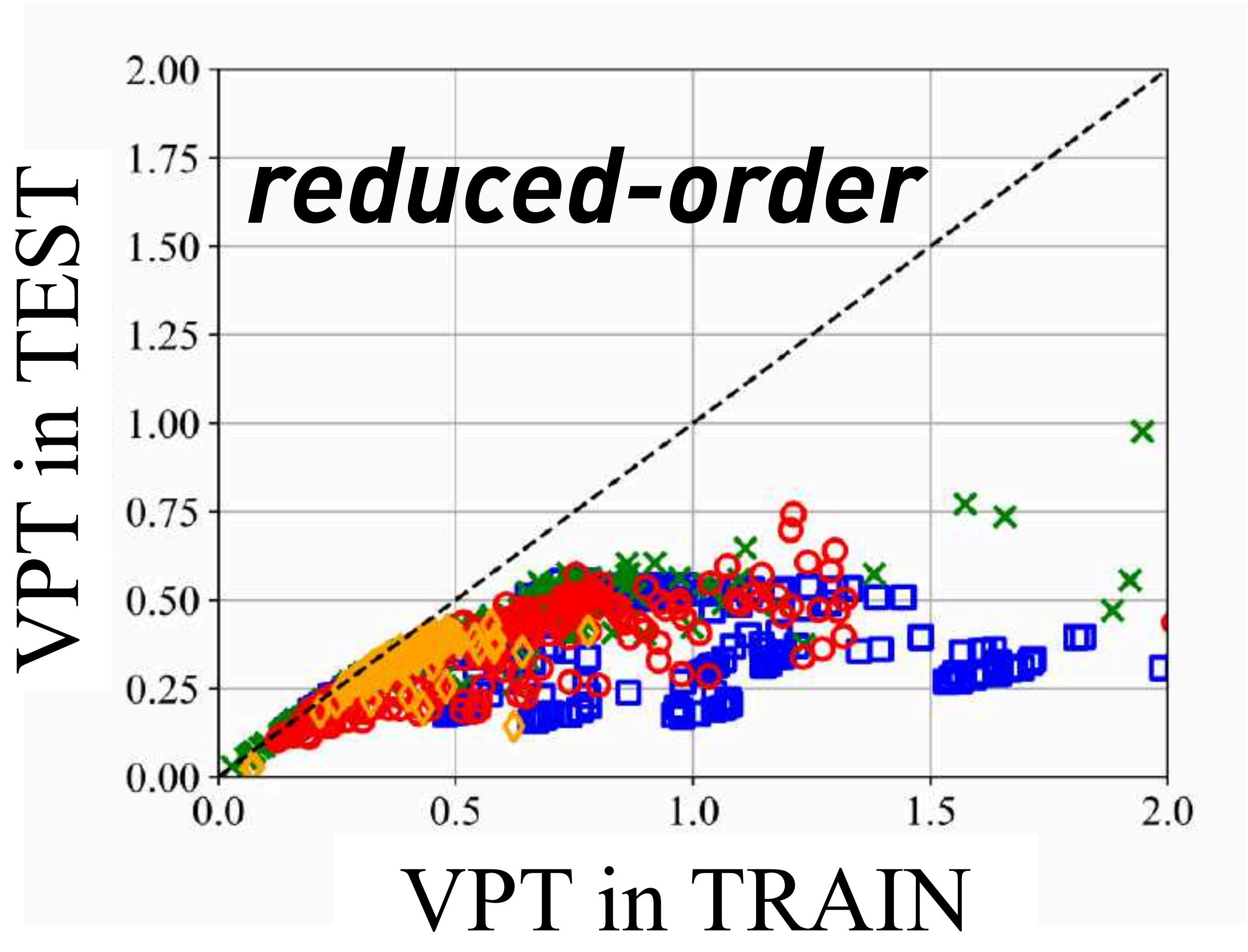

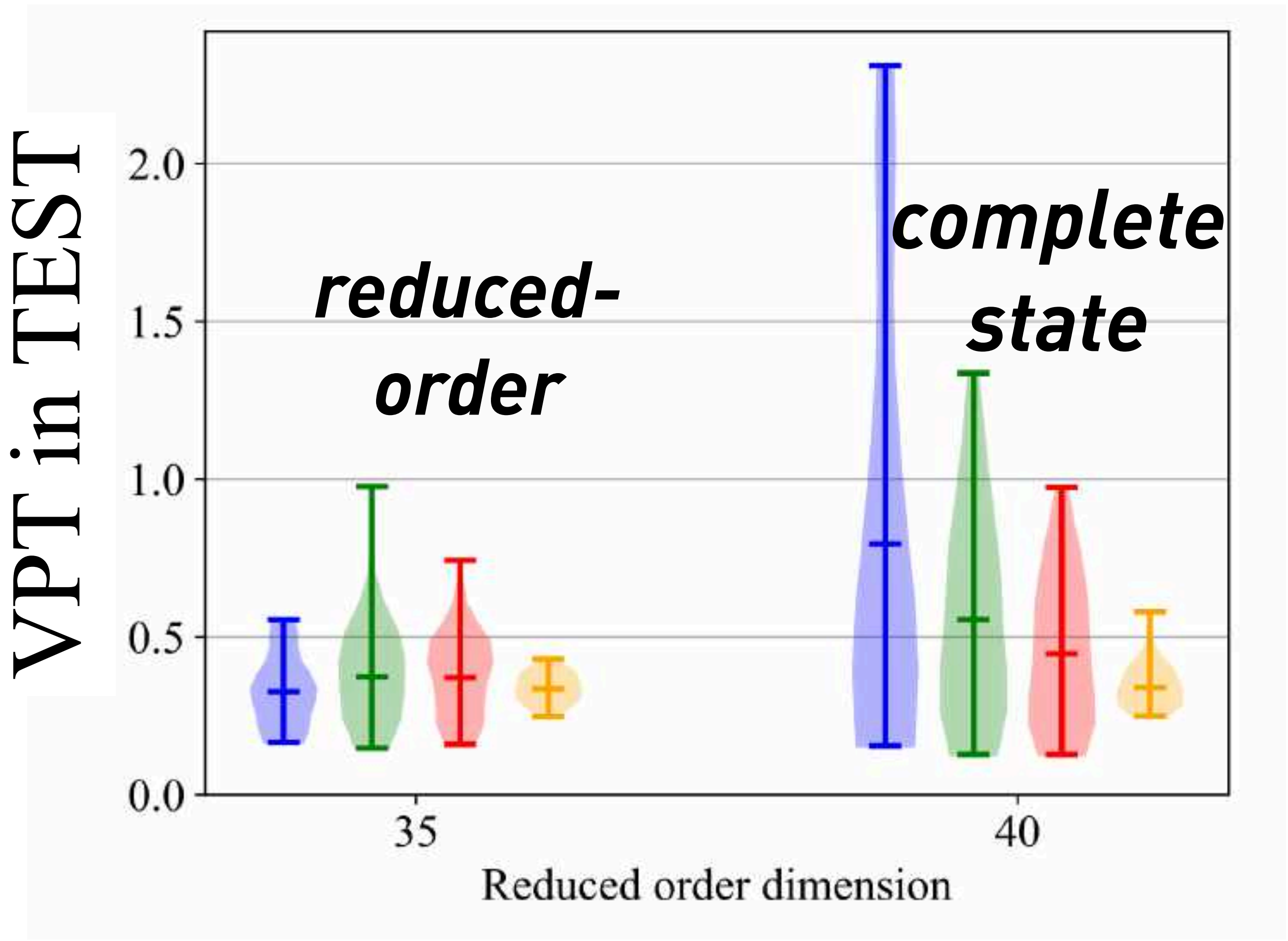

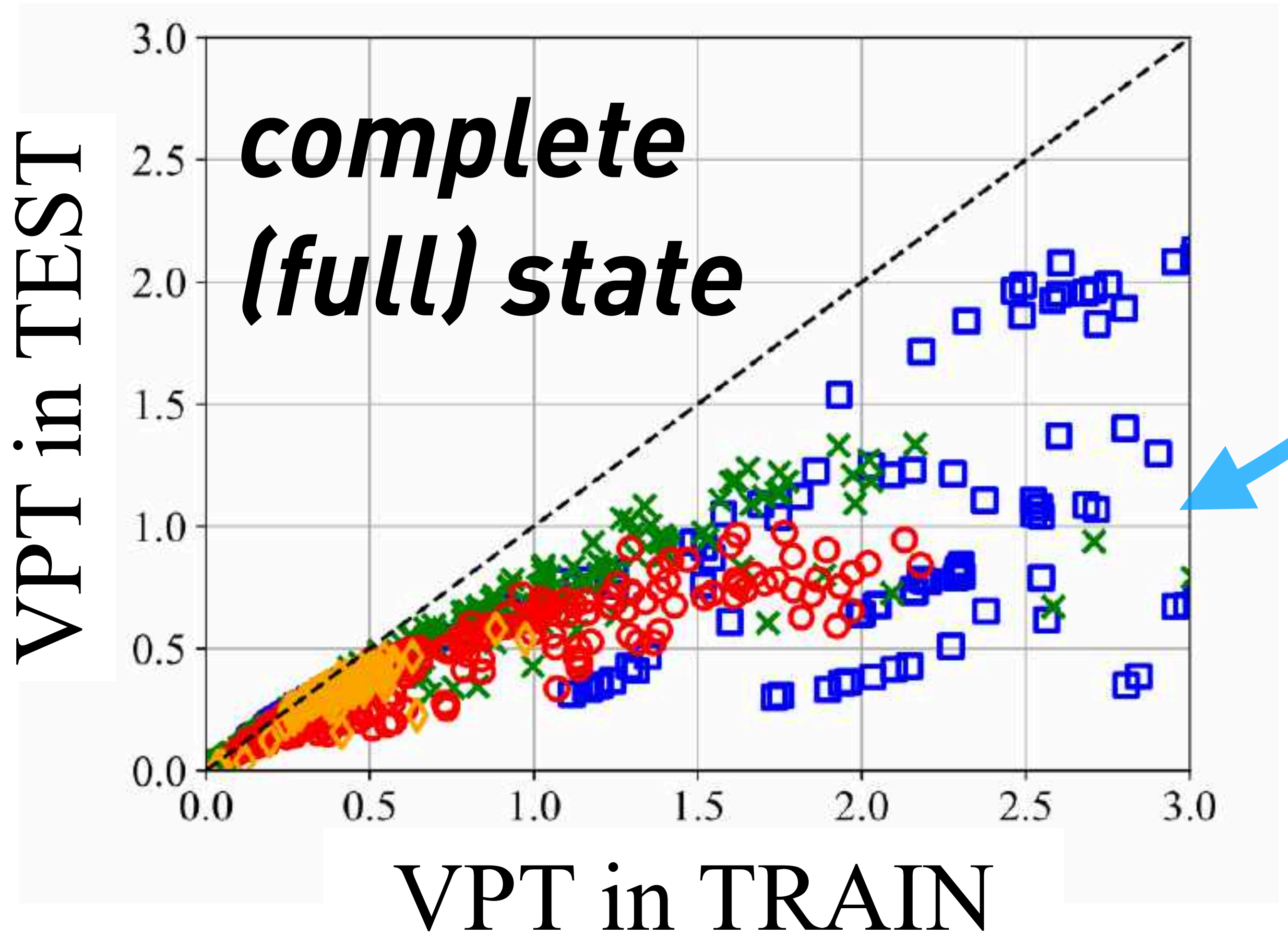

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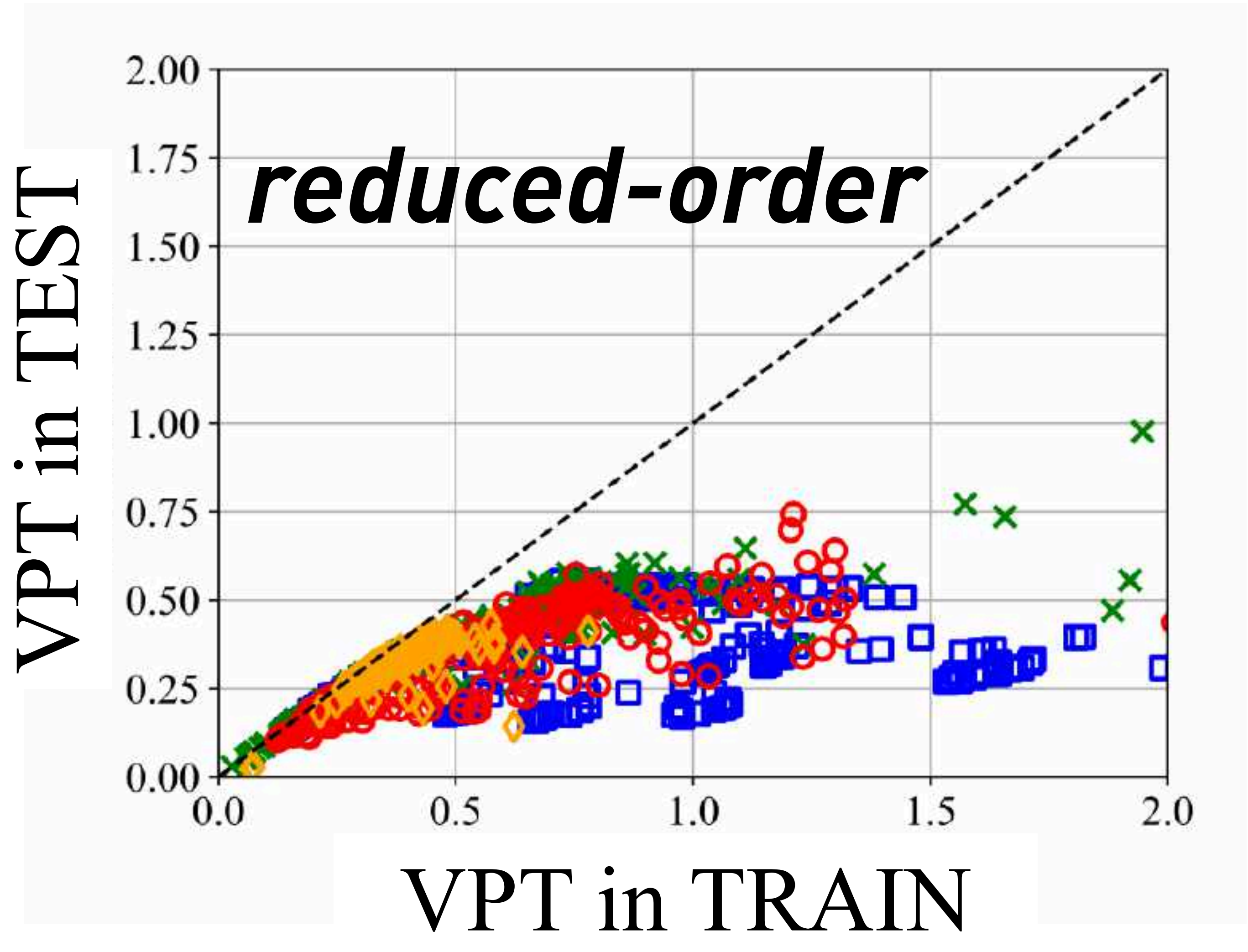

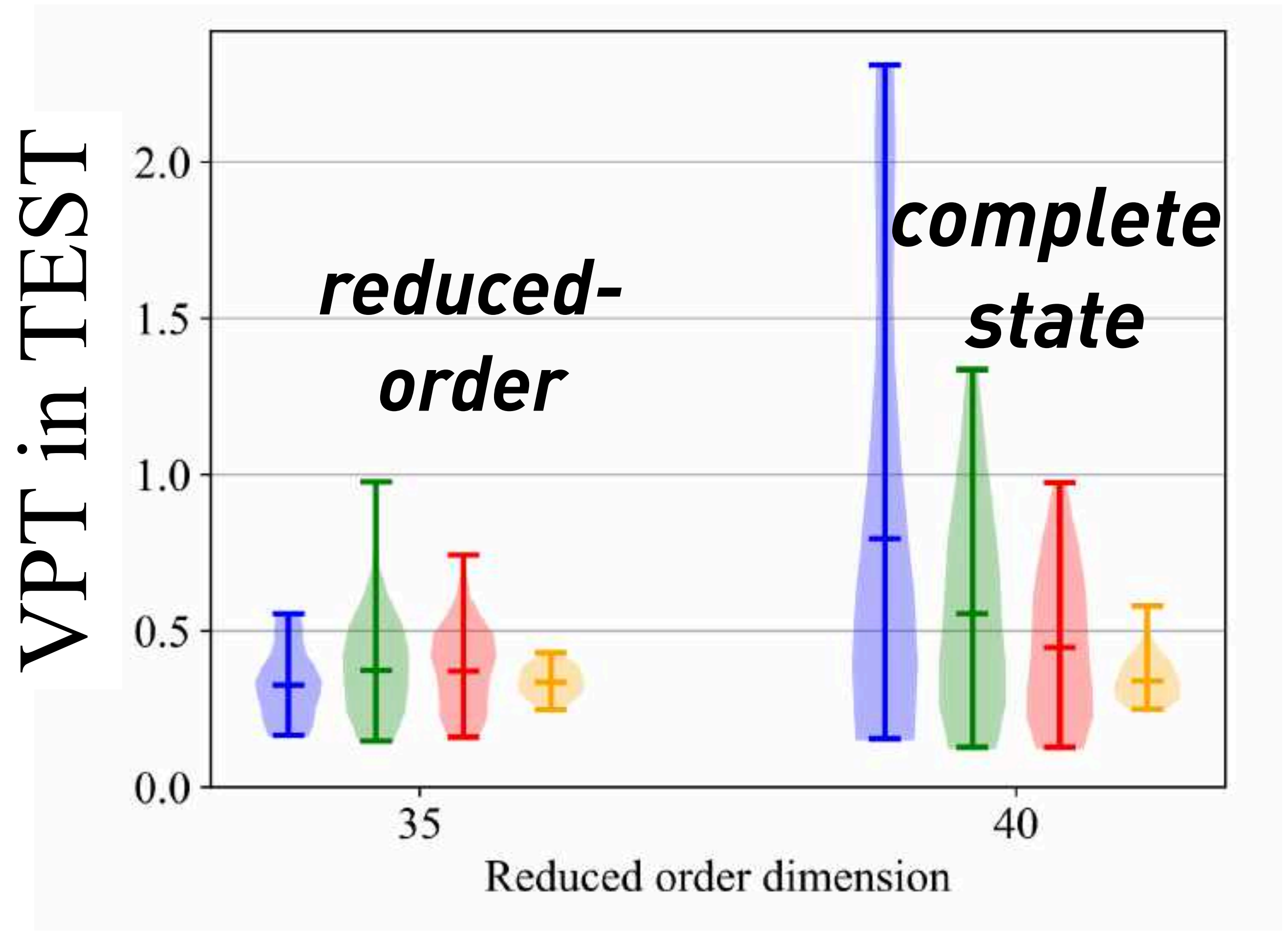

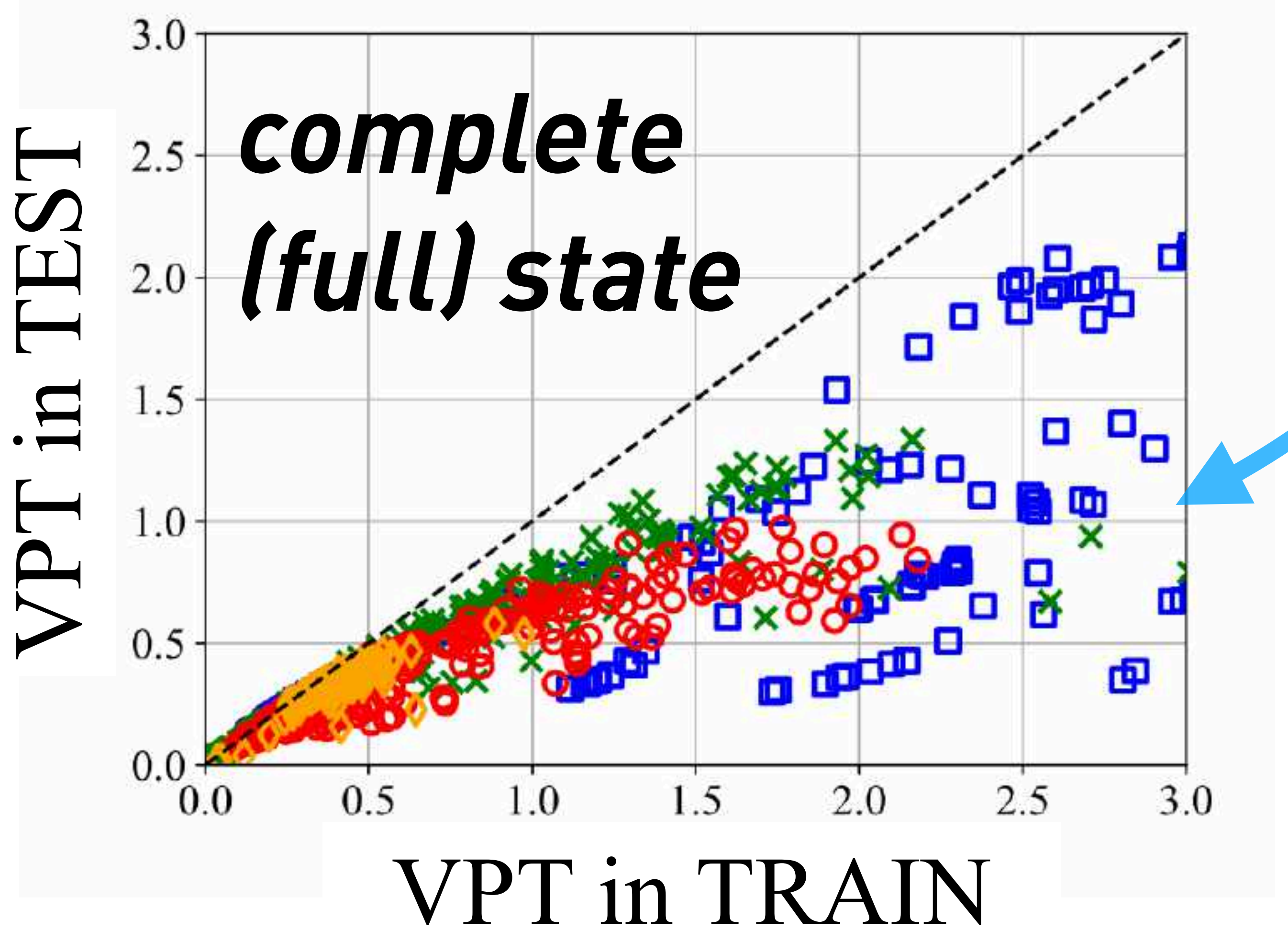

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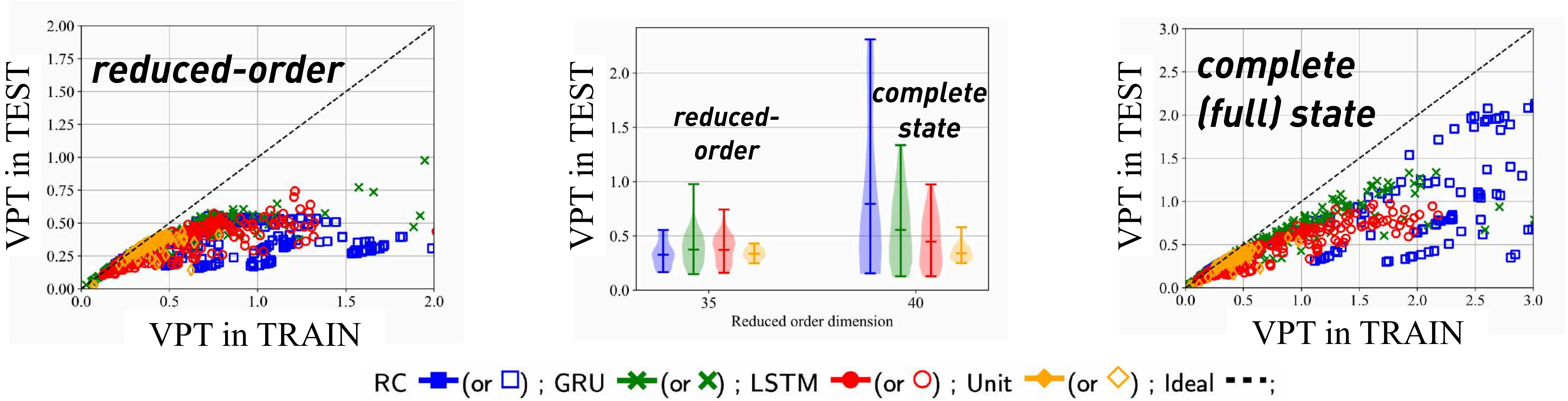
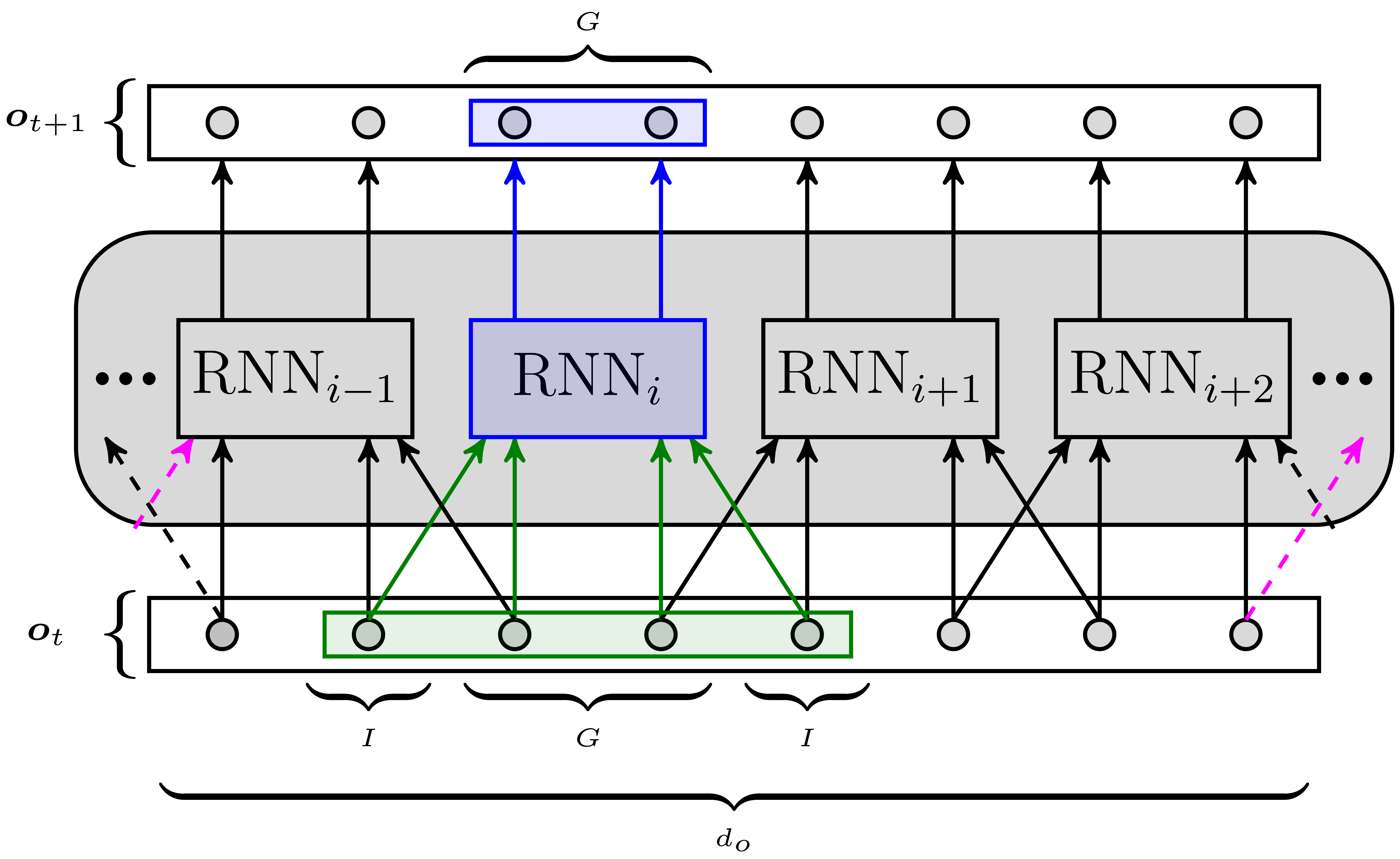


Lorenz 96, $F = 8$, *full state information & parallelism*



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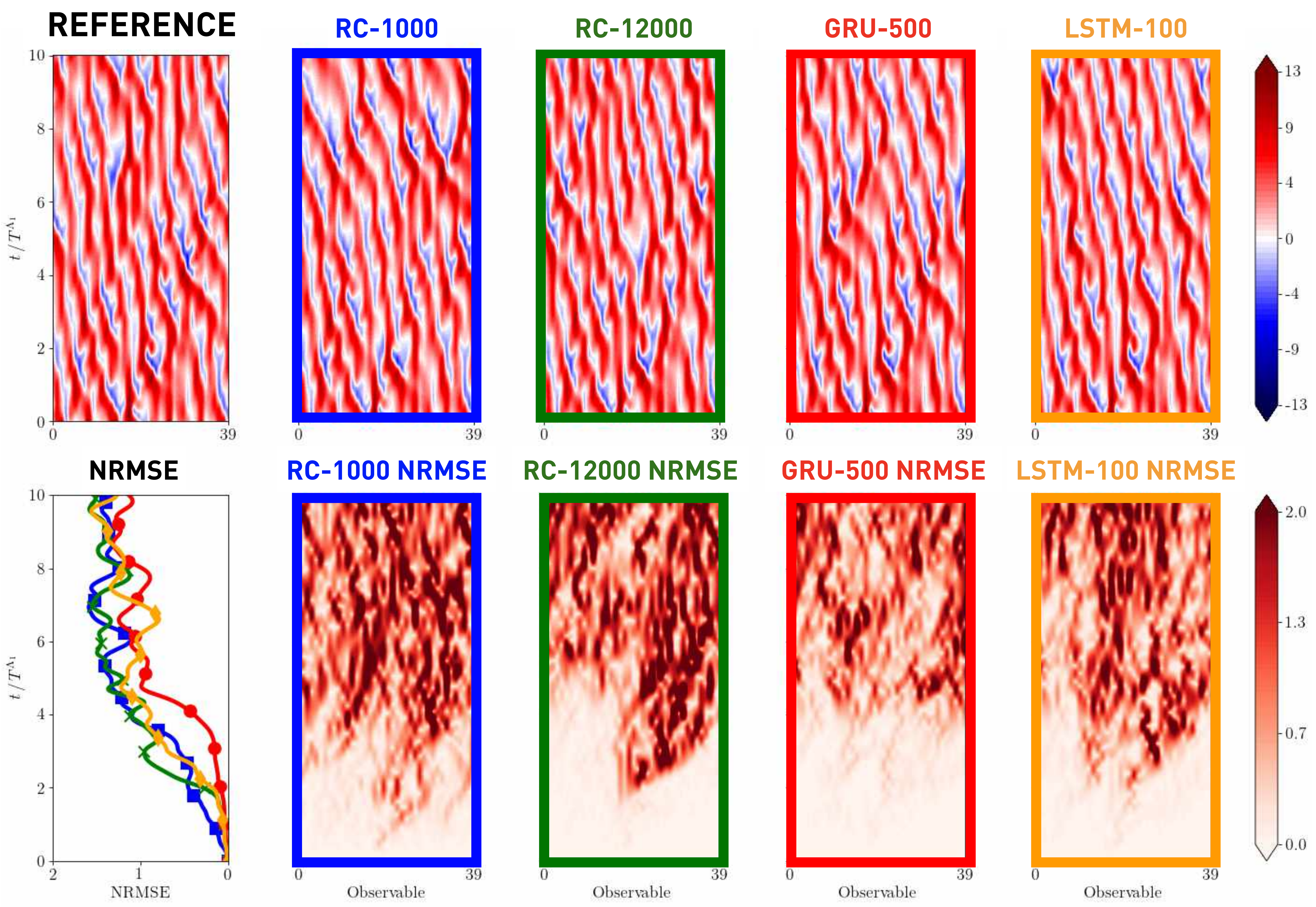

RC-1000; RC-12000; GRU-500; LSTM-100;

II

Learning Effective Dynamics

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

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- Complex Multiscale systems: ***Micro*** scale ("particles") and ***Macro*** scale ("continuum") dynamics

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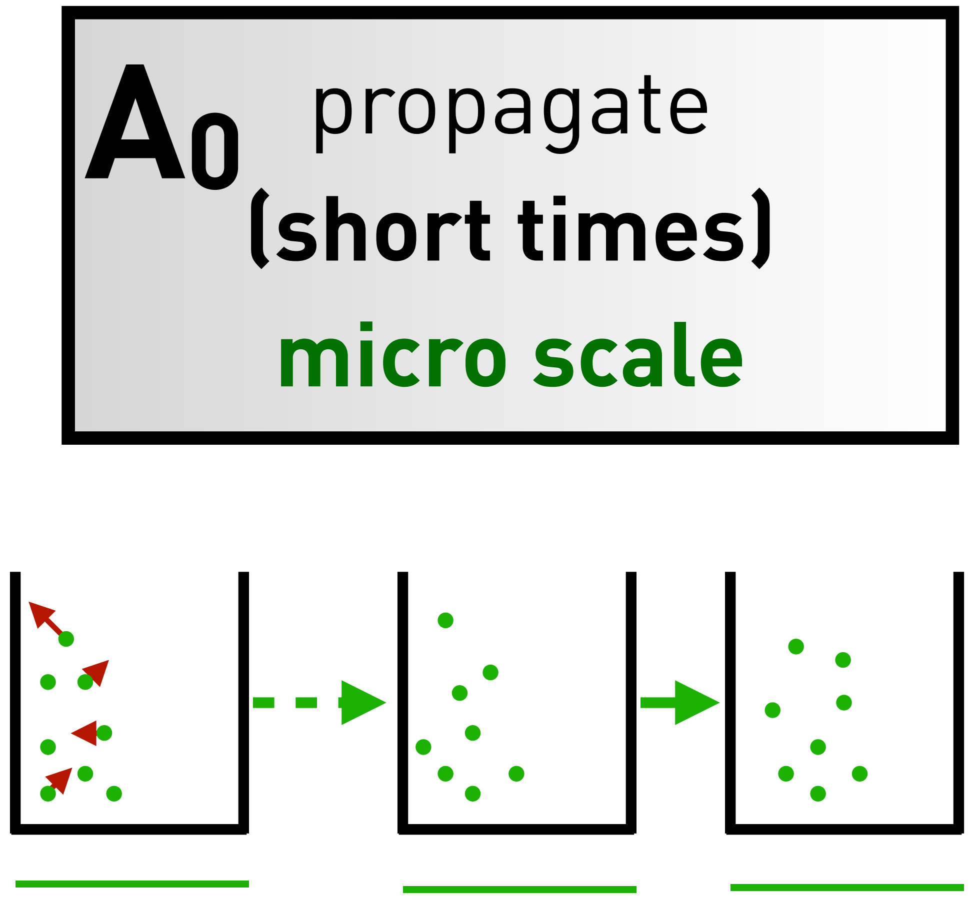
- **C Theodoropoulos, YH Qian, IG Kevrekidis,** *Coarse stability and bifurcation analysis using time-steppers: a reaction-diffusion example,* **Proc. Natl. Acad. Sci., 2000**
- **CW Gear, IG Kevrekidis, C Theodoropoulos,** *Coarse integration/bifurcation analysis via microscopic simulators: micro-Galerkin methods,* **Computers and Chemical Engineering, 2002**

AND MANY MANY MORE …

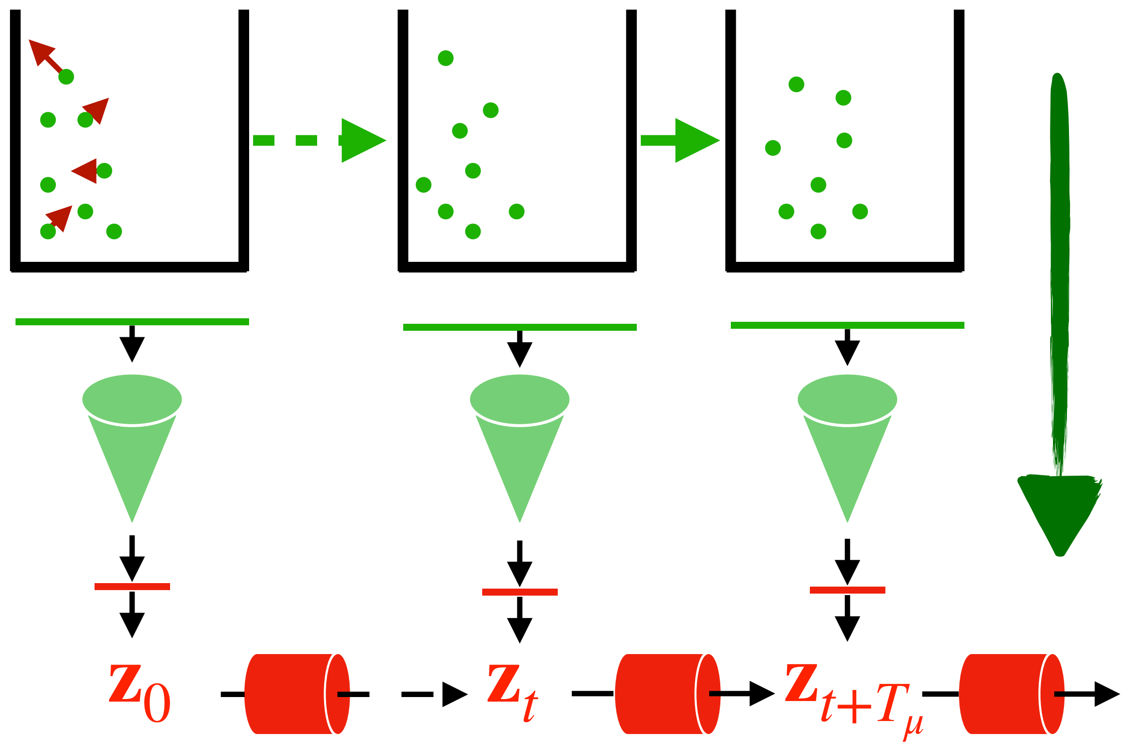
Equation Free Framework



A

Equation Free Framework

A0 propagate
(short times)
micro scale



B0 initialise
macro scale

Equation Free Framework

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

A0 propagate
(short times)
micro scale

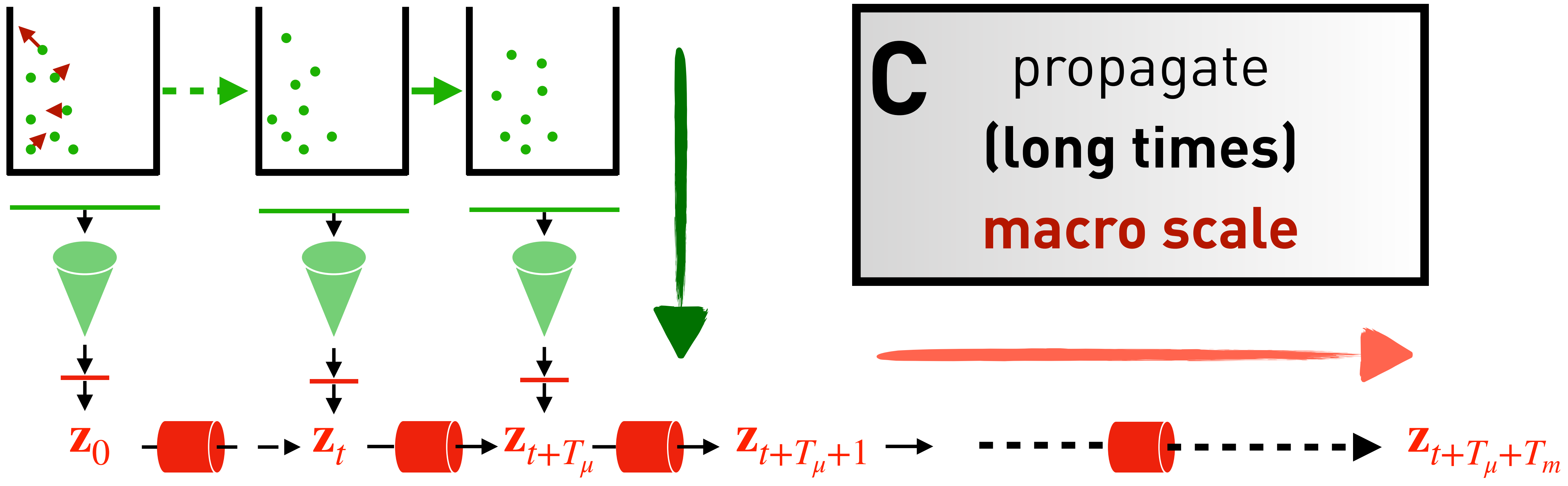
RESTRICTING /AVERAGING
(micro → macro)
e.g. PCA / DiffMaps / analytic

B

macro dynamics propagator
e.g. ODE / analytic

A → **B** → **C**

C propagate
(long times)
macro scale



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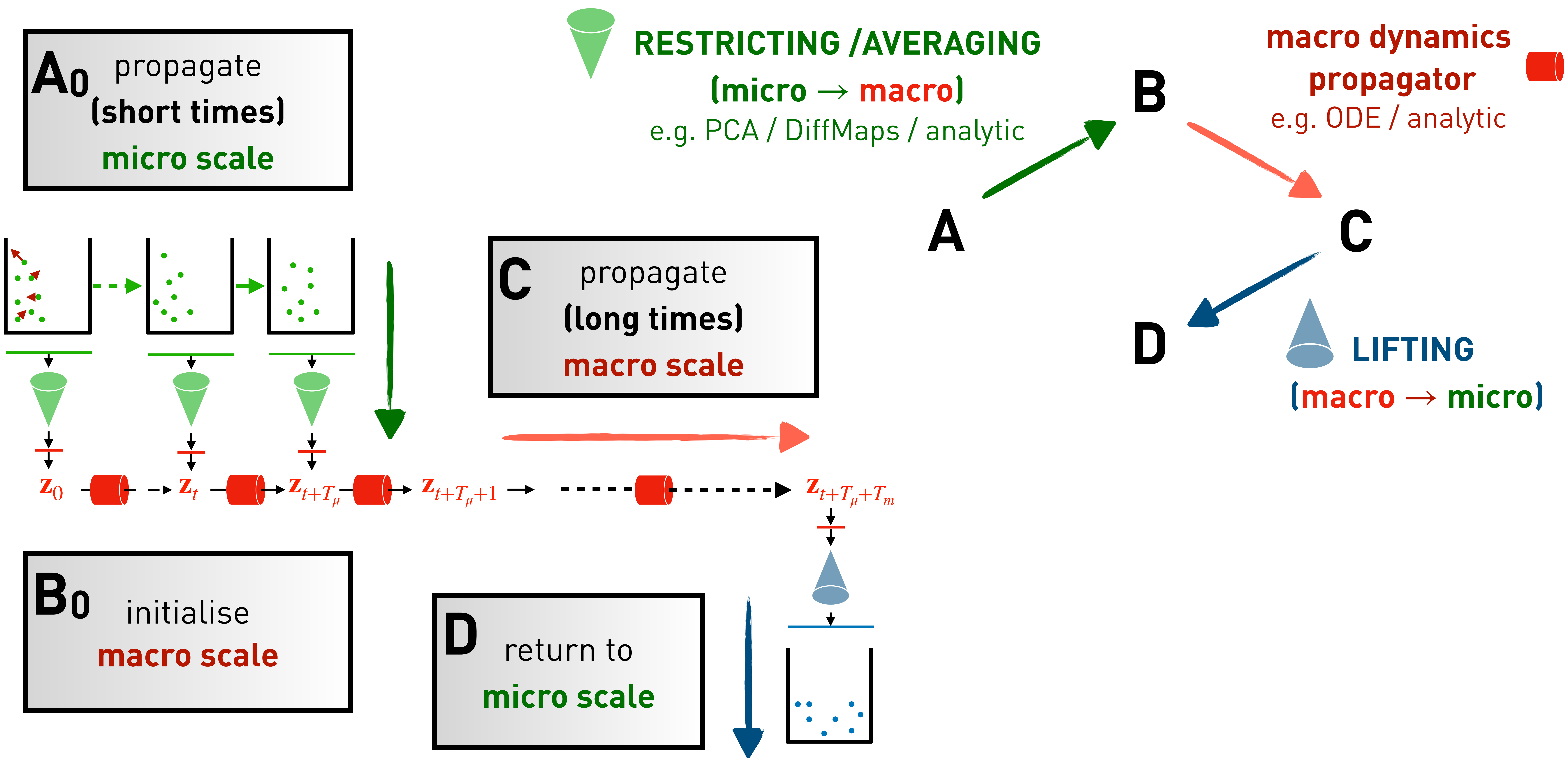

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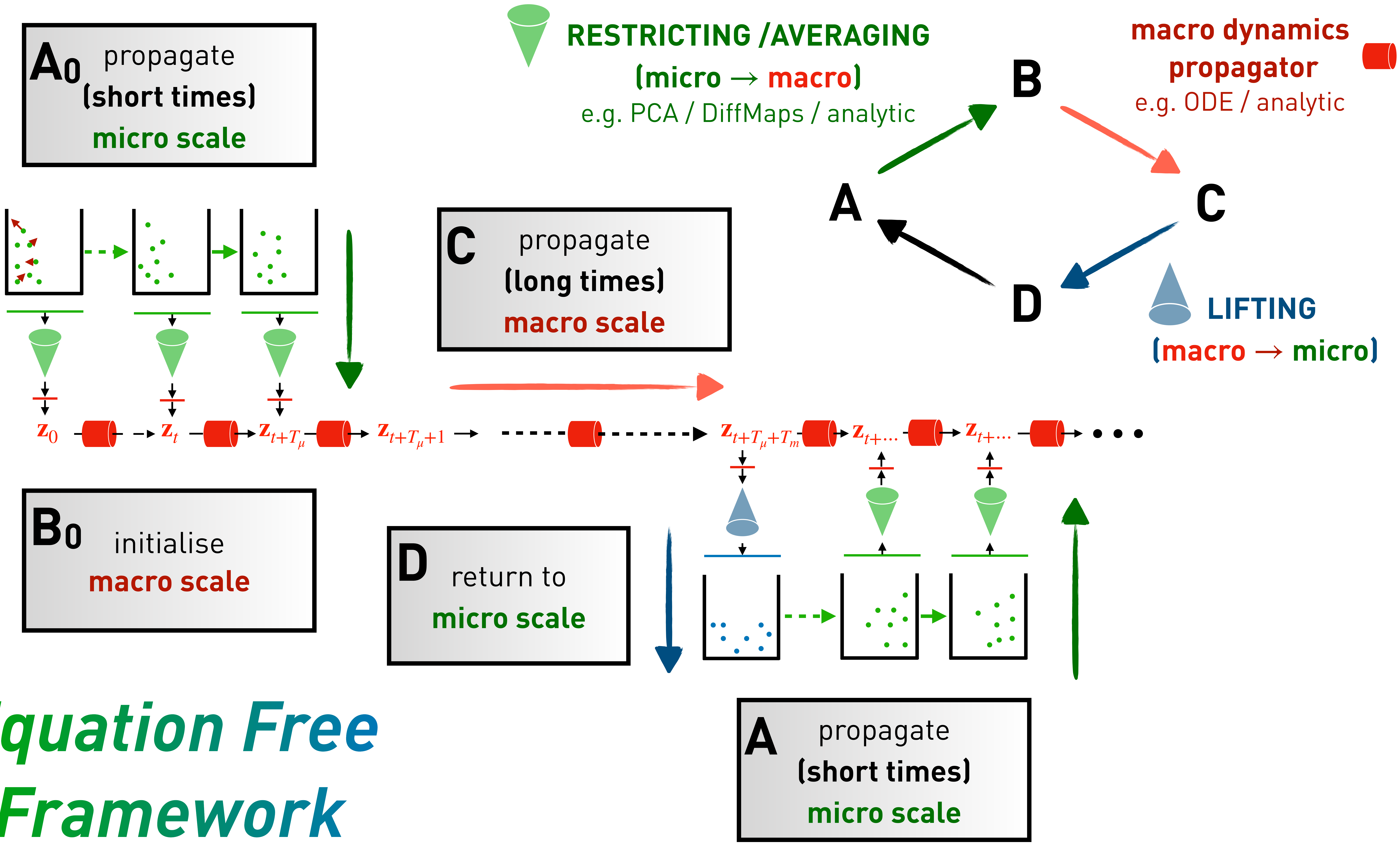

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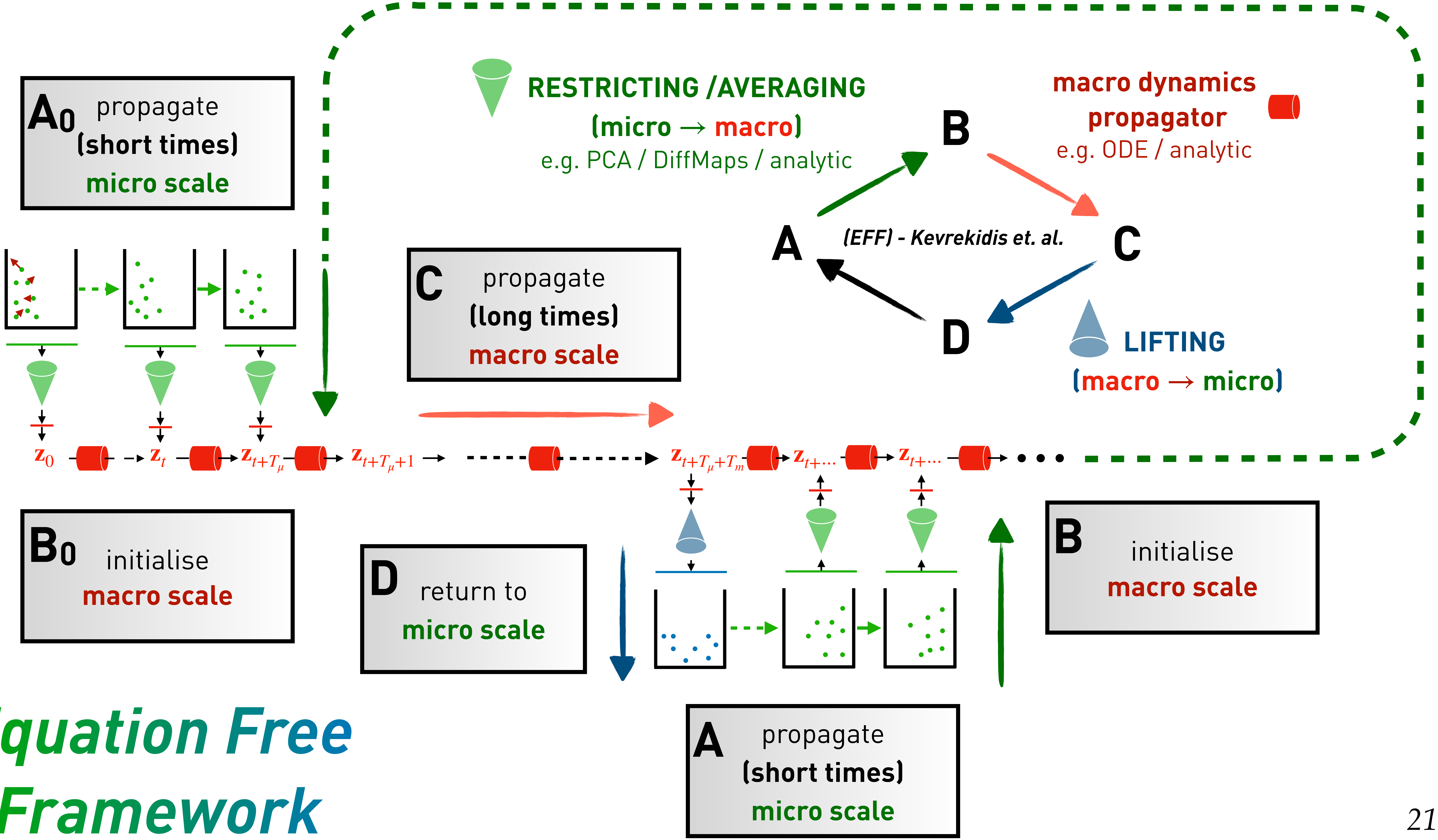

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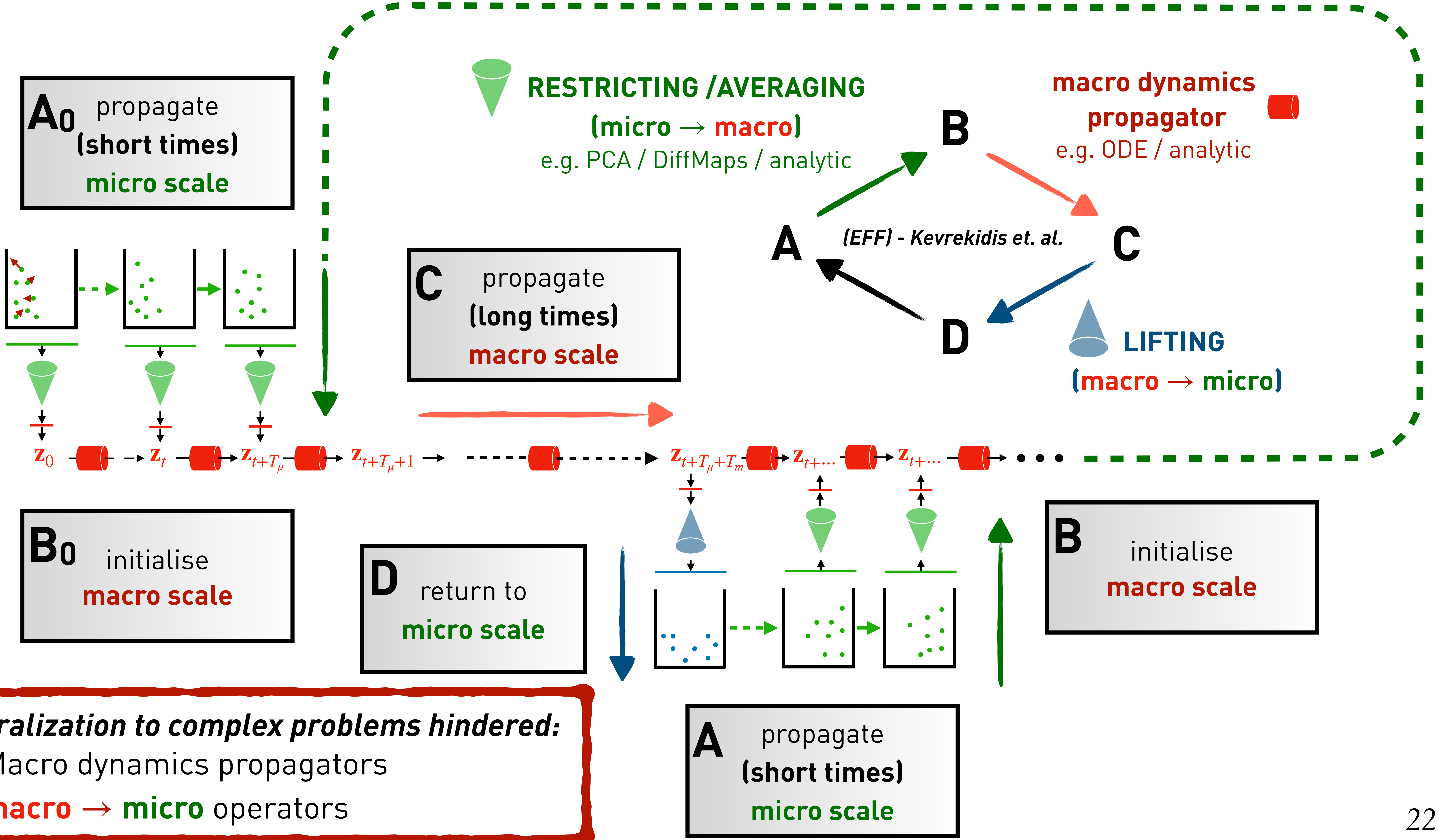


Generalization to complex problems hindered:

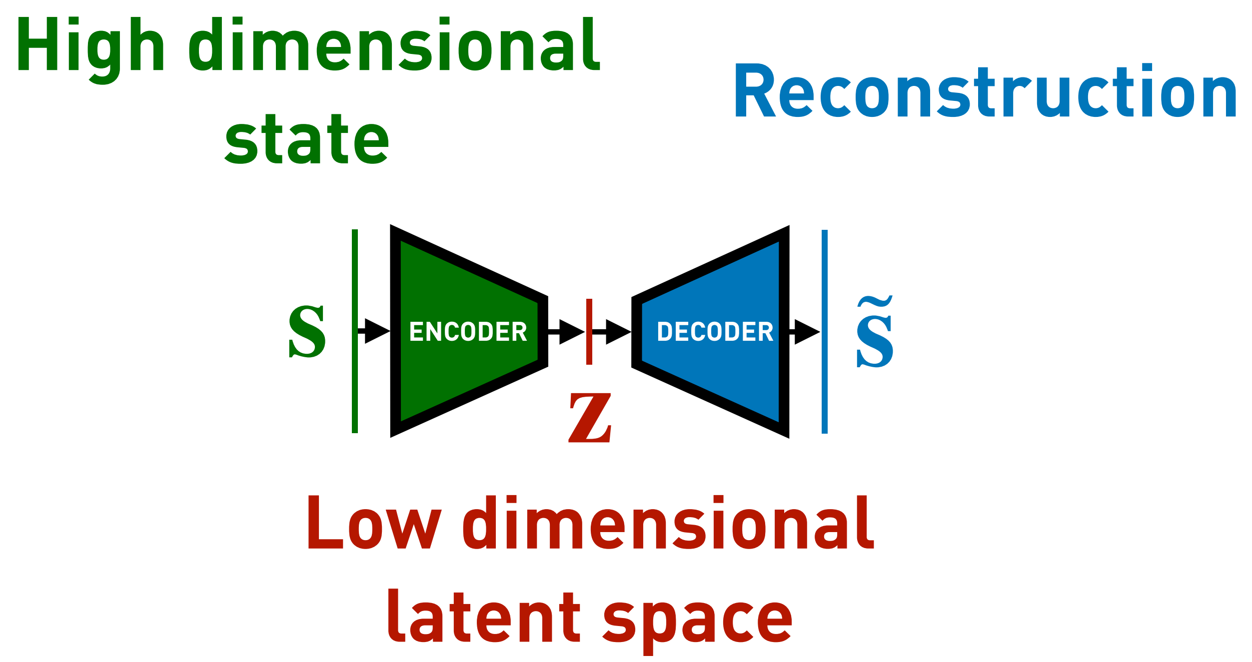
A. Macro dynamics propagators

B. **macro → micro** operators

Operators from Machine Learning

Operators from Machine Learning

(CONVOLUTIONAL) AUTOENCODERS

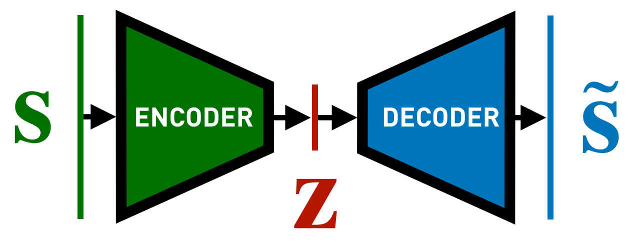


- Full high dimensional description of dynamical system system $\mathbf{s}$
- e.g. positions of atoms / micro scale / angles, bonds
- Loss Function $\mathscr{L} = |\mathbf{s} - \tilde{\mathbf{s}}|_2^2$
- Ideally after training $\mathbf{s} \approx \tilde{\mathbf{s}}$

Operators from Machine Learning

(CONVOLUTIONAL) AUTOENCODERS

High dimensional state **Reconstruction**



Low dimensional latent space

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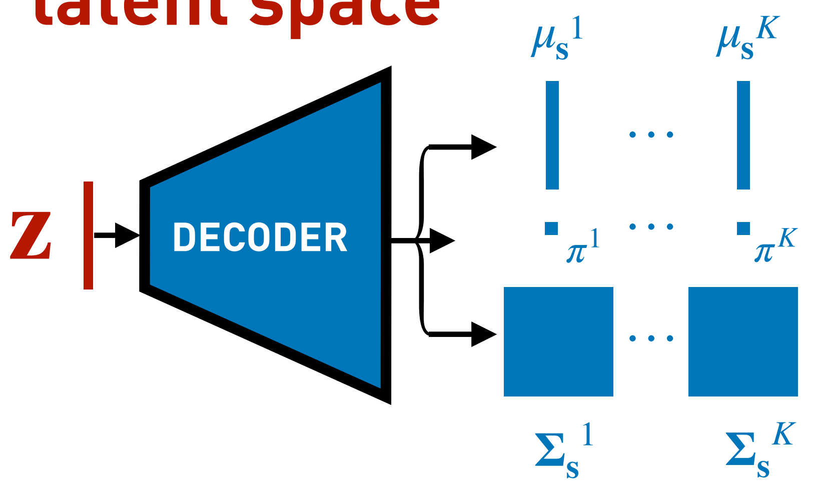
MIXTURE DENSITY NETWORKS

Low dimensional latent space



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

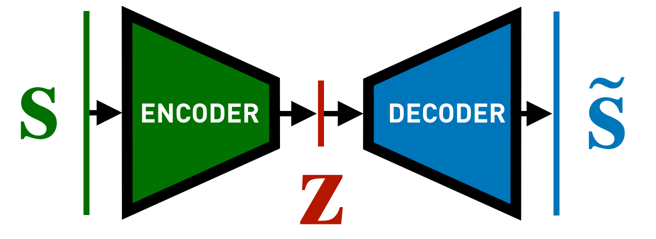
- Coarse (latent) representation has limited information
- Mapping $\mathbf{z} \to \mathbf{s}$ can be probabilistic !
- Generative network
- $p(\mathbf{s}\,|\,\mathbf{z})$ as **mixture model**
- $$p(\mathbf{s}\,|\,\mathbf{z}) = \sum_{k=1}^{K} \pi_k \mathcal{N}\left(\mu_{\mathbf{s}}^k, \Sigma_{\mathbf{s}}^k\right)$$

Operators from Machine Learning

(CONVOLUTIONAL) AUTOENCODERS

High dimensional state

Reconstruction



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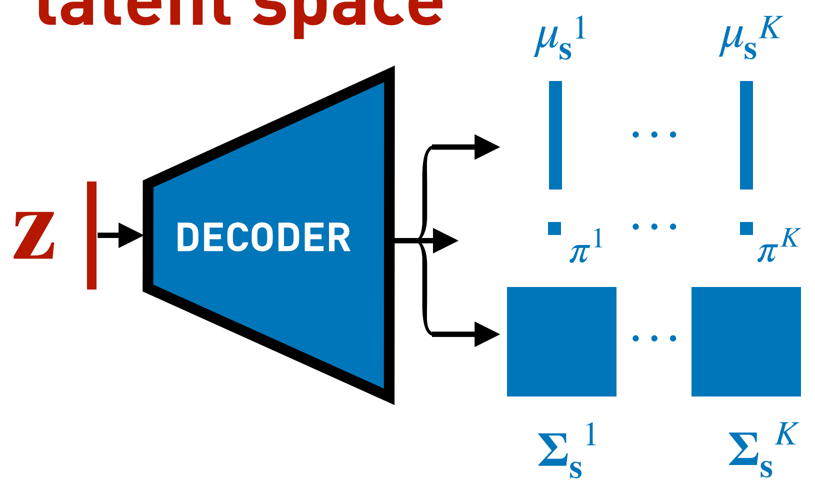

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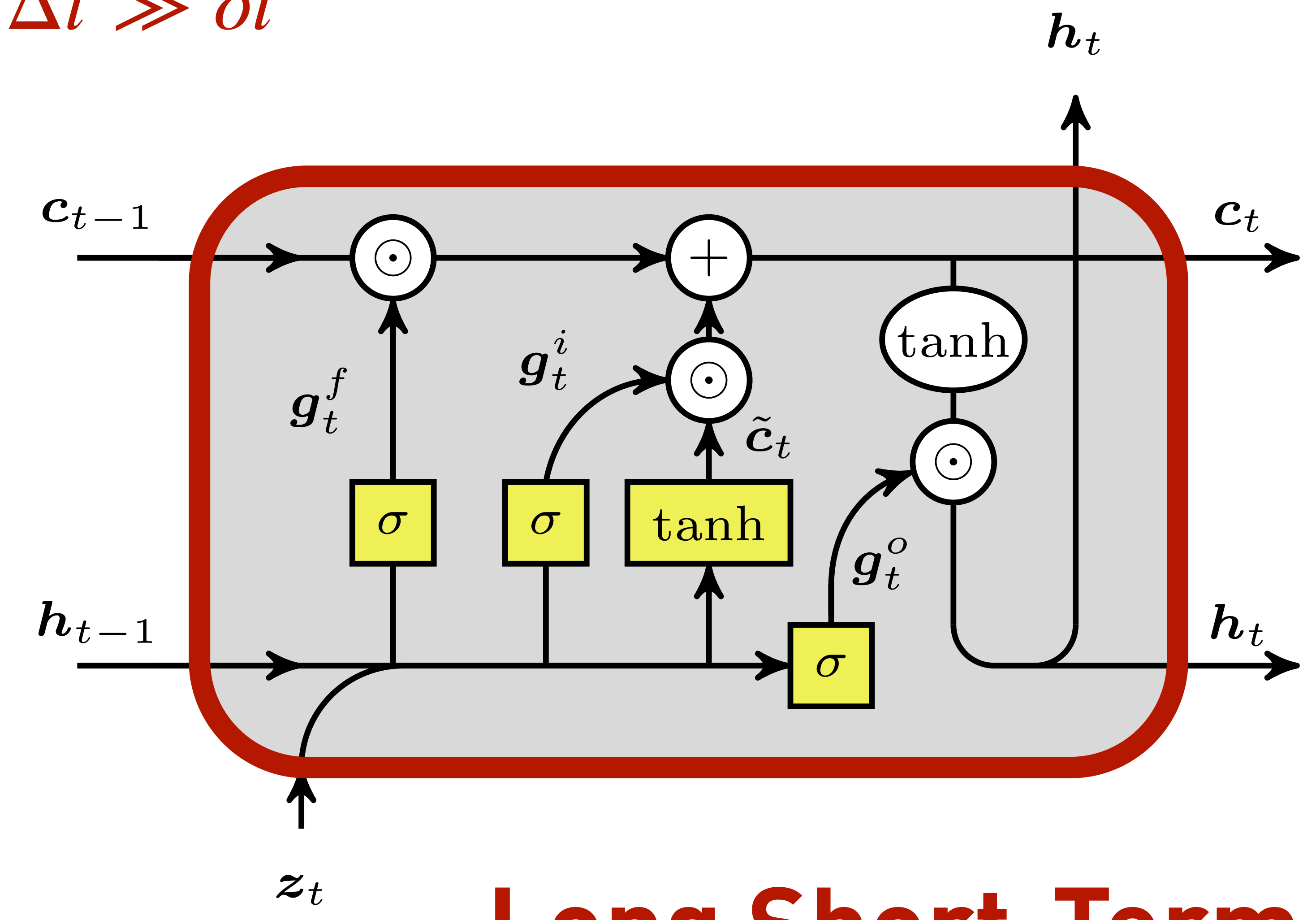


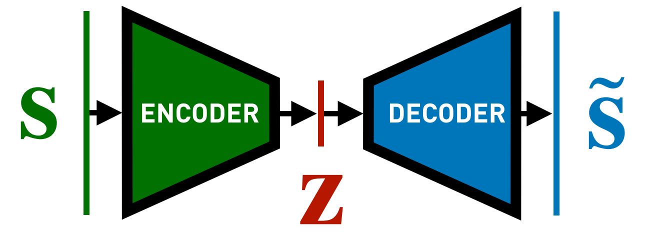
Long Short-Term Memory

Operators from Machine Learning

(CONVOLUTIONAL) AUTOENCODERS

High dimensional state

Reconstruction



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MIXTURE DENSITY NETWORKS

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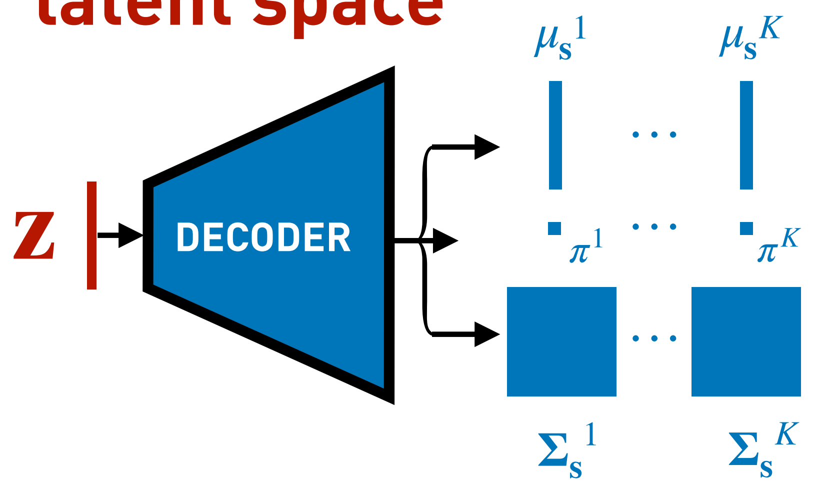

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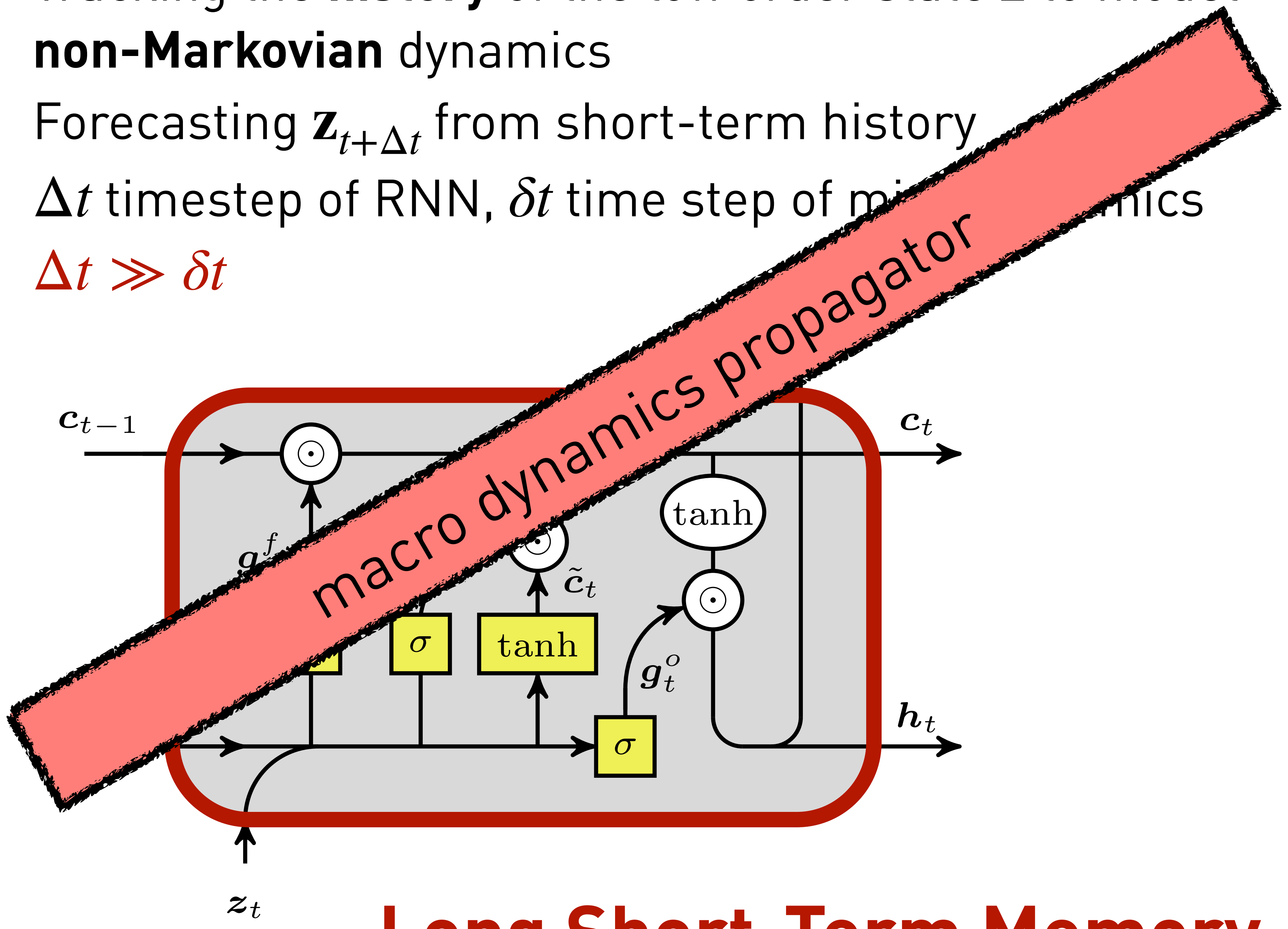


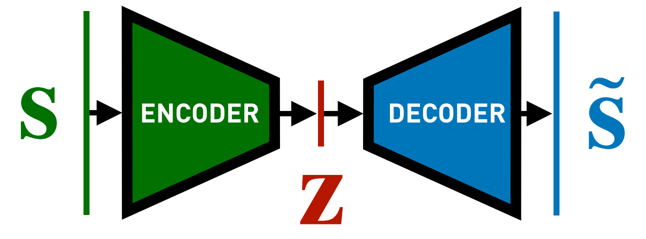
Long Short-Term Memory

Operators from Machine Learning

(CONVOLUTIONAL) AUTOENCODERS

High dimensional state

Reconstruction



Low dimensional latent spac

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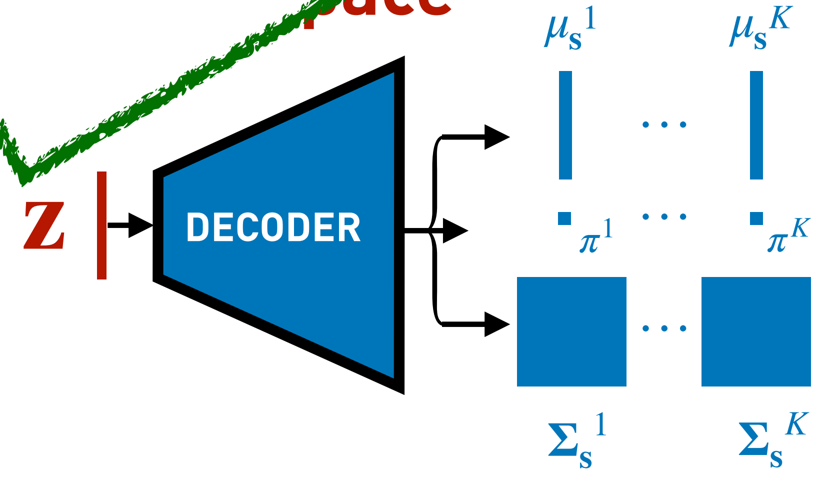
RESTRICTING/AVERAGING

(micro → macro)

...E DENSITY NETWORKS

...at ...ace



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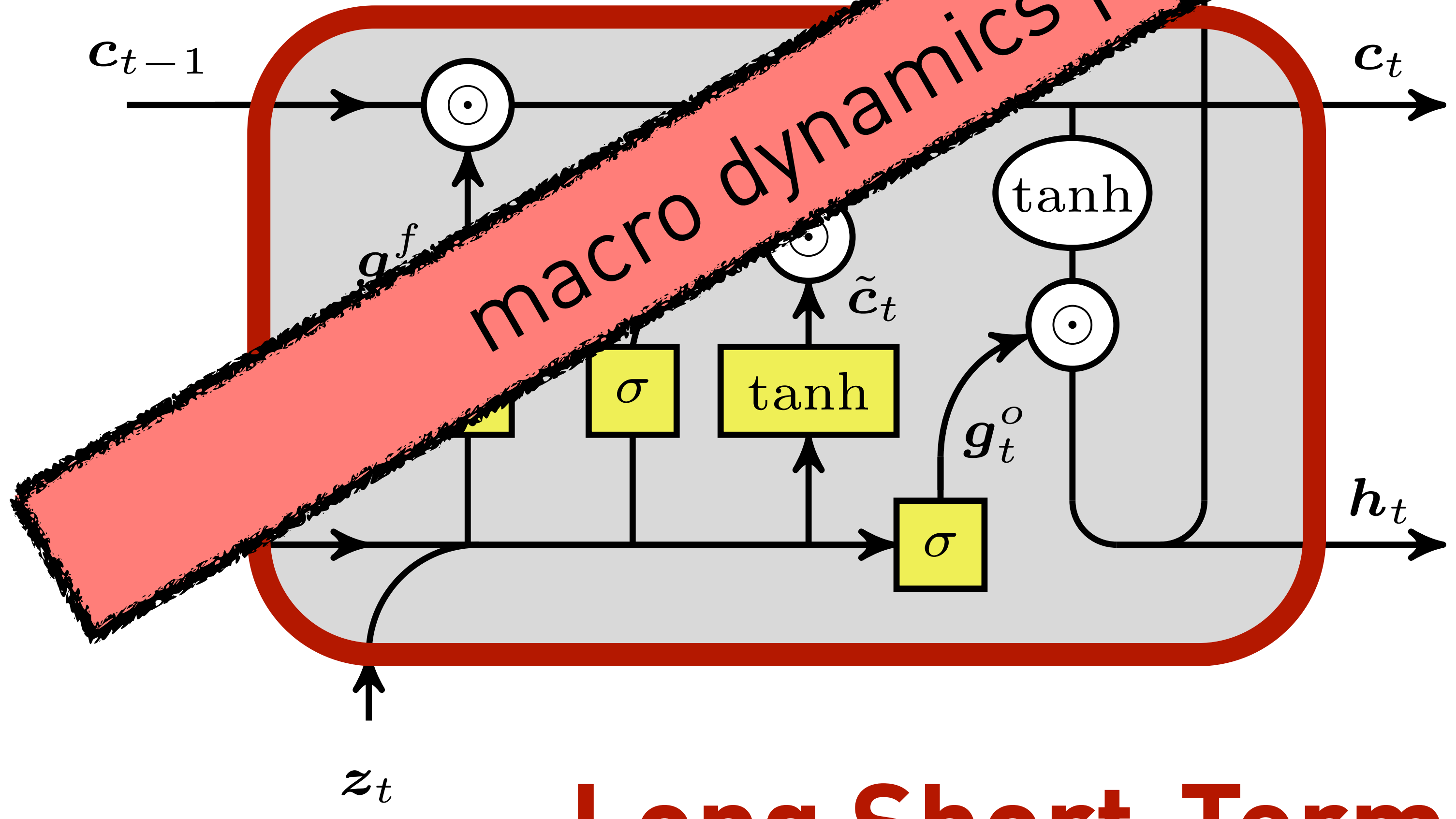
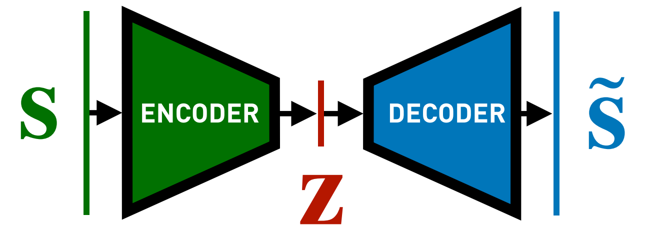


Long Short-Term Memory

Operators from Machine Learning

(CONVOLUTIONAL) AUTOENCODERS



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- ...of atoms / ...ate / angles ...
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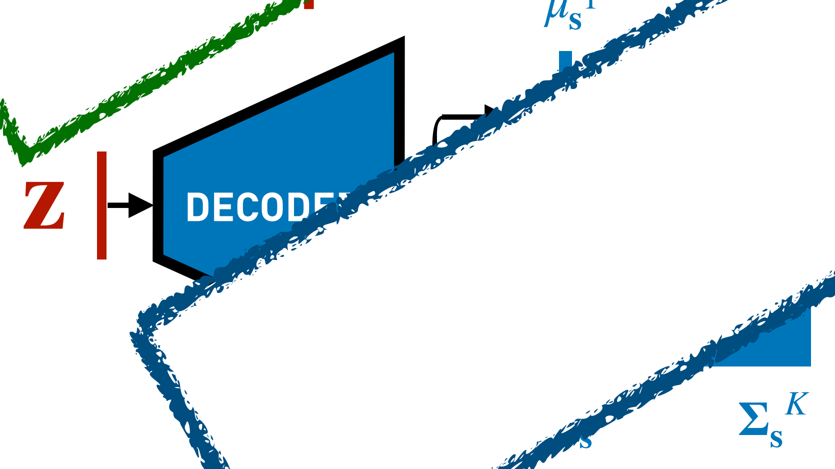
RESTRICTING/AVERAGING (micro → macro)

LIFTING (macro → micro)

...E DENSIT... ...RKS



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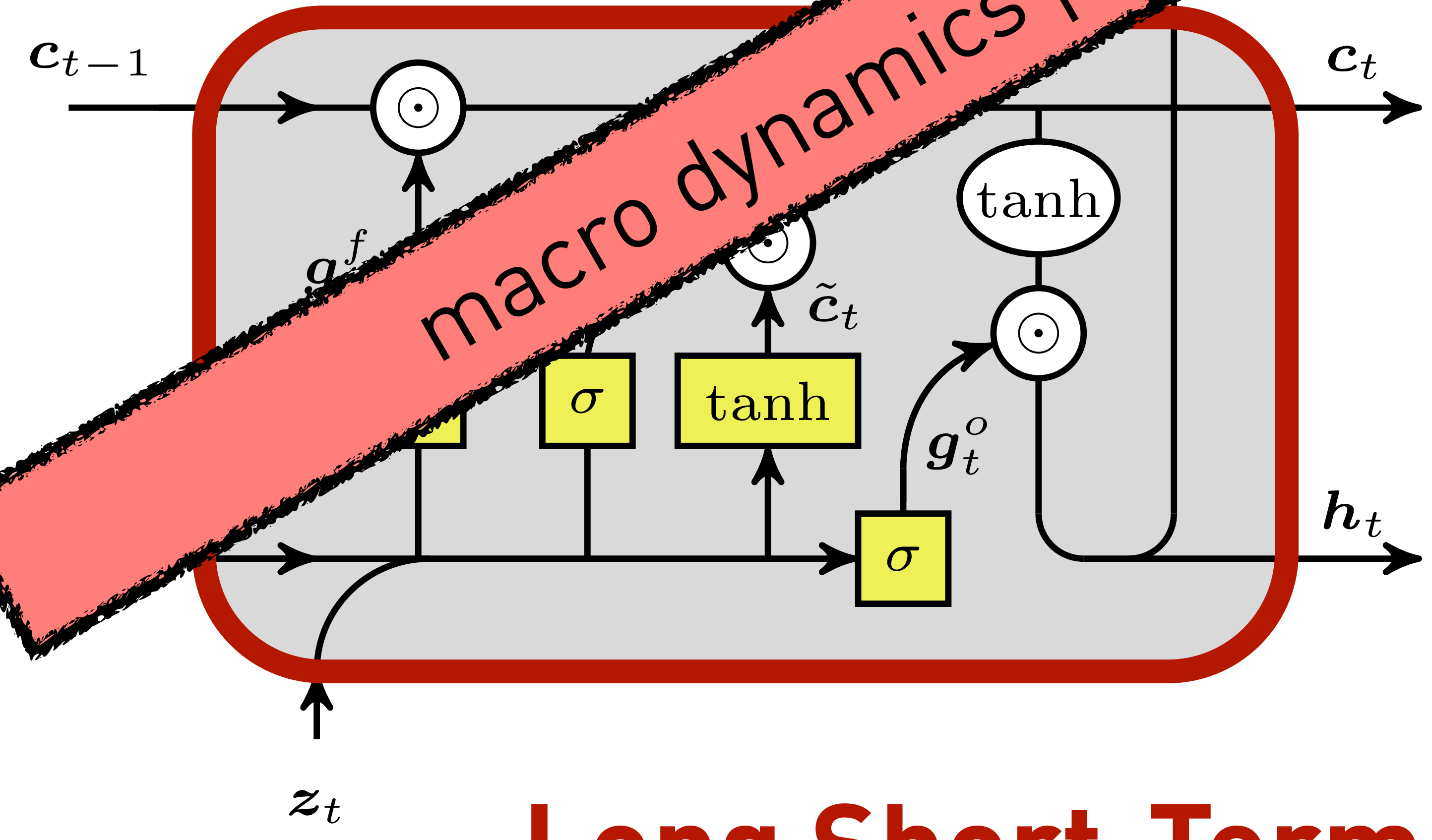
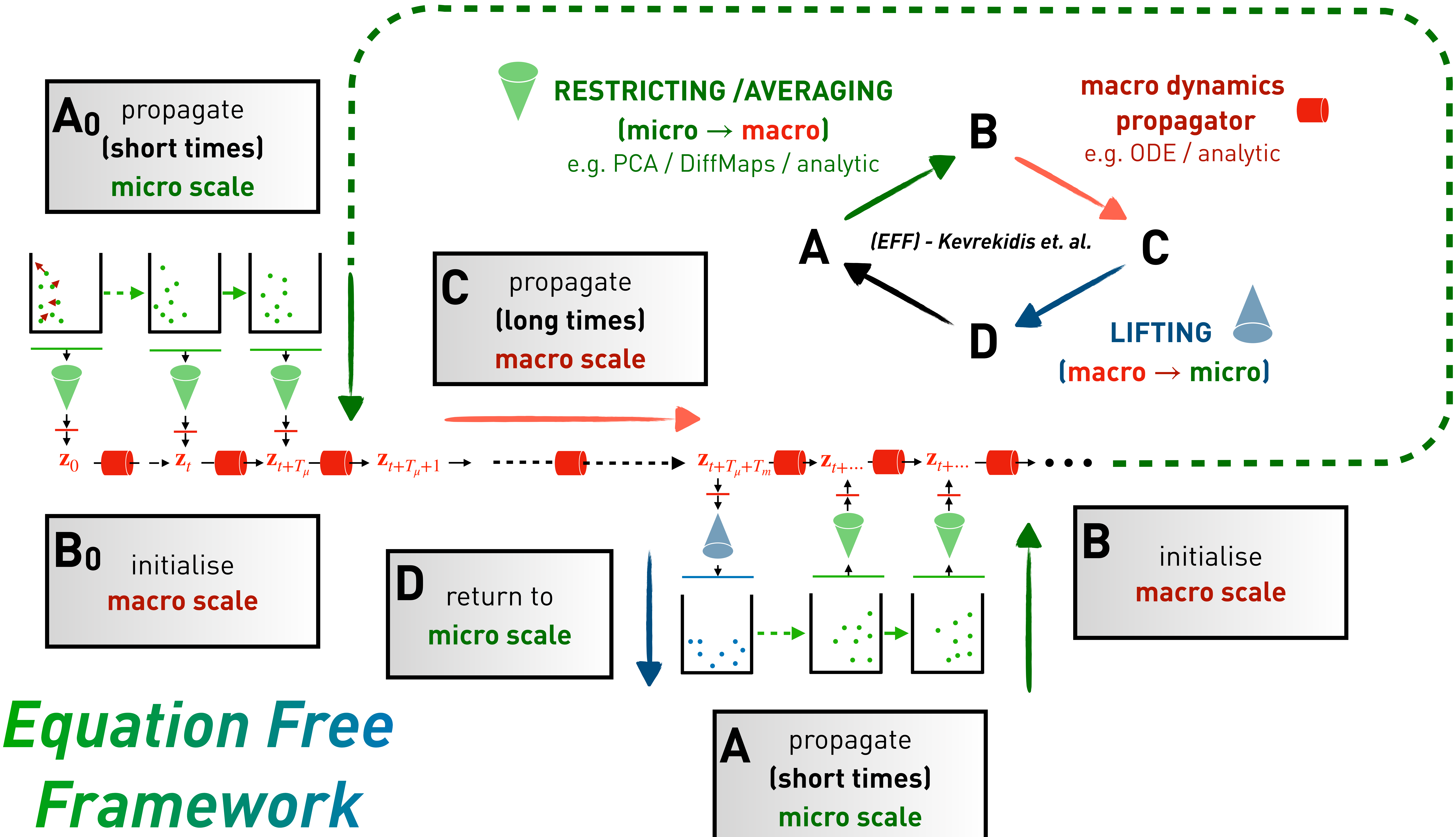
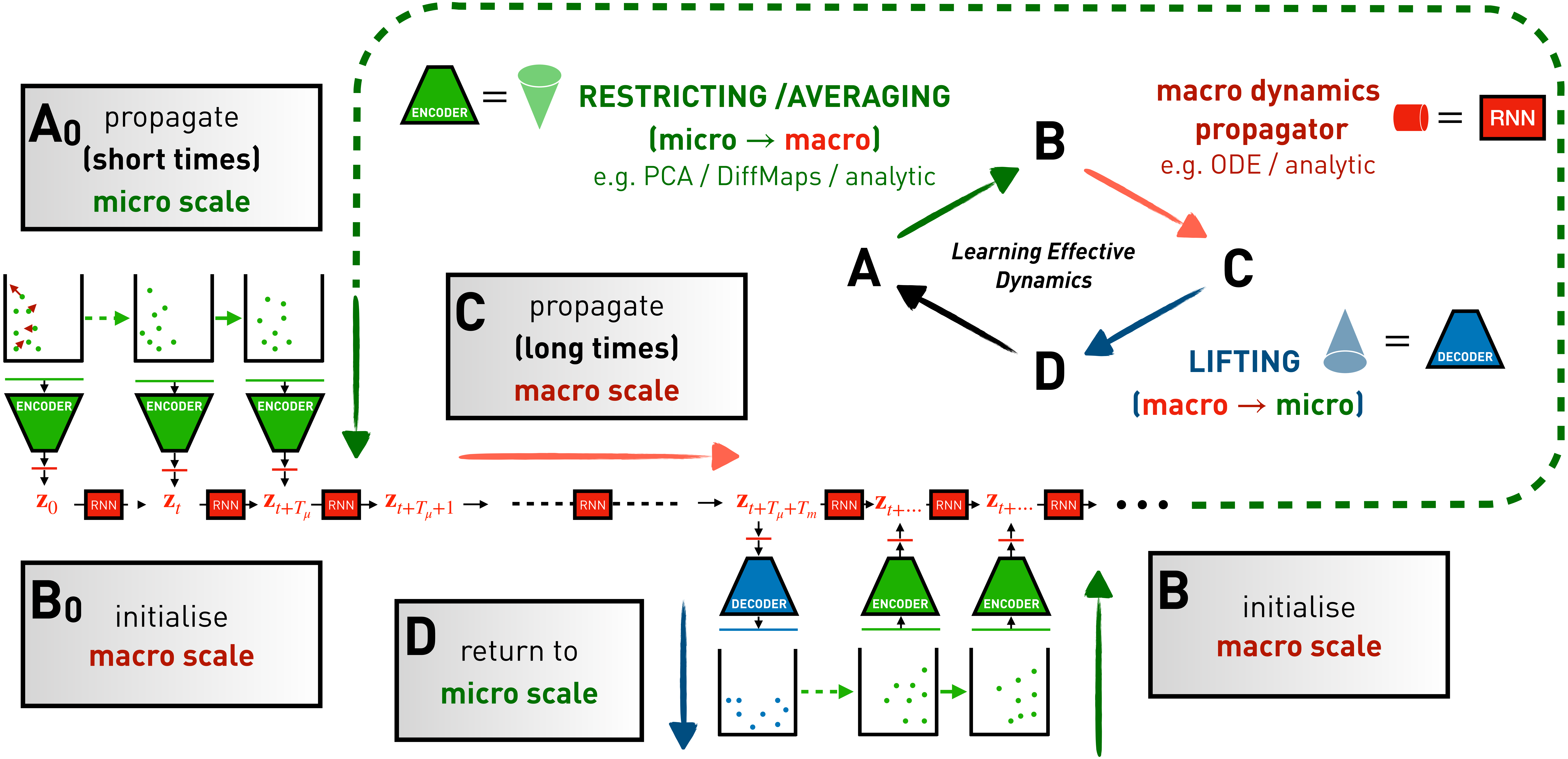
macro dynamics propagator



Long Short-Term Memory



RESTRICTING /AVERAGING
(micro → macro)
e.g. PCA / DiffMaps / analytic
macro dynamics
propagator
e.g. ODE / analytic
A
B
C
D
(EFF) - Kevrekidis et. al.
LIFTING
(macro → micro)
A0 propagate
(short times)
micro scale
C propagate
(long times)
macro scale
z_0
z_t
z_{t+T_μ}
$z_{t+T_\mu+1}$
$z_{t+T_\mu+T_m}$
$z_{t+\dots}$
$z_{t+\dots}$
B0 initialise
macro scale
D return to
micro scale
B initialise
macro scale
A propagate
(short times)
micro scale
Equation Free
Framework

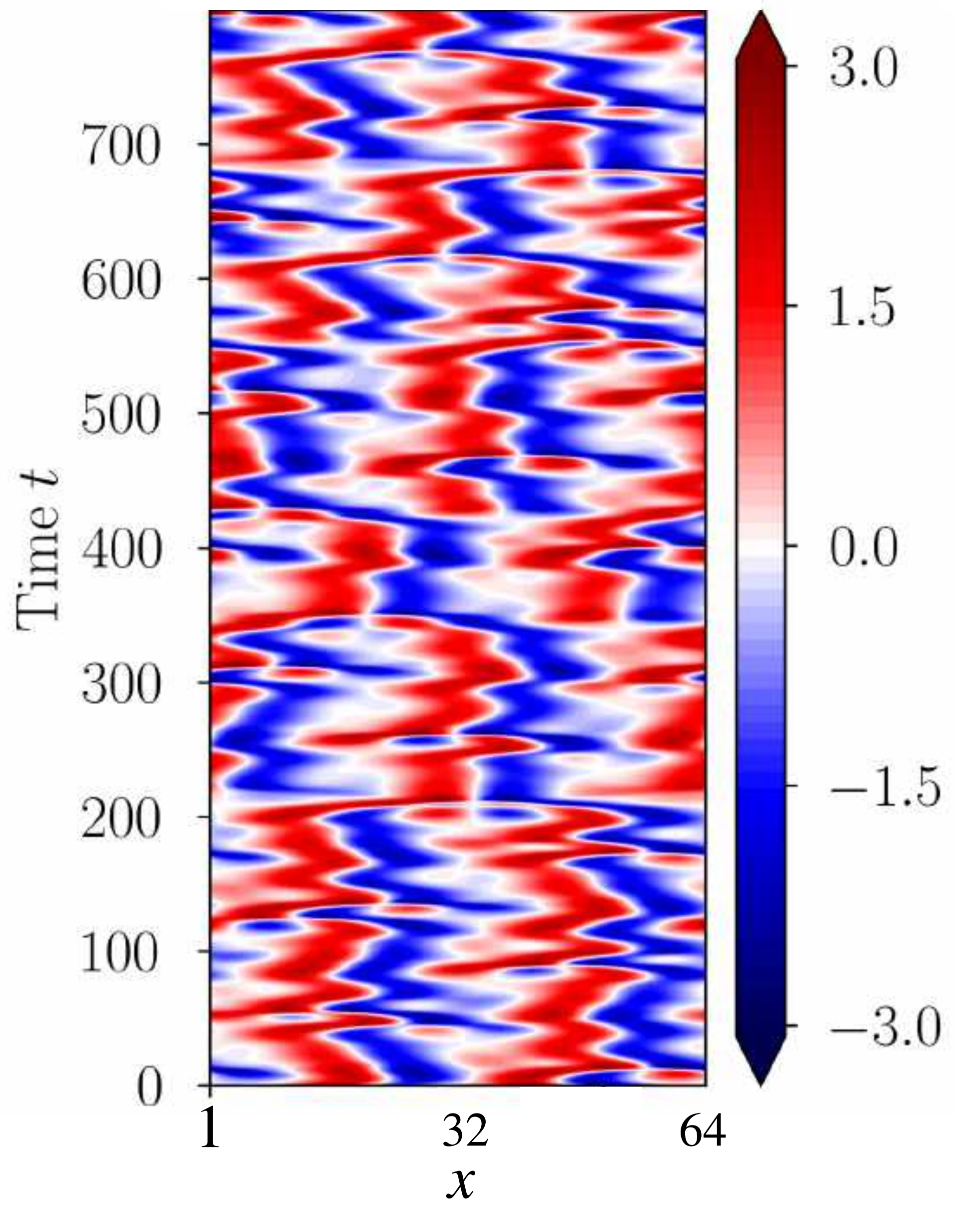


Learning Effective Dynamics (LED)

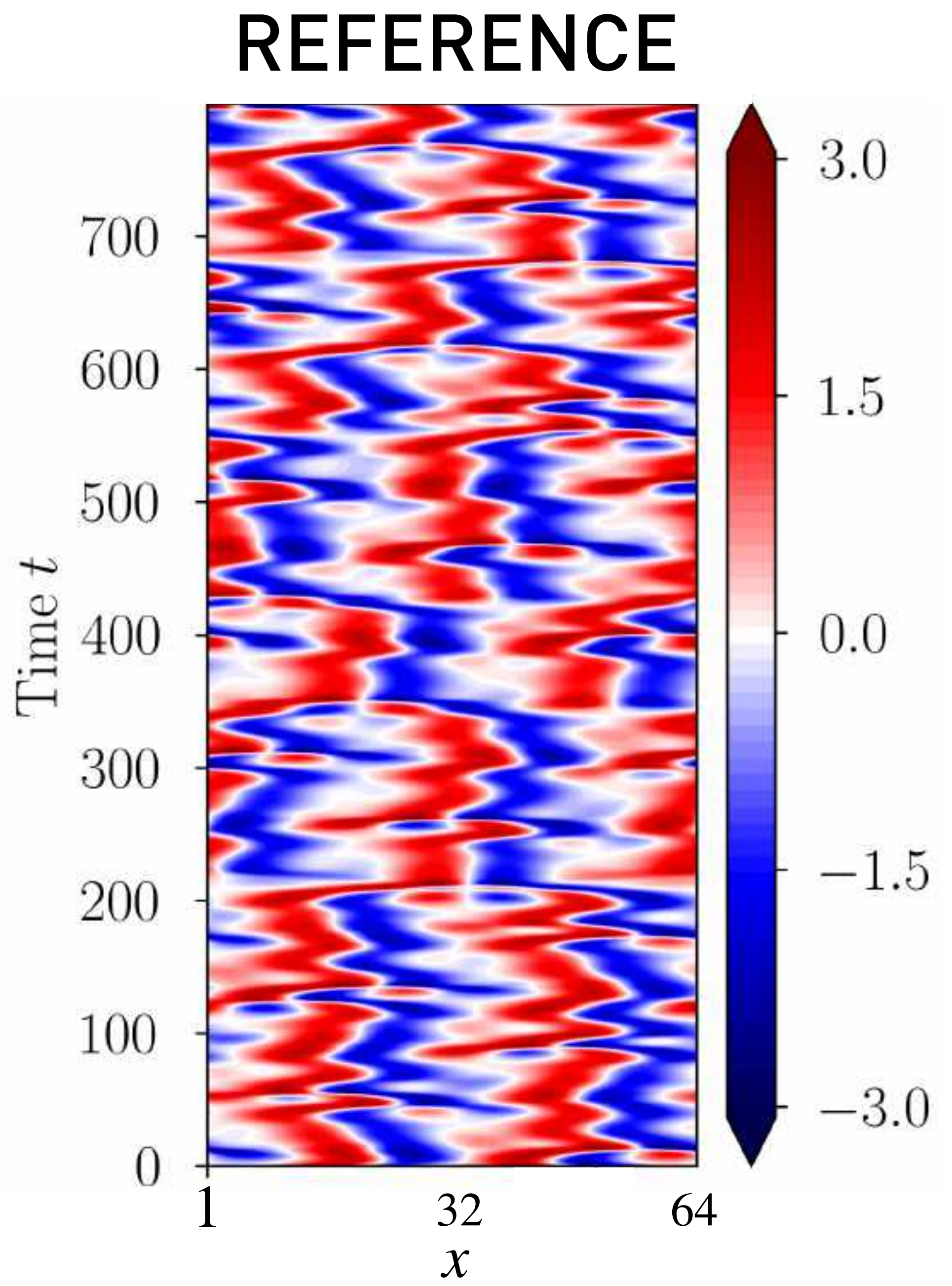
Kuramoto-Sivashinsky ($\tilde{L} \approx 3.5$)

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

REFERENCE



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



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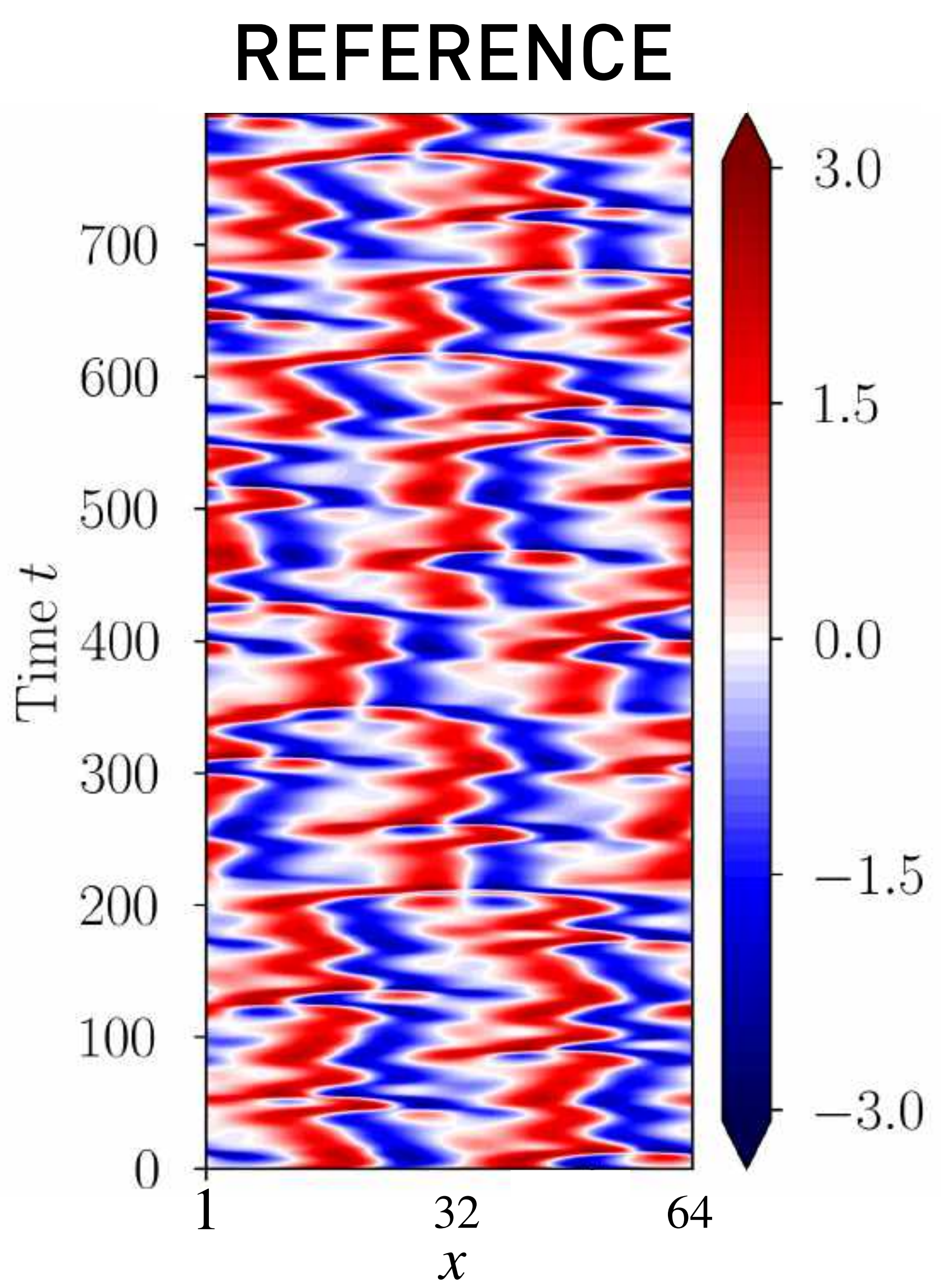

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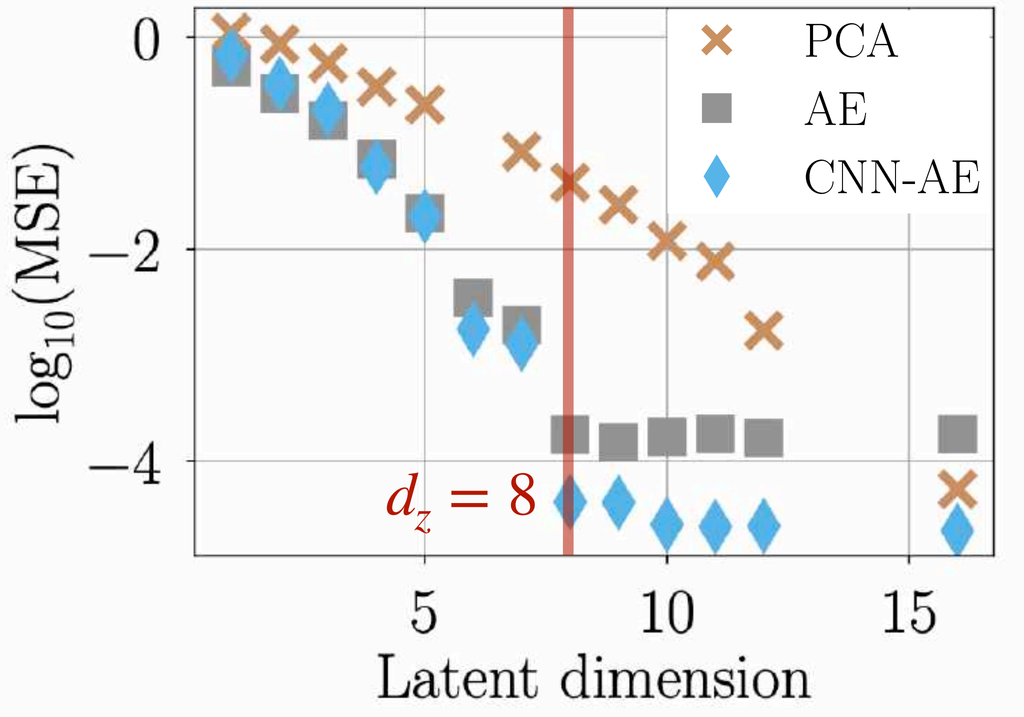
The AE error saturates after $d_z = 8$



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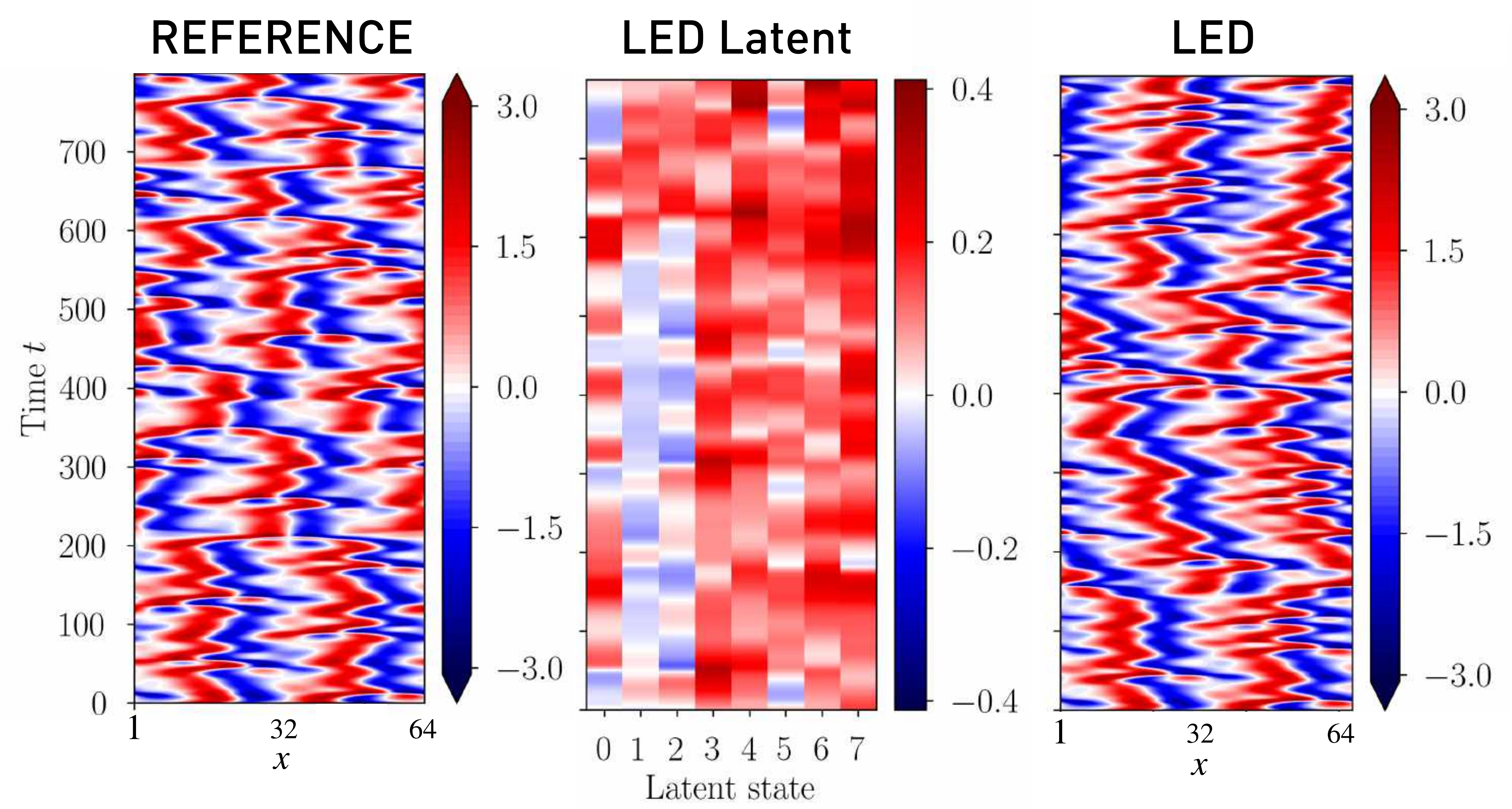

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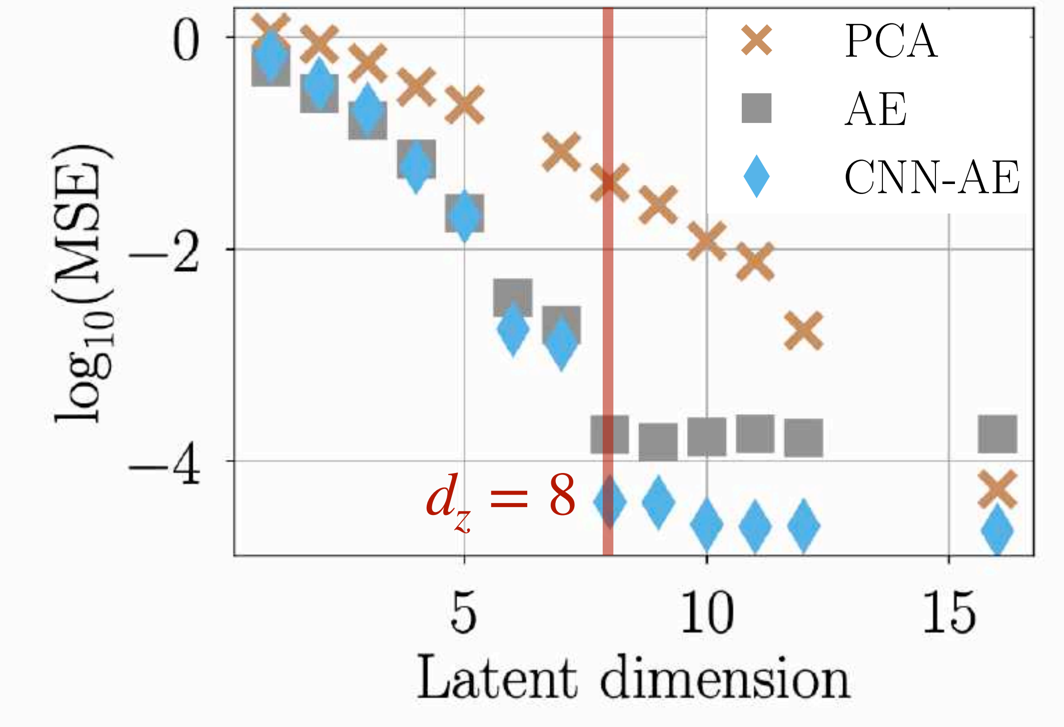

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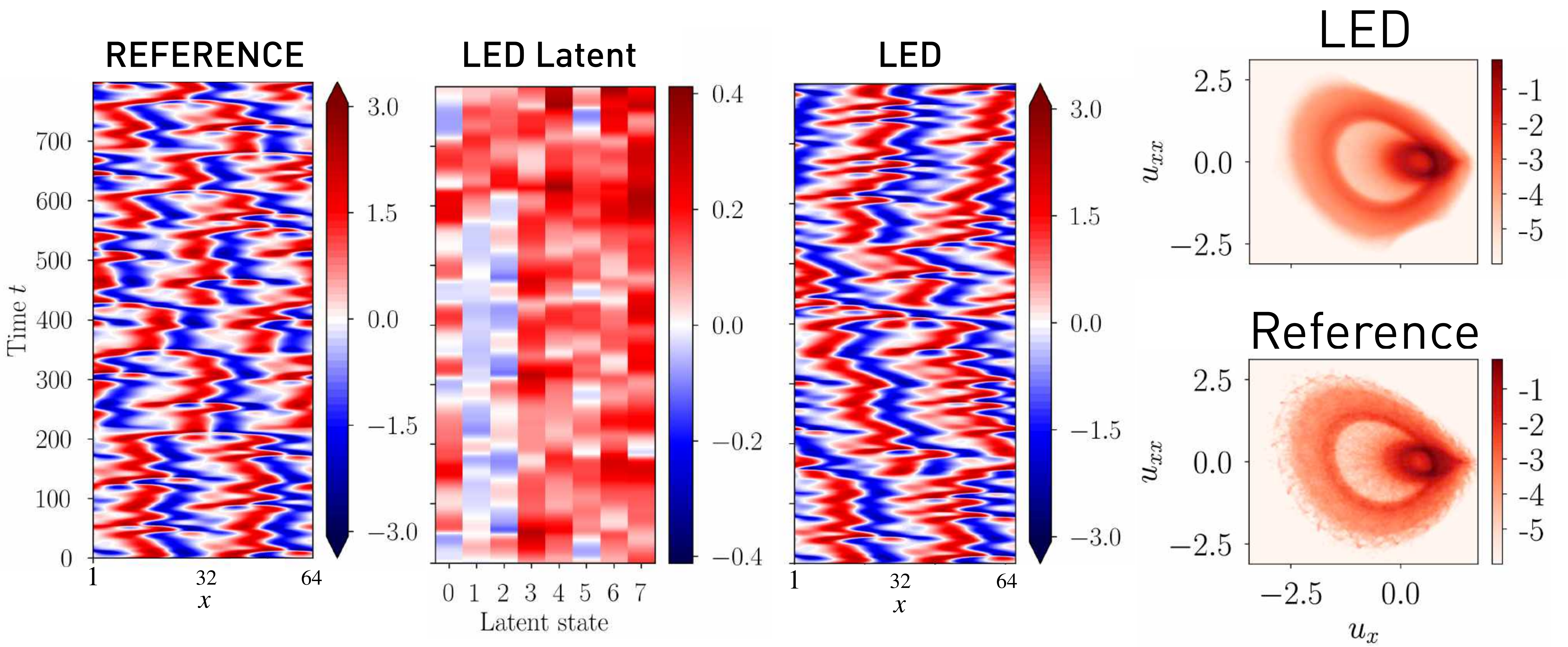

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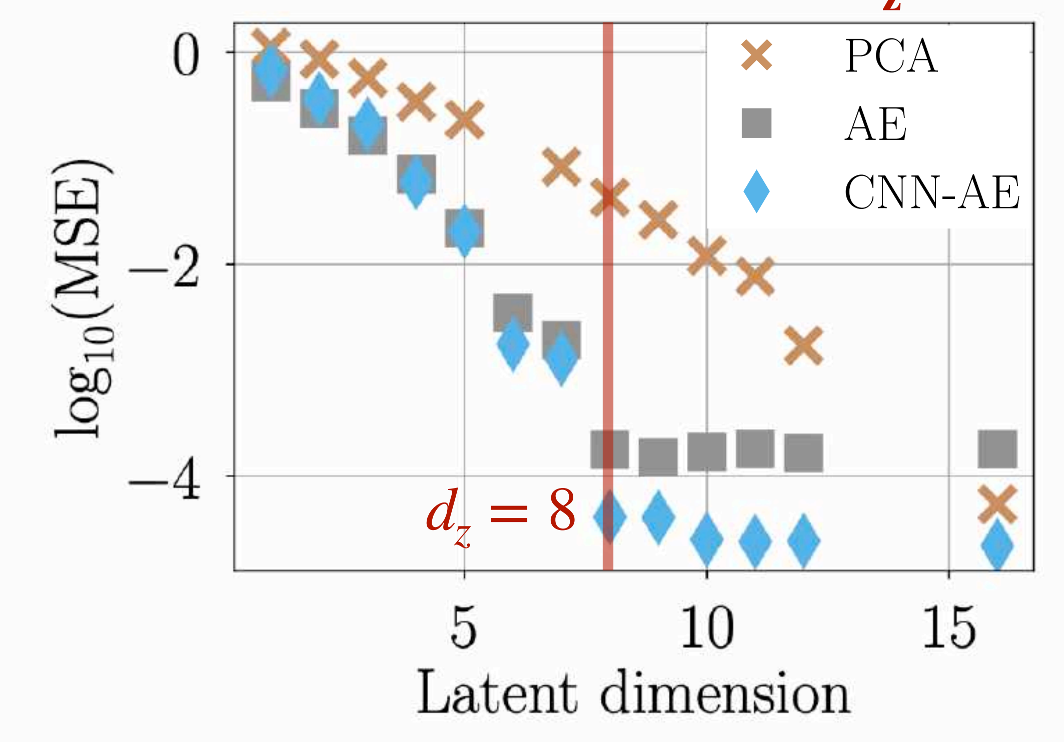

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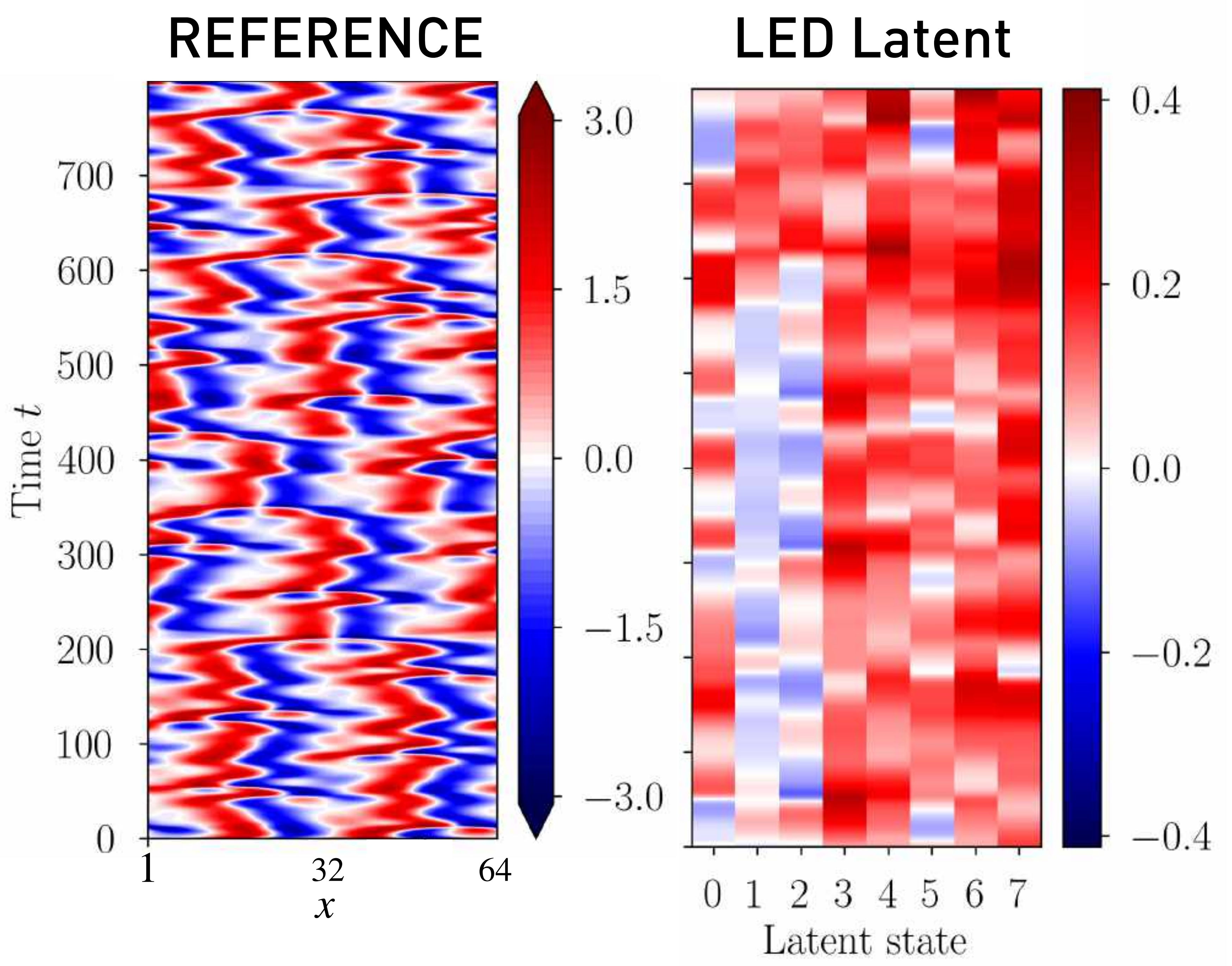

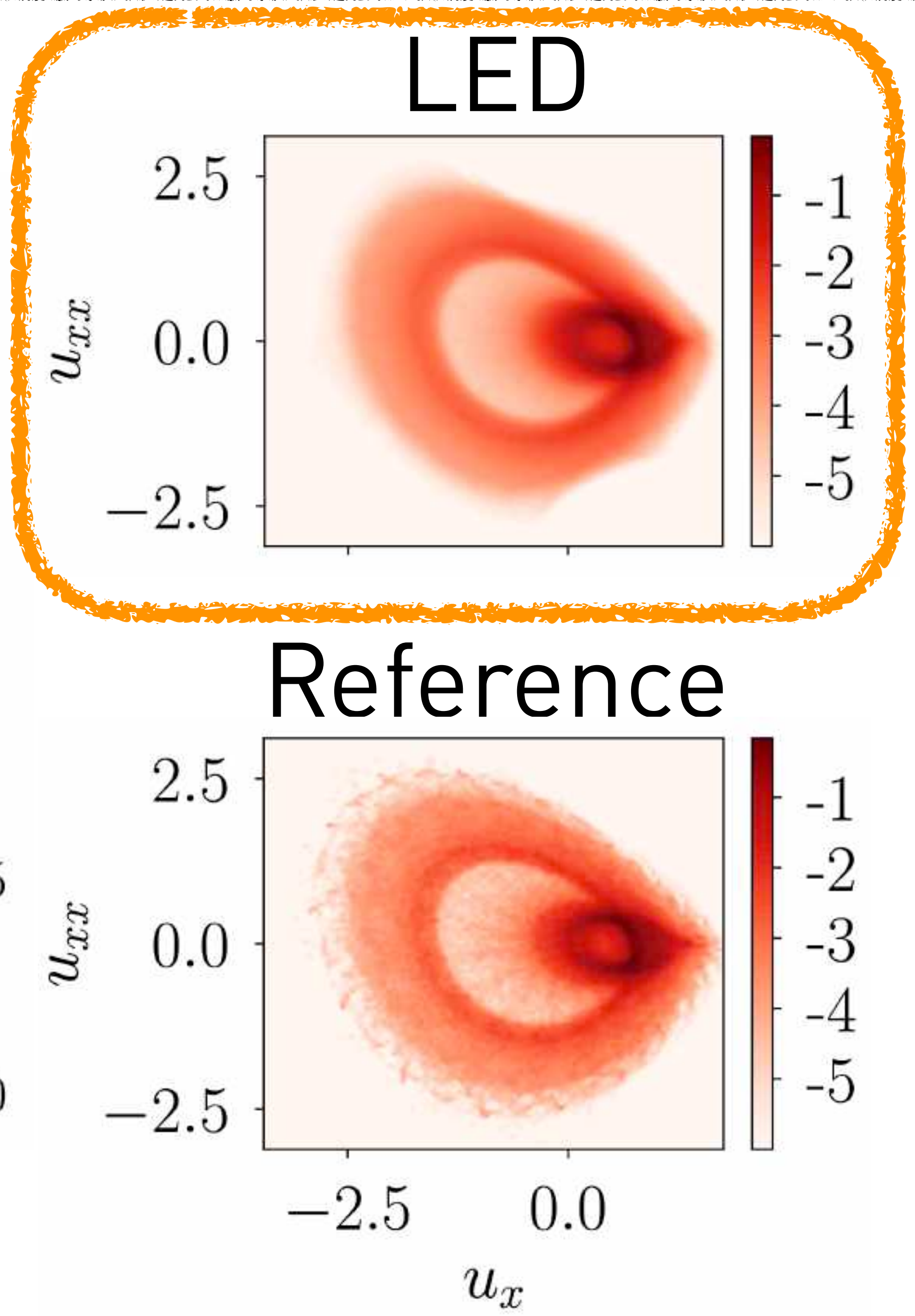

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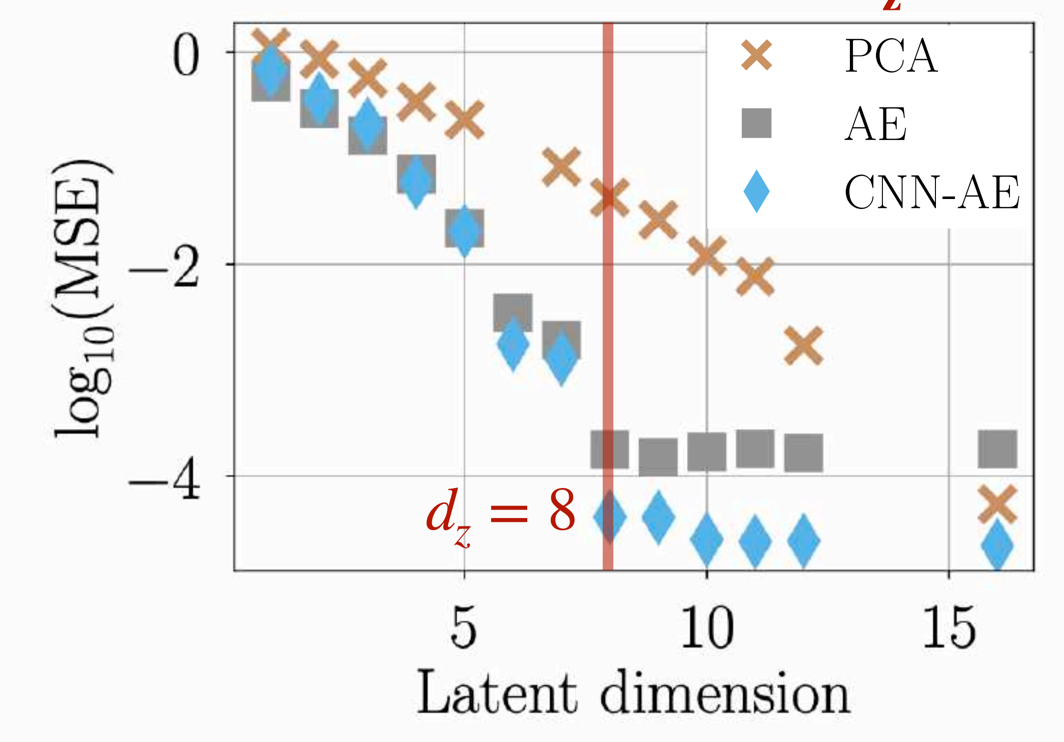

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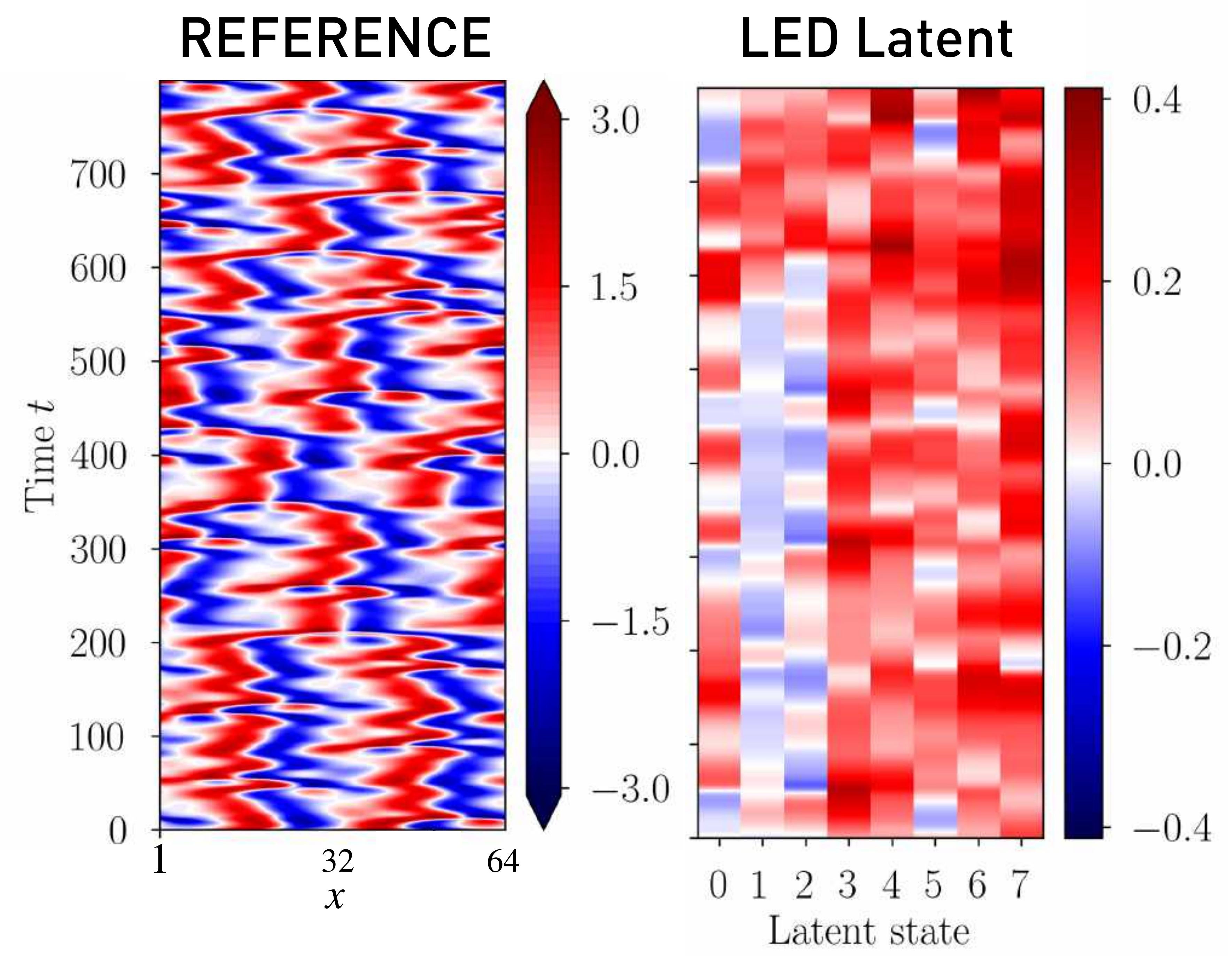

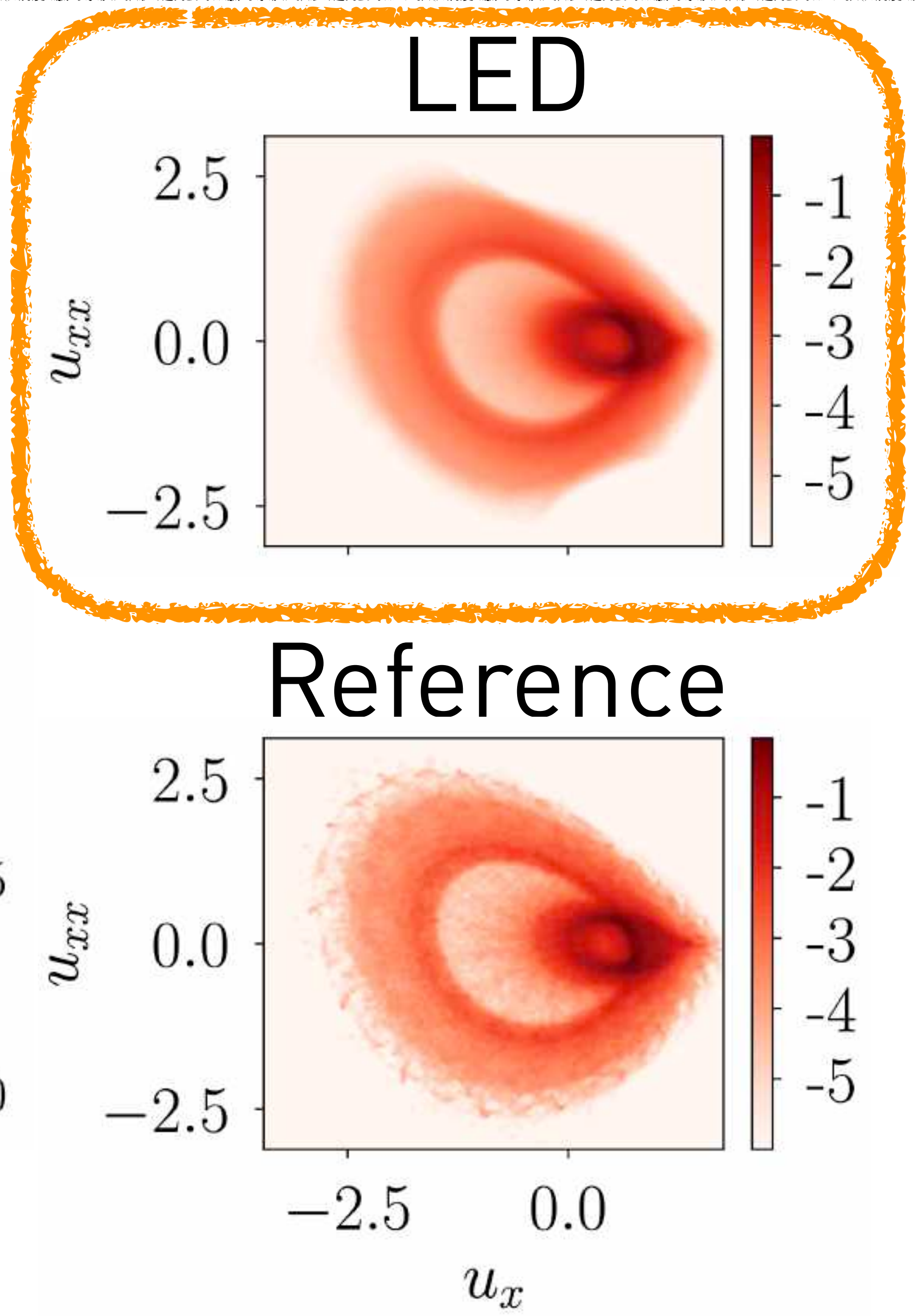

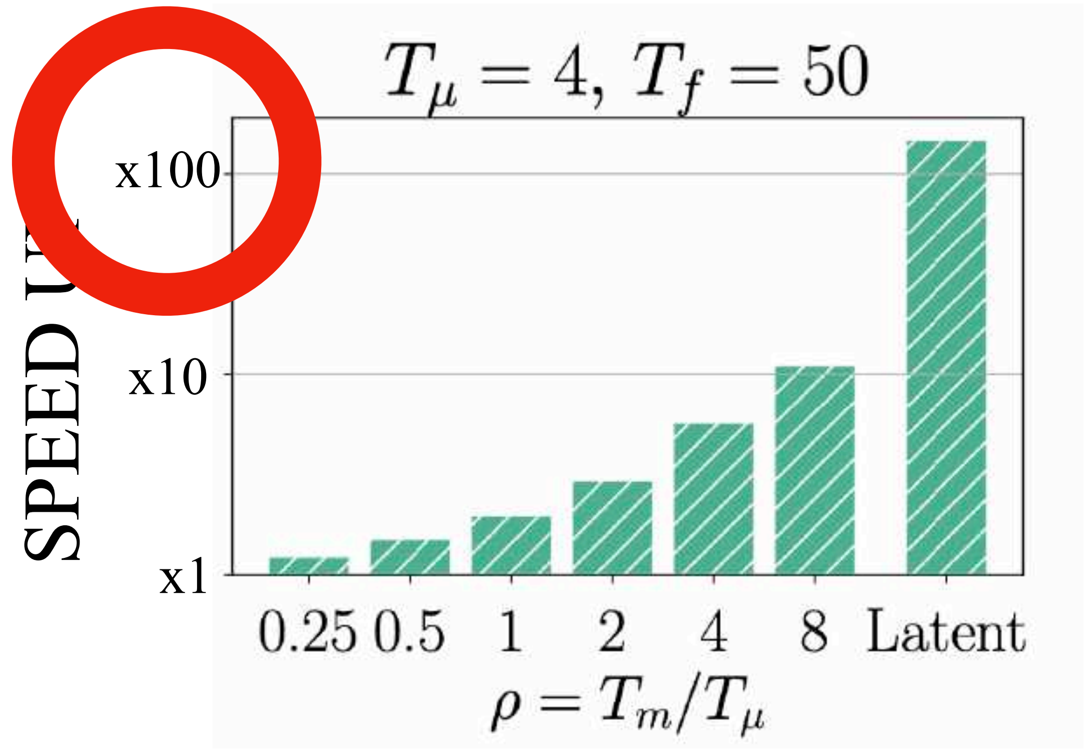

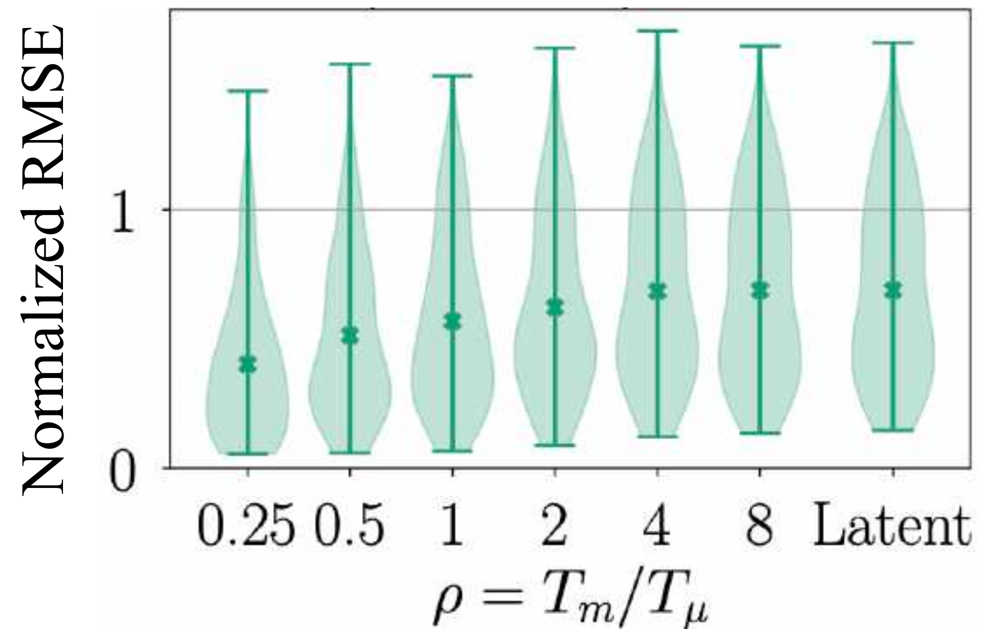

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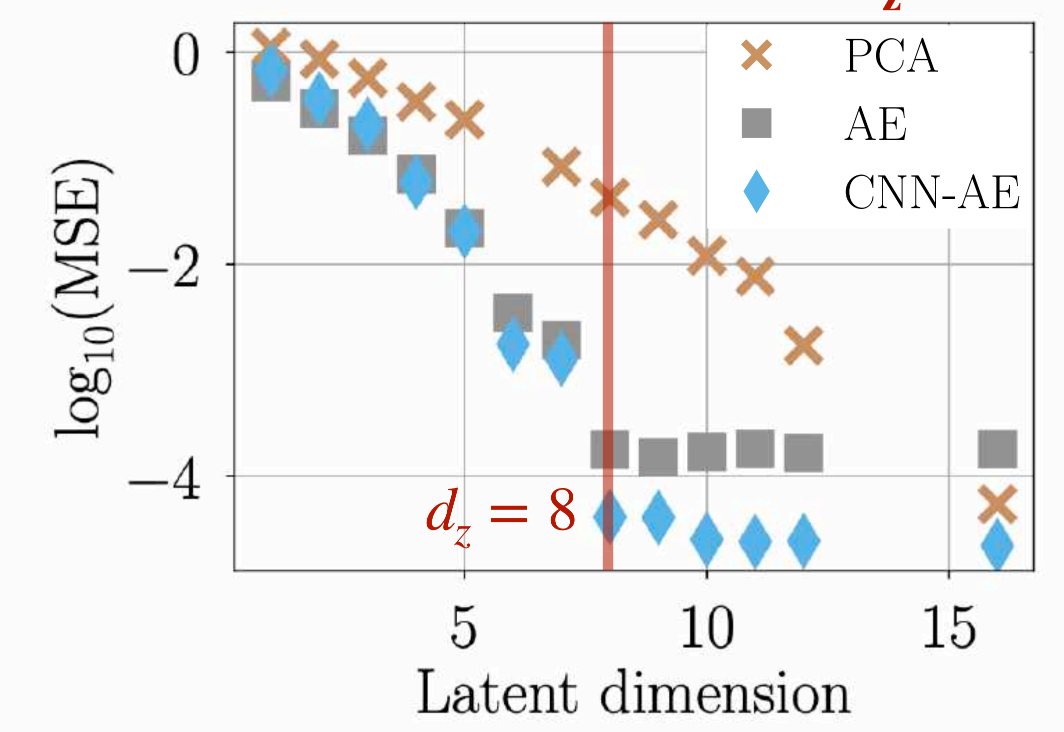

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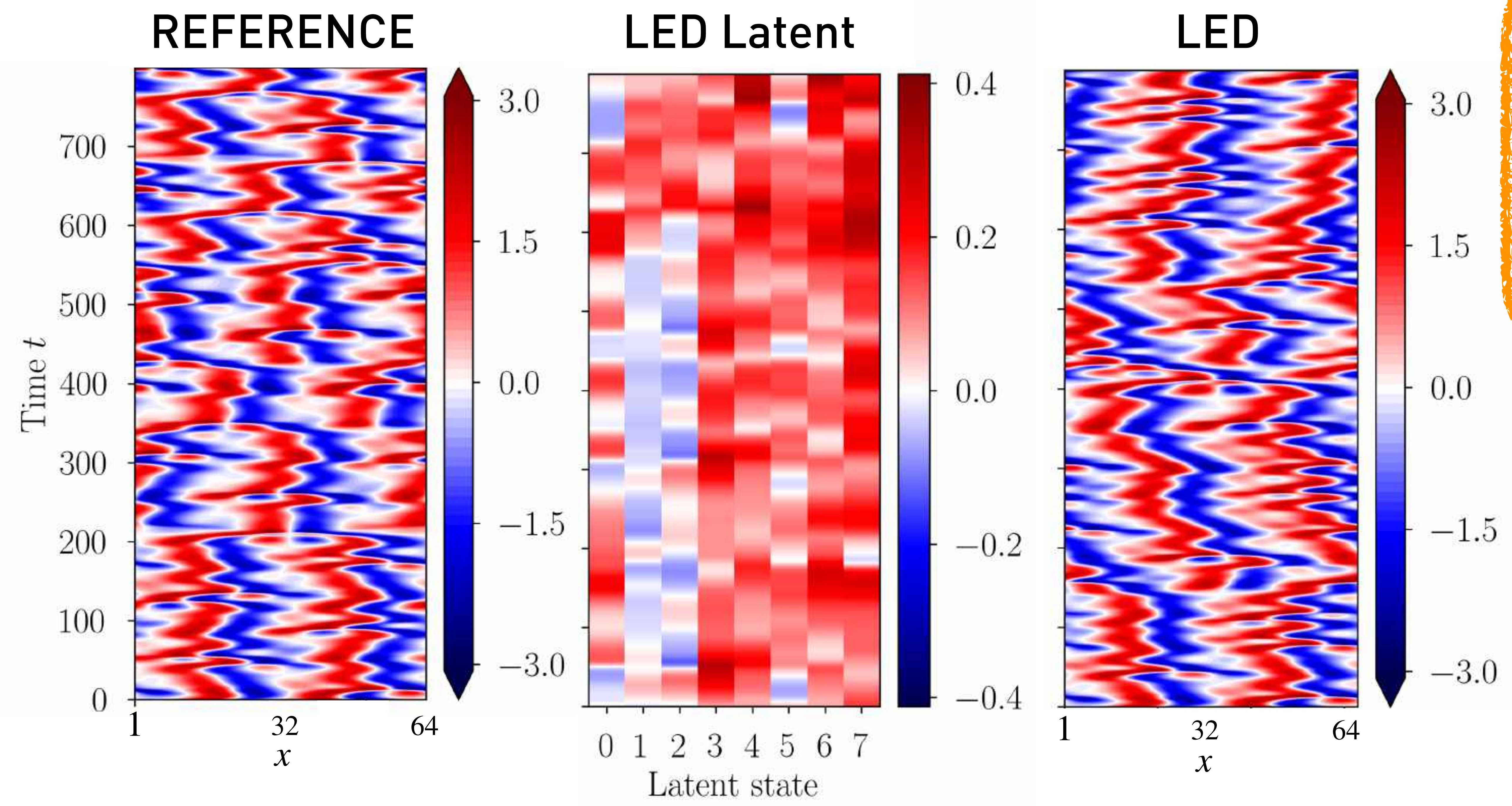

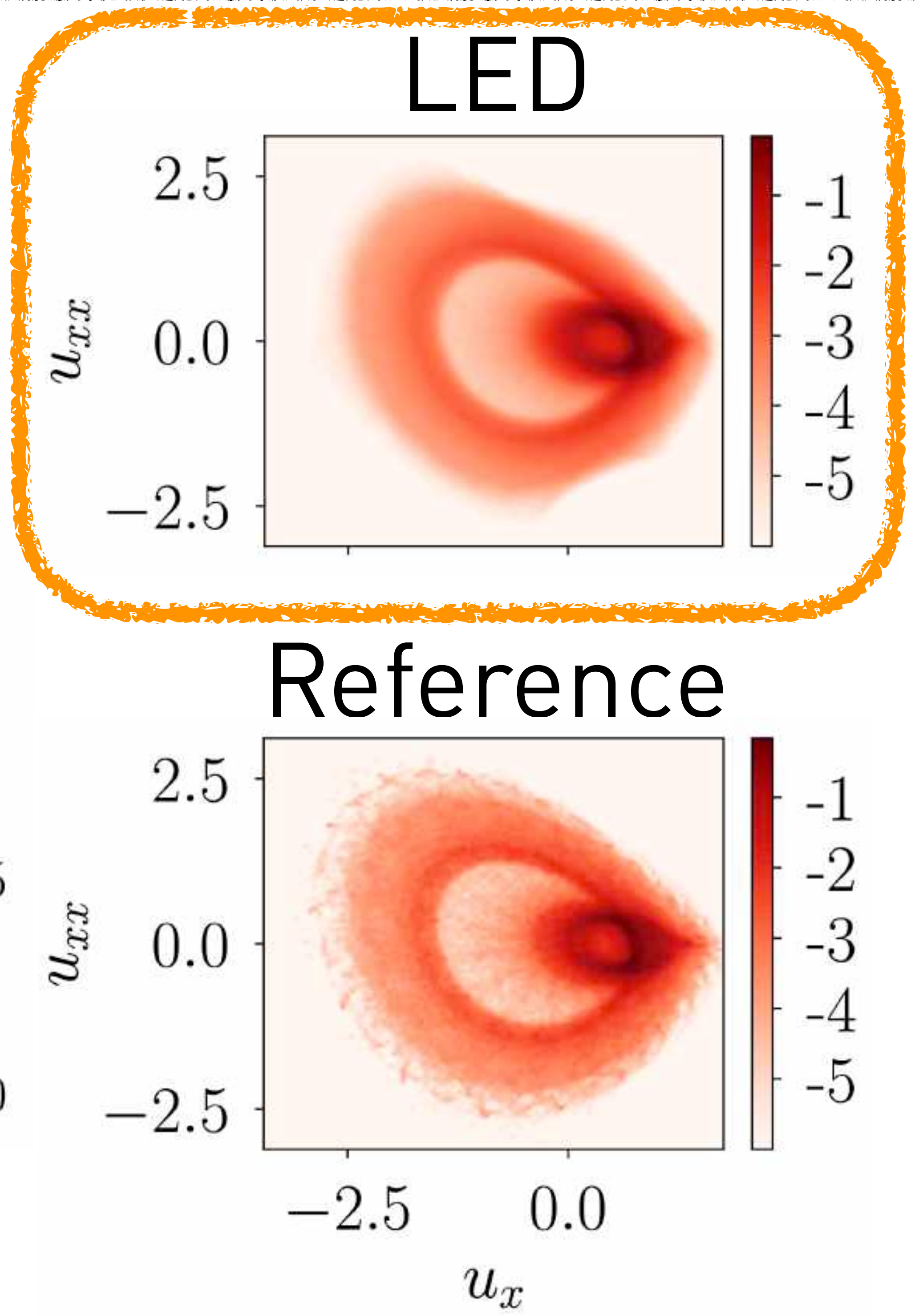

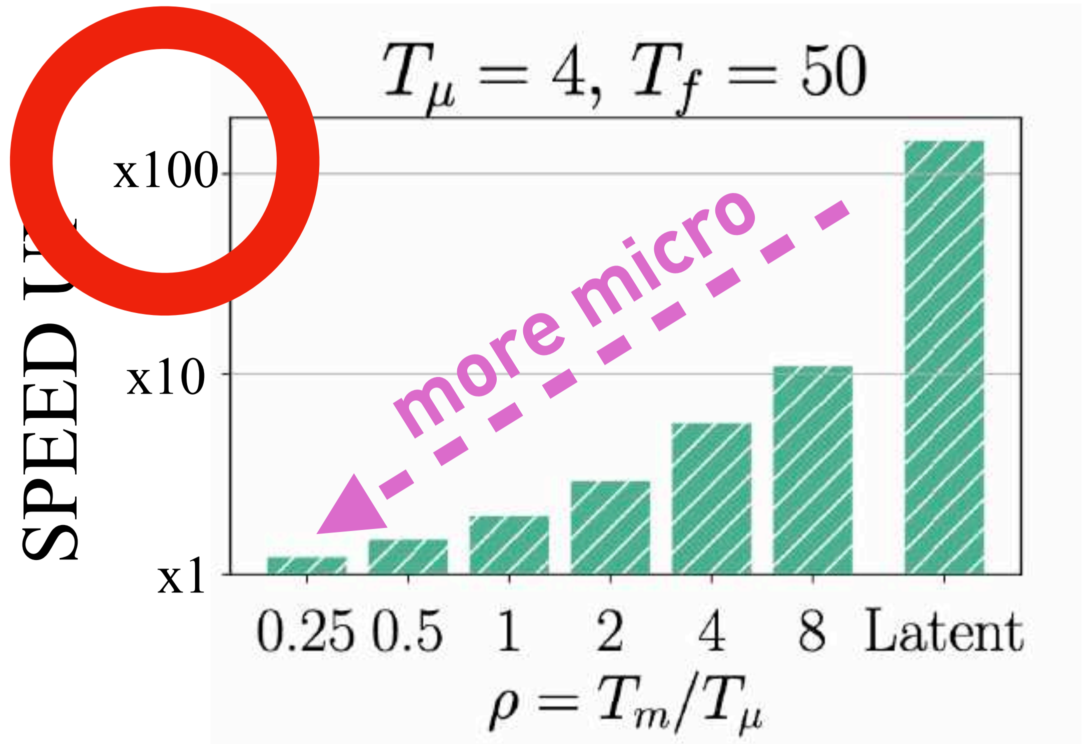

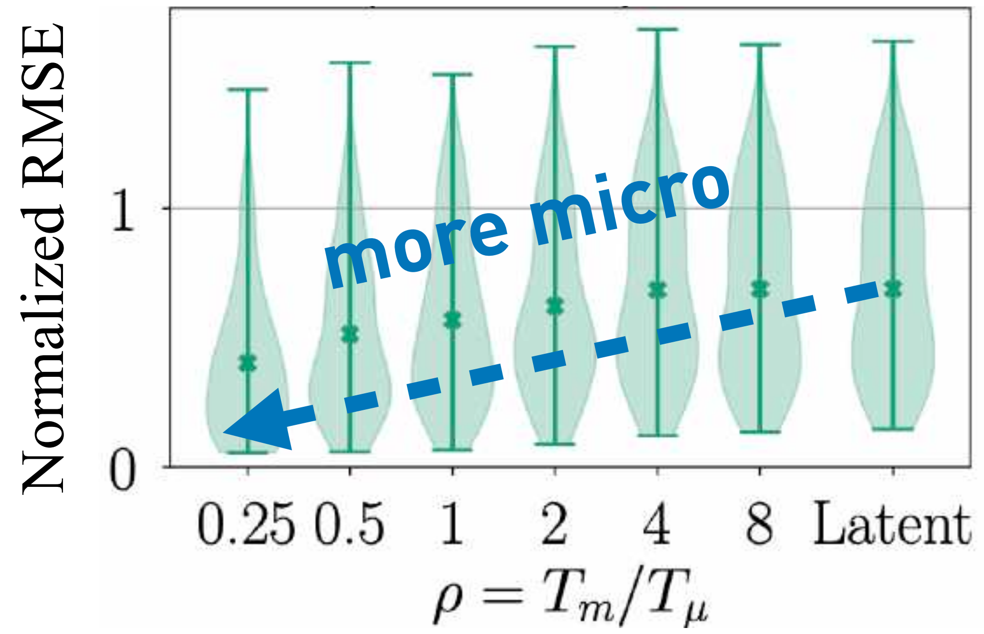

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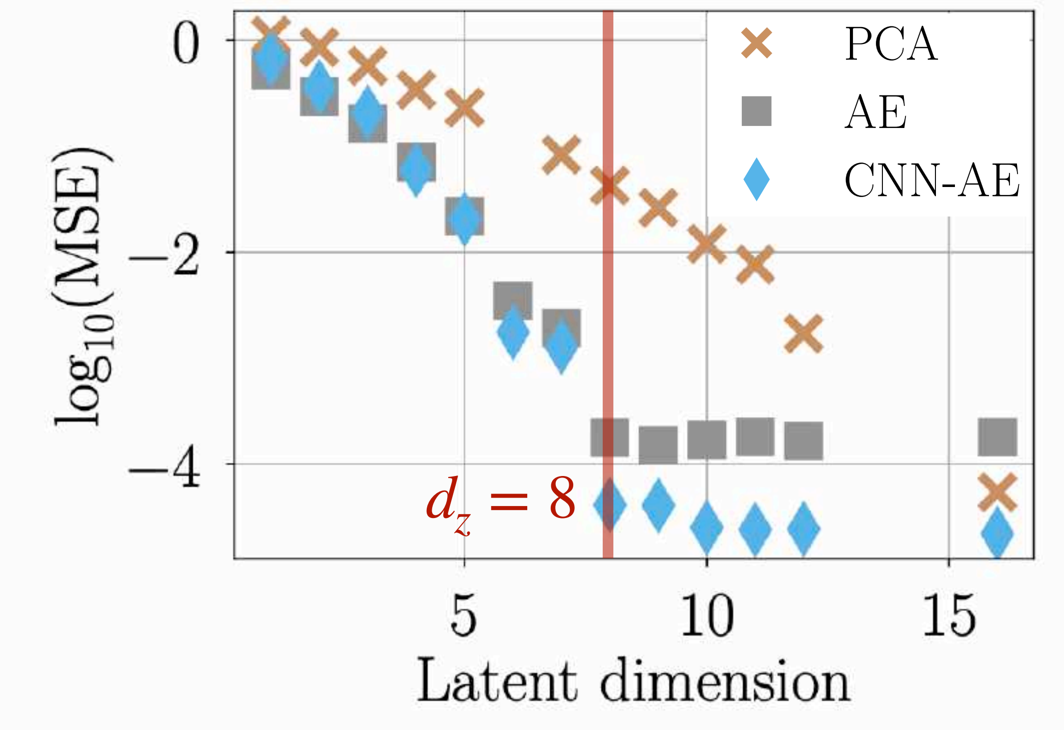

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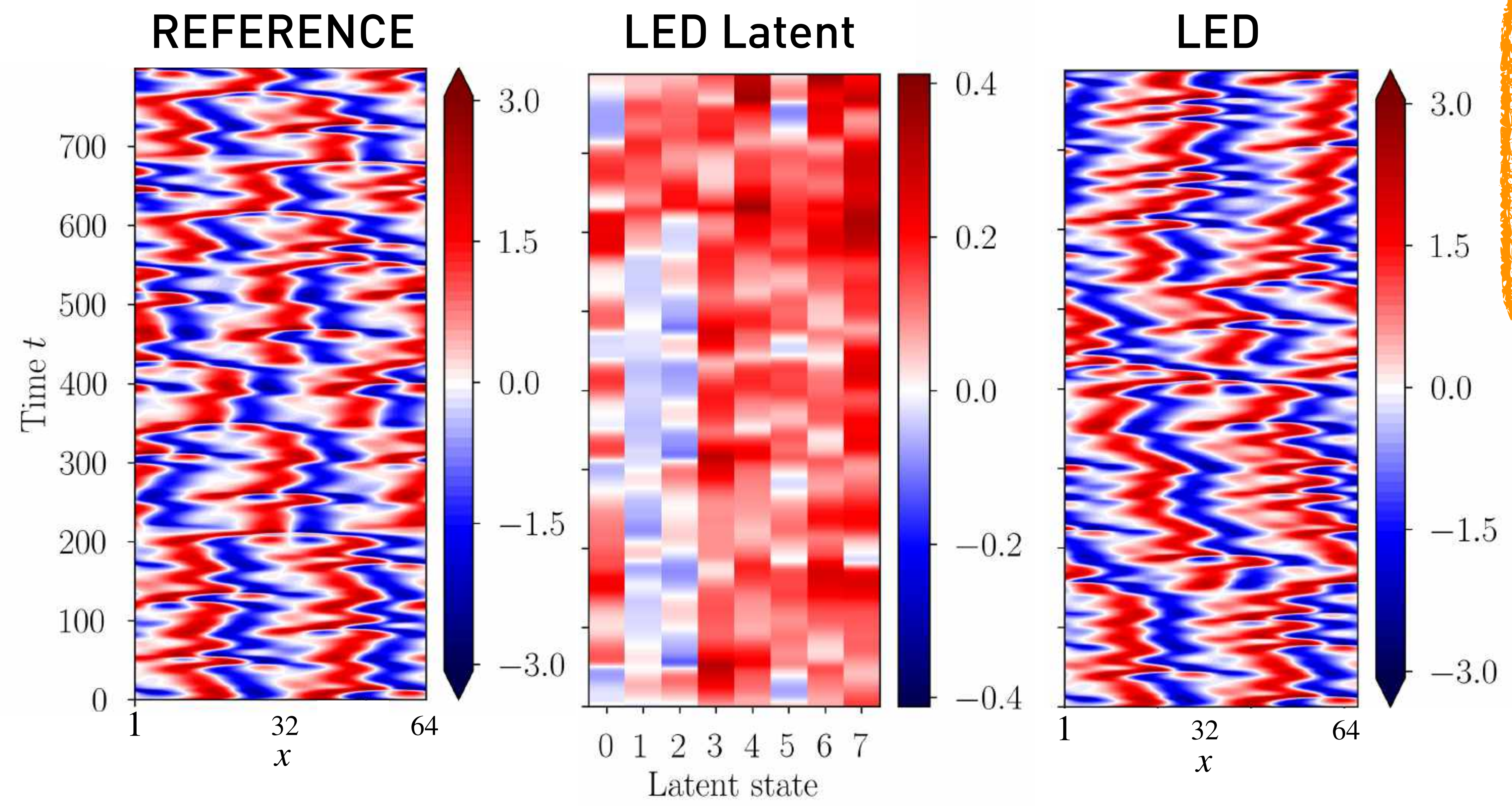

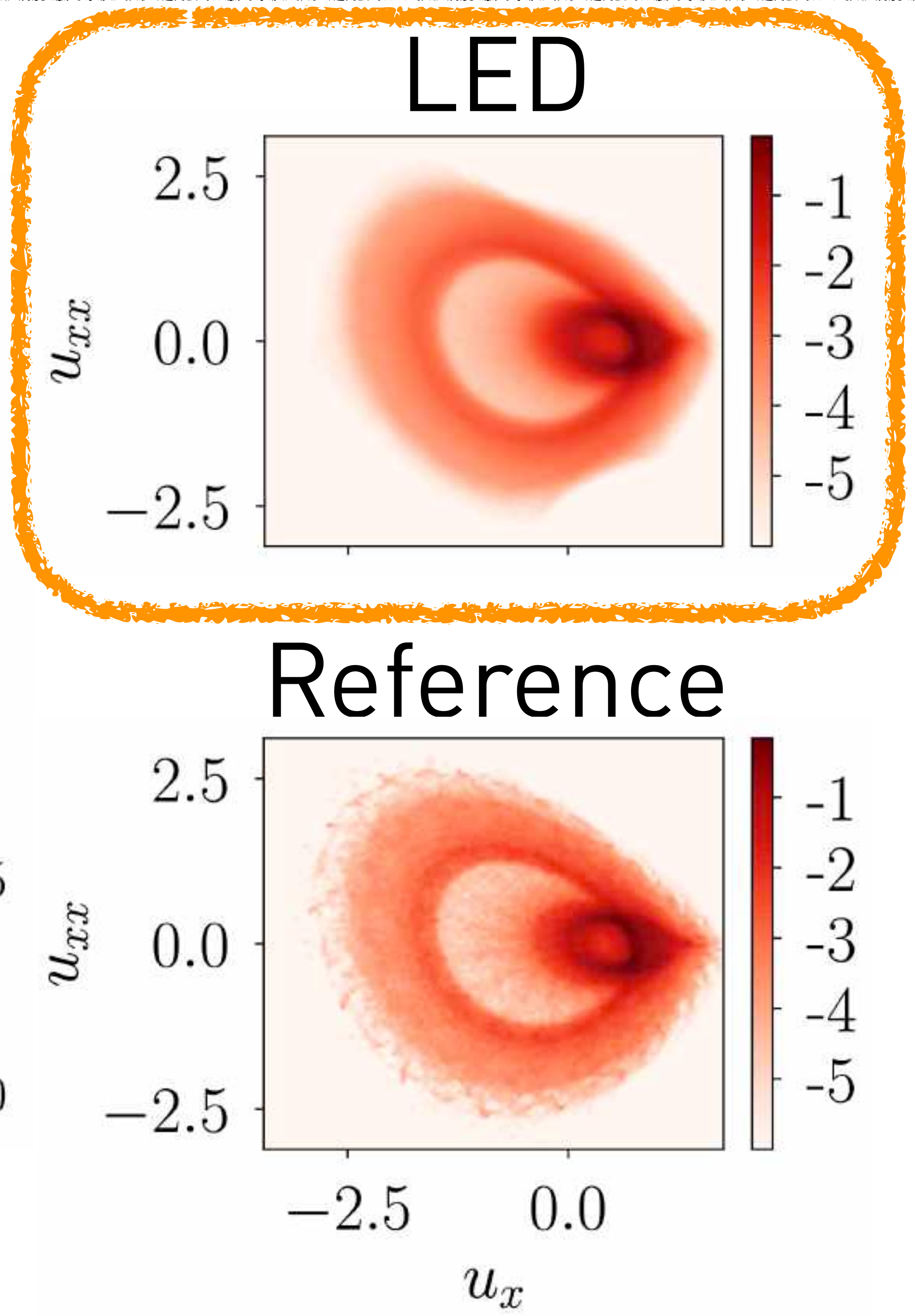

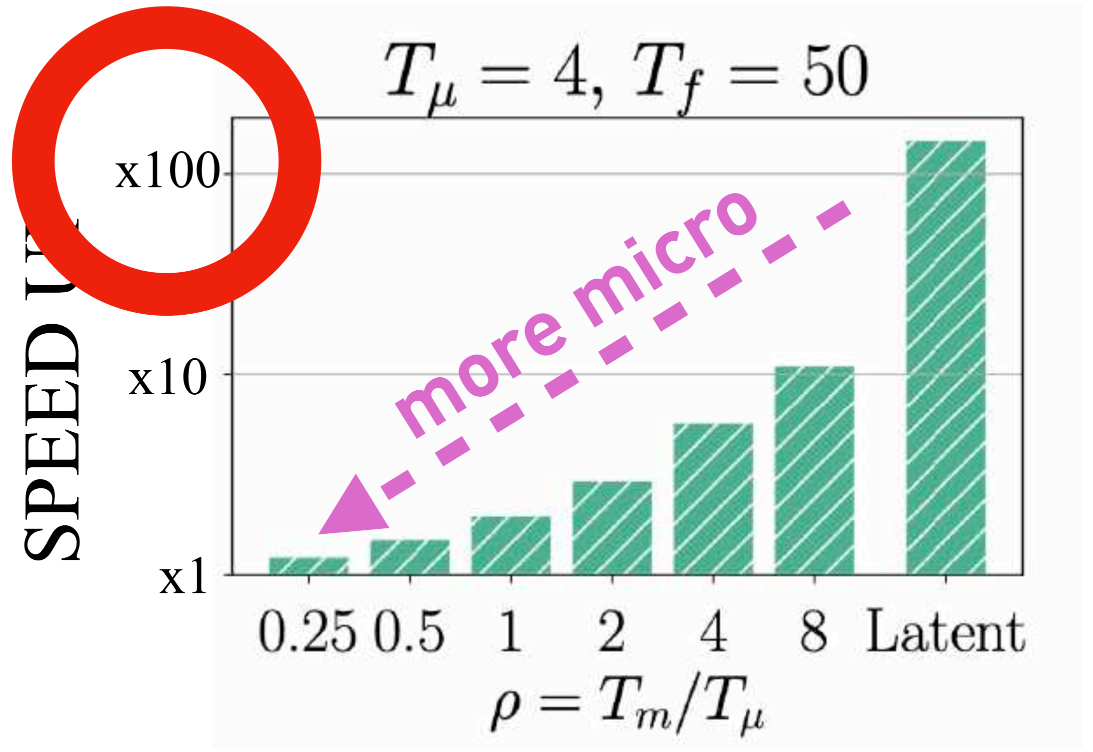

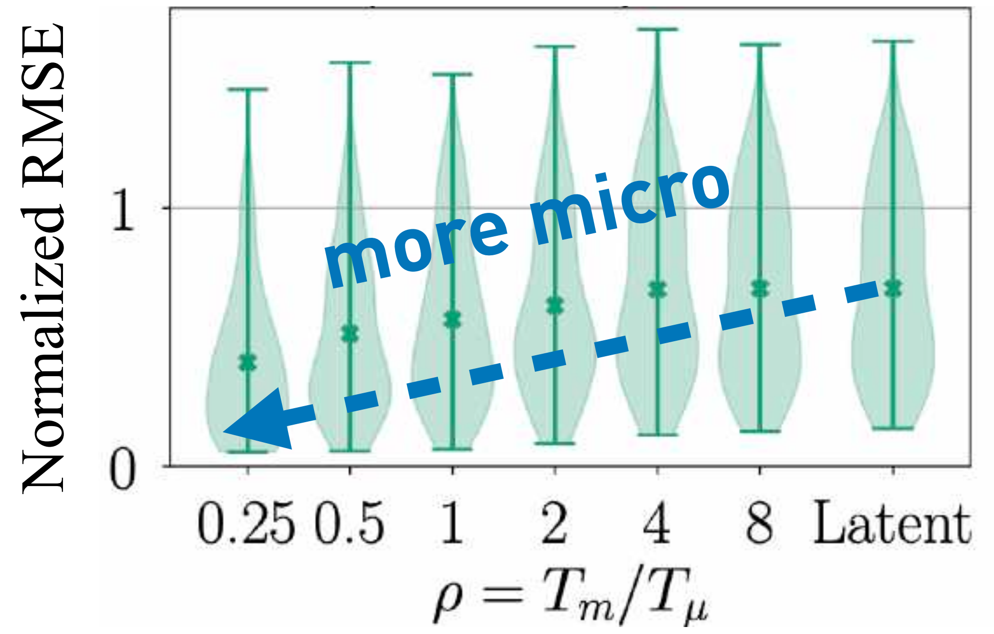

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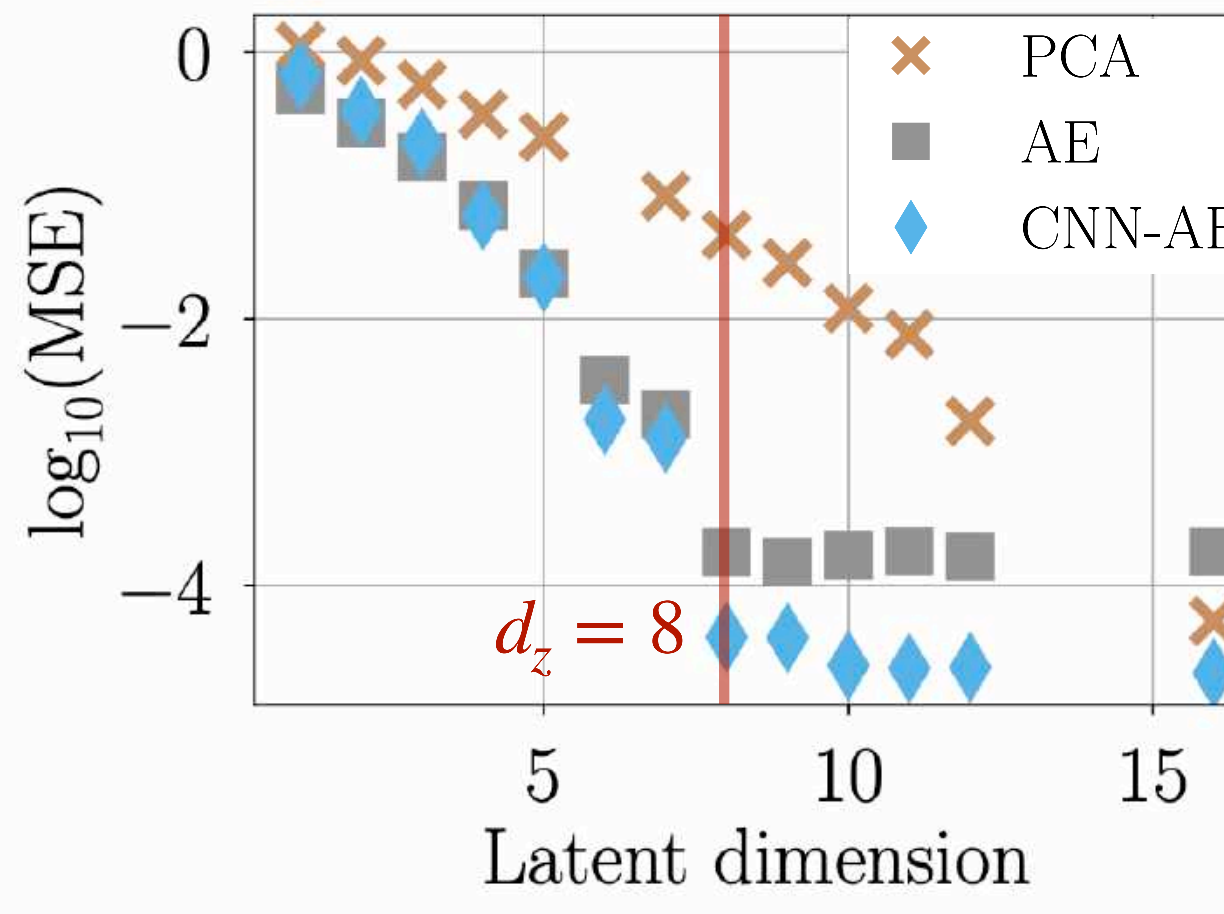

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Cylinder at $Re = 100$ - (LED $d_z = 4$)

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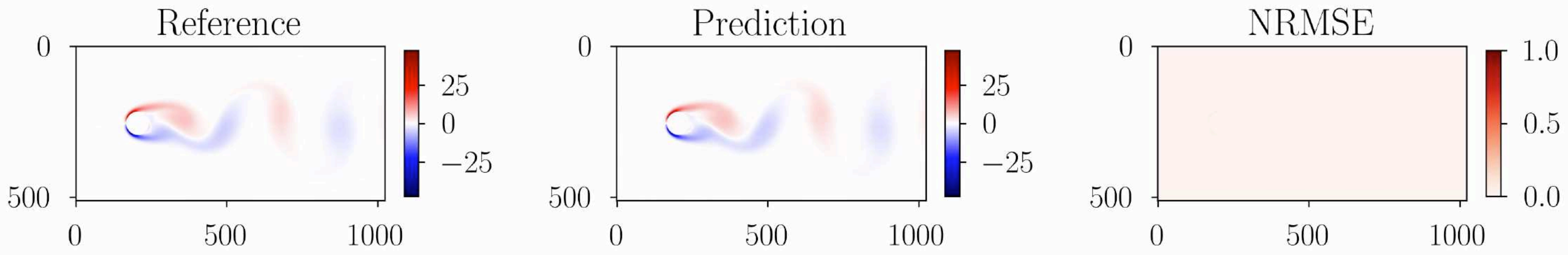

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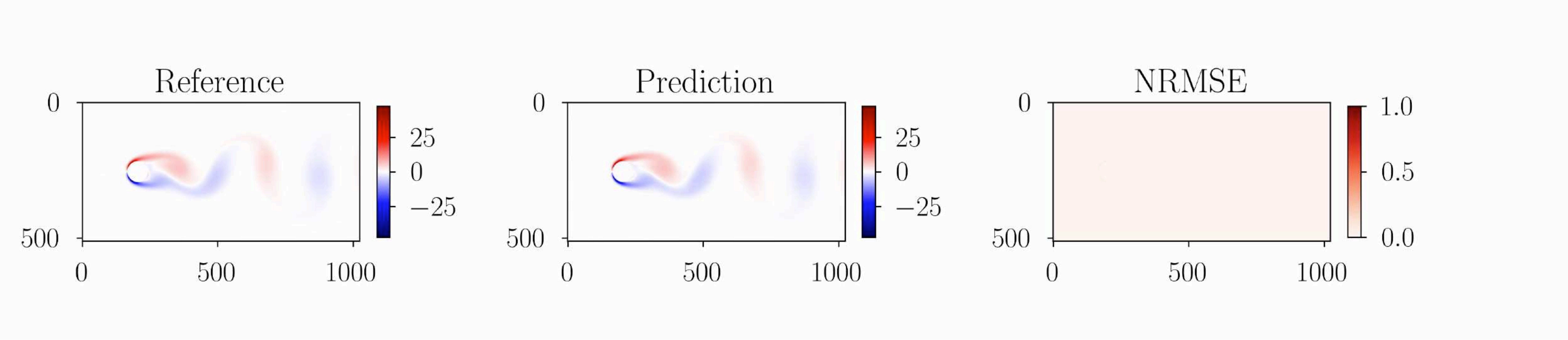

- Micro solver: Finite Differences (CubimUP2D) employing 12 cores

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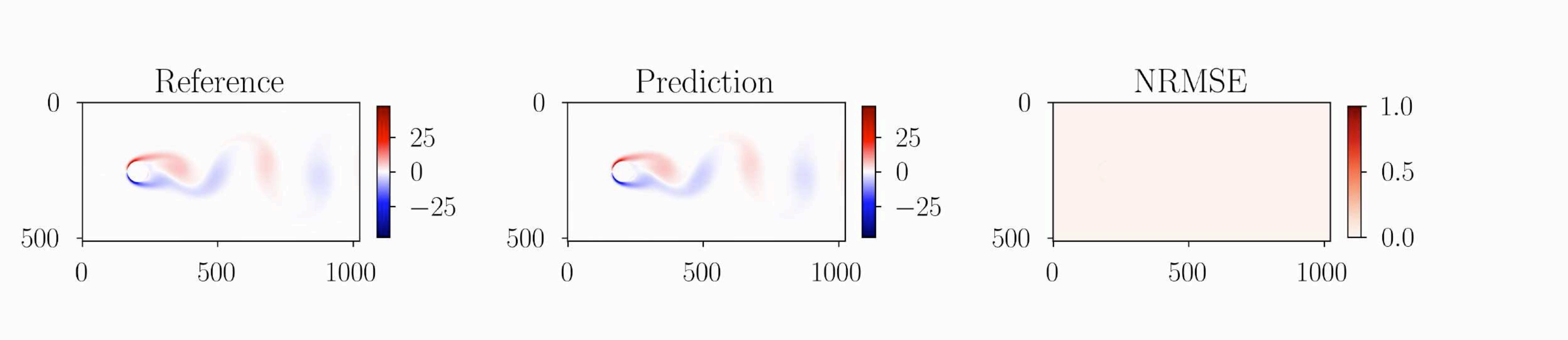

- Micro solver: Finite Differences (CubimUP2D) employing 12 cores
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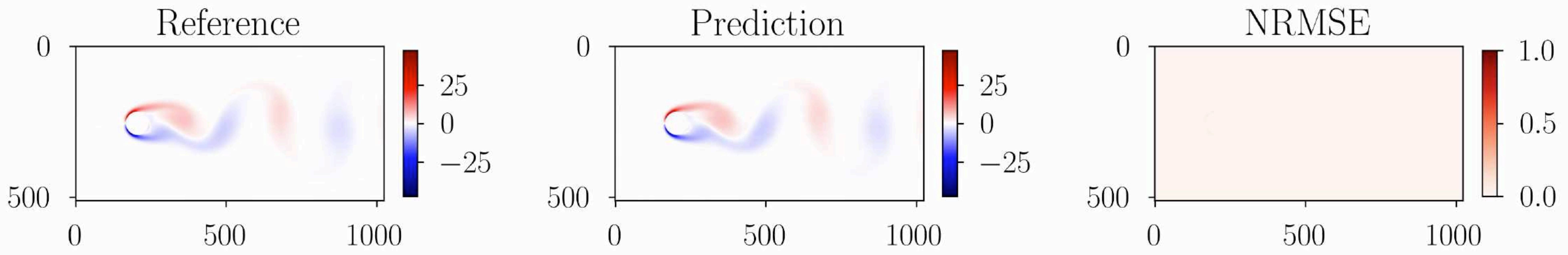

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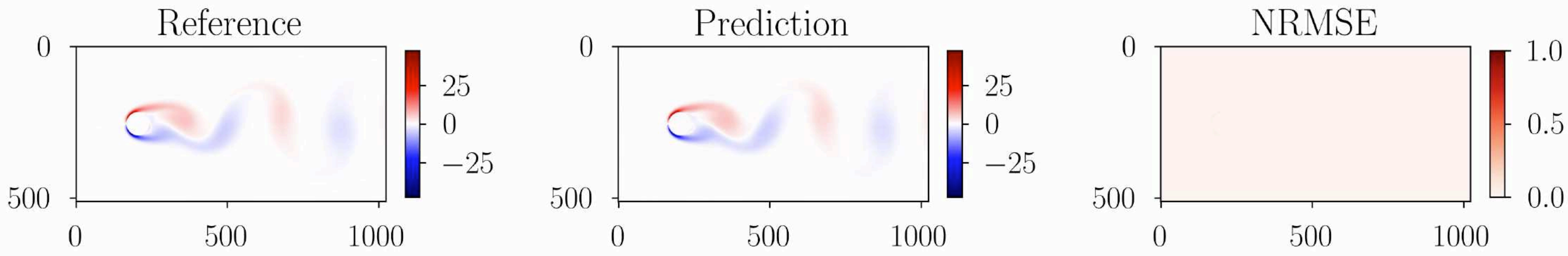

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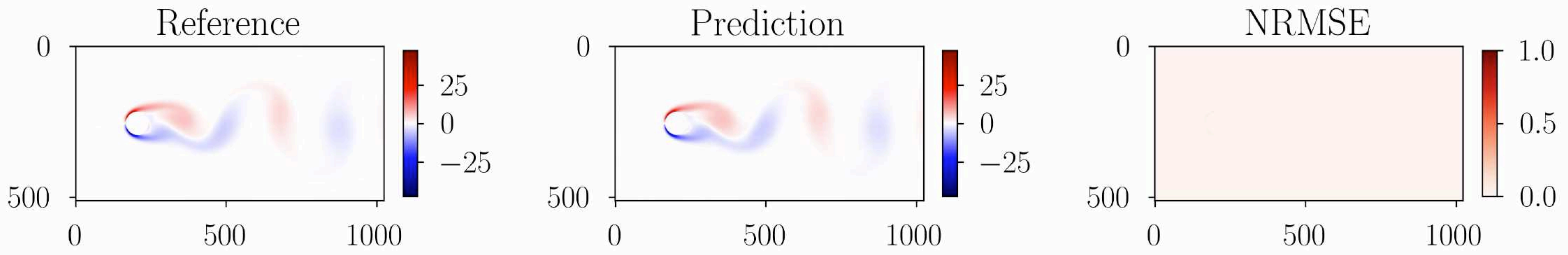

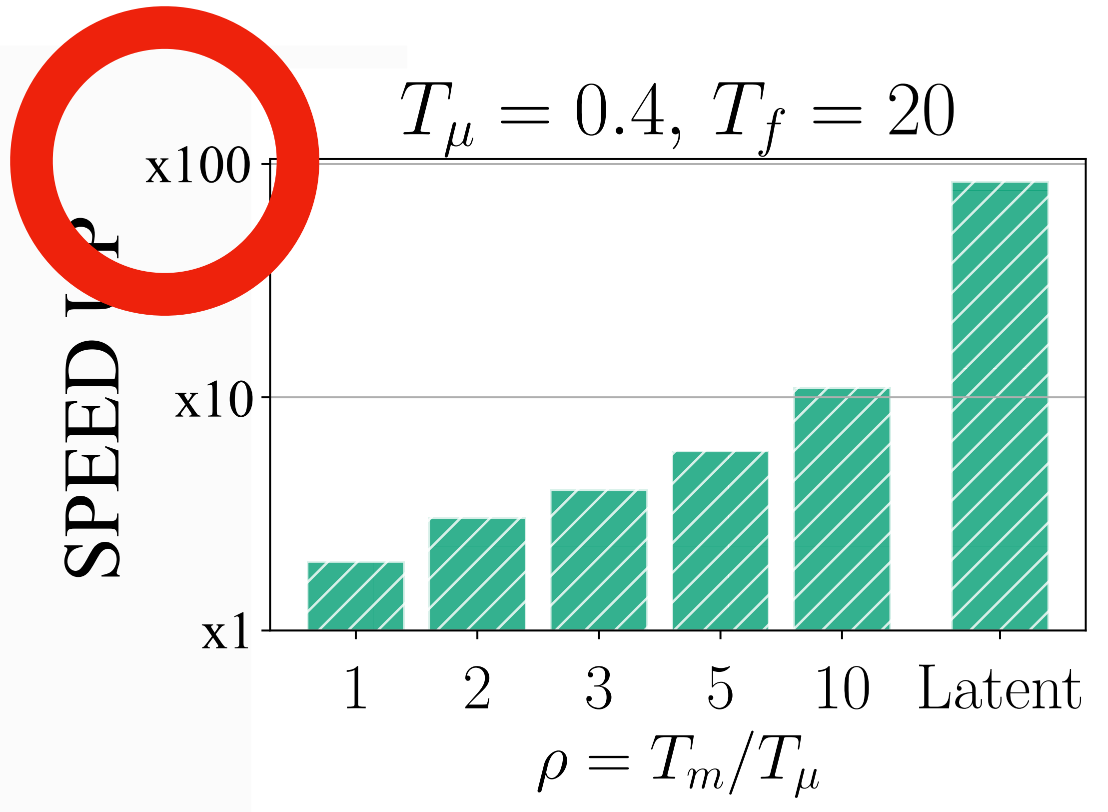

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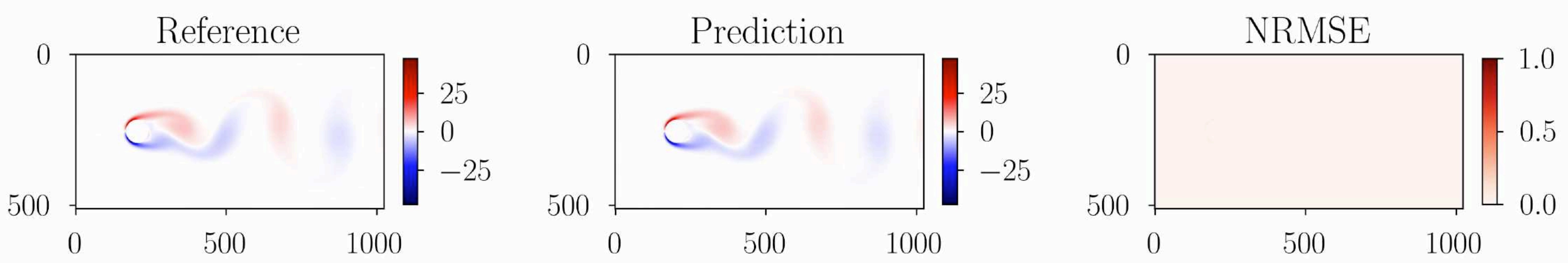

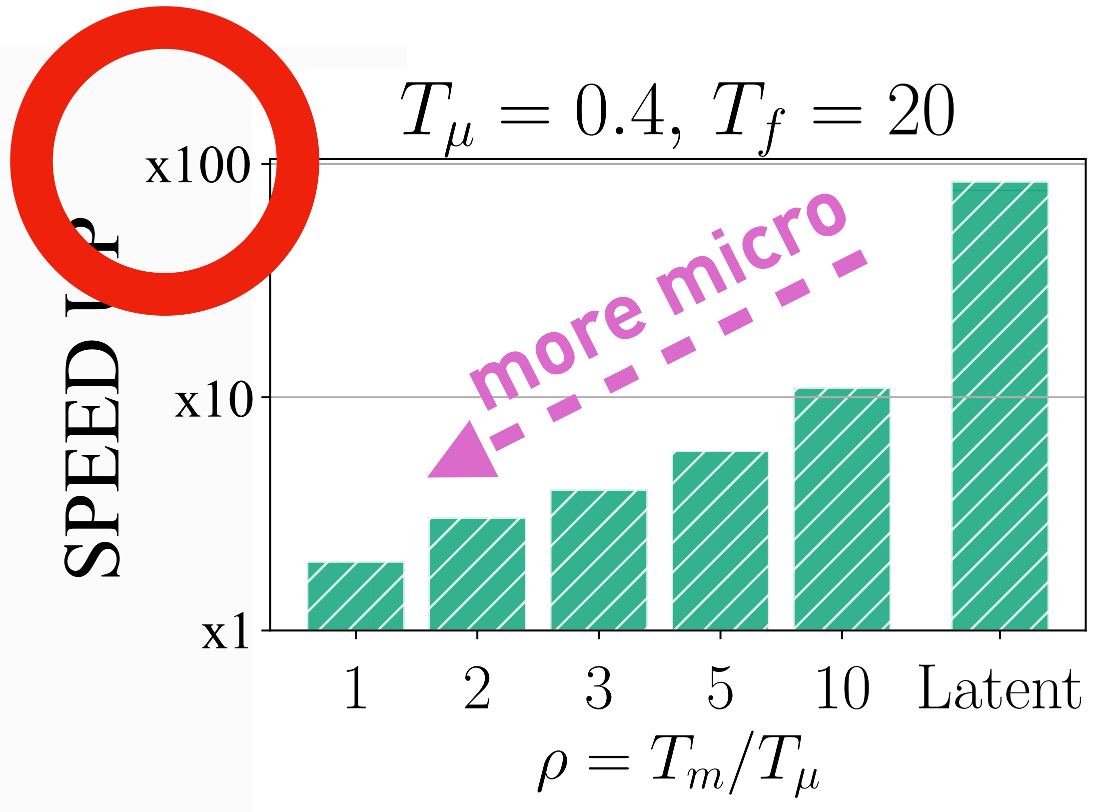

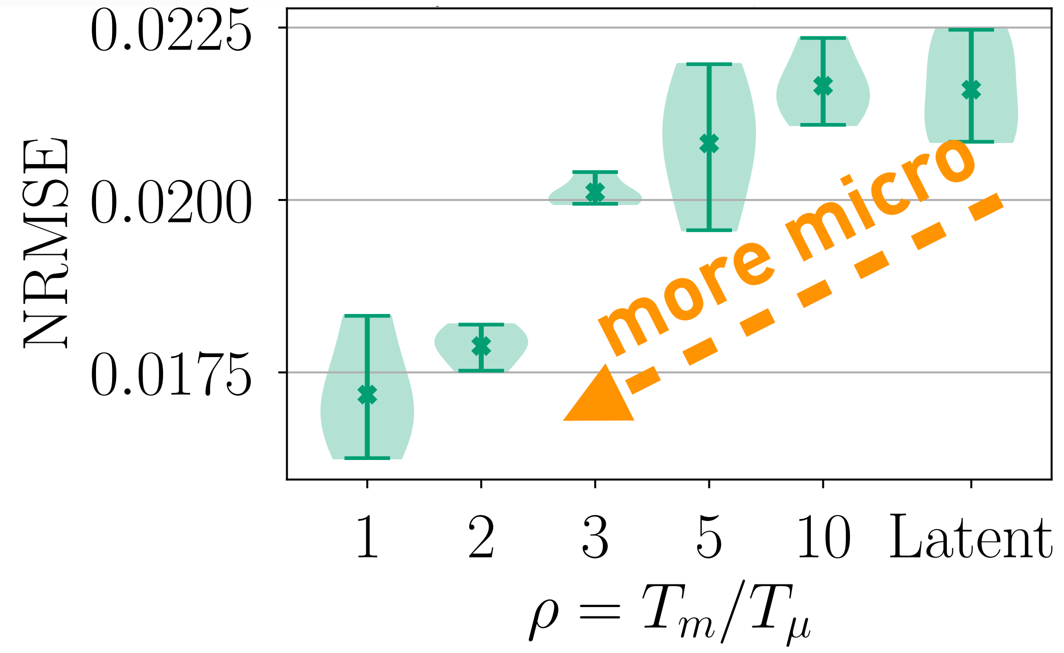

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- Multiscale LED reduces the approximation error at the cost of reduced speed-up

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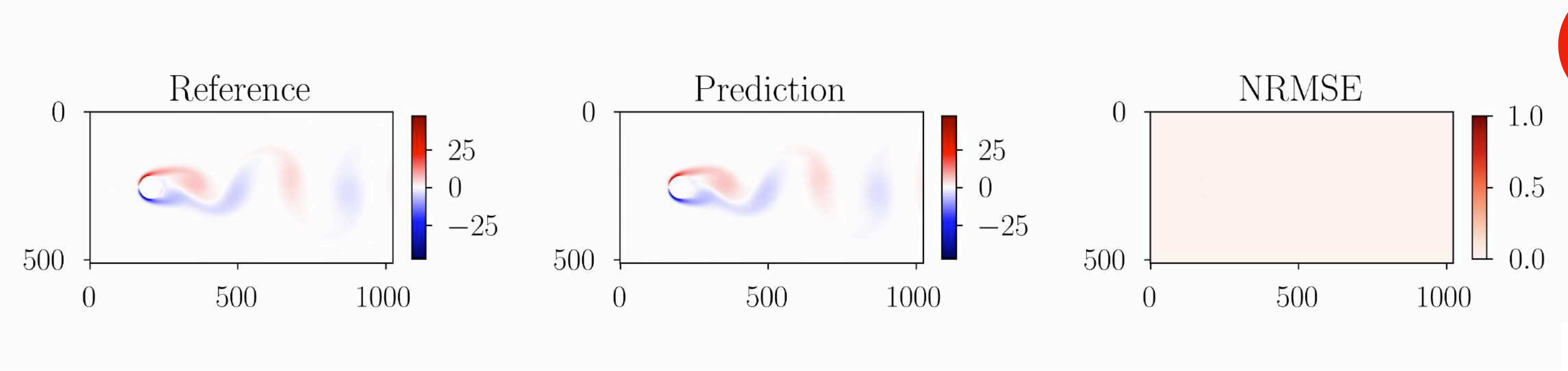

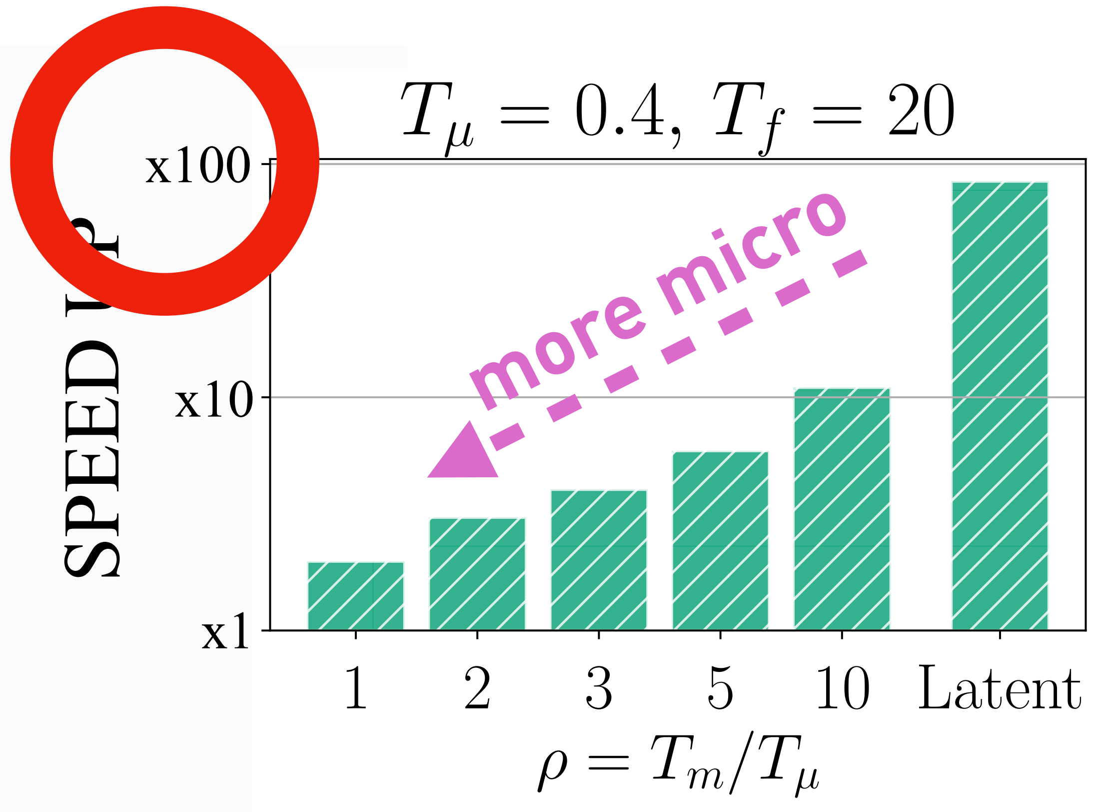

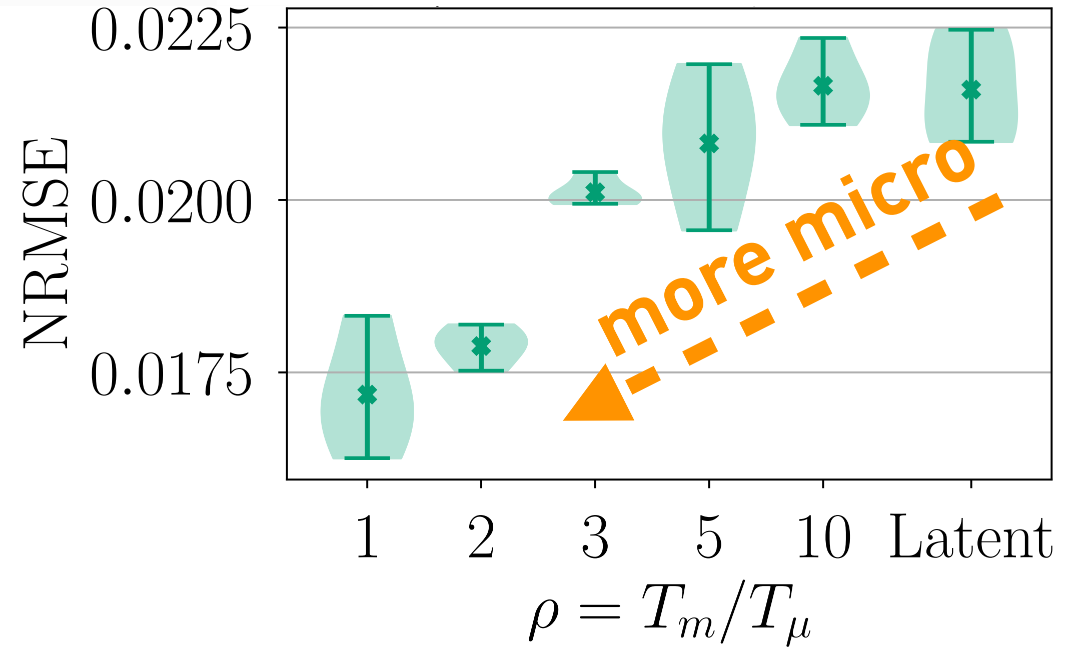

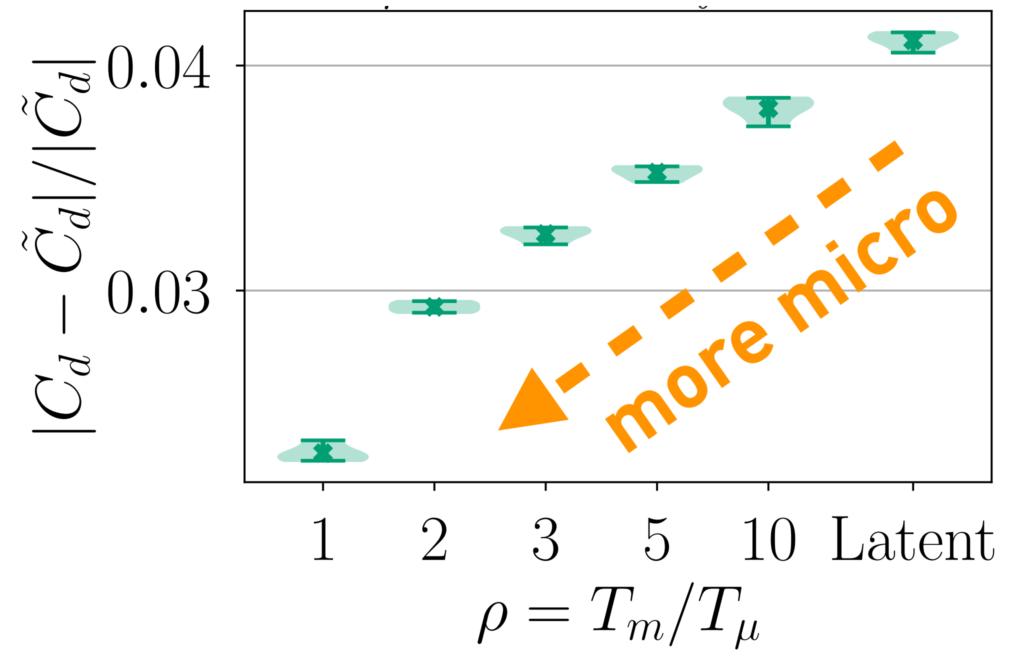

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- LED captures **long-term evolution** of velocity and pressure fields (low NRMSE)
- LED is up to **two orders of magnitude** faster than CubismUP2D
- Multiscale LED reduces the approximation error at the cost of reduced speed-up
- Recovers drag coefficient with $\approx 2 - 4\,\%$ error

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

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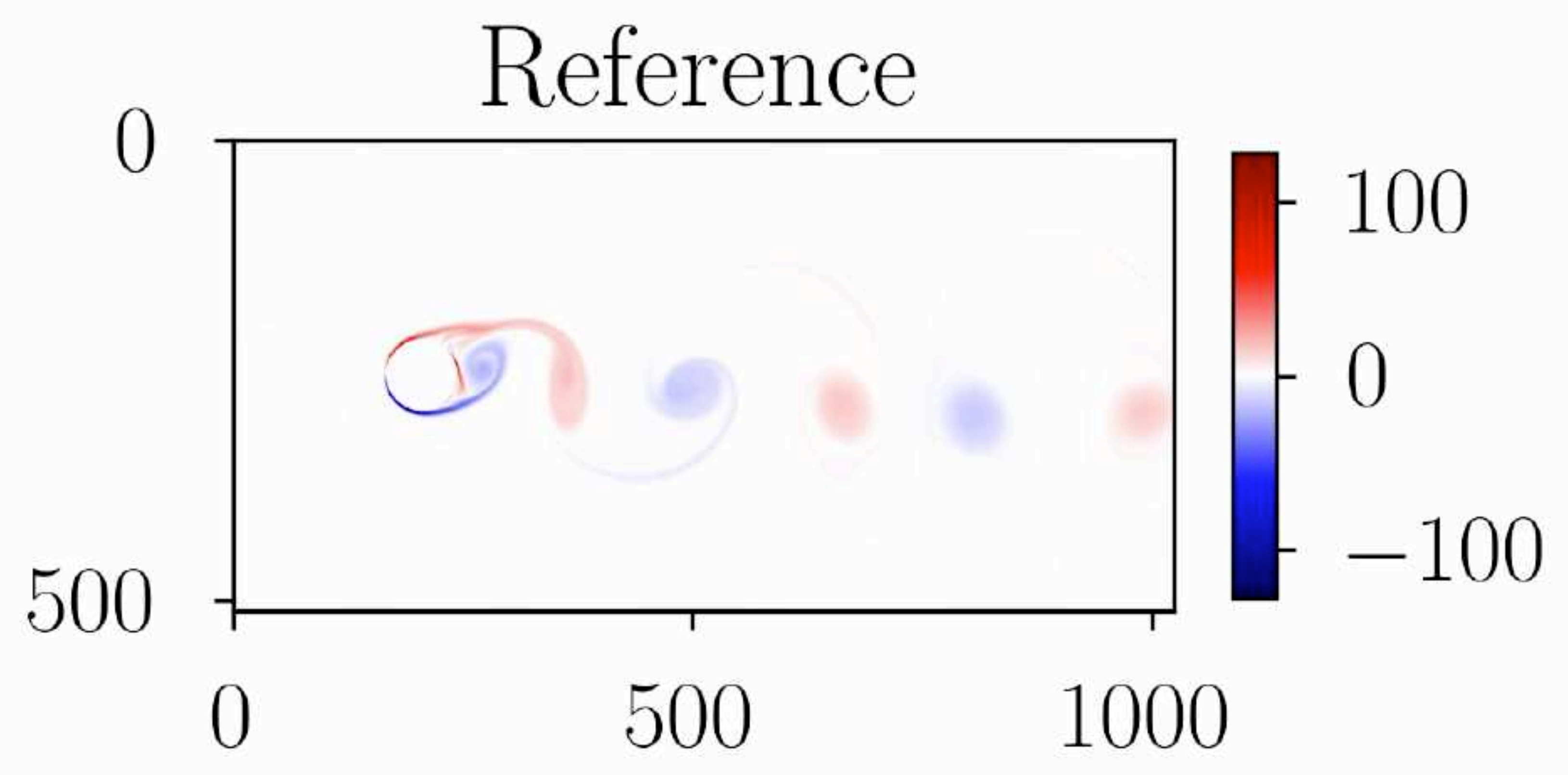

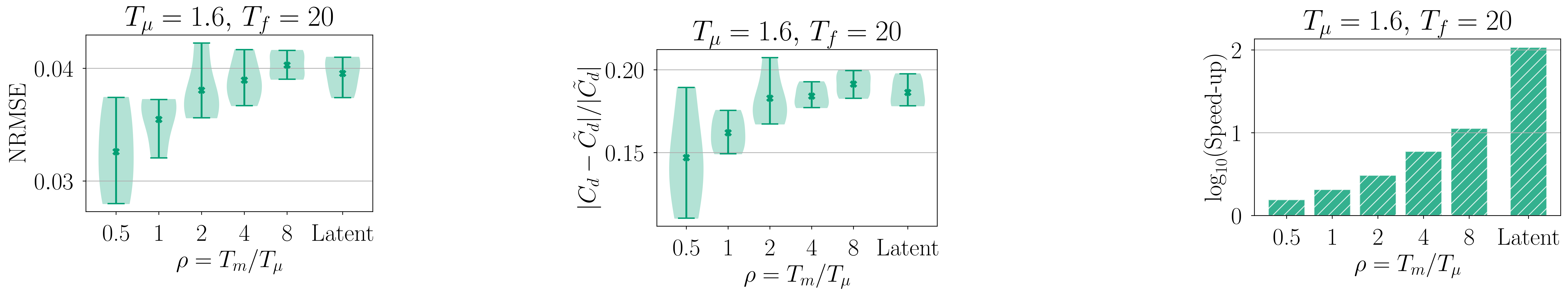

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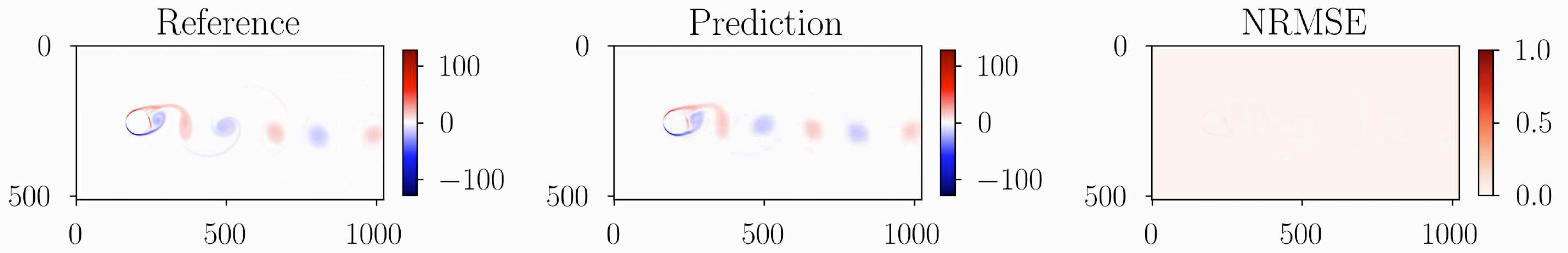

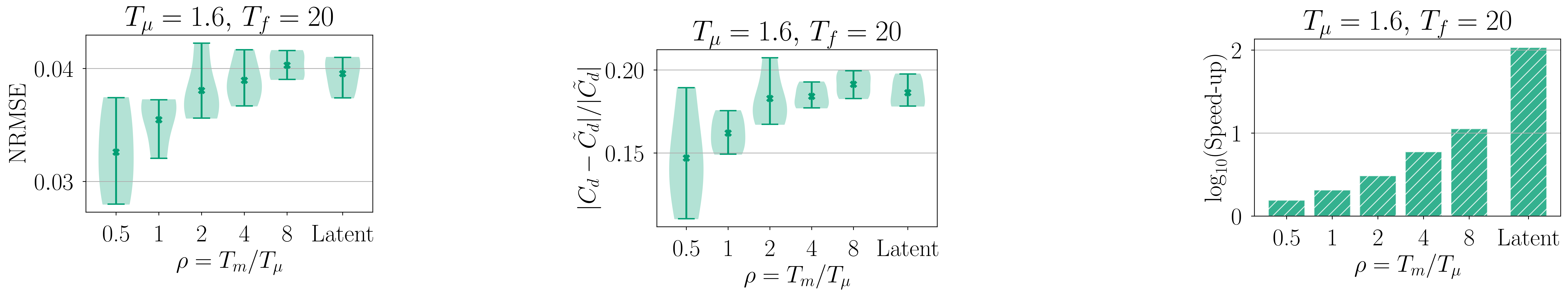

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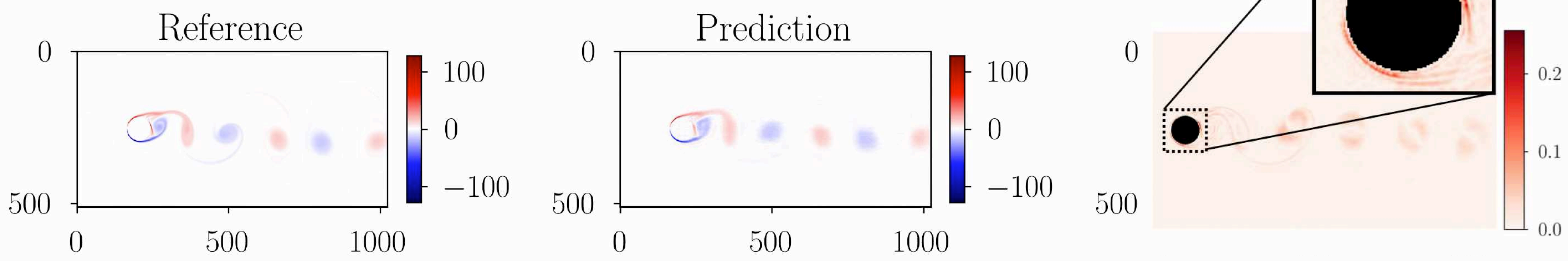
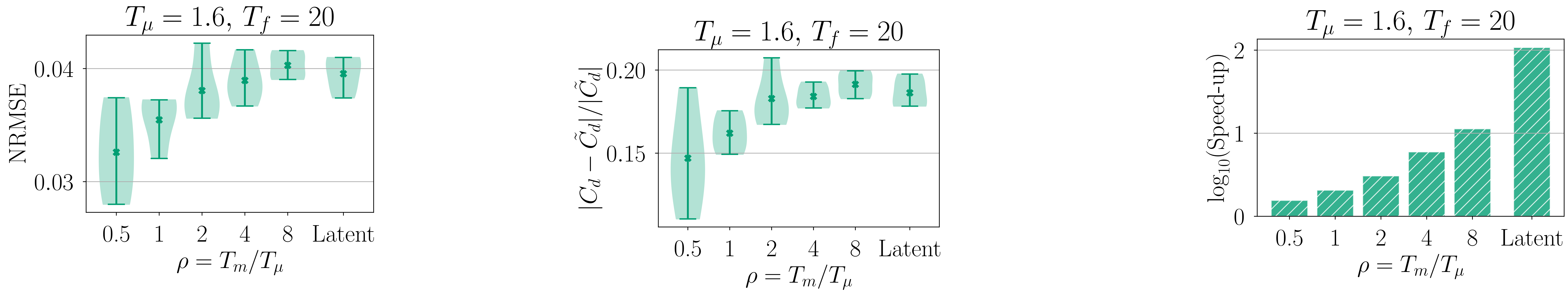
Most error is concentrated around the cylinder !





Comparisons of Latent Propagators

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

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

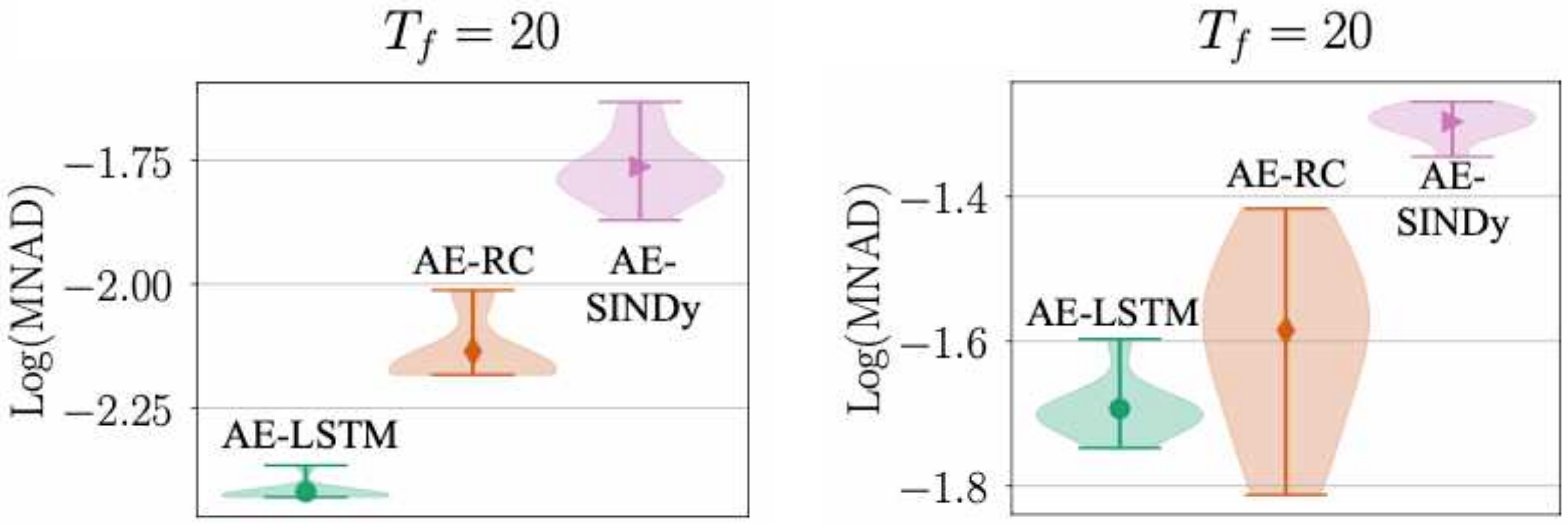
RC — **J Pathak, B Hunt, M Girvan, Z Lu, E Ott,** *Model-free prediction of large spatiotemporally chaotic systems from data: A reservoir computing approach,* **Physical review letters, 2018**

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

Mean normalised absolute difference:

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

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



$Re = 100$ $Re = 1000$

III

Learning Effective Dynamics for Molecular Systems

Alanine Dipeptide

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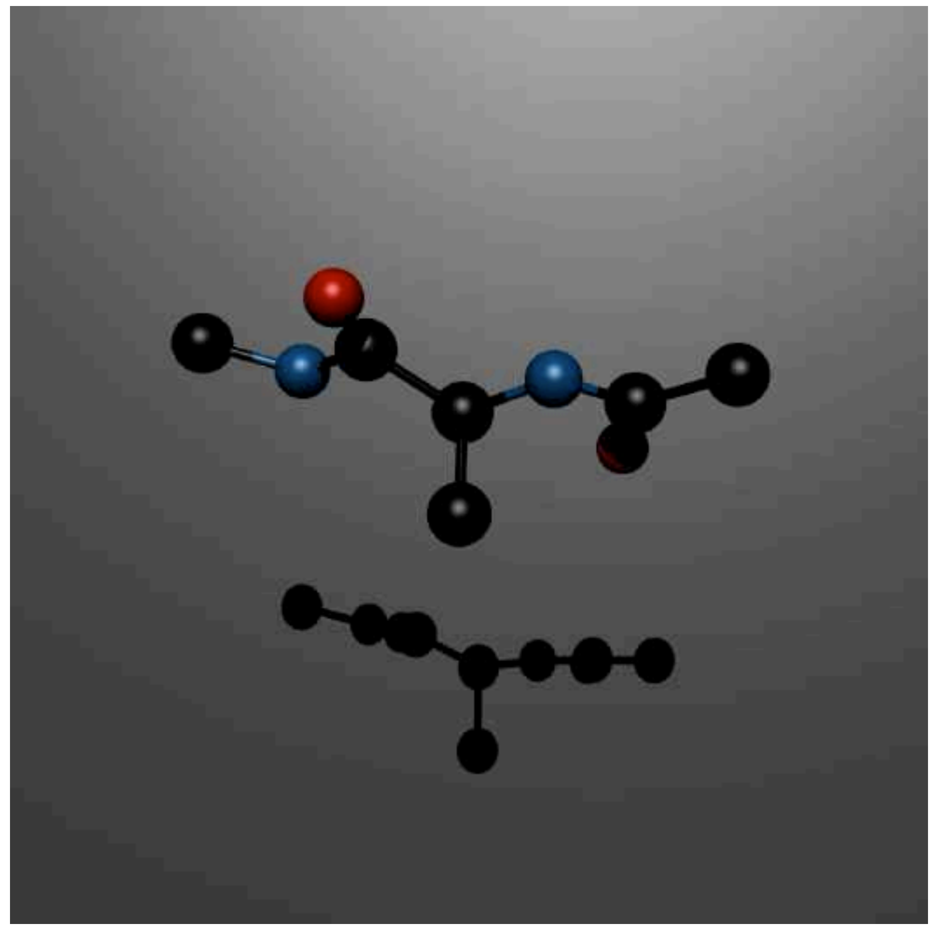
Journal of Chemical Theory & Computation, 2021



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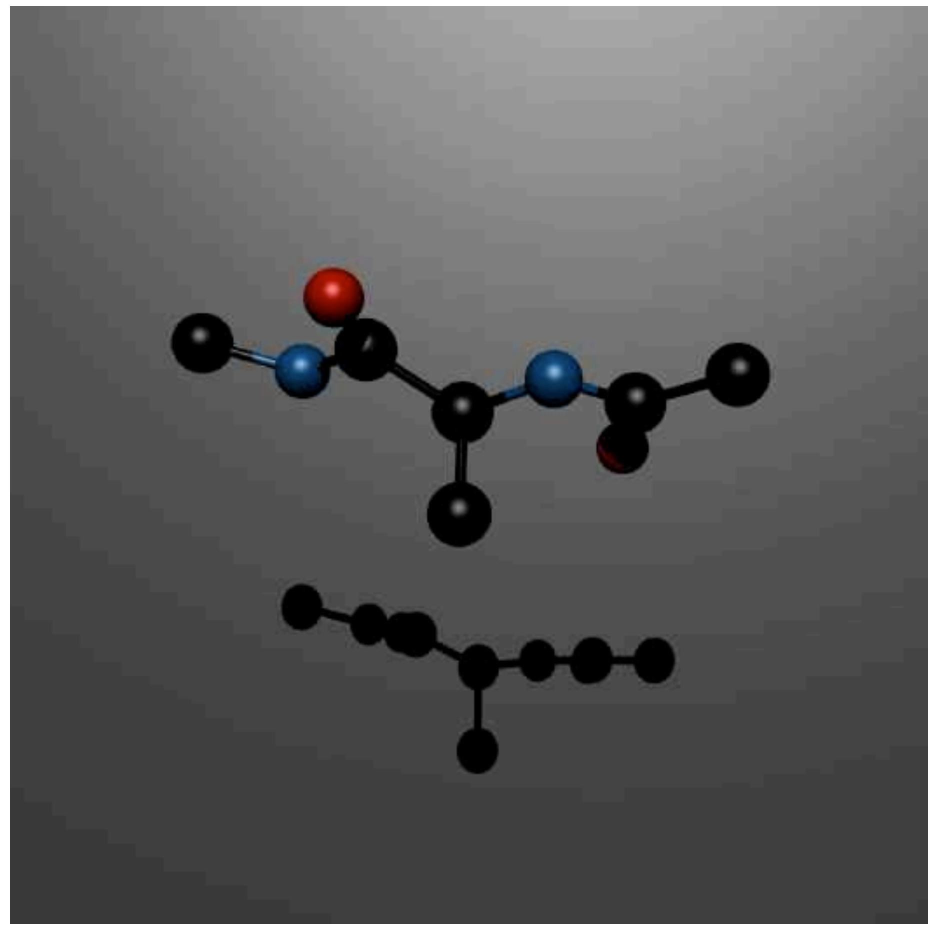

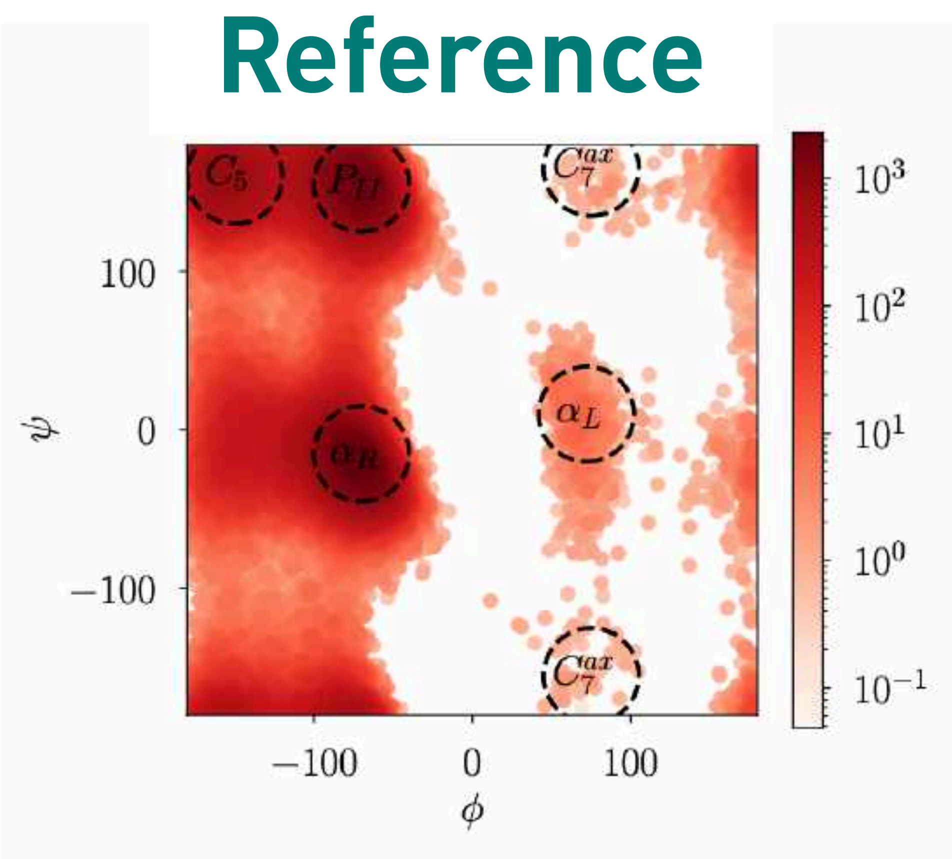

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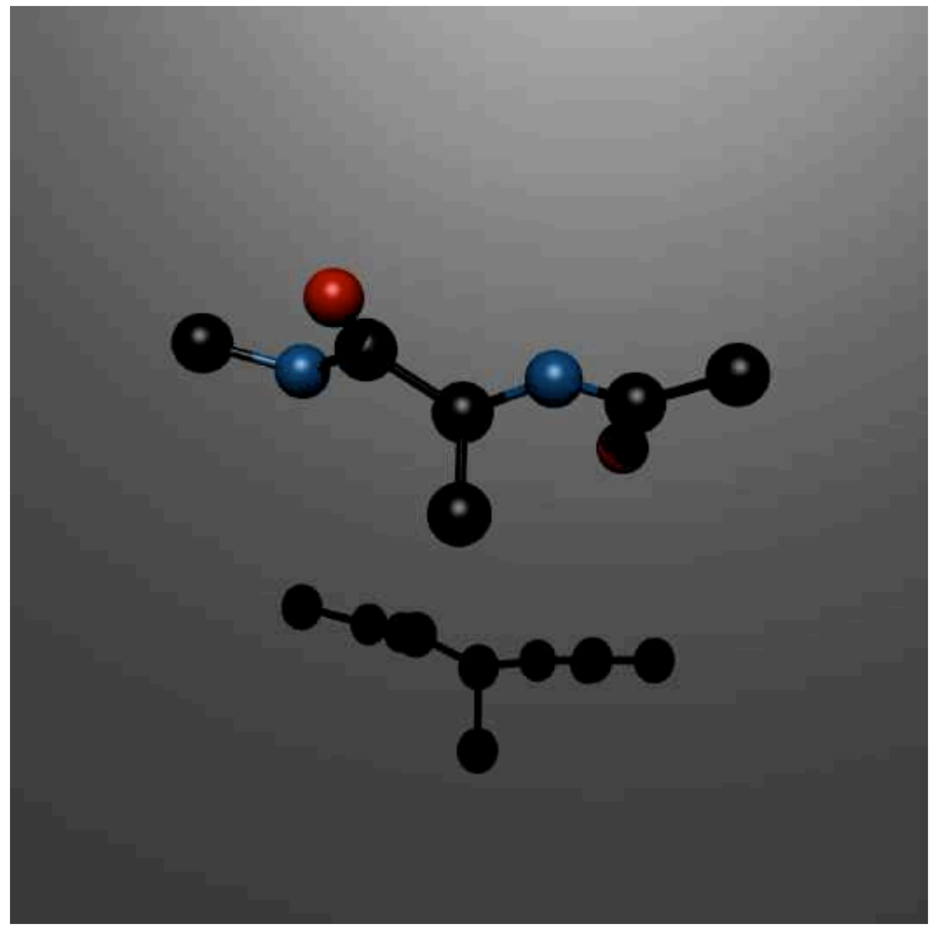

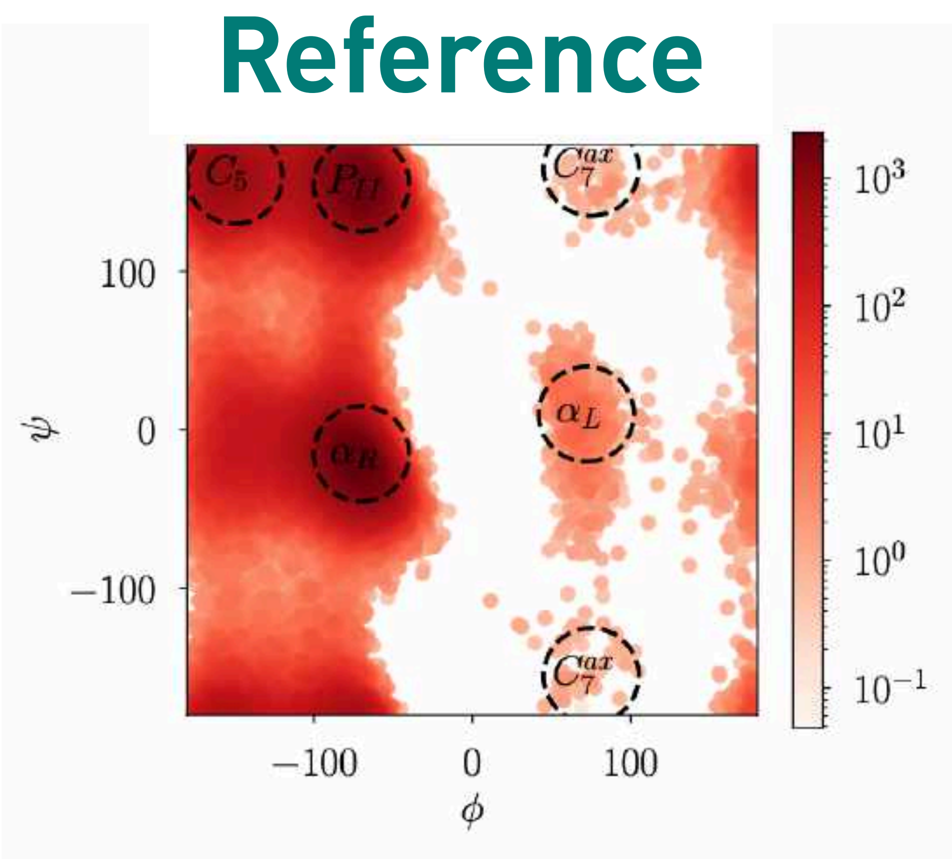

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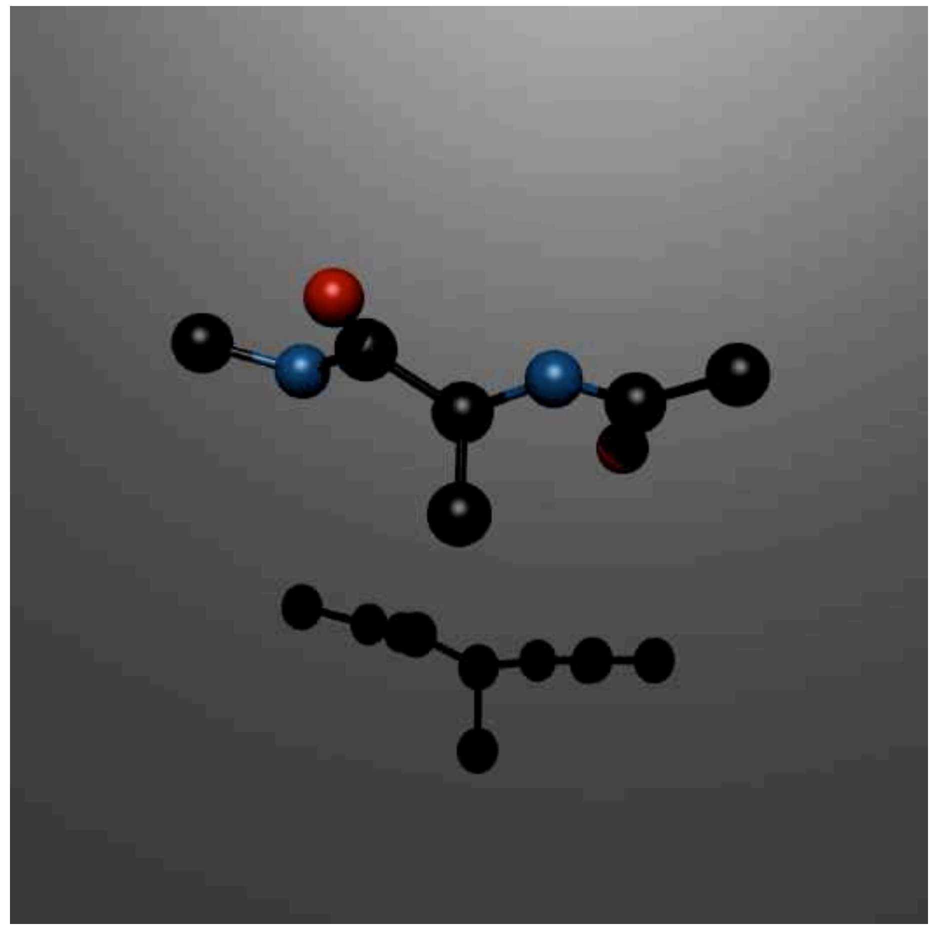

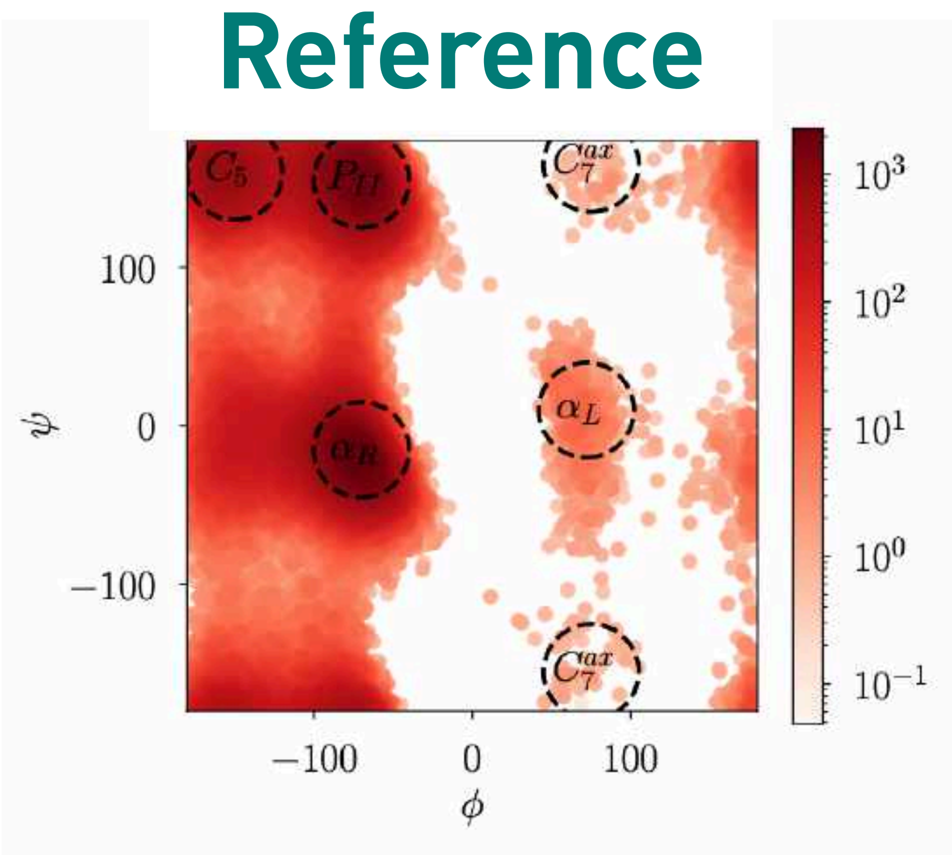

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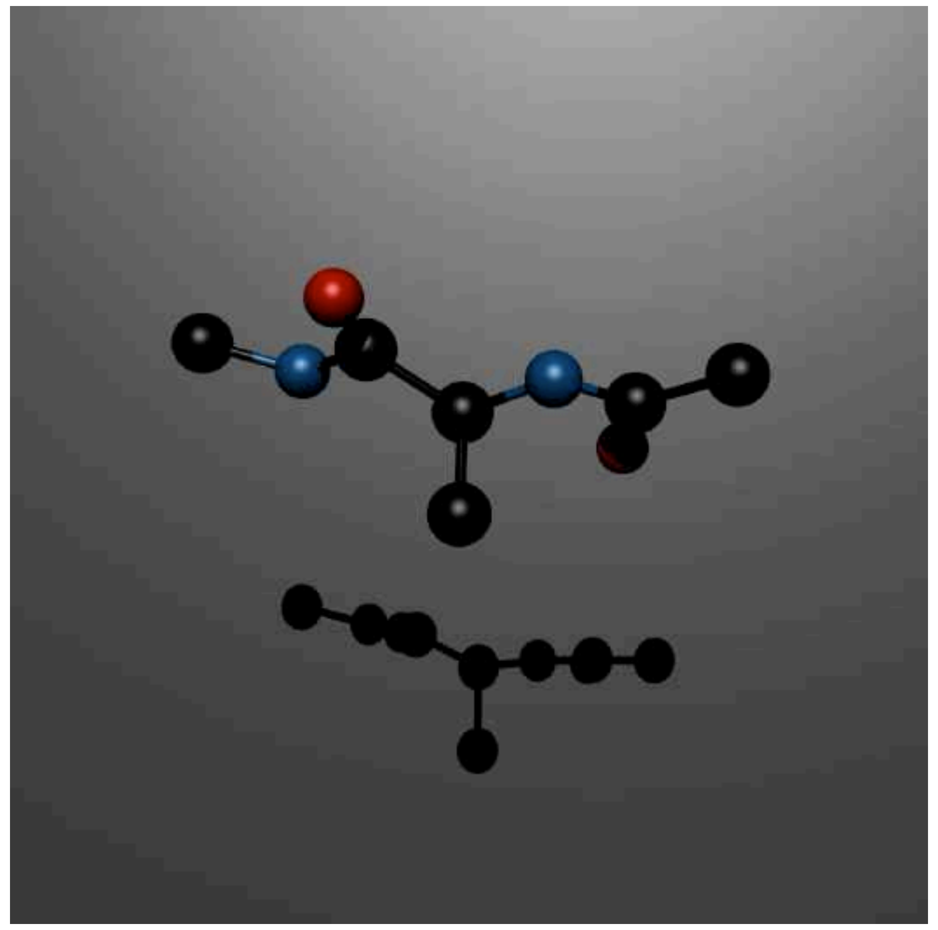

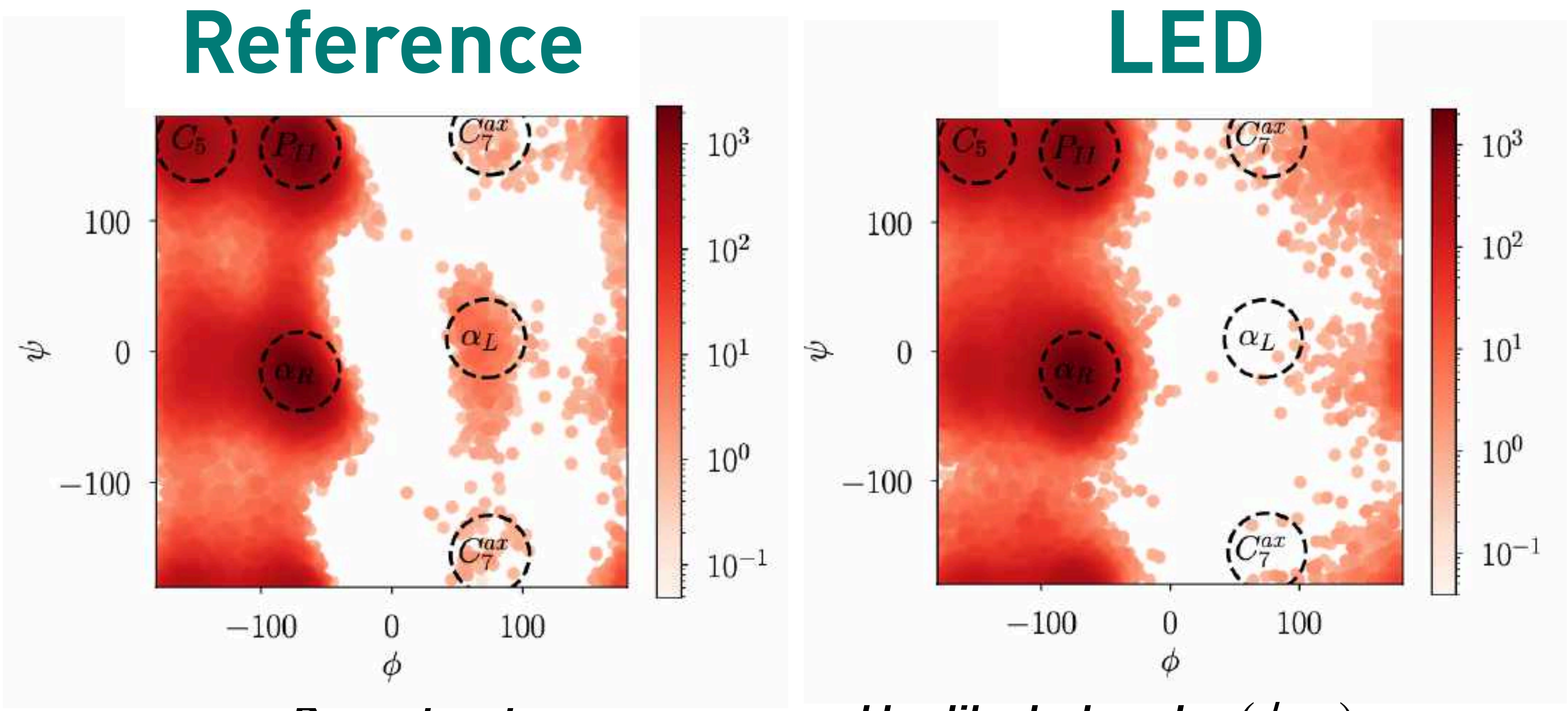

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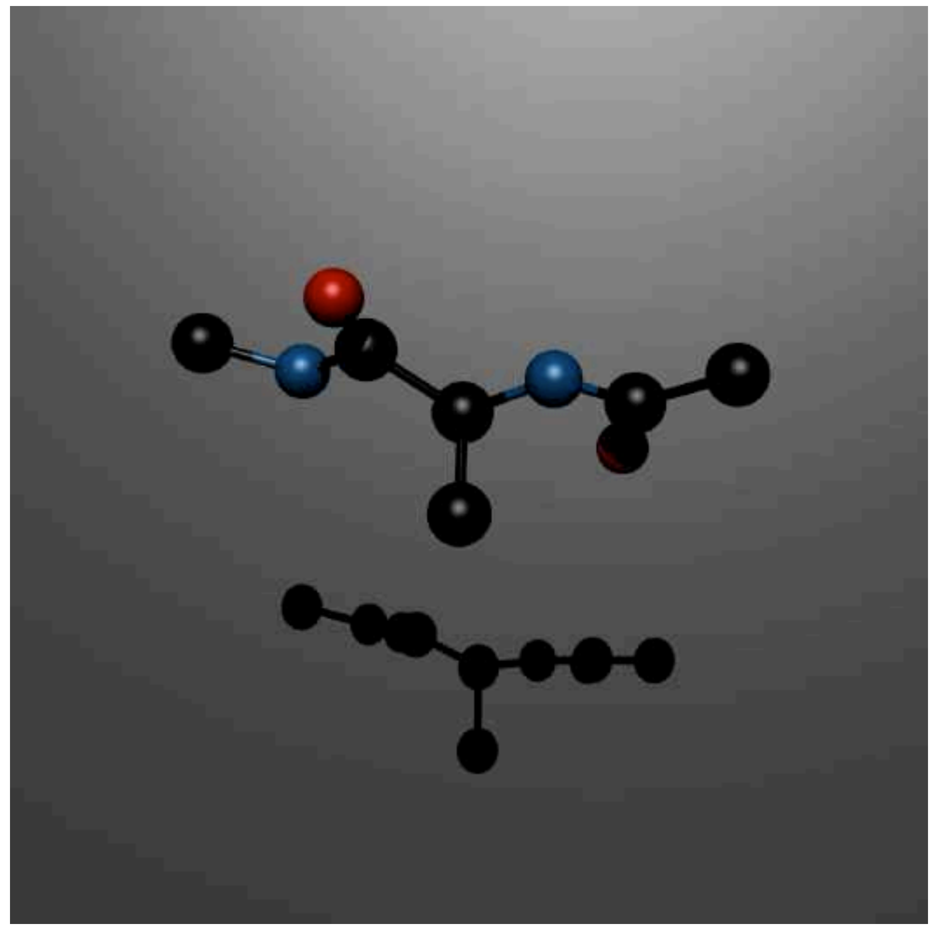

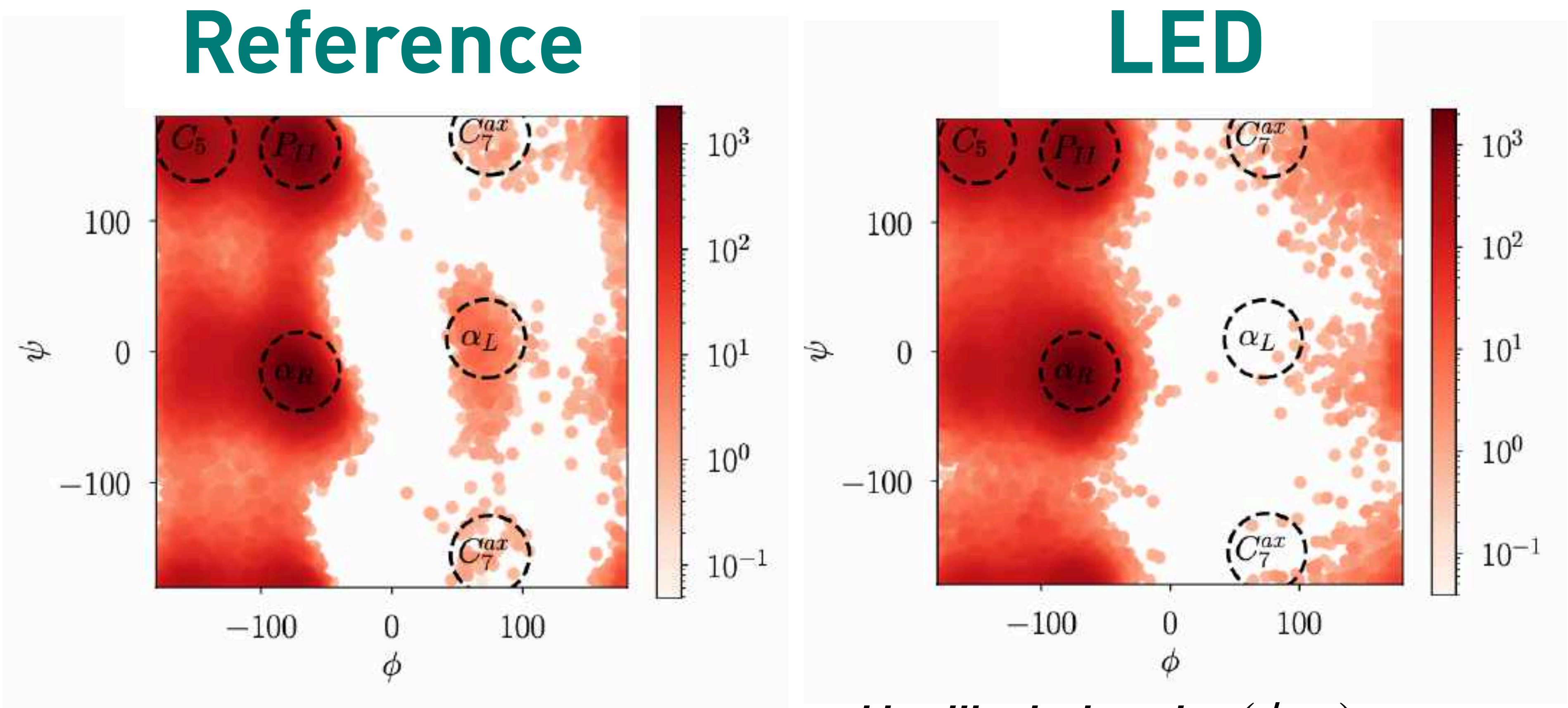

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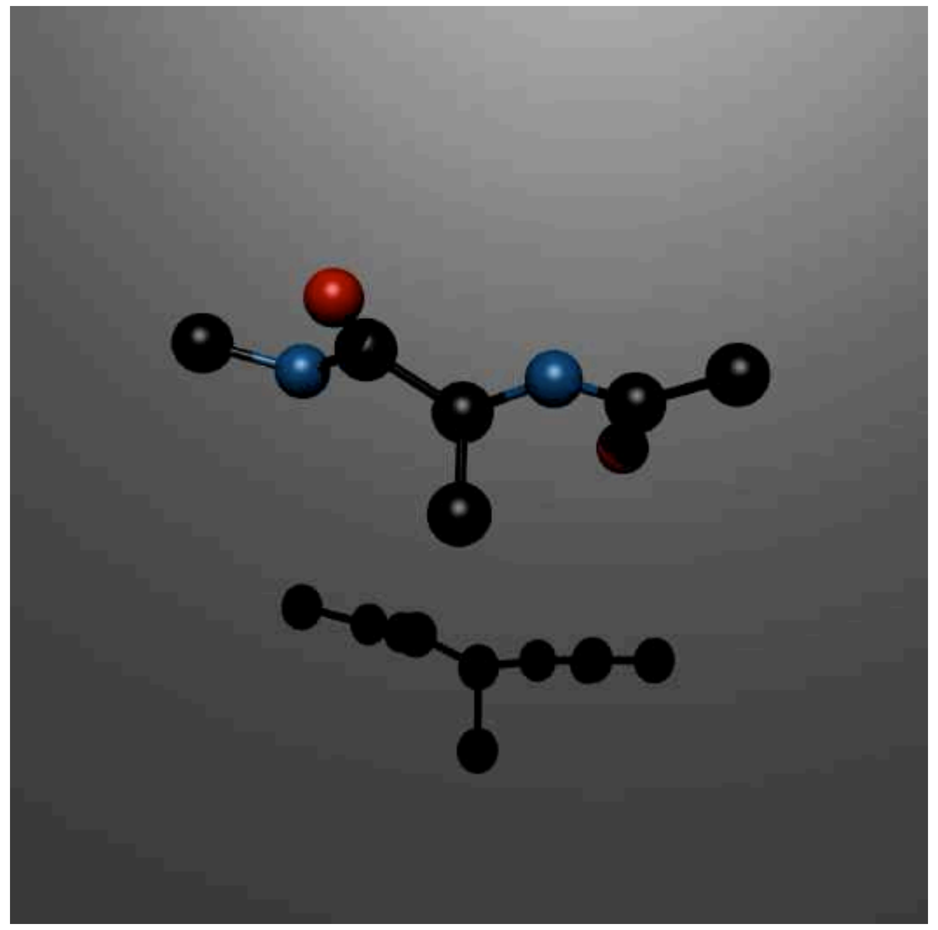

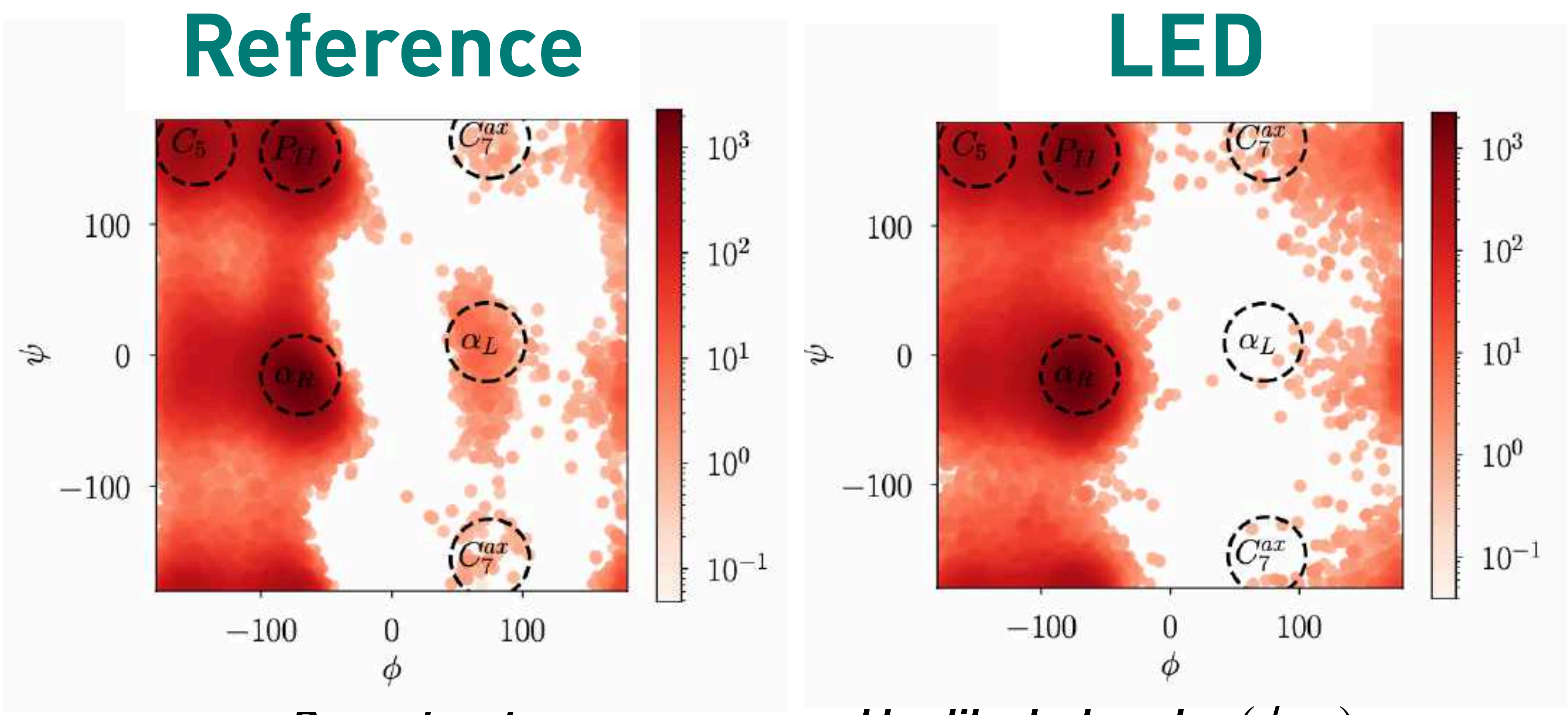

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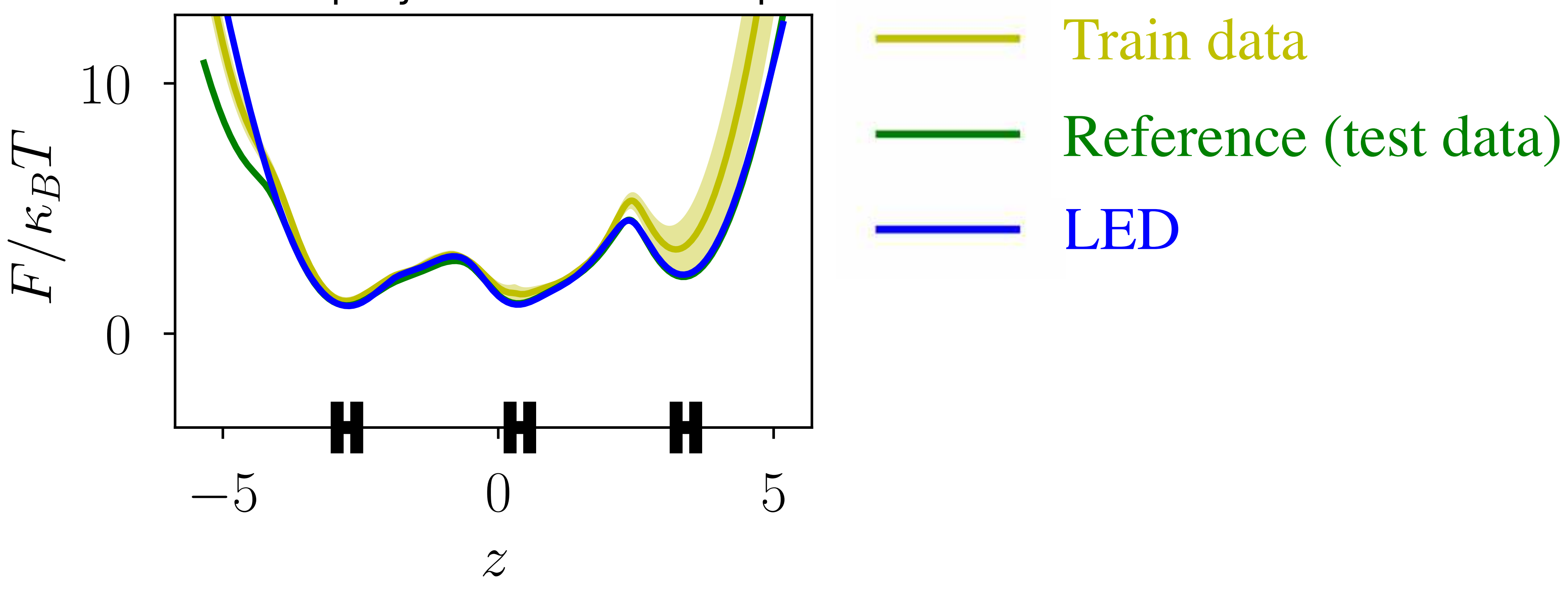

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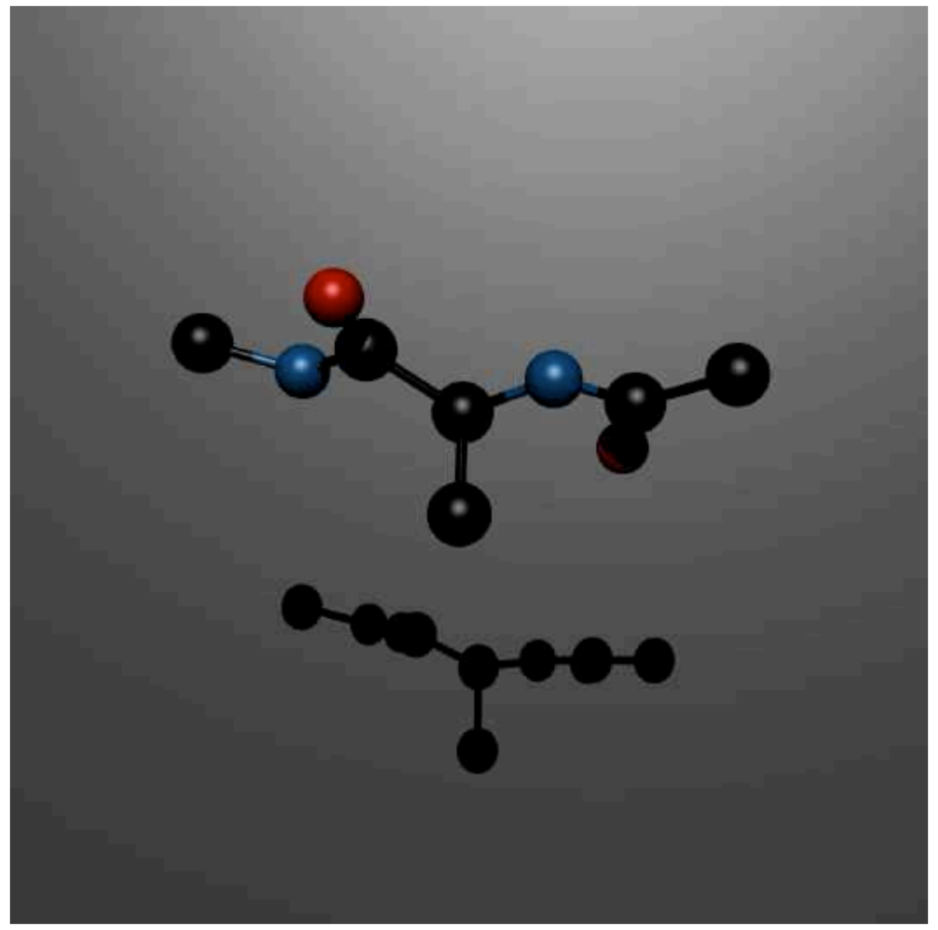

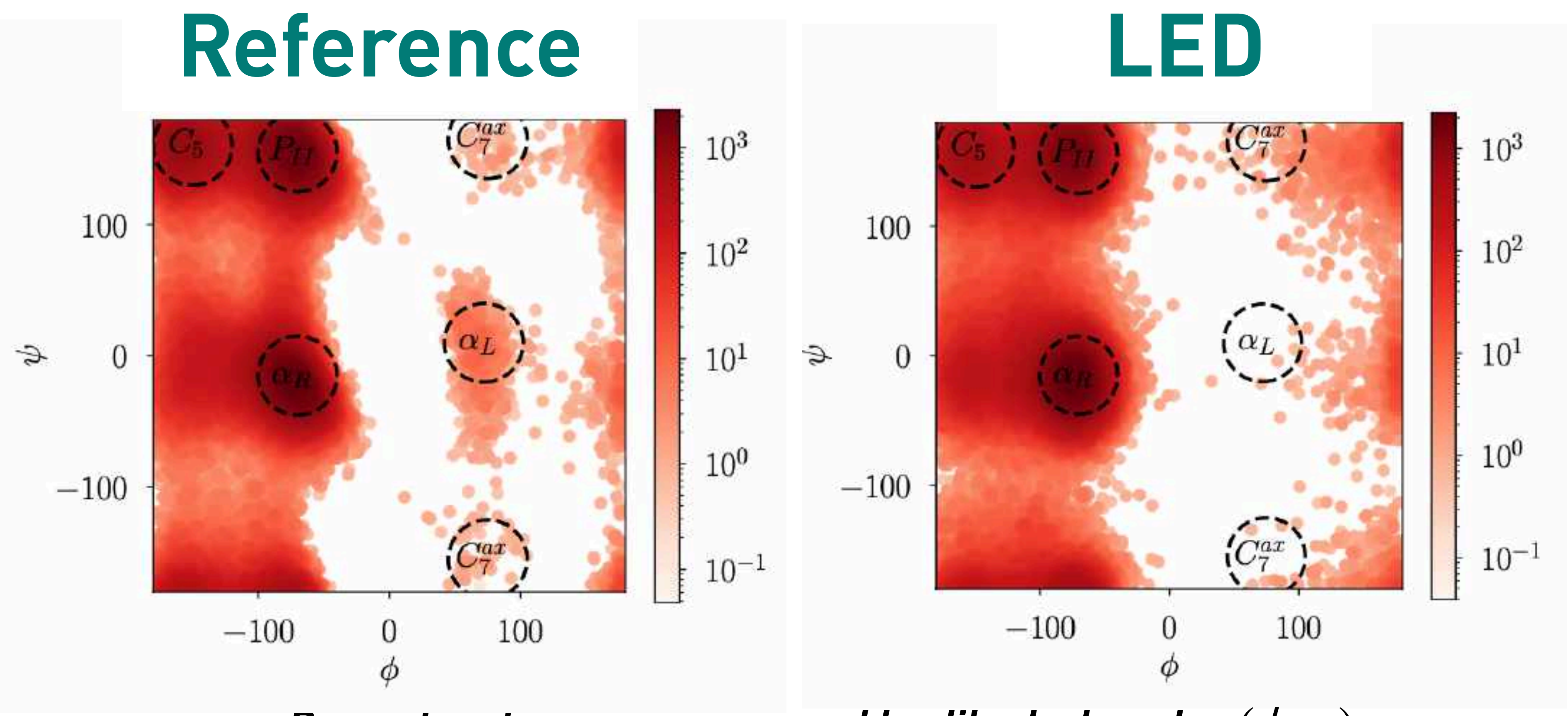

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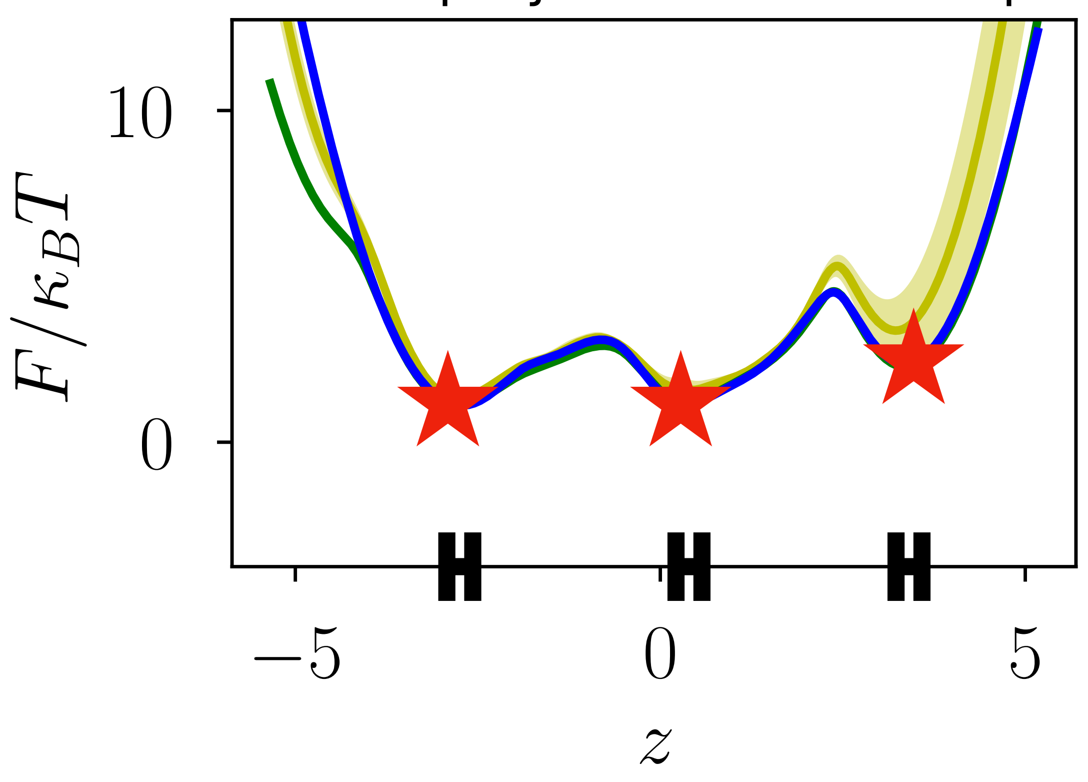

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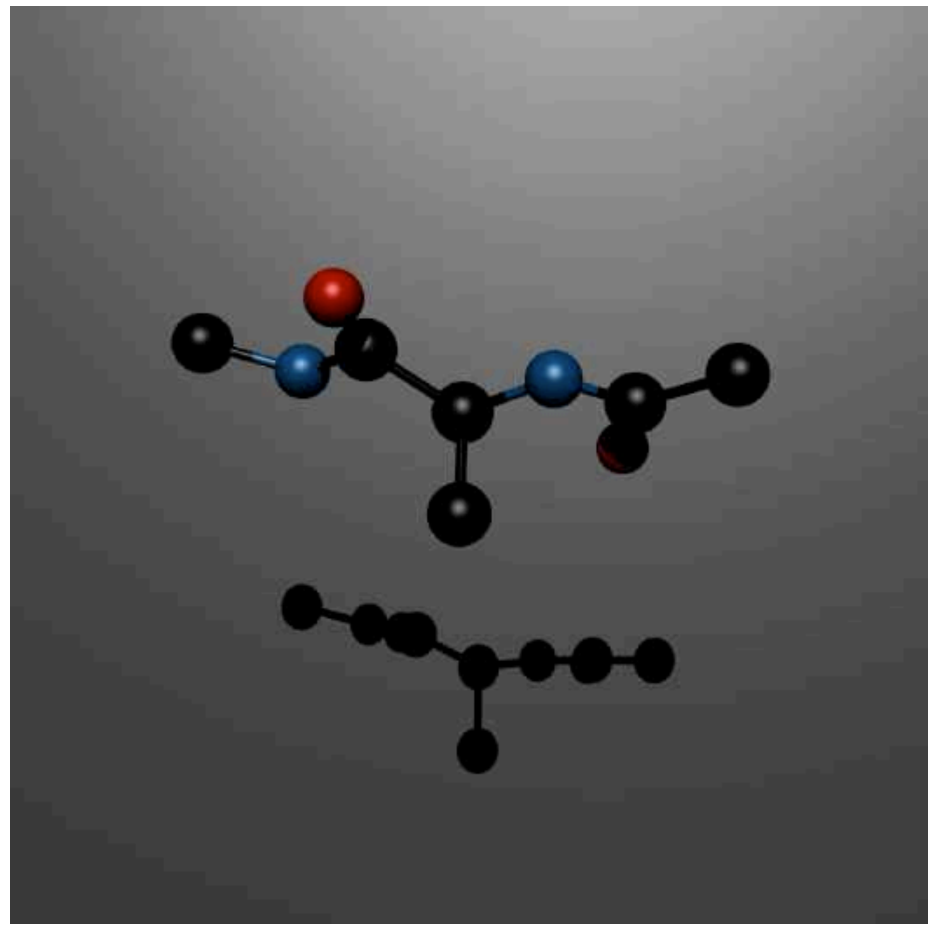

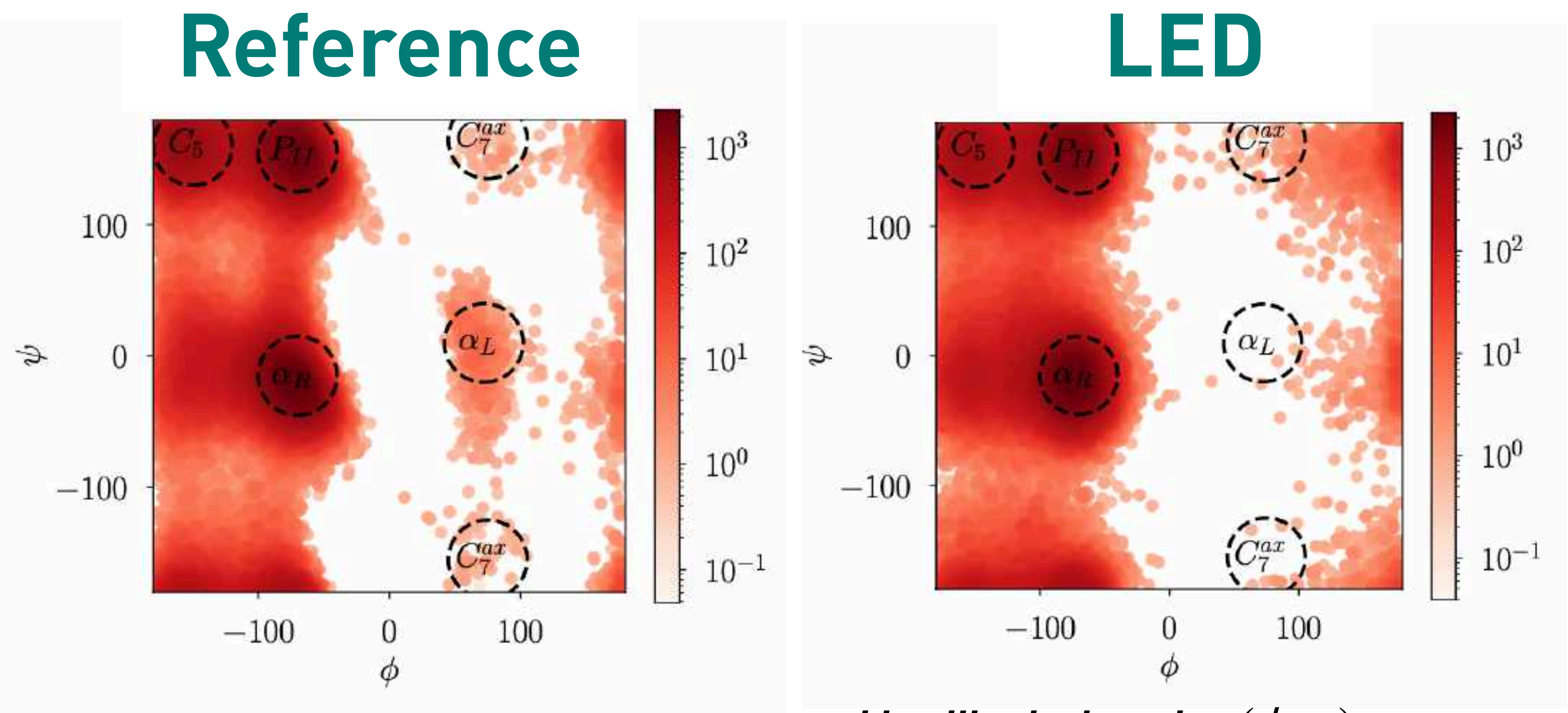

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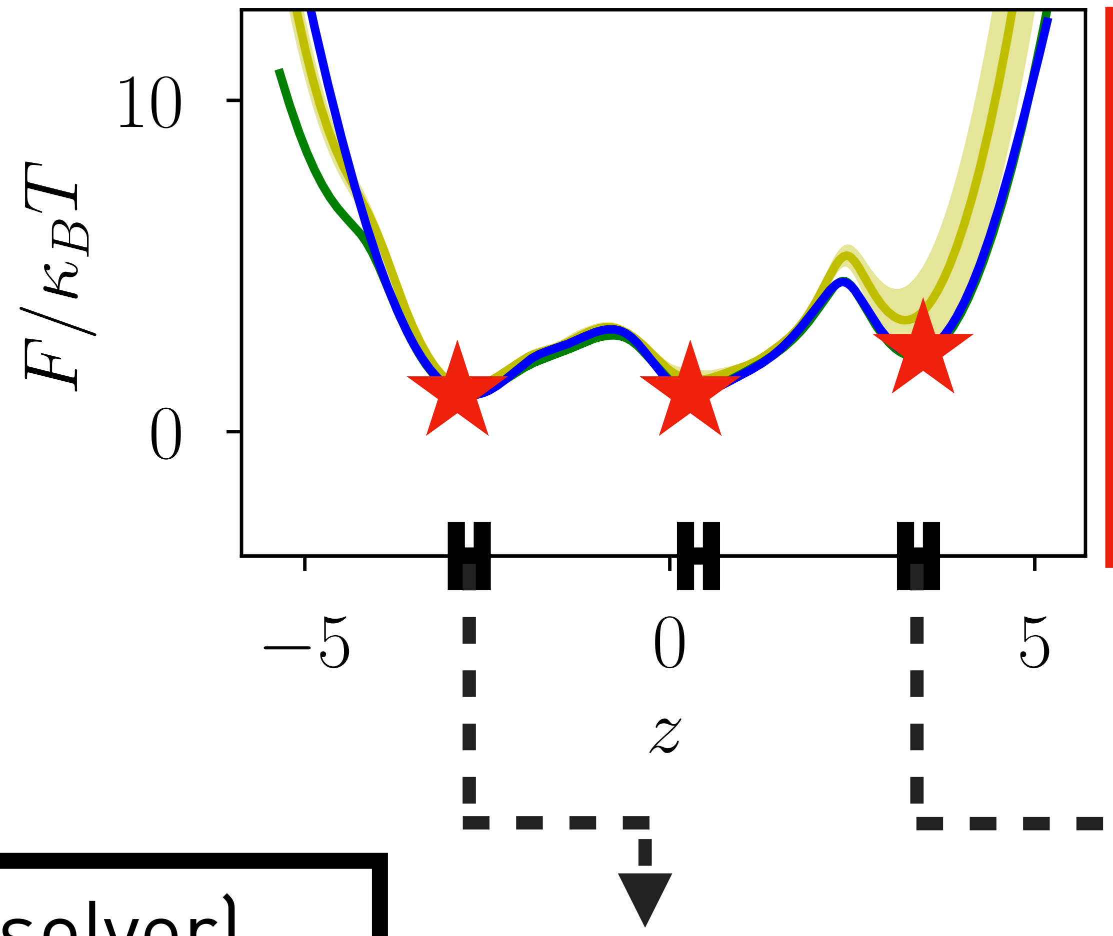

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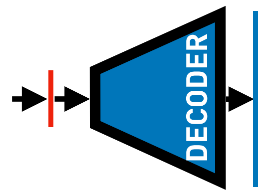

$\mathbf{z}_t \rightarrow$ DECODER $\sim \mathbf{s}_t$

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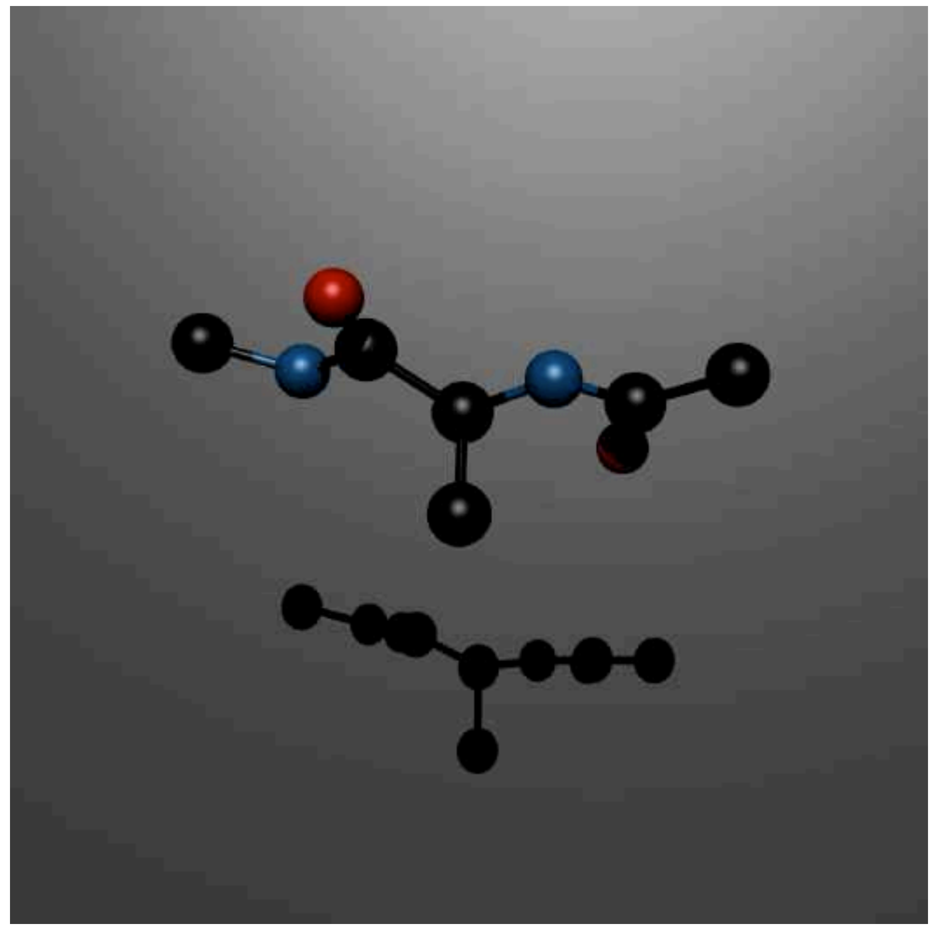

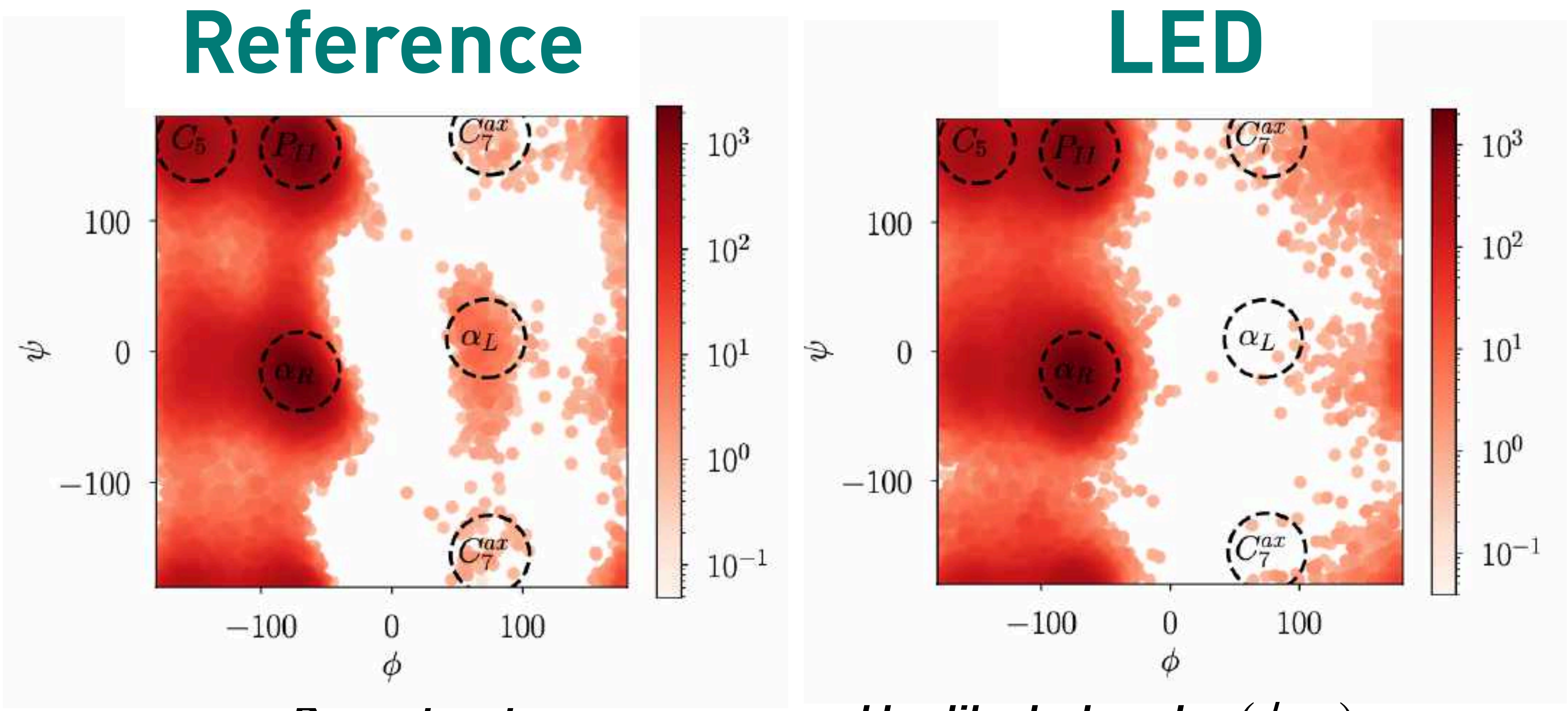

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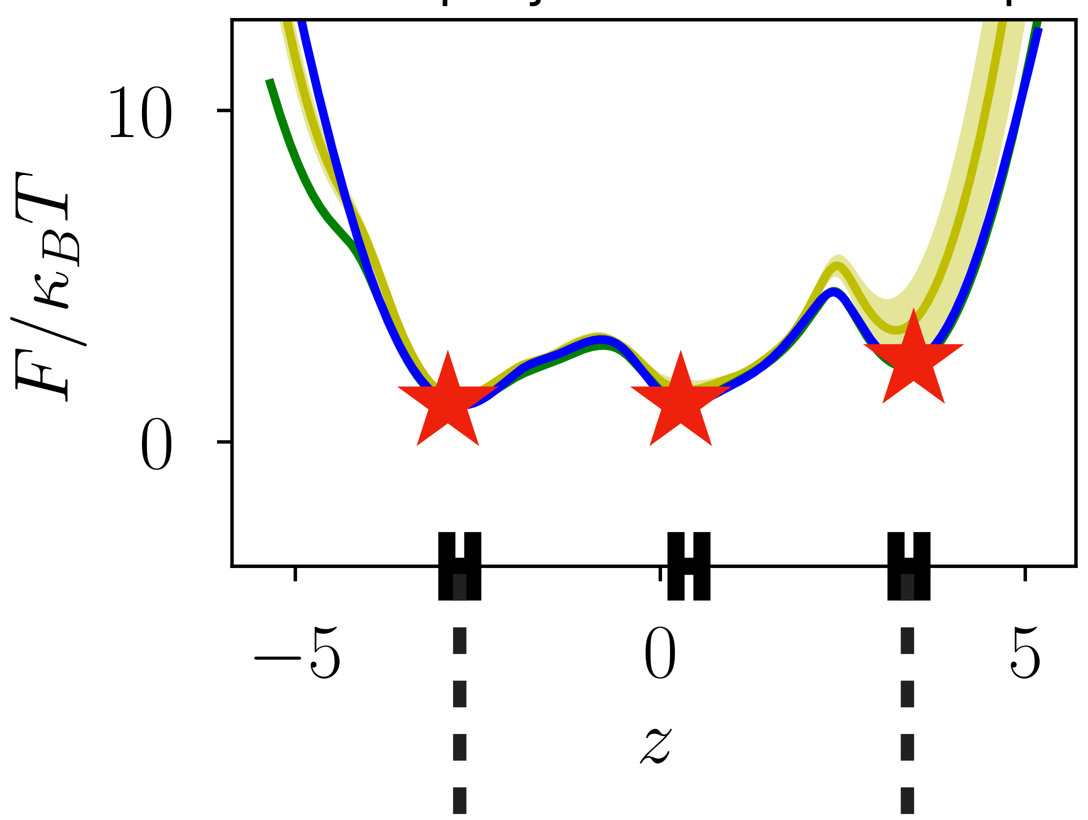

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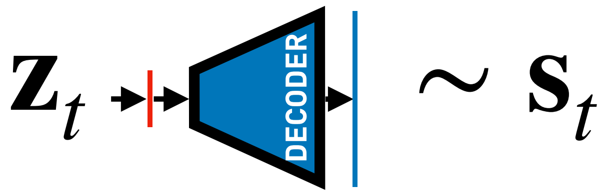

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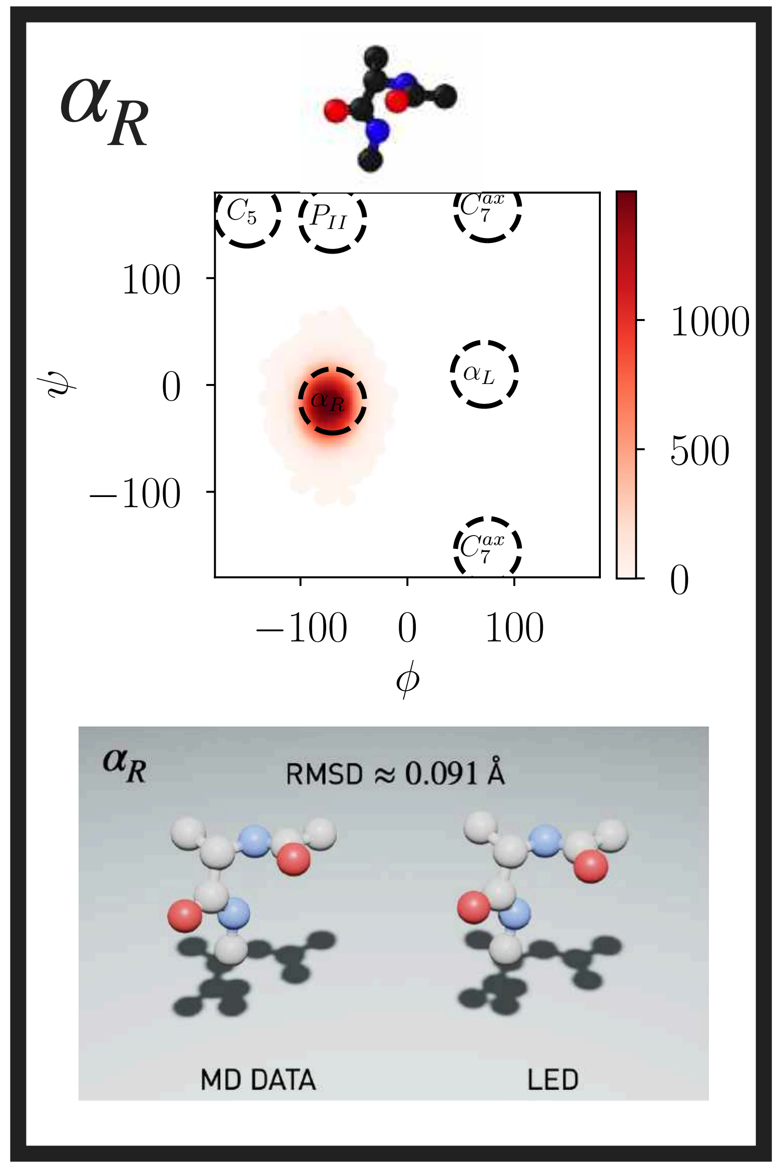

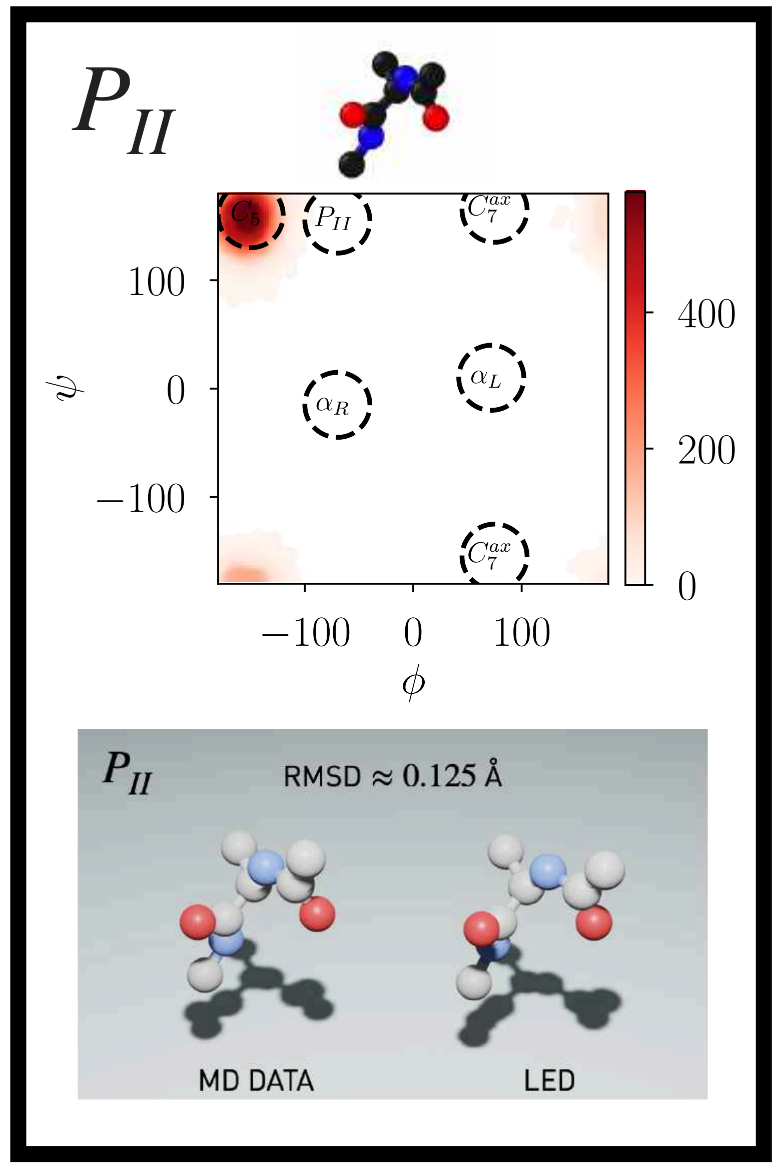

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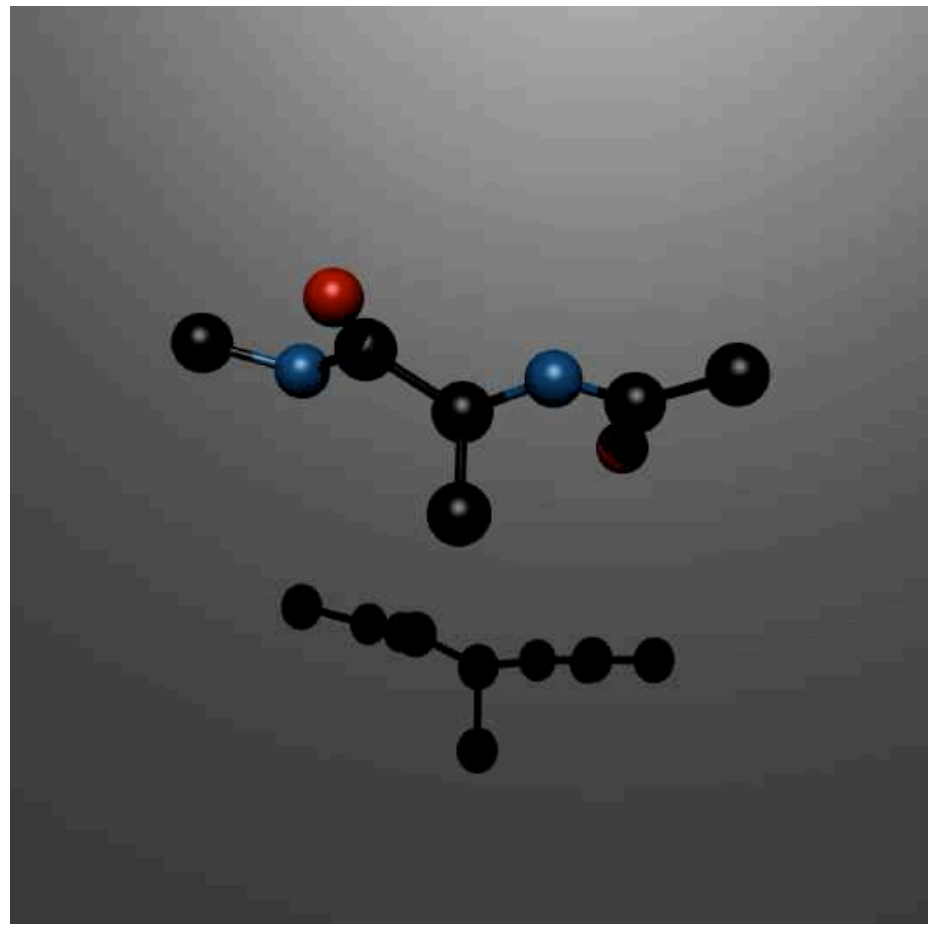

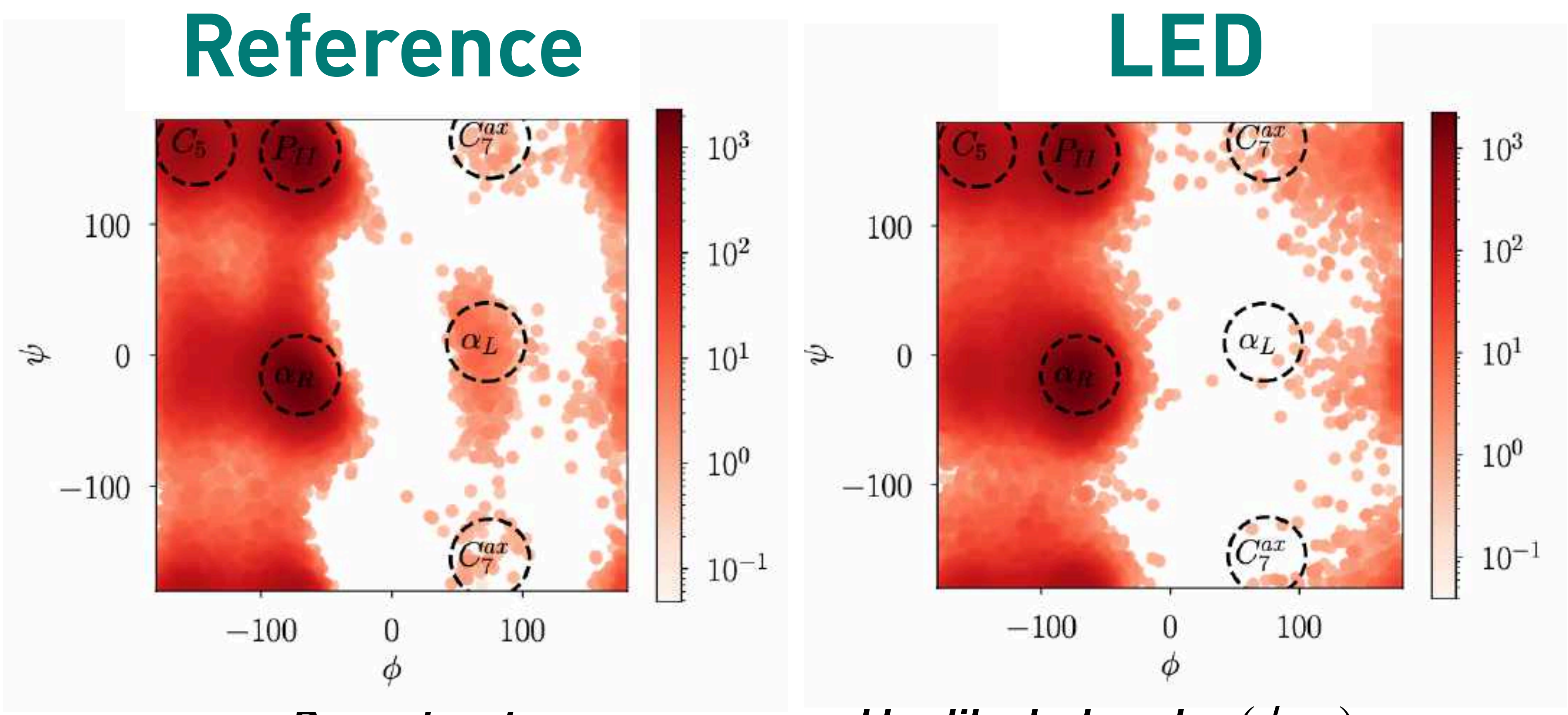

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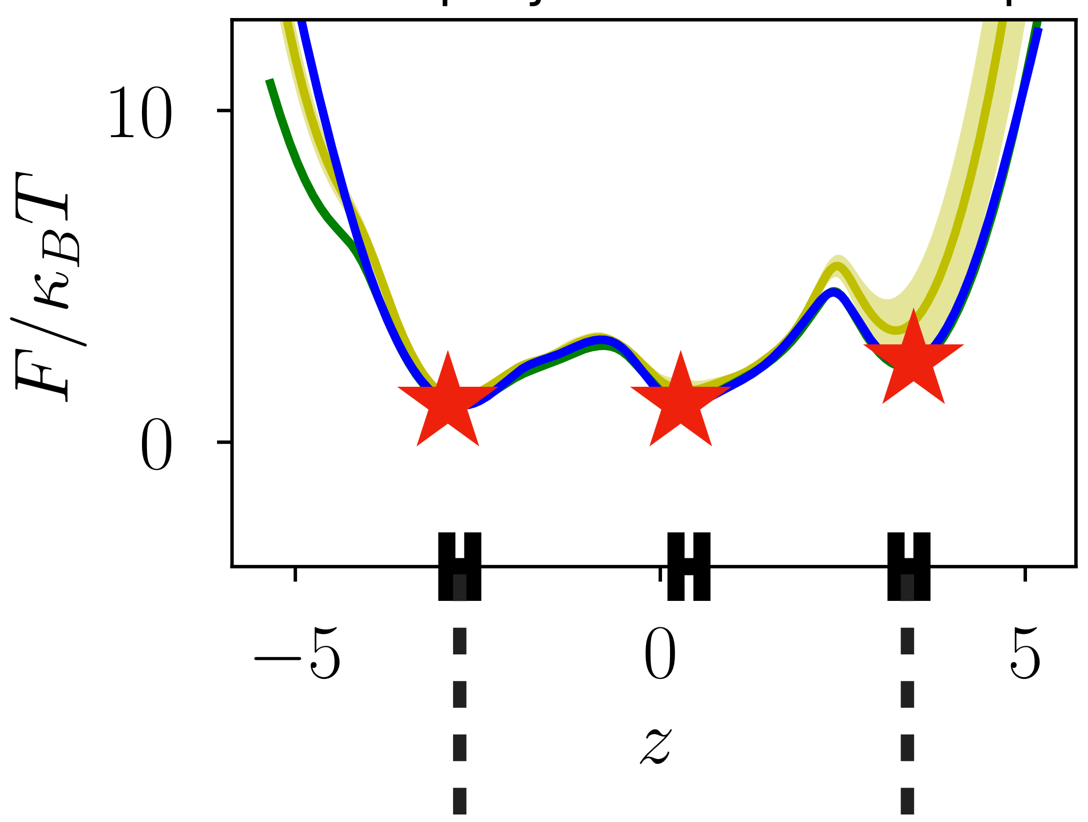

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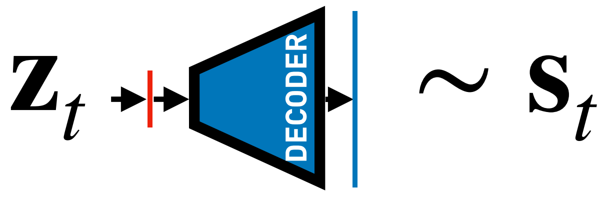

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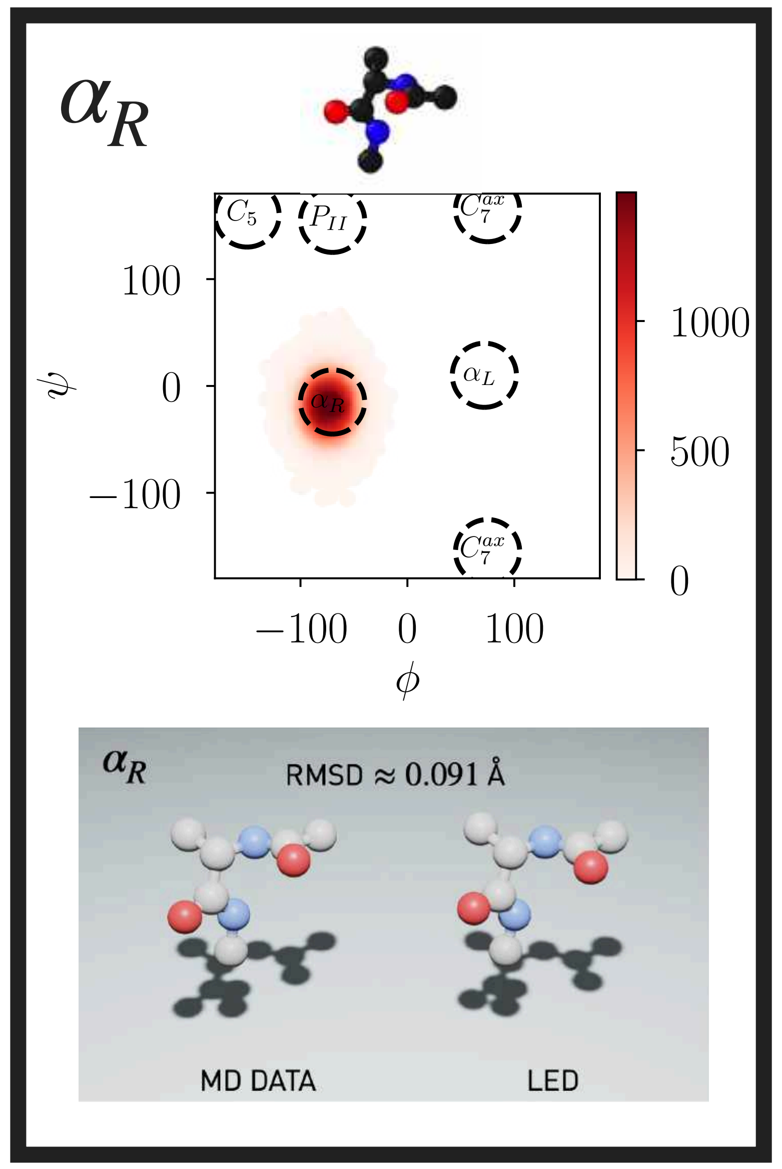

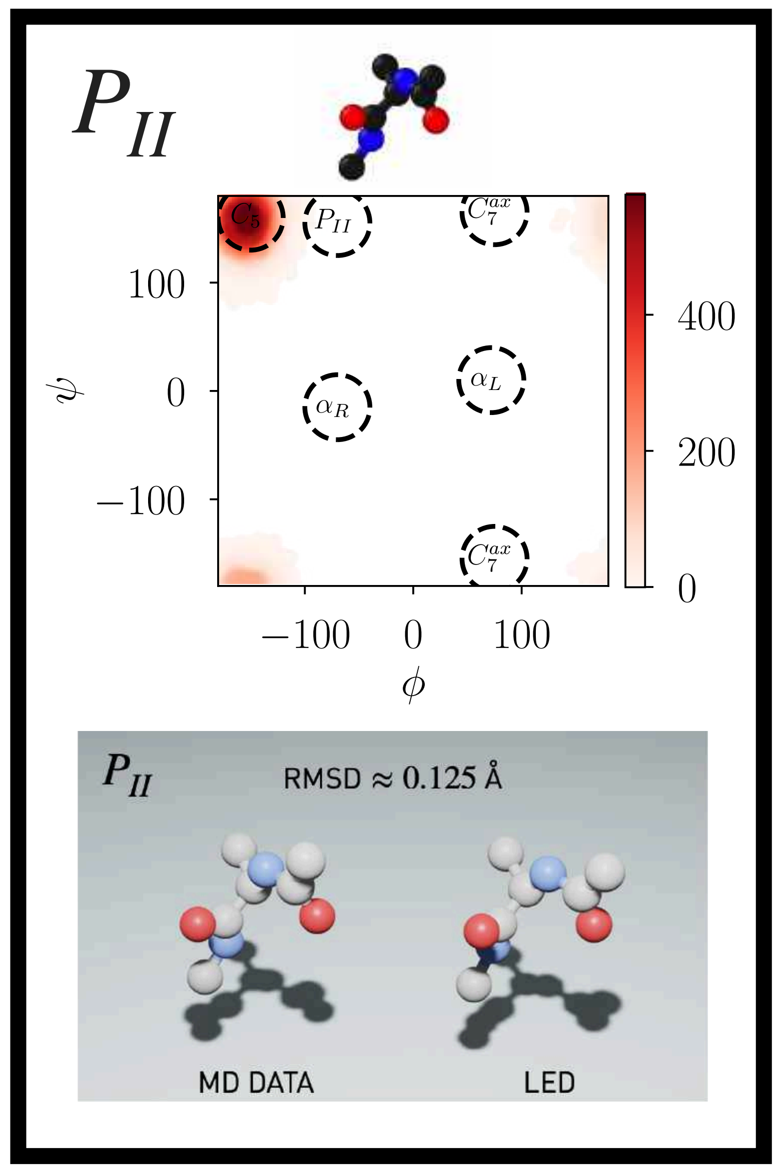

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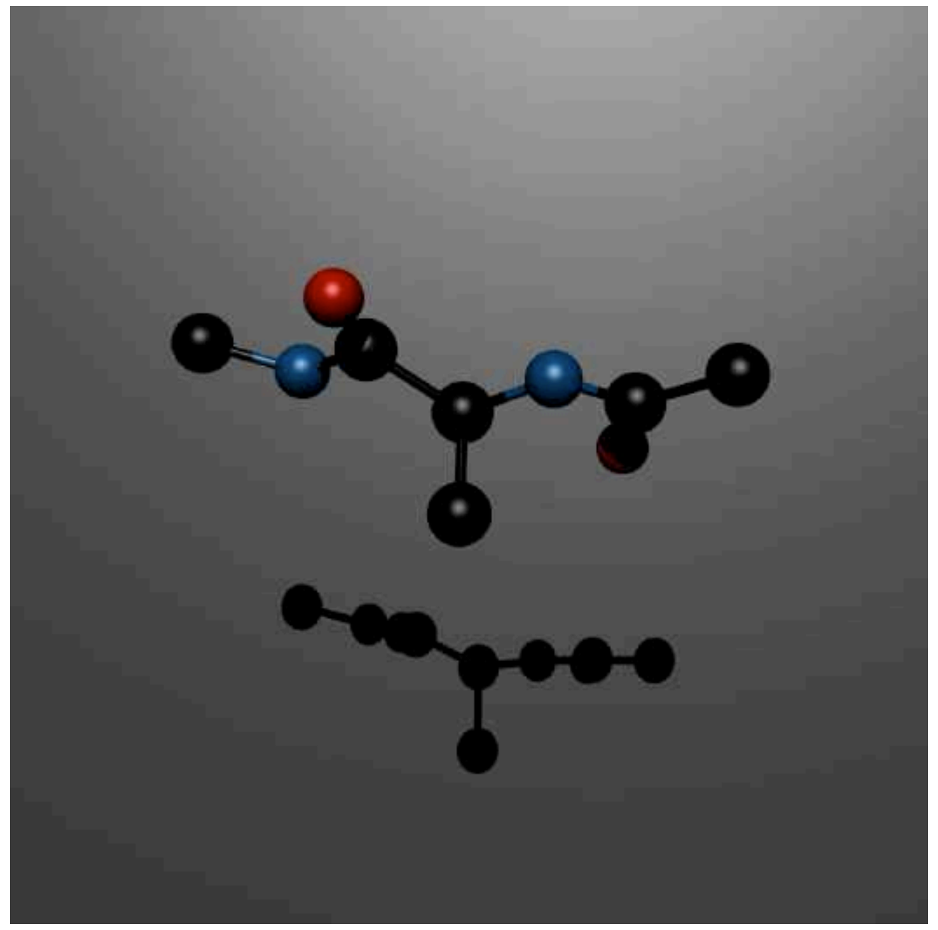

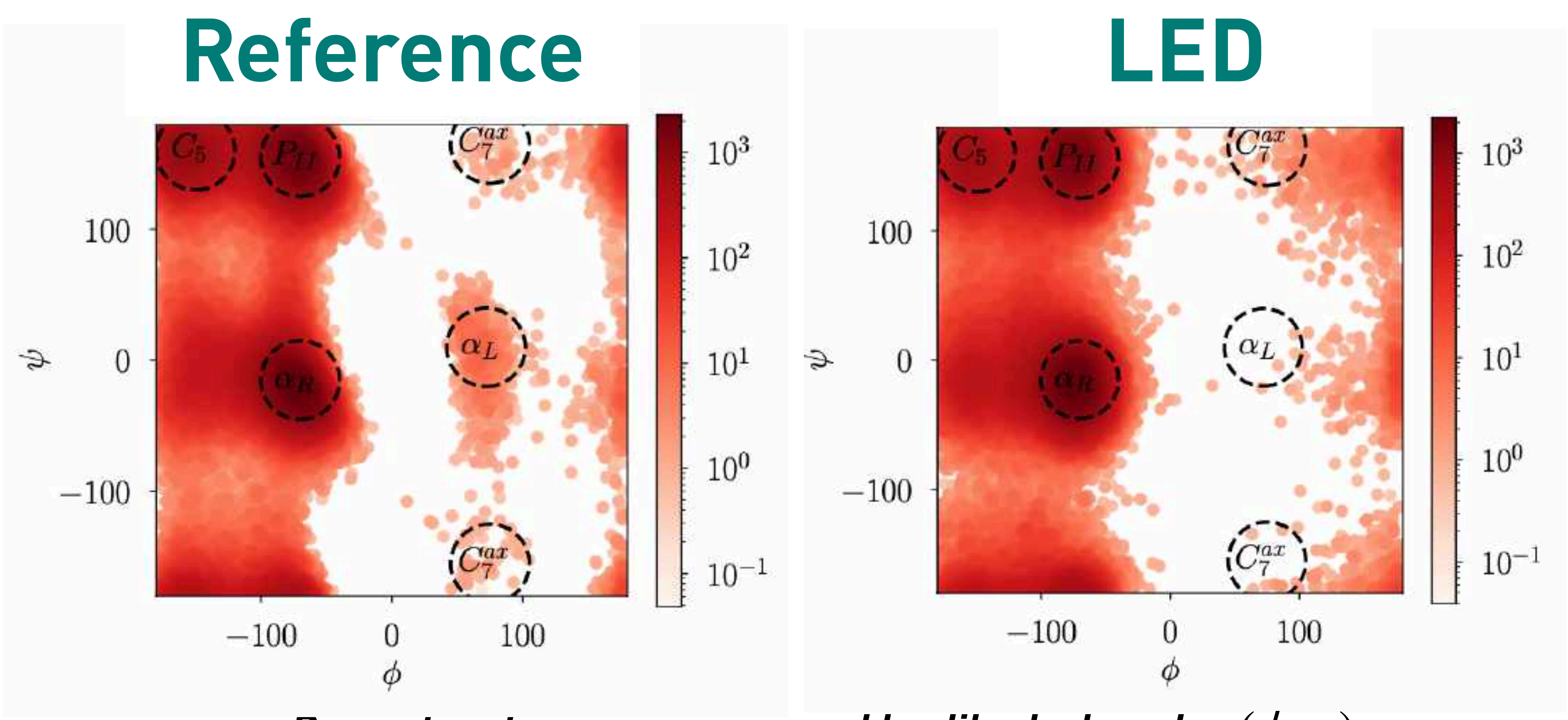

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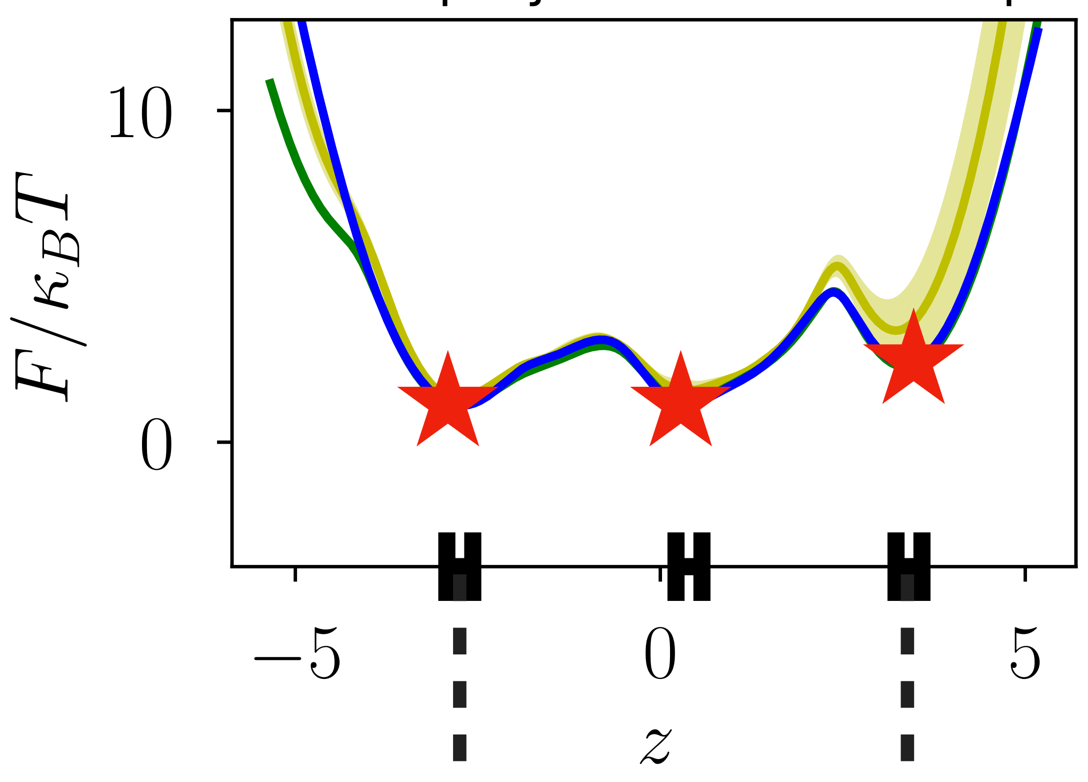

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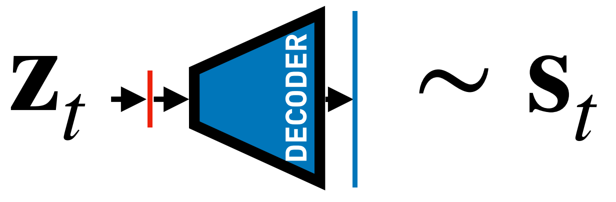

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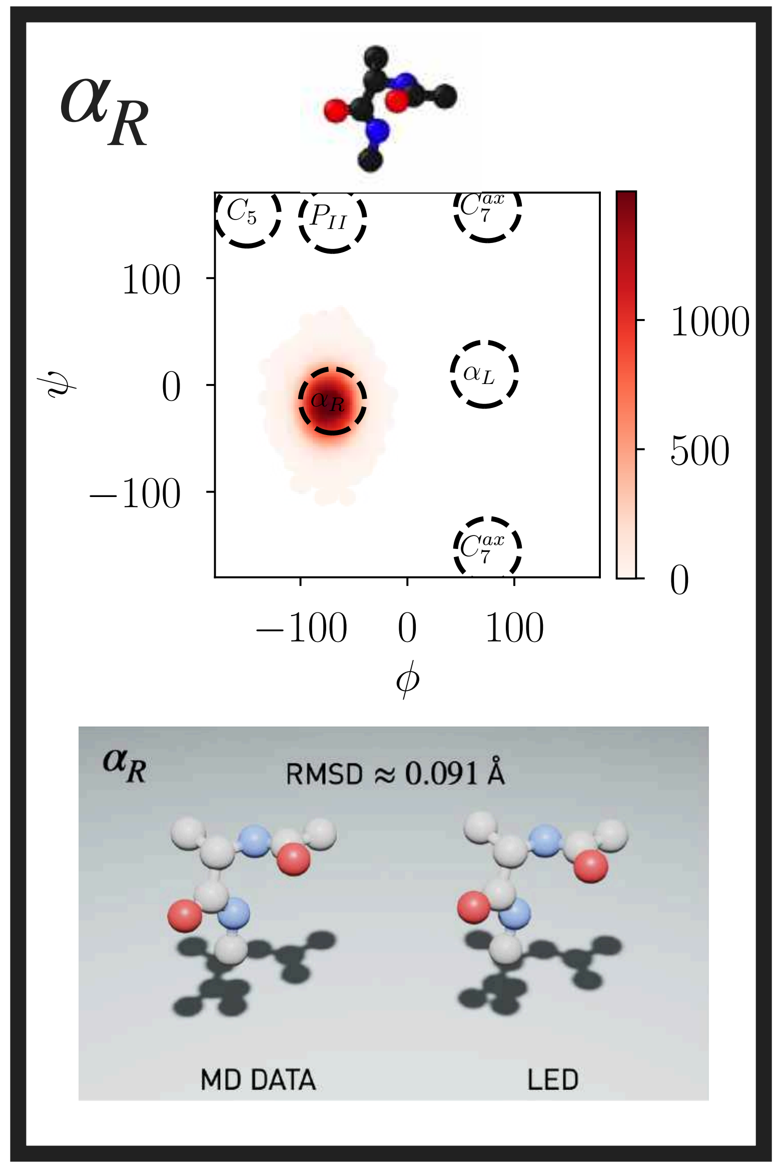

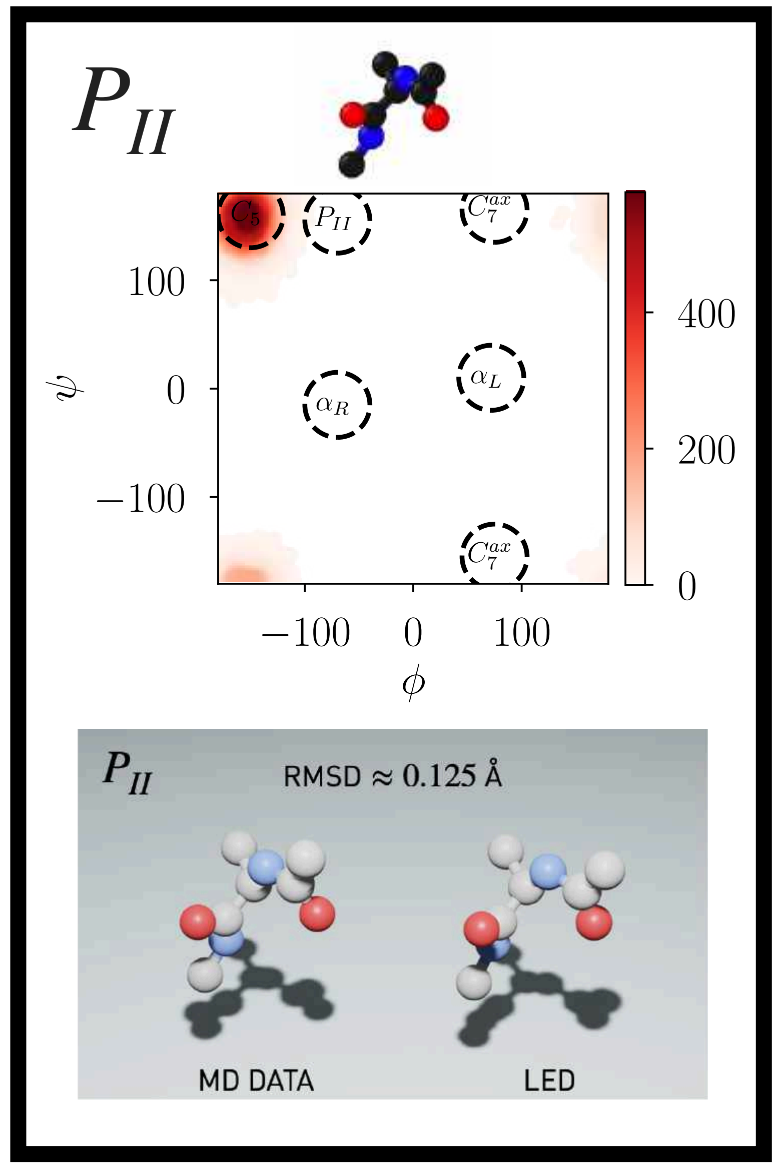

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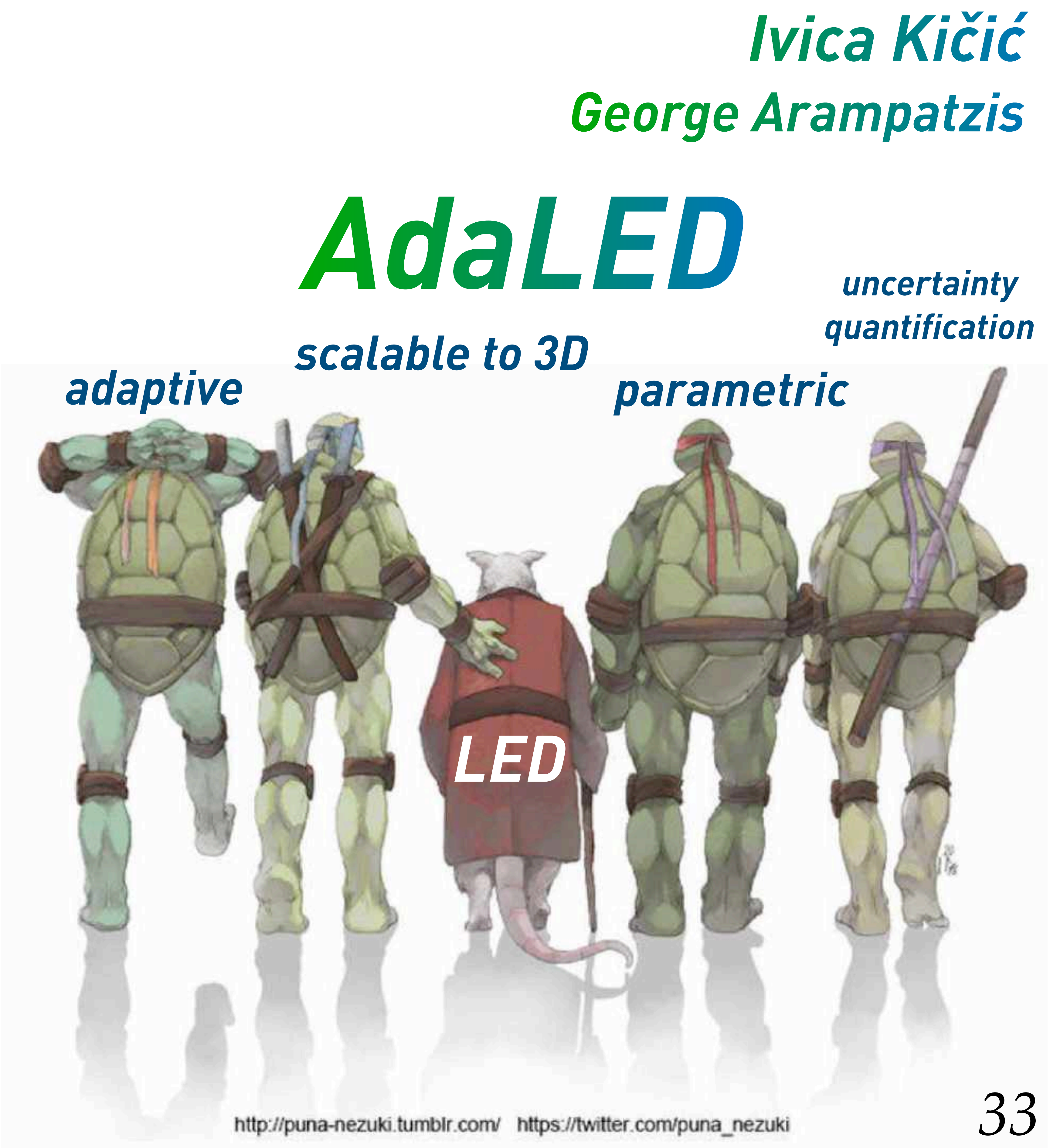

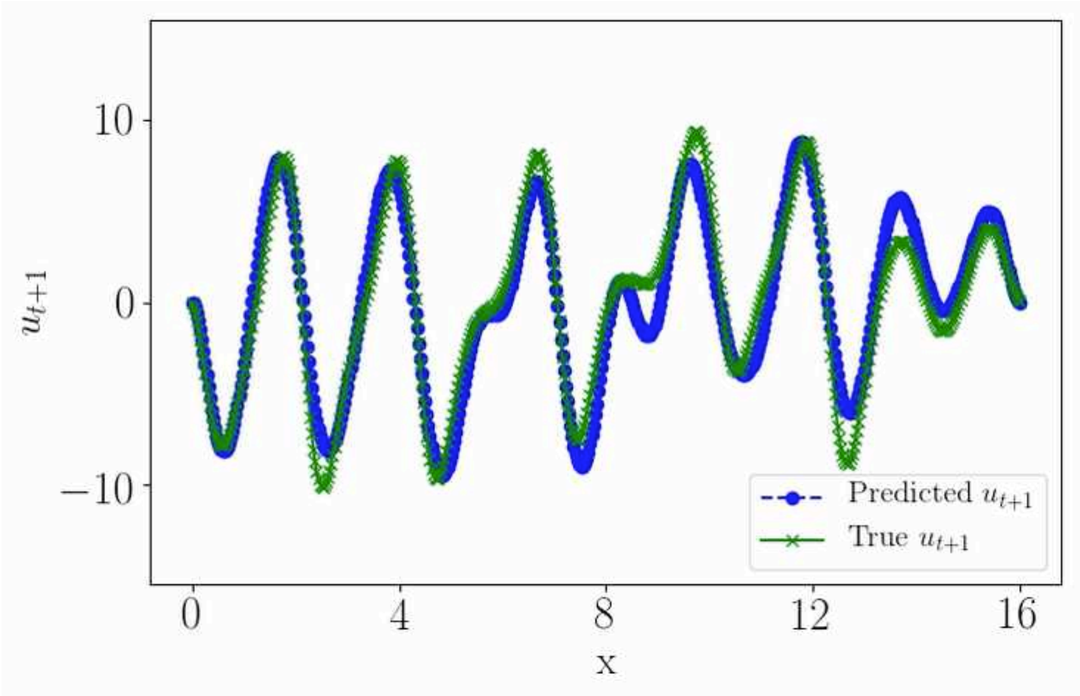

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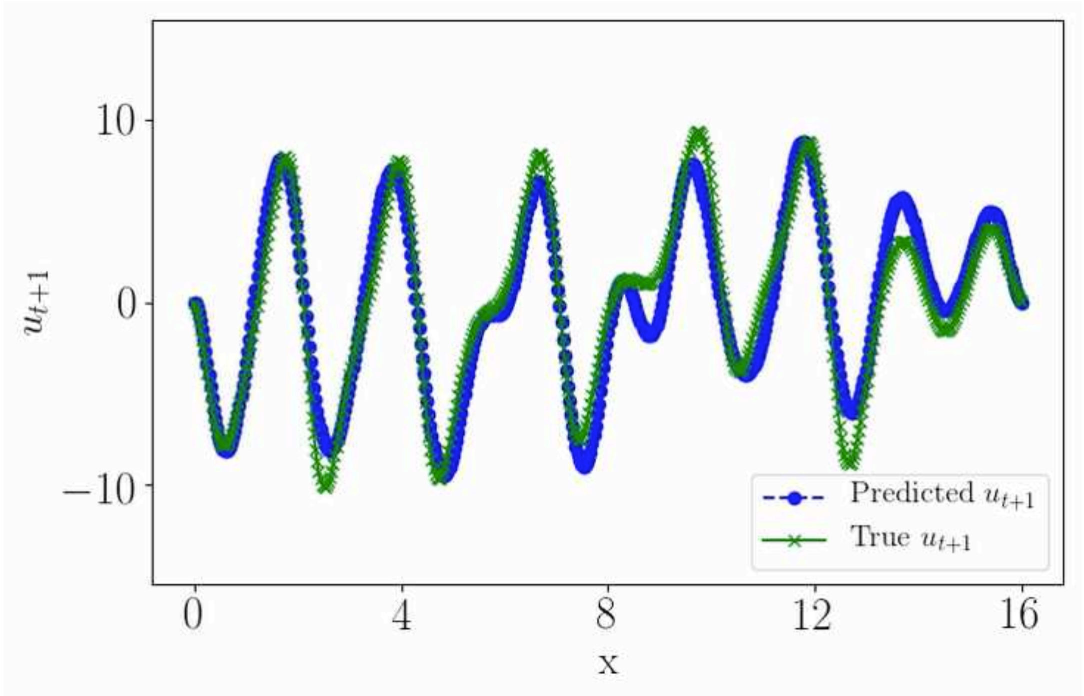

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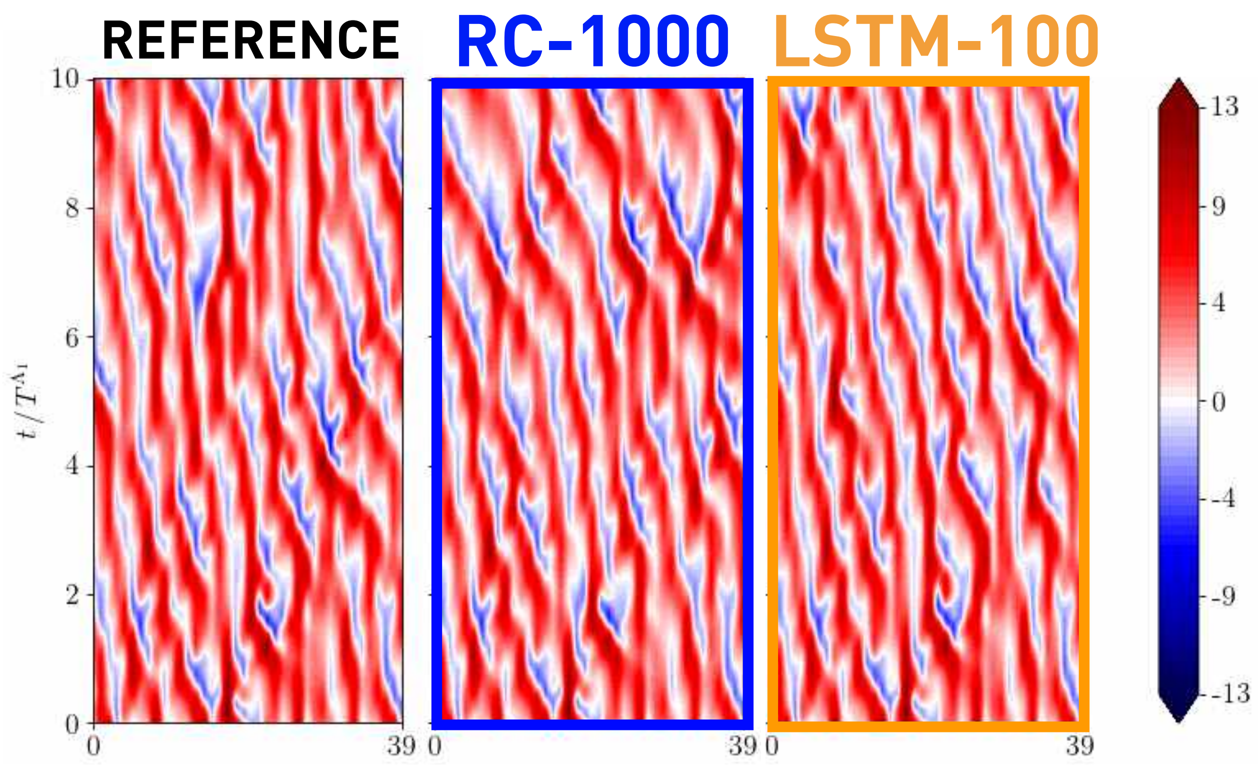

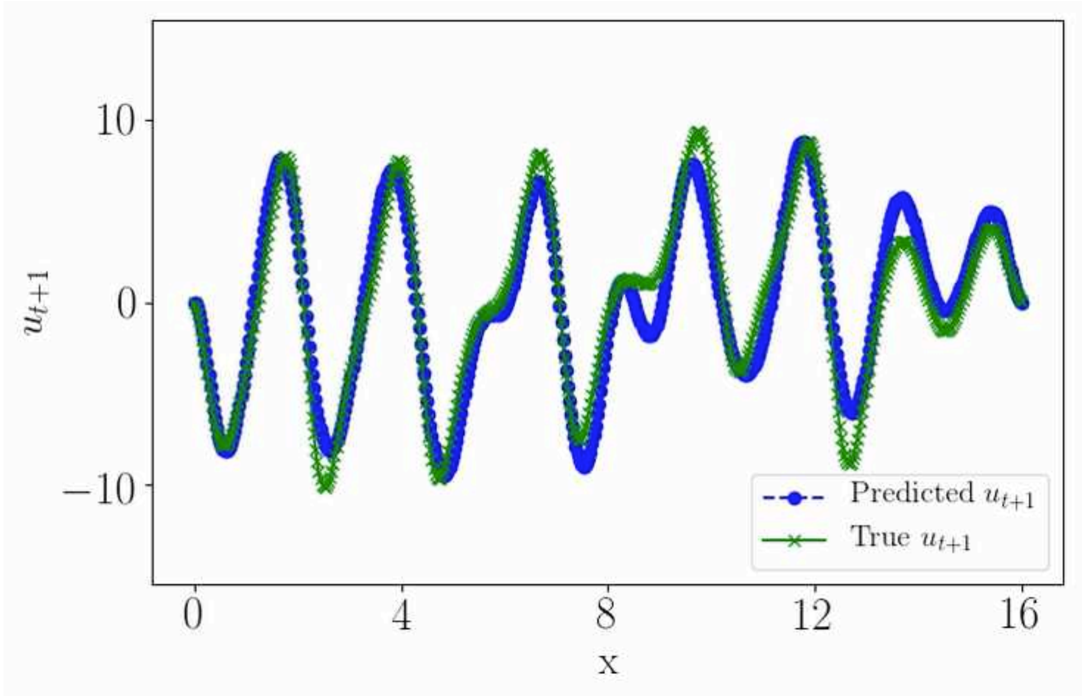

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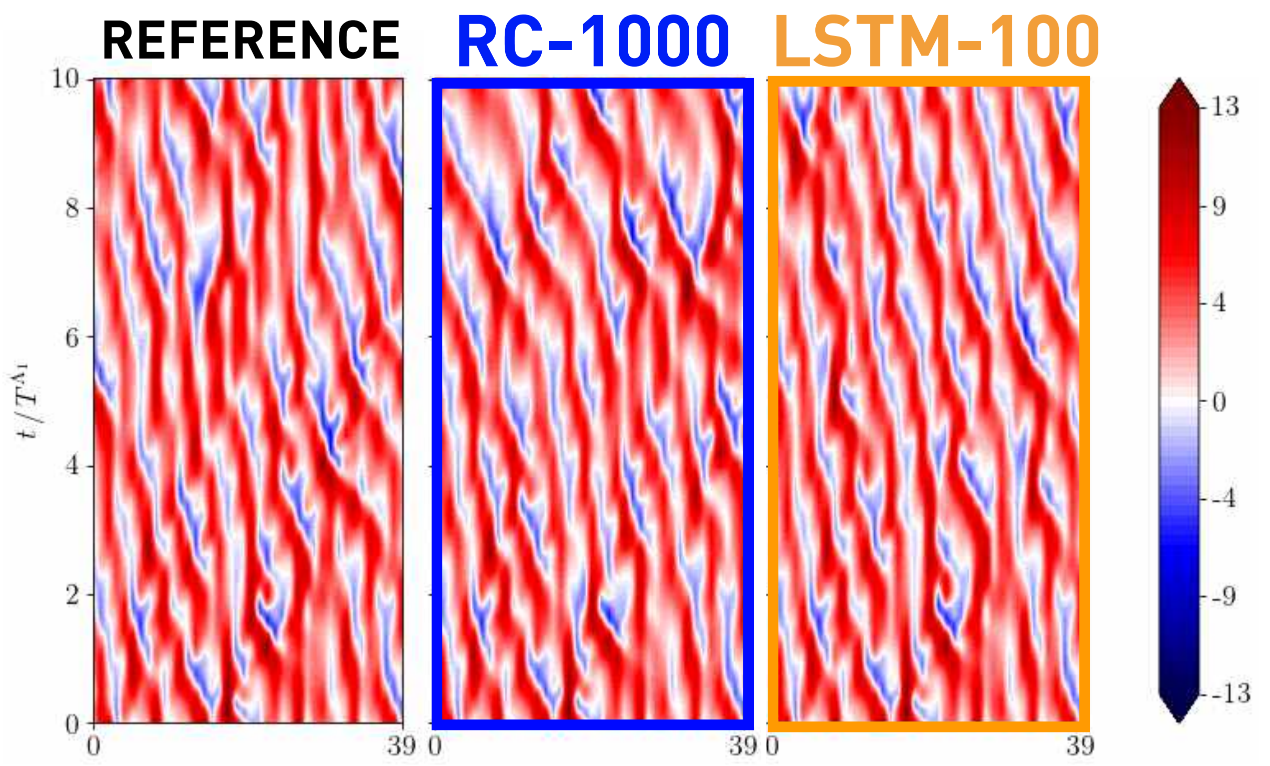

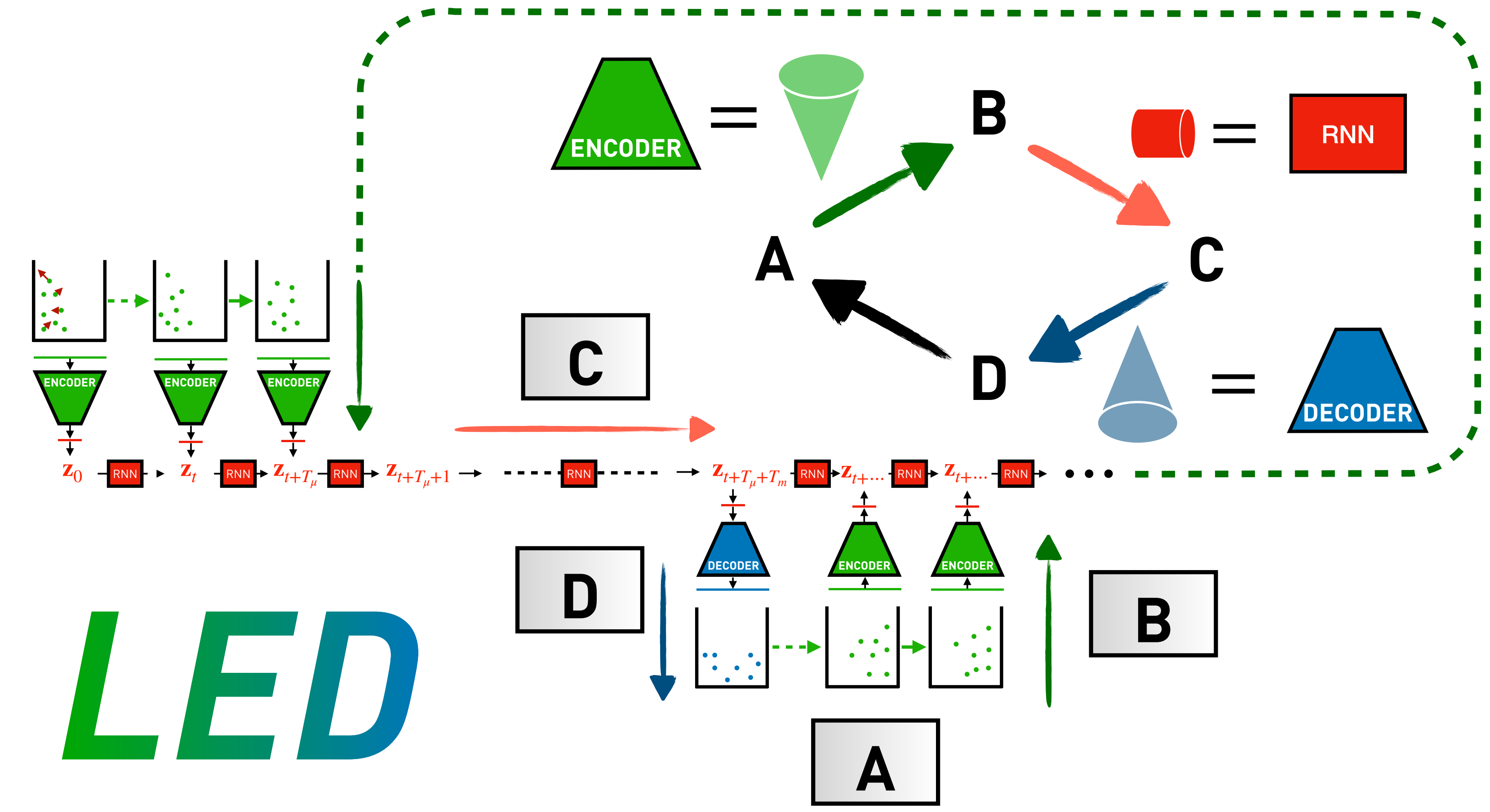

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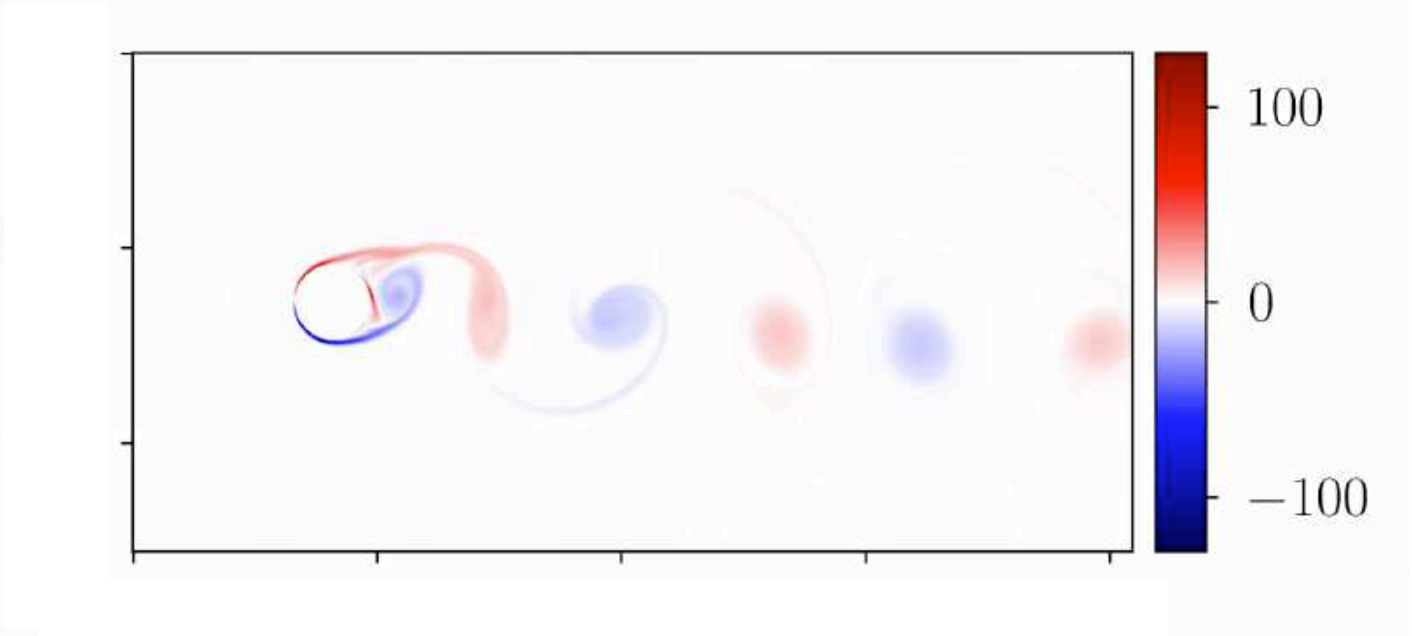

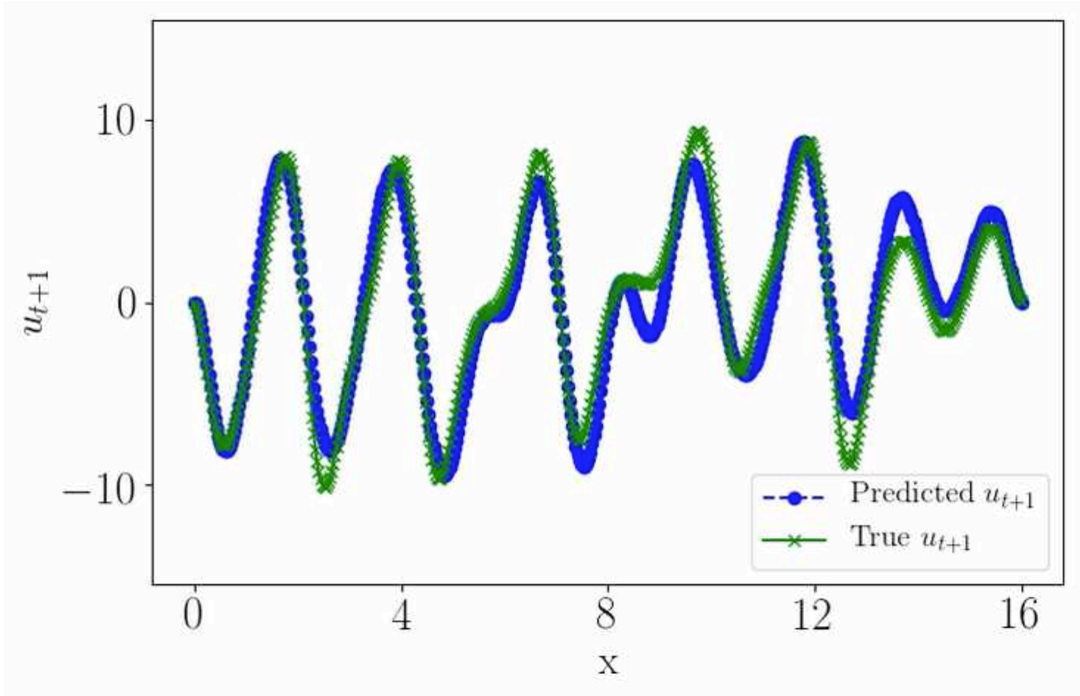

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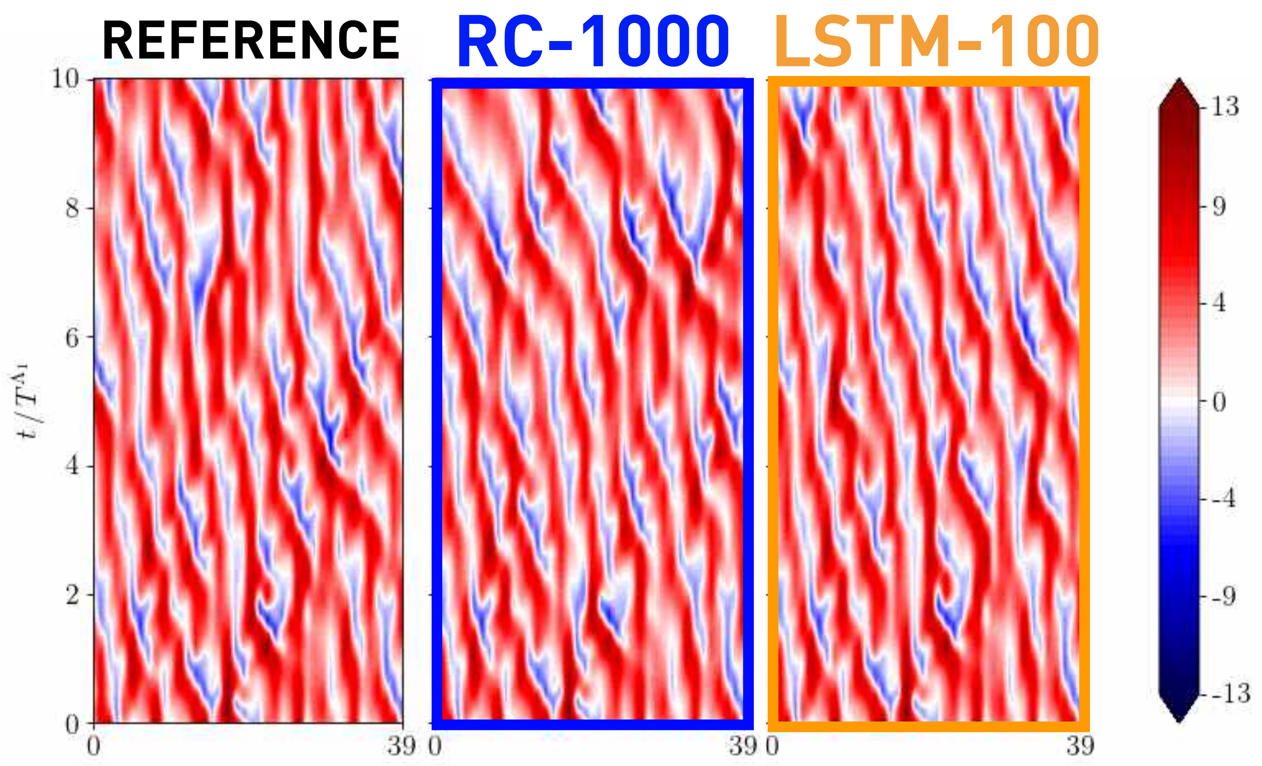

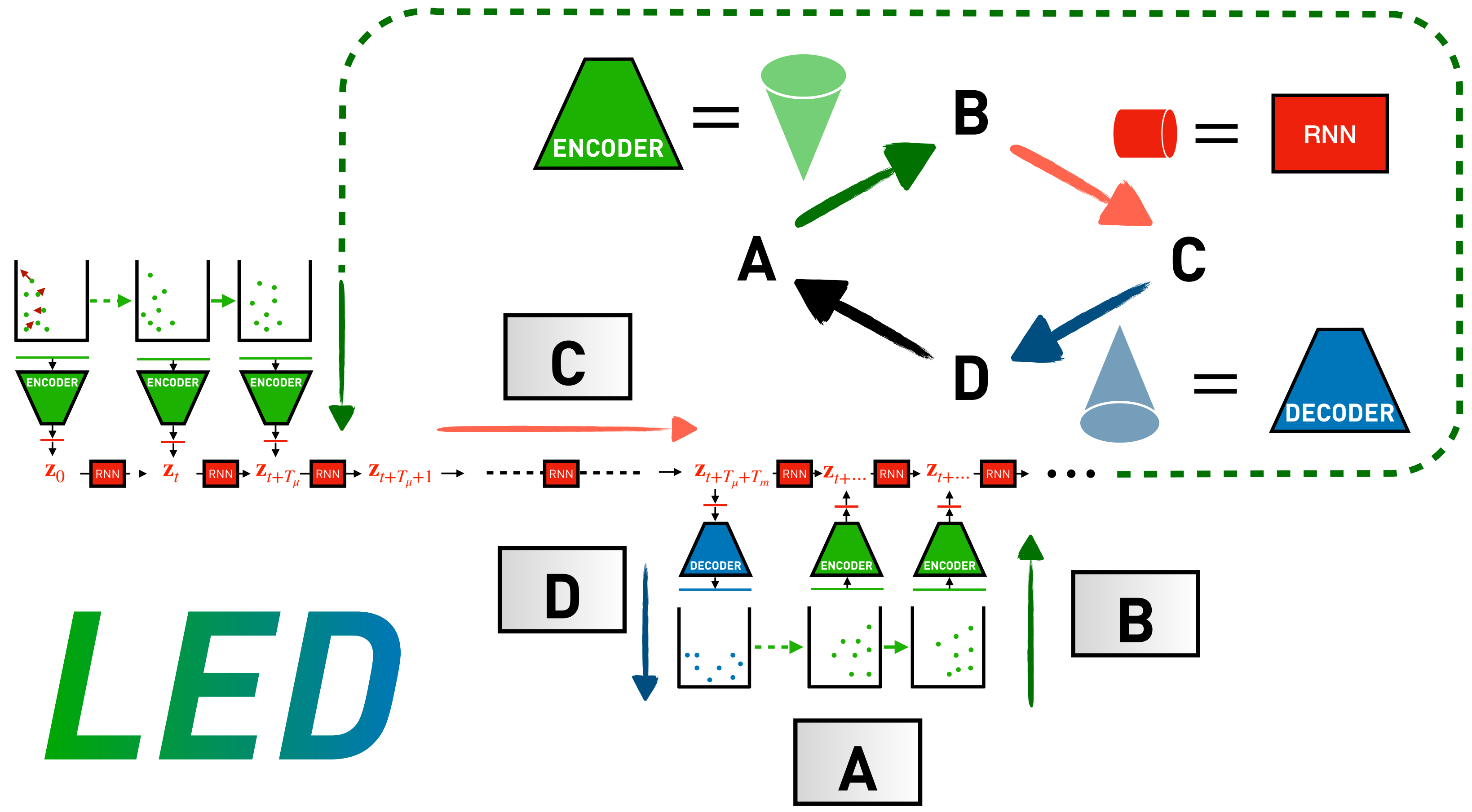

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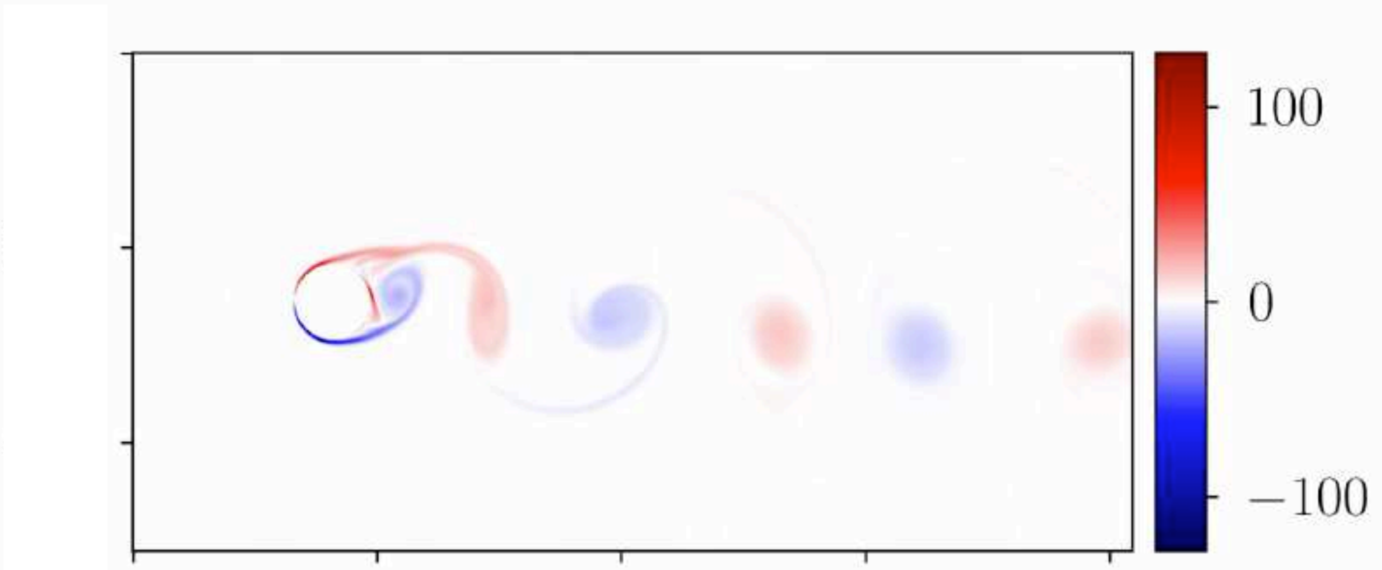

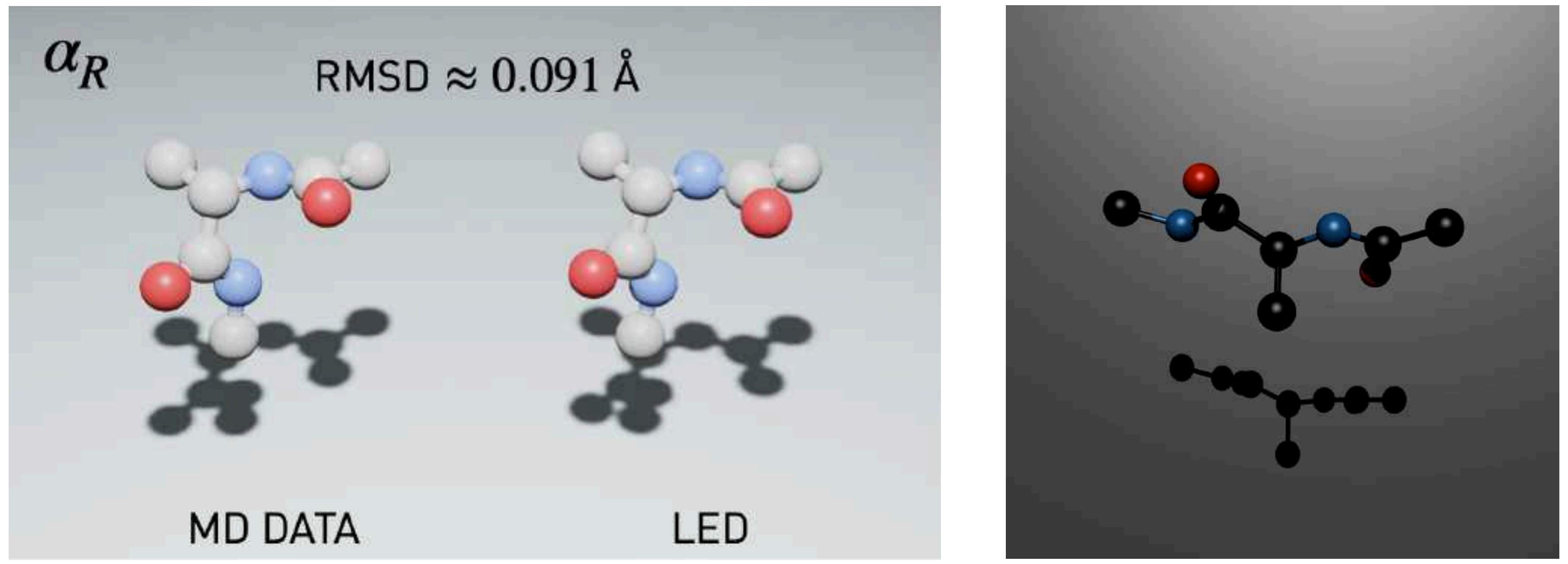

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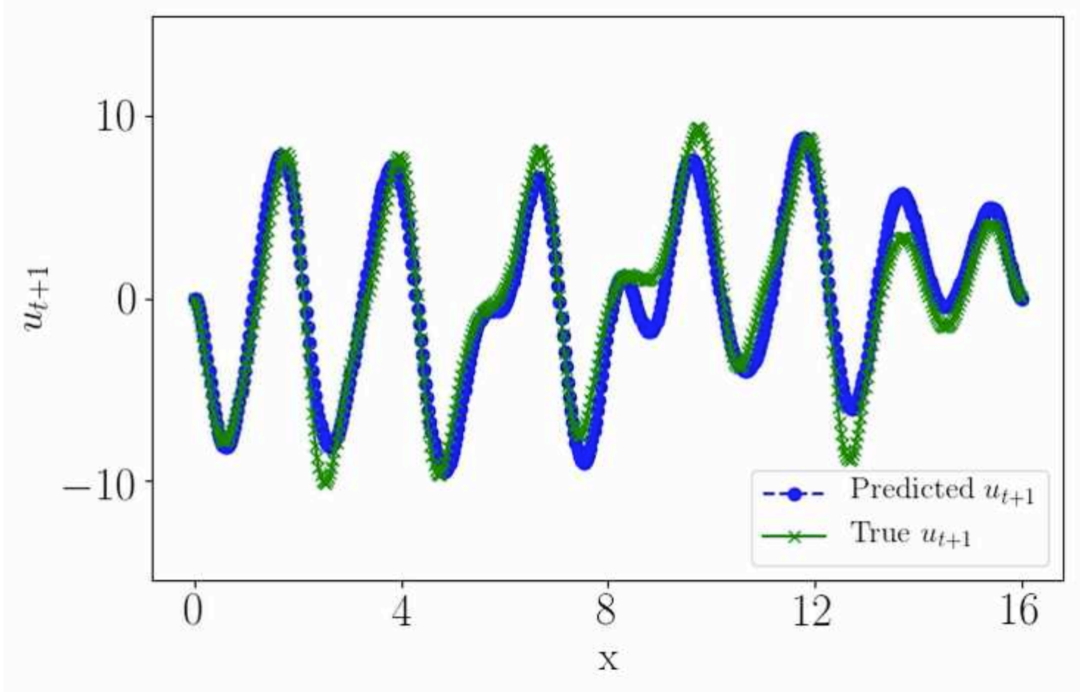

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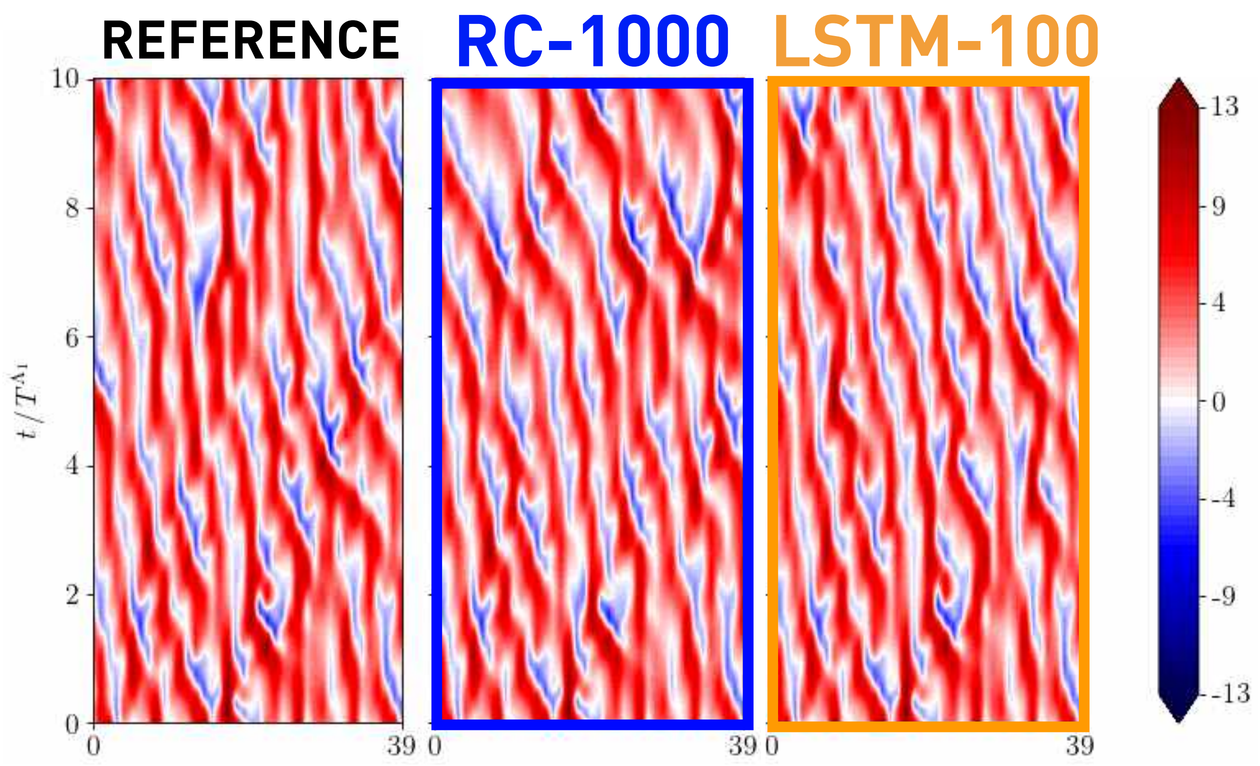

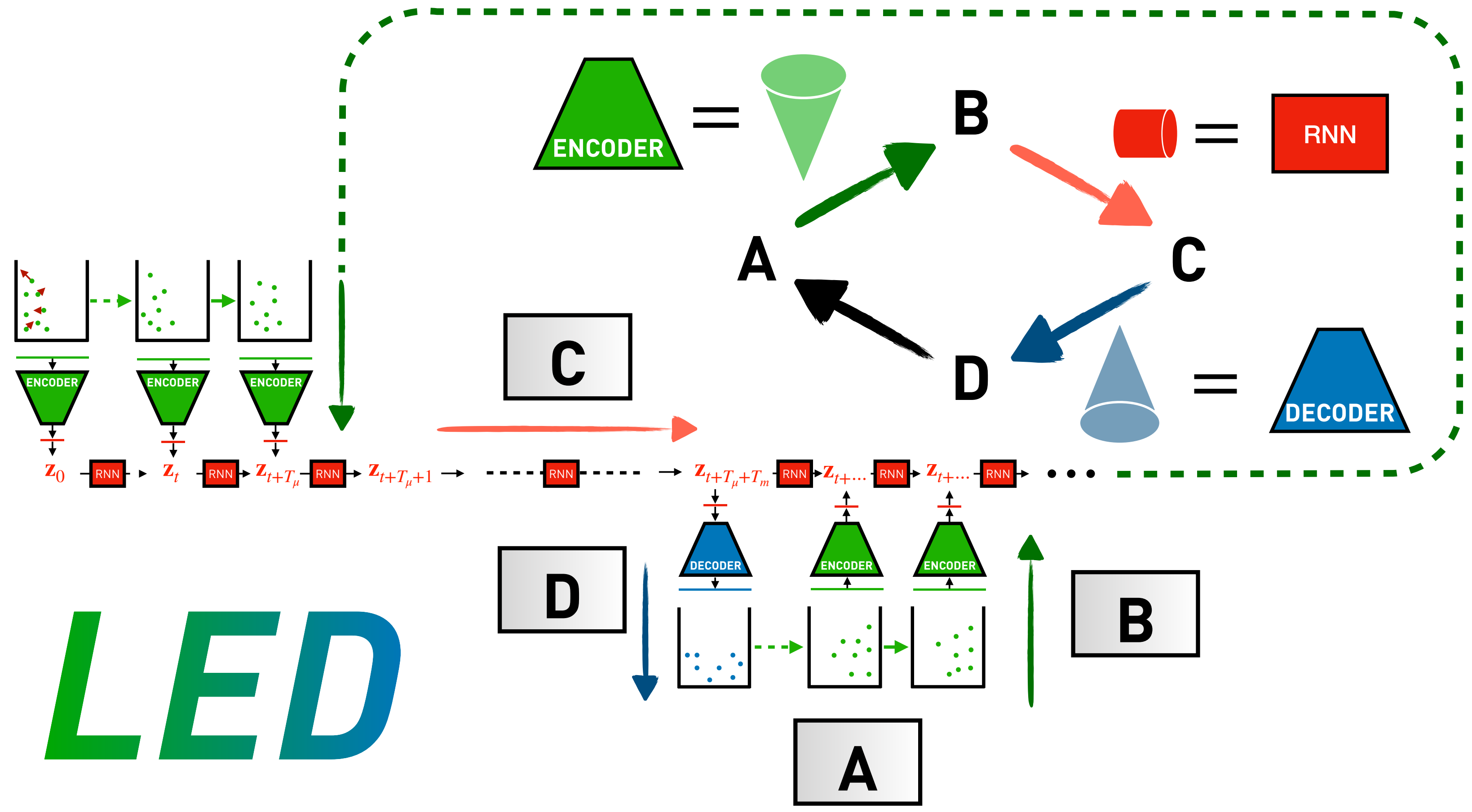

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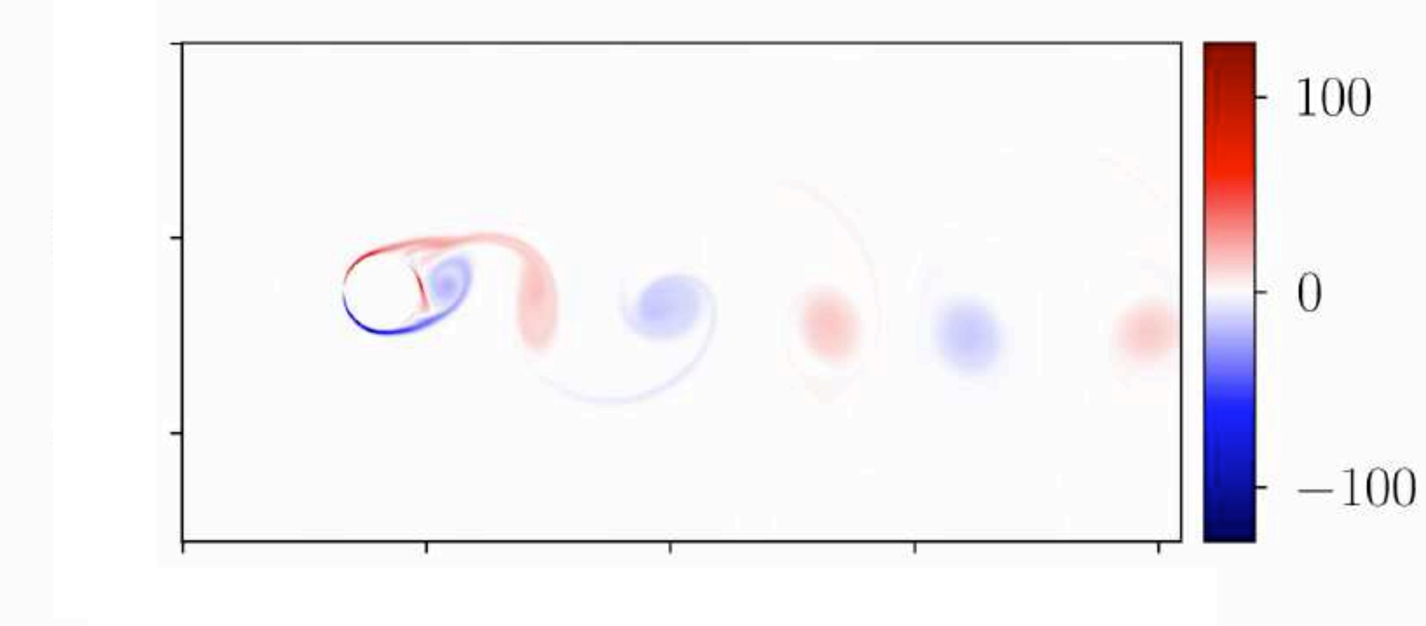

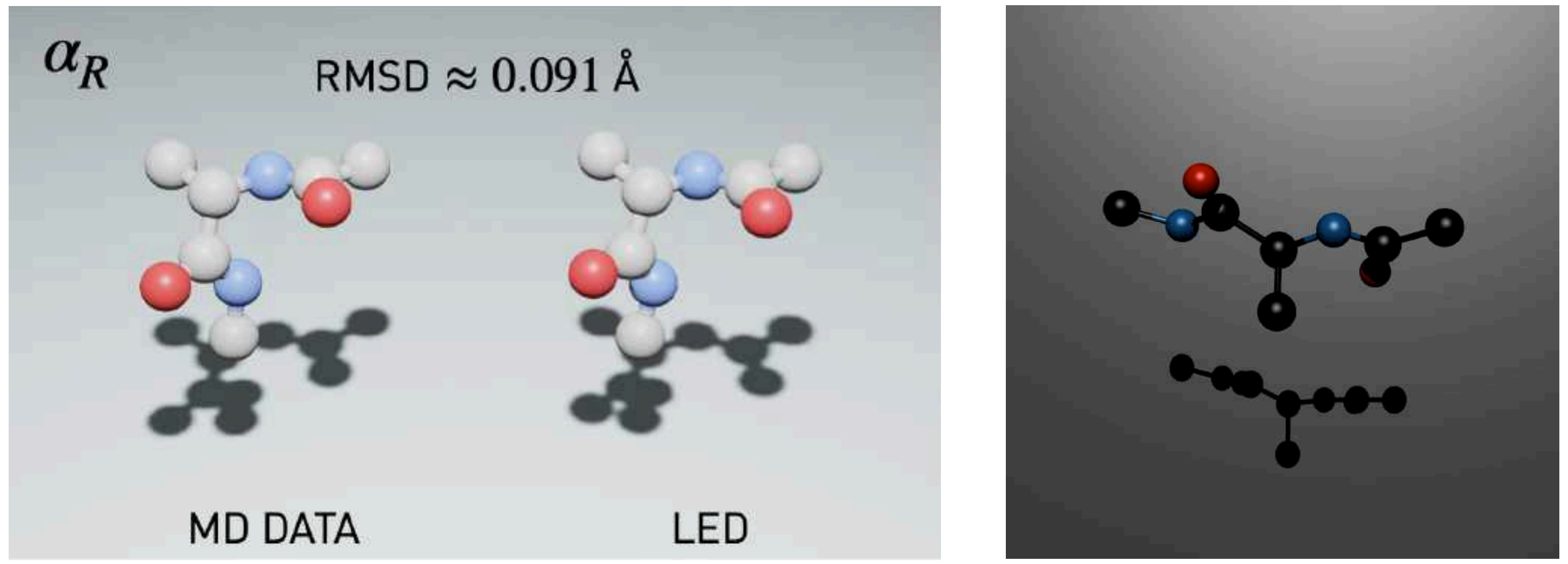

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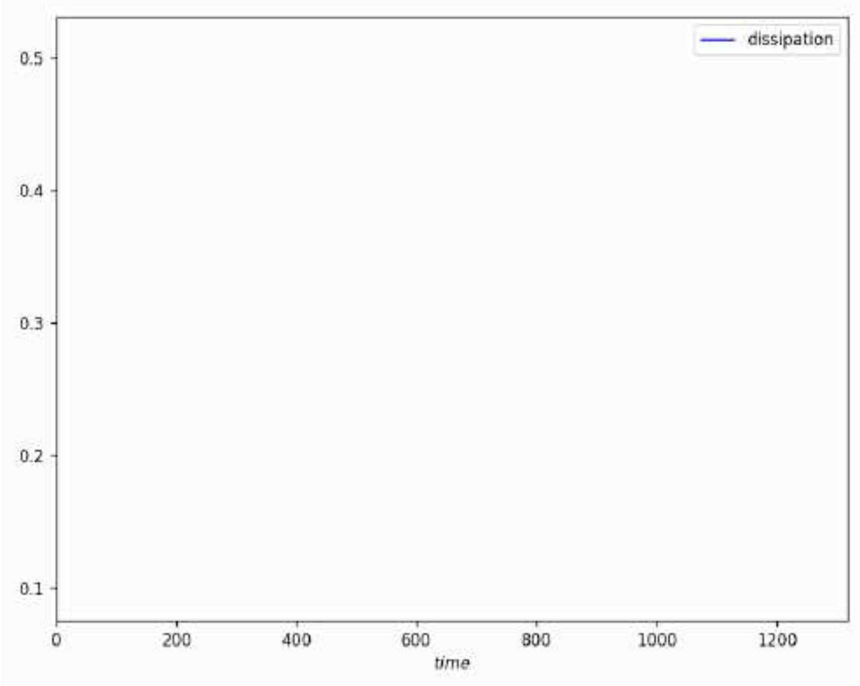

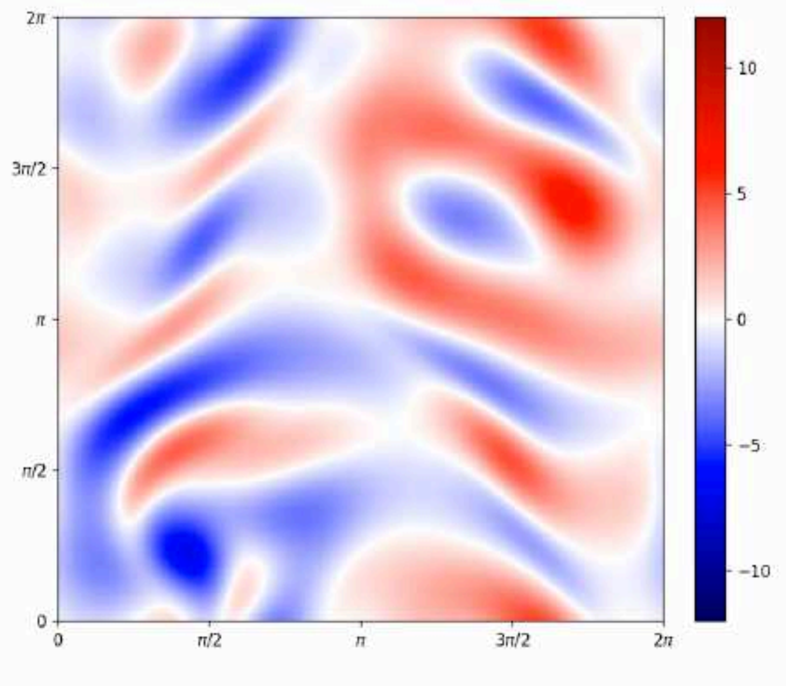

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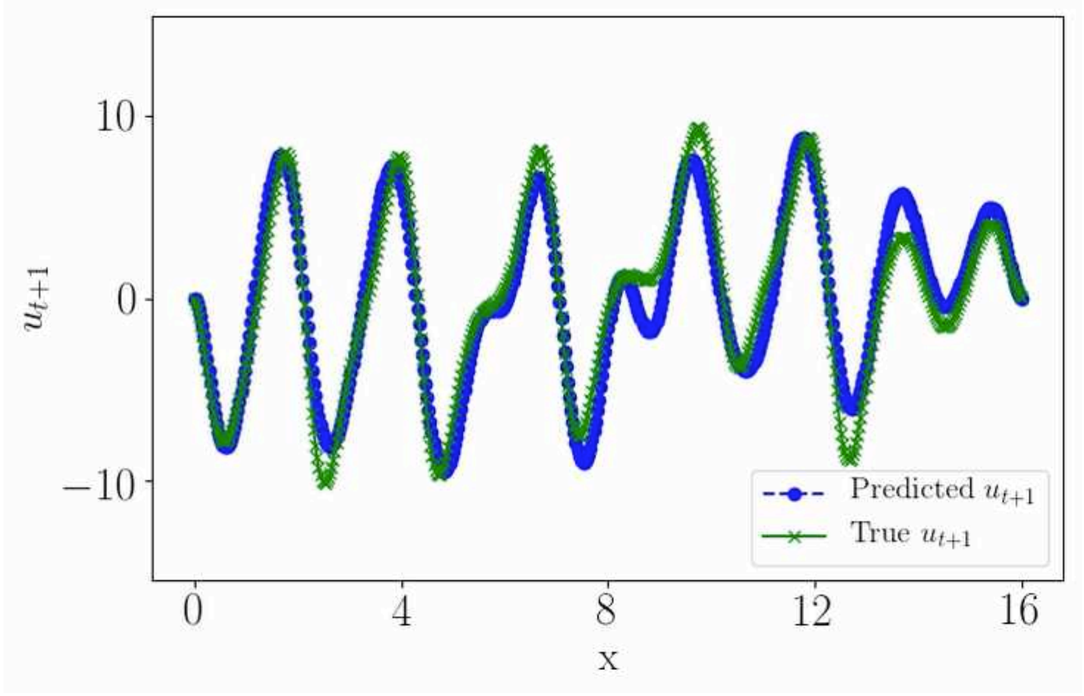

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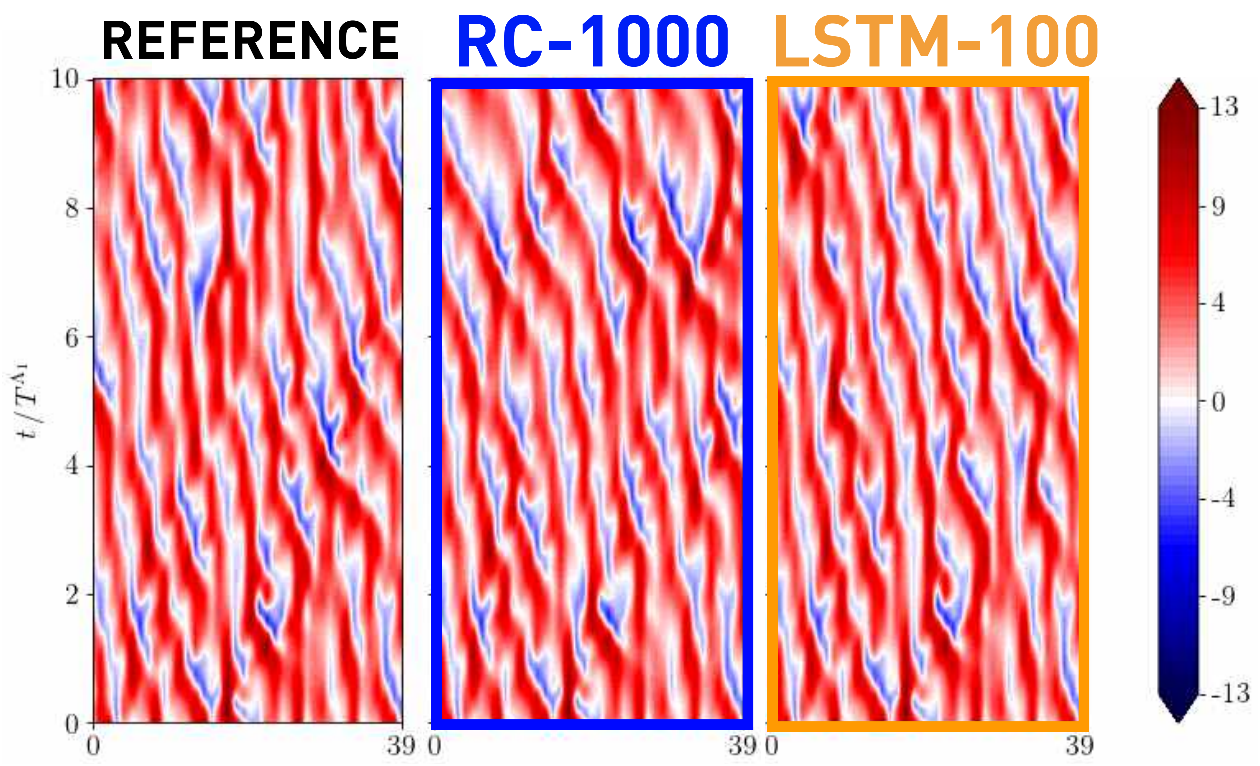

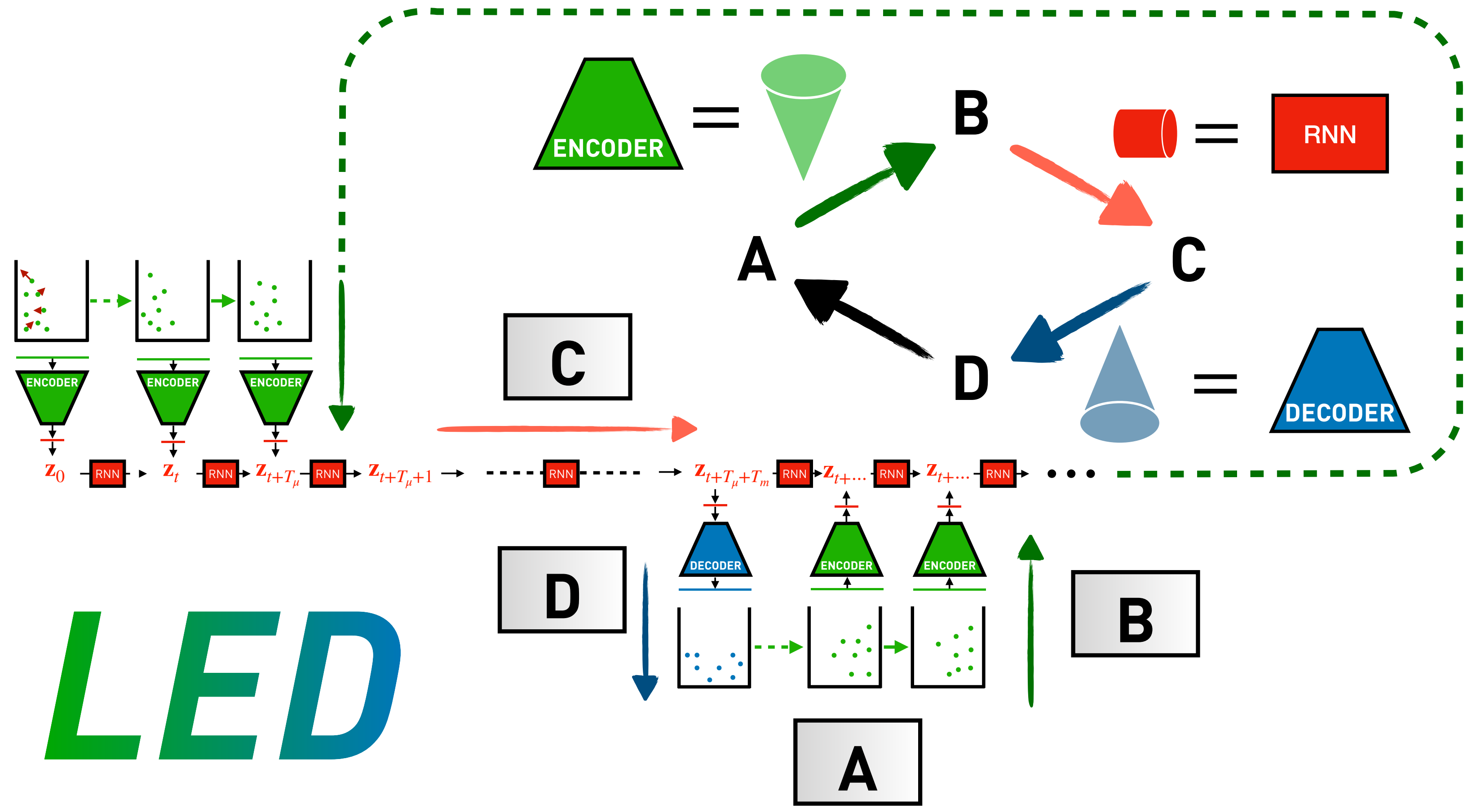

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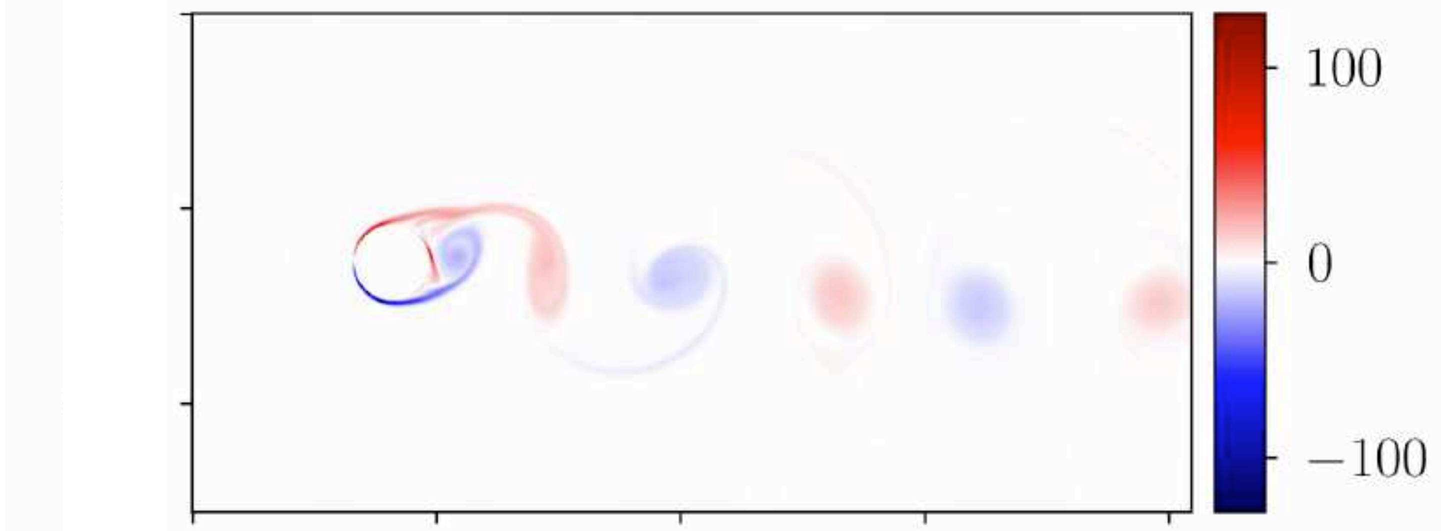

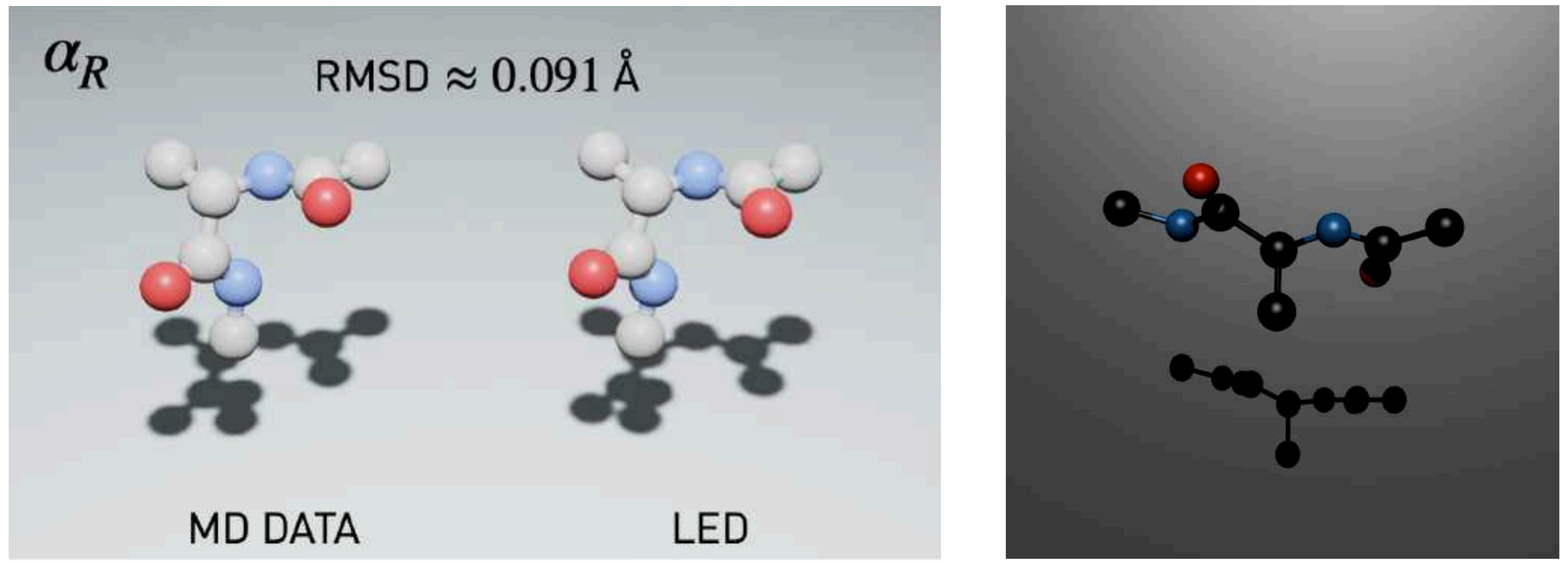

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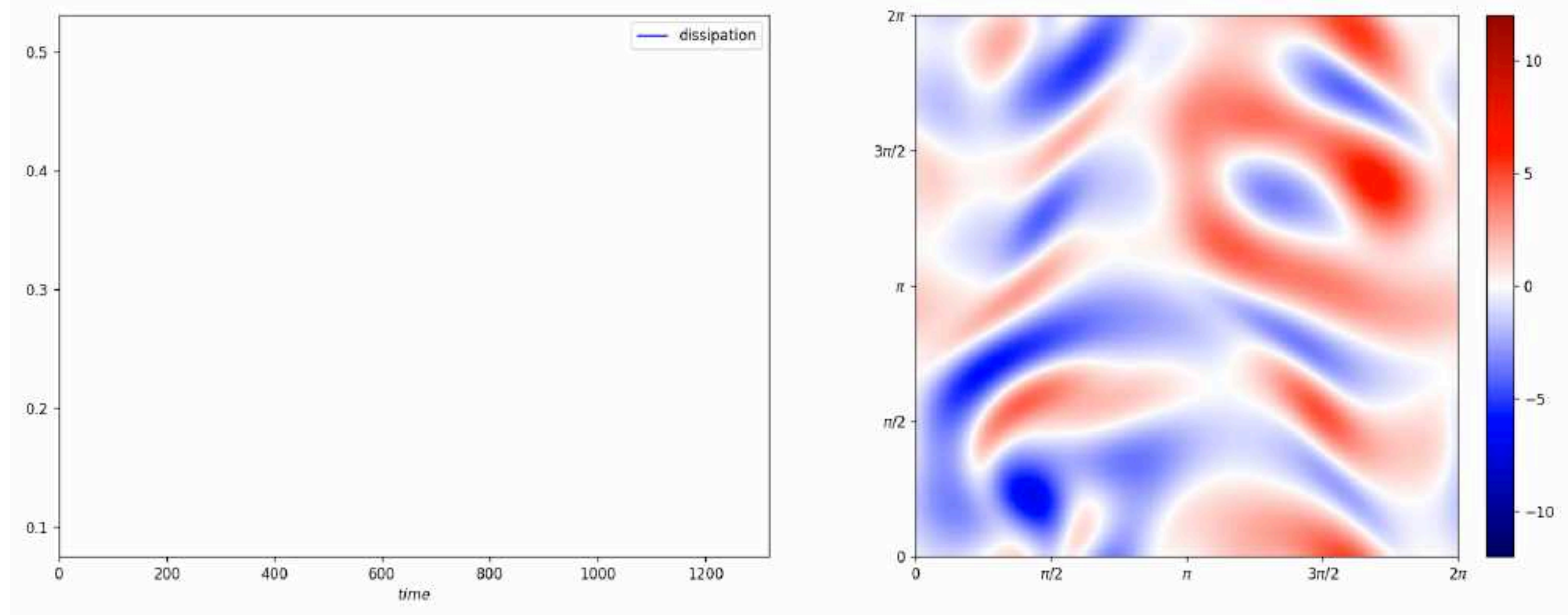

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