Machine Learning for Scientific Discovery

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University of Washington

(Video by Petros Vrellis)

Machine Learning for Scientific Discovery

Nathan Kutz

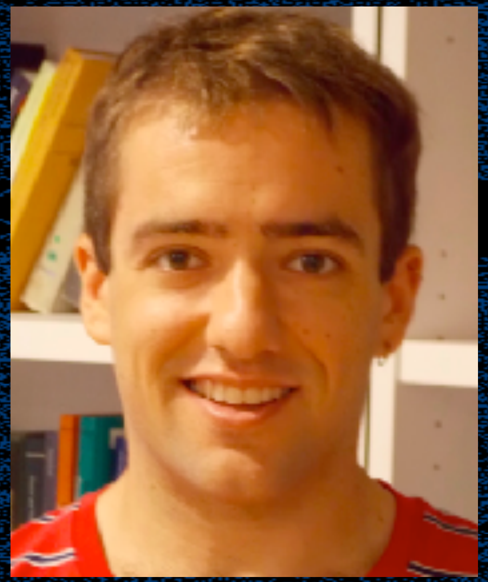
Urban Fasel

Eurika Kaiser

JC Loiseau

Kathleen Champion

Sam Rudy

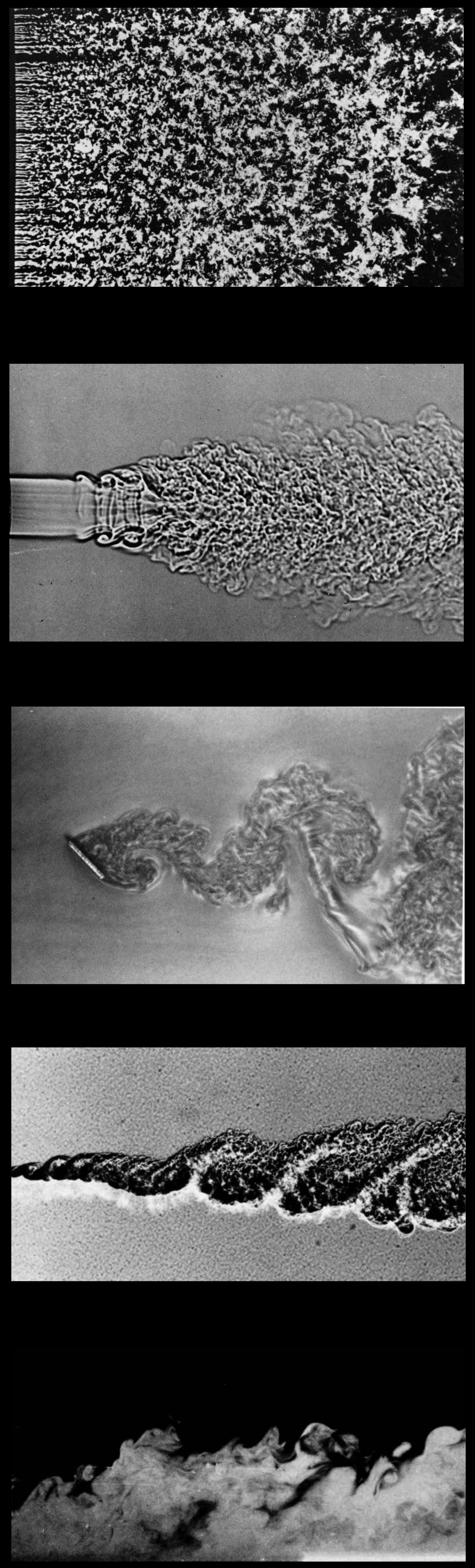


Jared Callaham

Bethany Lusch

Joe Bakarji

Machine Learning:
Models from Data via Optimization



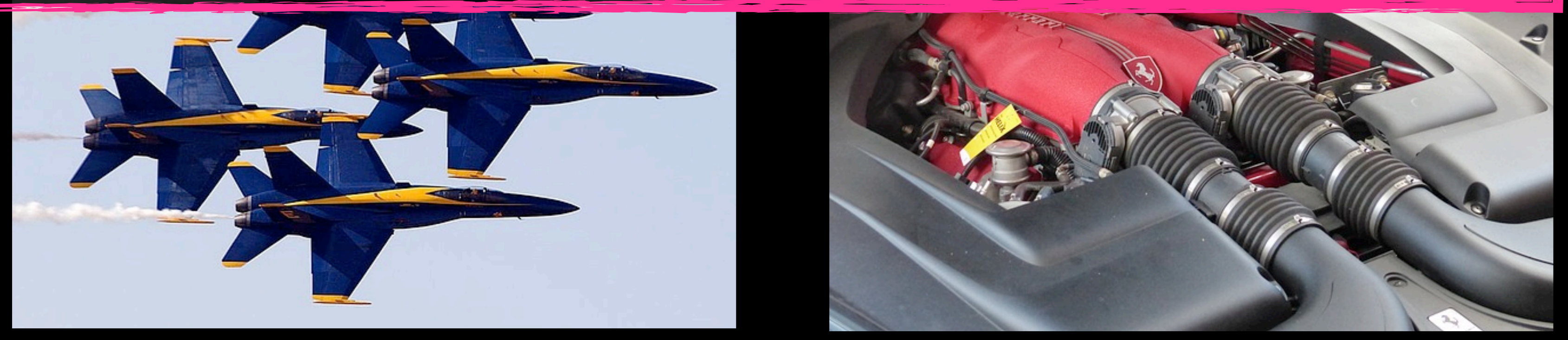
Optimization Problems:

- Nonlinear
- Multiscale

- High-dimensional
- Non-convex

Fluid Dynamics Tasks:

- Reduction
- Modeling
- Sensing
- Estimation
- Control

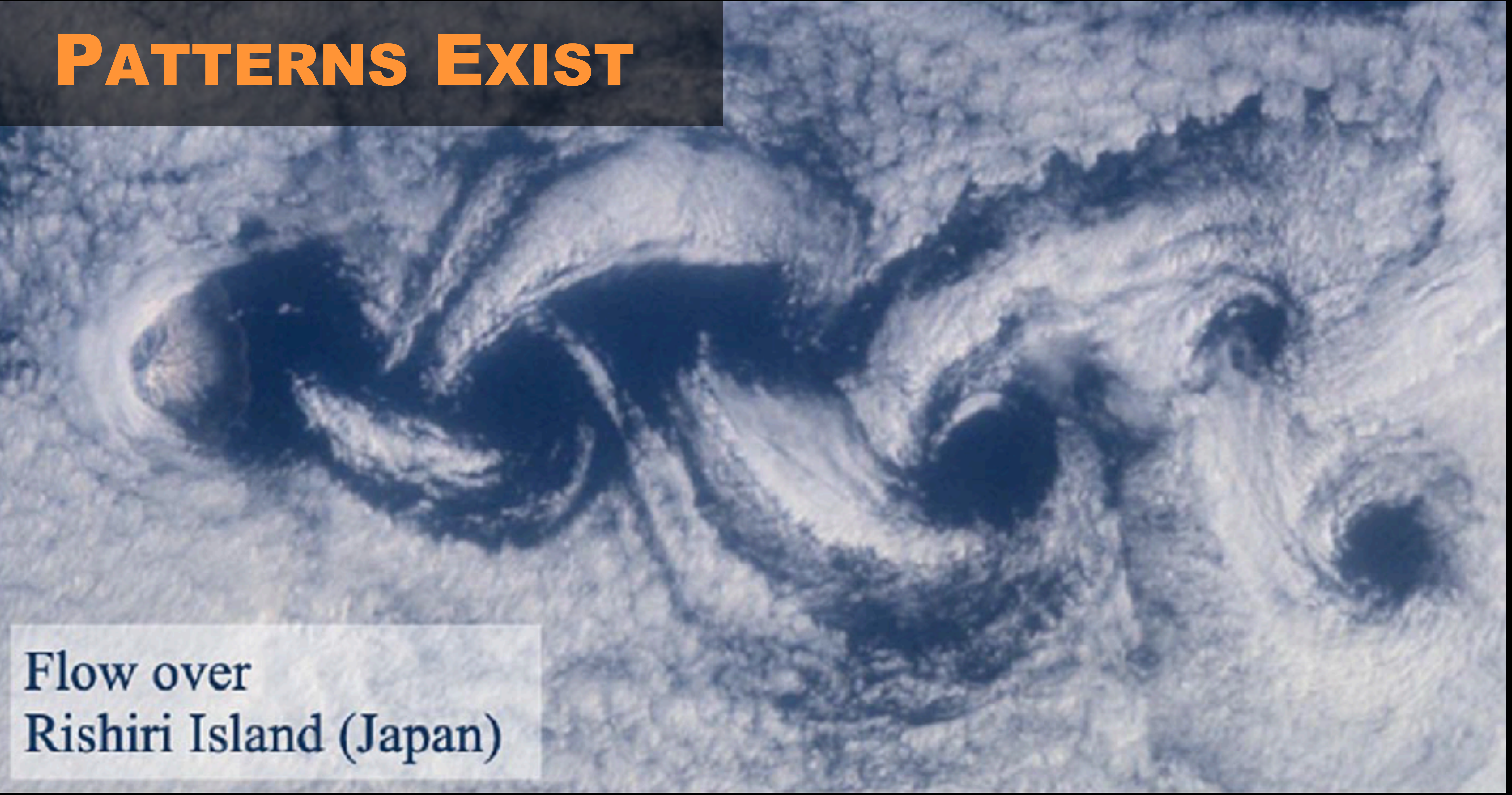


Patterns Exist

@CollinGrossWx

Guadalupe Island

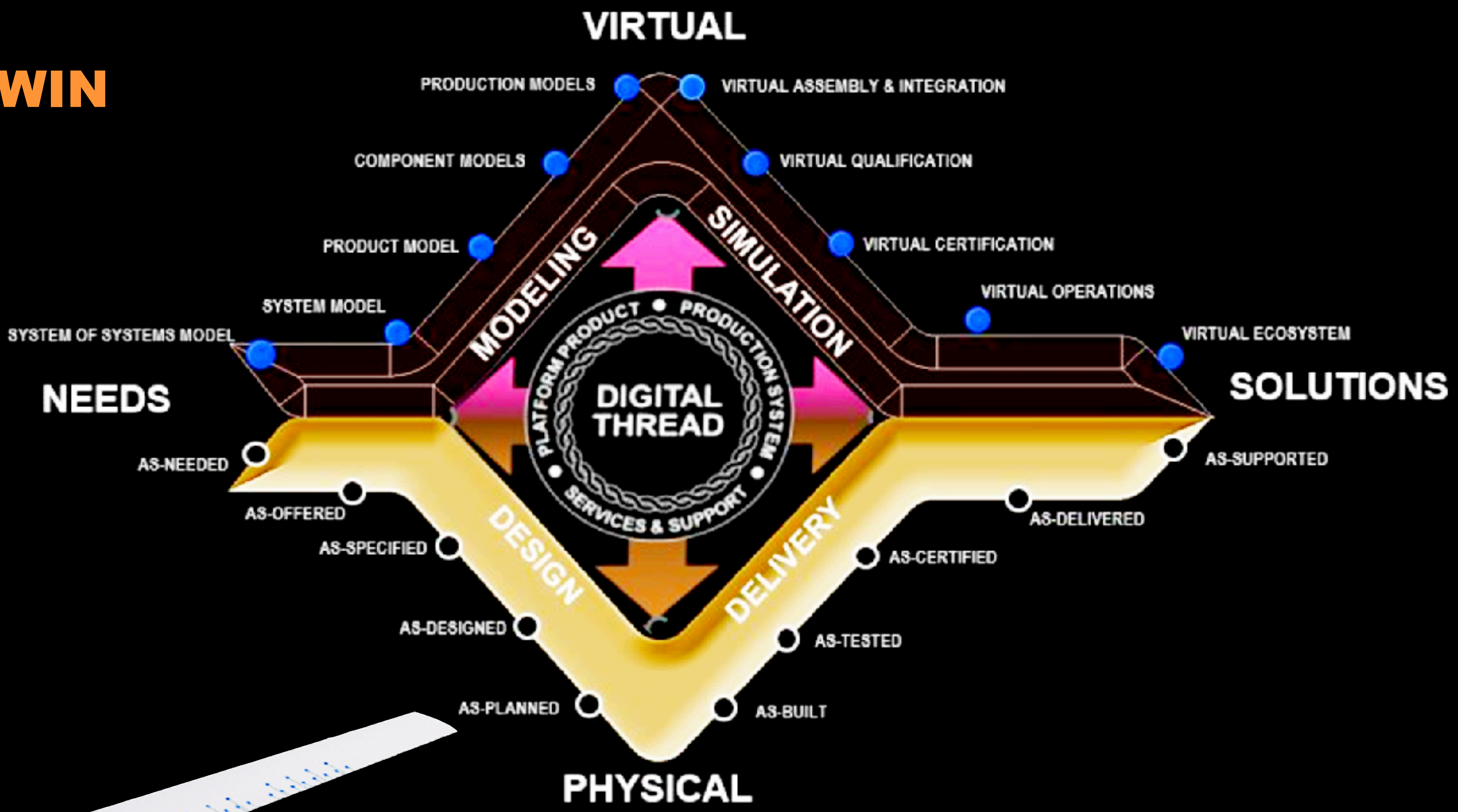
Patterns Exist

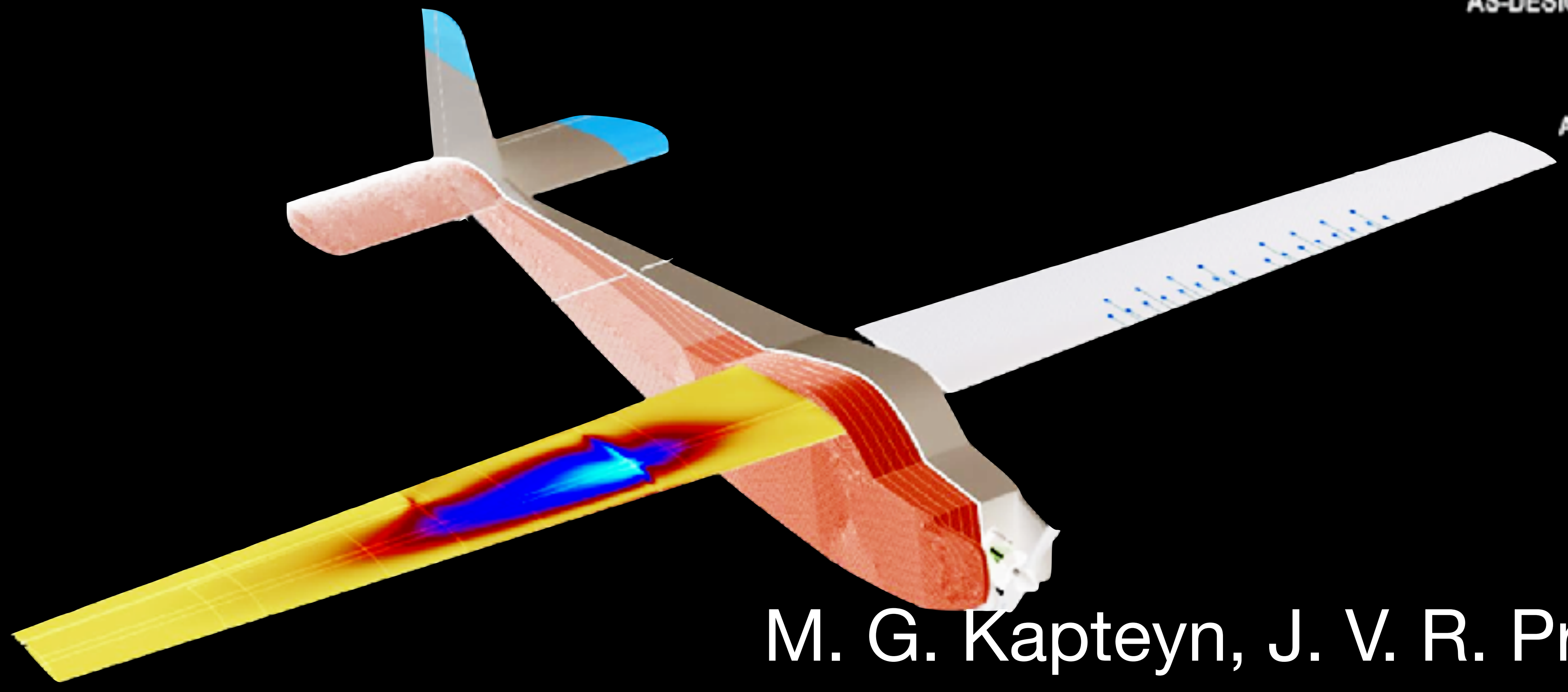


Patterns Enable:

- Sparse Sensing
- Reduced-Order Modeling
- Fast/Efficient Control

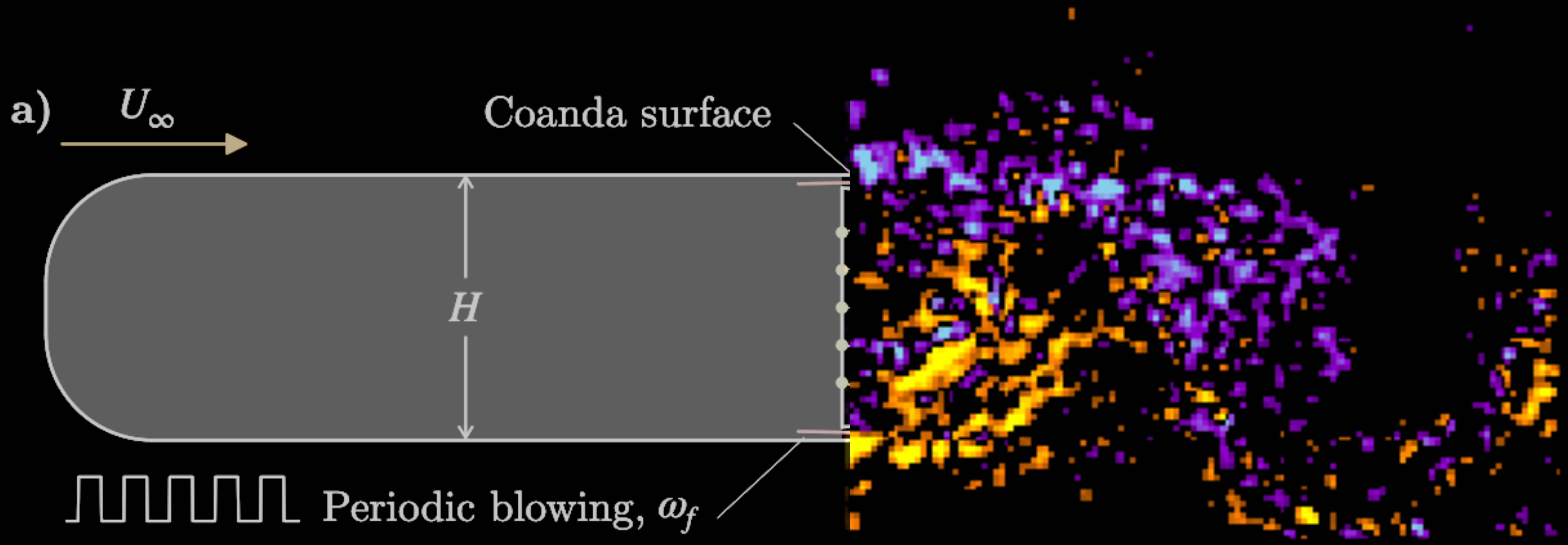
THE DIGITAL TWIN





M. G. Kapteyn, J. V. R. Pretorius, and K. E. Willcox, *Nat. Comp. Sci. 2021*
SLB et al. *AIAA J. 2021*

Reduced Order Models



$$\frac{d}{dt}\mathbf{x} = \mathbf{f}(\mathbf{x})$$

There is a need for INTERPRETABLE and GENERALIZABLE Machine Learning

$F = ma$

There is a need for

INTERPRETABLE and GENERALIZABLE

Machine Learning

EVERYTHING SHOULD BE MADE

AS SIMPLE AS POSSIBLE,

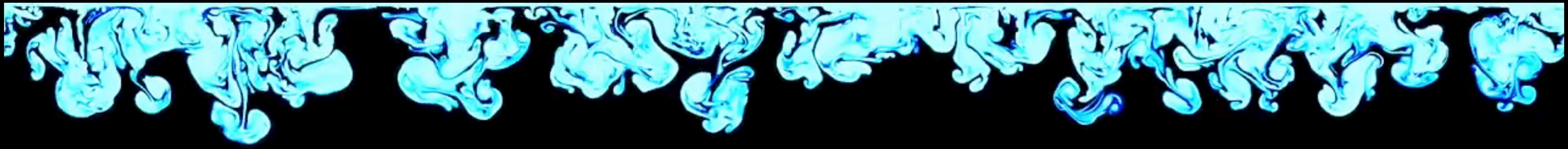
BUT NOT SIMPLER.

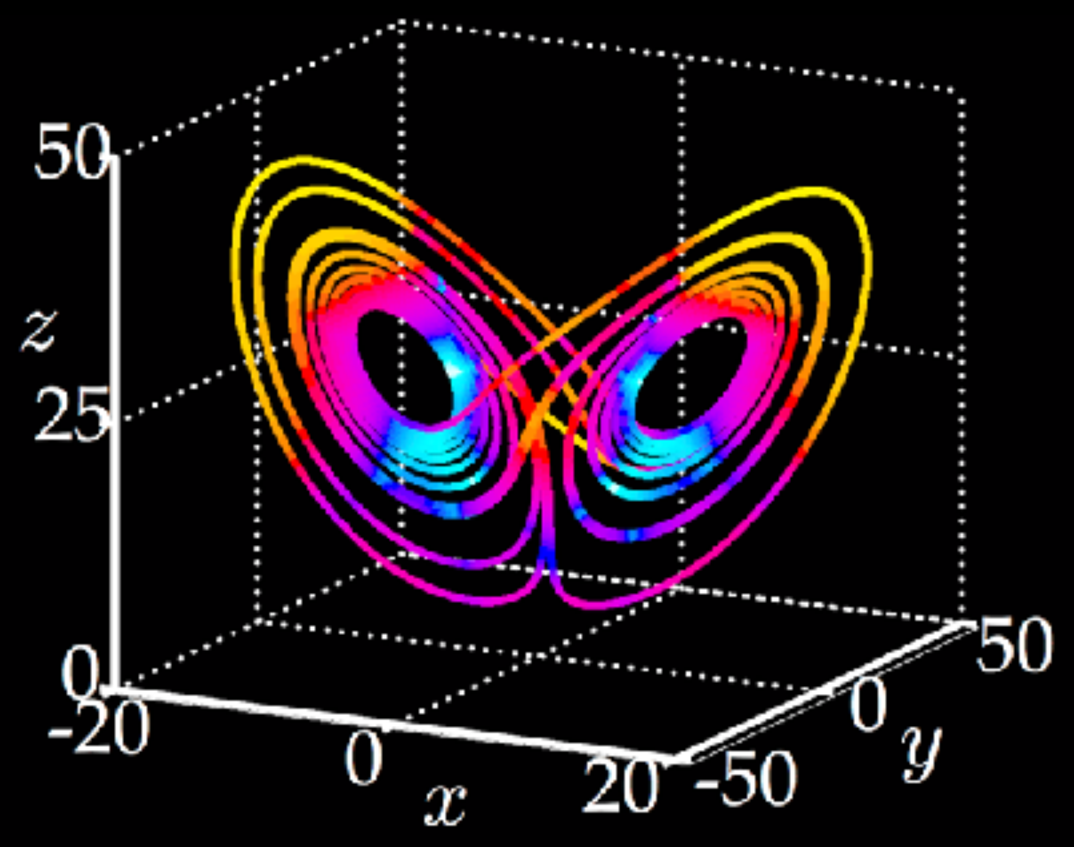
Albert Einstein

There is a need for INTERPRETABLE and GENERALIZABLE Machine Learning

- LOW-DIMENSIONAL
- SPARSE

Chaotic Thermal Convection



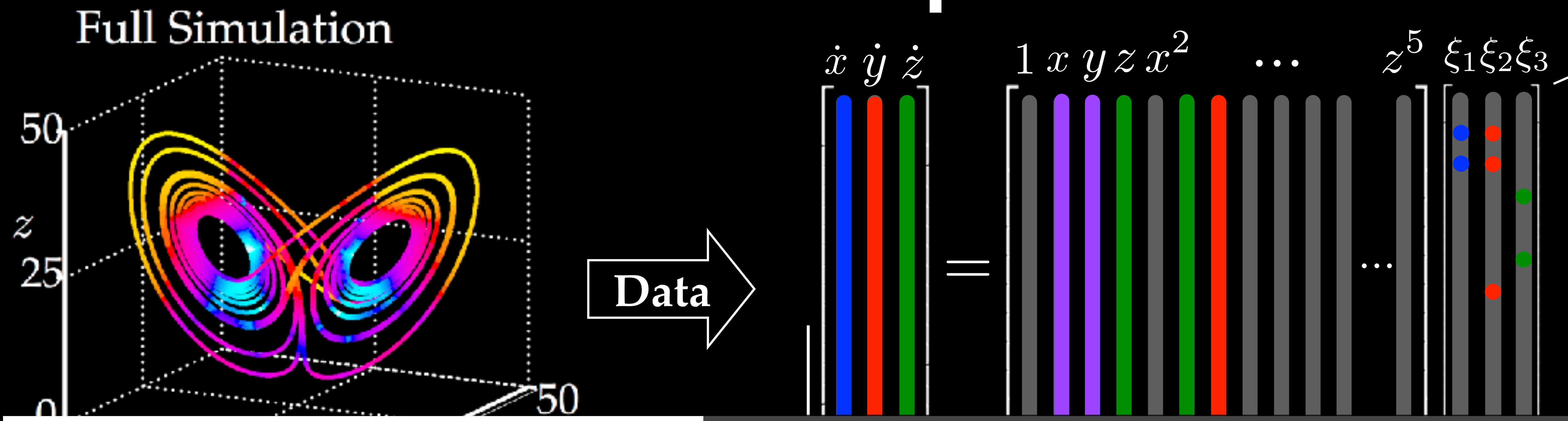


$$
\begin{aligned}
\dot{x} &= \sigma(y - x) \\
\dot{y} &= x(\rho - z) - y \\
\dot{z} &= xy - \beta z.
\end{aligned}
$$

YouTube: turbulenceteam

Lorenz, Fetter, Hamilton, 1963

Sparse Identification of Nonlinear Dynamics (SINDy)



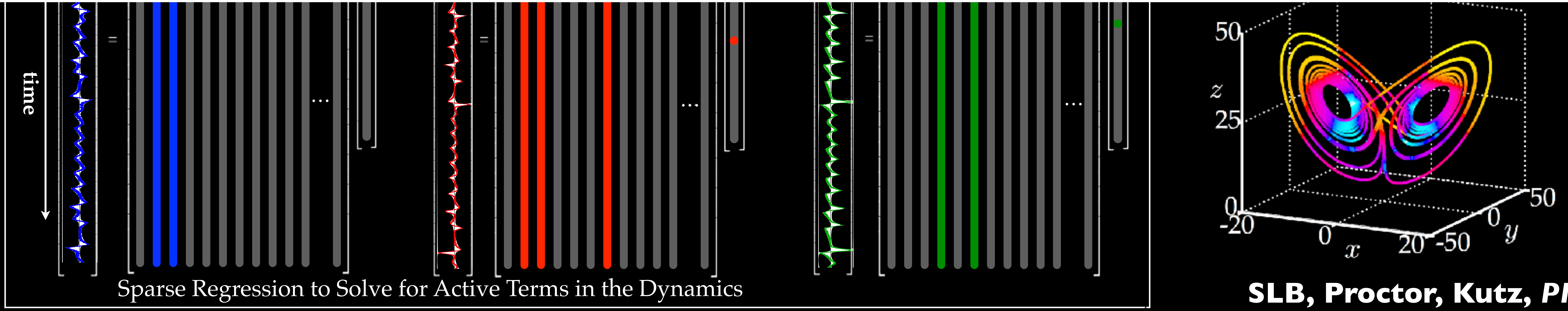
''	'xi_1'	'xi_2'	'xi_3'
'1'	[0]	[0]	[0]
'x'	[-9.9996]	[27.9980]	[0]
'y'	[9.9998]	[-0.9997]	[0]
'z'	[0]	[0]	[-2.6665]
'xx'	[0]	[0]	[0]
'xy'	[0]	[0]	[1.0000]
'xz'	[0]	[-0.9999]	[0]

PySINDy

Open-Source Software

Build CI passing | docs passing | pypi package 1.0.0 | codecov 95% | JOSS 10.21105/joss.02104 | DOI 10.5281/zenodo.3832319

PySINDy is a sparse regression package with several implementations for the Sparse Identification of Nonlinear Dynamical systems (SINDy) method introduced in Brunton et al. (2016a), including the unified optimization approach of Champion et al. (2019) and SINDy with control from Brunton et al. (2016b). A comprehensive literature review is given in de Silva et al. (2020).



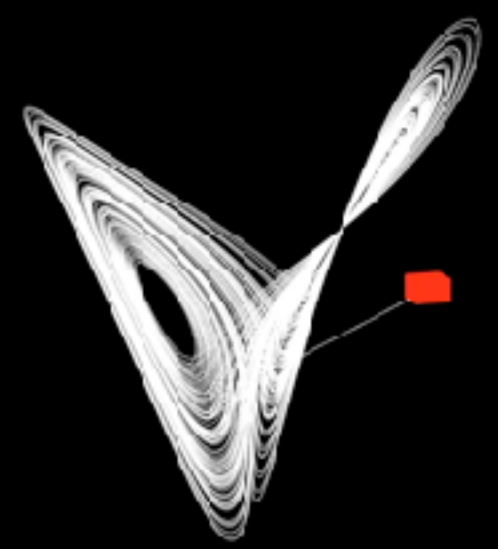
SLB, Proctor, Kutz, *PNAS* 2016.

PDEs

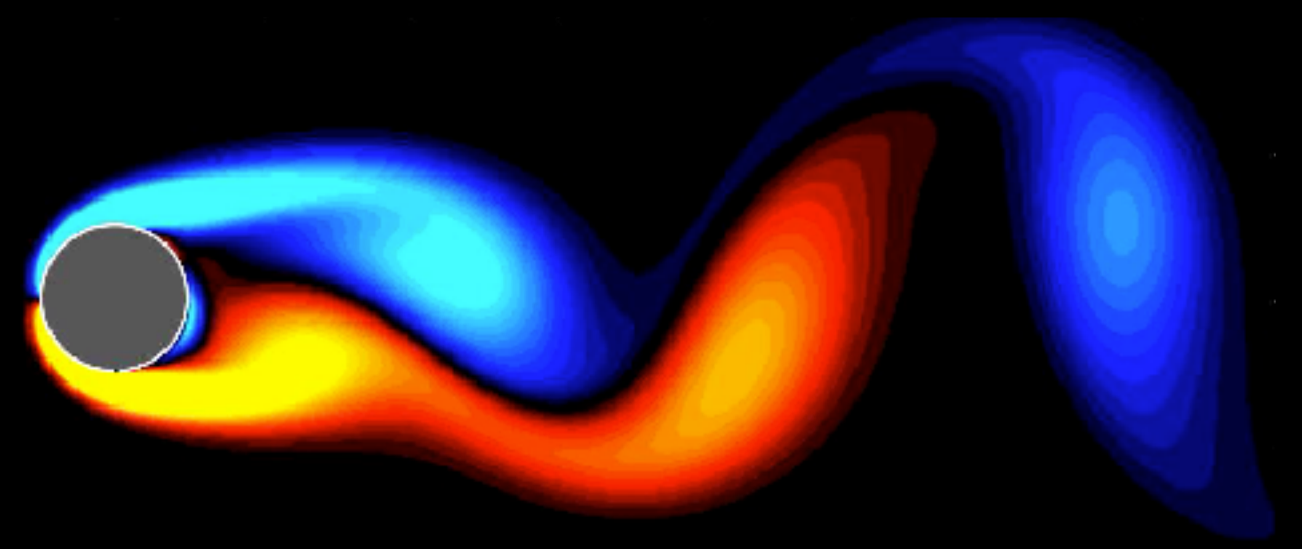
Rudy, SLB, Proctor, Kutz
Science Advances, 2017

Sparse Identification of Nonlinear Dynamics (SINDy)

Data → **Dynamics**



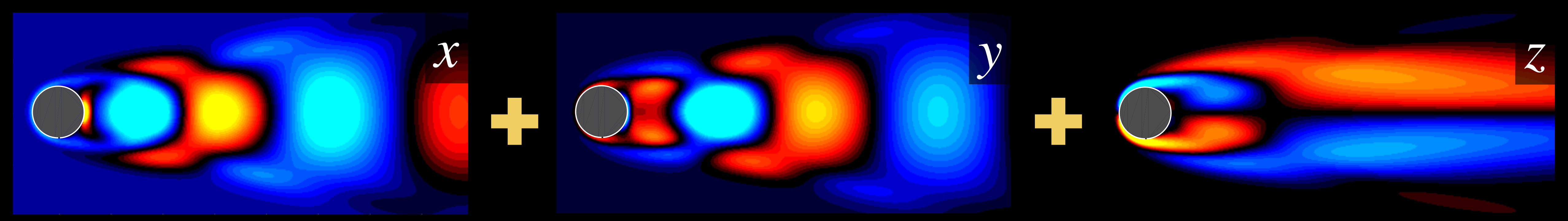
$$\begin{aligned} \dot{x} &= \sigma(y - x) \\ \dot{y} &= x(\rho - z) - y \\ \dot{z} &= xy - \beta z. \end{aligned}$$



$$\omega_t + (\mathbf{u}\cdot\nabla)\omega = \frac{1}{Re}\nabla^2\omega$$

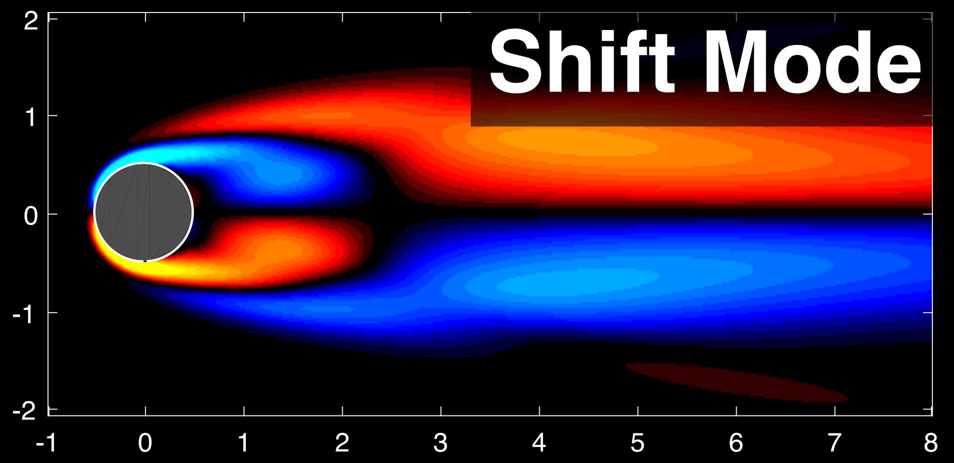
$$\frac{\partial \mathbf{u}}{\partial t} = \mathbf{N}(\mathbf{u})$$

$\approx$



$$\begin{aligned} \dot{x} &= \mu x - \omega y + Axz \\ \dot{y} &= \omega x + \mu y + Ayz \\ \dot{z} &= -\lambda(z - x^2 - y^2) \end{aligned}$$

Reduced Order Models



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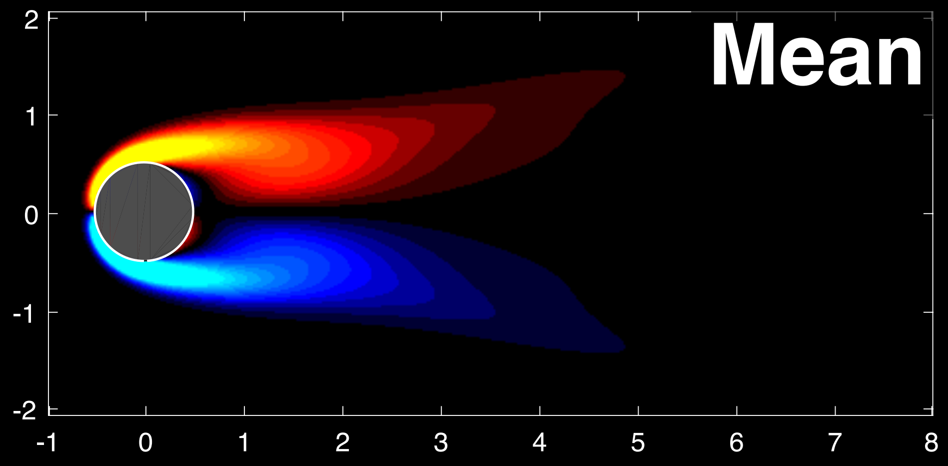
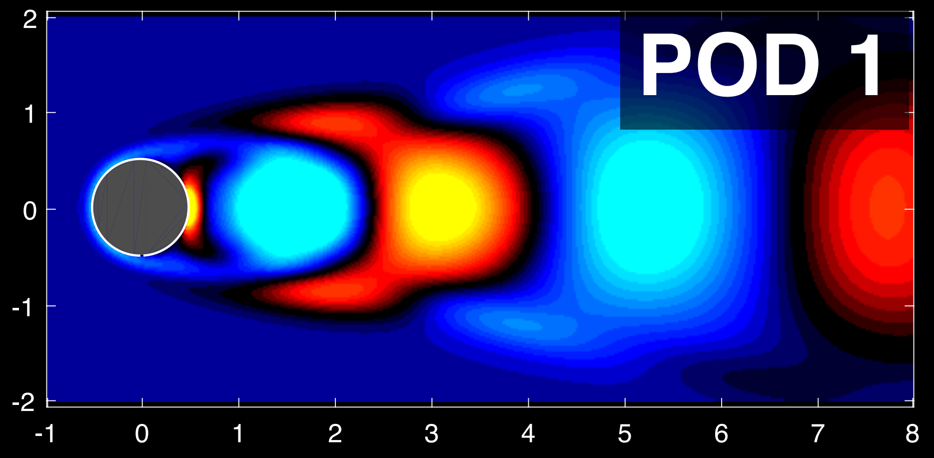
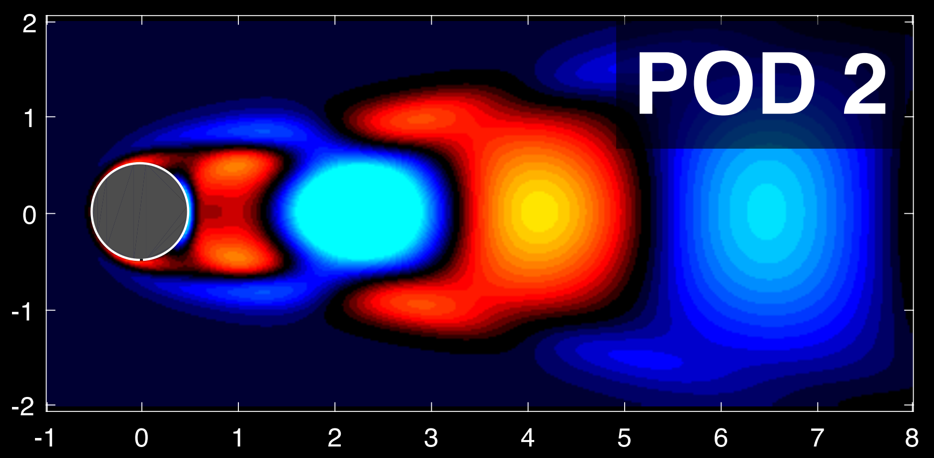
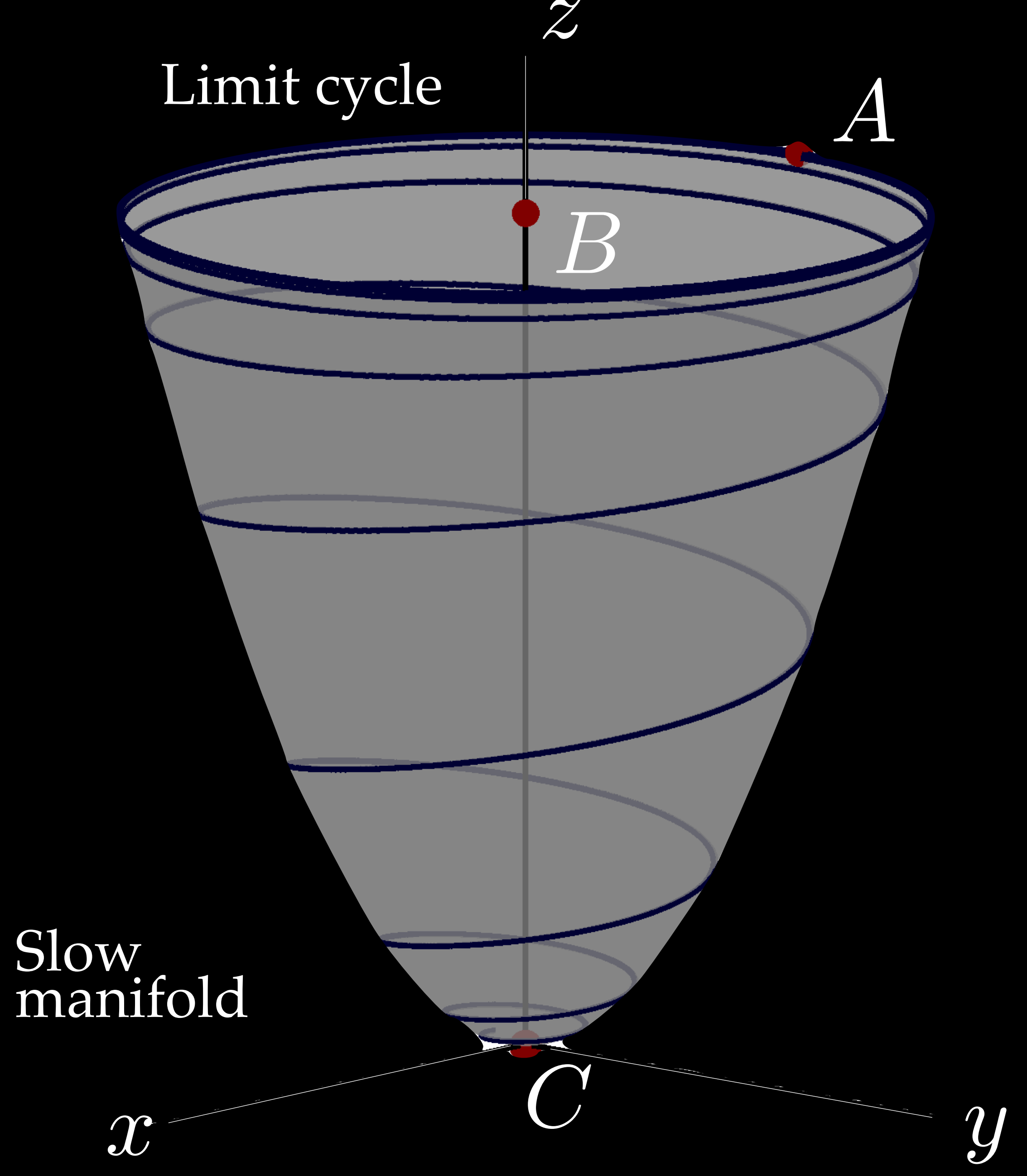
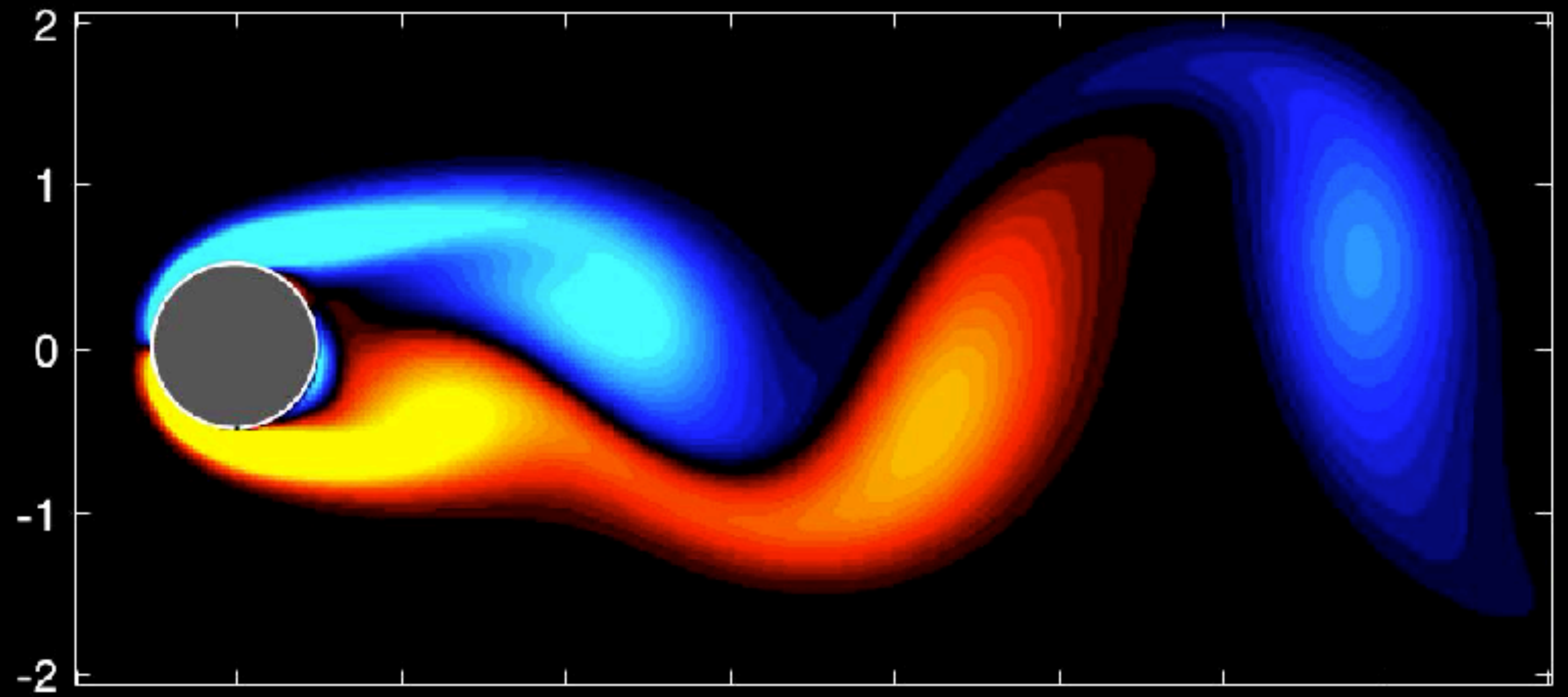






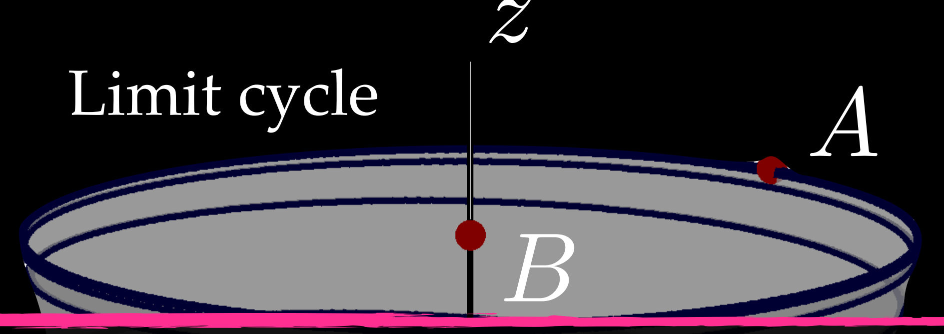


$$\begin{aligned}\dot{x} &= \mu x - \omega y + Axz\\ \dot{y} &= \omega x + \mu y + Ayz\\ \dot{z} &= -\lambda(z - x^2 - y^2).\end{aligned}$$

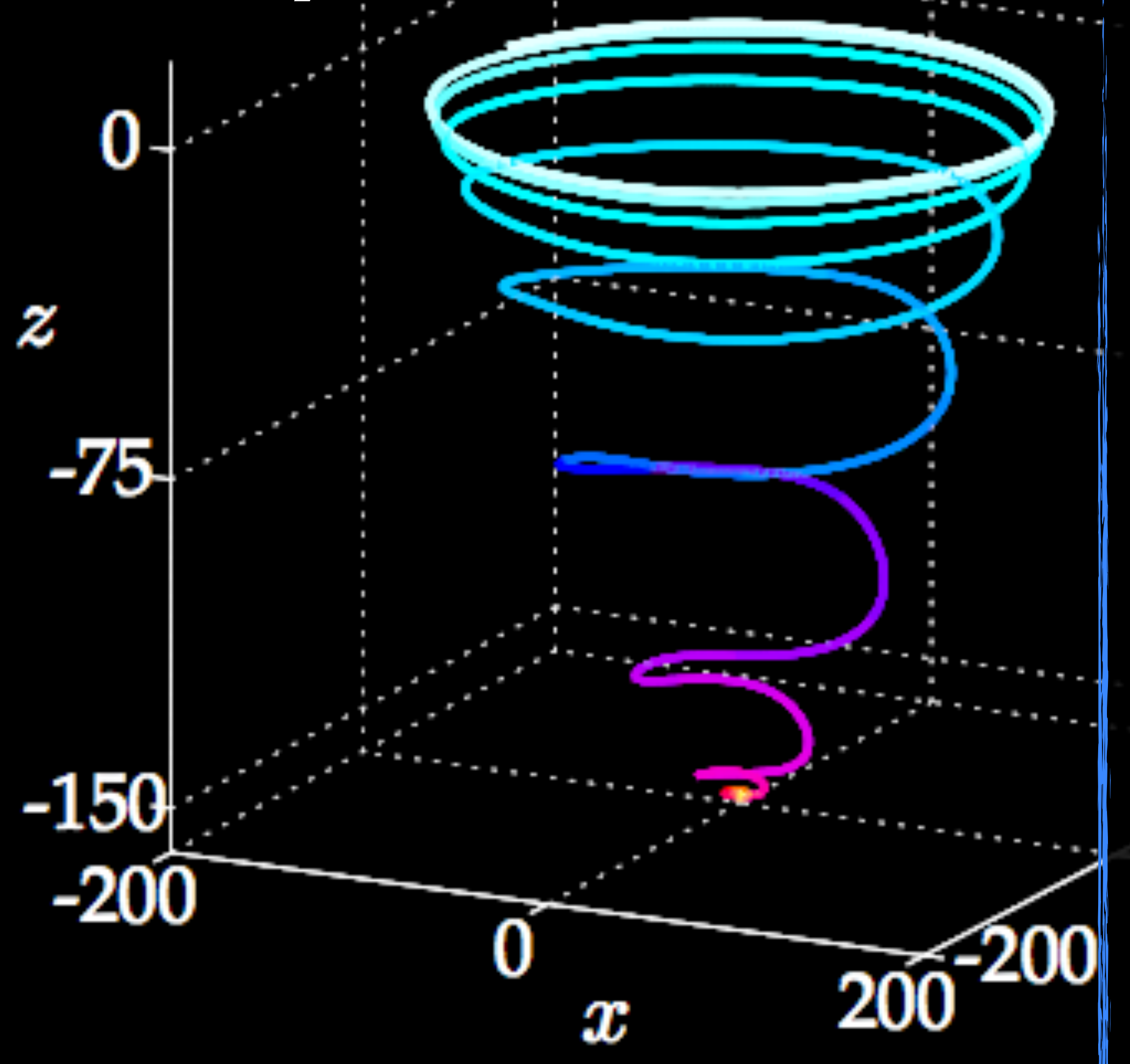


Noack *et al.*, JFM 2003.

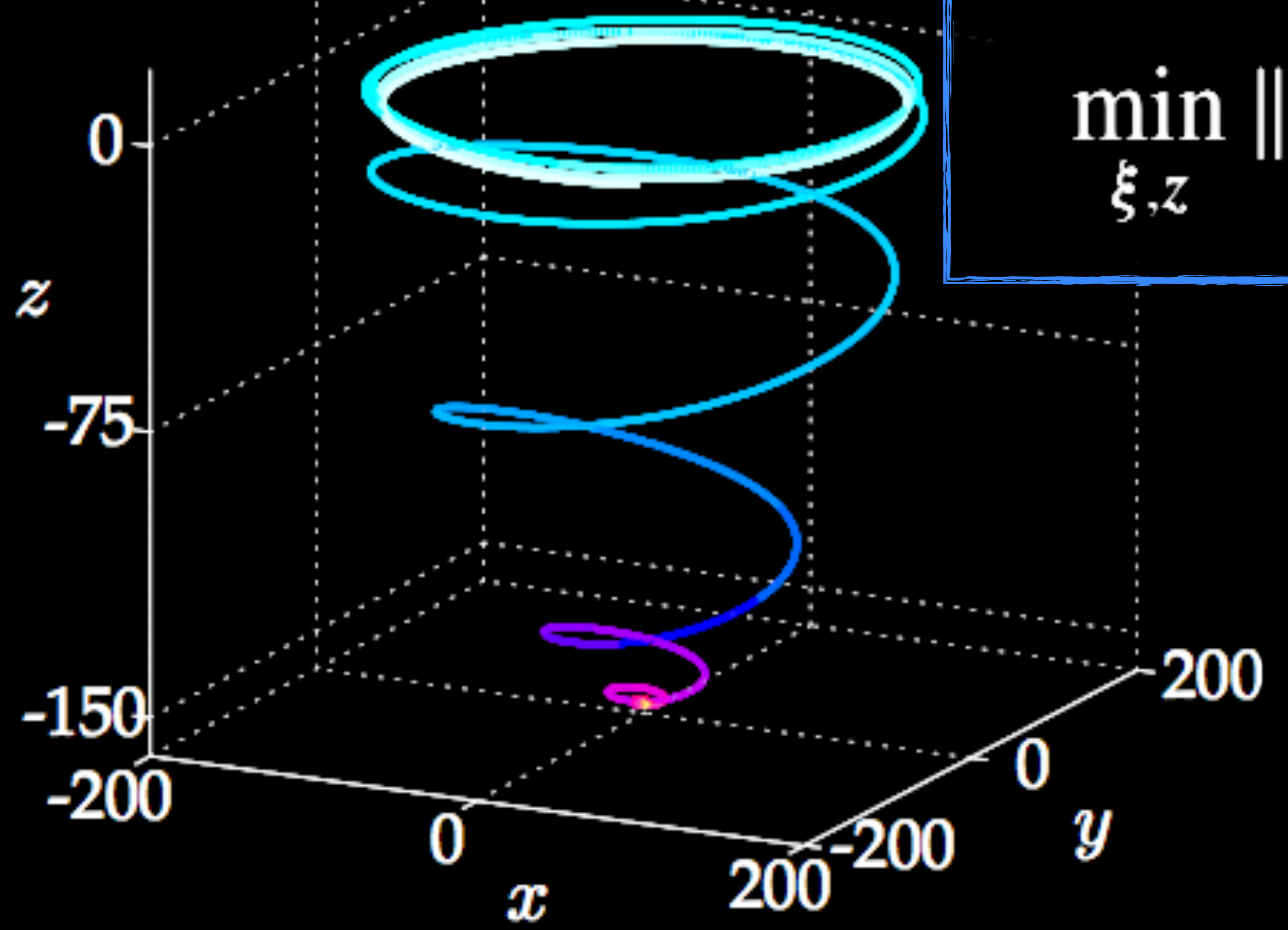
Sparse Identification of Nonlinear Dynamics (SINDy)



Full System



Identified System



Innovation 1: Enforcing known constraints

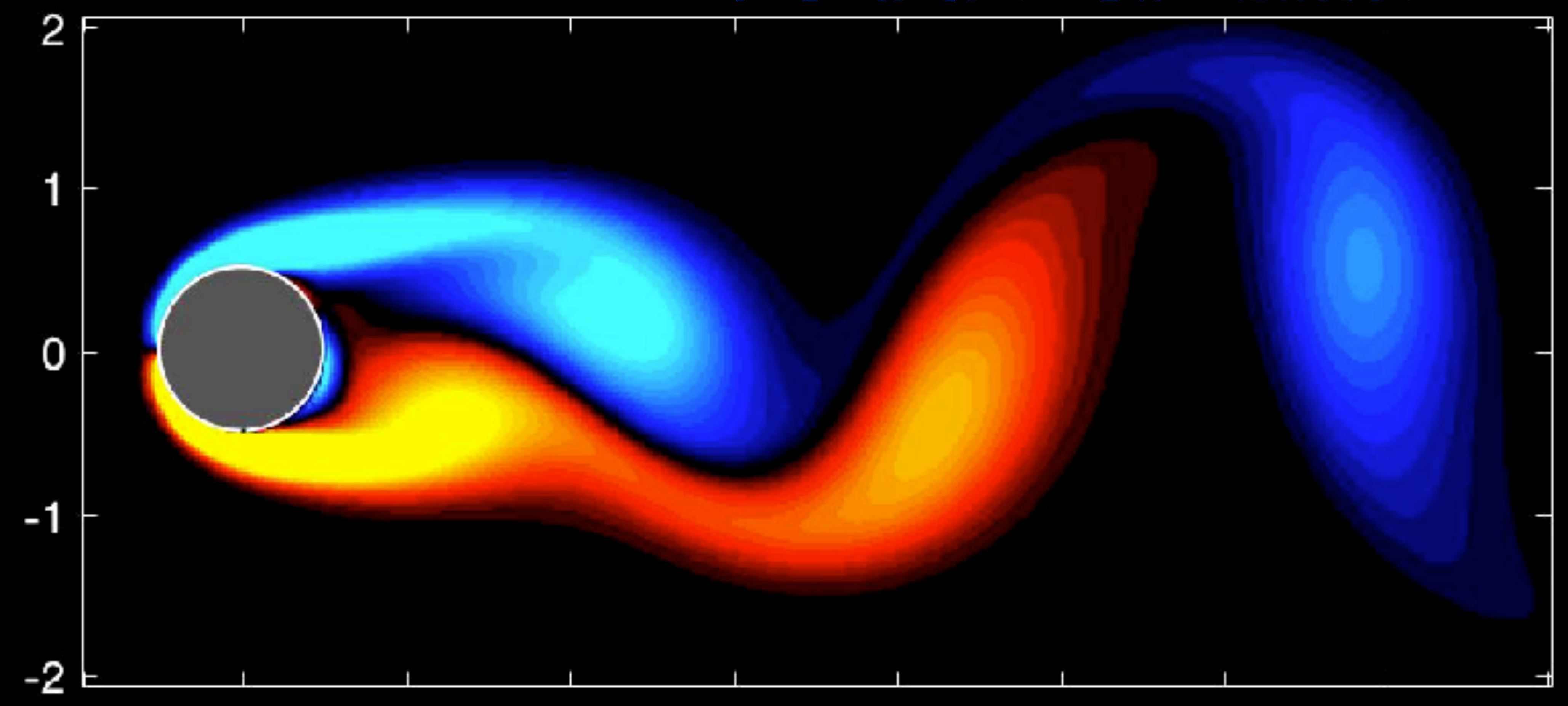
- Skew-symmetric quadratic nonlinearities to enforce energy conservation
- Improved stability

$$\min_{\xi,z} \|\Theta(X)\Xi - \dot{X}\|_2^2 + z^T(C\xi - d)$$

Innovation 2: Higher-order Nonlinearities

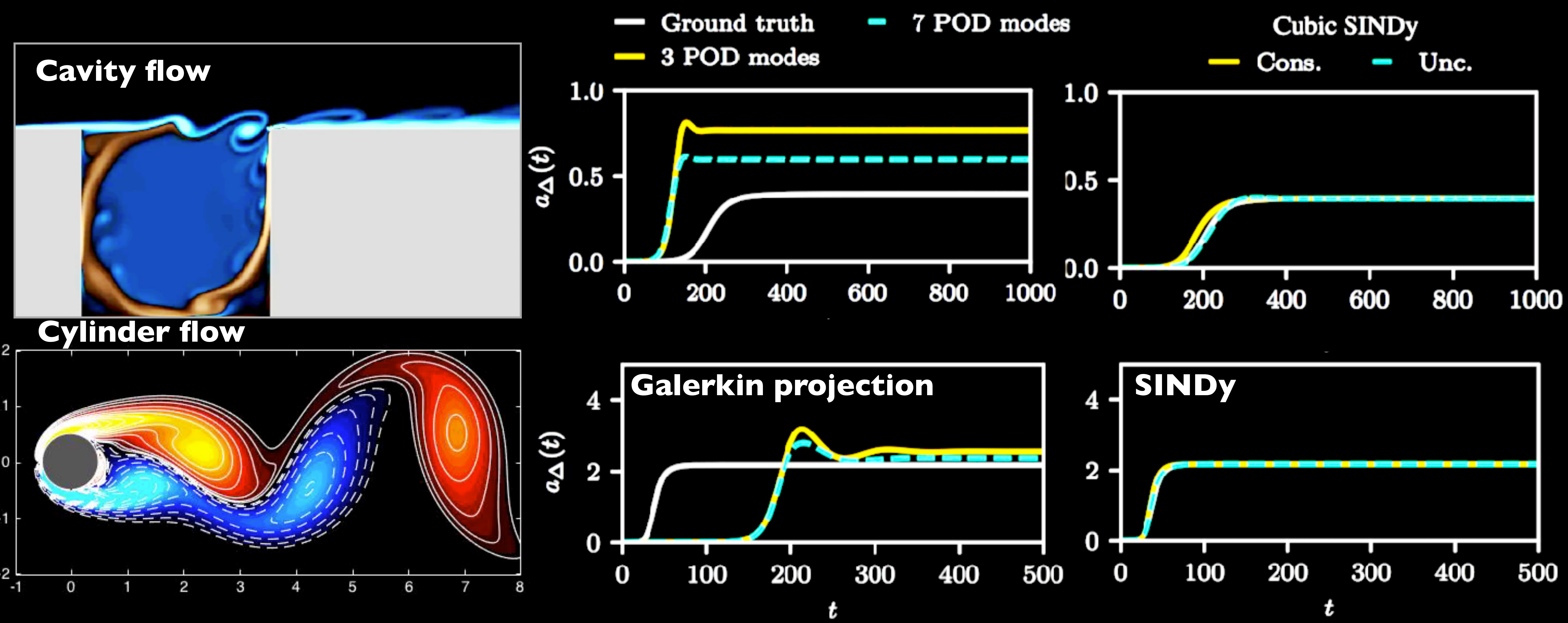
- Cubic, Quintic, Septic terms approximate truncated terms in Galerkin expansion

$$\begin{aligned}\dot{x} &= \mu x - \omega y + Axz\\ \dot{y} &= \omega x + \mu y + Ayz\\ \dot{z} &= -\lambda(z - x^2 - y^2).\end{aligned}$$



SLB, Proctor, Kutz, *PNAS* 2016.
Loiseau & SLB, *JFM* 838, 2018

Constrained Sparse Galerkin Regression

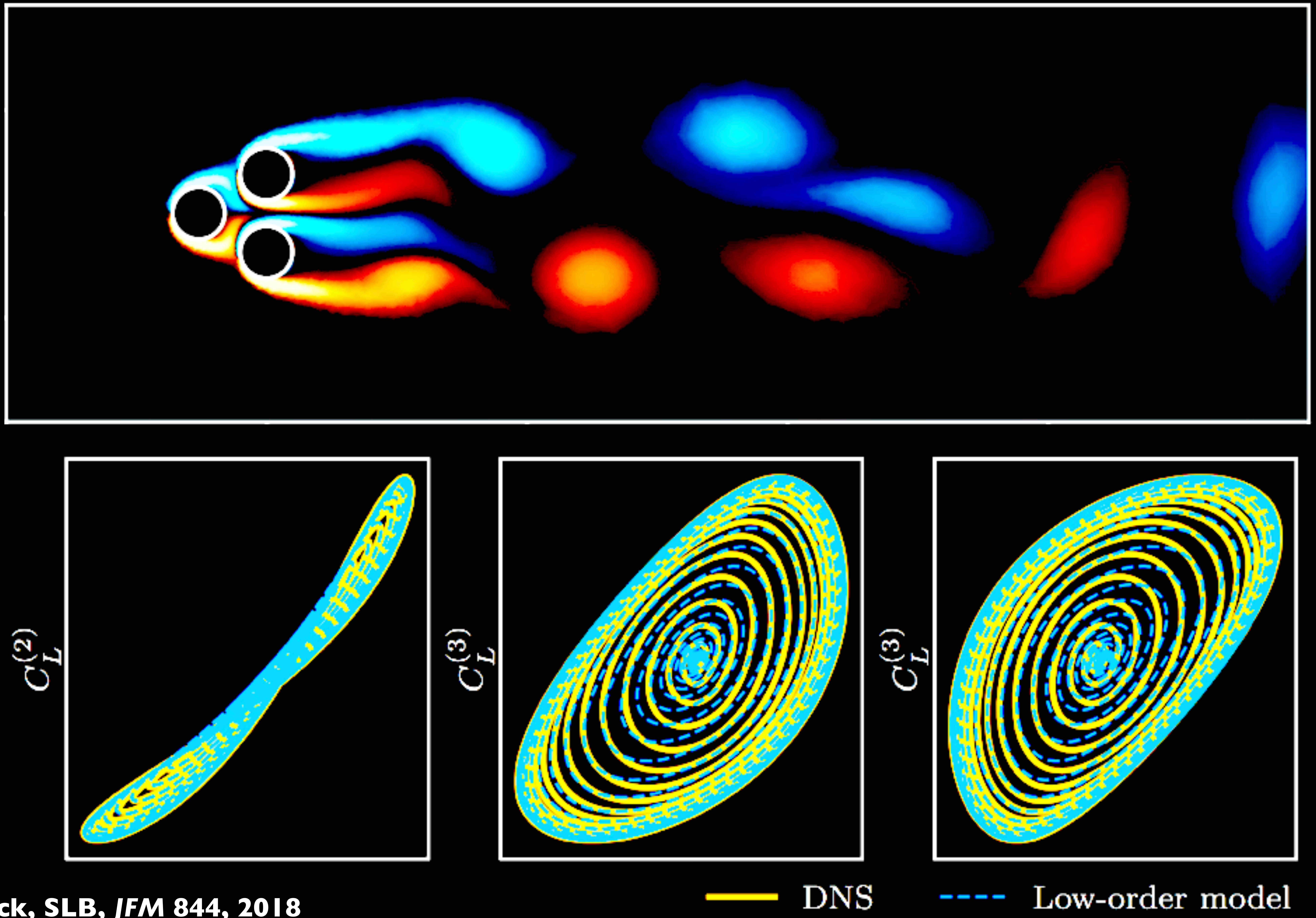


$$\boxed{\ddot{x} - \underbrace{\left(0.2 - 0.24x^2 - 0.15\dot{x}^2\right)}_{k(x,\dot{x})}\dot{x} + 1.26x = 0}$$

Spring-Mass Damper with Nonlinear Damping!

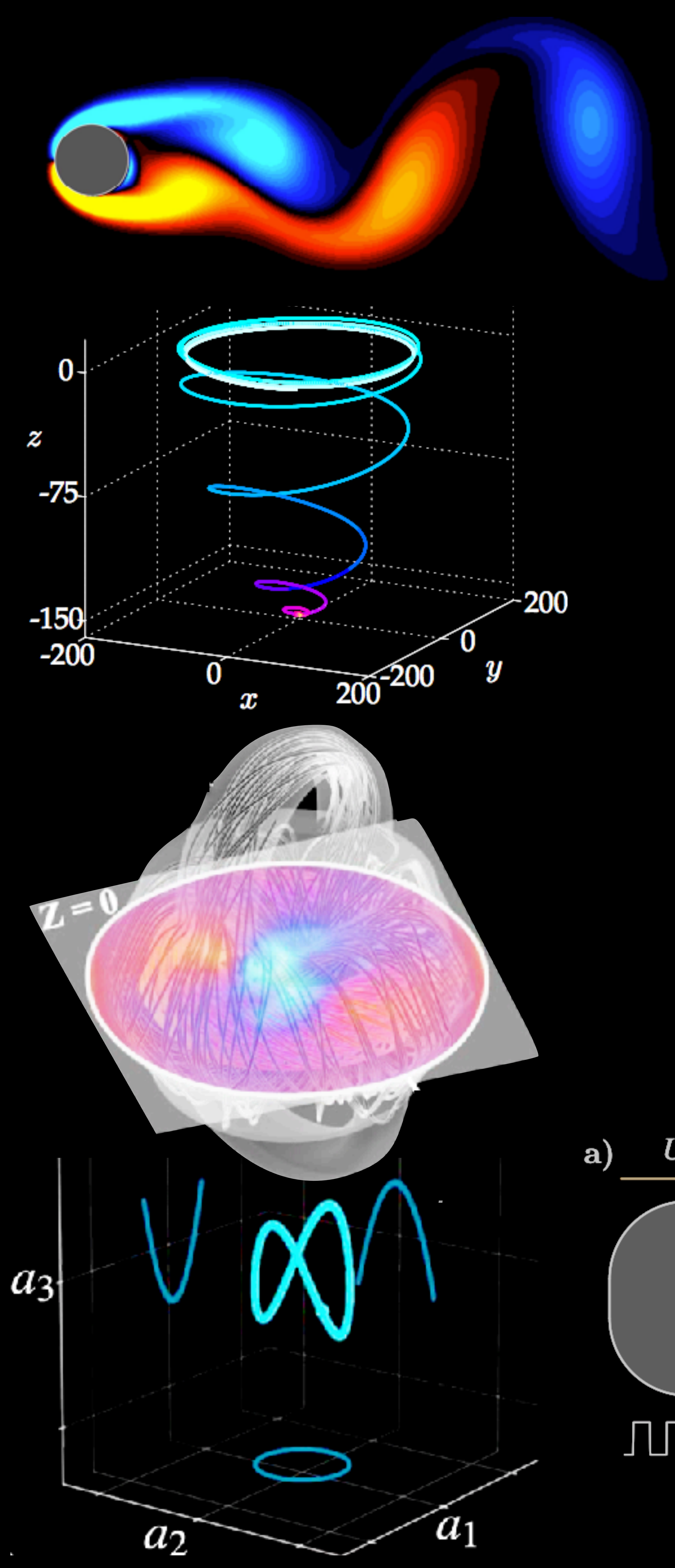
Loiseau & SLB, *JFM* 838, 2018

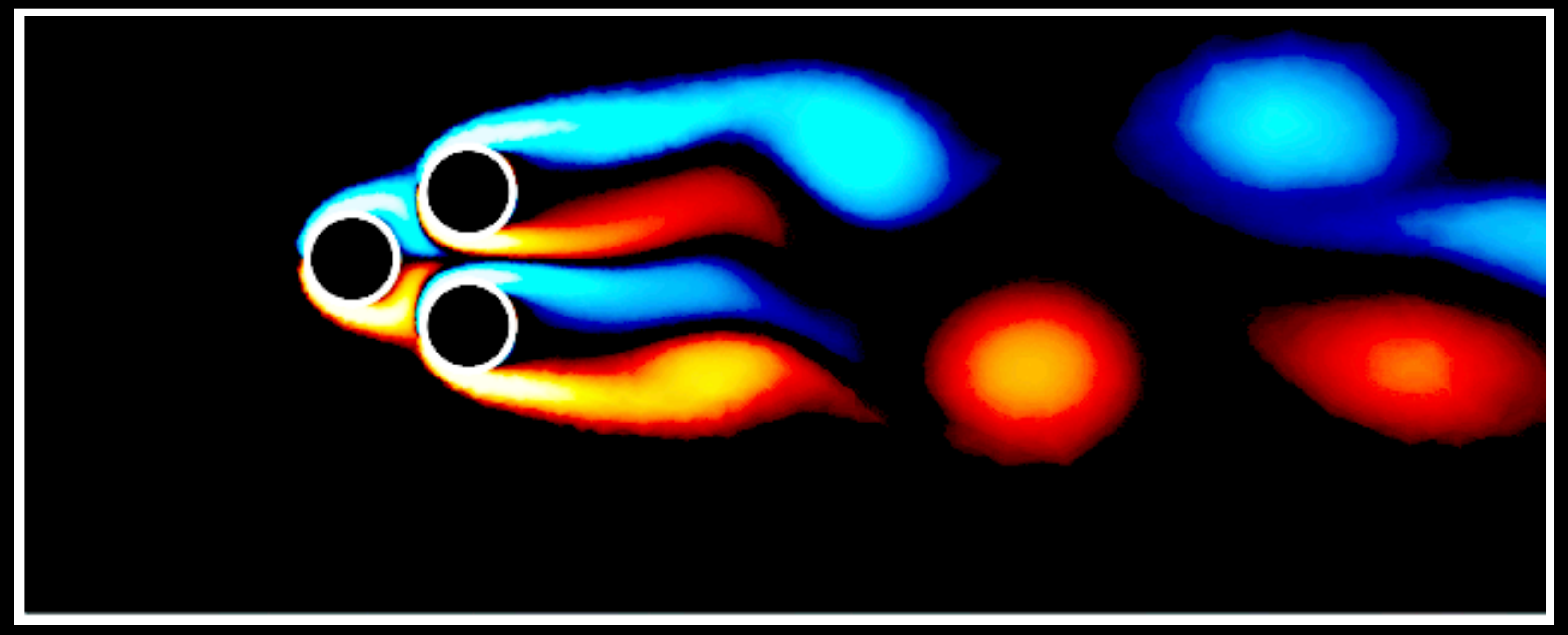
More Complex Flow: Fluidic Pinball

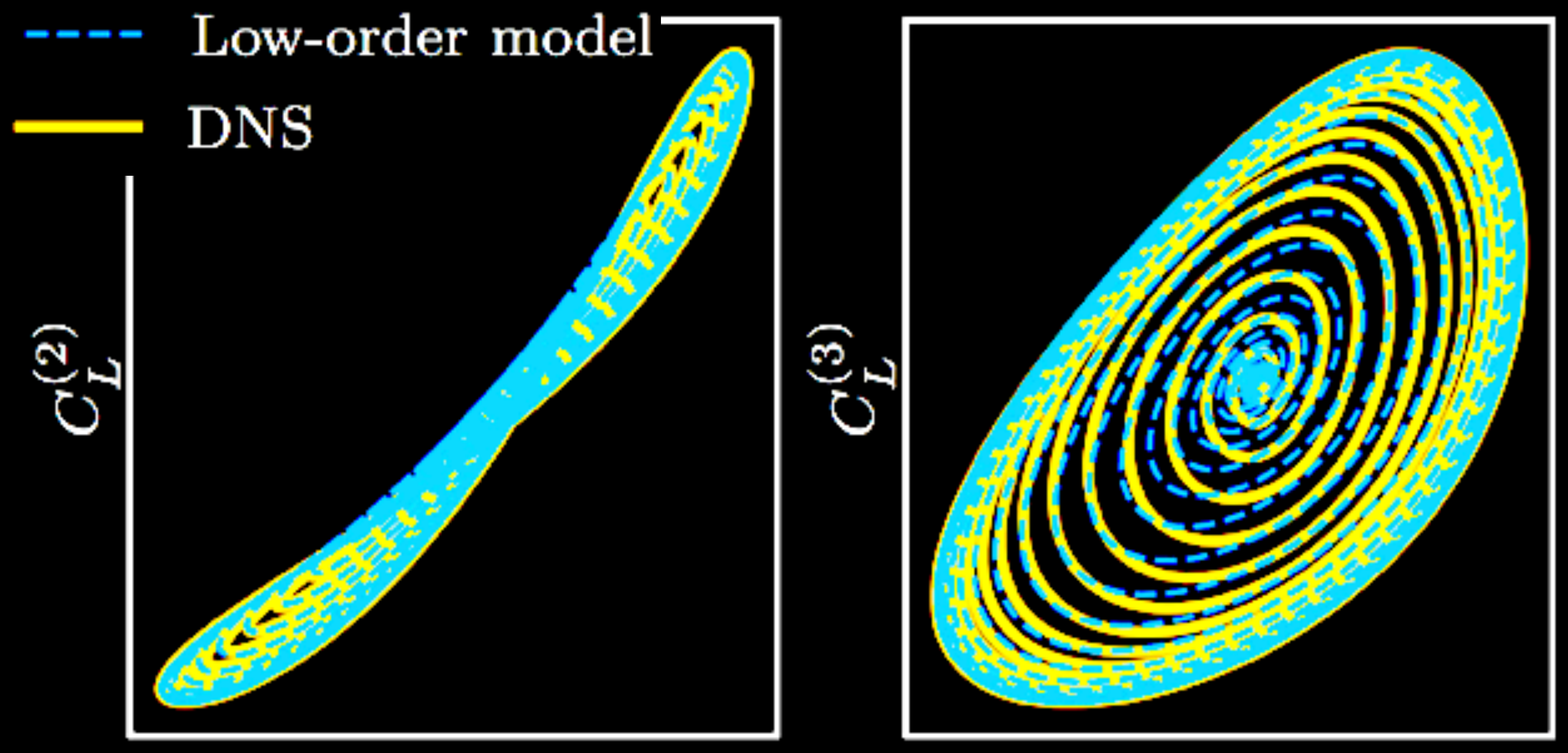


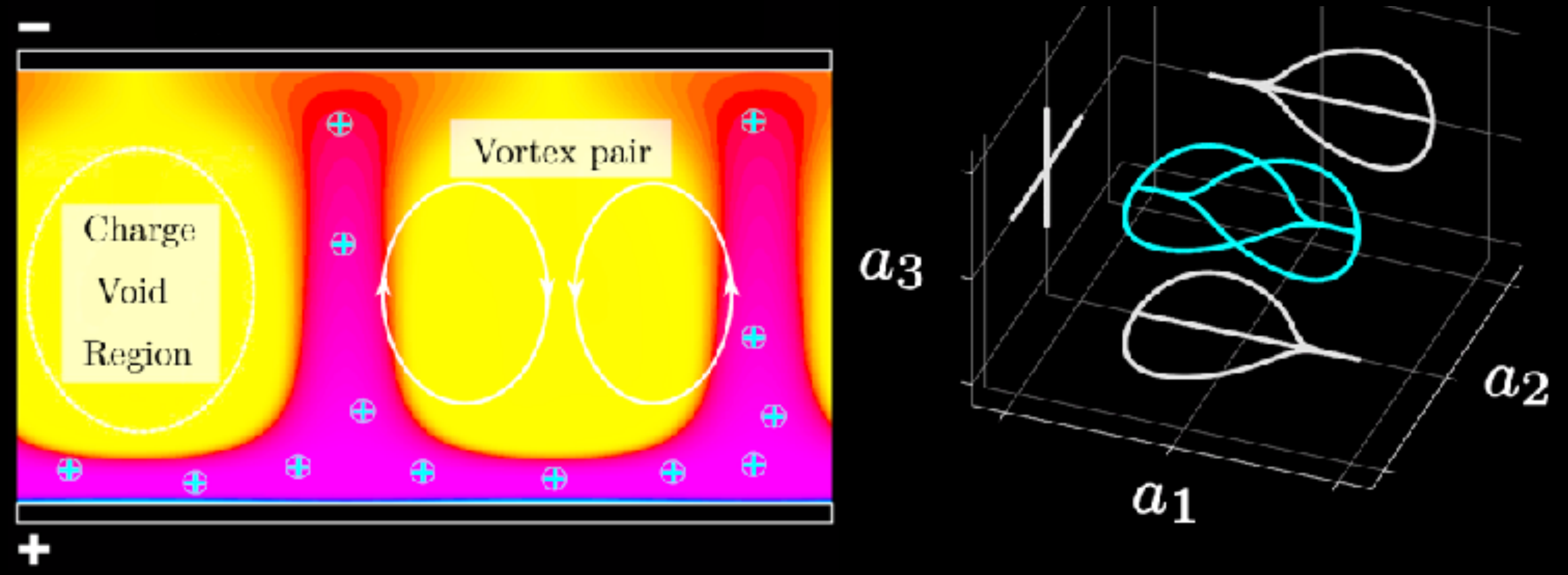
Loiseau, Noack, SLB, *JFM* 844, 2018

Sparse Nonlinear Models of Fluid Dynamics

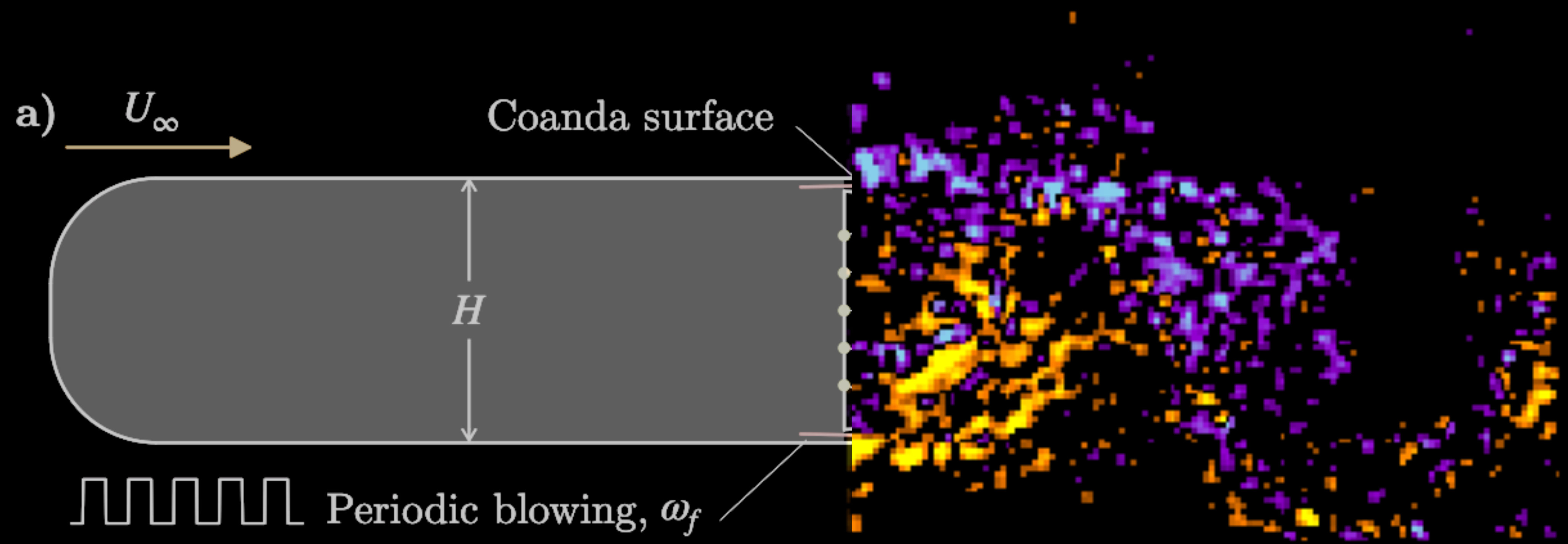


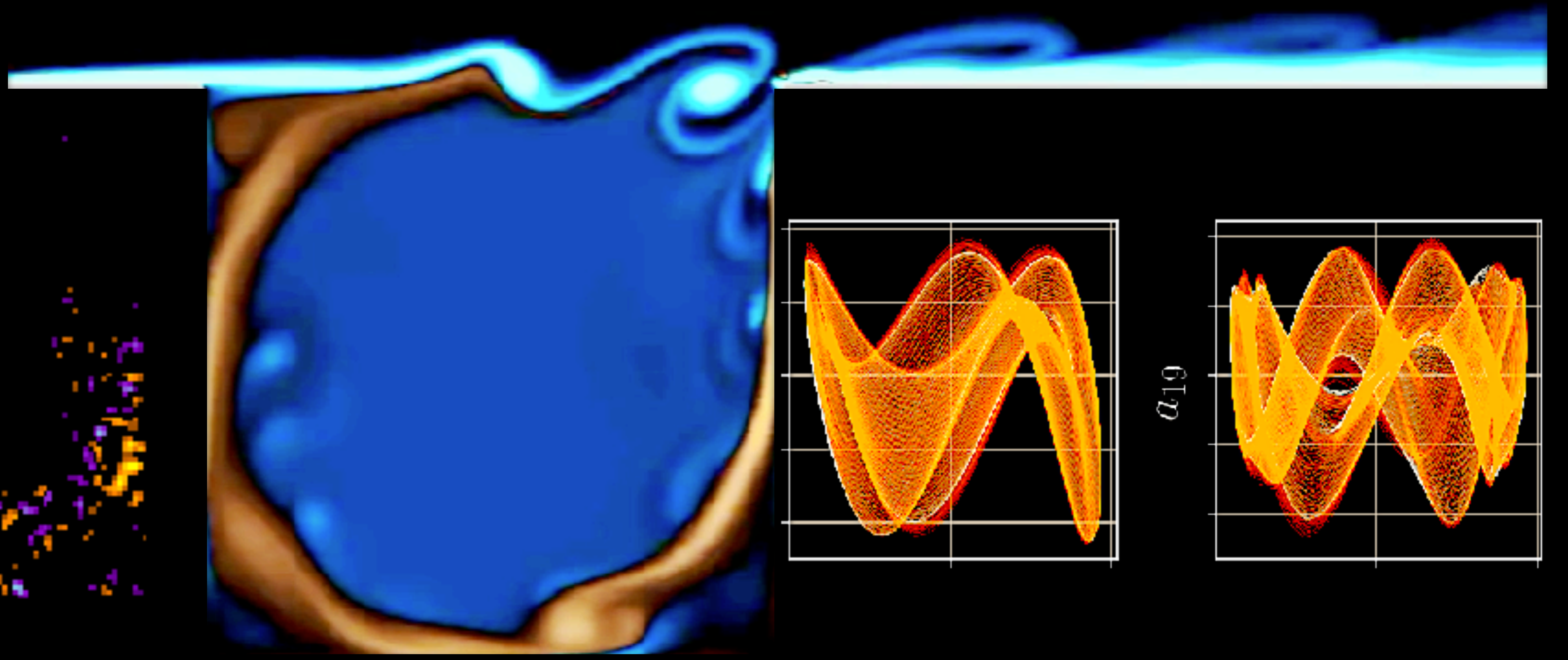




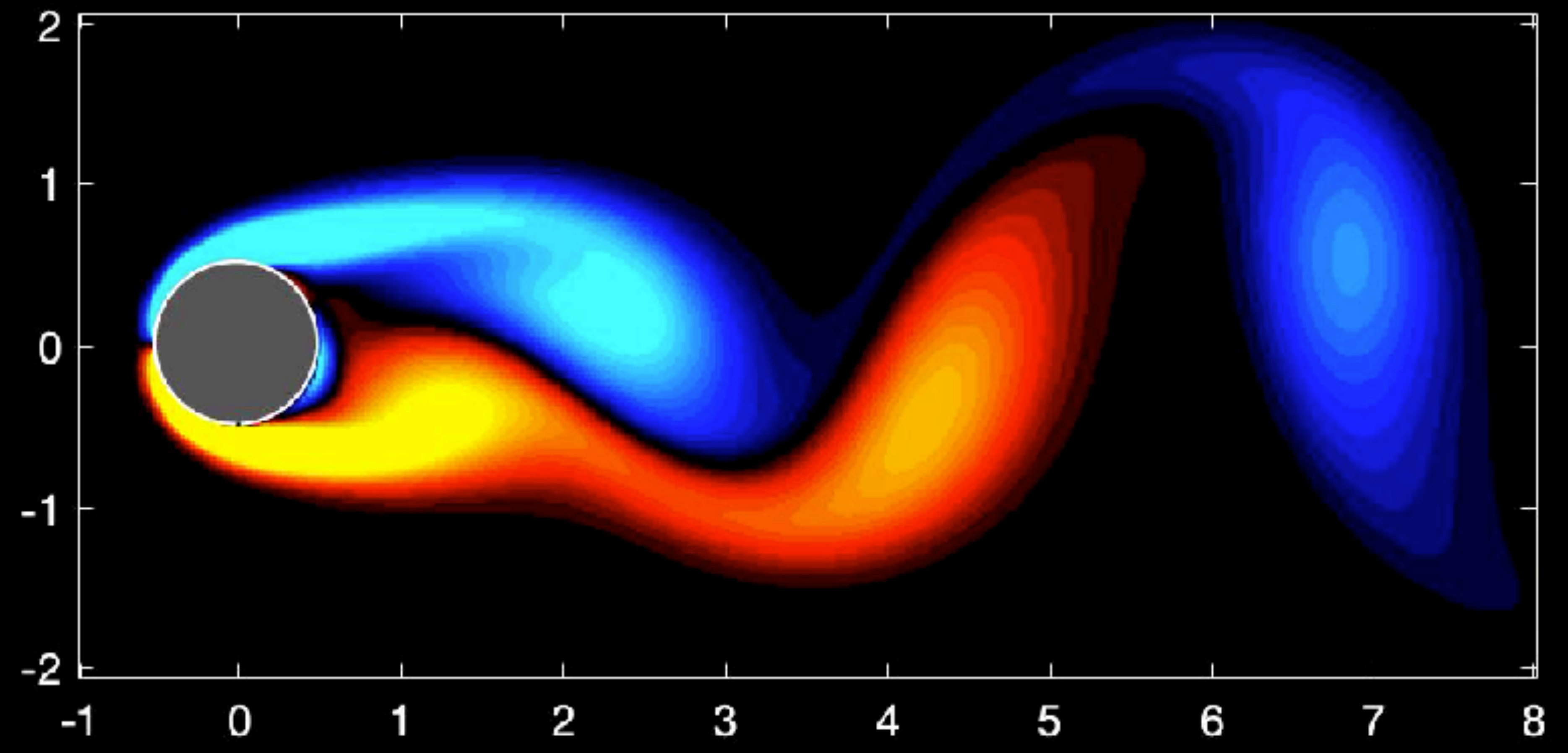


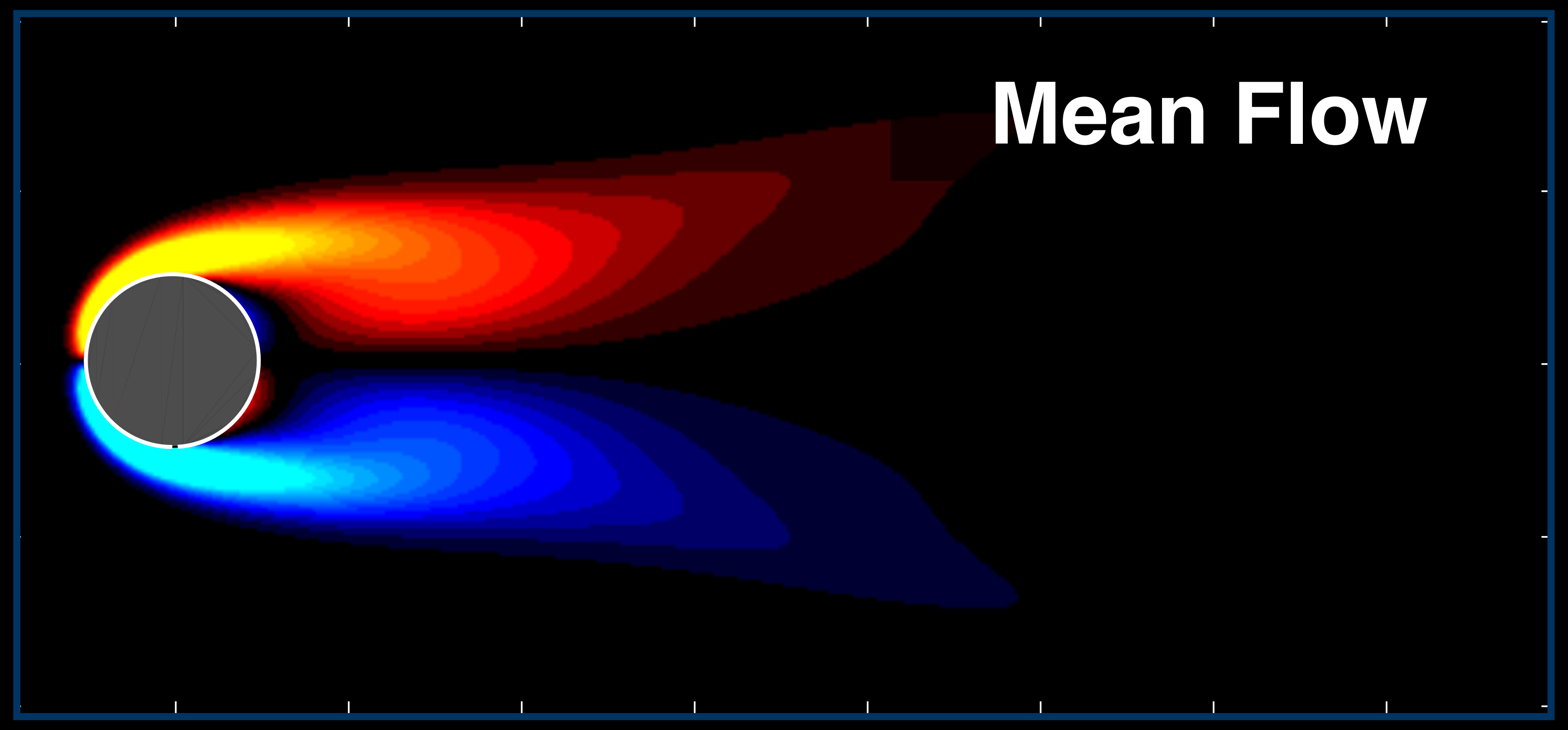
$$\frac{d}{dt}\mathbf{x} = \mathbf{f}(\mathbf{x})$$





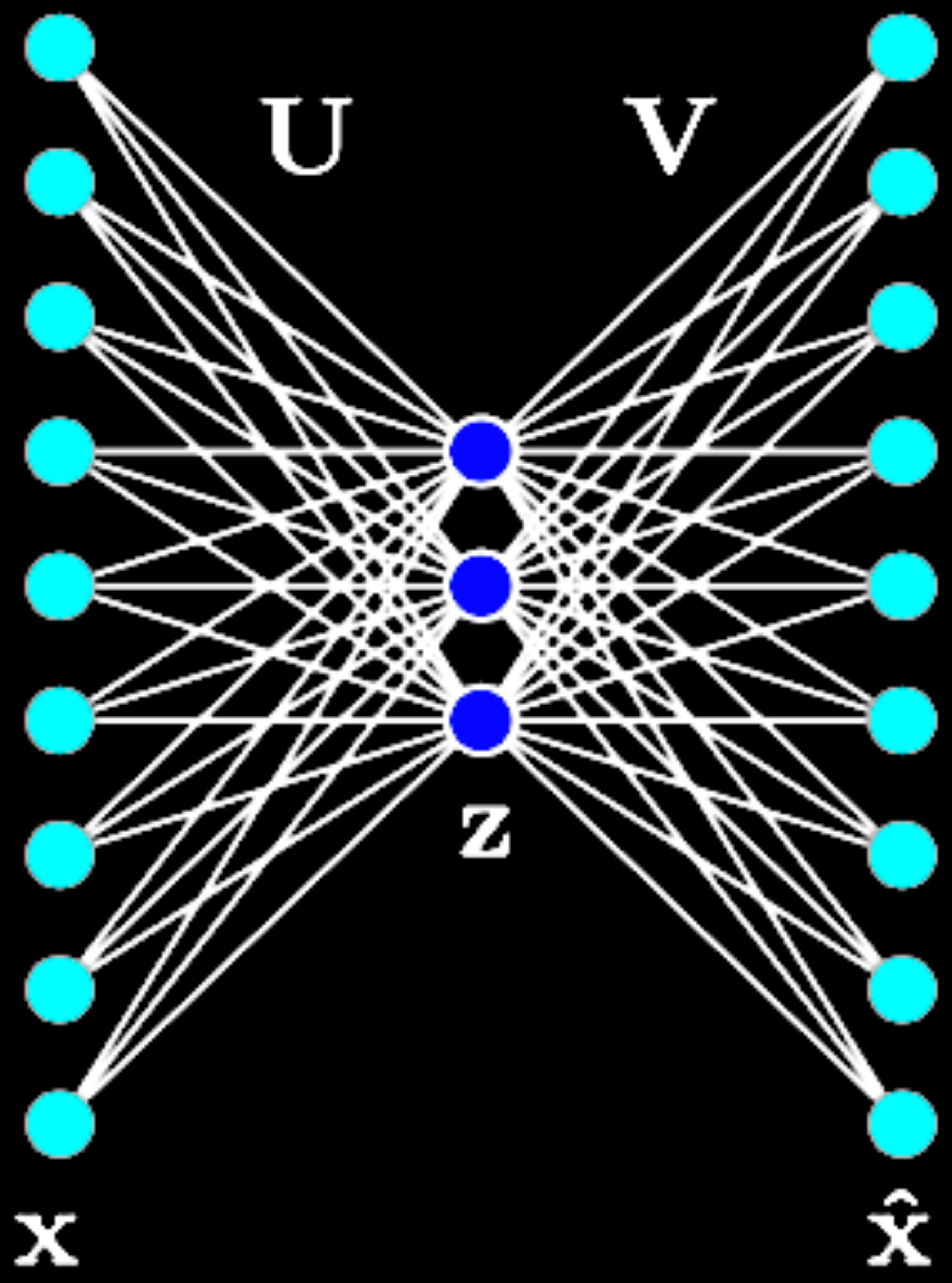
SVD
POD
PCA

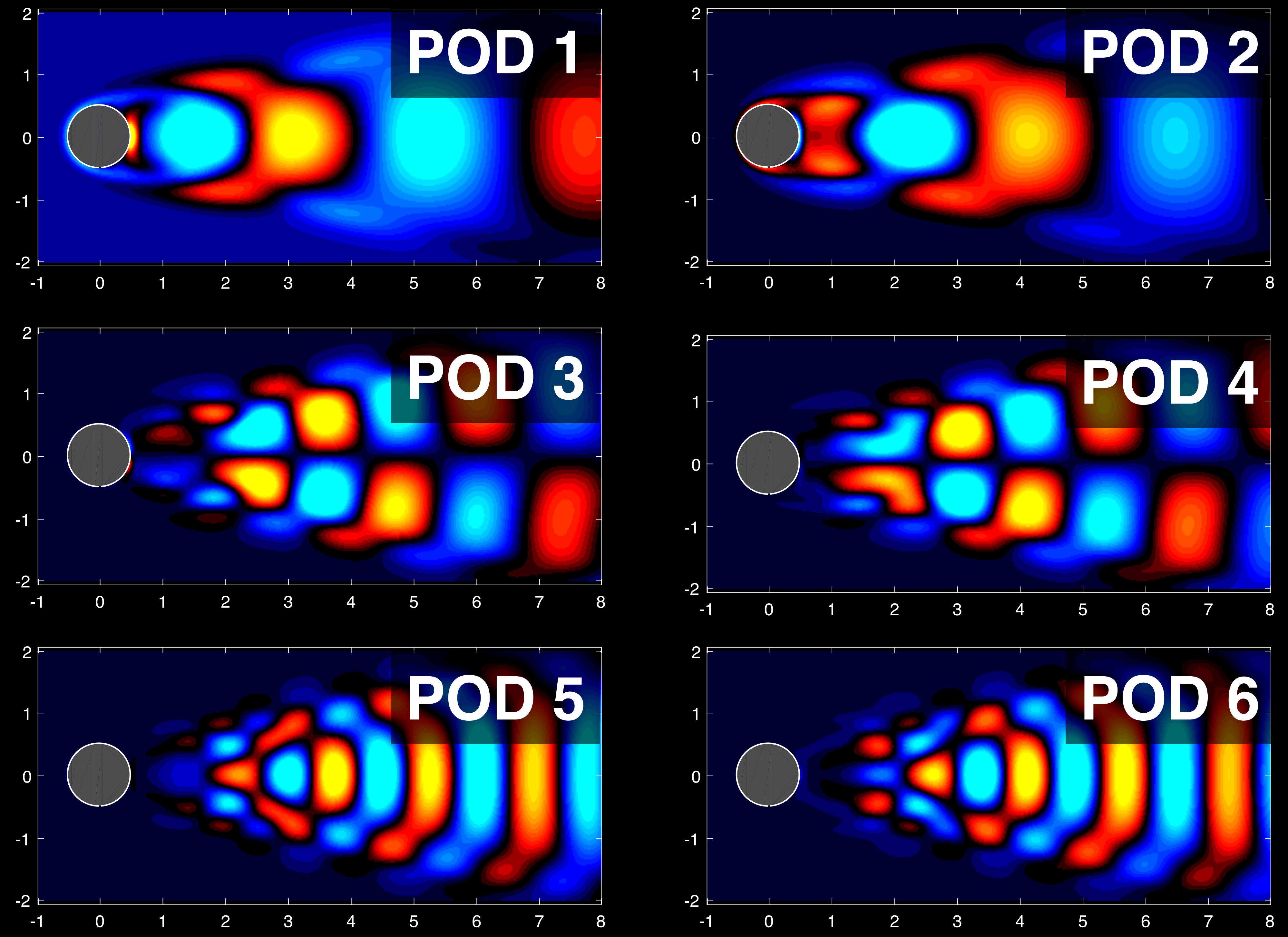




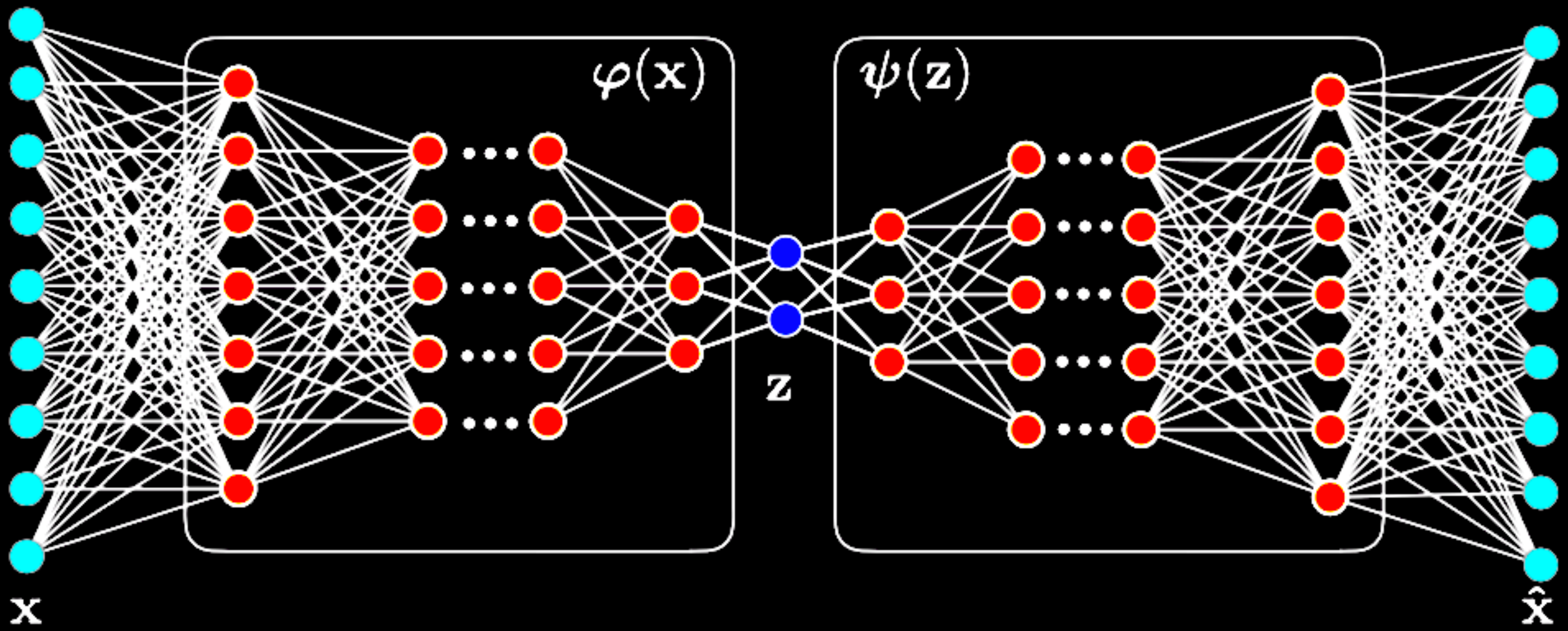
$$\mathbf{u}(\mathbf{x},t) \approx \bar{\mathbf{u}} + \sum_{k=1}^{r} \boldsymbol{\varphi}_k(\mathbf{x})\mathbf{a}_k(t)$$

Autoencoder (Shallow, linear)

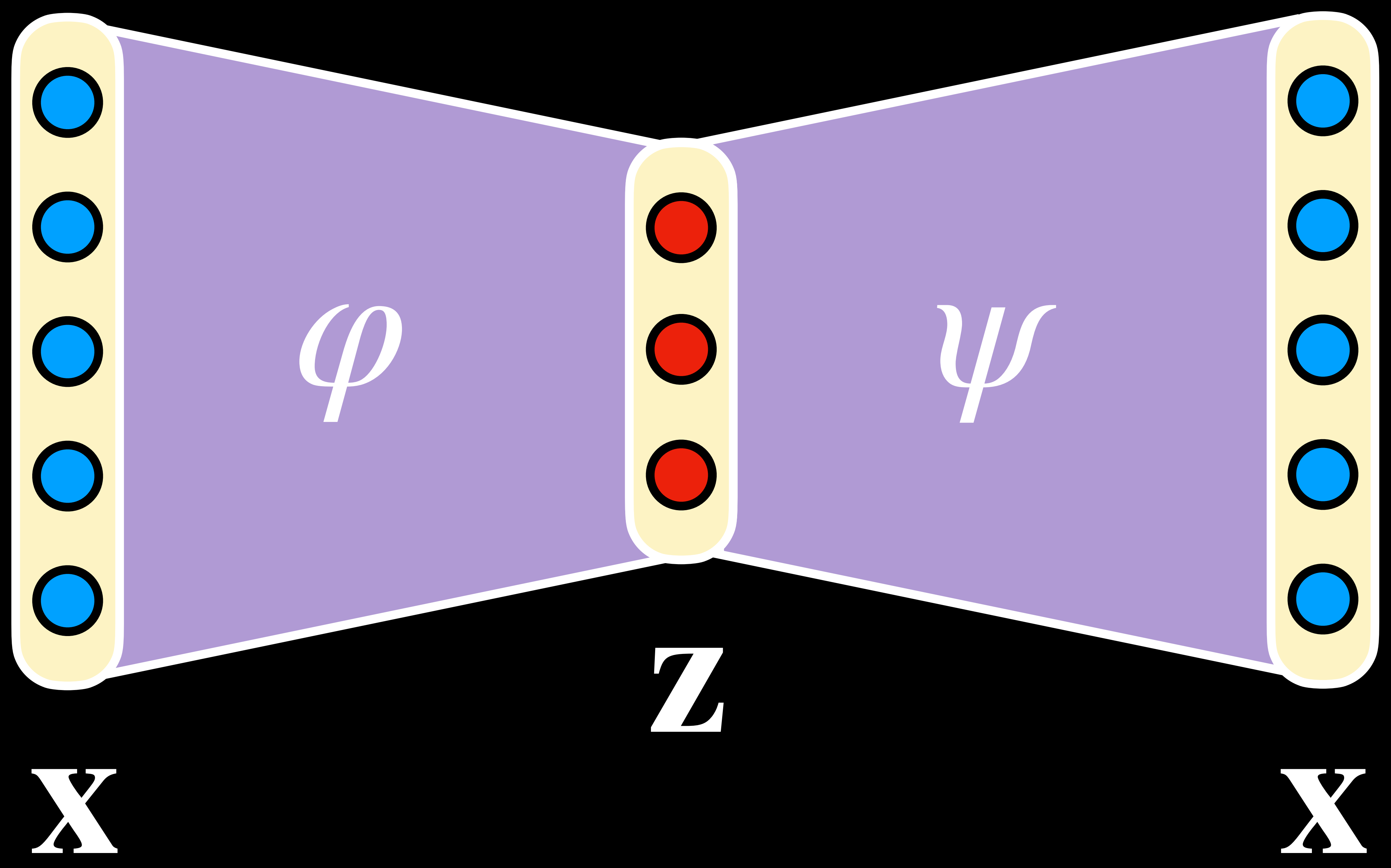




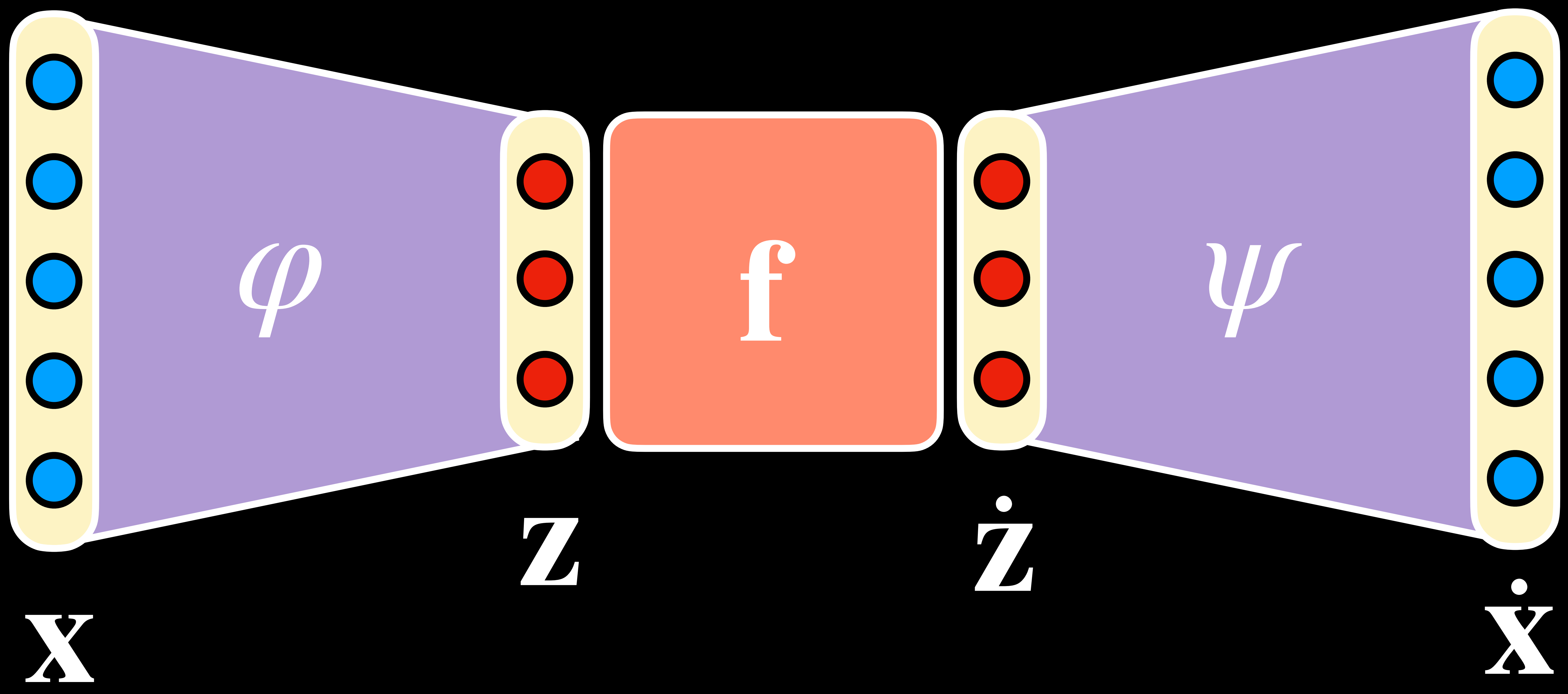
Deep Autoencoders



Deep Autoencoders



Deep Autoencoders for Dynamics

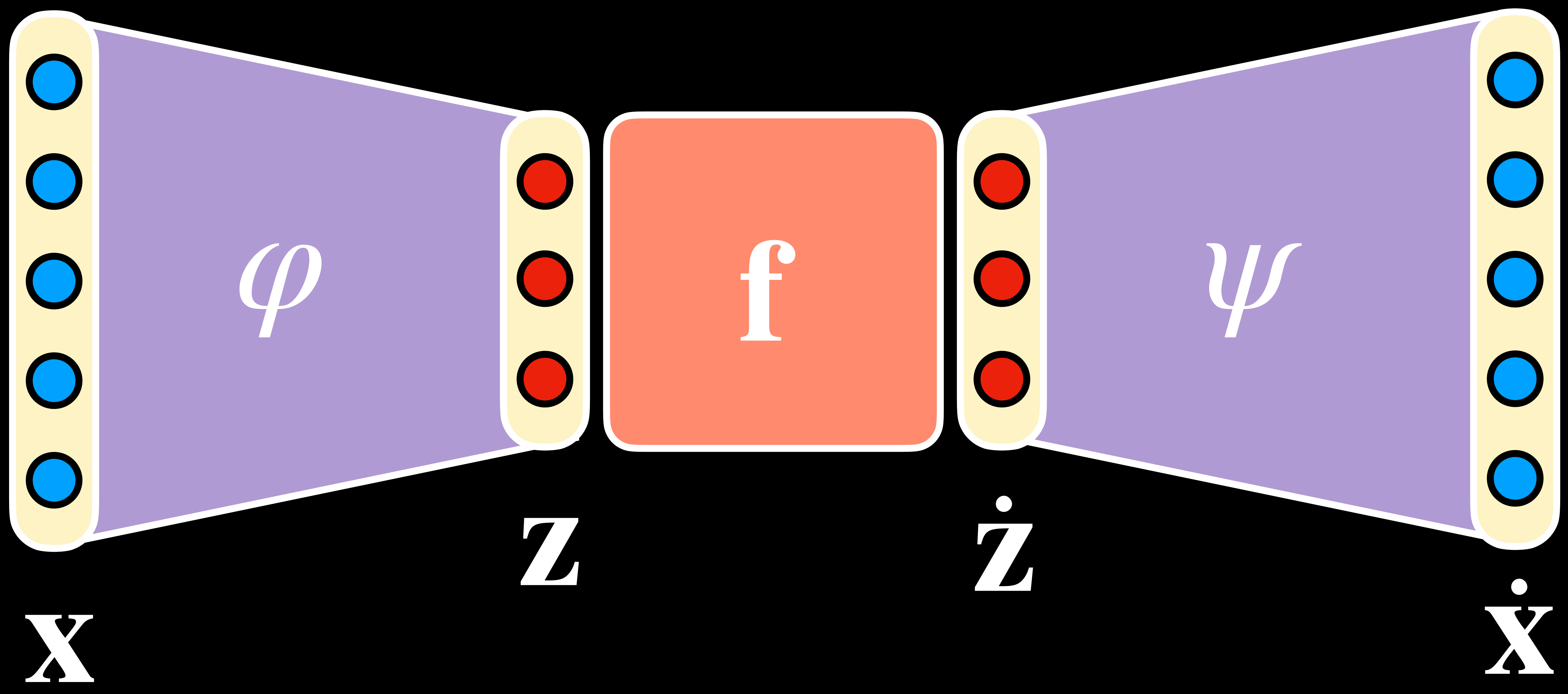


$$\frac{d}{dt}\mathbf{z} = \mathbf{f}(\mathbf{z})$$

Geocentrism

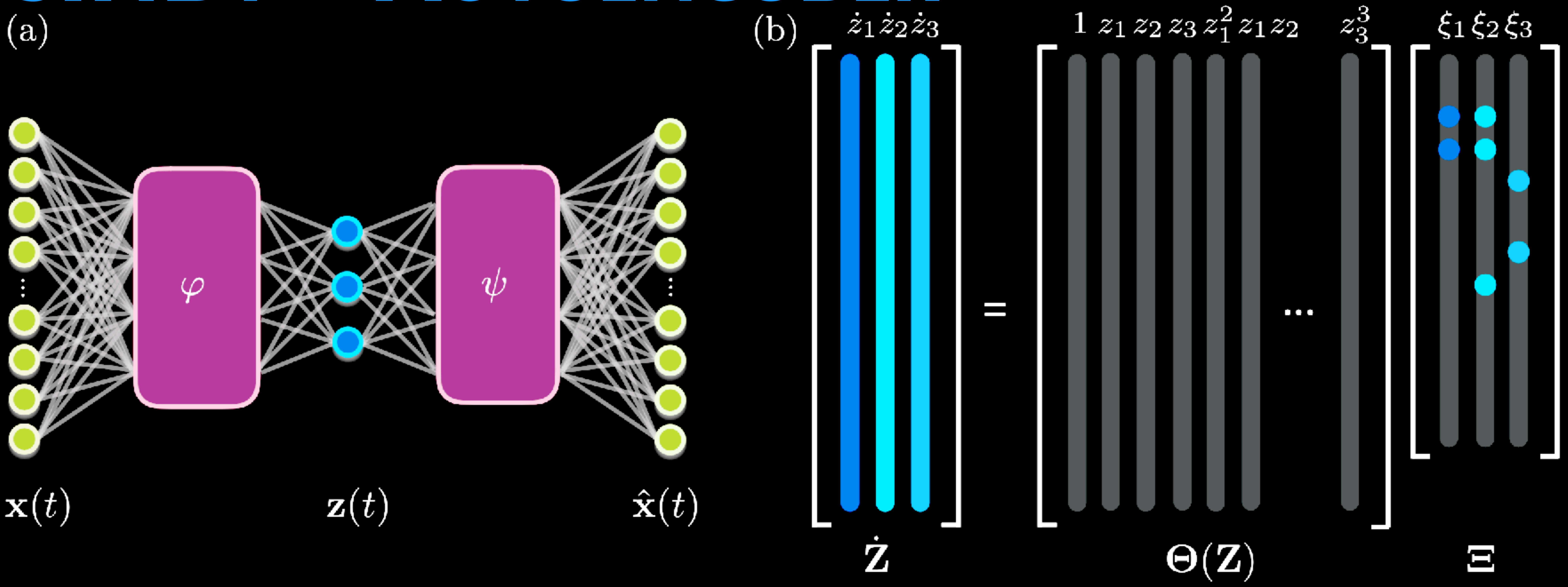
MALIN CHRISTERSSON

Deep Autoencoders for Dynamics



$$\frac{d}{dt}\mathbf{z} = \mathbf{f}(\mathbf{z})$$

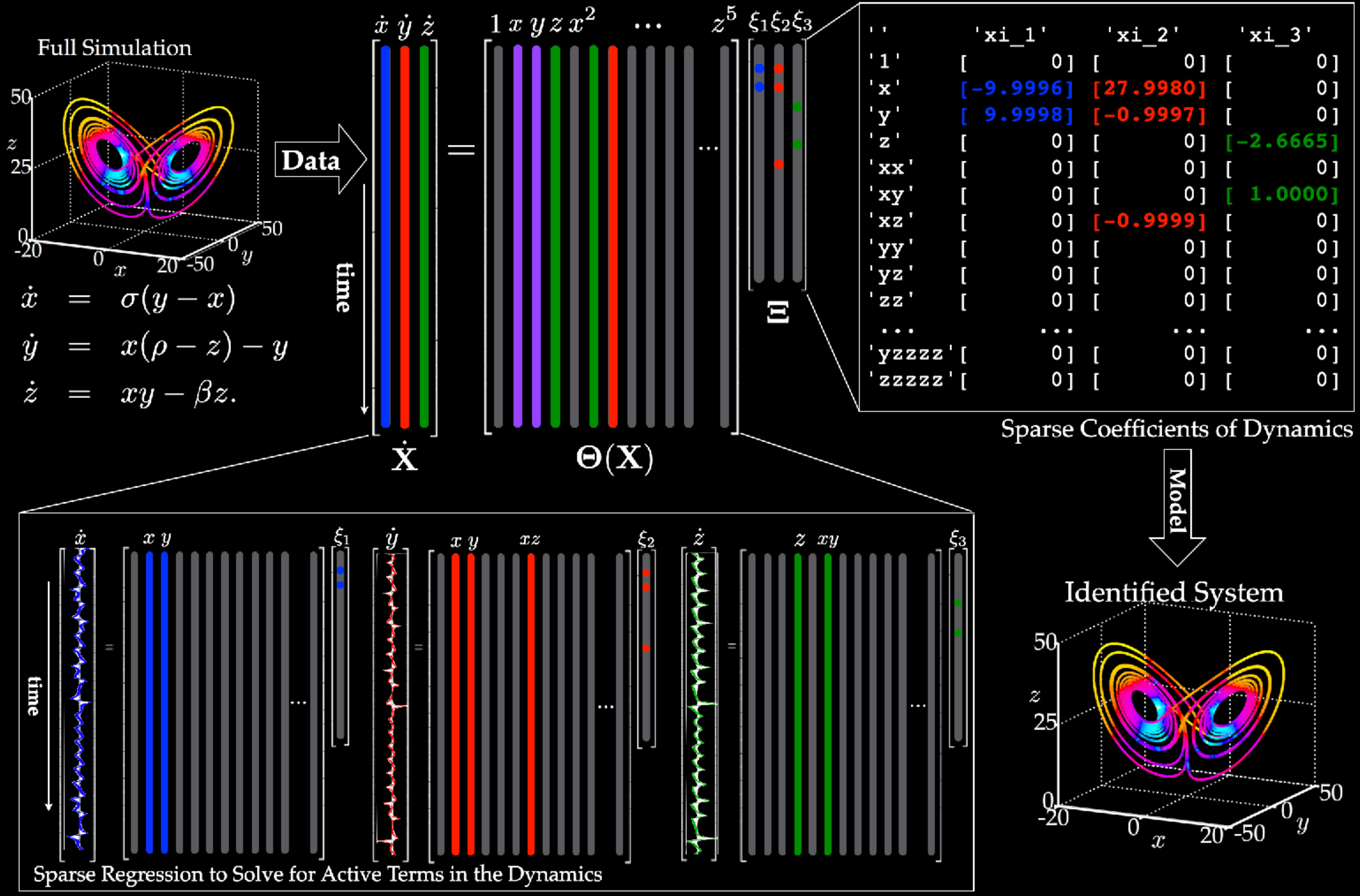
SINDy + Autoencoder



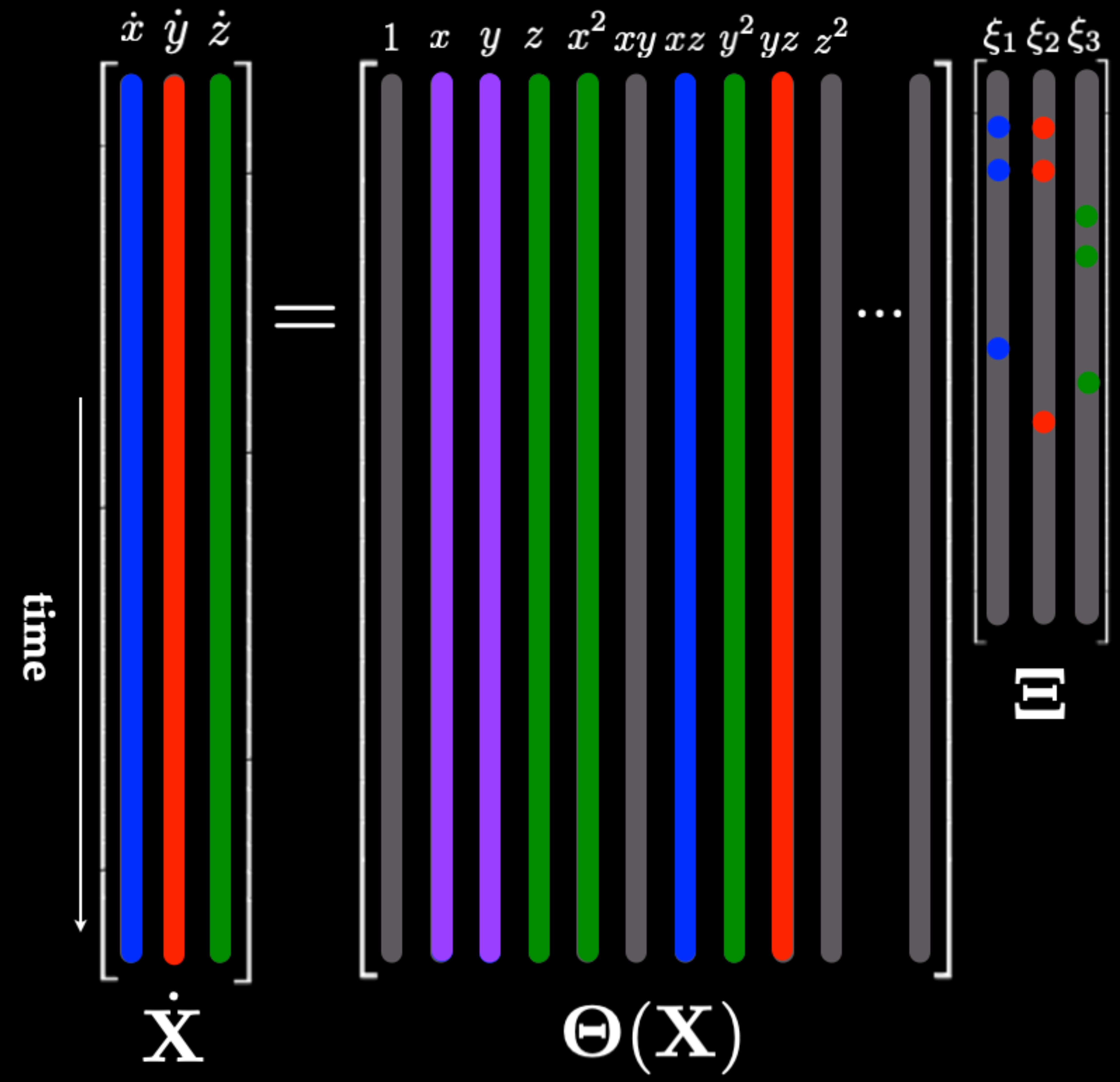
$$\dot{\mathbf{z}}_i = \nabla_{\mathbf{x}}\varphi(\mathbf{x}_i)\dot{\mathbf{x}}_i \qquad \boldsymbol{\Theta}(\mathbf{z}_i^T) = \boldsymbol{\Theta}(\varphi(\mathbf{x}_i)^T)$$

$$\underbrace{\|\mathbf{x}-\psi(\mathbf{z})\|_2^2}_{\text{reconstruction loss}} + \underbrace{\lambda_1 \left\|\dot{\mathbf{x}} - (\nabla_{\mathbf{z}}\psi(\mathbf{z}))\left(\boldsymbol{\Theta}(\mathbf{z}^T)\boldsymbol{\Xi}\right)\right\|_2^2}_{\text{SINDy loss in } \dot{\mathbf{x}}} + \underbrace{\lambda_2 \left\|(\nabla_{\mathbf{x}}\mathbf{z})\,\dot{\mathbf{x}} - \boldsymbol{\Theta}(\mathbf{z}^T)\boldsymbol{\Xi}\right\|_2^2}_{\text{SINDy loss in } \dot{\mathbf{z}}} + \underbrace{\lambda_3 \|\boldsymbol{\Xi}\|_1}_{\text{SINDy regularization}}$$

Champion, Lusch, Kutz, Brunton. *Proc. Nat. Acad. Sci*, 2019



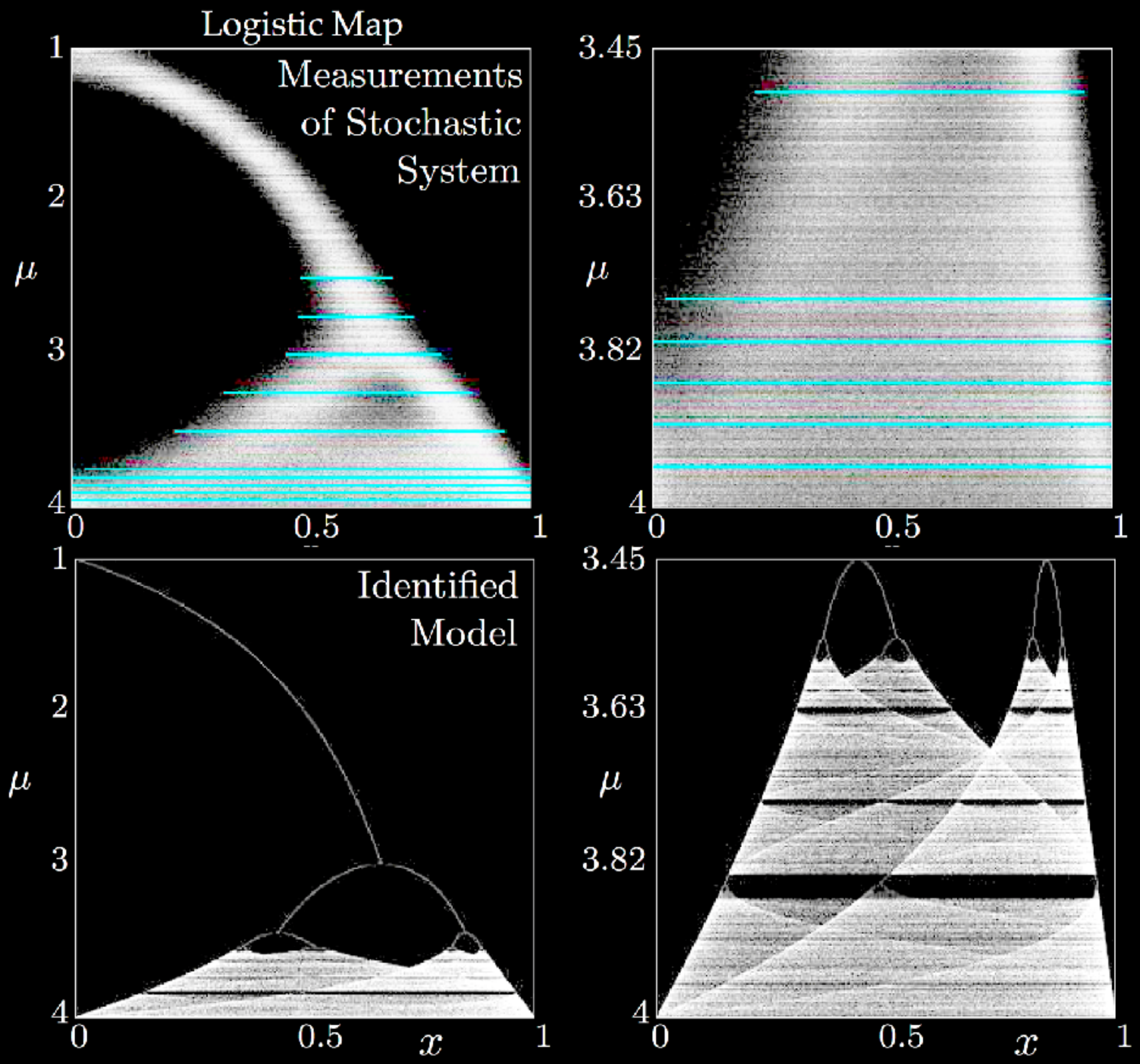
Full Simulation
$\dot{x} = \sigma(y - x)$
$\dot{y} = x(\rho - z) - y$
$\dot{z} = xy - \beta z.$
Data
time
$\dot{x}\ \dot{y}\ \dot{z}$
$1\ x\ y\ z\ x^2\ \cdots\ z^5$
$\xi_1 \xi_2 \xi_3$
$\dot{\mathbf{X}}$
$\Theta(\mathbf{X})$
Ξ
'' 'xi_1' 'xi_2' 'xi_3'
'1' [0] [0] [0]
'x' [-9.9996] [27.9980] [0]
'y' [9.9998] [-0.9997] [0]
'z' [0] [0] [-2.6665]
'xx' [0] [0] [0]
'xy' [0] [0] [1.0000]
'xz' [0] [-0.9999] [0]
'yy' [0] [0] [0]
'yz' [0] [0] [0]
'zz' [0] [0] [0]
... ...
'yzzzz'[0] [0] [0]
'zzzzz'[0] [0] [0]
Sparse Coefficients of Dynamics
Model
Identified System
time
$\dot{x}$ $x\ y$ ξ_1
$\dot{y}$ $x\ y$ xz ξ_2
$\dot{z}$ z xy ξ_3
Sparse Regression to Solve for Active Terms in the Dynamics



$\dot{x}$ $\dot{y}$ $\dot{z}$
time
$=$
1 x y z x^2 xy xz y^2 yz z^2 $\cdots$
ξ_1 ξ_2 ξ_3
$\dot{\mathbf{X}}$
$\boldsymbol{\Theta}(\mathbf{X})$
$\boldsymbol{\Xi}$

SINDy: Bifurcation Parameters and Forcing

$$x_{k+1} = \mu x_k(1 - x_k) + \eta_k.$$

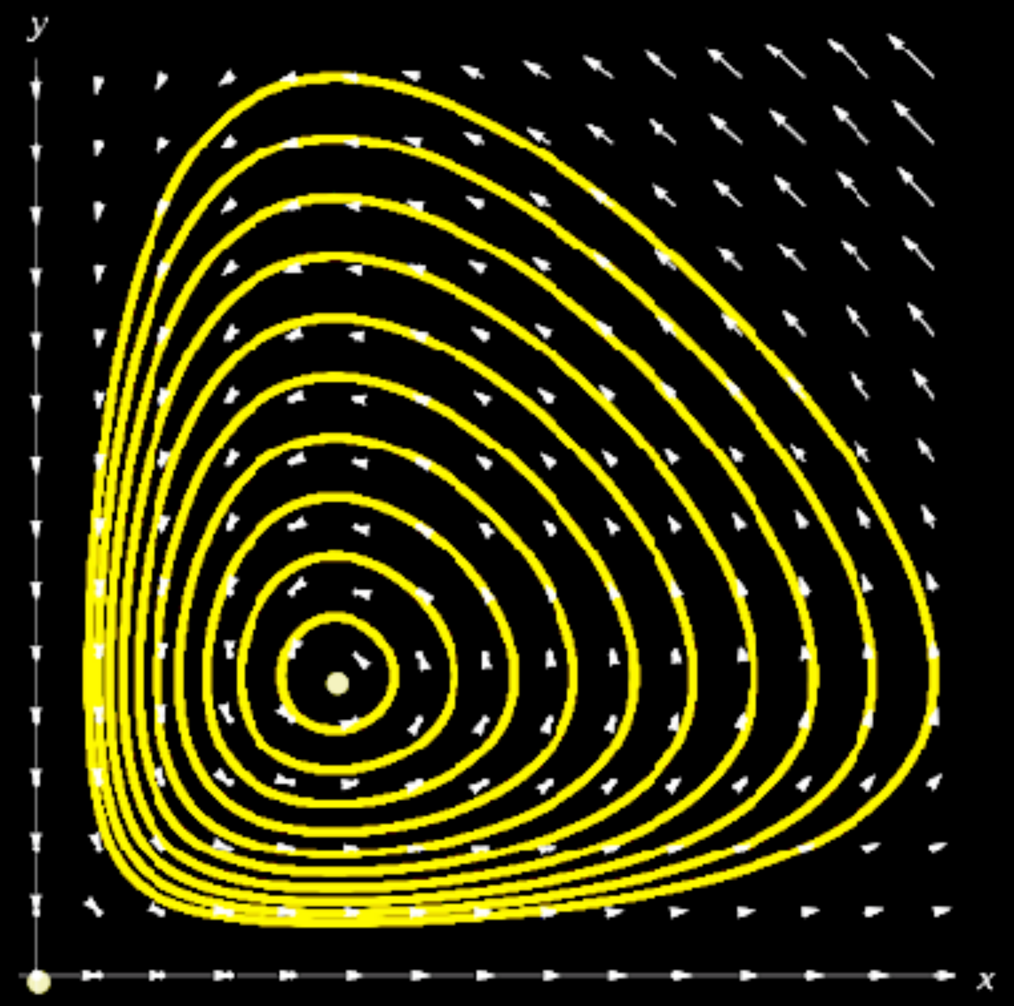


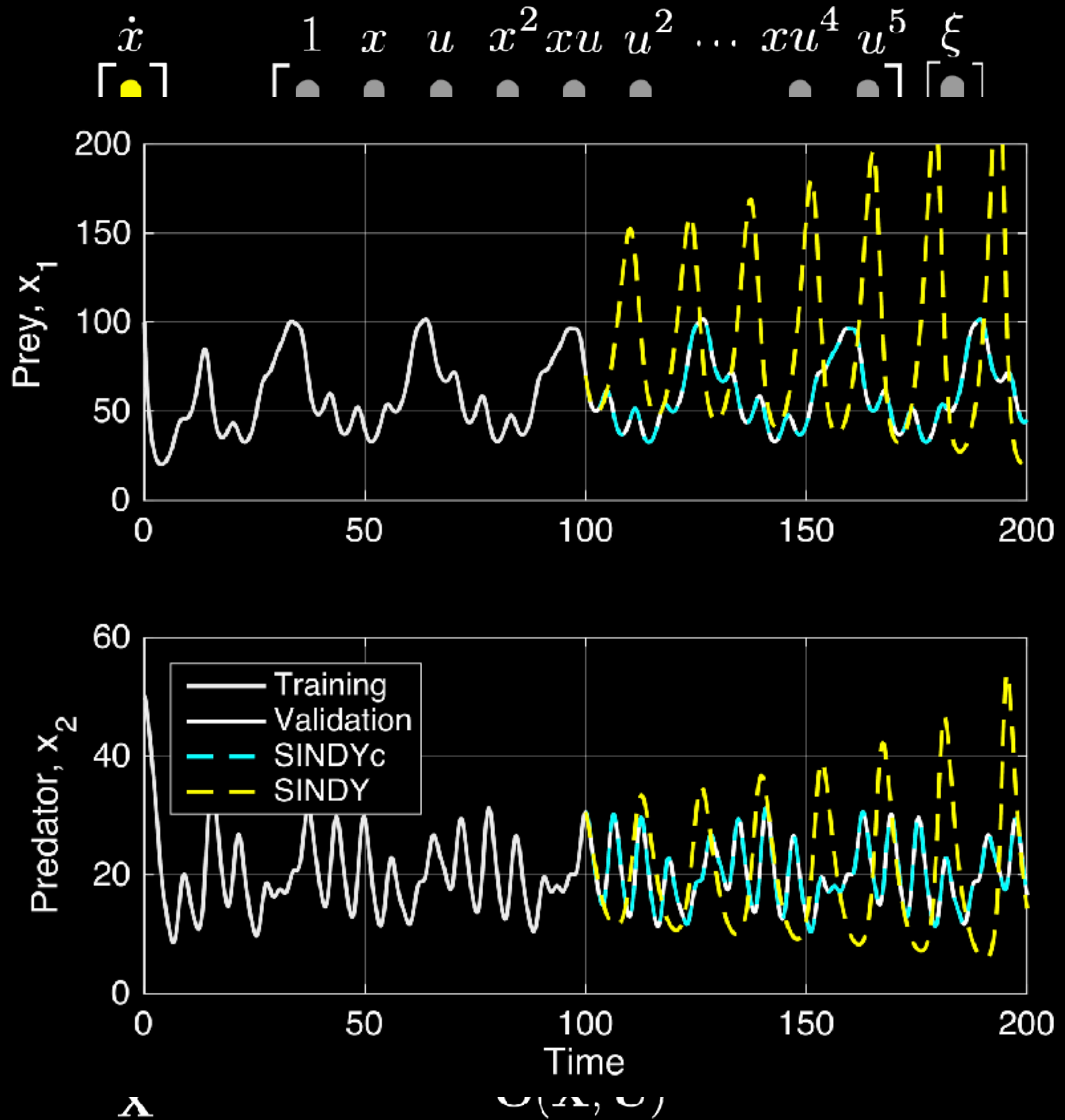
$$\begin{aligned}\dot{\mathbf{x}} &= \mathbf{f}(\mathbf{x}; \mu)\\ \dot{\mu} &= 0.\end{aligned}$$

Brunton, Proctor, Kutz, *PNAS* 2016.

SINDy with Control

Predator Prey System





Kaiser, Kutz, Brunton, *Proc. Roy. Soc. A*, 2018.

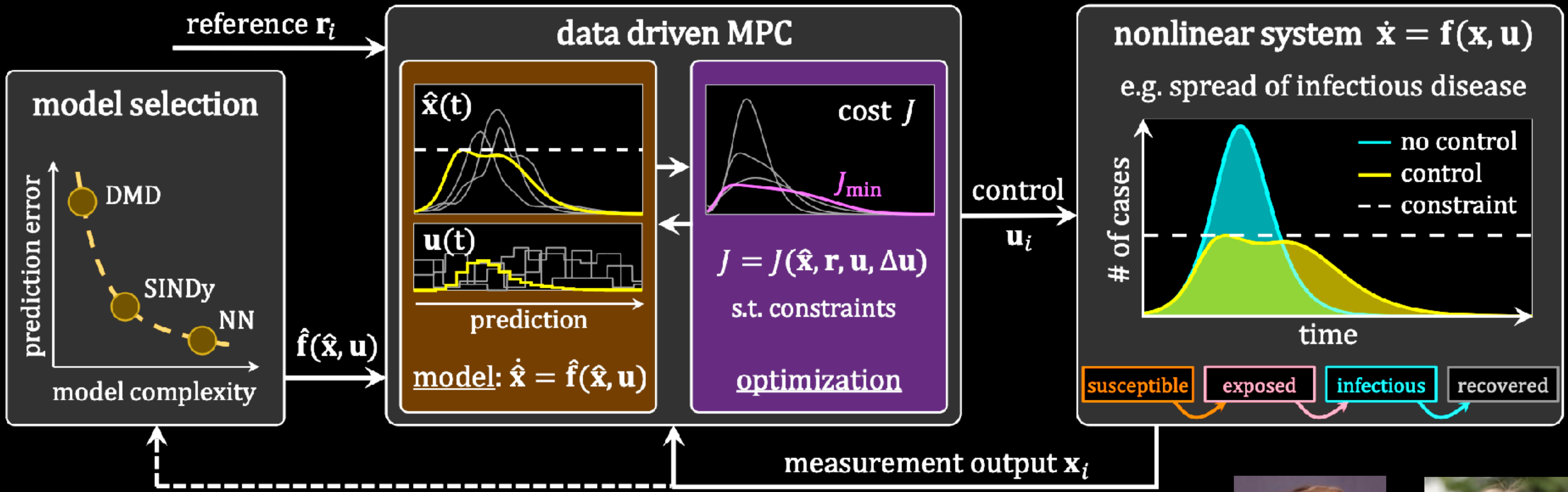
SINDy with Control: A Tutorial

Urban Fasel, Eurika Kaiser, J. Nathan Kutz, Bingni W. Brunton, and Steven L. Brunton

***Abstract*—Many dynamical systems of interest are nonlinear, with examples in turbulence, epidemiology, neuroscience, and finance, making them difficult to control using linear approaches. Model predictive control (MPC) is a powerful model-based optimization technique that enables the control of such nonlinear systems with constraints. However, modern systems often lack computationally tractable models, motivating the use of system identification techniques to learn accurate and efficient models for real-time control. In this tutorial article, we review emerging data-driven methods for model discovery and how they are used for nonlinear MPC. In particular, we focus on the sparse identification of nonlinear dynamics (SINDy) algorithm and show how it may be used with MPC on an infectious disease control example. We compare the performance against MPC based on a linear dynamic mode decomposition (DMD) model. Code is provided to run the tutorial examples and may be modified to extend this data-driven control framework to arbitrary nonlinear systems.**

disciplines that lack known governing equations. Generally, MPC also suffers from the curse of dimensionality, requiring large computational effort and limiting the applicability to low-dimensional problems, often based on locally linear models. Increasingly, data-driven approaches are providing a hierarchy of models of various fidelity and complexity, which may be used for MPC.

System identification has a long and rich history in control theory, and it has a close connection with machine learning, as it builds models from data via regression and optimization [4]. A wide range of data-driven system identification techniques exist in literature, including state-space models from the eigensystem realization algorithm (ERA) [7] and other subspace identification methods, Volterra series [8], [9], autoregressive models [10] (e.g. ARX, ARMA, NARX and NARMAX [11] models), and neural network (NN)


reference $\mathbf{r}_i$
data driven MPC
nonlinear system $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u})$
e.g. spread of infectious disease
model selection
prediction error
DMD
SINDy
NN
model complexity
$\hat{\mathbf{f}}(\hat{\mathbf{x}}, \mathbf{u})$
$\hat{\mathbf{x}}(t)$
$\mathbf{u}(t)$
prediction
model: $\dot{\hat{\mathbf{x}}} = \hat{\mathbf{f}}(\hat{\mathbf{x}}, \mathbf{u})$
cost J
$J_{\min}$
$J = J(\hat{\mathbf{x}}, \mathbf{r}, \mathbf{u}, \Delta\mathbf{u})$
s.t. constraints
optimization
control
$\mathbf{u}_i$
# of cases
no control
control
constraint
time
susceptible
exposed
infectious
recovered
measurement output $\mathbf{x}_i$



A Hierarchy of Models for Control

$$\frac{d}{dt}\mathbf{x} = \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u}$$

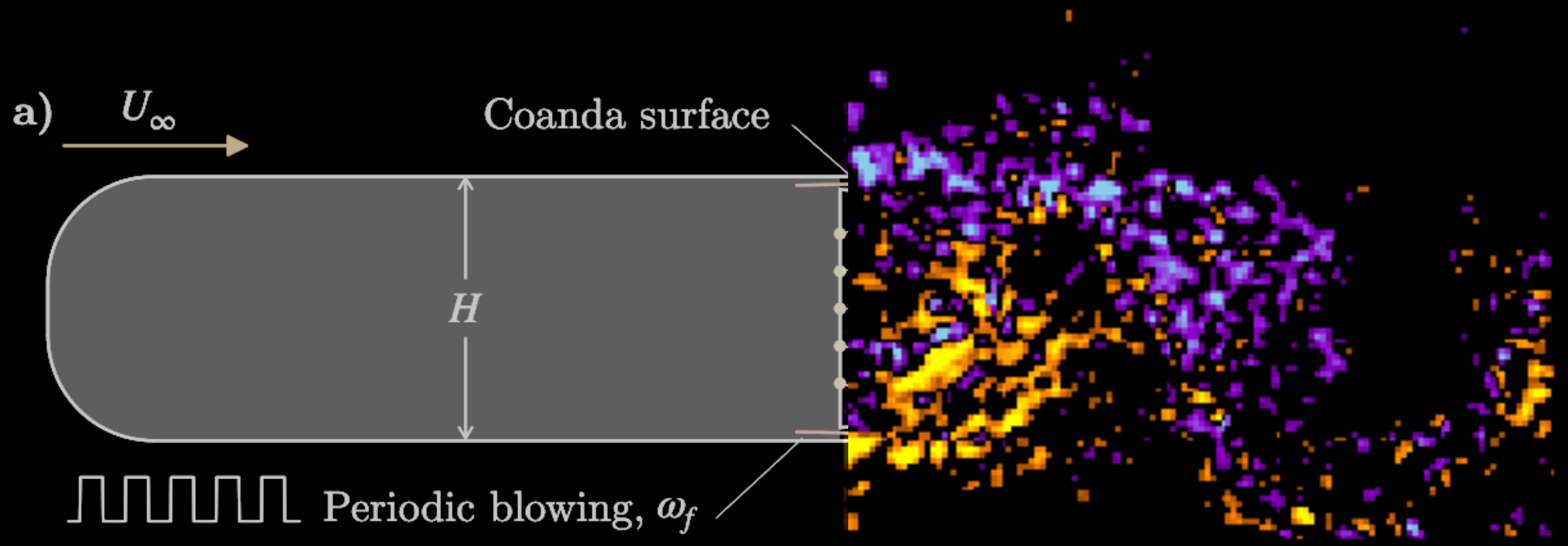
Linear (DMD)

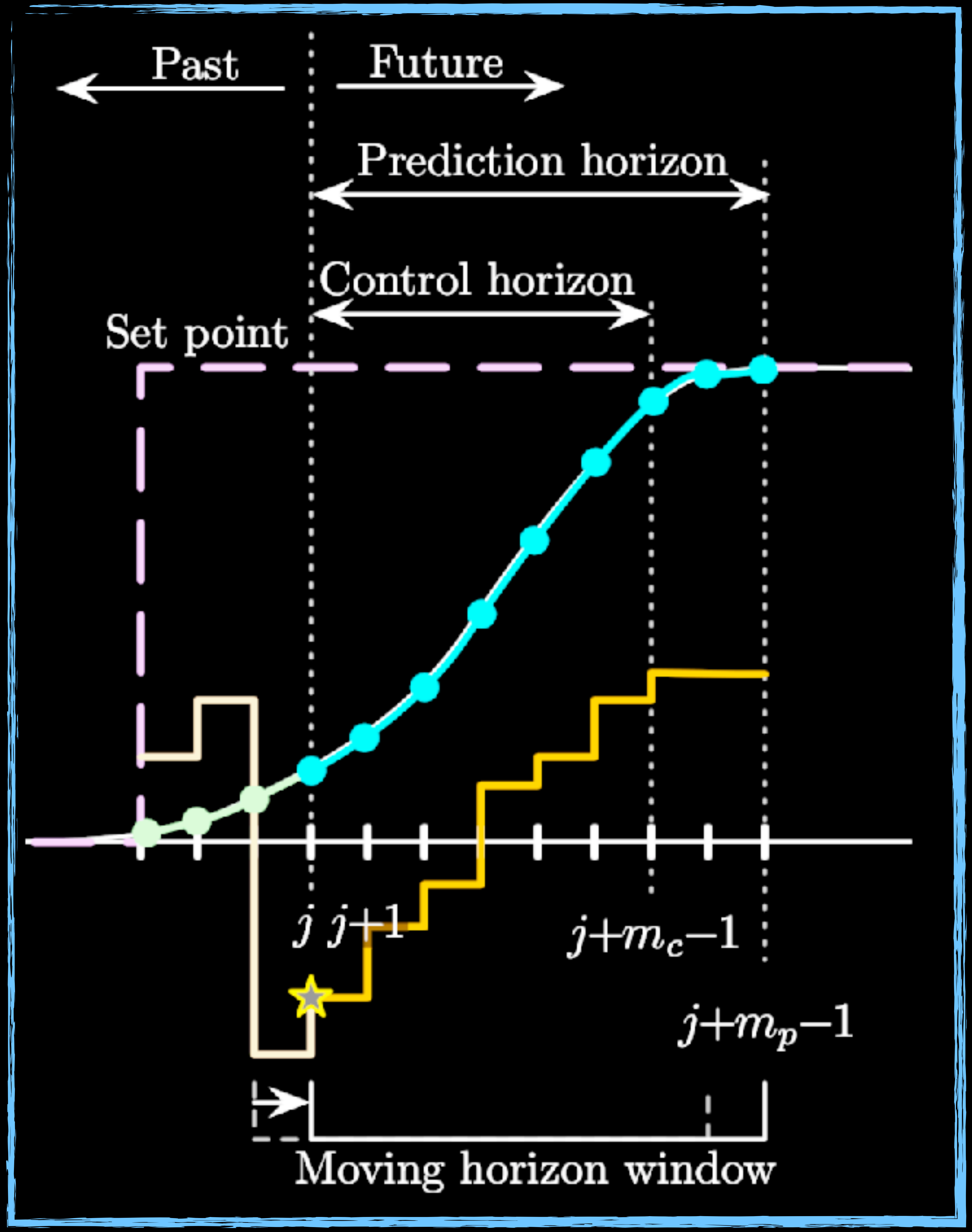
$$\frac{d}{dt}\mathbf{x} = \mathbf{f}(\mathbf{x}, \mathbf{u})$$

Sparse Nonlinear (SINDy)

$$\frac{d}{dt}\mathbf{x} = \mathcal{N}(\mathbf{x}, \mathbf{u})$$

Neural Network





Kaiser, Kutz, Brunton, *Proc. Roy. Soc. A*, 2018.

Machine Learning for Scientific Discovery

Questions?