

USING MACHINE LEARNING FOR ANALYSIS AND PREDICTION OF HIGH-DIMENSIONAL SPATIOTEMPORAL CHAOTIC DYNAMICAL SYSTEMS

10th October 2018

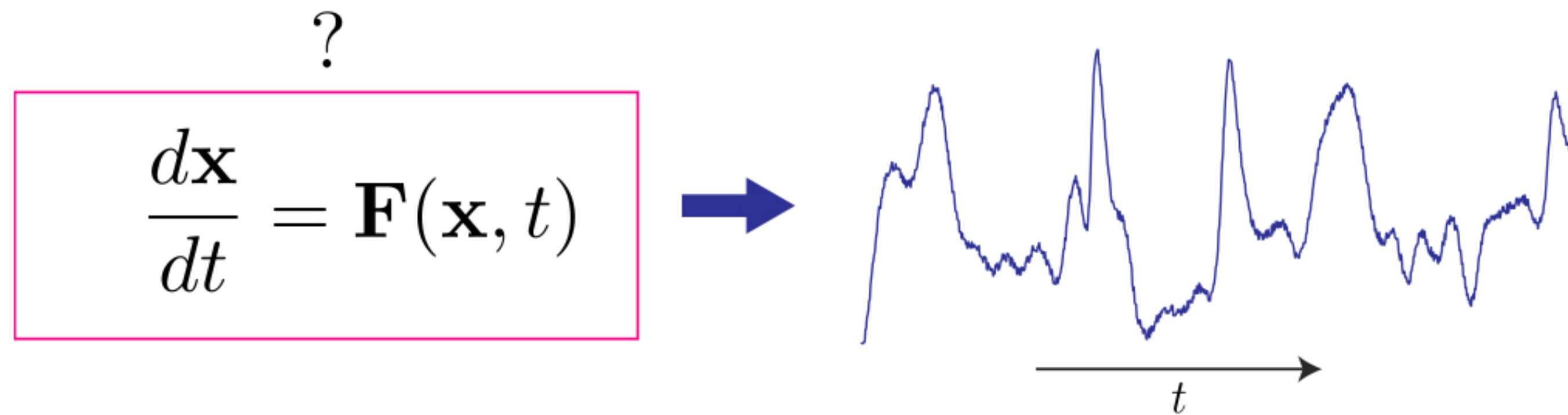
APS Physics Next - Machine Learning (Eastern Long Island, NY)

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Brian Hunt, Michelle Girvan, Zhixin Lu, Edward Ott

University of Maryland, College Park

Given some data from a dynamical system, what can we say about the dynamical process that generated this data?



OUTLINE

Prediction

Given a limited time series of past measurements **can we predict the future state** of the dynamical system, at least in the short term?

Reconstructing the attractor

Can we learn something about the long-term dynamics of the system? Specifically, can we use our setup to **understand the ergodic properties** of a high-dimensional dynamical system?

Scalability

Can we use our setup for **very high-dimensional attractors**?

INTRODUCTION

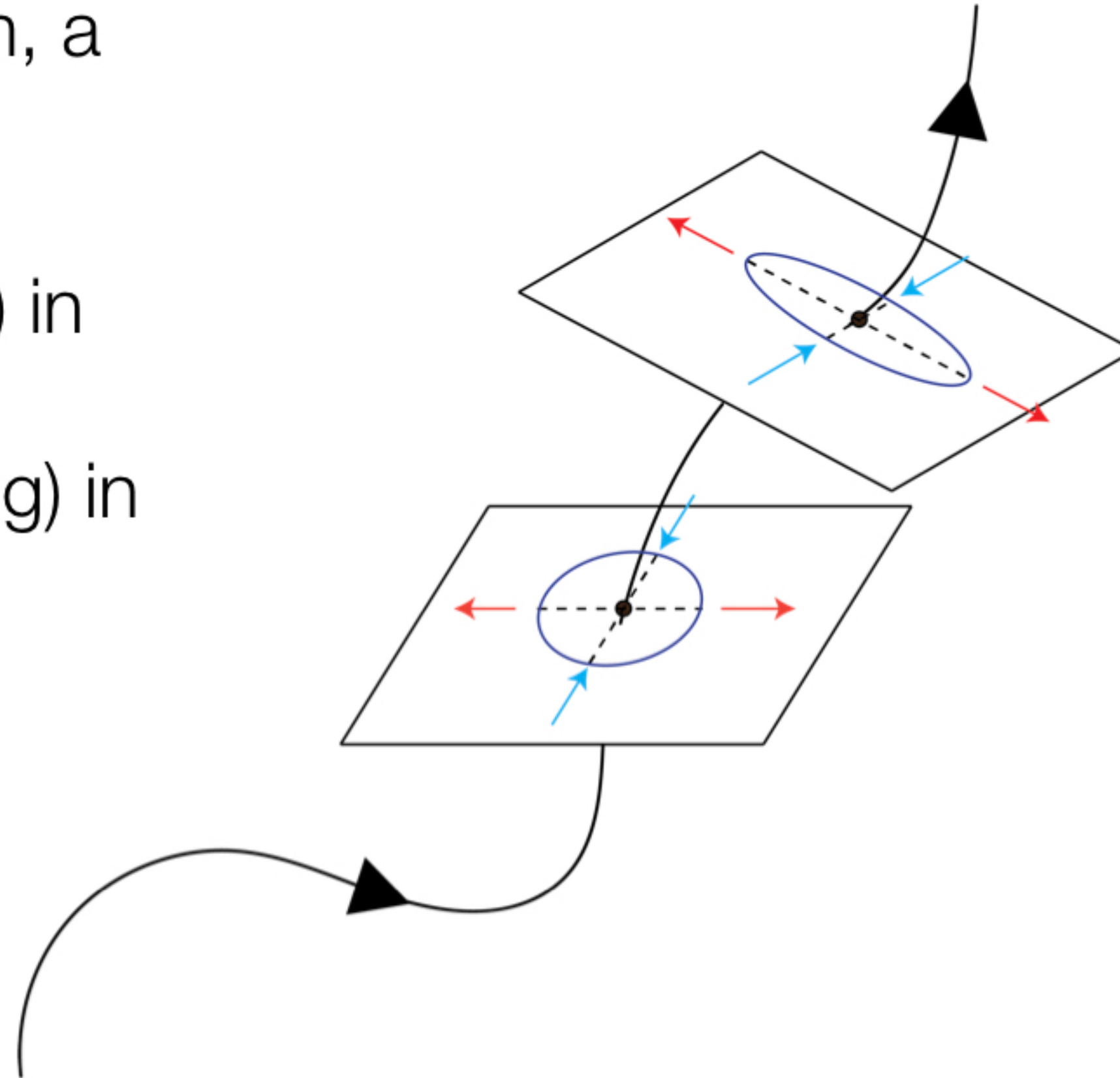
Operationally, we say a dynamical system is **chaotic** if, in a bounded phase space, two nearby **trajectories** **diverge exponentially**.

$$\mathbf{x}_1(t) - \mathbf{x}_2(t) = \delta\mathbf{x}(t)$$

$$\|\delta\mathbf{x}(t)\| \sim \|\delta\mathbf{x}(0)\| \exp(\Lambda t)$$

INTRODUCTION

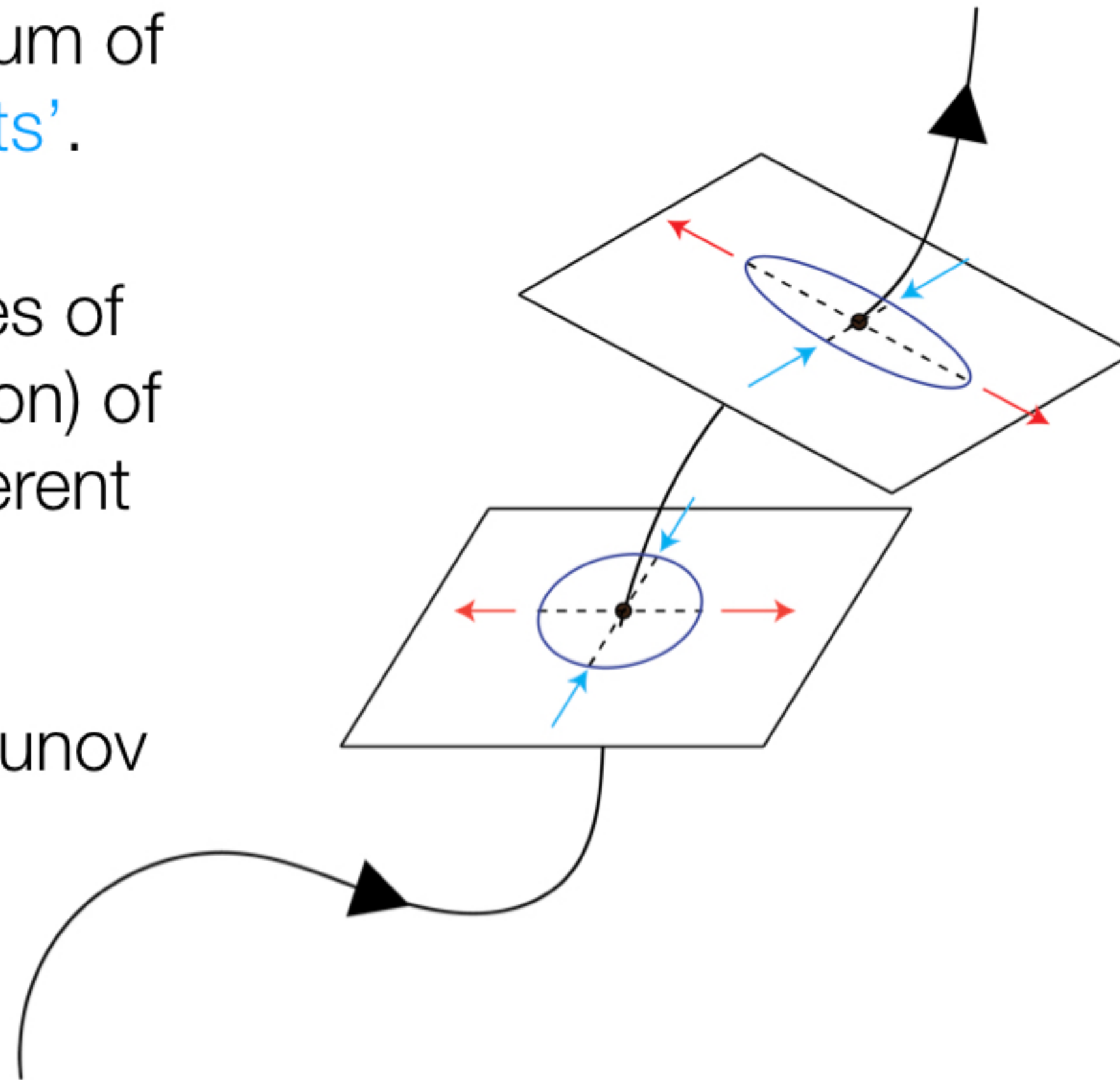
In a chaotic system, a perturbation to the trajectory may be **stable** (contracting) in some directions, **unstable** (expanding) in some directions.



INTRODUCTION

This leads to the concept of a spectrum of 'Lyapunov exponents'.

The exponential rates of growth (or contraction) of perturbations in different directions are characterized by corresponding Lyapunov exponents.



INTRODUCTION

The Lyapunov exponents of a dynamical system are an important characteristic and provide us with a lot of useful information.

Is a system chaotic?

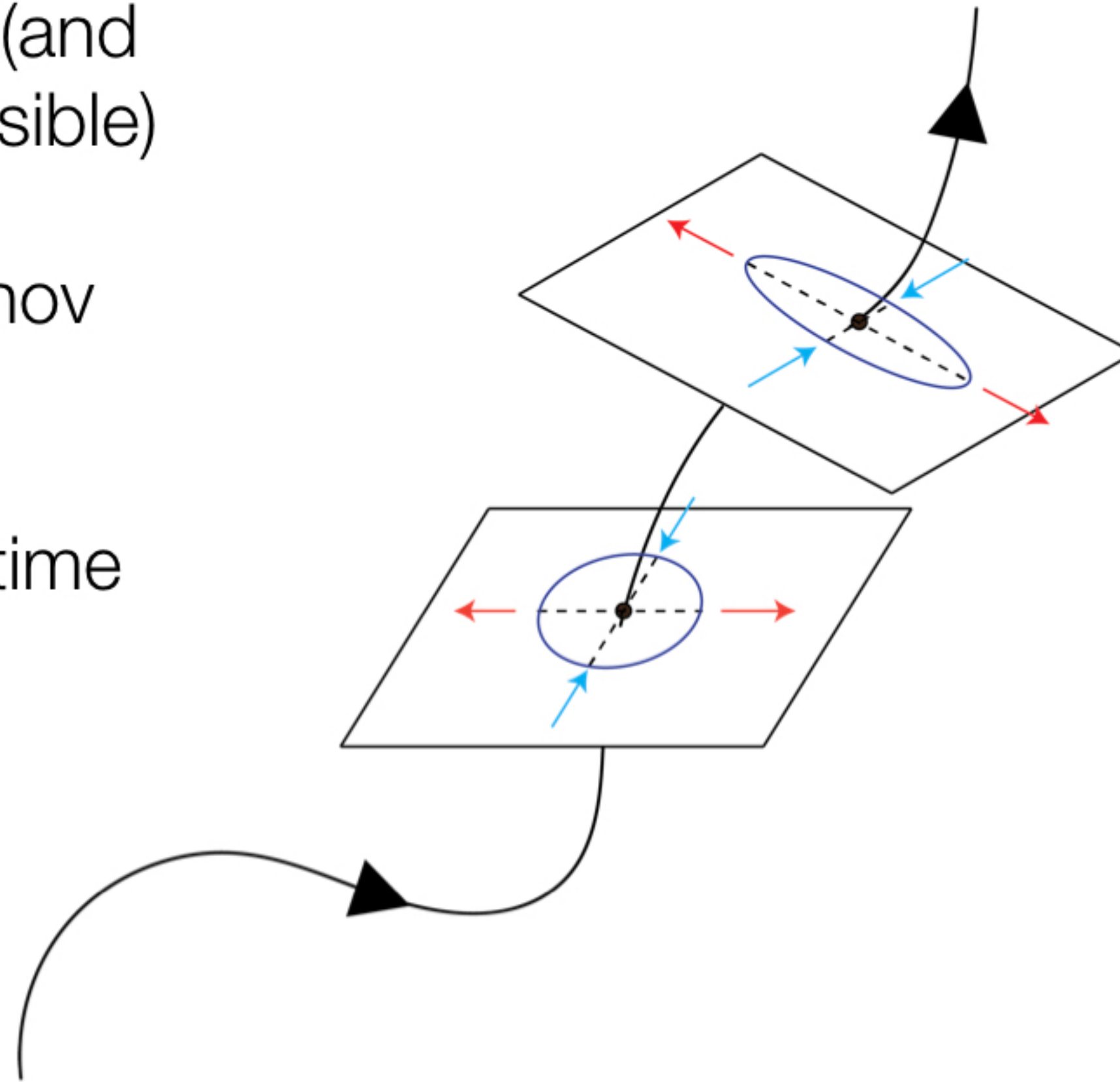
What is the 'complexity' of the system

What is the effective dimension of the chaotic attractor of the system (via the 'Kaplan-Yorke conjecture')?

What is the possible prediction horizon?

INTRODUCTION

In general, in the past it has proven difficult (and sometimes not possible) to estimate the spectrum of Lyapunov exponents of a dynamical system purely from limited time series data.



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MACHINE LEARNING TECHNIQUE: RESERVOIR COMPUTING

Provides a way to train Recurrent Neural Networks.

Independently introduced by Jaeger (2001), and Maass et al. (2002).

Main component is a **very high-dimensional system**, called the **reservoir** (not to be confused with the measured dynamical system).

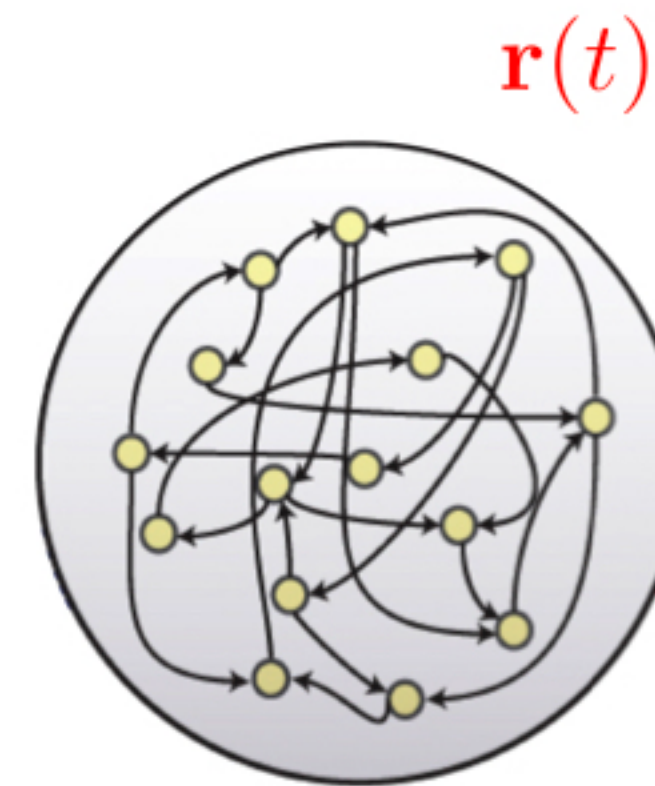
The reservoir provides a rich repository of dynamics.

RESERVOIR COMPUTING

The reservoir in our setup is a network of D_r nodes.

Each node i has multiple inputs and outputs and a scalar state denoted by $r_i(t)$.

The weighted connections between the nodes can be represented by an adjacency matrix $\mathbf{A}$.



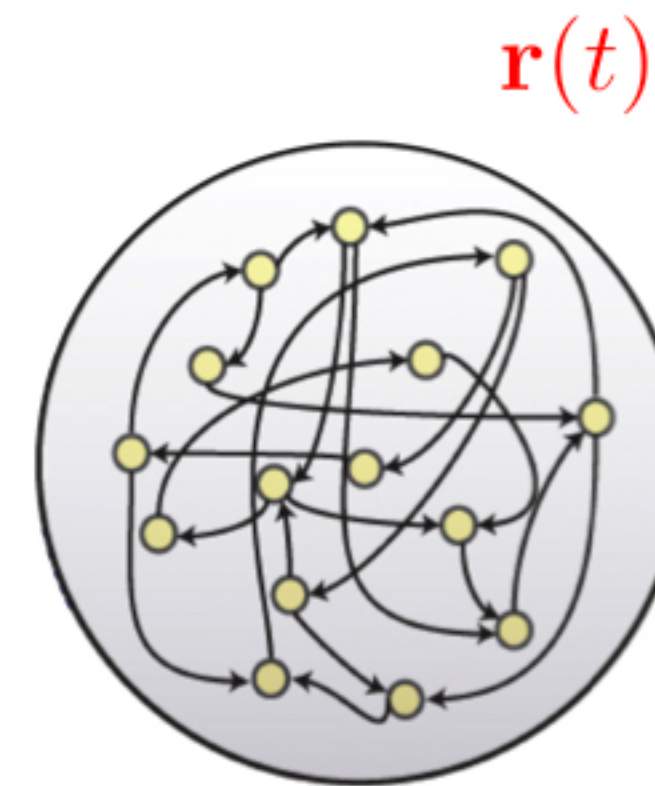
$$\mathbf{A} : D_r \times D_r$$

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$$\mathbf{A} : D_r \times D_r$$

- Sparse.
- Randomly Generated.
- Fixed.

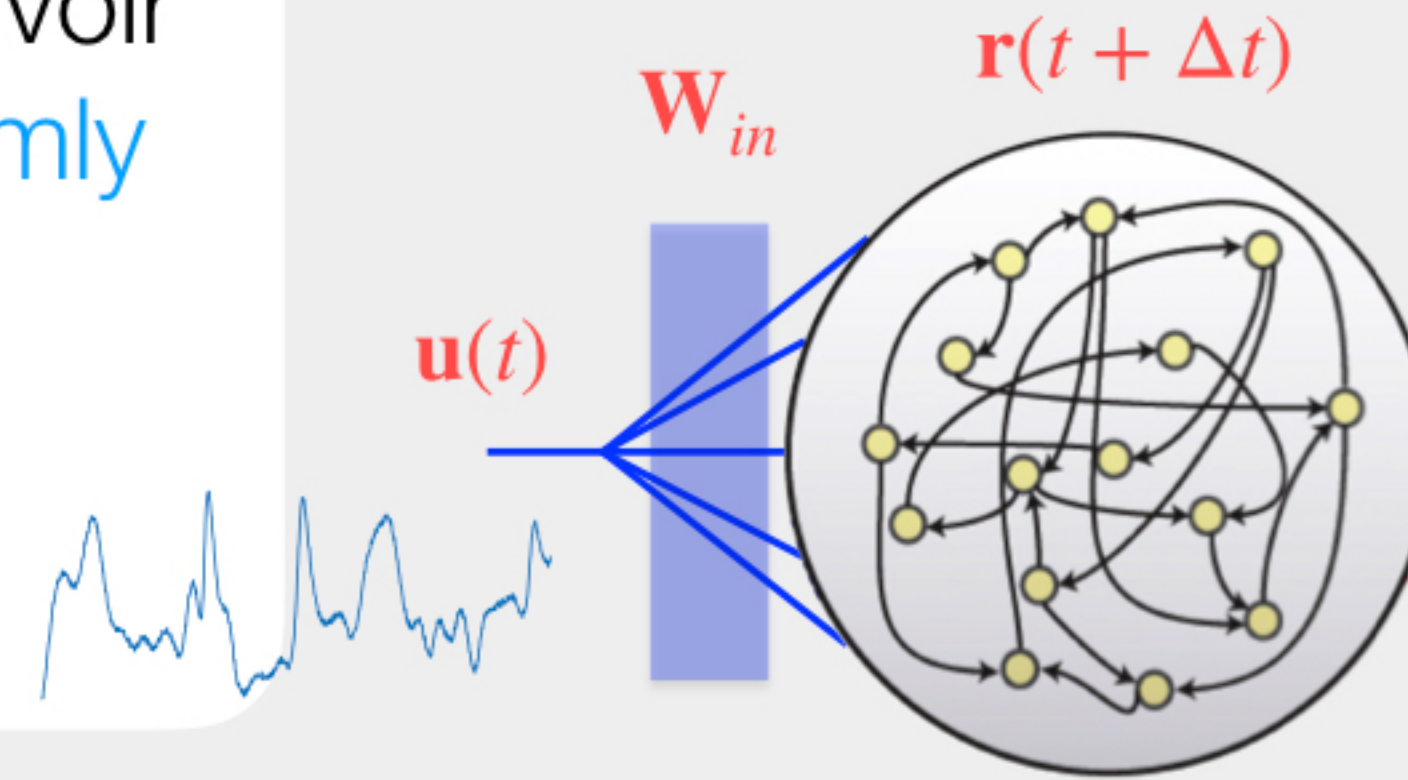
RESERVOIR NEURAL NETWORK IMPLEMENTATION

FEED DATA

An input is coupled to the reservoir network through a **fixed, randomly generated** input matrix.

$$\mathbf{r}(t + \Delta t) = \tanh (\mathbf{A}\mathbf{r}(t) + \mathbf{W}_{in}\mathbf{u}(t))$$

$$-T \leq t \leq 0$$



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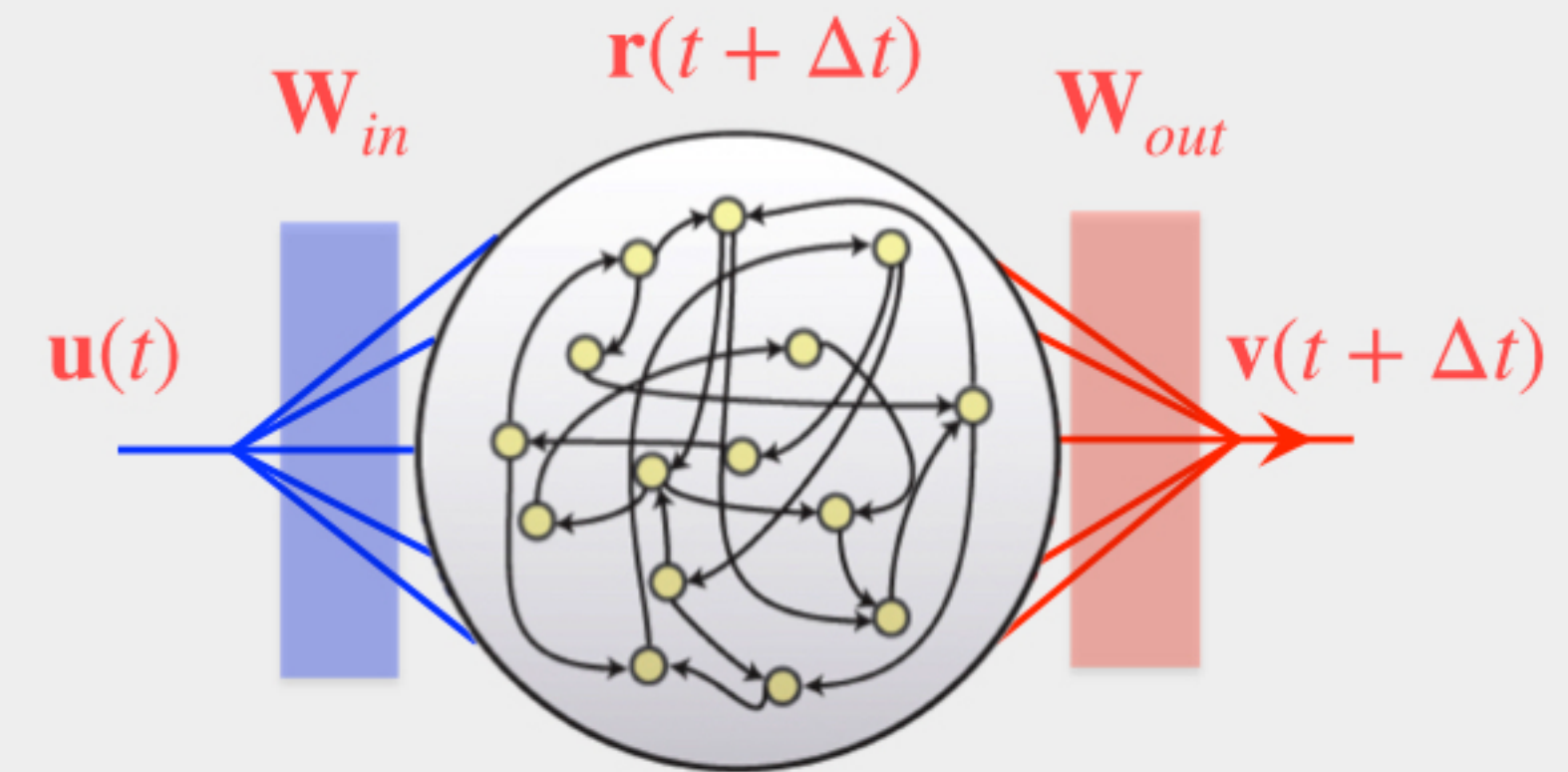
LINEAR FIT

Find the output weight matrix that minimizes the following loss function

$$\mathcal{L}(\mathbf{W}_{out}) = \sum_{t=-T}^0 \|\mathbf{W}_{out}\mathbf{r}(t) - \mathbf{u}(t)\|^2$$

$$\mathbf{v}(t) = \mathbf{W}_{out}\mathbf{r}(t)$$

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TRAINING IS A SIMPLE LINEAR REGRESSION PROBLEM.

INSTEAD OF GRADIENT DESCENT, WE HAVE A SIMPLER PROBLEM OF MATRIX INVERSION.



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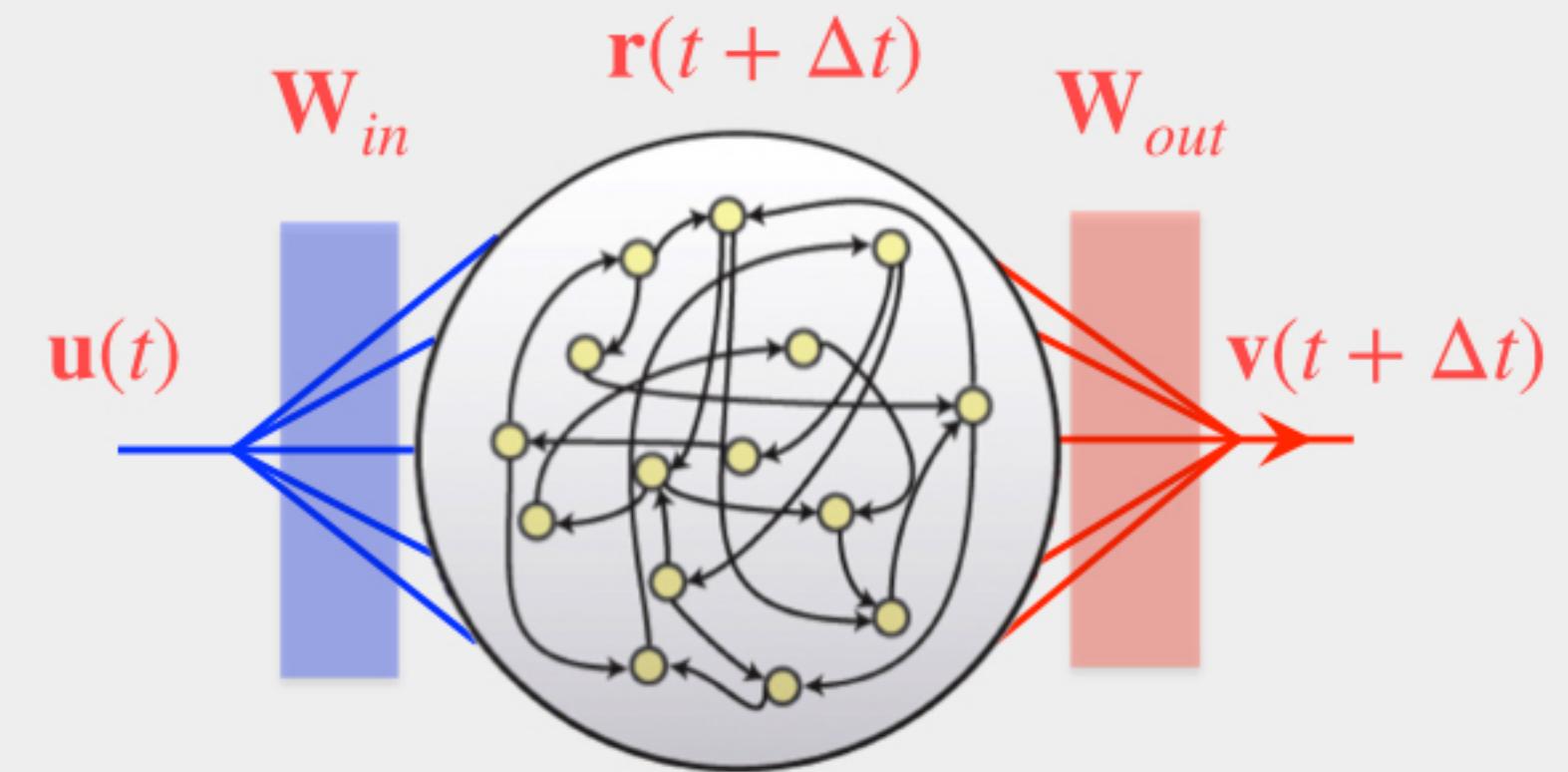
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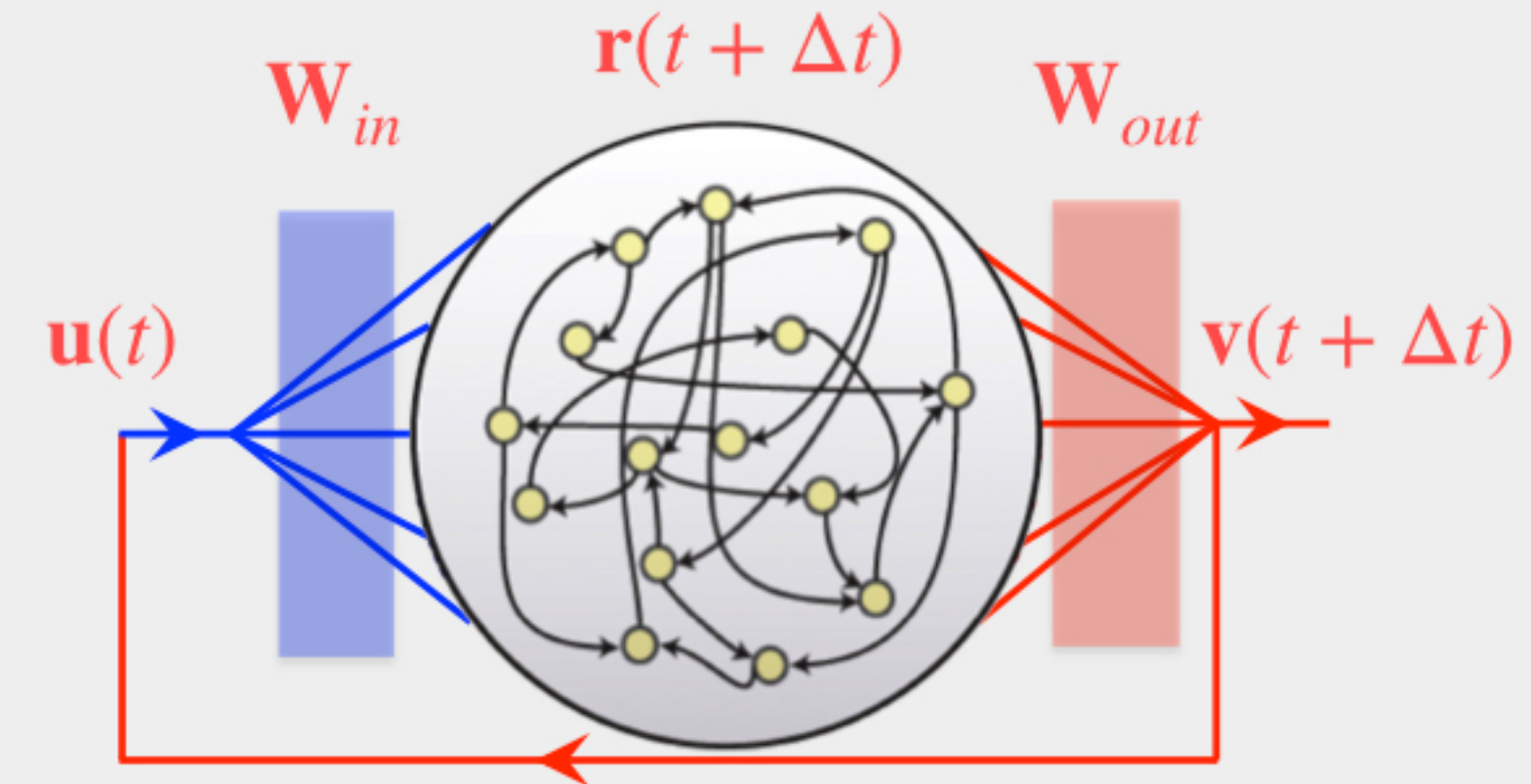
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PREDICTION

$$t > 0$$

$$\mathbf{v}(t) = \mathbf{W}_{out}\mathbf{r}(t)$$

$$\mathbf{r}(t + \Delta t) = \tanh (\mathbf{A}\mathbf{r}(t) + \mathbf{W}_{in}\mathbf{v}(t))$$

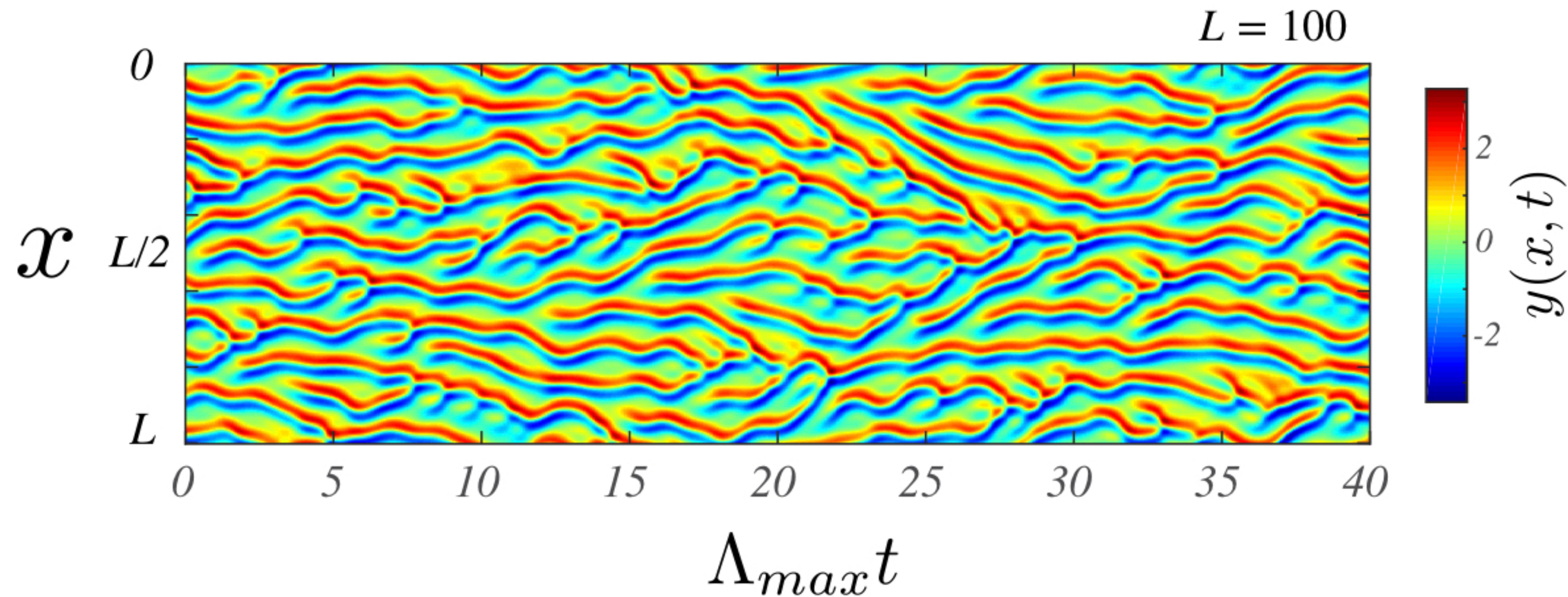
THE KURAMOTO-SIVASHINSKY (KS) SYSTEM

A nonlinear, spatiotemporal chaotic PDE

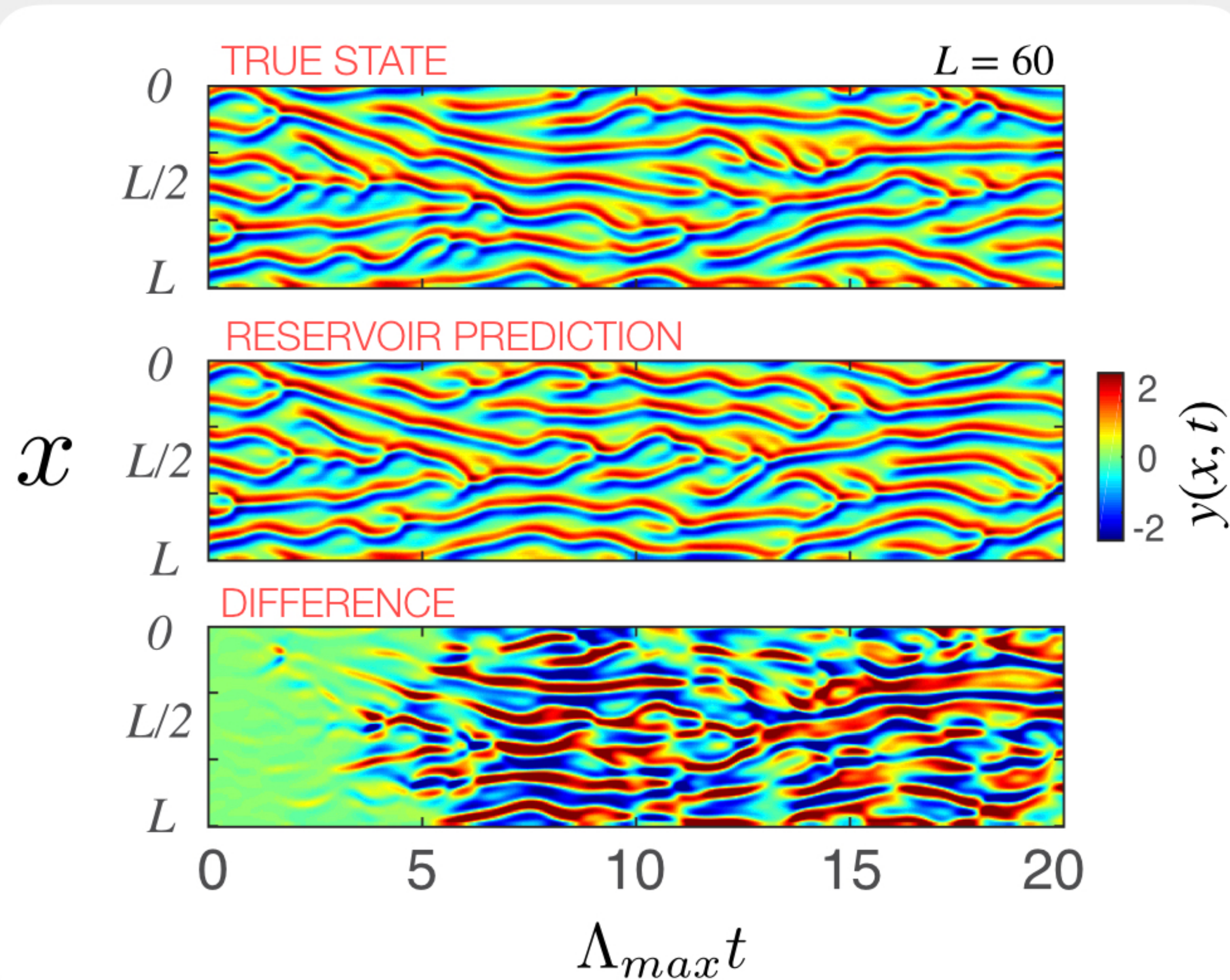
$$y_t = -yy_x - y_{xx} - y_{xxxx}$$

$$x \in [0, L)$$

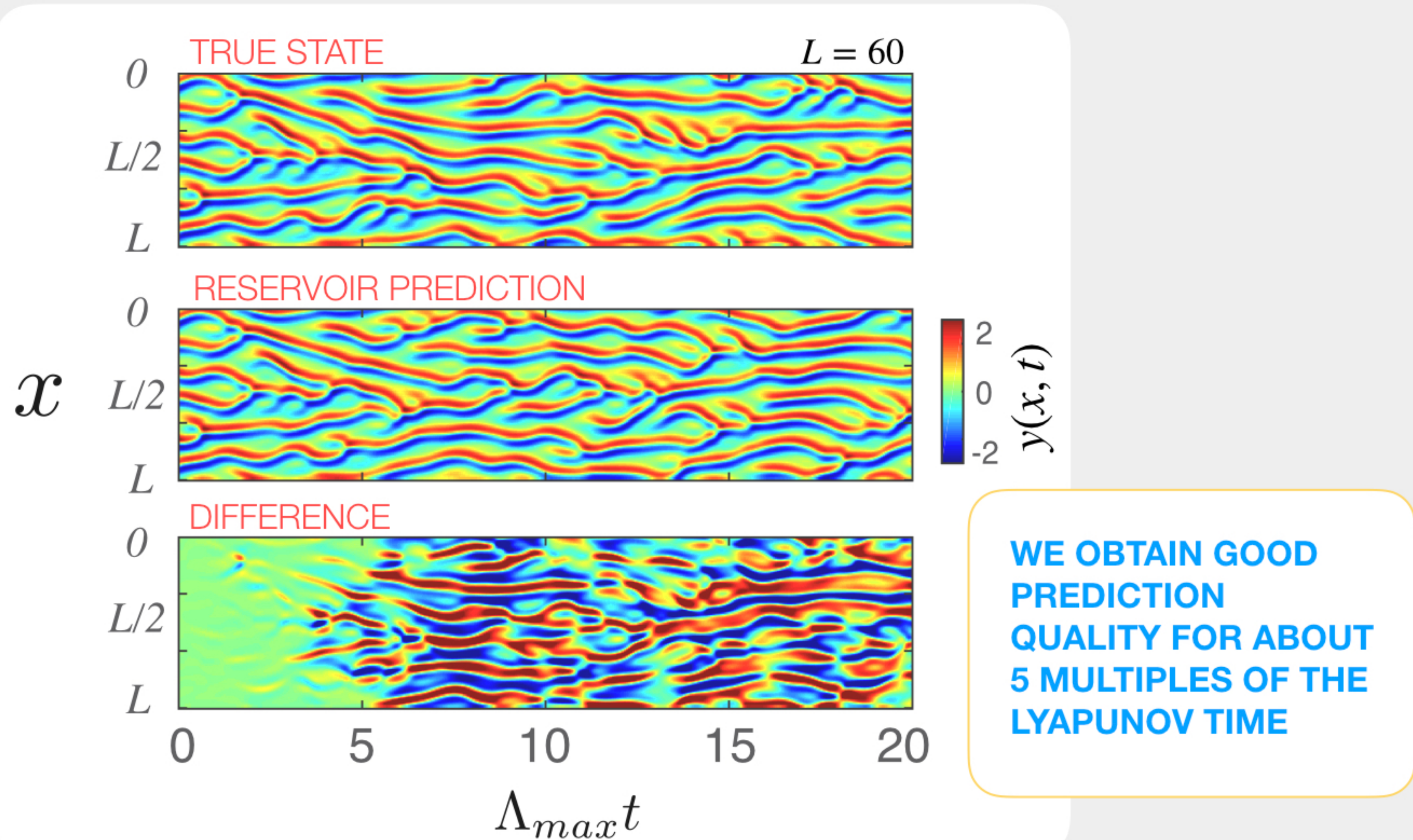
$$y(x + L) = y(x)$$



SHORT-TERM FORECASTING OF CHAOS: KURAMOTO-SIVASHINSKY EQUATION



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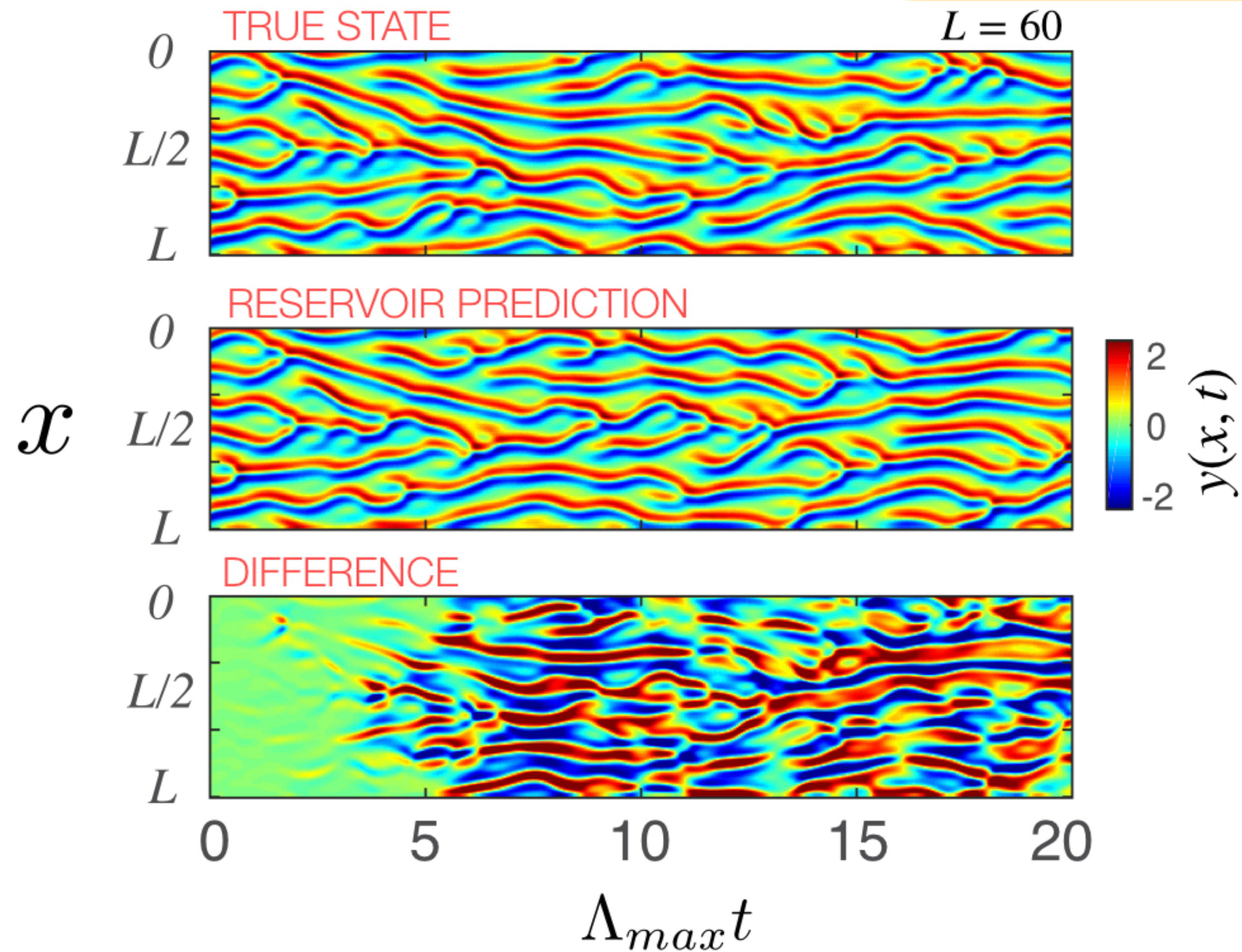


SHORT-TERM FORECASTING OF CHAOS: KURAMOTO-SIVASHINSKY EQUATION

The reservoir computer is really good at learning the dynamics from data alone.

It is capable of making high quality short term predictions when the system dynamics is unknown.

NOTICE THAT THE DYNAMICS
LOOKS 'KS LIKE' EVEN WHEN
THE PREDICTION HAS
DIVERGED FROM THE TRUE
STATE



'CLIMATE' OF THE RESERVOIR DYNAMICS

Has the reservoir truly learned the dynamical behavior of the Kuramoto-Sivashinsky system?

If it has, the ergodic properties of the autonomous reservoir dynamical system should resemble those of the true system.

Is there a way to verify this?

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LYAPUNOV EXPONENTS FROM DATA

We know the evolution equation of the post-training autonomous reservoir system.

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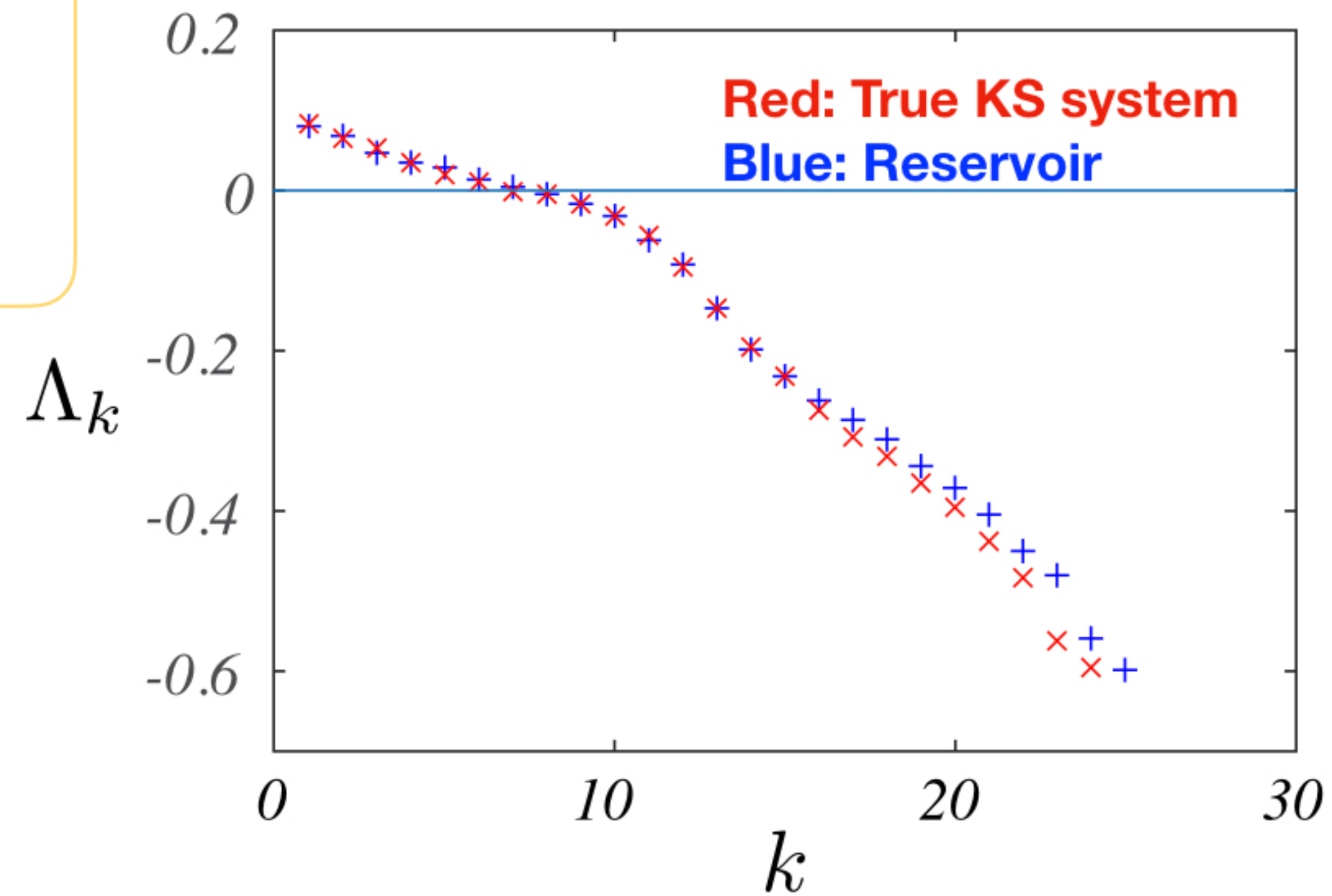
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Are the Lyapunov exponents of the reservoir same as those of the data generating system?

LYAPUNOV EXPONENTS FROM DATA

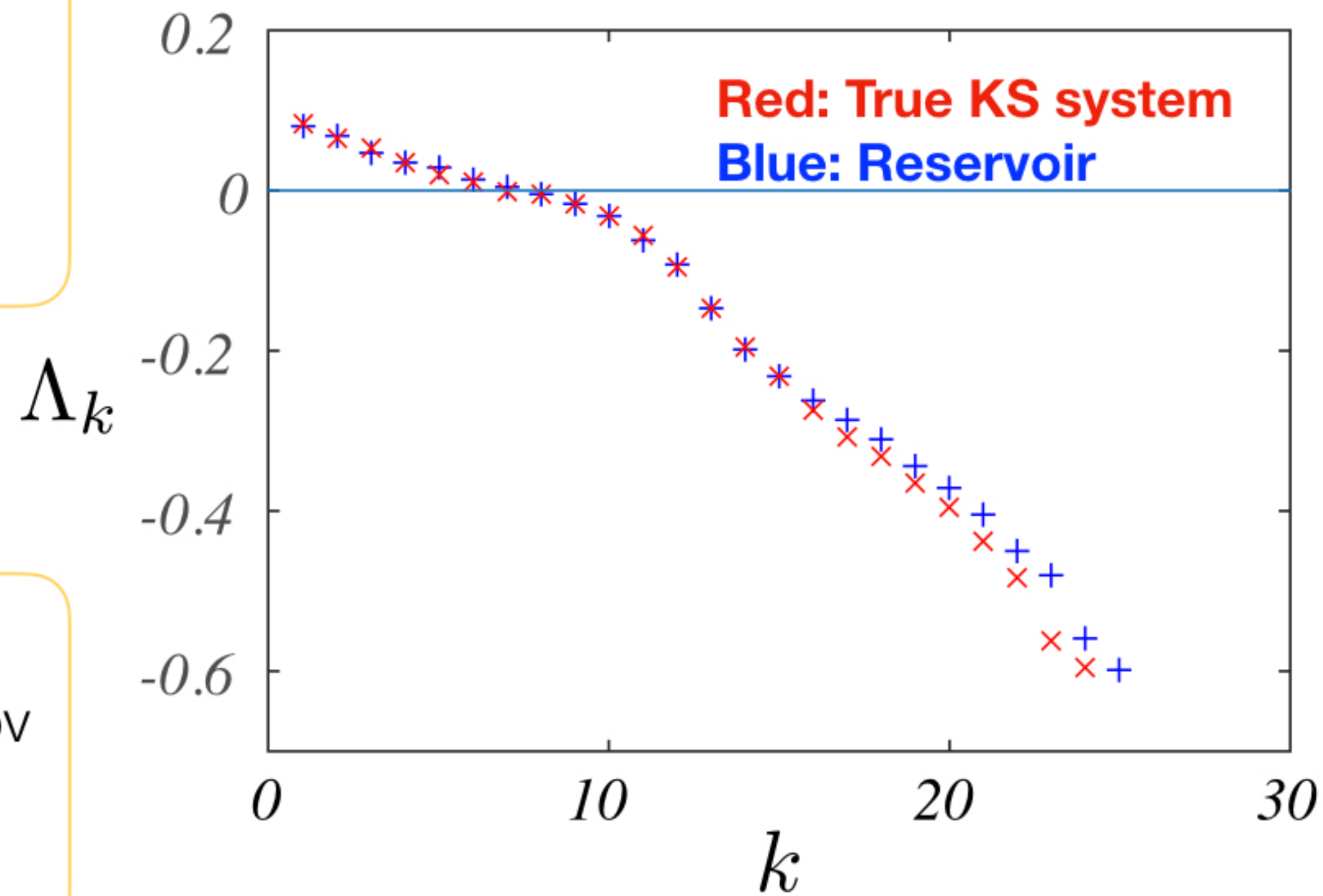
The Lyapunov exponents of the KS system are indeed accurately reproduced by the reservoir!



LYAPUNOV EXPONENTS FROM DATA

The Lyapunov exponents of the KS system are indeed accurately reproduced by the reservoir!

The reservoir fails at obtaining symmetry-related zero Lyapunov exponents. This aspect is discussed further in our paper.



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VERY HIGH-DIMENSIONAL DYNAMICAL SYSTEMS

Can machine learning be useful for studying **very high dimensional dynamical systems**?

As you **increase the size/complexity** of the dynamical system, you need a **bigger reservoir**.

If we keep increasing the nodes, the training problem becomes intractable.

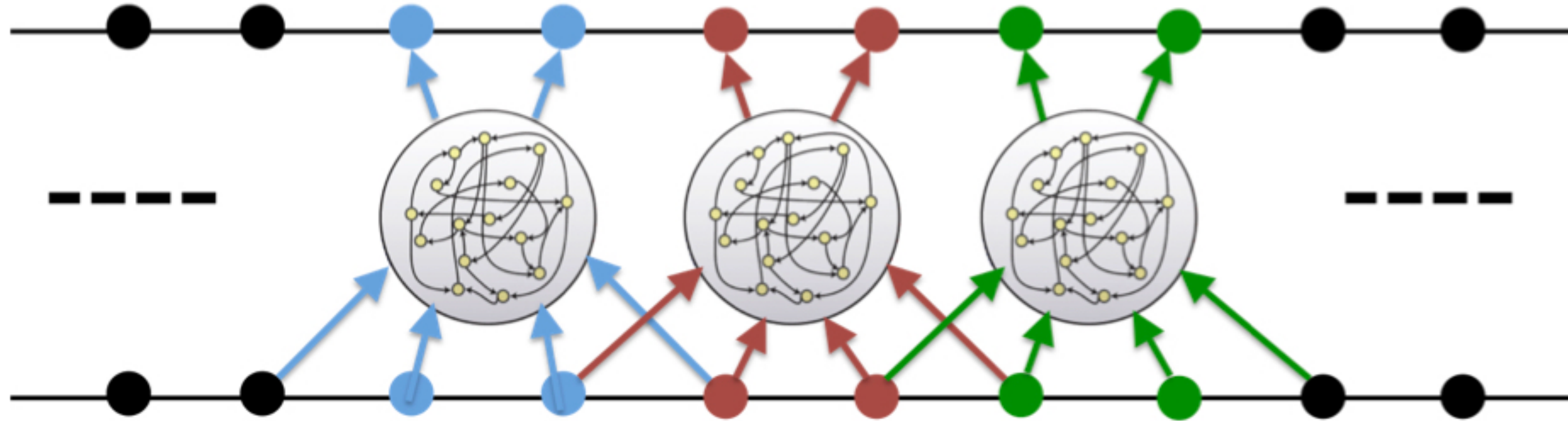
VERY HIGH-DIMENSIONAL DYNAMICAL SYSTEMS

We use some knowledge of the physics of spatiotemporal systems: our system has short-range spatial correlations.

The training and prediction of spatiotemporal chaos can be very effectively parallelized

VERY HIGH-DIMENSIONAL DYNAMICAL SYSTEMS

Training



Multiple reservoirs,
parallel computing
on a cluster.

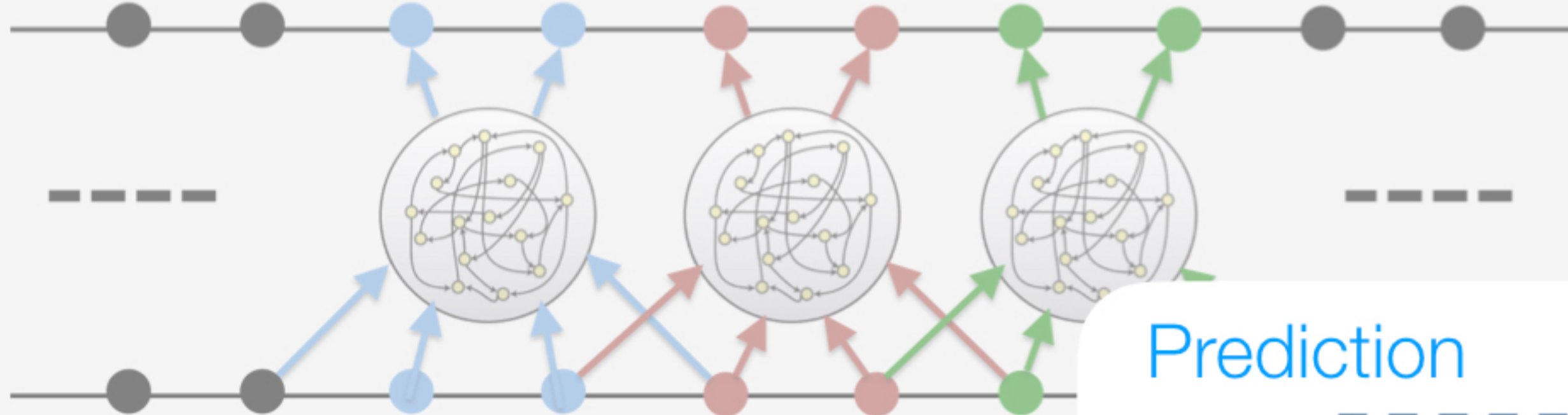
Each reservoir is assigned to [a local neighborhood](#) on the spatial grid and is trained to predict a subset of its inputs.

The local neighborhood consists of the grid points to be predicted plus [buffer zones](#) on each side.

Each of the relatively small parallel reservoirs has its own relatively small [independently trained](#) output matrix.

VERY HIGH-DIMENSIONAL DYNAMICAL SYSTEMS

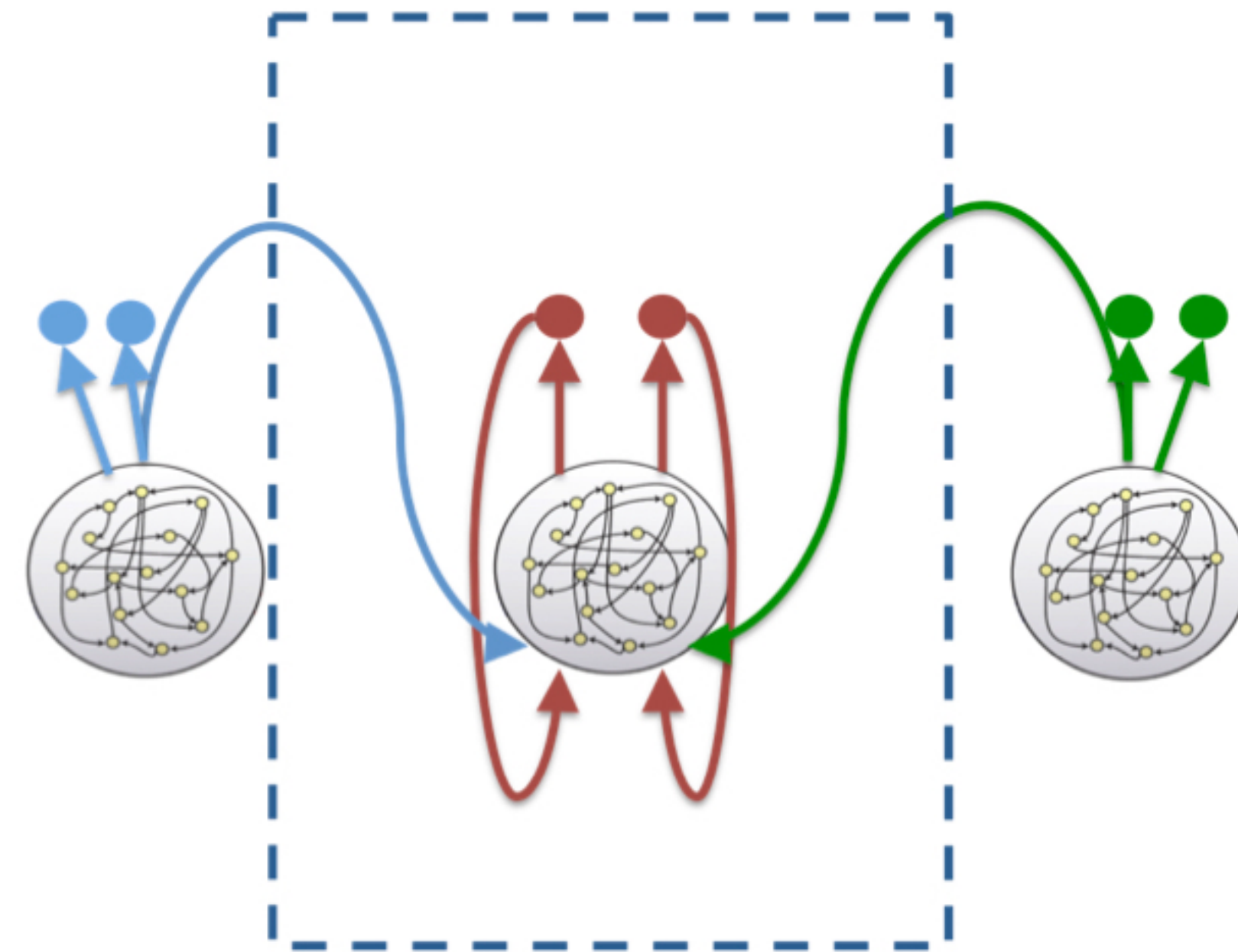
Training



Multiple reservoirs,
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on a cluster.

During the prediction phase, a given reservoir has feedbacks from its own outputs and from the outputs of neighboring reservoirs on each side to account for the buffer zones/overlaps.

Prediction



VERY HIGH-DIMENSIONAL DYNAMICAL SYSTEMS

We use a KS type system with periodic boundary conditions $y(x + L, t) = y(x, t)$.

The attractor dimension of this system increases linearly with the periodicity length L .

L	D_{KY}
100	23
200	43
400	85
800	167
1600	338

D_{KY} : Kaplan-Yorke Dimension of the Chaotic Attractor (Measure of Complexity)

VERY HIGH-DIMENSIONAL DYNAMICAL SYSTEMS: KURAMOTO-SIVASHINSKY

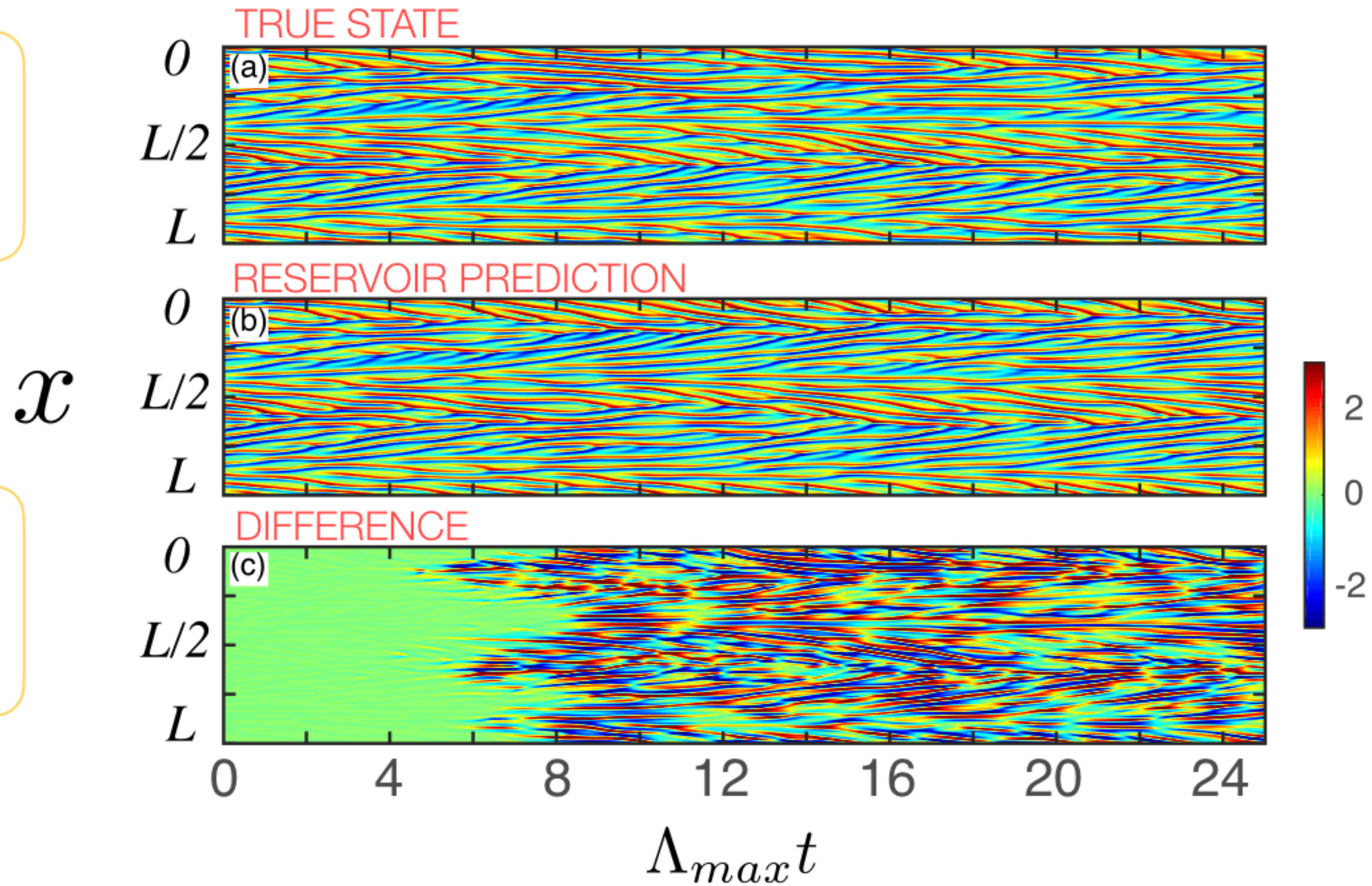
Model Parameters:

$$L = 200$$

$$D_{KY} = 43$$

Reservoir:

$$(D_r = 5000) \times 64$$

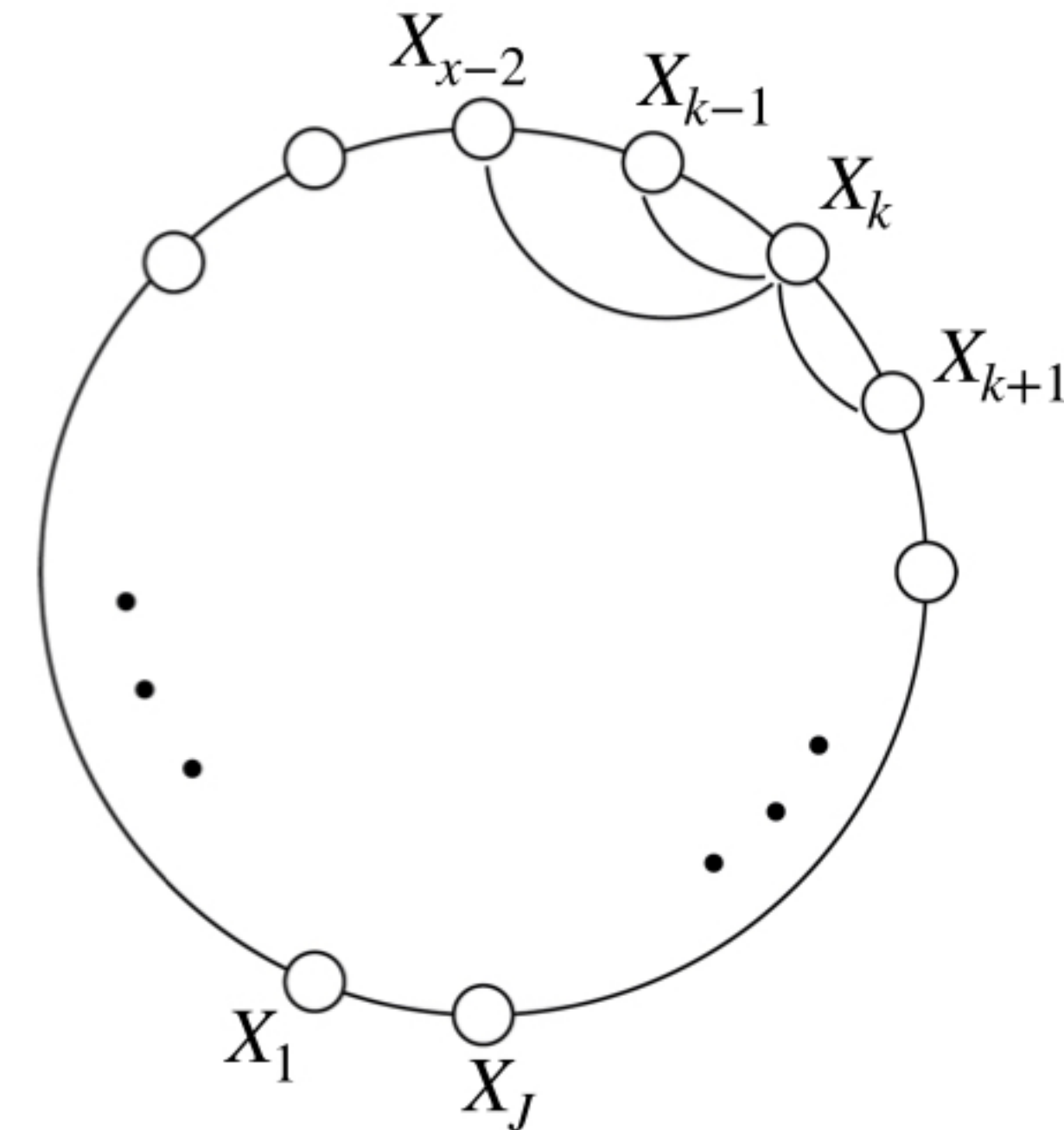


VERY HIGH-DIMENSIONAL DYNAMICAL SYSTEMS: THE LORENZ 1996 TOY WEATHER MODEL

As another example, we consider the Lorenz 1996 model of atmospheric dynamics often used for testing techniques in weather prediction.

$$\frac{dX_k}{dt} = -X_k + (X_{k+1} - X_{k-2})X_{k-1} + F$$

$$k = 1, 2, \dots, J$$



VERY HIGH-DIMENSIONAL DYNAMICAL SYSTEMS: THE LORENZ 1996 TOY WEATHER MODEL

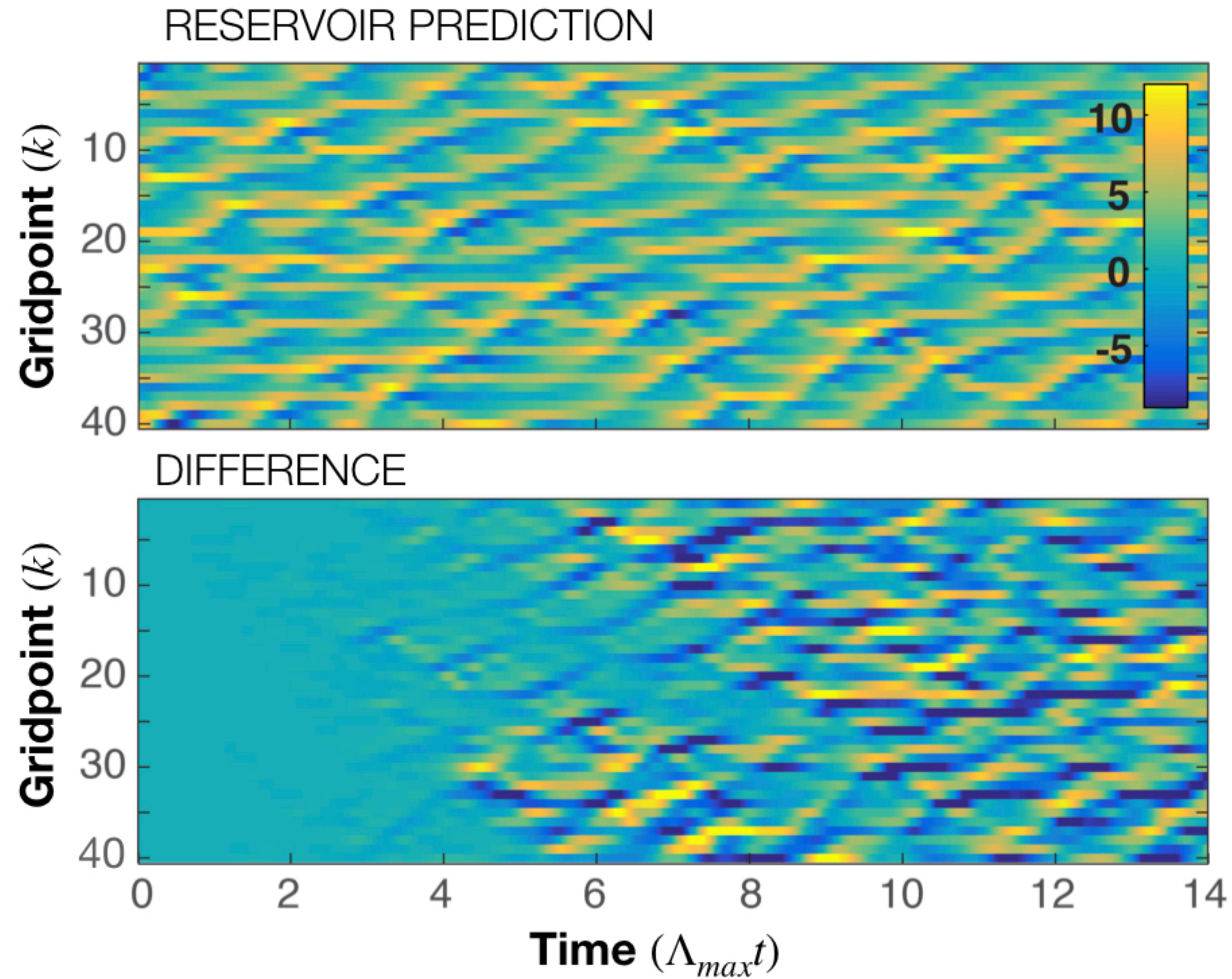
Model Parameters:

$$J = 40$$

$$F = 8$$

Reservoir:

$$(D_r = 5000) \times 20$$



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RESERVOIR COMPUTING AND OTHER RNN ARCHITECTURES

Reservoir computers/ Echo state networks offer very quick and cheap training as compared to Recurrent Neural Networks trained using gradient descent (e.g. LSTM networks). Systematic comparisons currently underway.

Training time for the examples shown today is approximately ~10 min on our cluster of CPUs. Although this is at the cost of using hundreds of cores for large spatiotemporal systems.

FUTURE DIRECTIONS OF OUR RESEARCH

'Hybrid' forms of machine learning that incorporate physics-based models, data-assimilation techniques.

Theoretical insight into prediction of chaotic systems. Lu et al. is a good start in this direction.

Combine with more sophisticated sequence models for learning systems with long-range correlations in space and time.

May be possible to implement ESNs/Reservoir Computing very efficiently on specialized hardware such as FPGAs or opto-electronic systems

CONCLUSIONS

Machine Learning can be a very effective tool for studying high dimensional chaos, including problems which are difficult to tackle with traditional tools.

Potential applications include weather prediction, understanding neural activity, control of chaos, improved simulation techniques for PDEs.

REFERENCES

Jaeger et al. "Harnessing nonlinearity: Predicting chaotic systems and saving energy in wireless communication." *Science* 304.5667 (2004): 78-80.

[A paper that introduced reservoir computing.](#)

Pathak et al. "Model-free prediction of large spatiotemporally chaotic systems from data: a reservoir computing approach." *Physical Review Letters* 120.2 (2018): 024102.

[Prediction of high dimensional attractors.](#)

Pathak et al. "Using machine learning to replicate chaotic attractors and calculate Lyapunov exponents from data." *Chaos* 27.12 (2017): 121102.

[Estimating Lyapunov exponents.](#)

Pathak et al. "Hybrid forecasting of chaotic processes: using machine learning in conjunction with a knowledge-based model." *Chaos* 28.4 (2018): 041101.

[Machine learning in conjunction with incomplete knowledge-based models.](#)

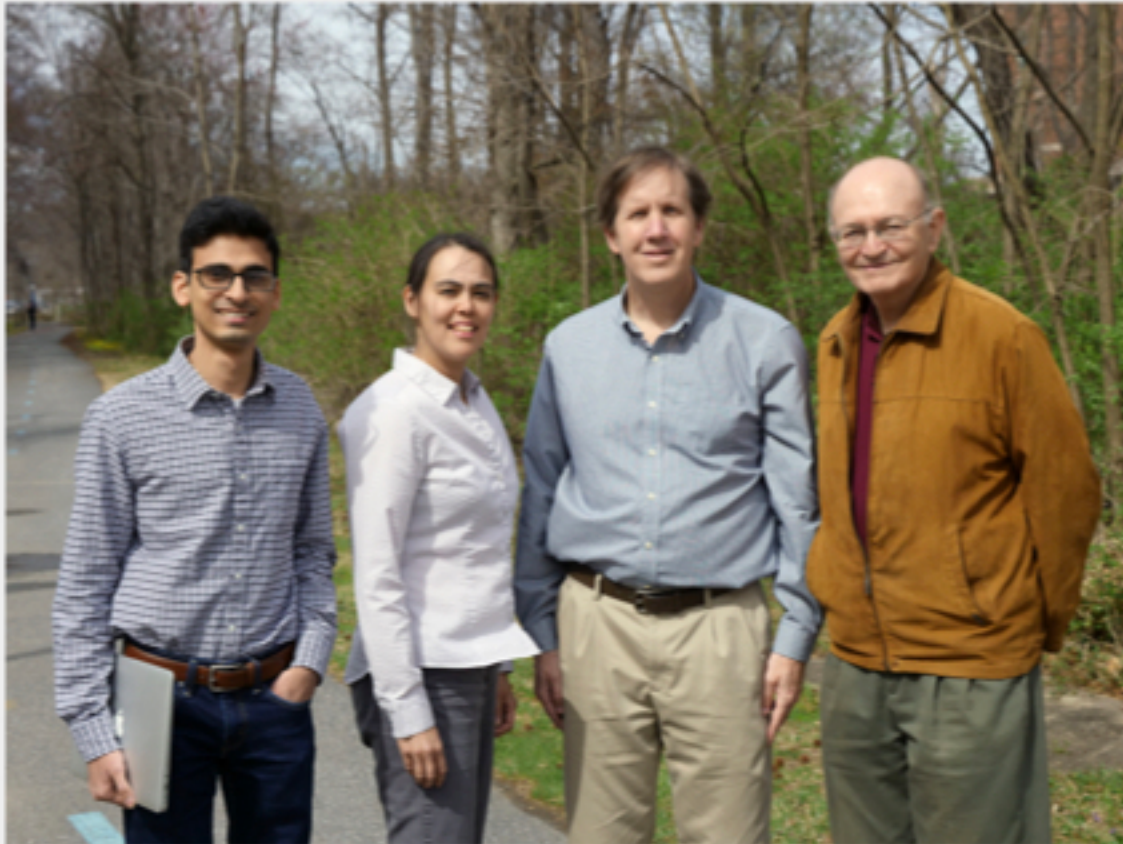
Lu et al. "Attractor reconstruction by machine learning." *Chaos* 28.6 (2018): 061104.

[An attempt to understand attractor reconstruction through the lens of generalized synchronization.](#)

THANK YOU!

The organizers and speakers of the APS Physics Next Workshop.

My Collaborators:



Dr. Michelle Girvan
Dr. Brian Hunt
Dr. Edward Ott
(University of Maryland, College Park)



Dr. Zhixin Lu
(University of
Pennsylvania)



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(University of
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Supported by:

U.S. Army Research Office.

DARPA.

Laboratory of Telecommunication Sciences.