Machine Learning for Scientific Discovery

Steve Brunton
University of Washington

(Video by Petros Vrellis)

Machine Learning for Scientific Discovery

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Beverley McKeon

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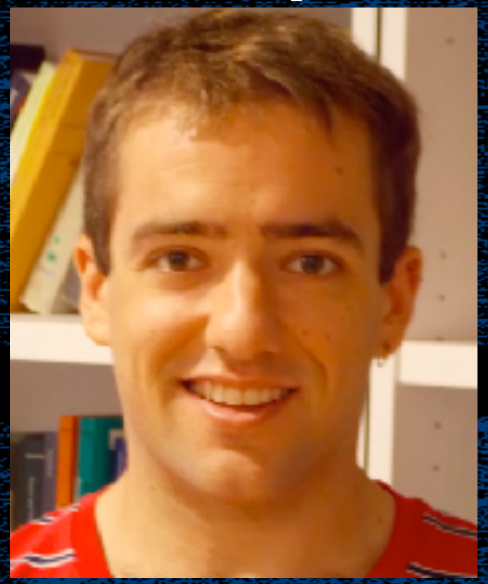

Kathleen Champion

Bethany Lusch

Benjamin Herrmann

Peter Baddoo

Joe Bakarji

Science to Shape the Future of the Army · Army Research Office · 1951

Air Force Research Laboratory

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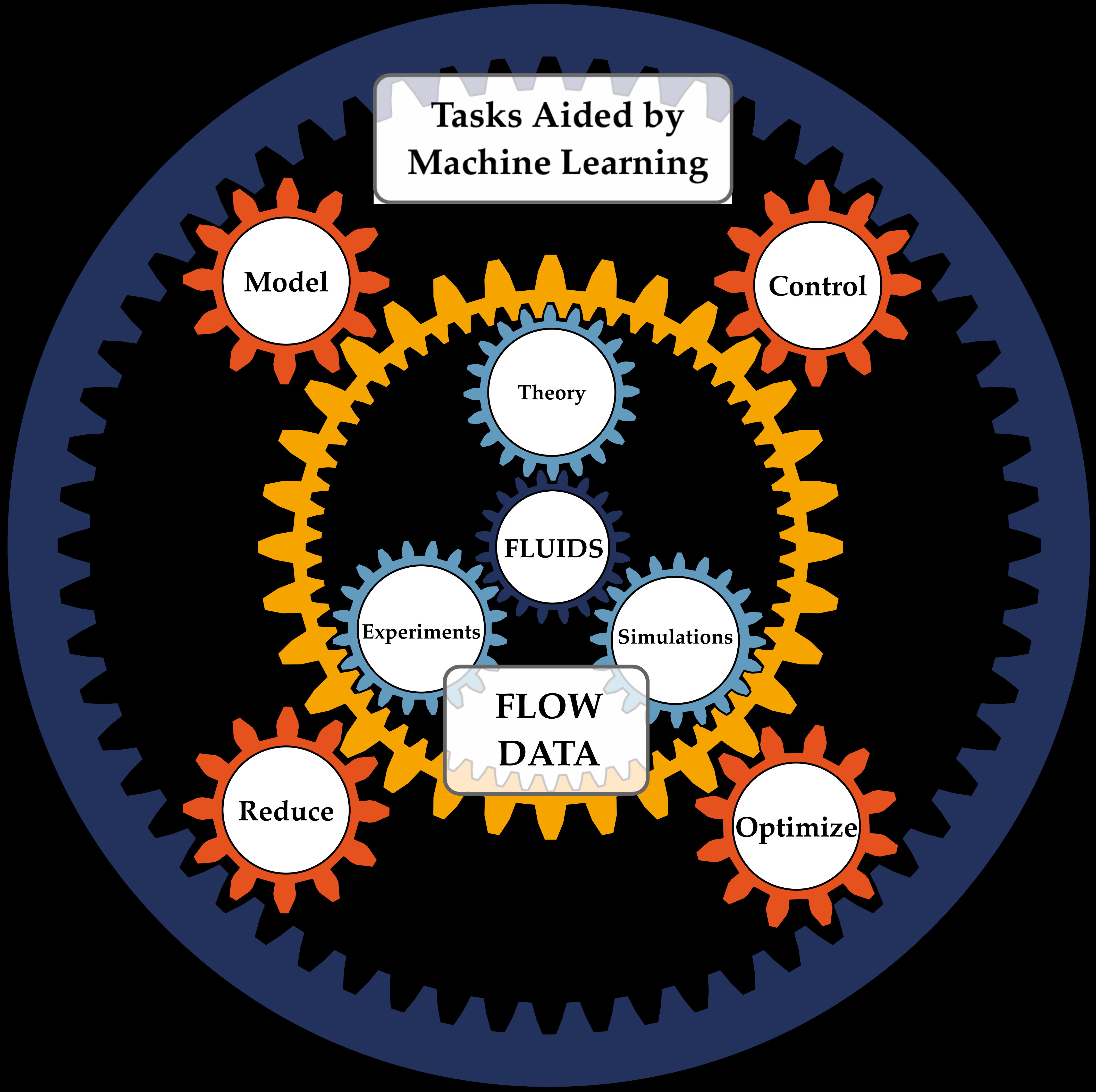
DARPA

BOEING



Machine Learning for Fluid Mechanics

Steven L. Brunton,[1] Bernd R. Noack,[2] and Petros Koumoutsakos[3],[4]

Keywords

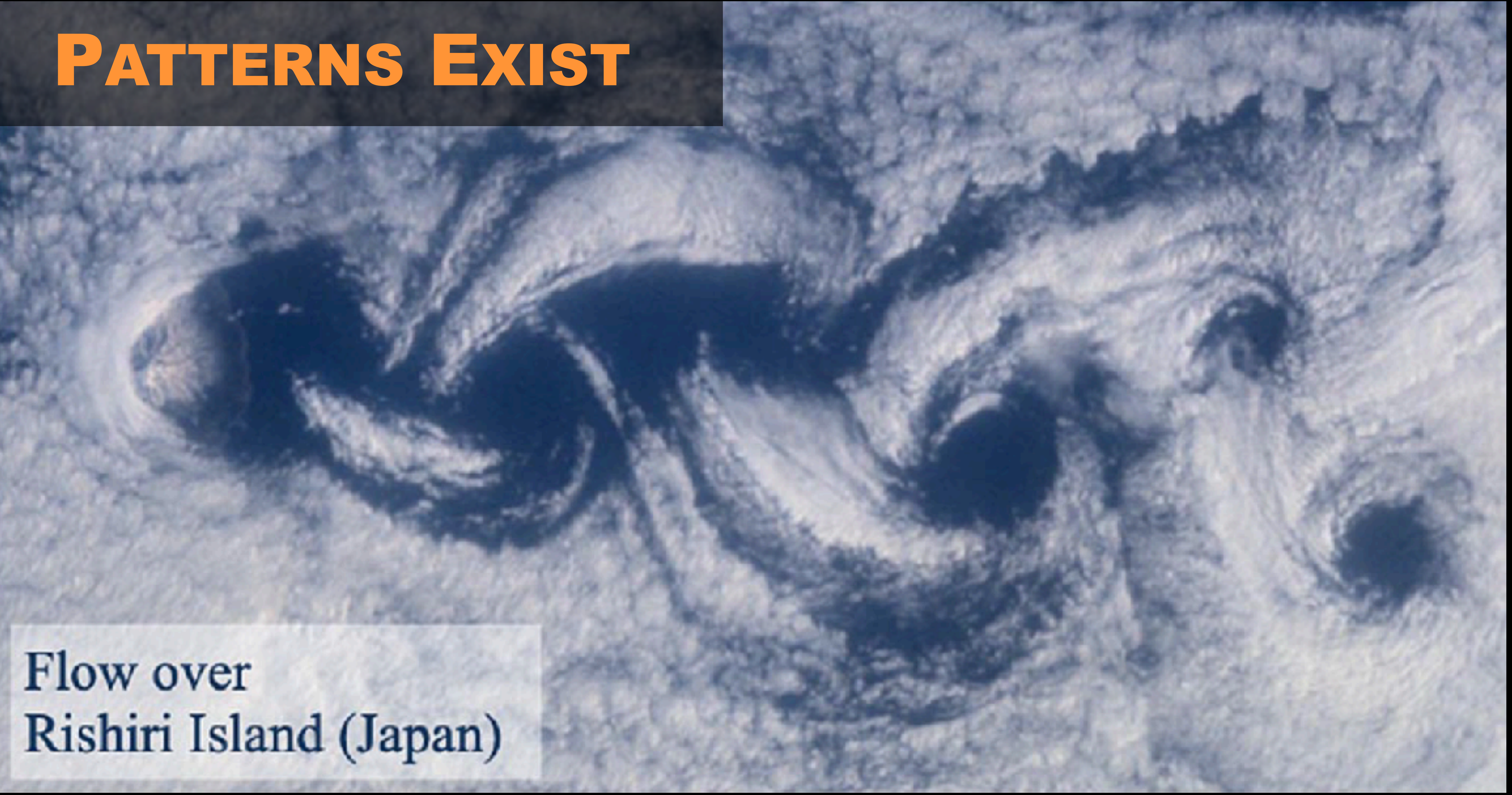
machine learning, data-driven modeling, optimization, control

Abstract

The field of fluid mechanics is rapidly advancing, driven by unprecedented volumes of data from experiments, field measurements, and large-scale simulations at multiple spatiotemporal scales. Machine learning presents us with a wealth of techniques to extract information from data that can be translated into knowledge about the underlying fluid mechanics. Moreover, machine learning algorithms can augment domain knowledge and automate tasks related to flow control and optimization. This article presents an overview of past history, current developments, and emerging opportunities of machine learning for fluid mechanics. We outline fundamental machine learning methodologies and discuss their uses for understanding, modeling, optimizing, and controlling fluid flows. The strengths and limitations of these methods are addressed from the perspective of scientific inquiry that links data with modeling, experiments, and simulations. Machine learning provides a powerful information processing framework that can augment, and possibly even transform, current lines of fluid mechanics research and industrial applications.

Patterns Exist

PATTERNS EXIST



Taira et al., AIAA J. 2017

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,

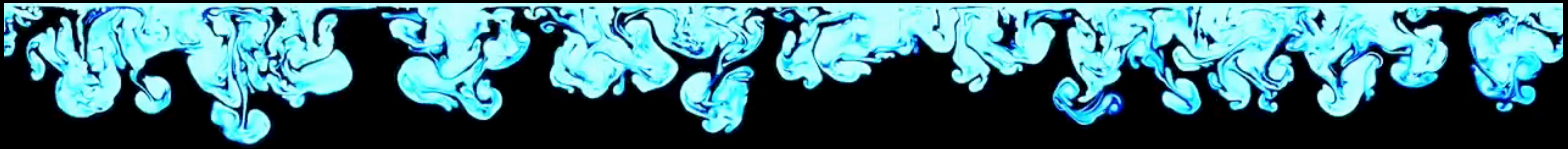
BUT NOT SIMPLER.

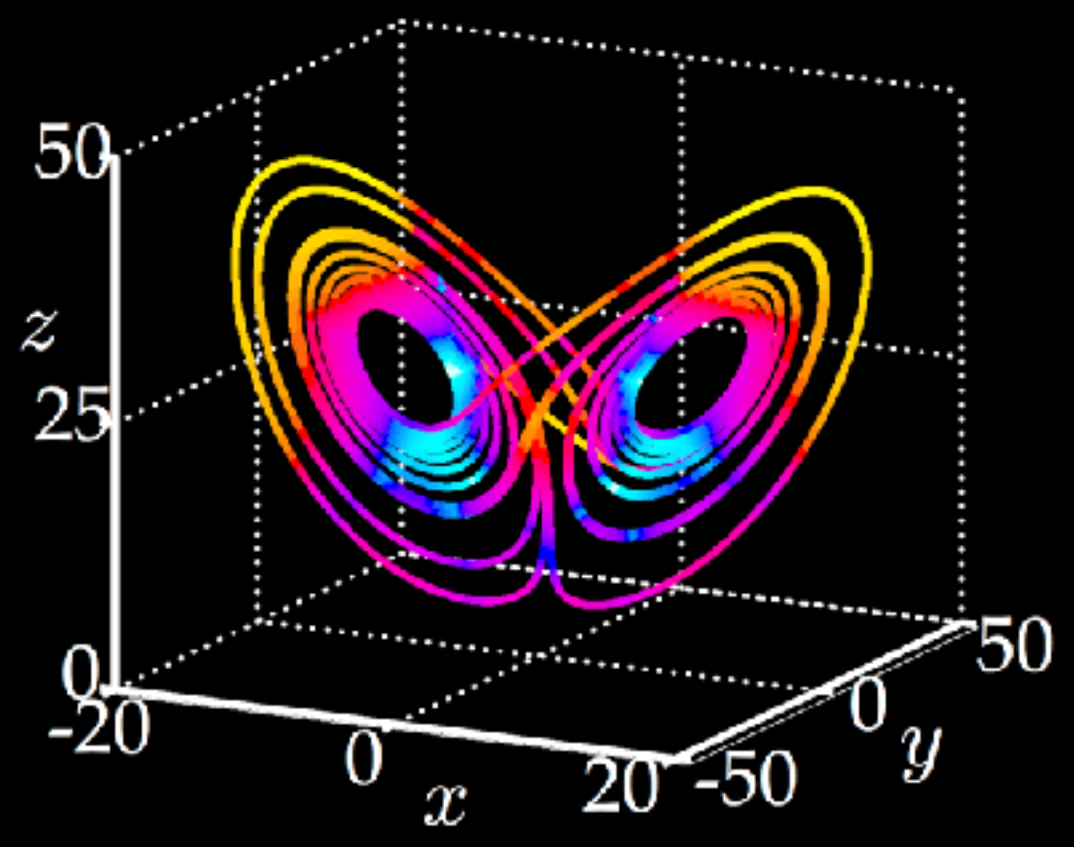
Albert Einstein

There is a need for
Interpretable and Generalizable
Machine Learning

- Low-Dimensional
- Sparse

Chaotic Thermal Convection



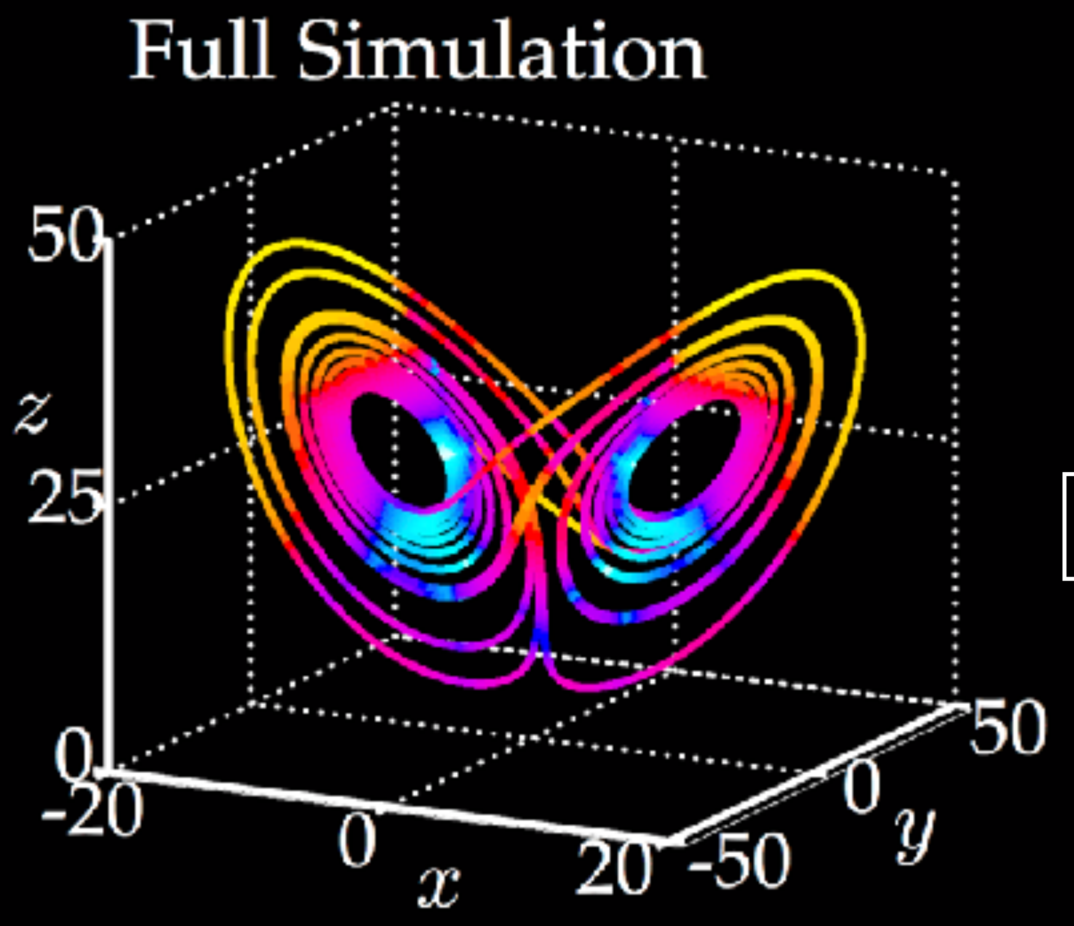


$$\begin{aligned}\dot{x} &= \sigma(y-x)\\ \dot{y} &= x(\rho-z)-y\\ \dot{z} &= xy-\beta z.\end{aligned}$$

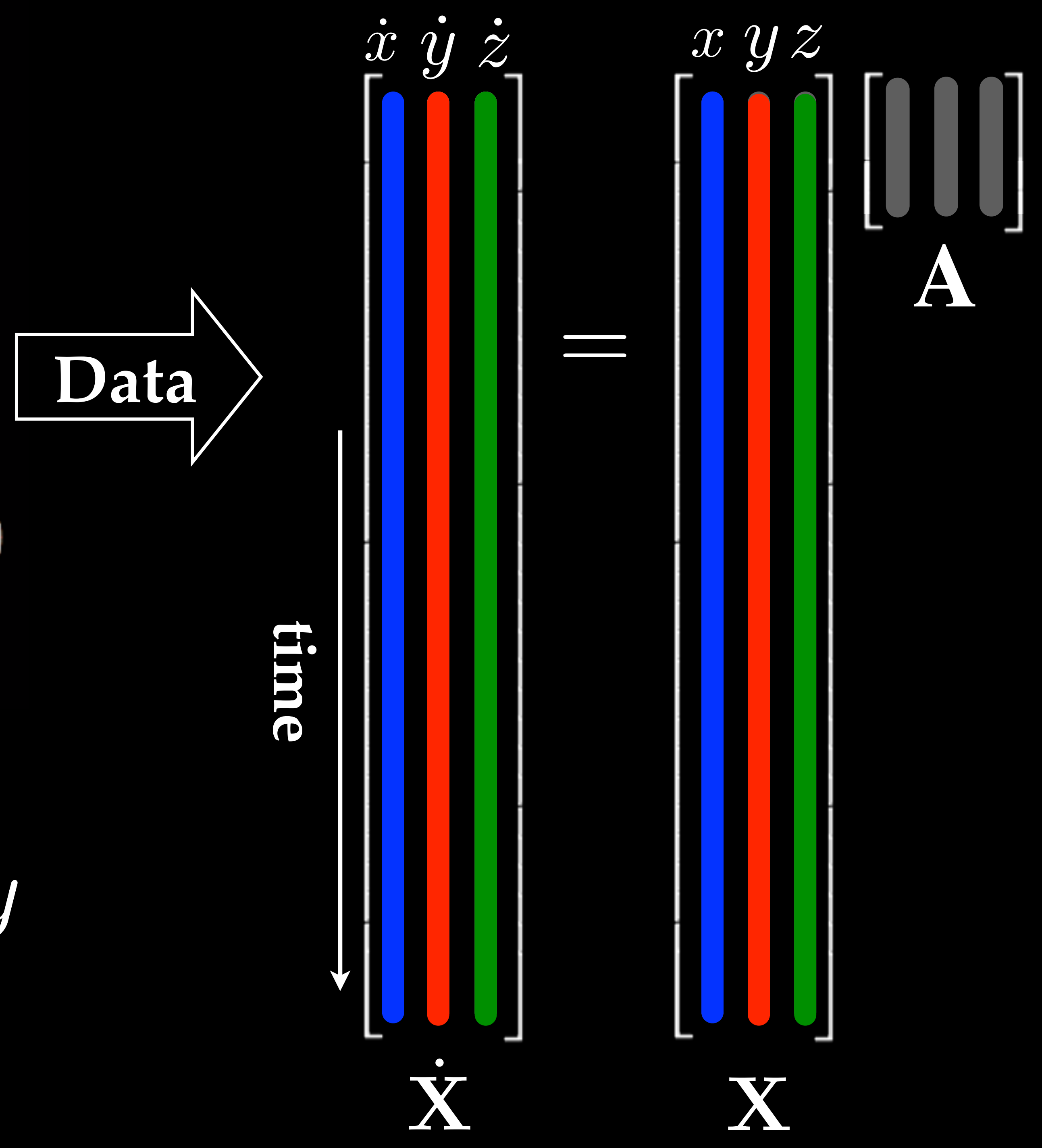
YouTube: turbulenceteam

Lorenz, Fetter, Hamilton, 1963

Sparse Identification of Nonlinear Dynamics (SINDy)



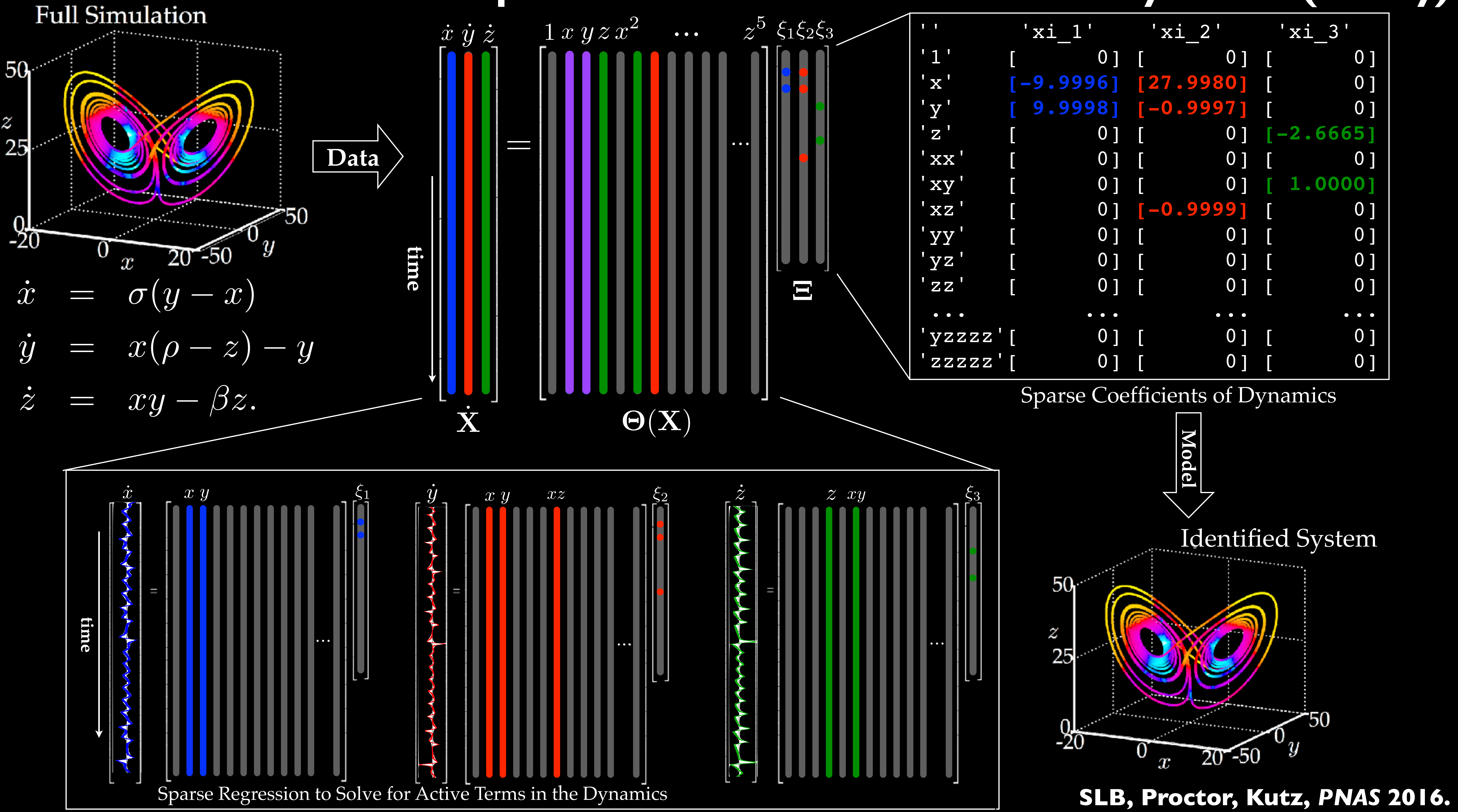
$$\dot{x} = \sigma(y - x)$$
$$\dot{y} = x(\rho - z) - y$$
$$\dot{z} = xy - \beta z.$$



DMD

SLB, Proctor, Kutz, *PNAS* 2016.

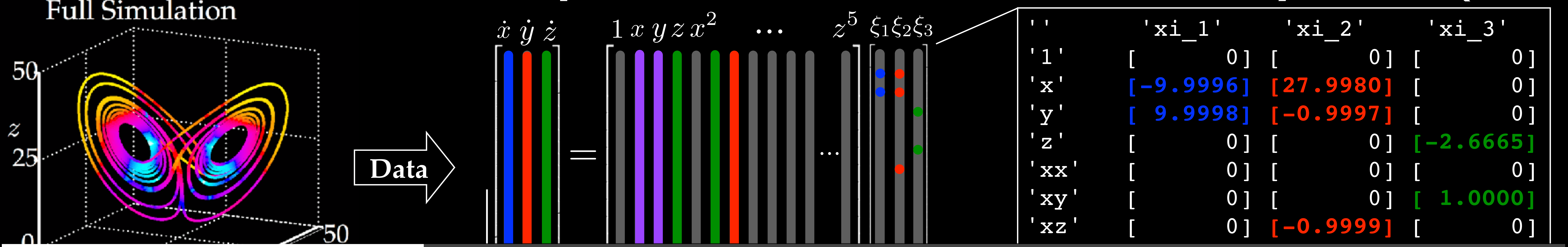
Sparse Identification of Nonlinear Dynamics (SINDy)



''	'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]
'yy'	[0]	[0]	[0]
'yz'	[0]	[0]	[0]
'zz'	[0]	[0]	[0]
...	...	...	...
'yzzzz'	[0]	[0]	[0]
'zzzzz'	[0]	[0]	[0]

SLB, Proctor, Kutz, *PNAS* 2016.

Sparse Identification of Nonlinear Dynamics (SINDy)

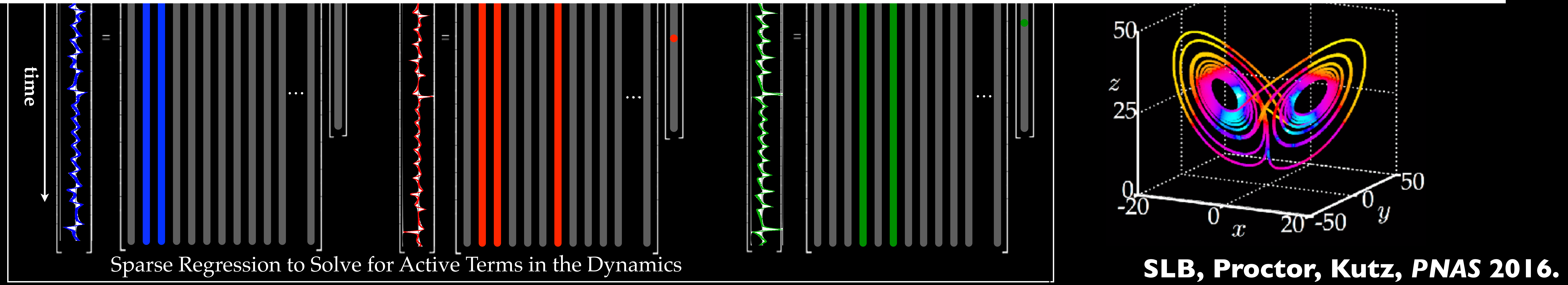


PySINDy

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).



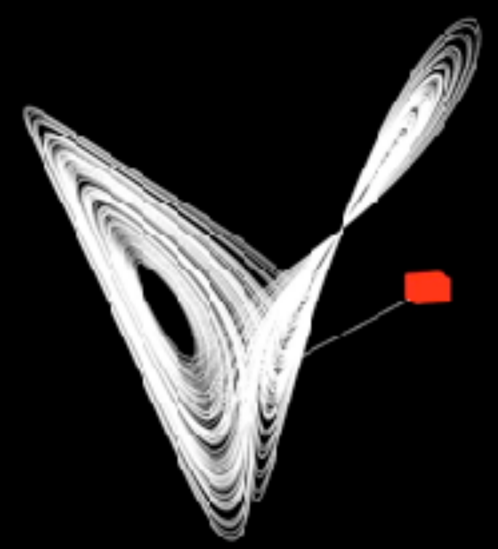
SLB, Proctor, Kutz, *PNAS* 2016.

PDEs

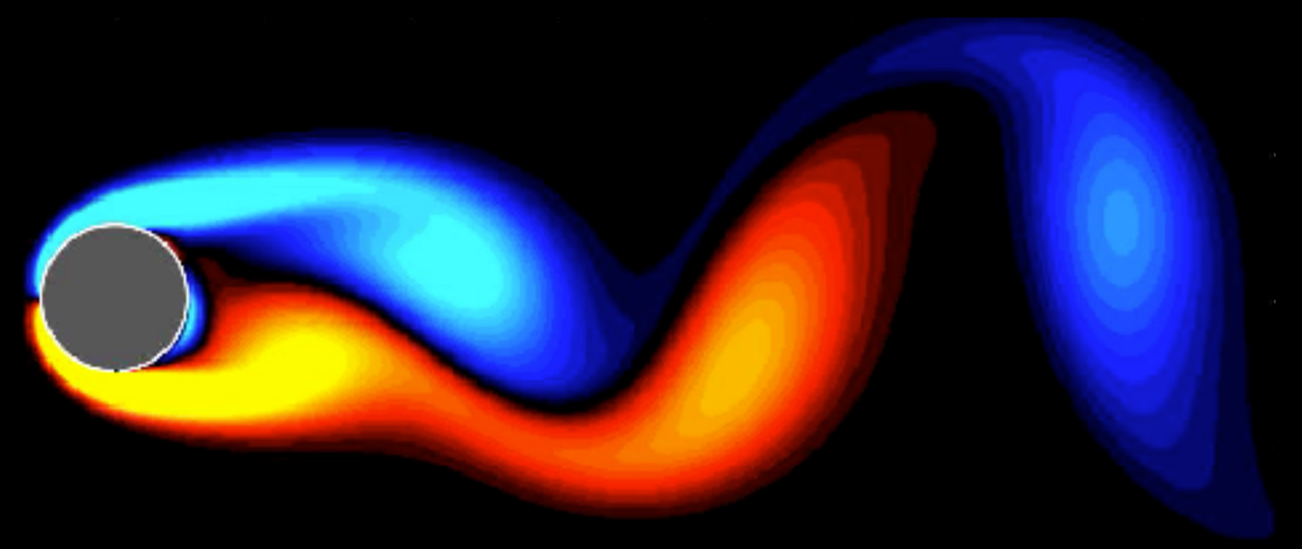
Rudy, SLB, Proctor, Kutz
Science Advances, 2017

Sparse Identification of Nonlinear Dynamics (SINDy)

Data → **Dynamics**

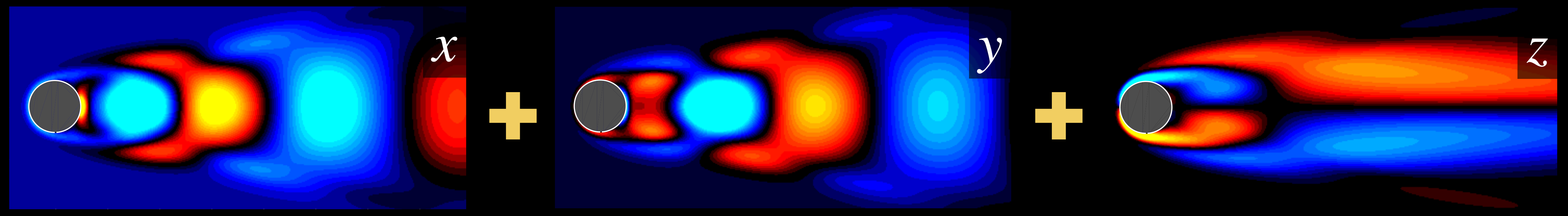


$$\begin{aligned}\dot{x} &= \sigma(y - x)\\ \dot{y} &= x(\rho - z) - y\\ \dot{z} &= xy - \beta z.\end{aligned}$$



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

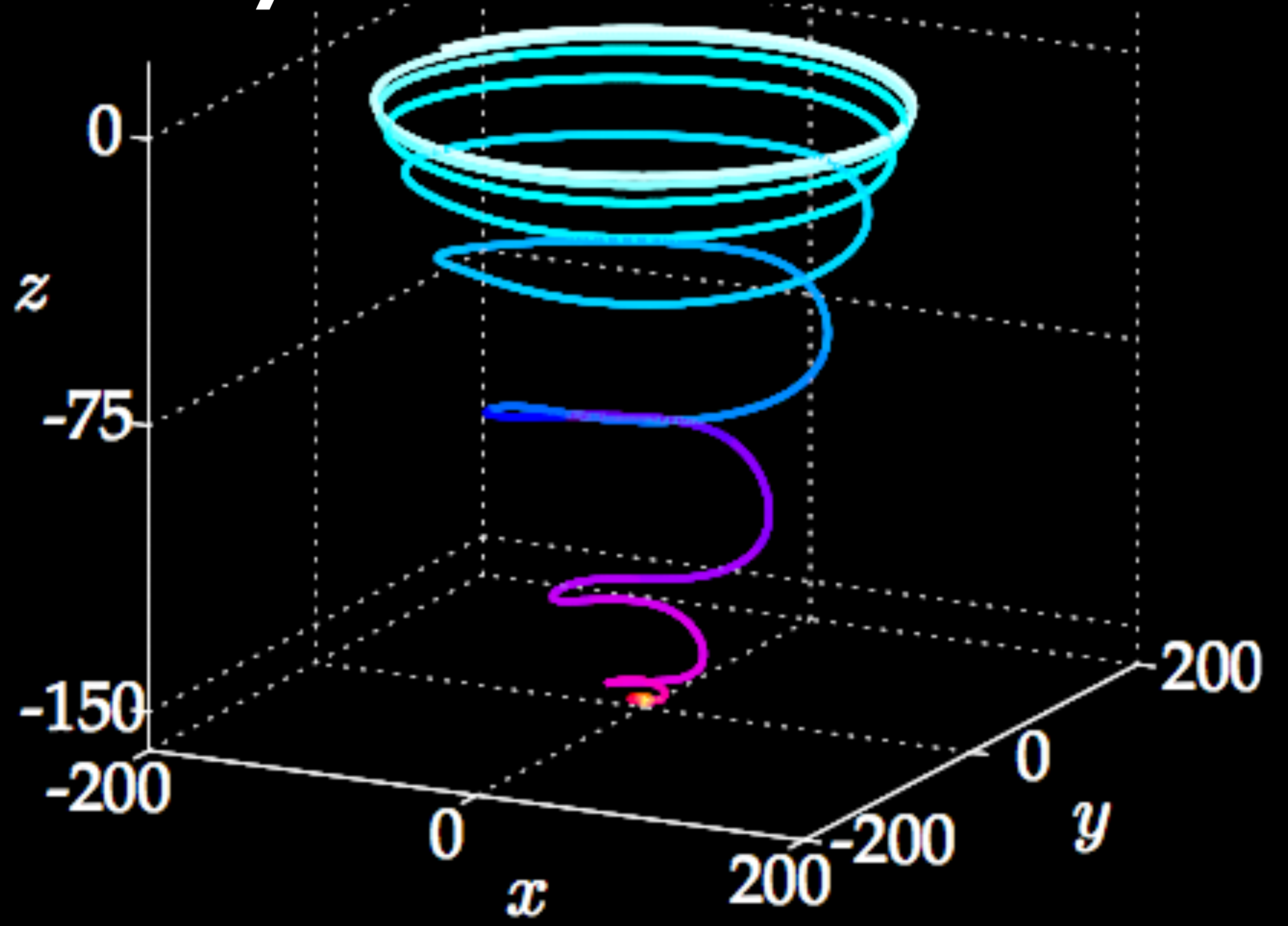
$\approx$



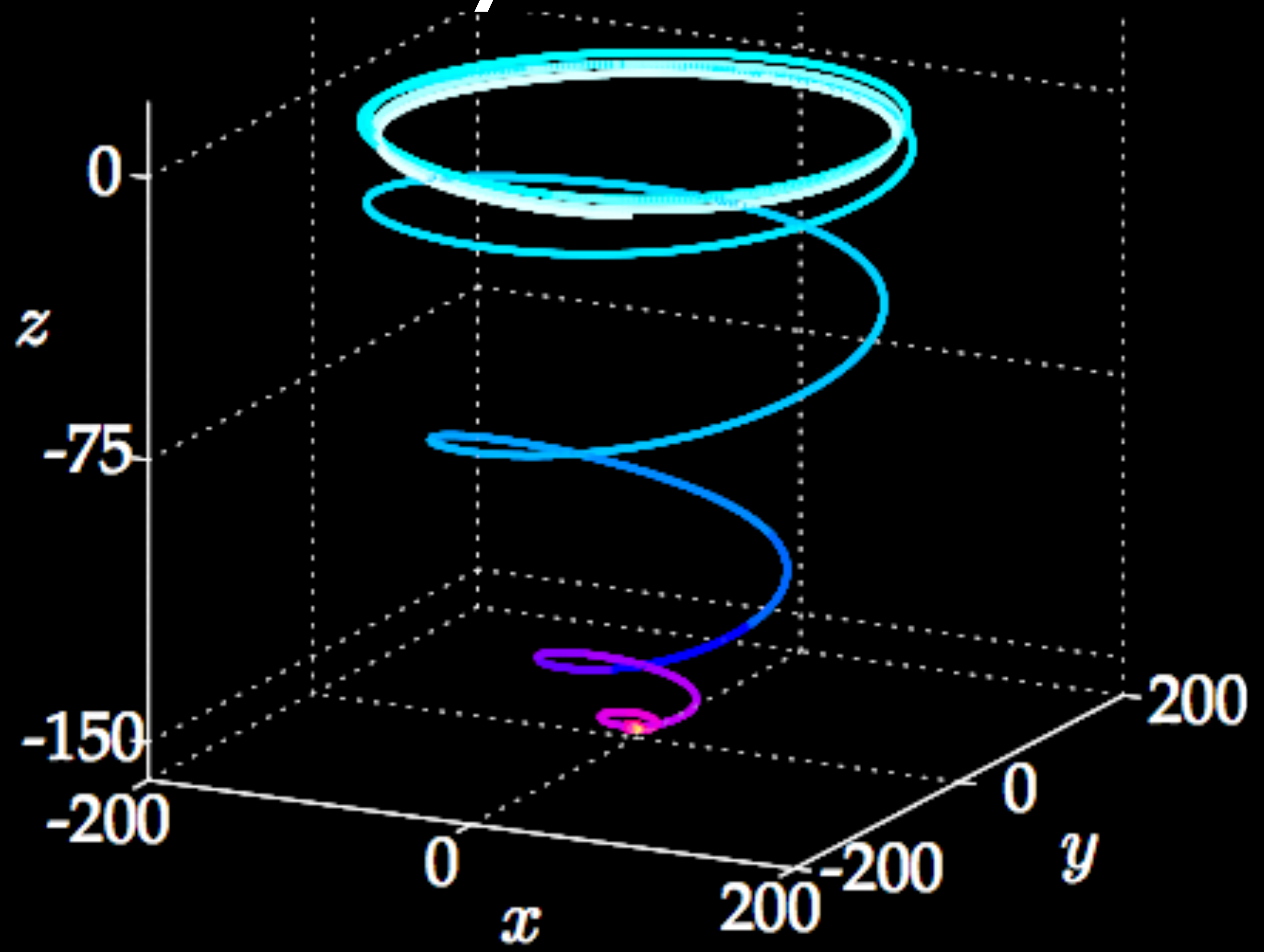
$$\begin{aligned}\dot{x} &= \mu x - \omega y + Axz\\ \dot{y} &= \omega x + \mu y + Ayz\\ \dot{z} &= -\lambda(z - x^2 - y^2)\end{aligned}$$

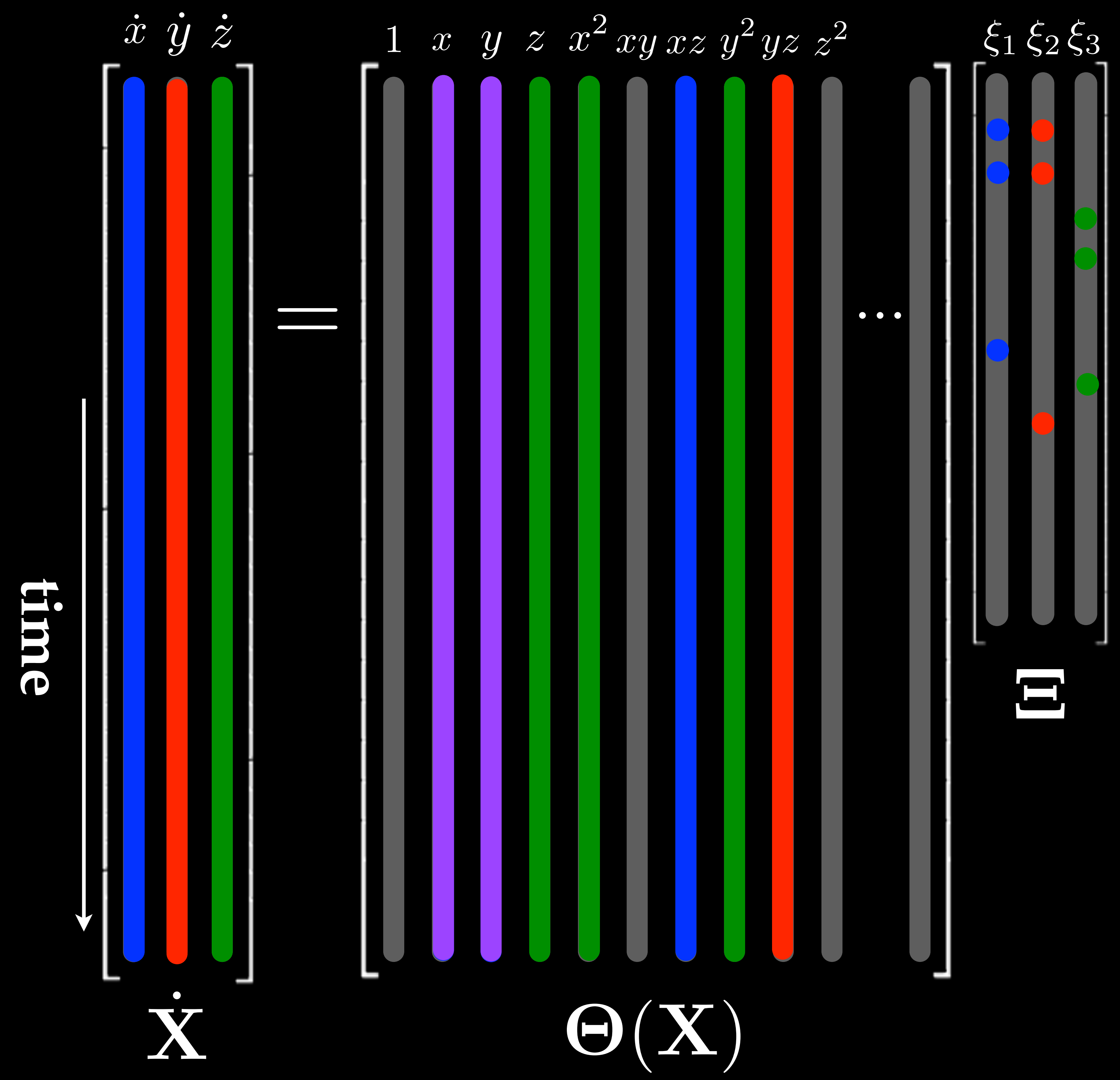
Sparse Identification of Nonlinear Dynamics (SINDy)

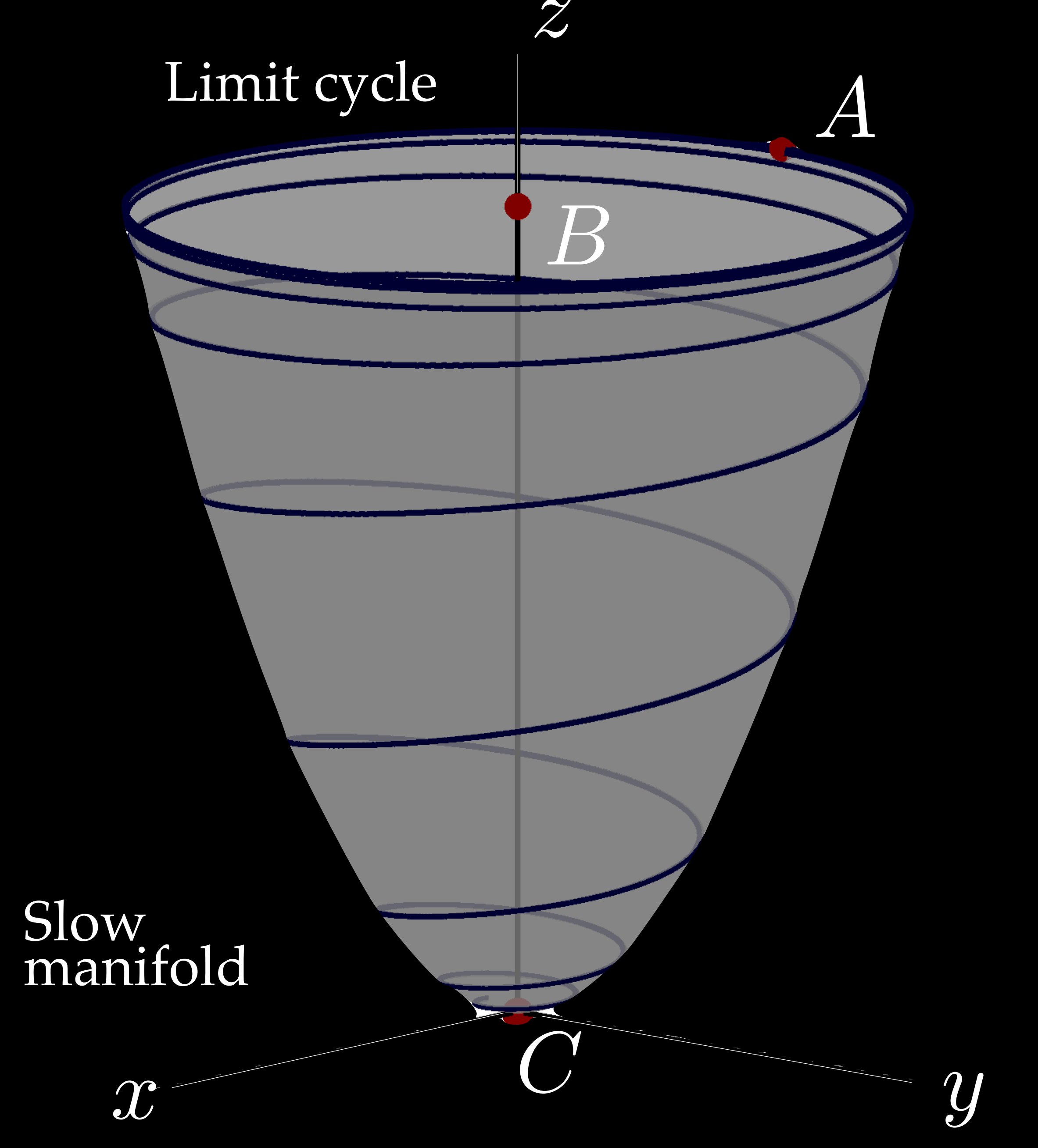
Full System



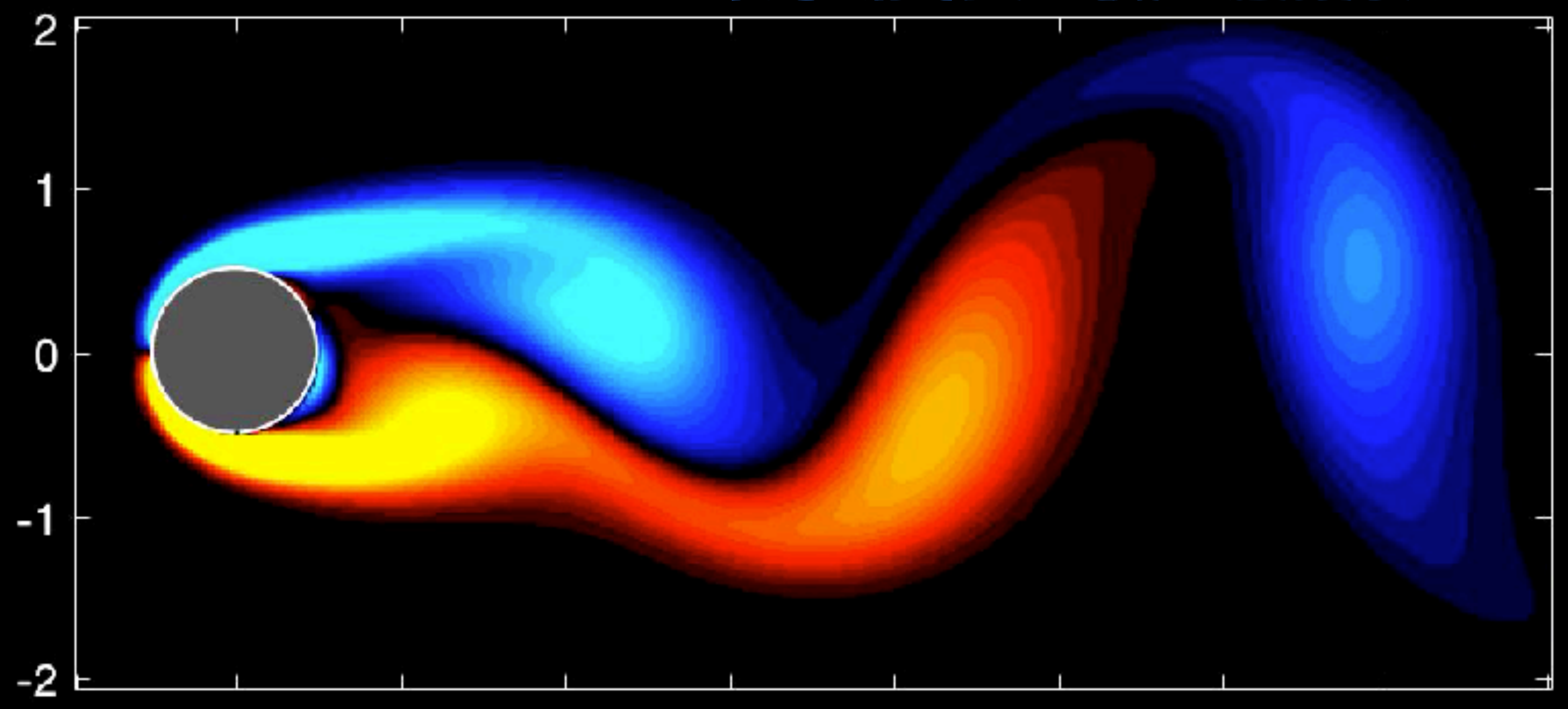
Identified System







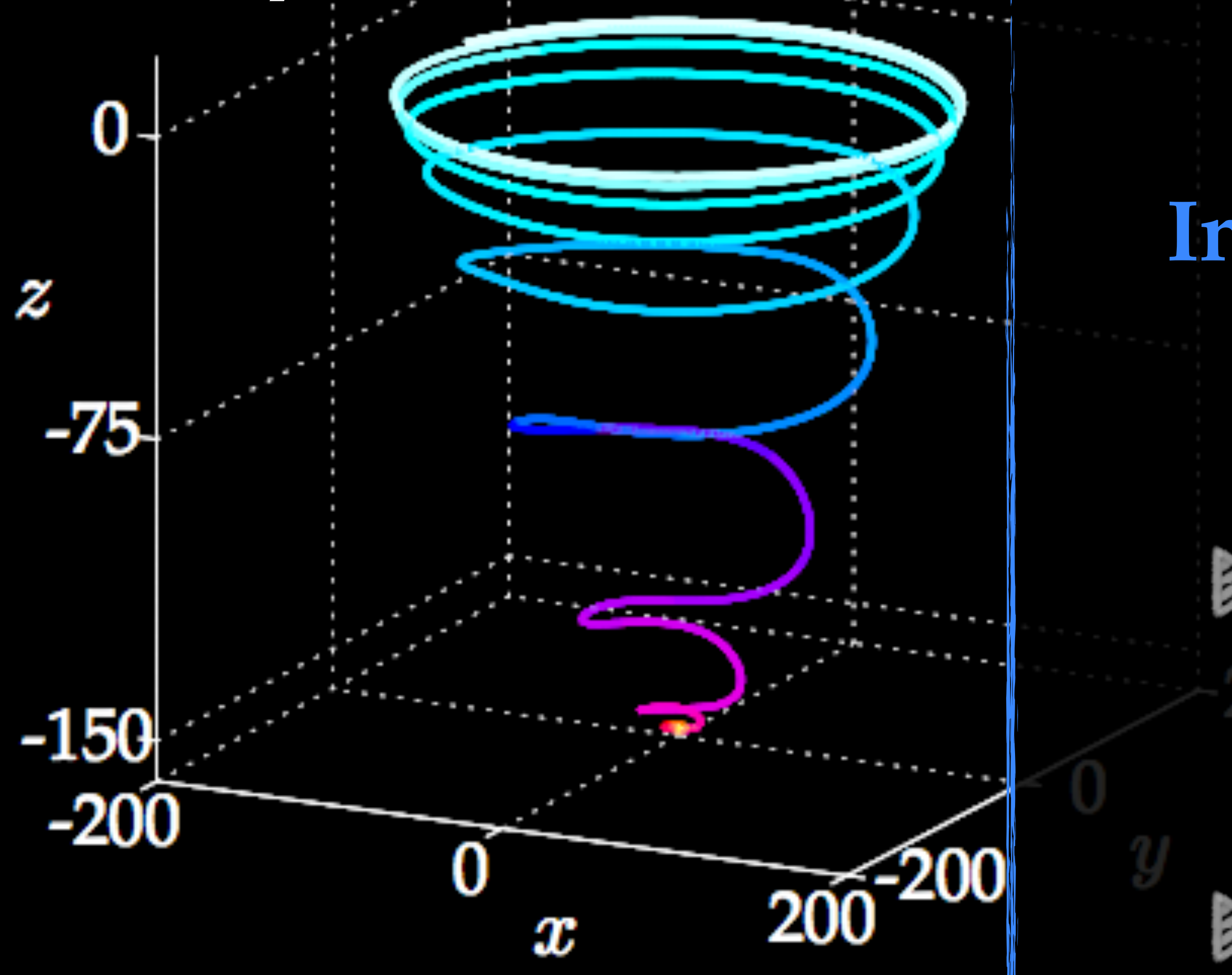
$$\dot{x} = \mu x - \omega y + Axz$$
$$\dot{y} = \omega x + \mu y + Ayz$$
$$\dot{z} = -\lambda(z - x^2 - y^2).$$



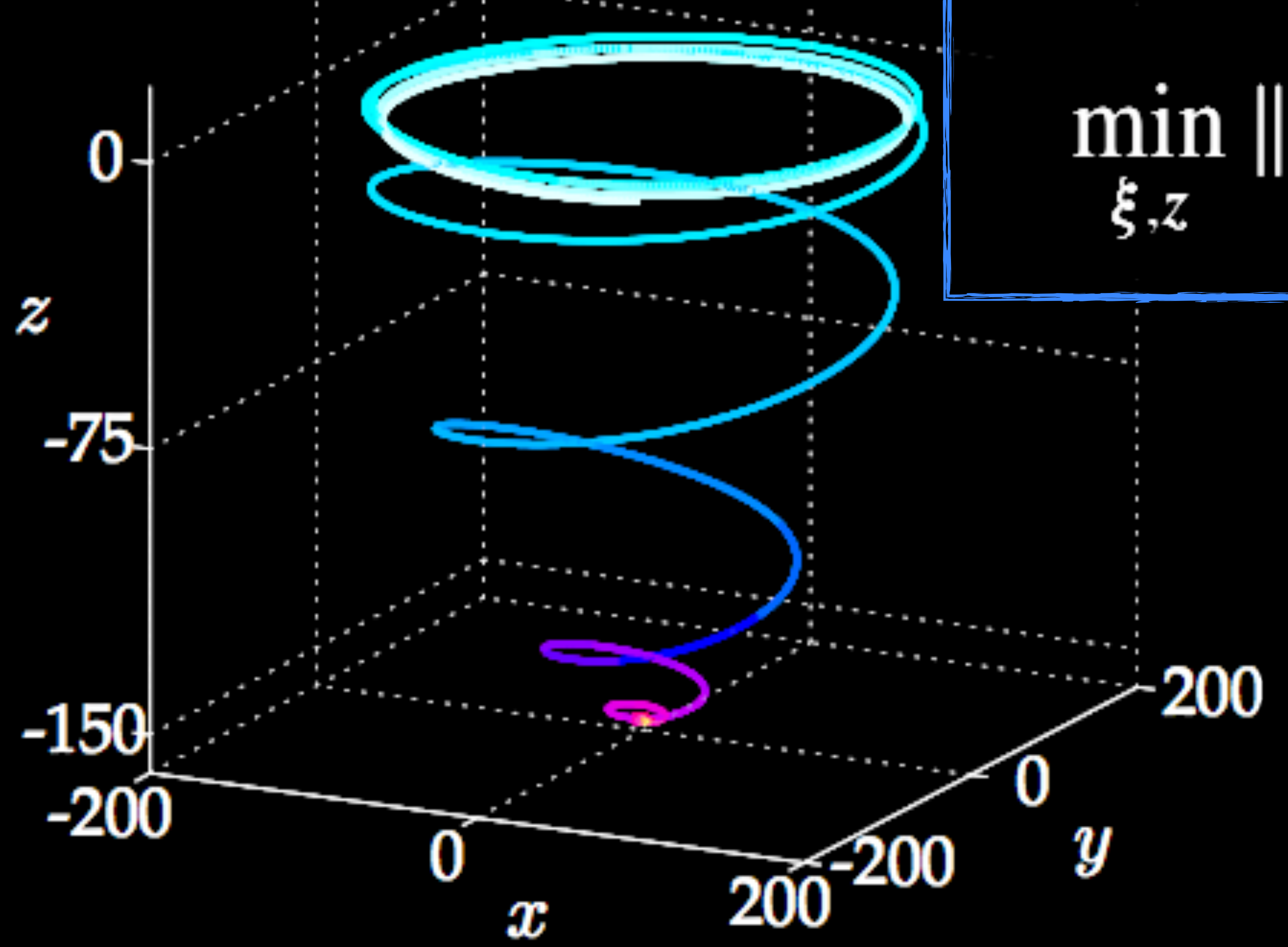
SLB, Proctor, Kutz, *PNAS* 2016.
Loiseau & SLB, *JFM* 838, 2018

Sparse Identification of Nonlinear Dynamics (SINDy)

Full System



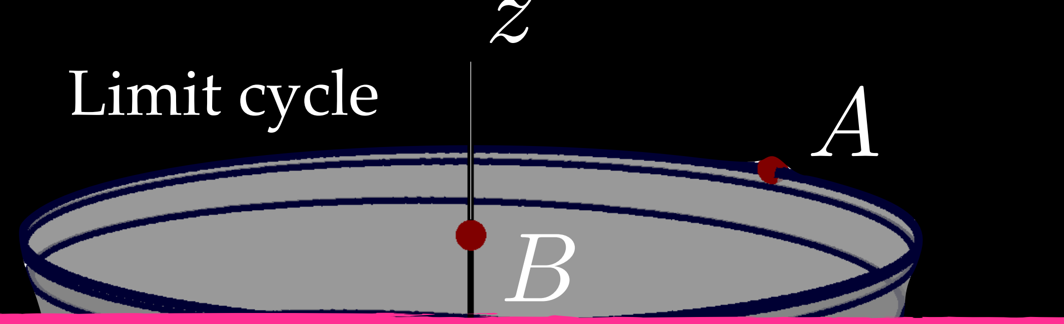
Identified System



Innovation 1: Enforcing known constraints

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

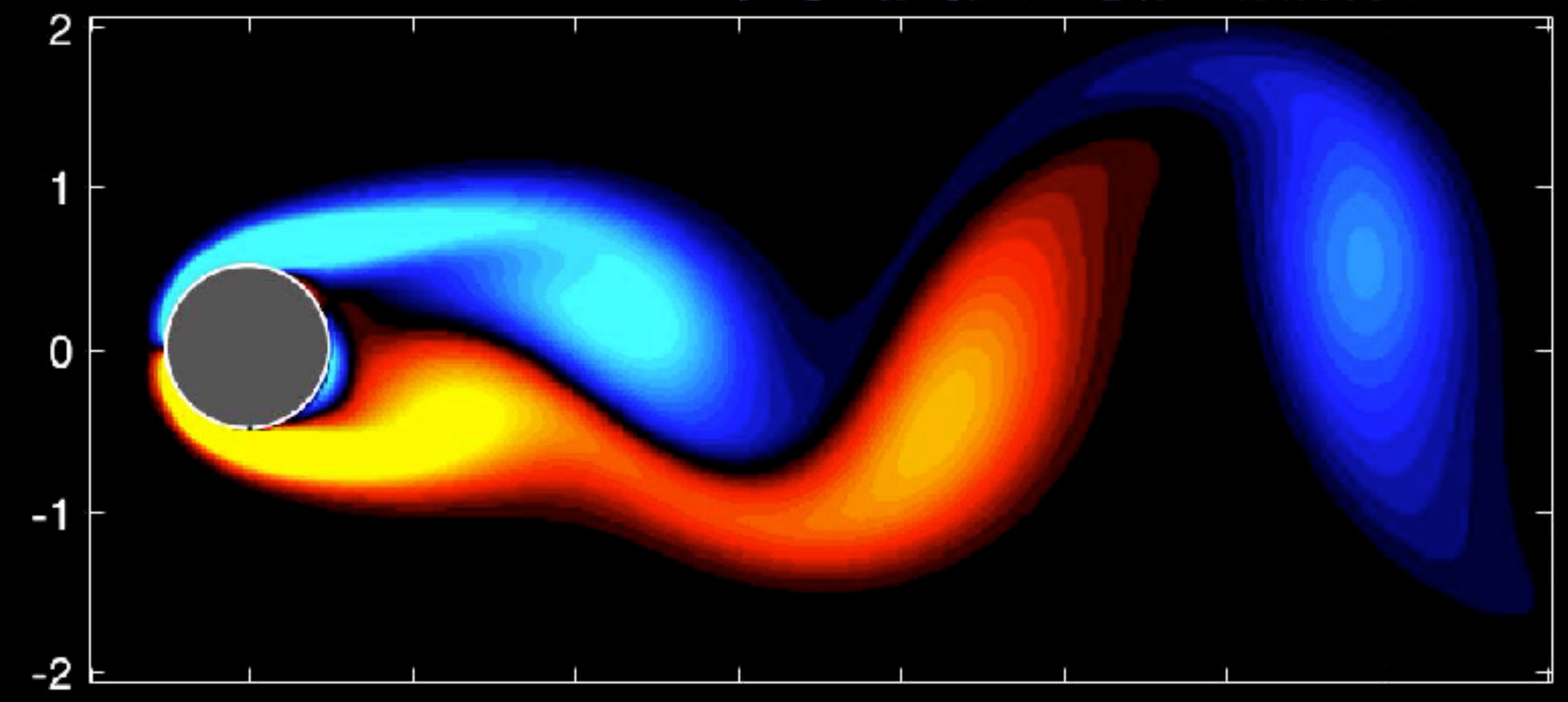
$$\min_{\xi, z} \|\Theta(X)\Xi - \dot{X}\|_2^2 + z^T(C\xi - d)$$



Innovation 2: Higher-order Nonlinearities

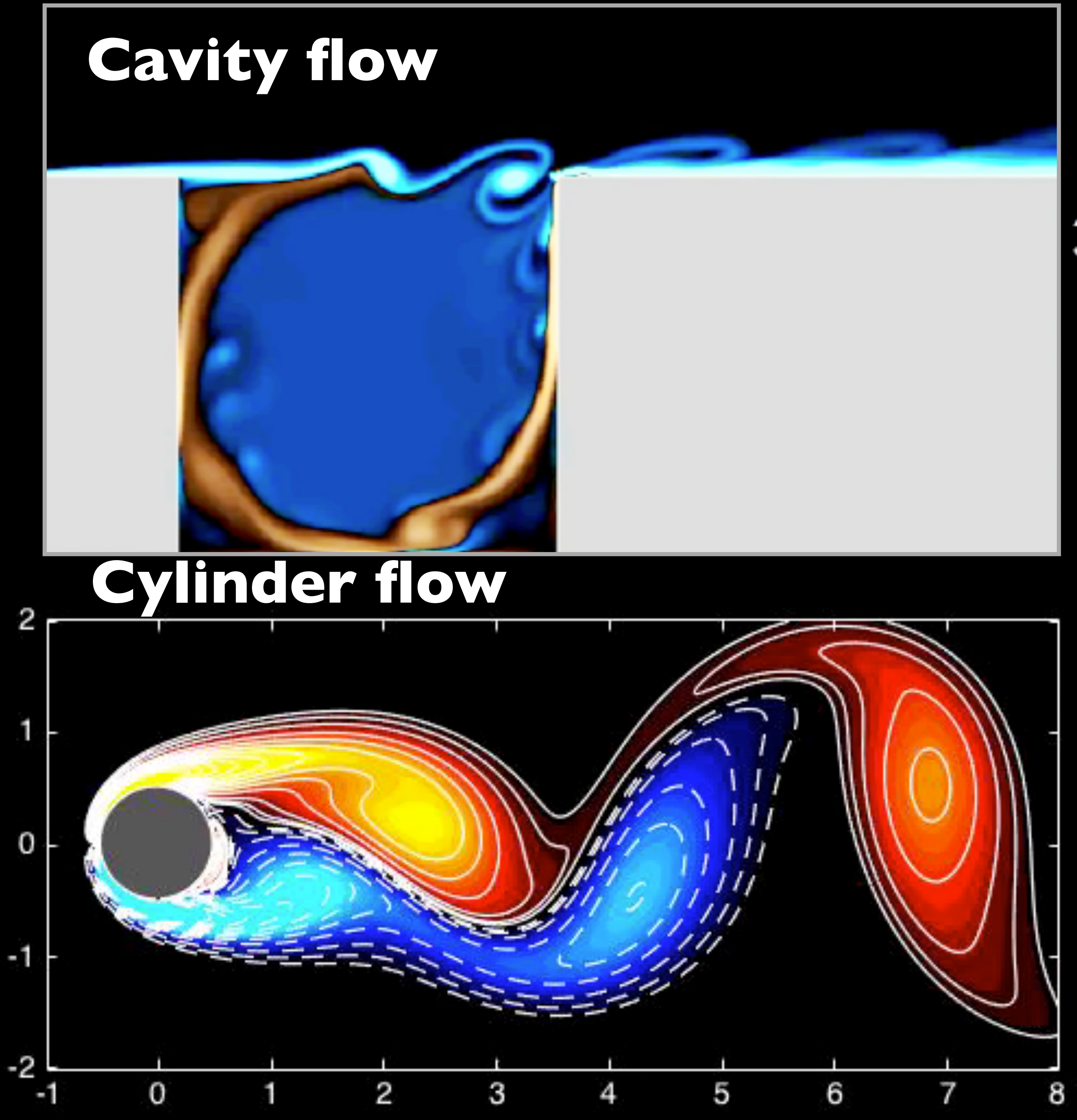
- Cubic, Quintic, Septic terms approximate truncated terms in Galerkin expansion

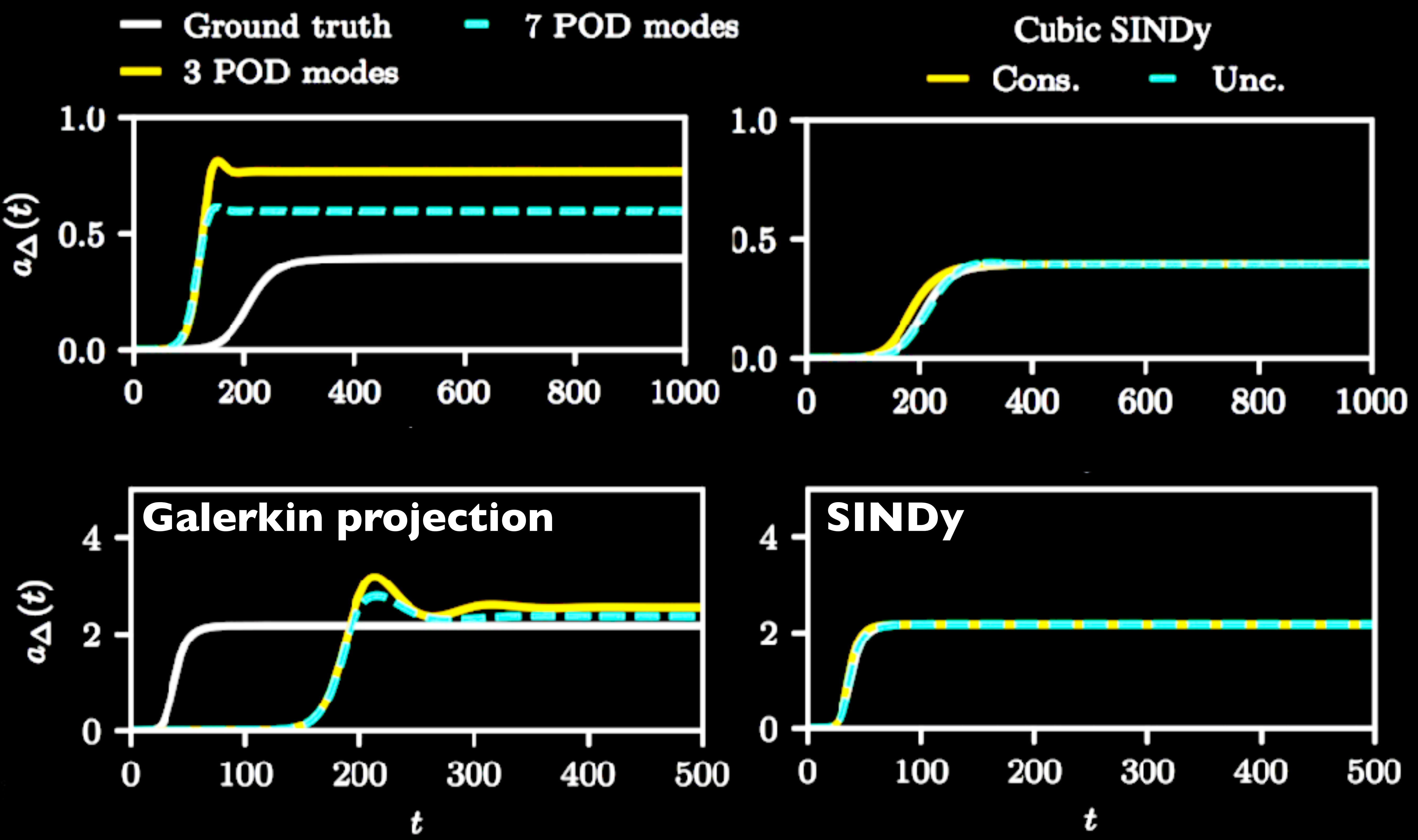
$$\begin{aligned}
\dot{x} &= \mu x - \omega y + Axz \\
\dot{y} &= \omega x + \mu y + Ayz \\
\dot{z} &= -\lambda(z - x^2 - y^2).
\end{aligned}$$



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

Constrained Sparse Galerkin Regression



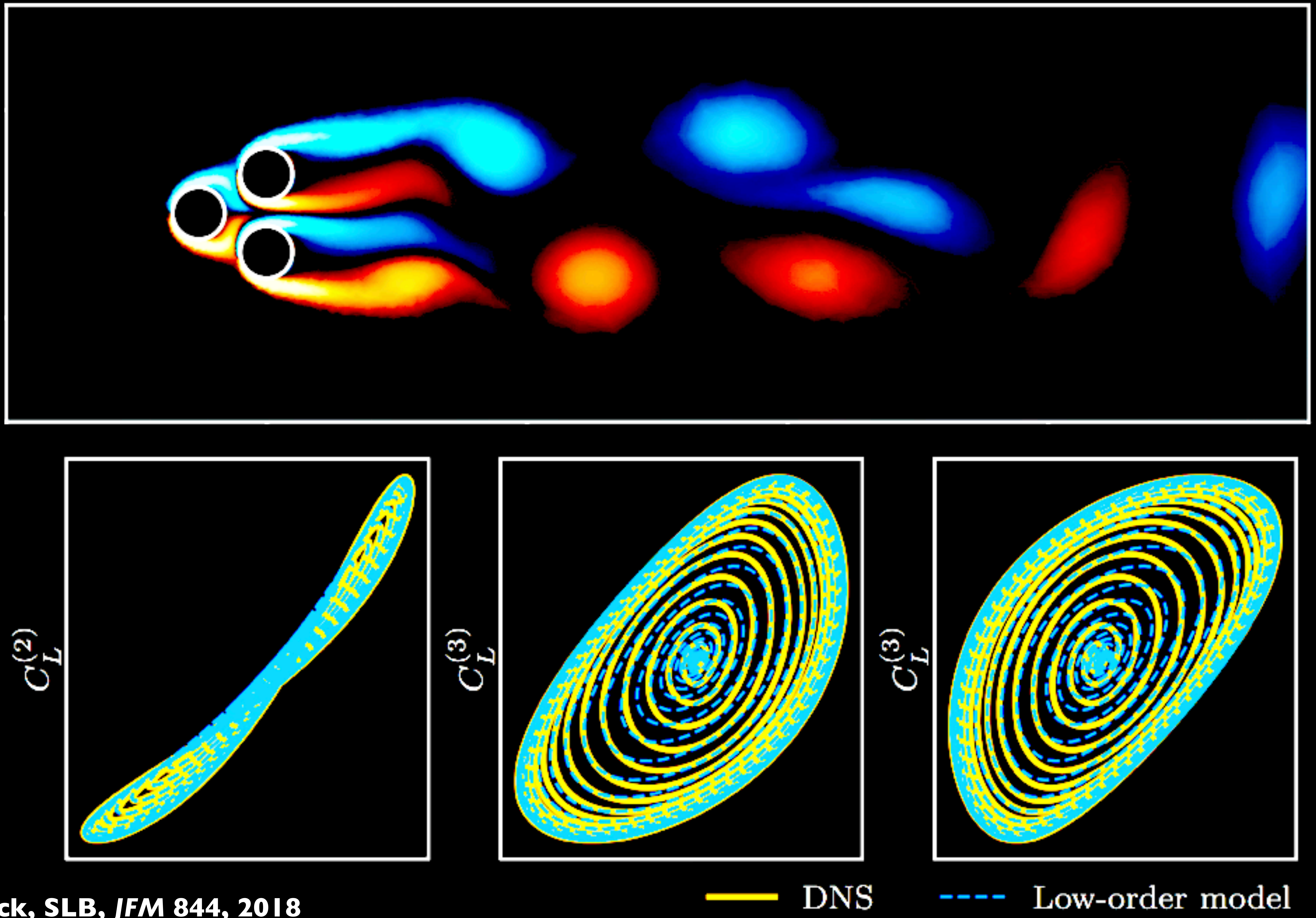


$$\ddot{x} - \underbrace{\left(0.2 - 0.24x^2 - 0.15\dot{x}^2\right)}_{k(x,\dot{x})}\dot{x} + 1.26x = 0$$

Spring-Mass Damper with Nonlinear Damping!

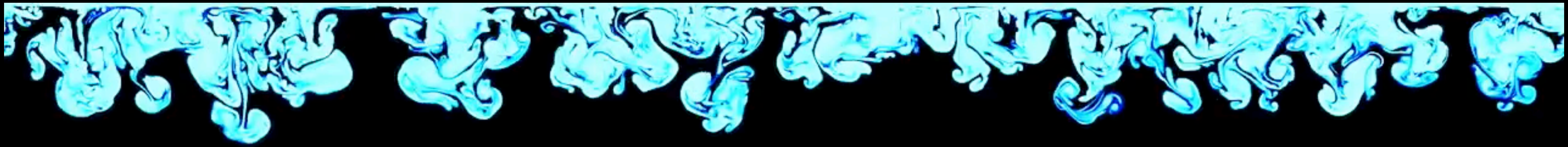
Loiseau & SLB, *JFM* 838, 2018

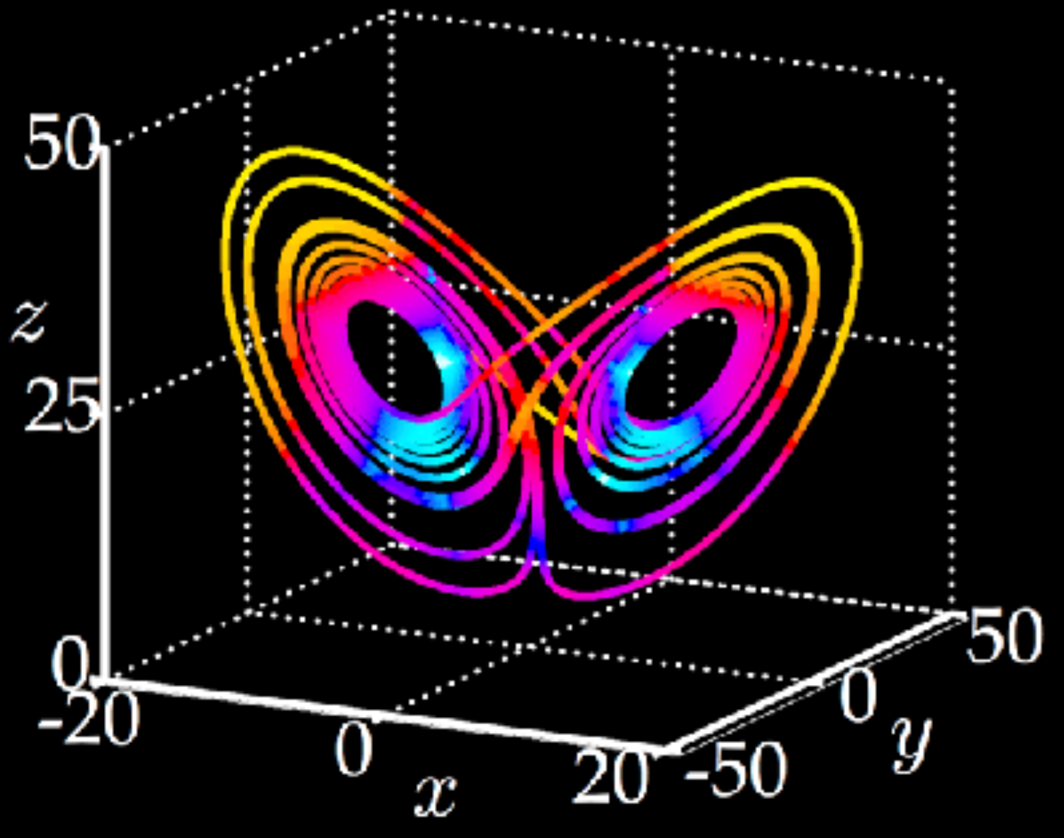
More Complex Flow: Fluidic Pinball



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

Chaotic Thermal Convection



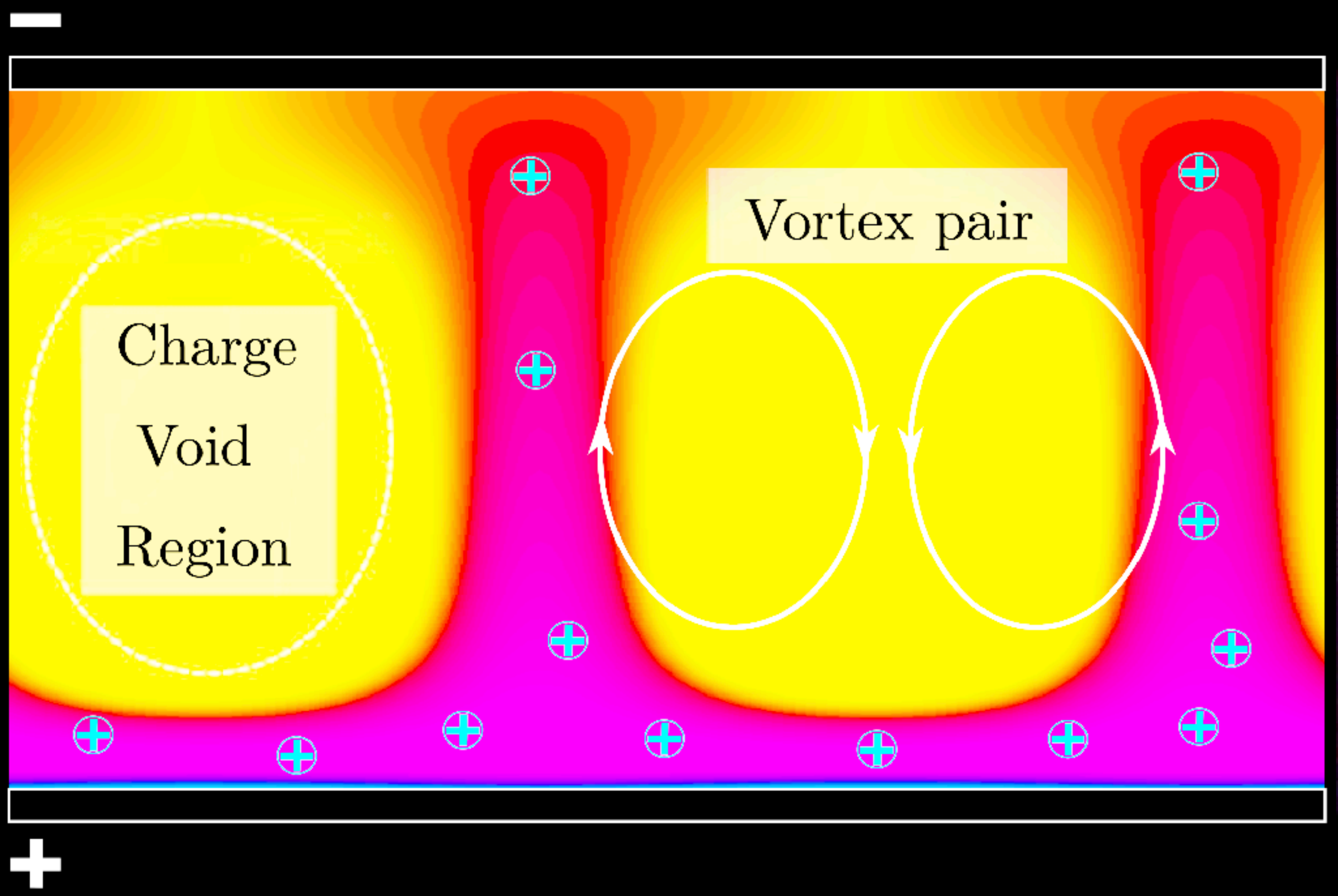


$$
\begin{aligned}
\dot{x} &= \sigma(y - x) \\
\dot{y} &= x(\rho - z) - y \\
\dot{z} &= xy - \beta z.
\end{aligned}
$$

YouTube: turbulenceteam

Lorenz, Fetter, Hamilton, 1963

CHAOTIC ELECTROCONVECTION



Three way coupling:

- **Fluid flow**
- **Charge density**
- **Electric field**

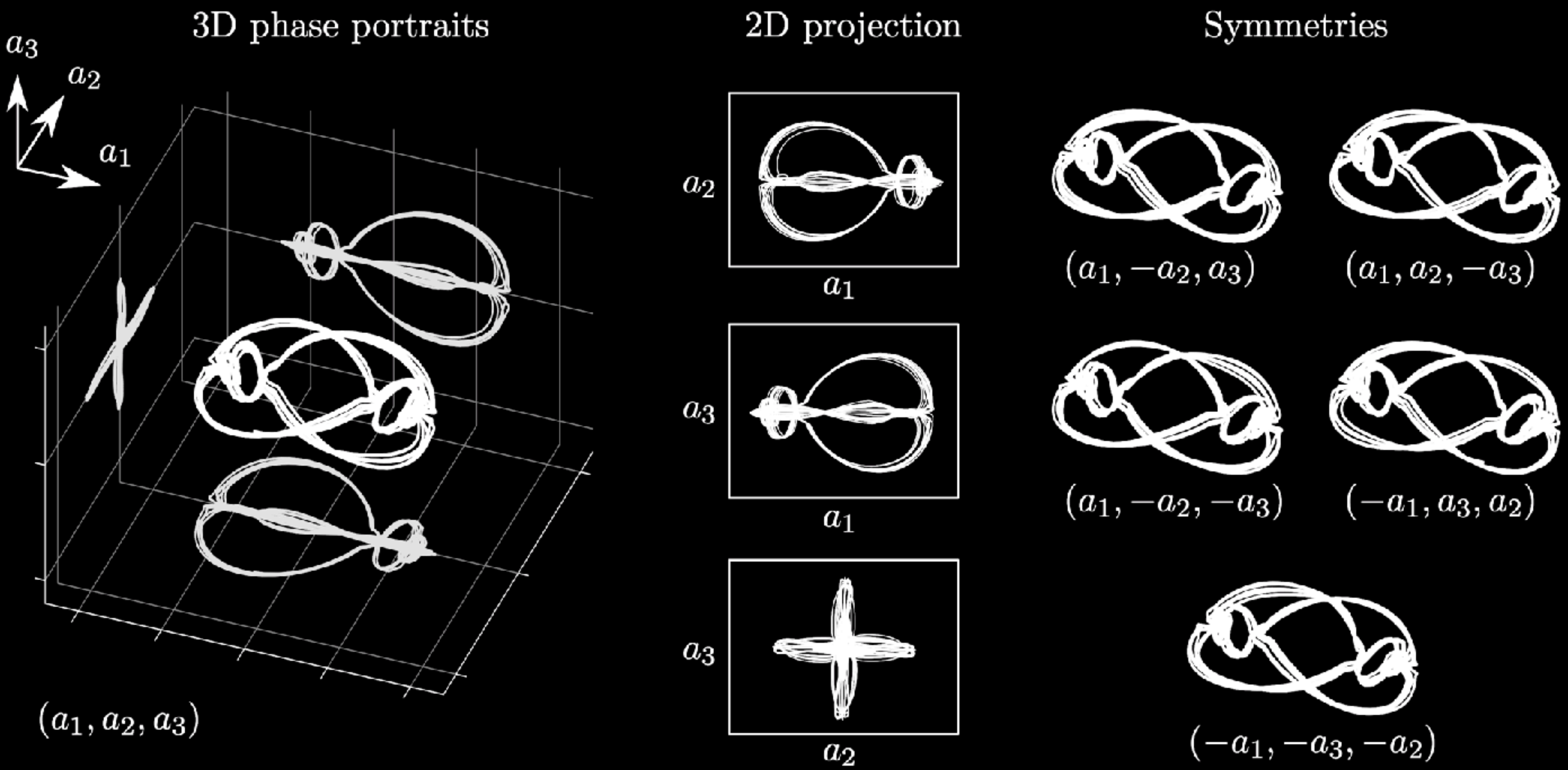
$$\begin{aligned}
\nabla \cdot \mathbf{u}^* &= 0 \\
\rho \frac{D\mathbf{u}^*}{Dt^*} &= -\nabla P^* + \mu \nabla^2 \mathbf{u}^* - \rho_c^* \nabla \phi^* \\
\frac{\partial \rho_c^*}{\partial t^*} &= -\nabla \cdot [(\mathbf{u}^* - \mu_b \nabla \phi^*)\rho_c^* - D_c \nabla \rho_c^*] \\
\nabla^2 \phi^* &= -\frac{\rho_c^*}{\epsilon}
\end{aligned}$$

Guan, SLB, Novosselov, *arXiv 2020*

CHAOTIC ELECTROCONVECTION

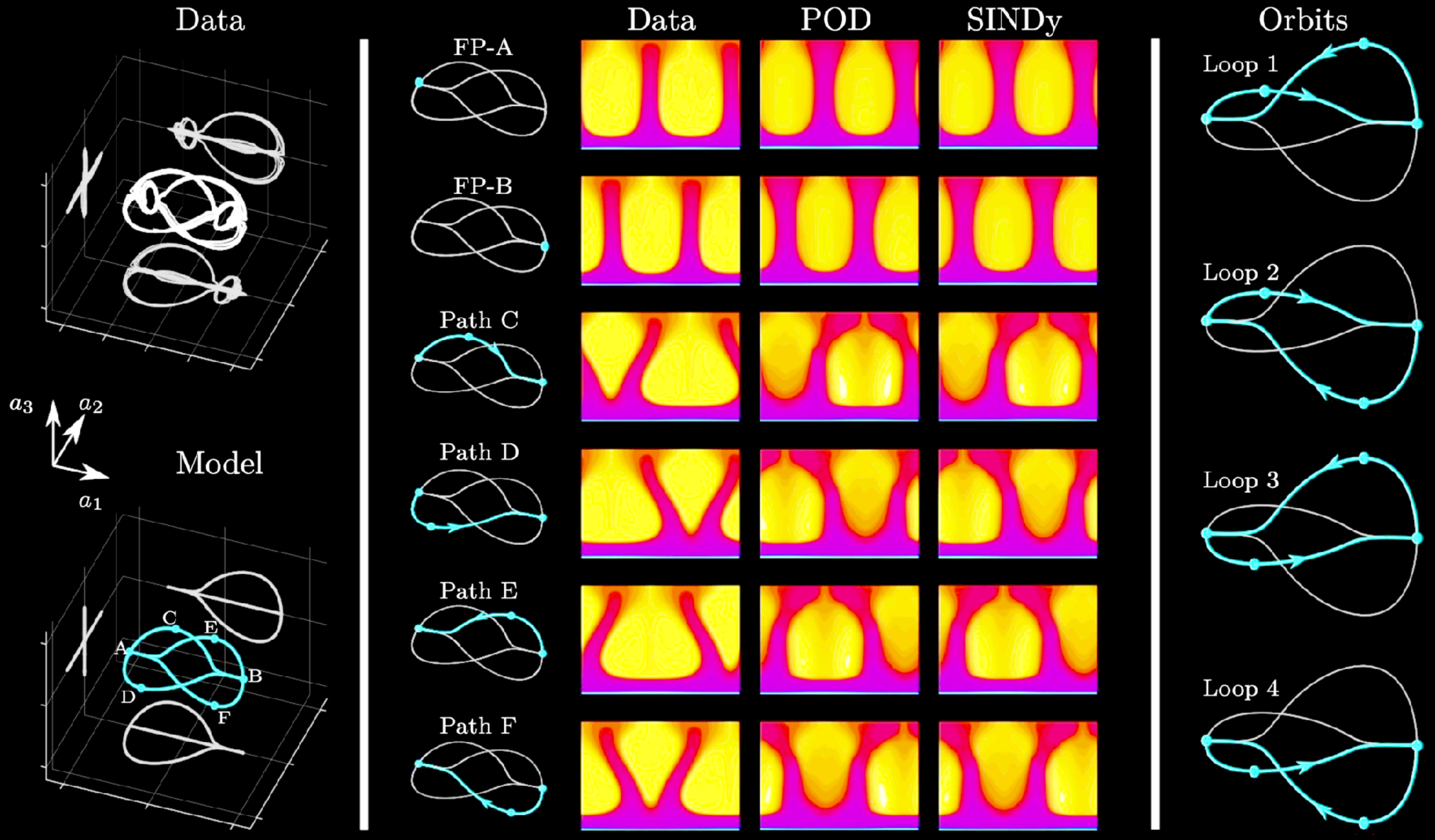
Guan, SLB, Novosselov, *arXiv 2020*

Symmetry in the Data



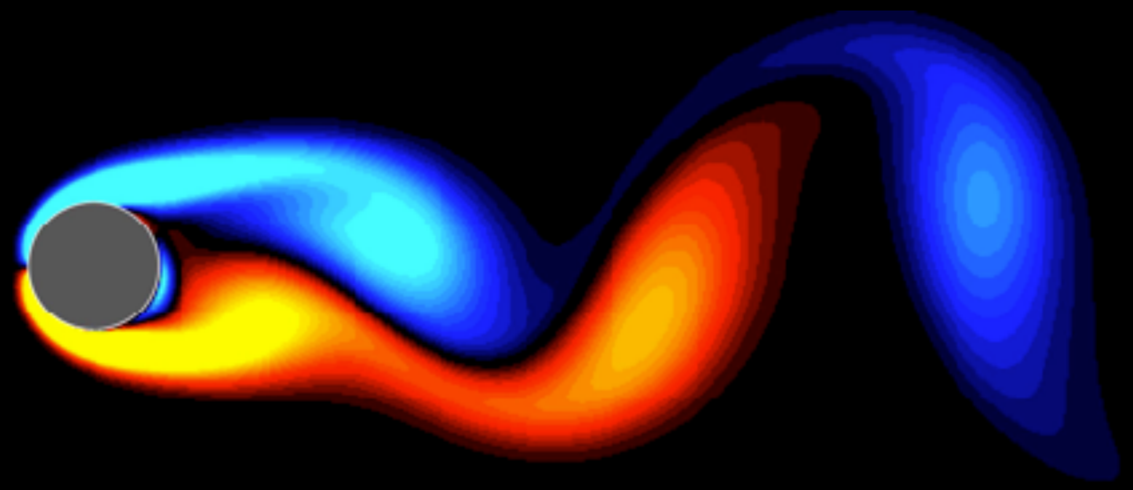
	a_1	a_2	a_3	a_1^2	a_1a_2	a_1a_3	a_2^2	a_2a_3	a_3^2	a_1^3	$a_1^2a_2$	$a_1^2a_3$	$a_1a_2^2$	$a_1a_2a_3$	$a_1a_3^2$	a_2^3	$a_2^2a_3$	$a_2a_3^2$	a_3^3
$\dot{a}_1$	ξ_1						ξ_2		$-\xi_2$	ξ_3			ξ_4		ξ_4				
$\dot{a}_2$		ξ_5			$-\xi_2$						ξ_6					ξ_7		ξ_8	
$\dot{a}_3$			ξ_5			ξ_2						ξ_6					ξ_8		ξ_7

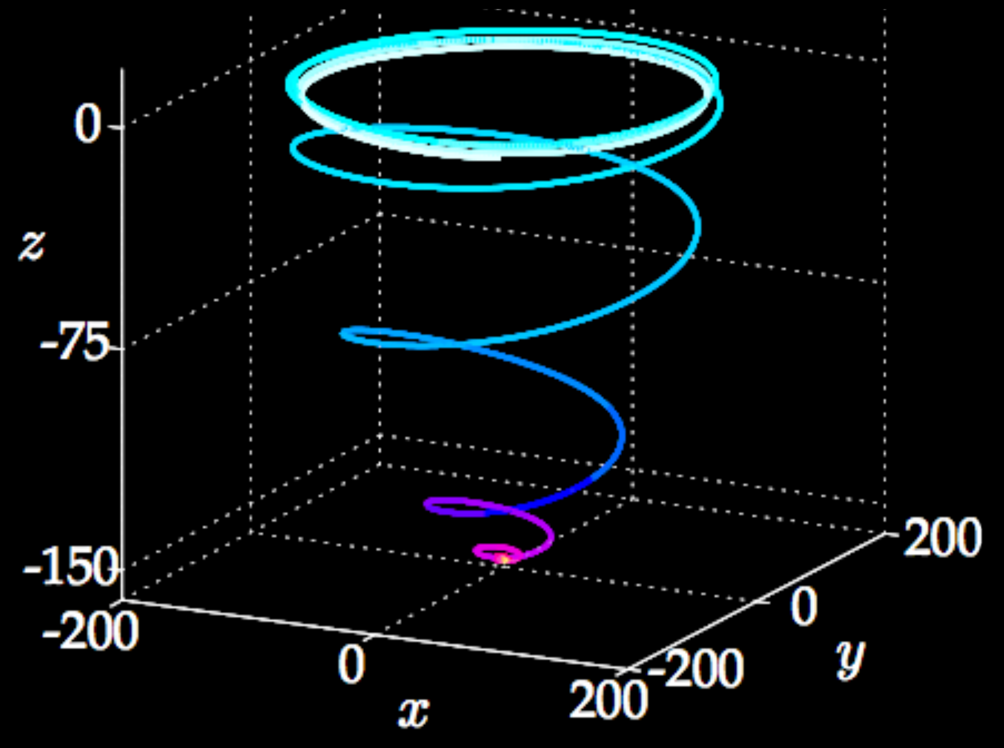
Guan, SLB, Novosselov, *arXiv 2020*

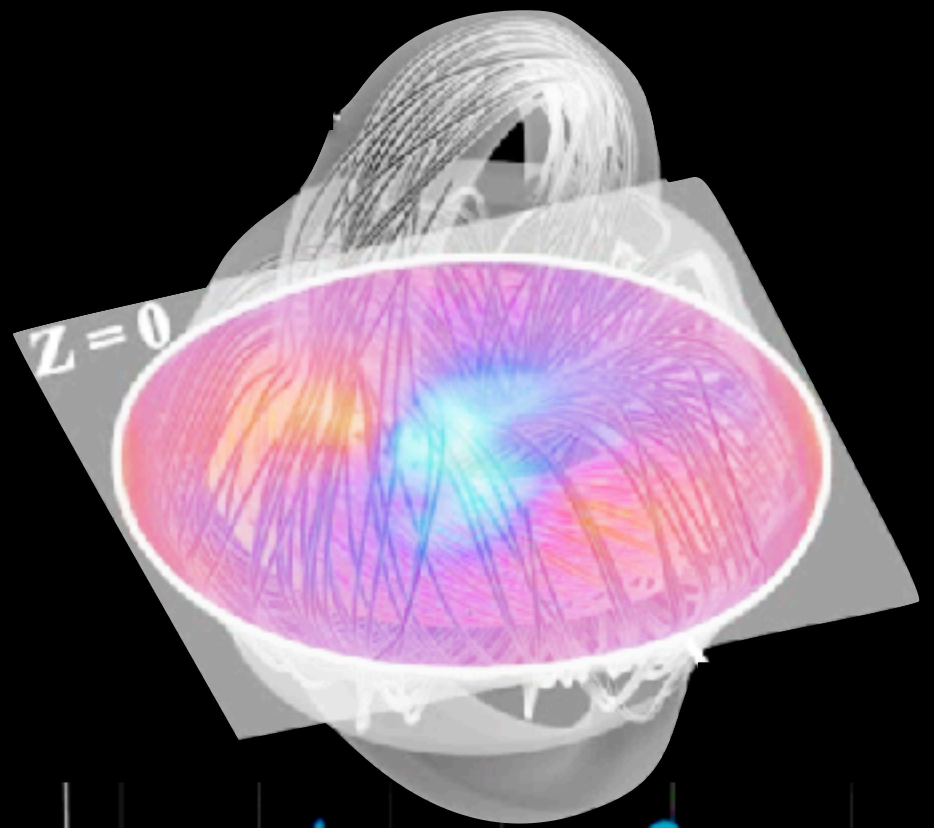


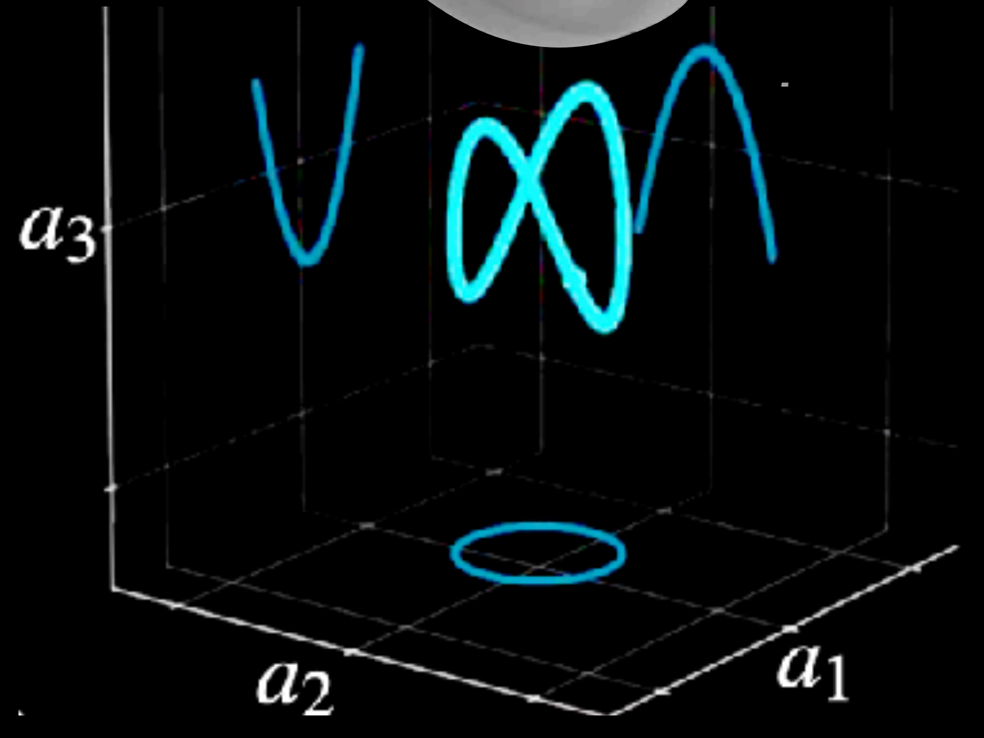
Guan, SLB, Novosselov, *arXiv 2020*

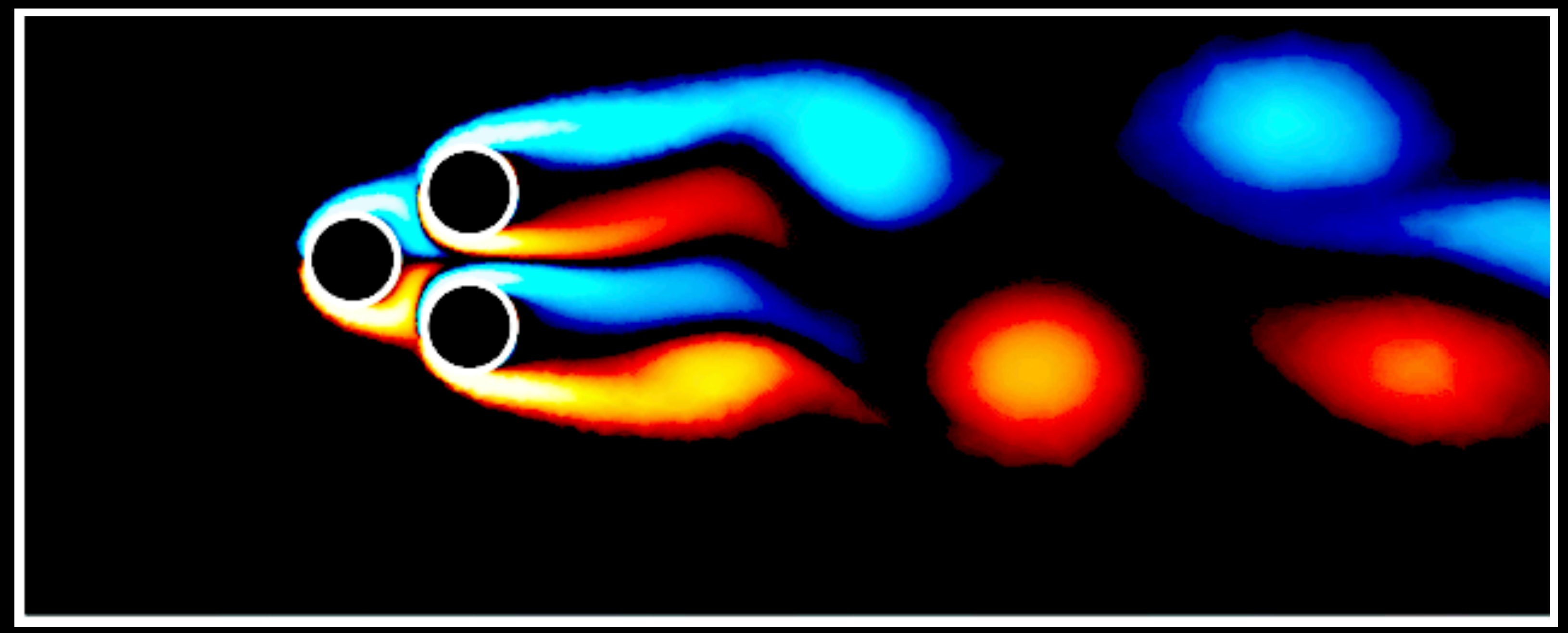
Sparse Nonlinear Models of Fluid Dynamics

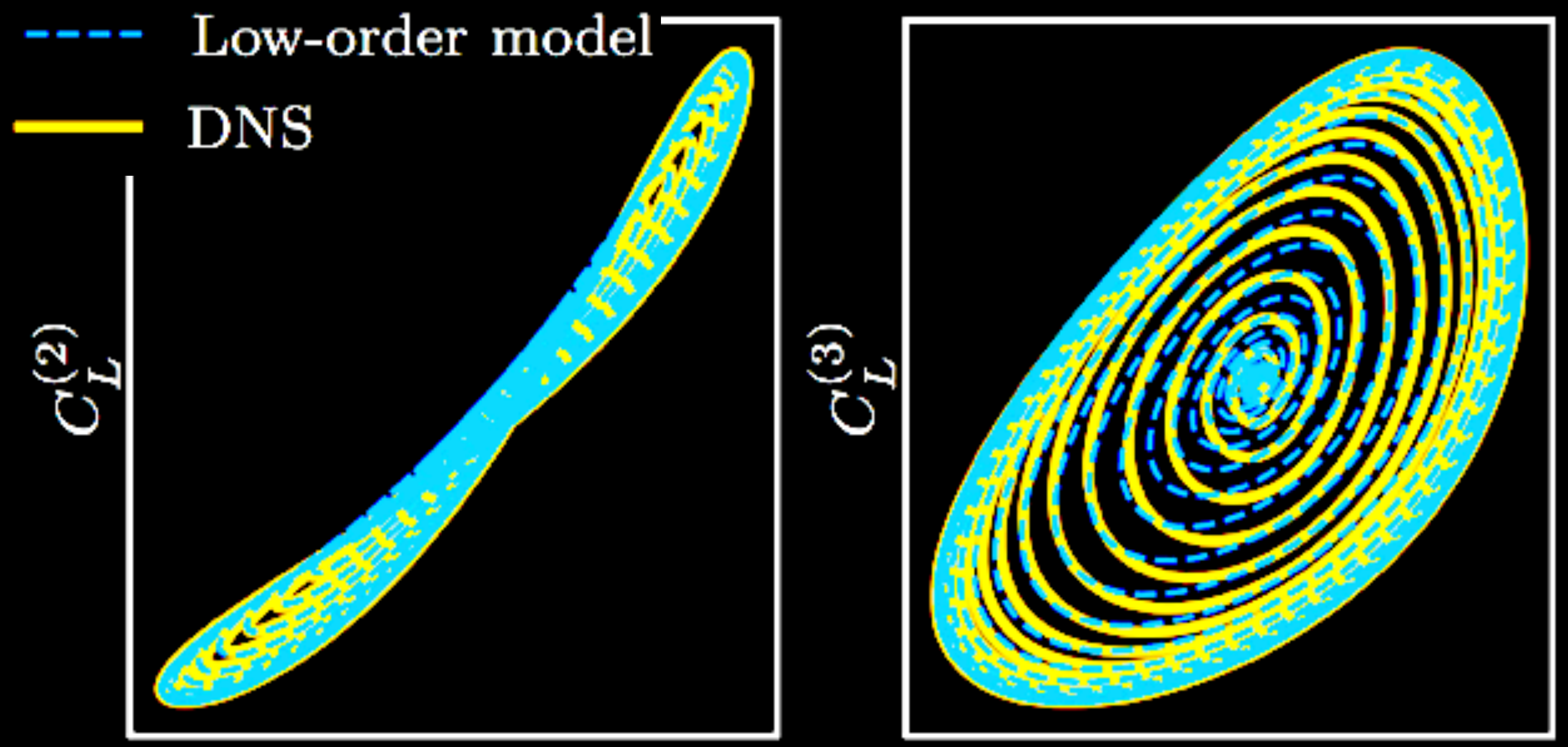


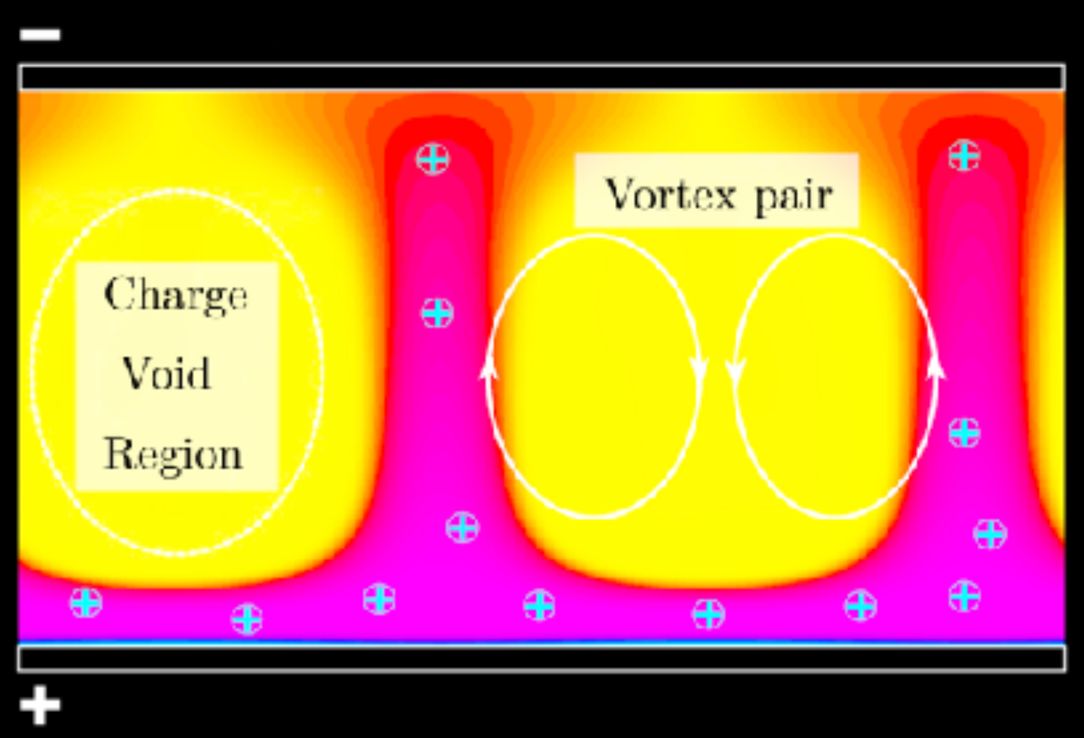


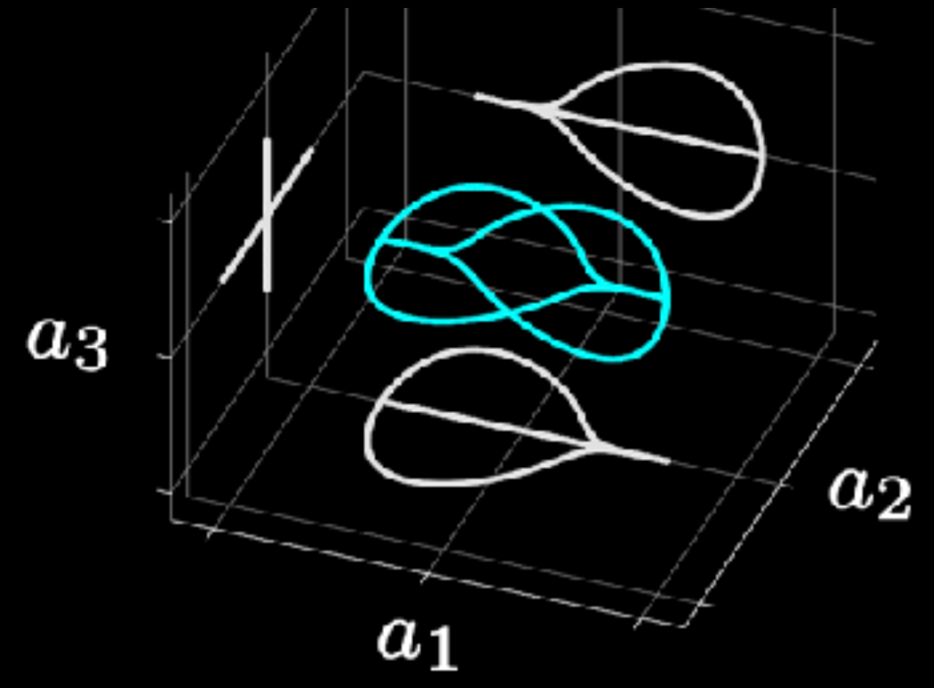




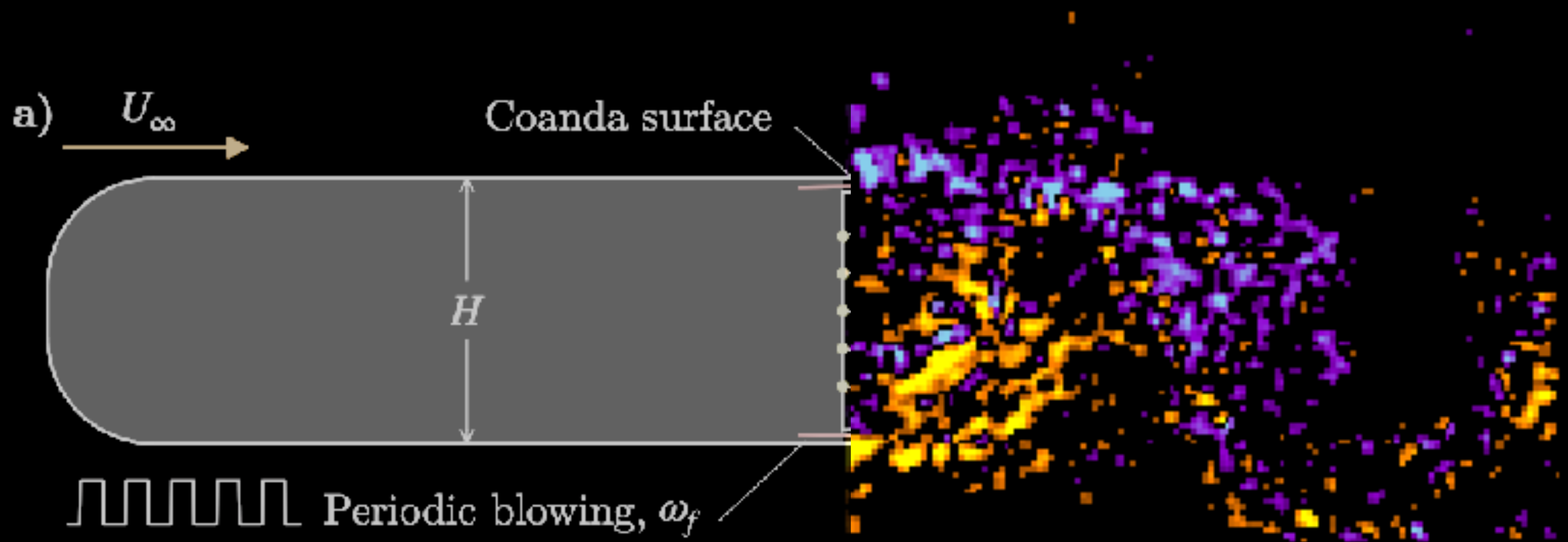


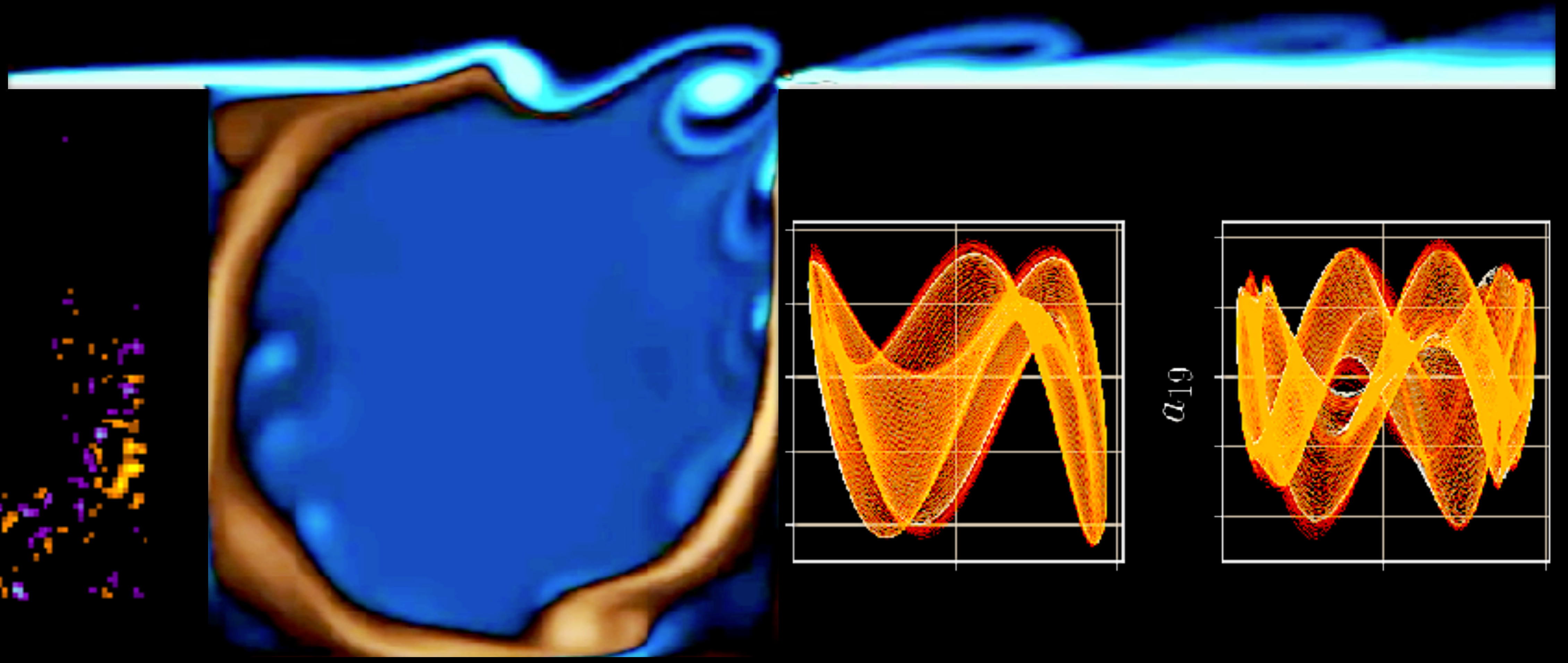




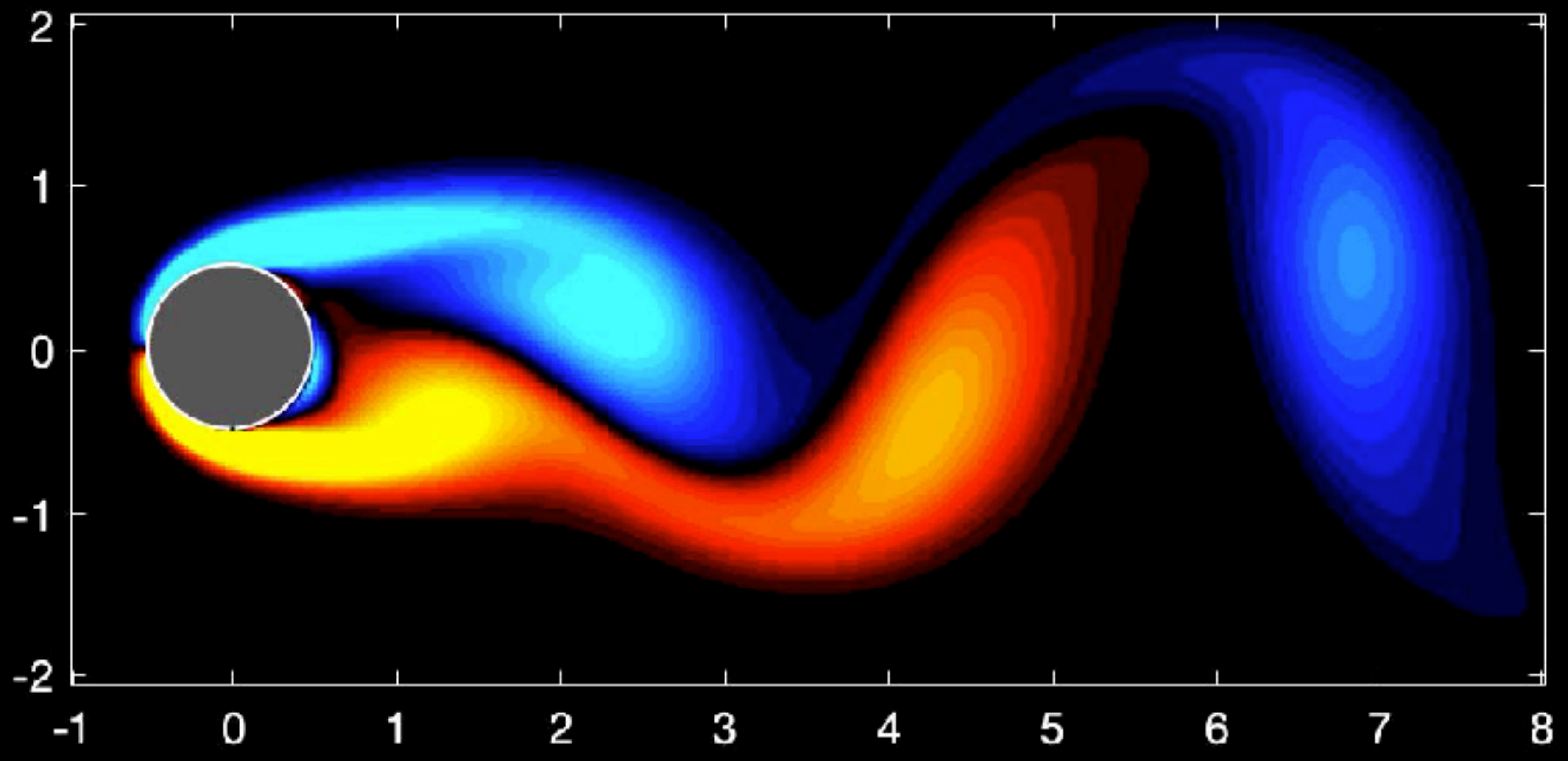


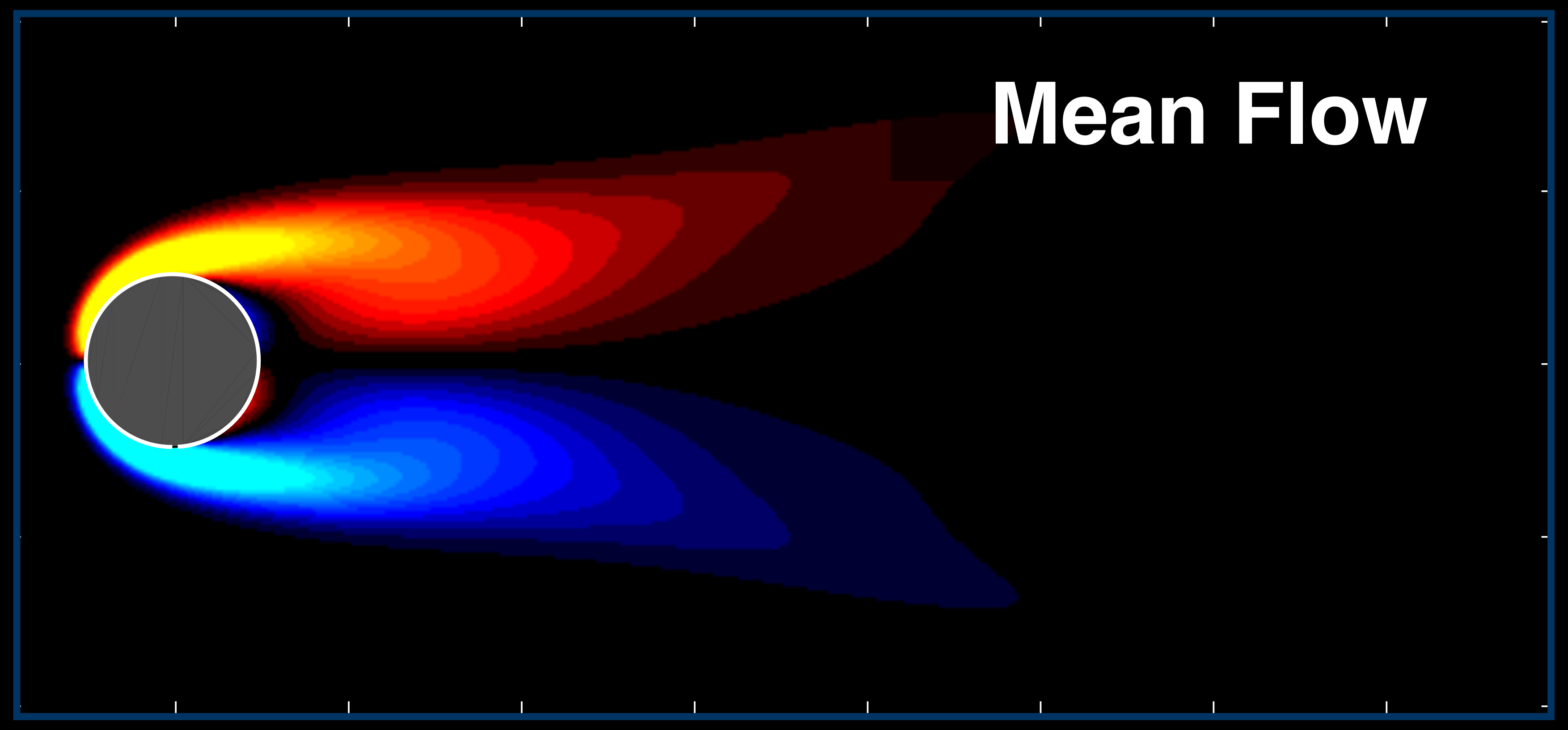
$$\frac{d}{dt}\mathbf{x} = \mathbf{f}(\mathbf{x})$$





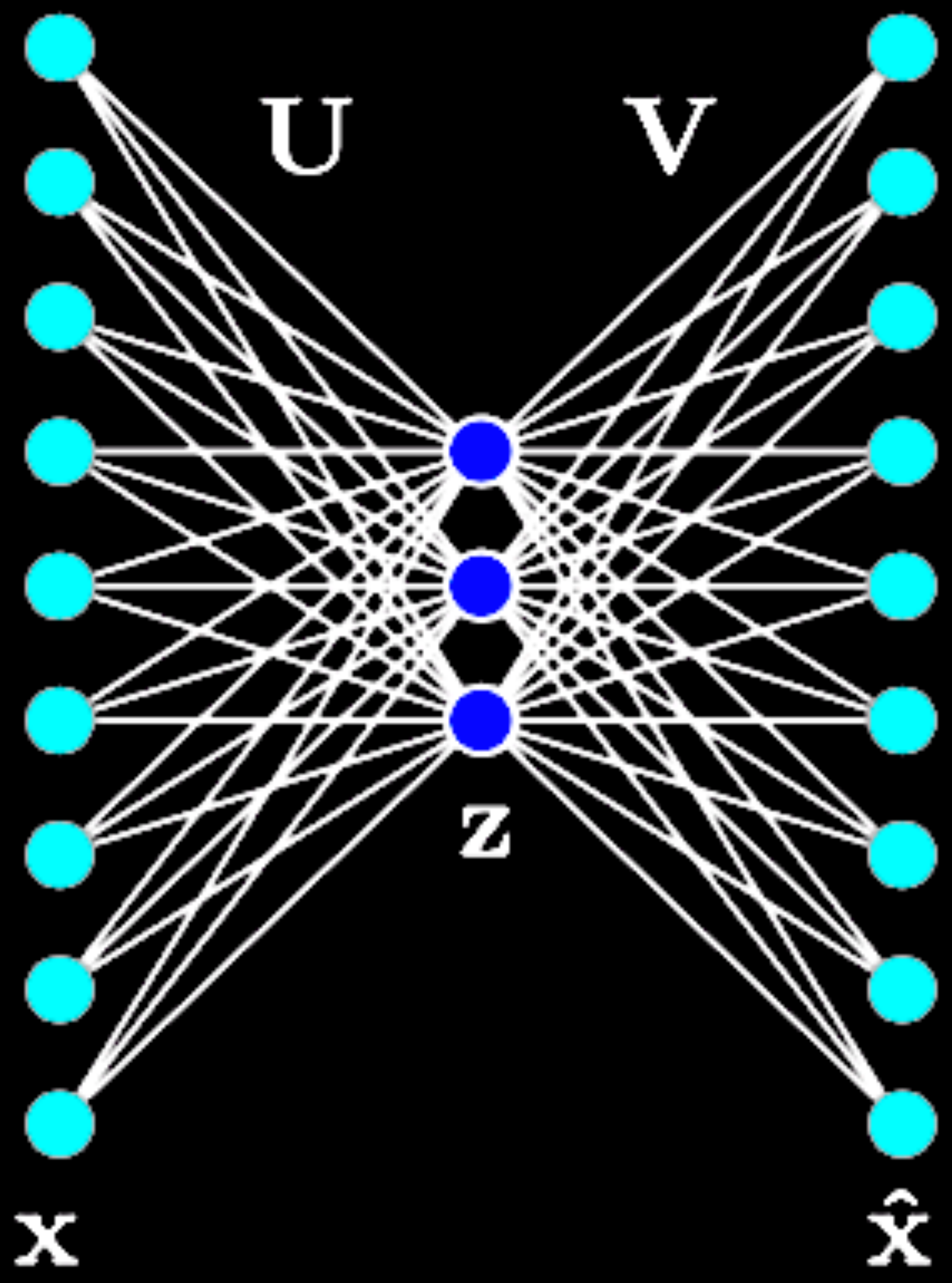
POD
PCA

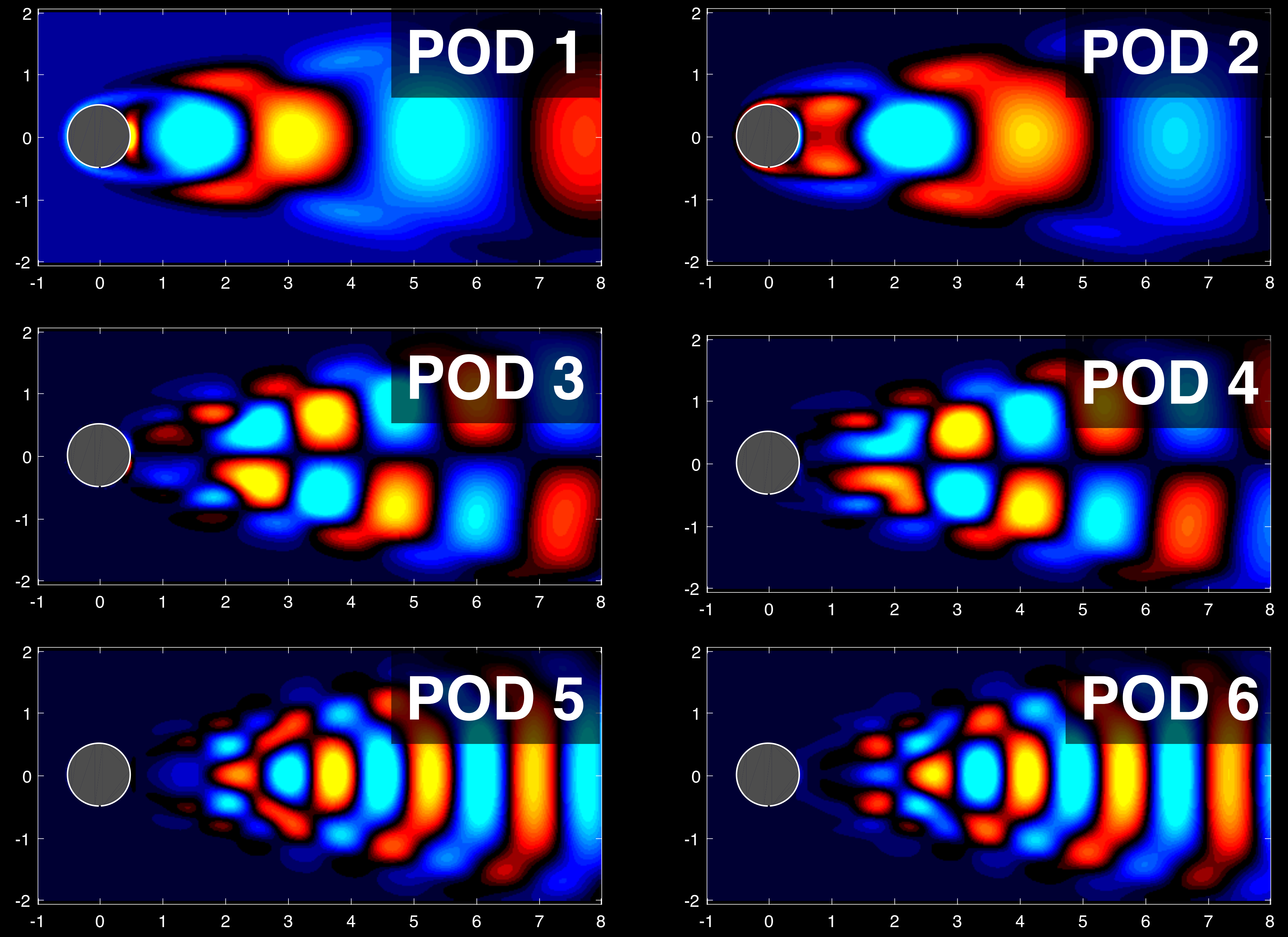




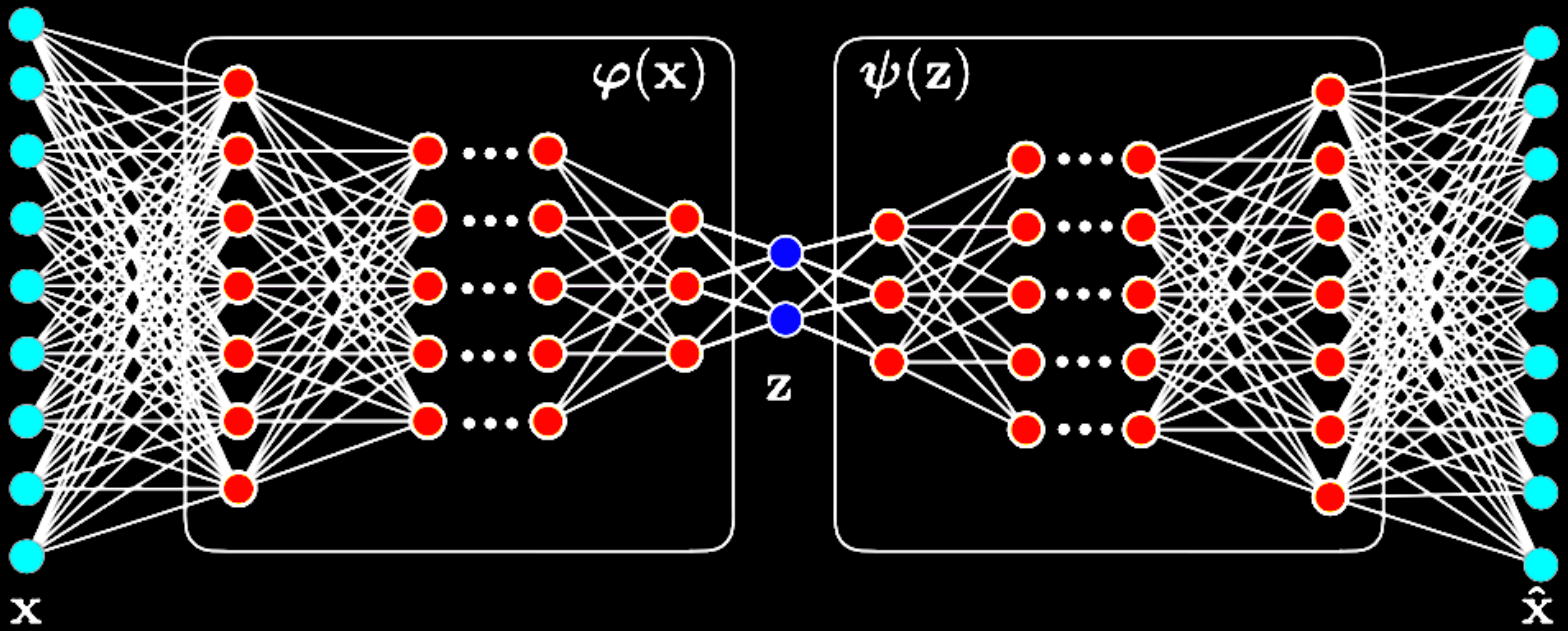
$$\mathbf{u}(\mathbf{x},t) \approx \bar{\mathbf{u}} + \sum_{k=1}^{r} \boldsymbol{\varphi}_k(\mathbf{x})\mathbf{a}_k(t)$$

Autoencoder (Shallow, linear)

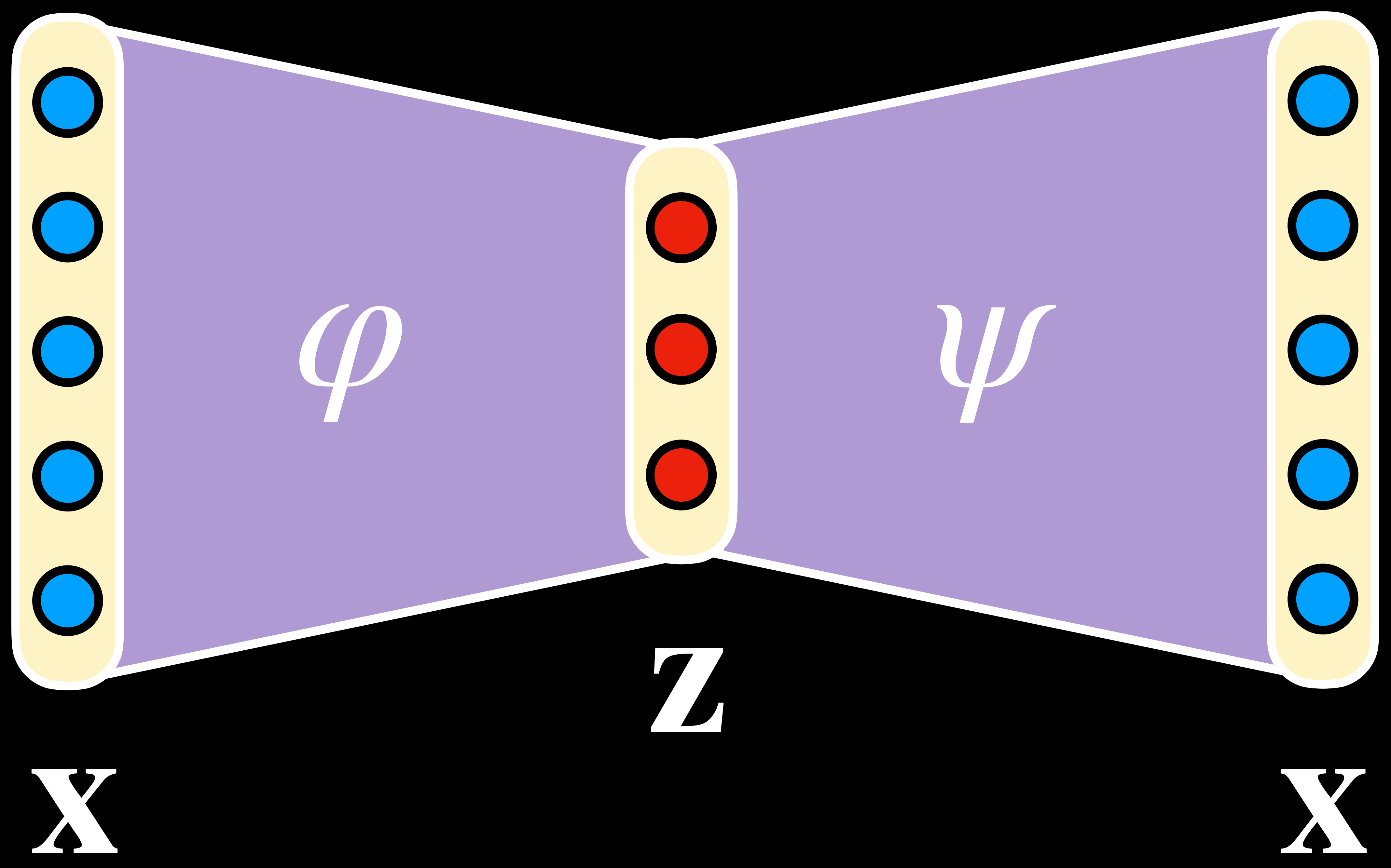




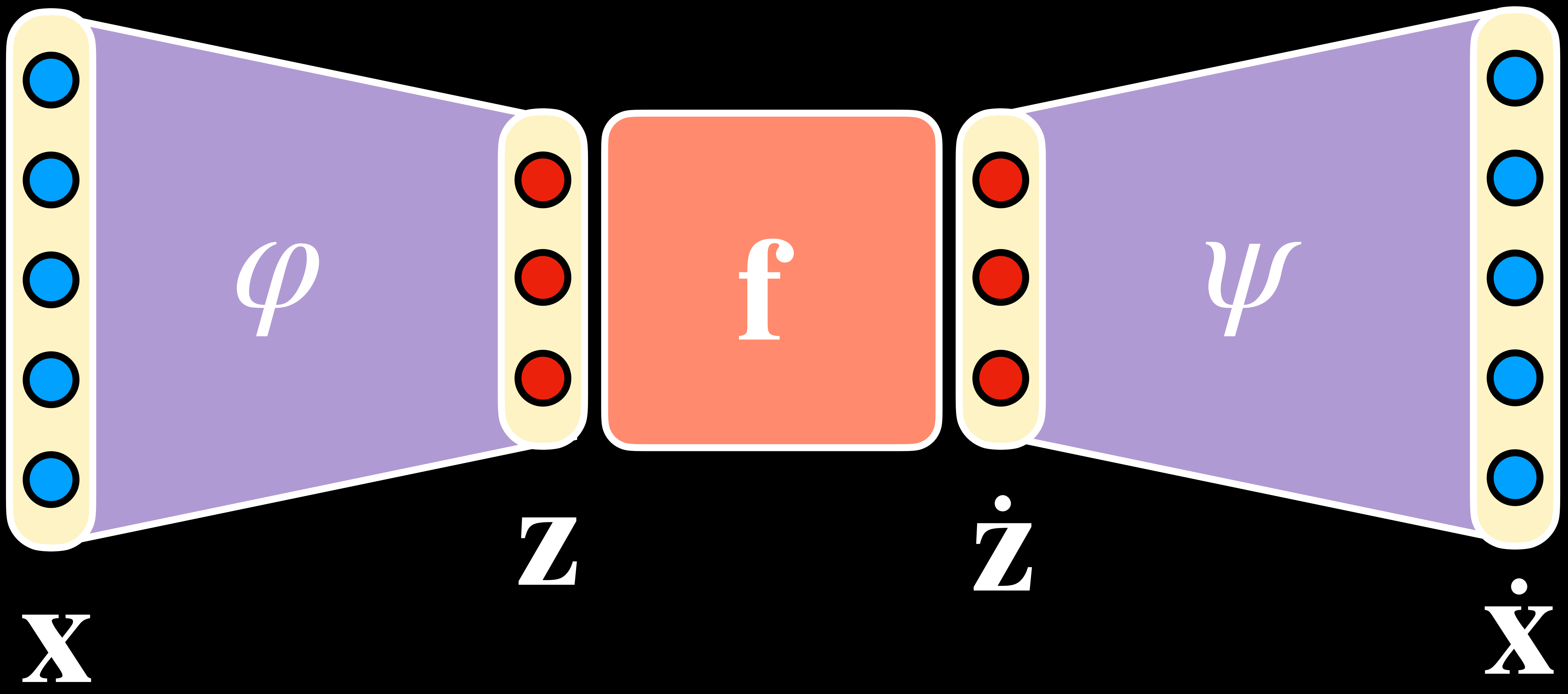
Deep Autoencoders



Deep Autoencoders



Deep Autoencoders for Dynamics



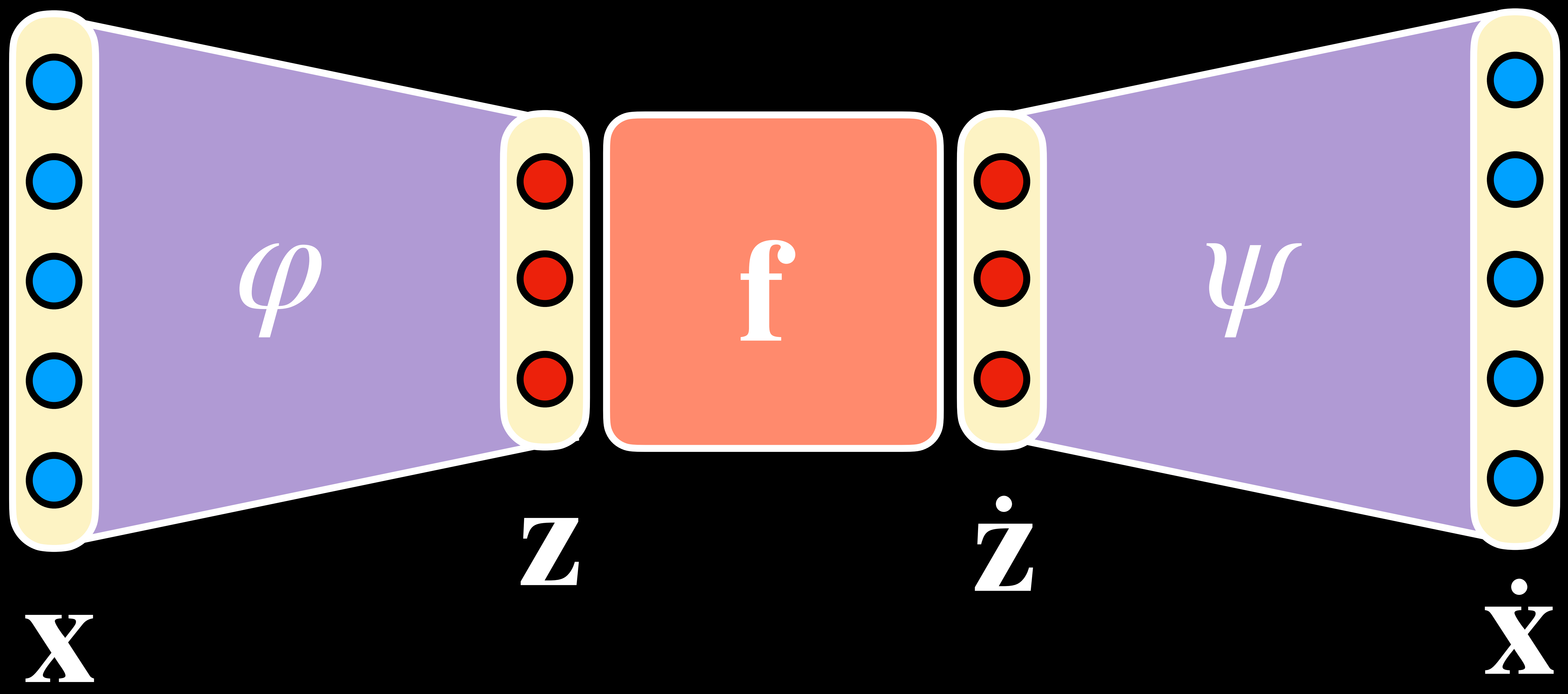
$$\frac{d}{dt}\mathbf{z} = \mathbf{f}(\mathbf{z})$$

Heliocentrism

Geocentrism

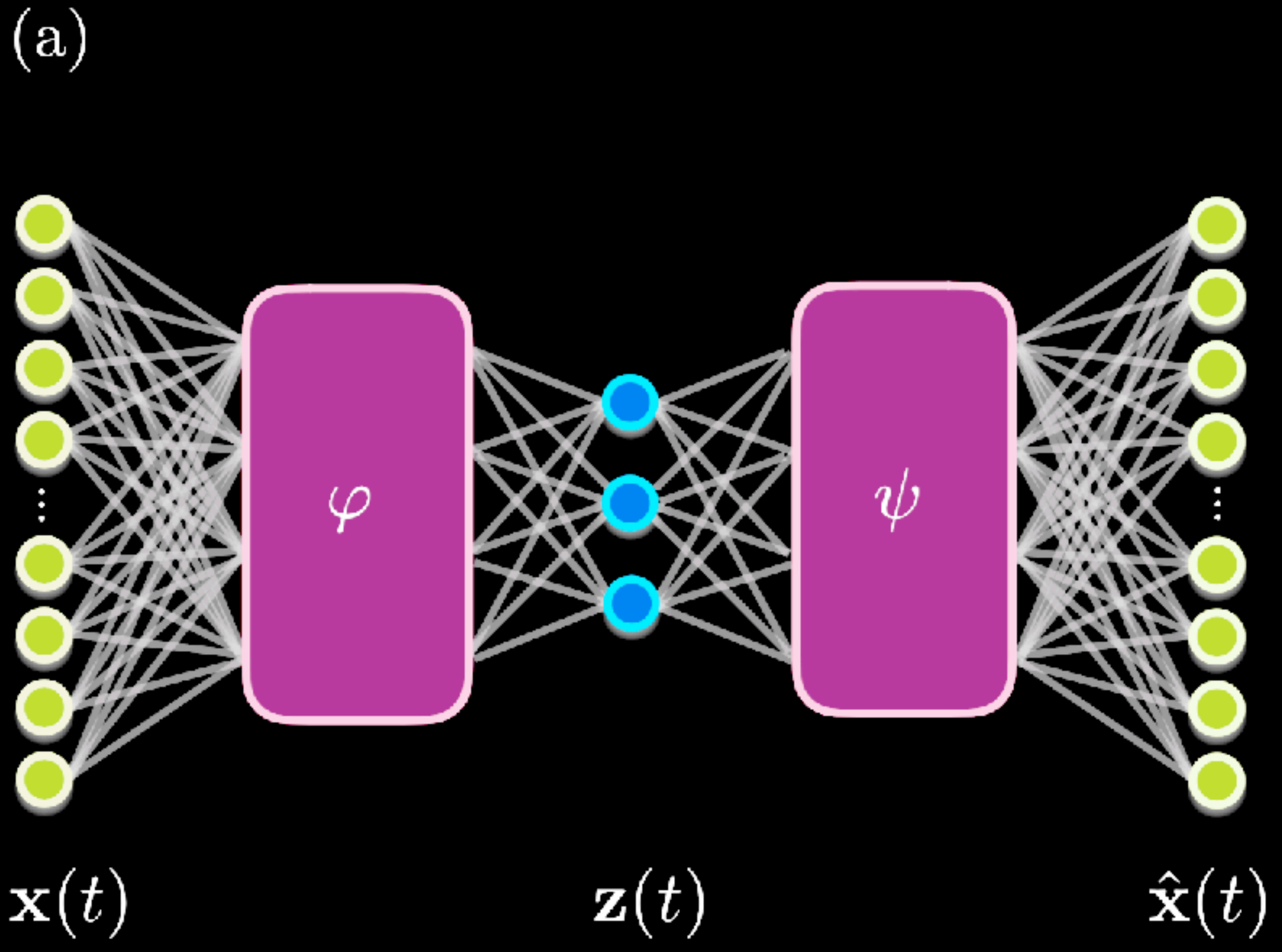
MALIN CHRISTERSSON

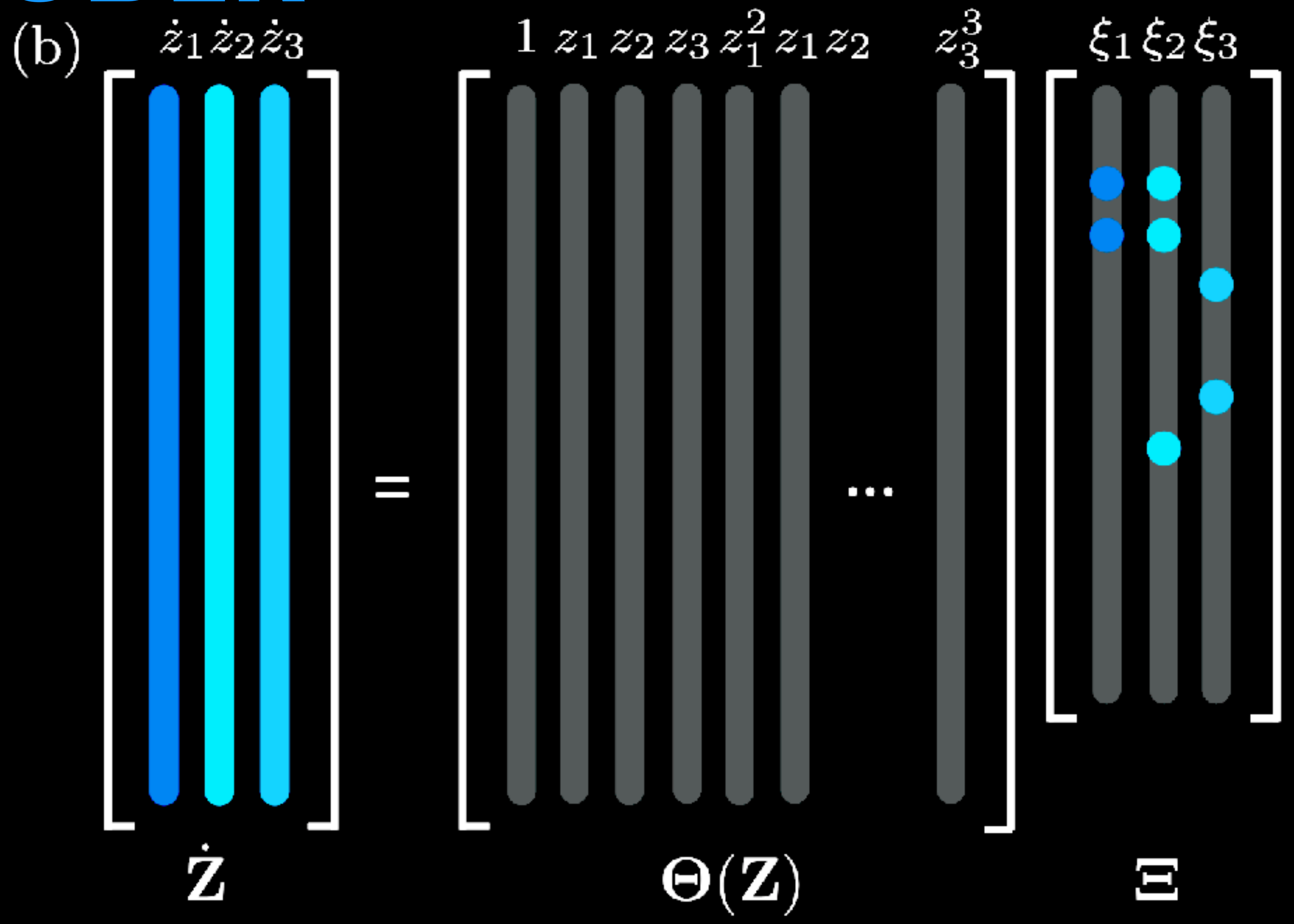
Deep Autoencoders for Dynamics



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

SINDy + Autoencoder





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

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

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