Interpretable & Generalizable Machine Learning for Fluid Dynamics

Steve Brunton
University of Washington

(Video by Petros Vrellis)

Interpretable & Generalizable Machine Learning for Fluid Dynamics

Nathan Kutz

Josh Proctor

Bernd Noack

JC Loiseau

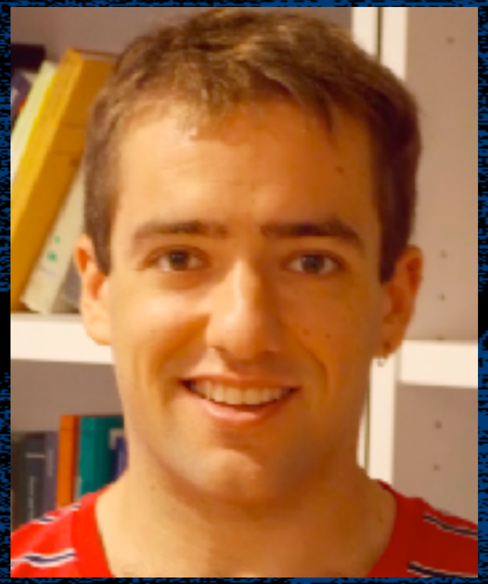
Eurika Kaiser

Bethany Lusch

Alan Kaptanoglu

Isabel Scherl

Sam Rudy



Jared Callaham

Benjamin Herrmann

Kathleen Champion

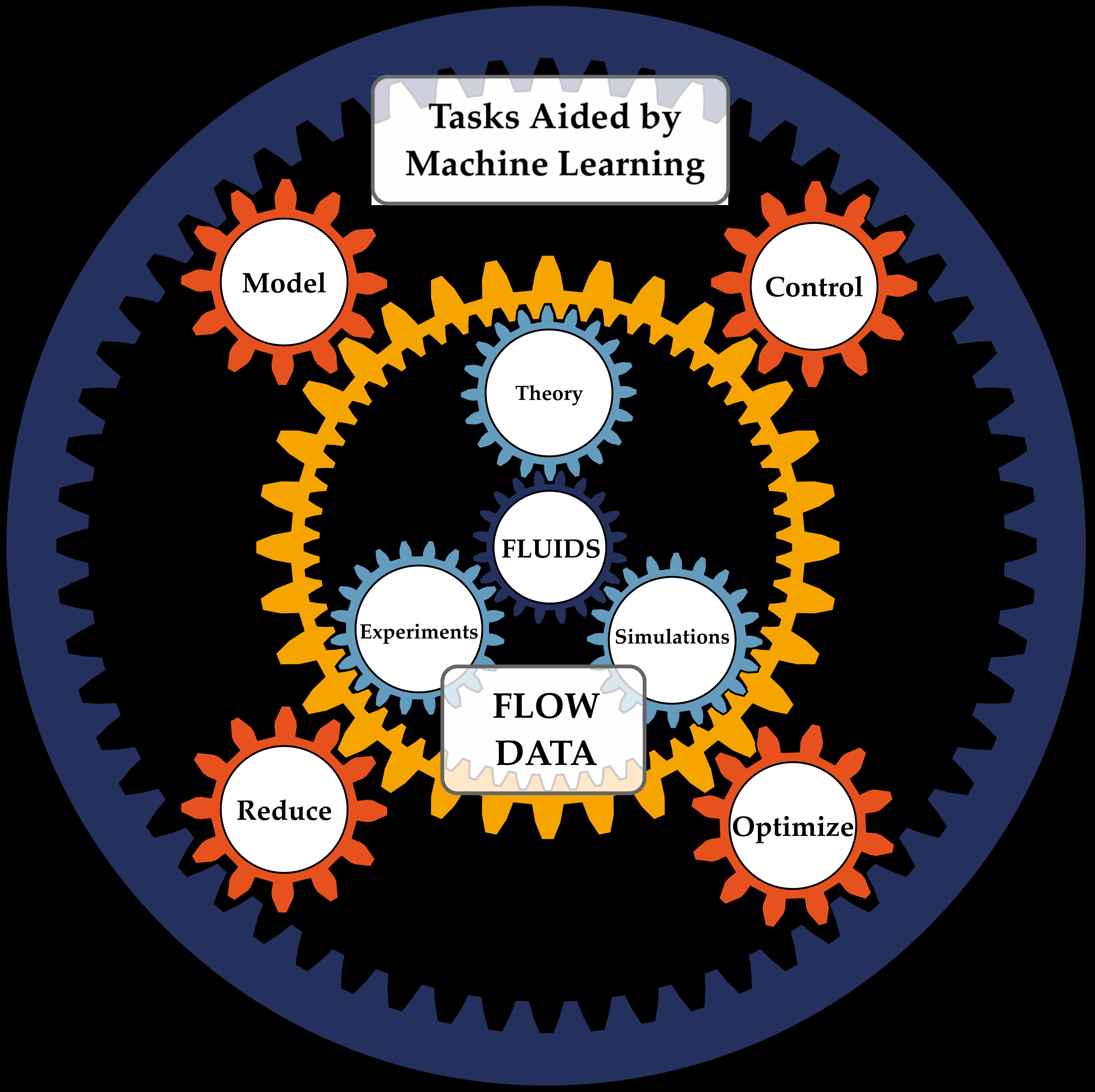
Science to Shape the Future of the Army · Army Research Office · 1951

Air Force Research Laboratory

Air Force Office of Scientific Research · United States Air Force

DARPA

BOEING



Machine Learning for Fluid Mechanics

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

Keywords

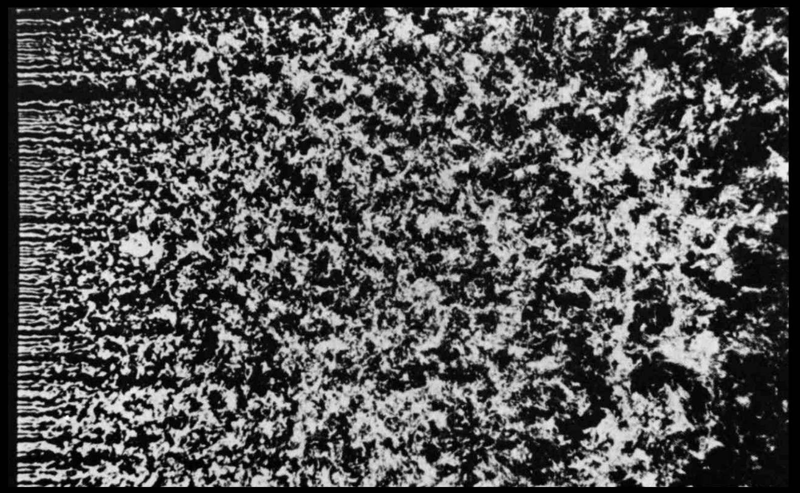
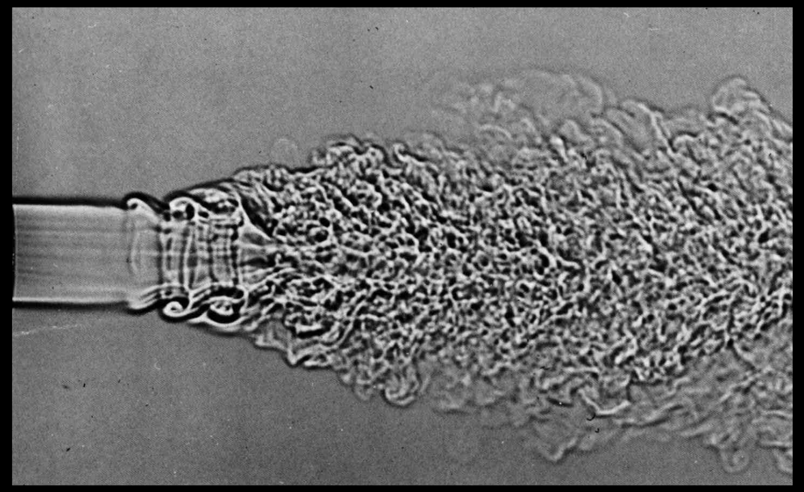
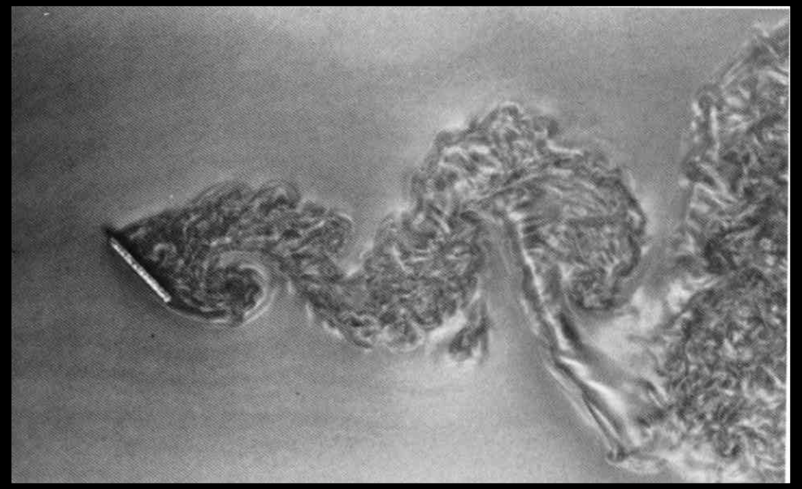
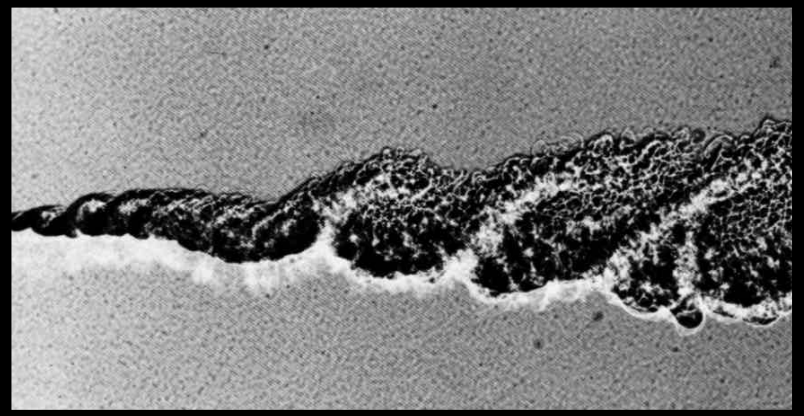
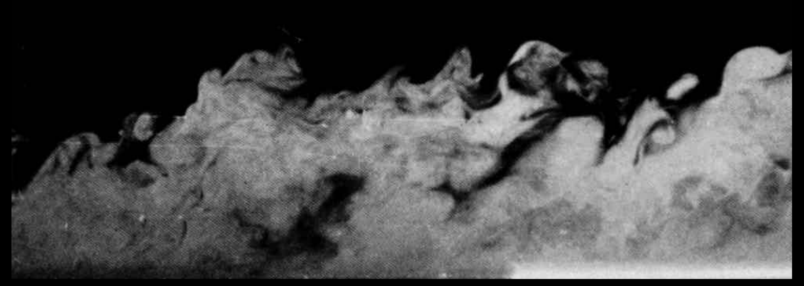
machine learning, data-driven modeling, optimization, control

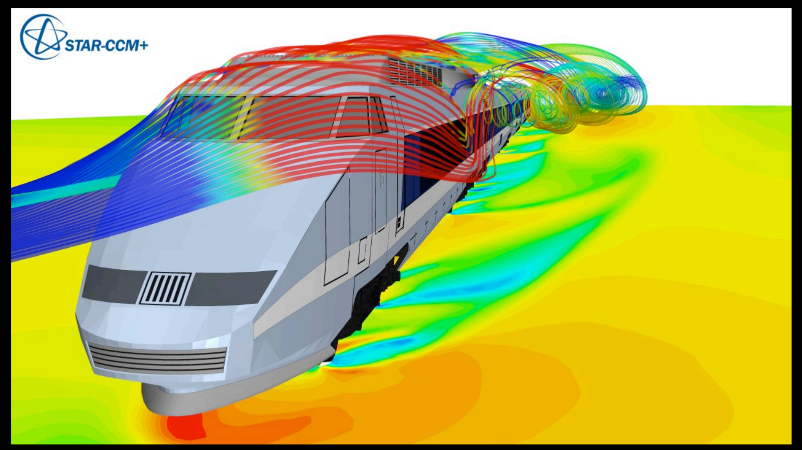
Abstract

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.

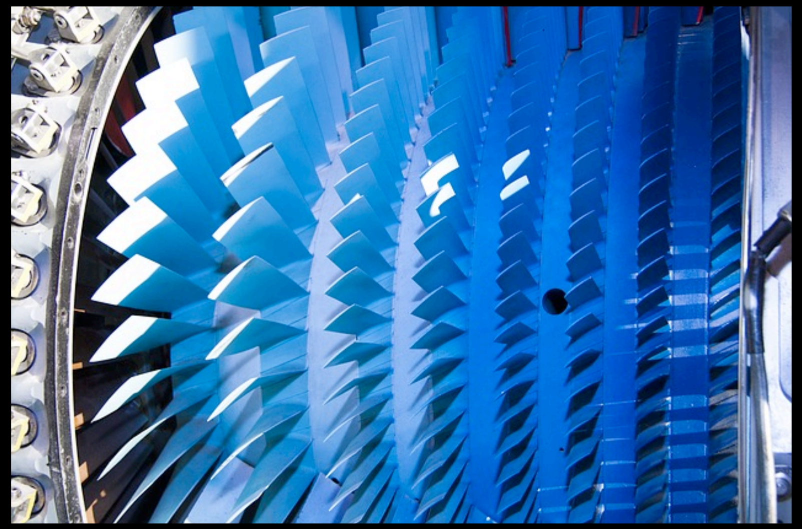
ANY SUFFICIENTLY ADVANCED TECHNOLOGY IS INDISTINGUISHABLE FROM MAGIC.

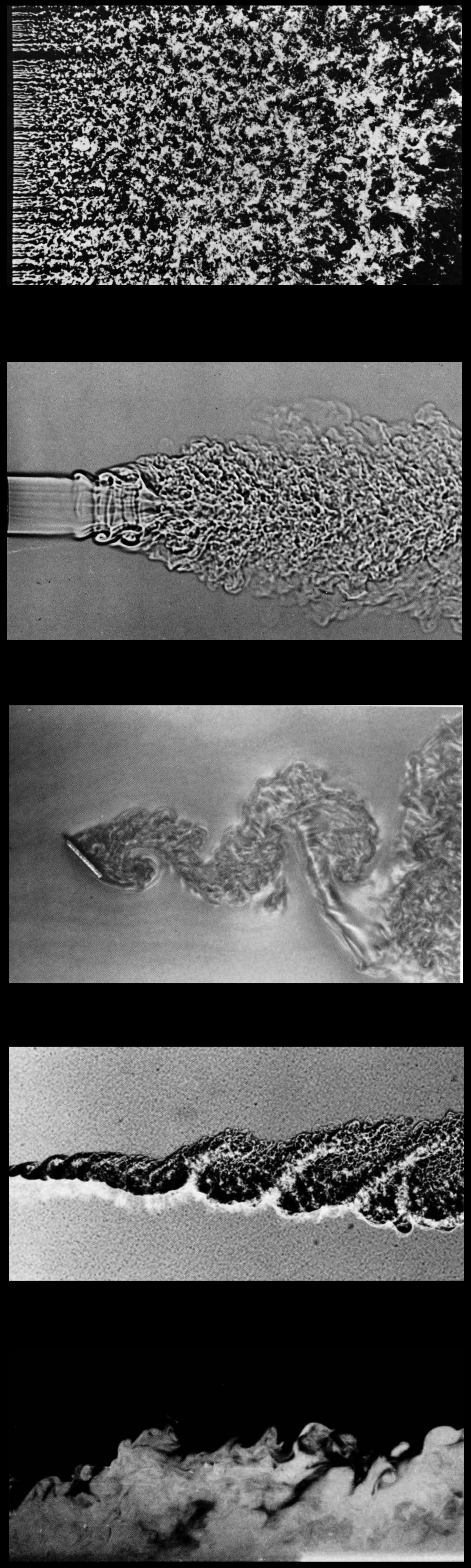
Arthur C. Clarke

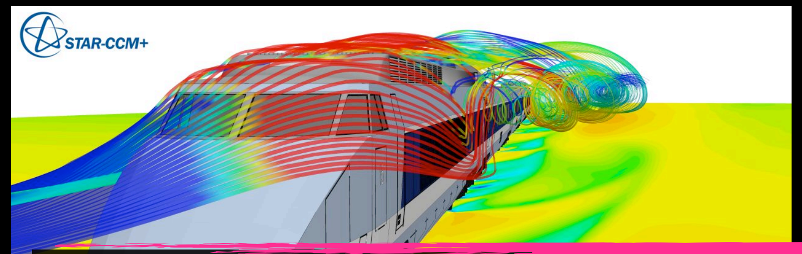

STAR-CCM+





Machine Learning:
Models from Data via Optimization

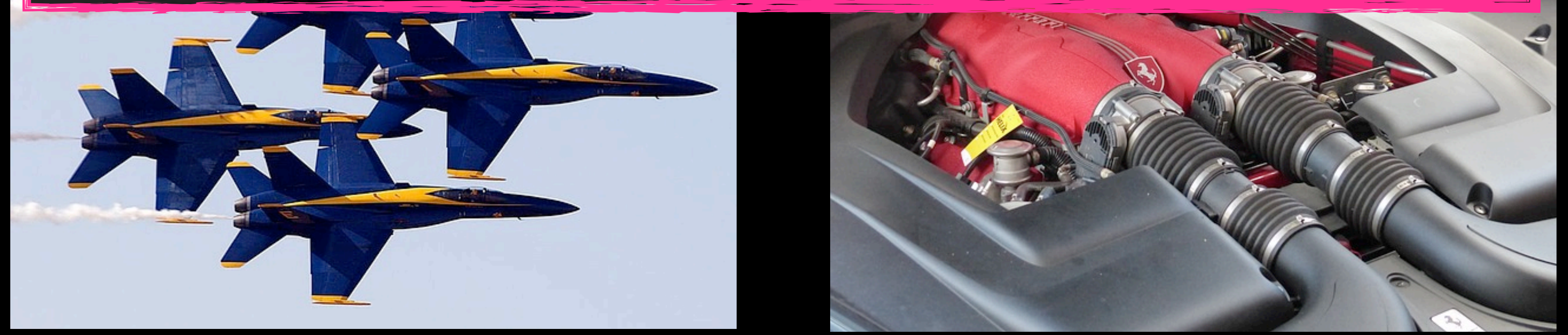


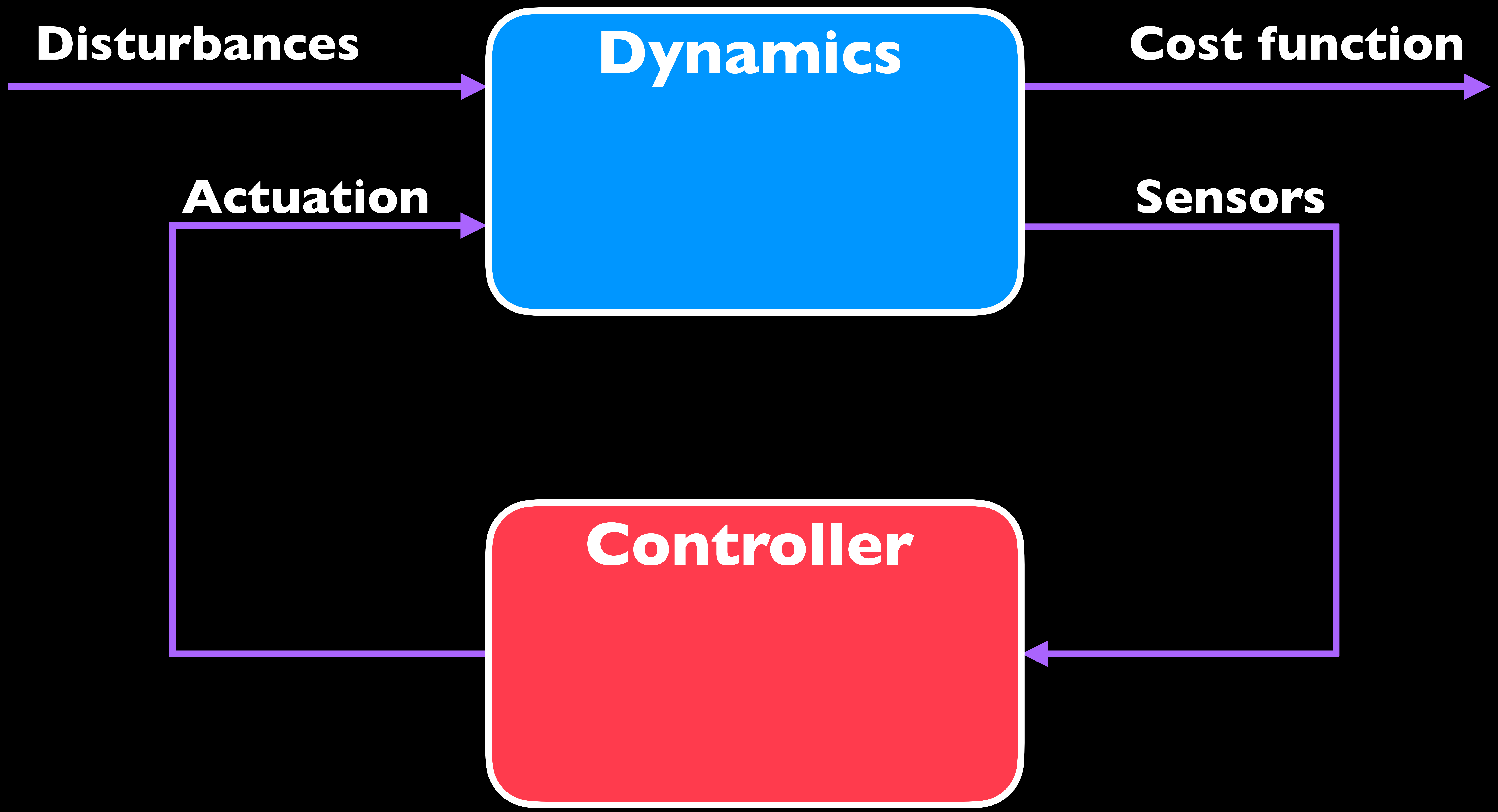
Optimization Problems:

- High-dimensional
- Nonlinear
- Non-convex
- Multiscale

Fluid Dynamics Tasks:

- Reduction
- Modeling
- Sensing
- Control




Disturbances
Dynamics
Cost function
Actuation
Sensors
Controller

Disturbances

Dynamics

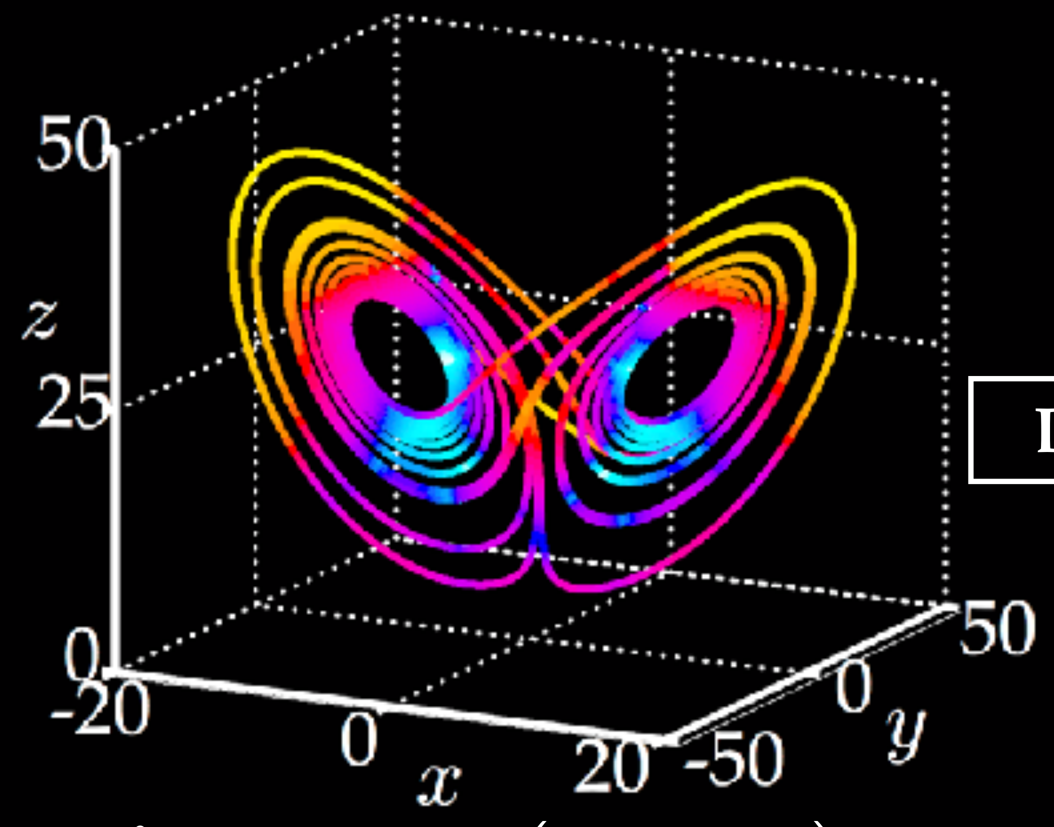
Cost function

Actuation

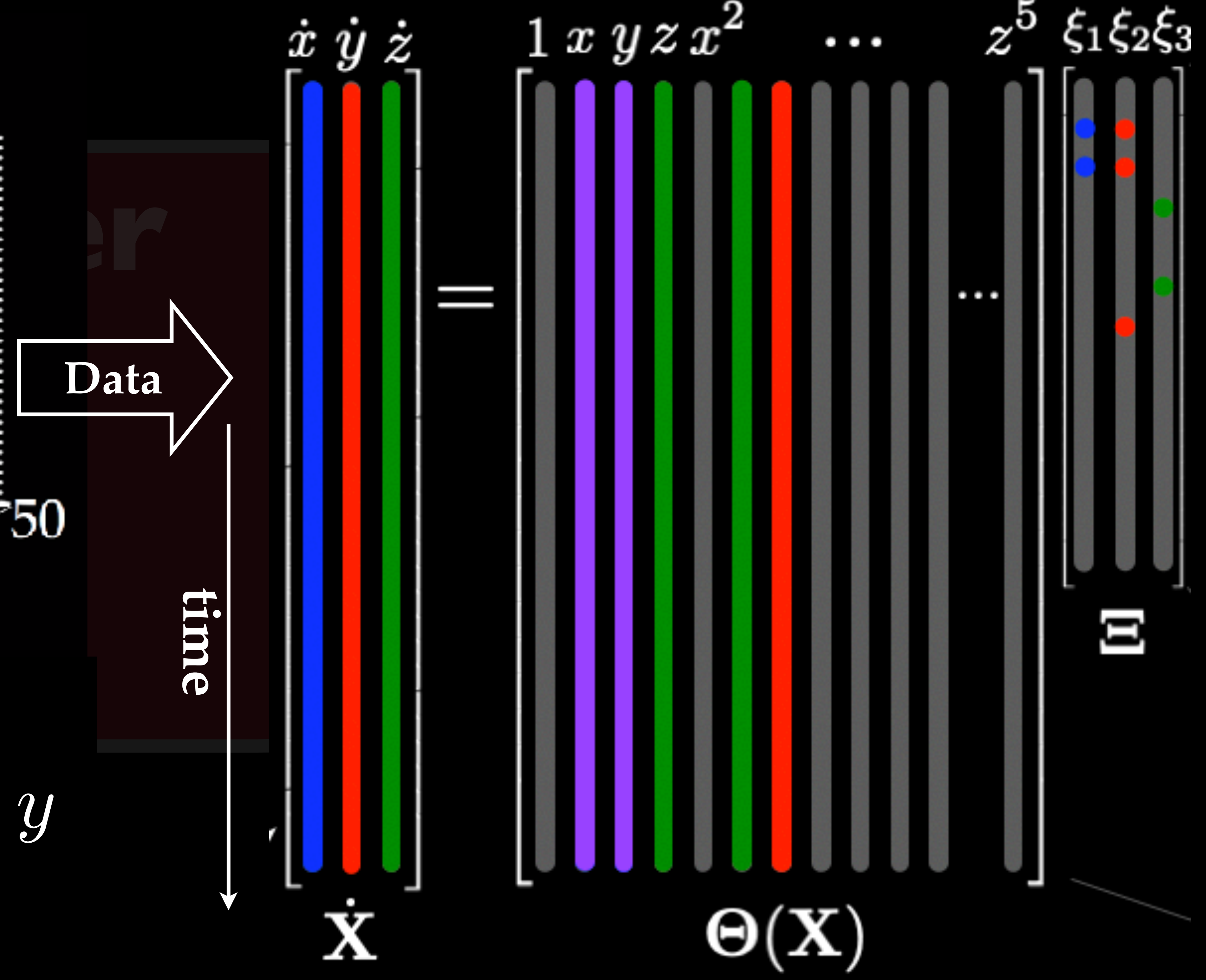
Sensors

LEARNING PHYSICS FROM DATA:

- Interpretable
- Generalizable



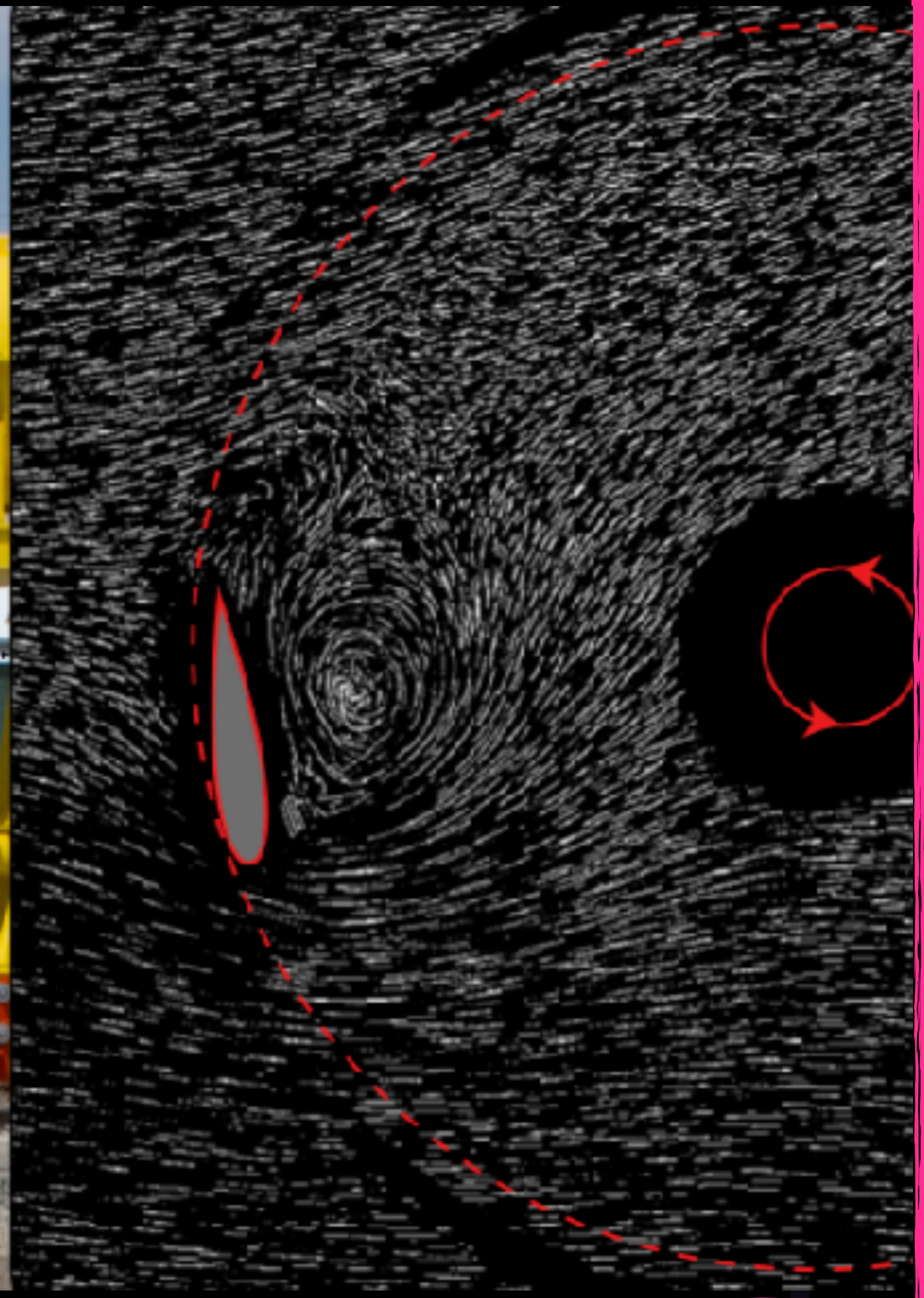
$$\dot{x} = \sigma(y - x)$$
$$\dot{y} = x(\rho - z) - y$$
$$\dot{z} = xy - \beta z.$$



SLB, Proctor, Kutz, *PNAS* 2016.

Control and Optimization:

- Nonlinear
- Use ML



Strom, SLB, Polagye, *Nature Energy* 2017.

Disturbances

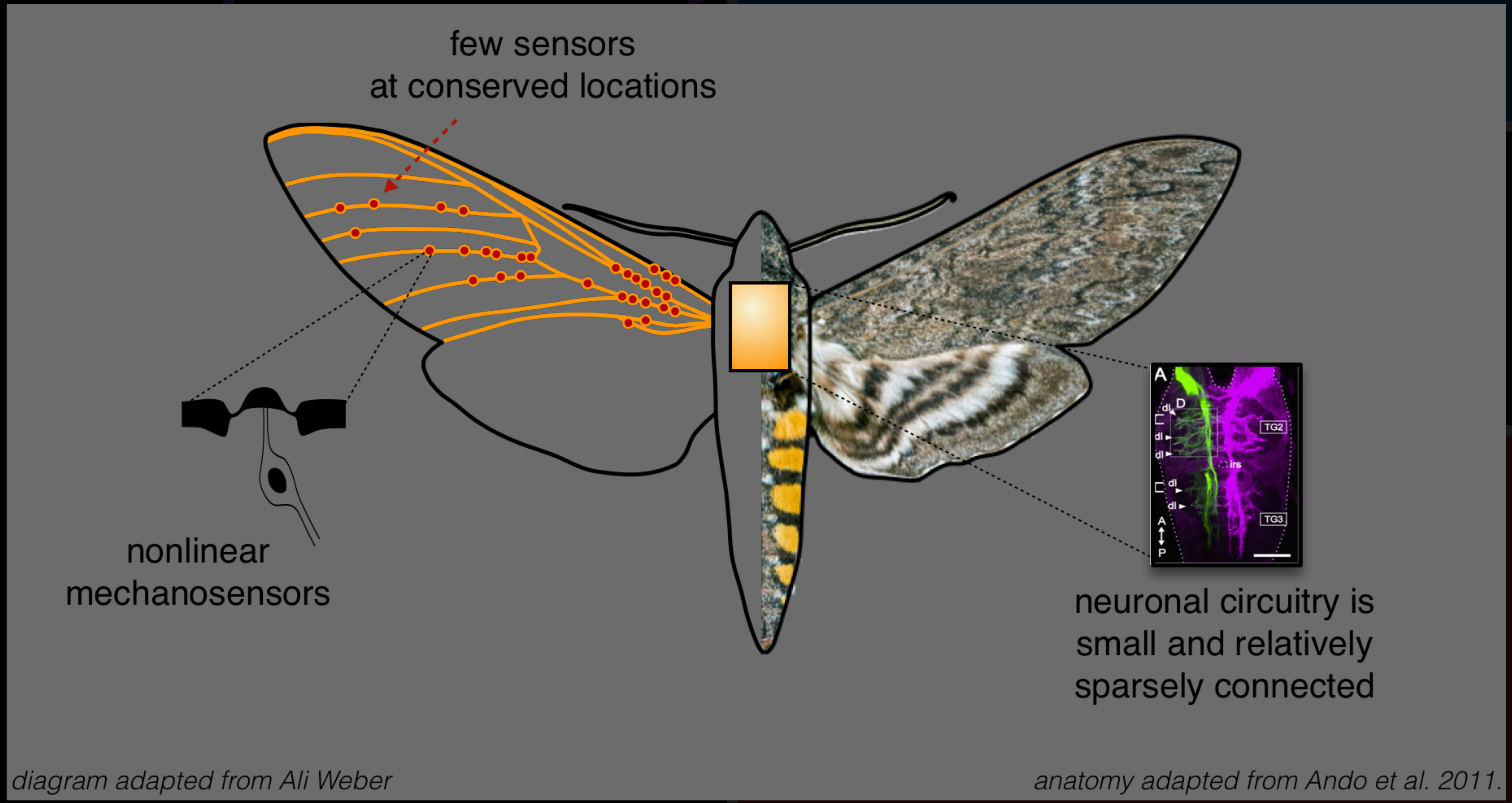
Actuation

...tion

Controller

Sparse Sensor Optimization:

- **Patterns facilitate sparse sampling**

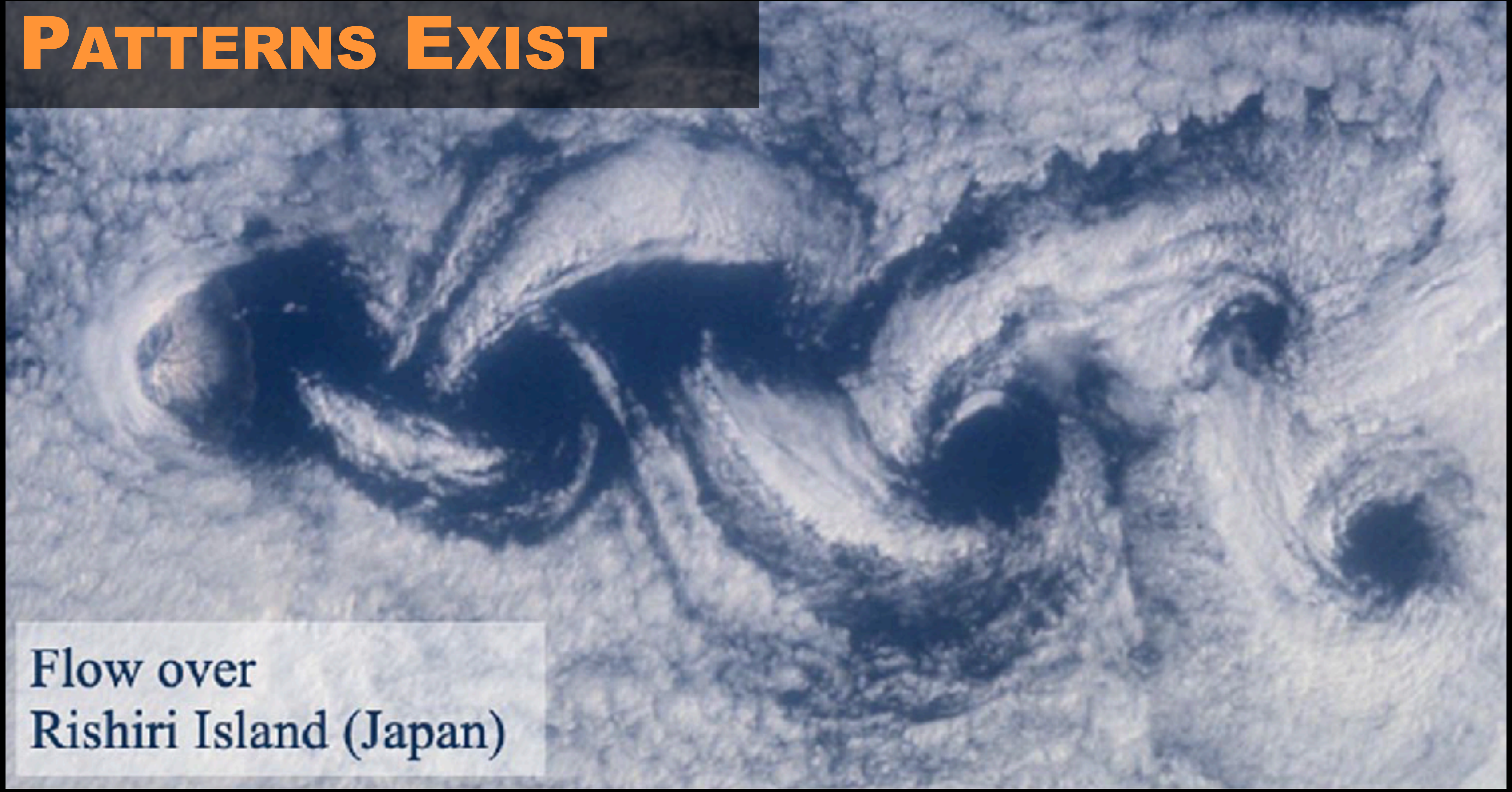


B. Brunton, SLB, Proctor, Kutz, *SIAM SIAP* 2016.
Manohar, B Brunton, Kutz, SLB, *IEEE CSM* 2017.

Cost function

Sensors

Patterns Exist



ROBUST PROPER ORTHOGONAL DECOMPOSITION

$$\min_{L,S} \textbf{rank}(L) + \|S\|_0 \ \ \textbf{subject to} \ \ L + S = X$$

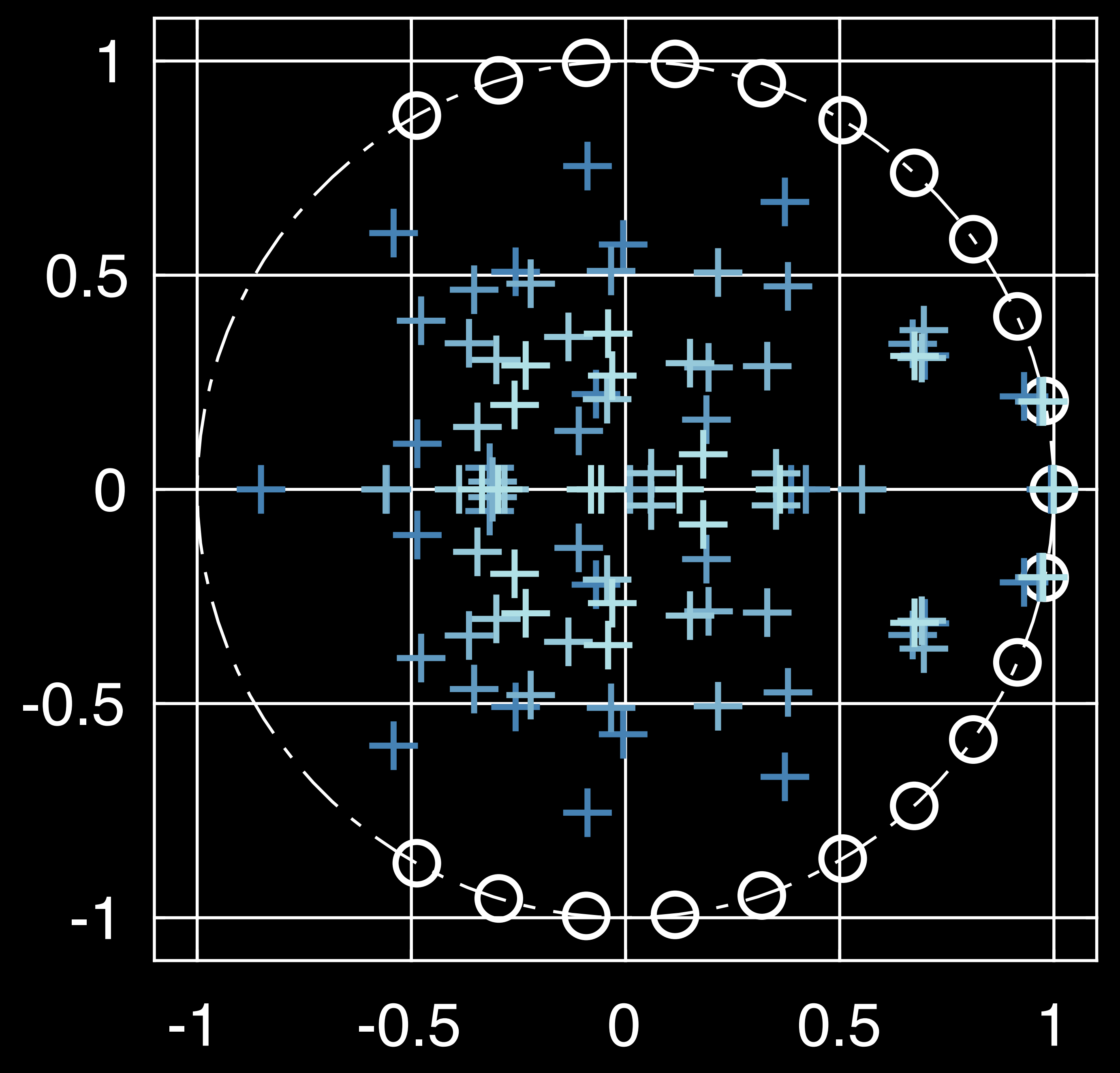
Convex Relaxation

$$\min_{L,S} \|L\|_* + \lambda_0 \|S\|_1 \ \ \textbf{subject to} \ \ L + S = X$$

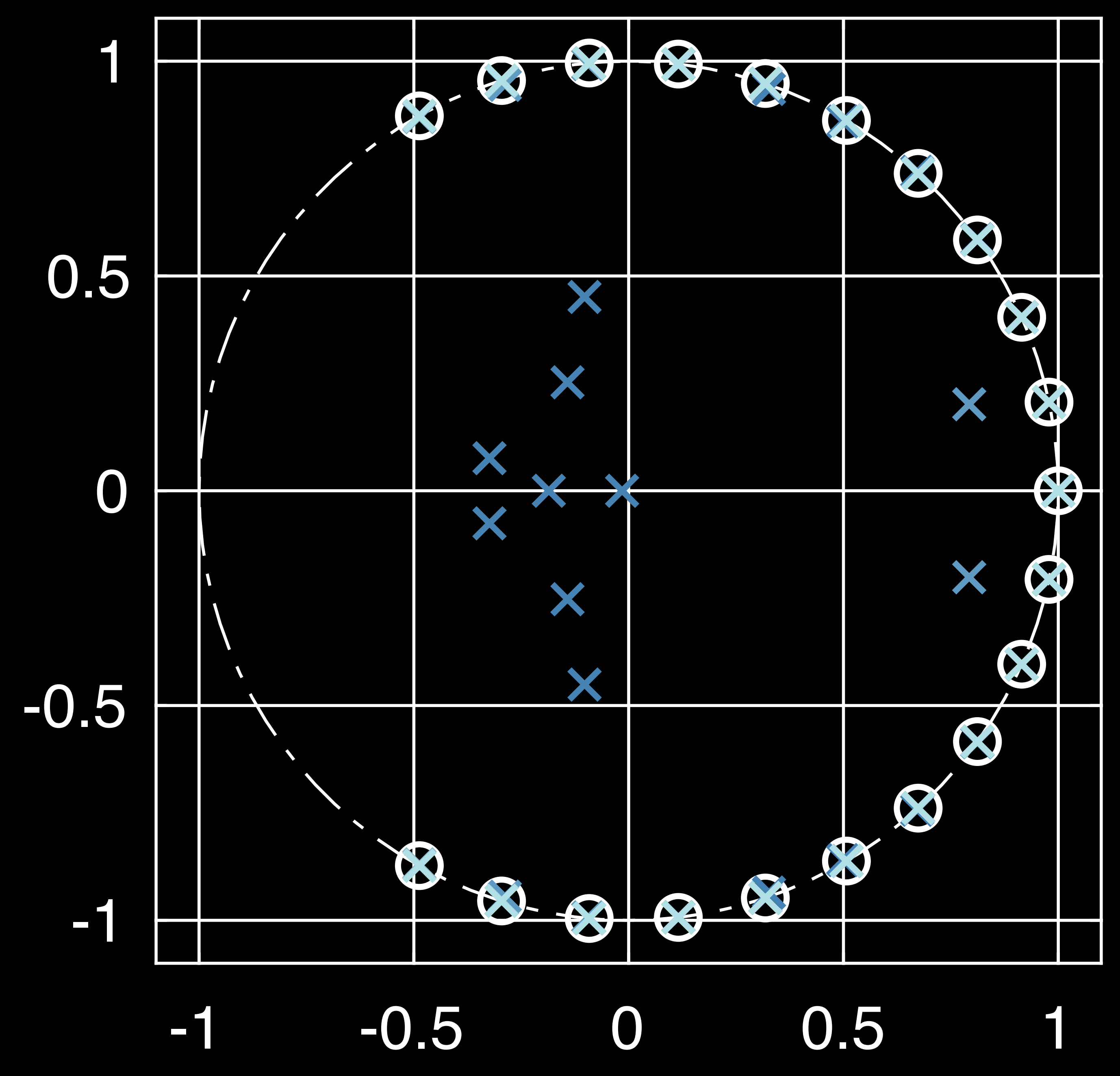
Candes et *al.*, *J. ACM*, 2011
Scherl et *al.*, *Phys Rev Fluids*, 2020

ROBUST PROPER ORTHOGONAL DECOMPOSITION

DMD Before



DMD After RPCA

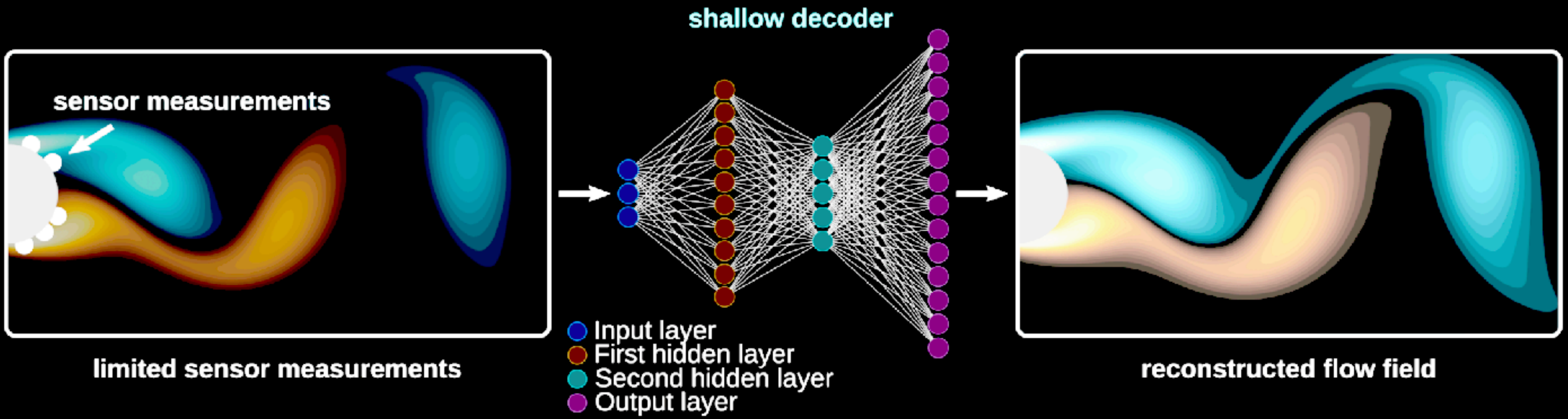


Candes *et al.*, *J. ACM*, 2011
Scherl *et al.*, *Phys Rev Fluids*, 2020

SUPER RESOLUTION

SUPER RESOLUTION

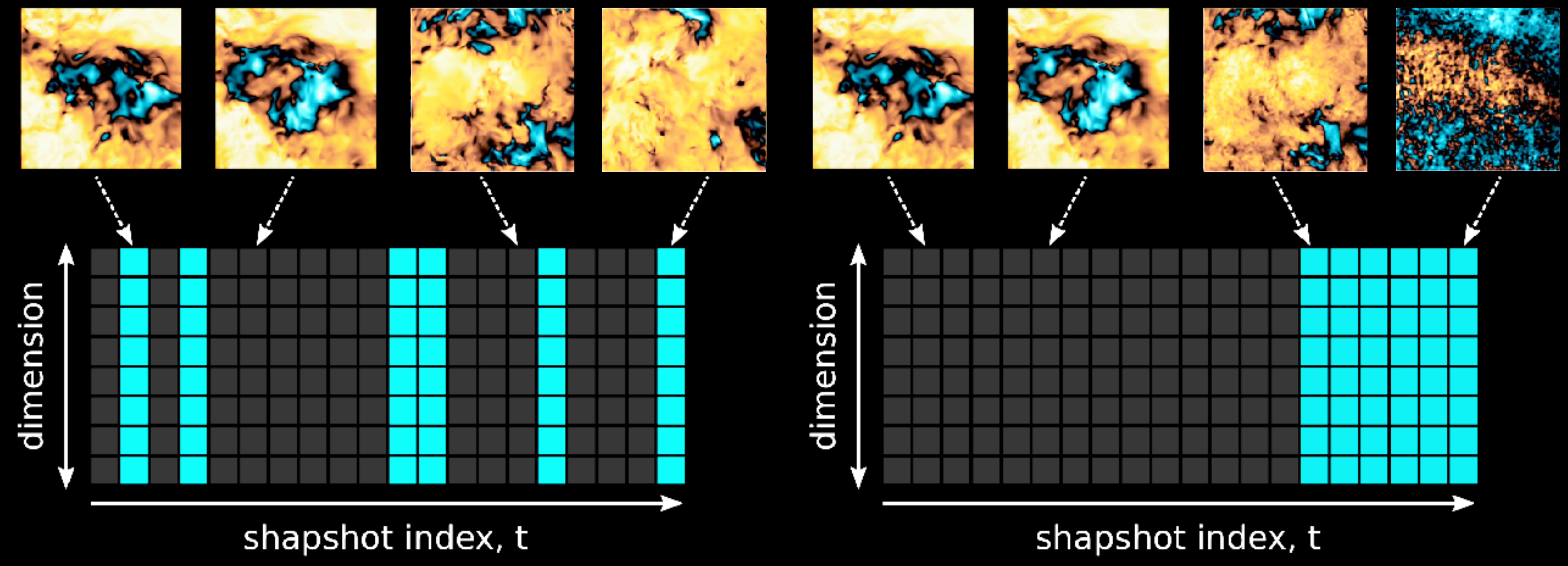
(a) Snapshot (b) Low resolution (c) Shallow Decoder



Erichson et al, *Proc. Roy. Soc. A*, 2020

SUPER RESOLUTION

(a) Snapshot (b) Low resolution (c) Shallow Decoder

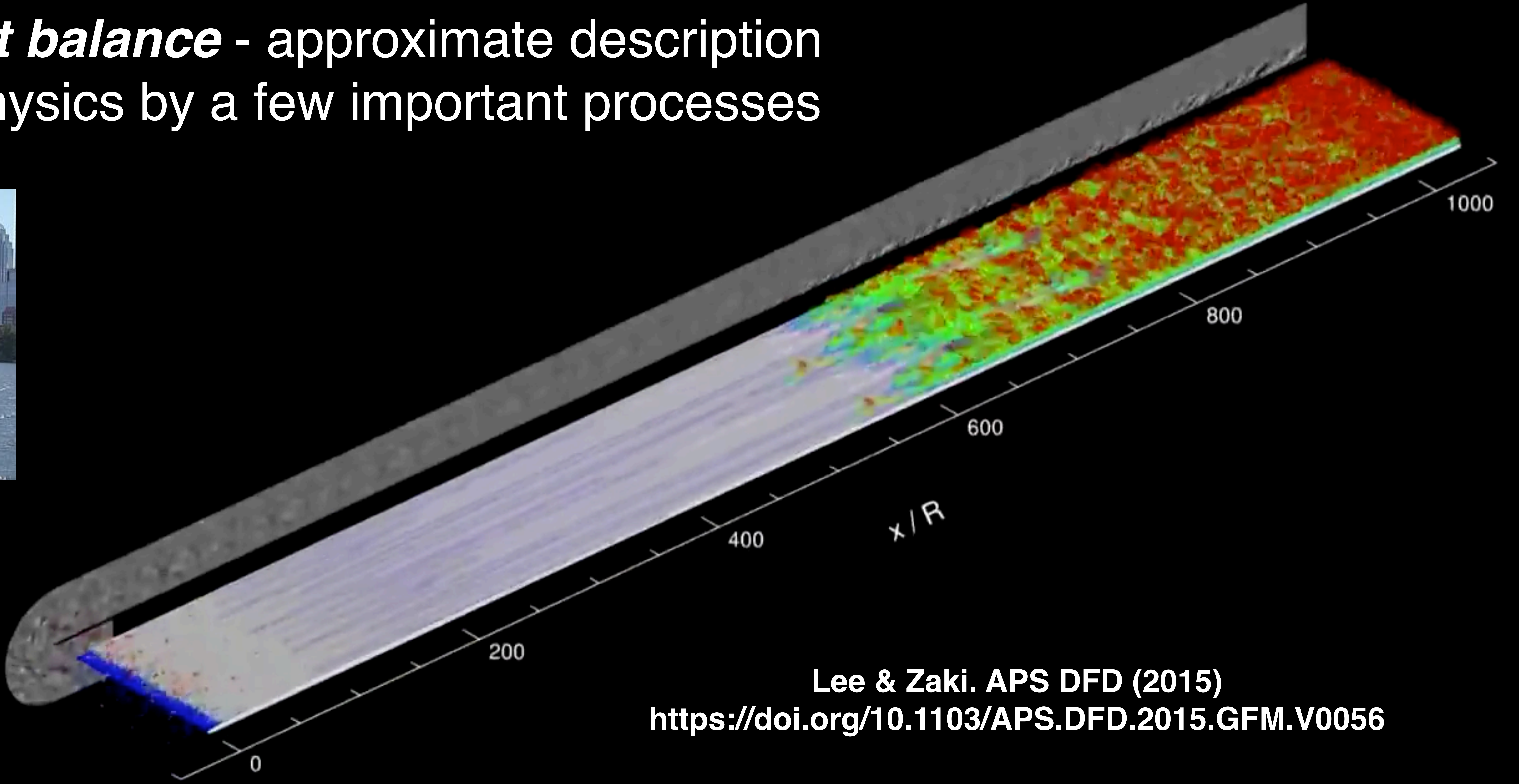


(a) Interpolation (b) Extrapolation

Erichson et al, *Proc. Roy. Soc. A*, 2020

DOMINANT BALANCE

Dominant balance - approximate description of local physics by a few important processes



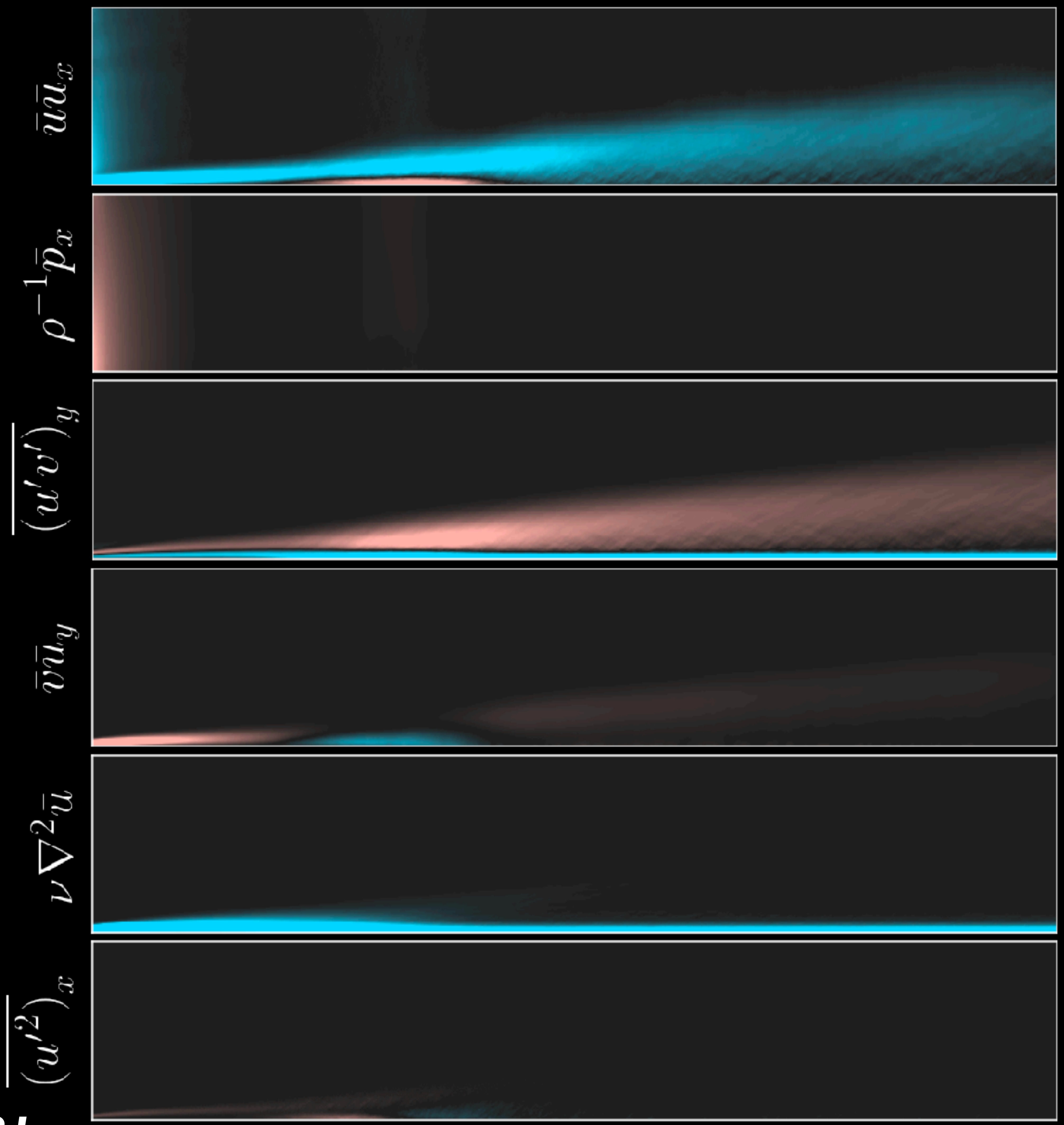
Lee & Zaki. APS DFD (2015)
https://doi.org/10.1103/APS.DFD.2015.GFM.V0056

Callaham, Koch, Brunton, Kutz, SLB, *To appear Nat Comm 2021*

Reynolds-averaged Navier-Stokes equations

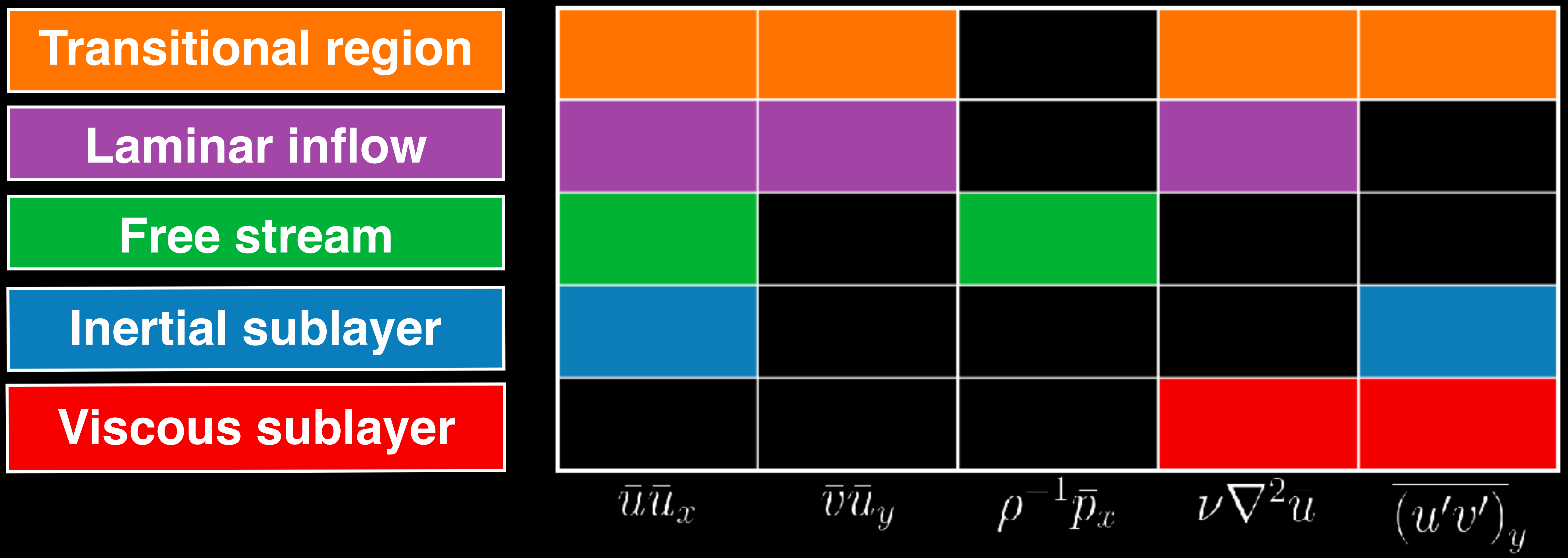
$$\bar{u}\bar{u}_x + \bar{v}\bar{u}_y + (\overline{u'^2})_x + (\overline{u'v'})_y = -\rho^{-1}\bar{p}_x + \nu\nabla^2\bar{u}$$

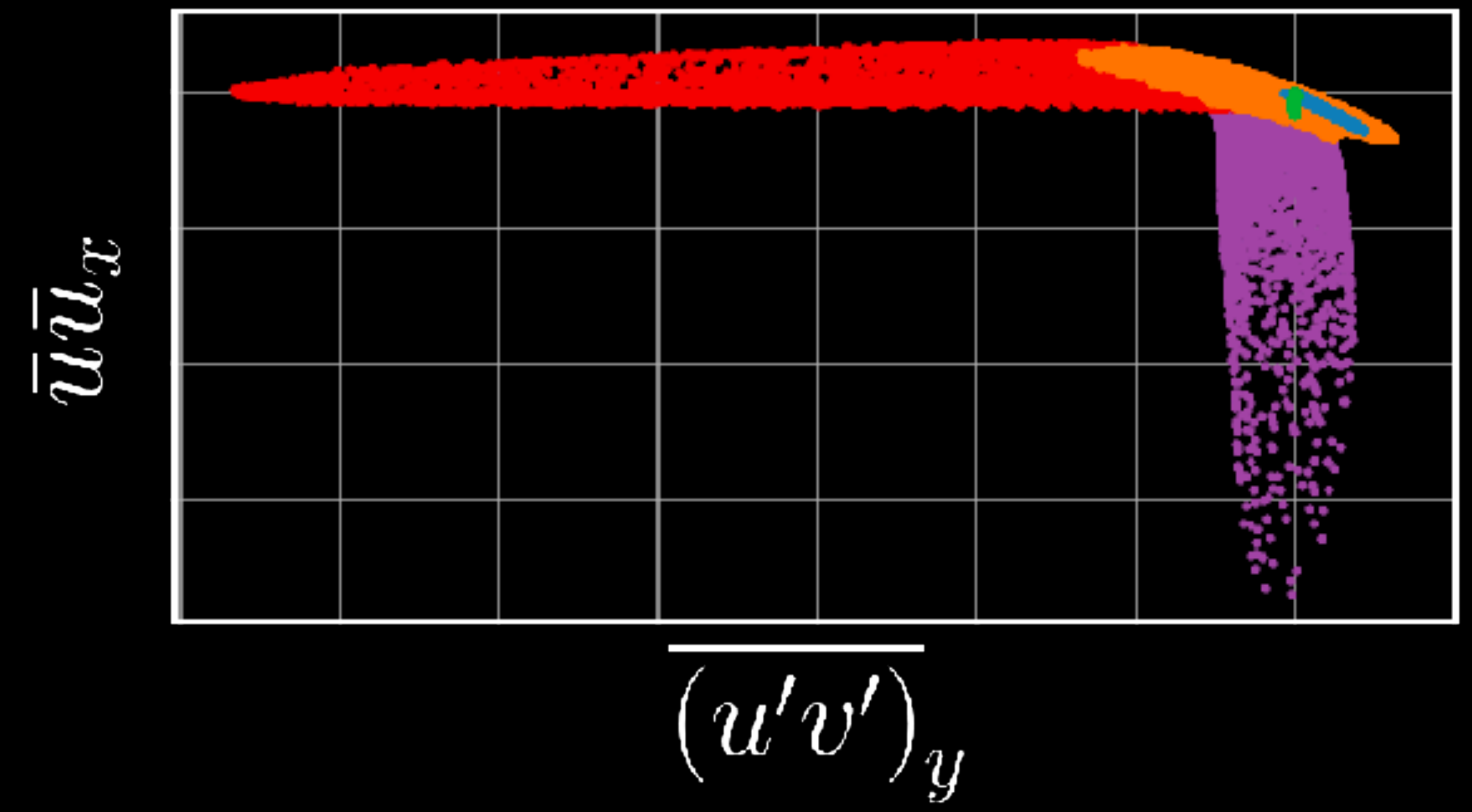
$$u(x,t) = \bar{u}(x) + u'(x,t)$$

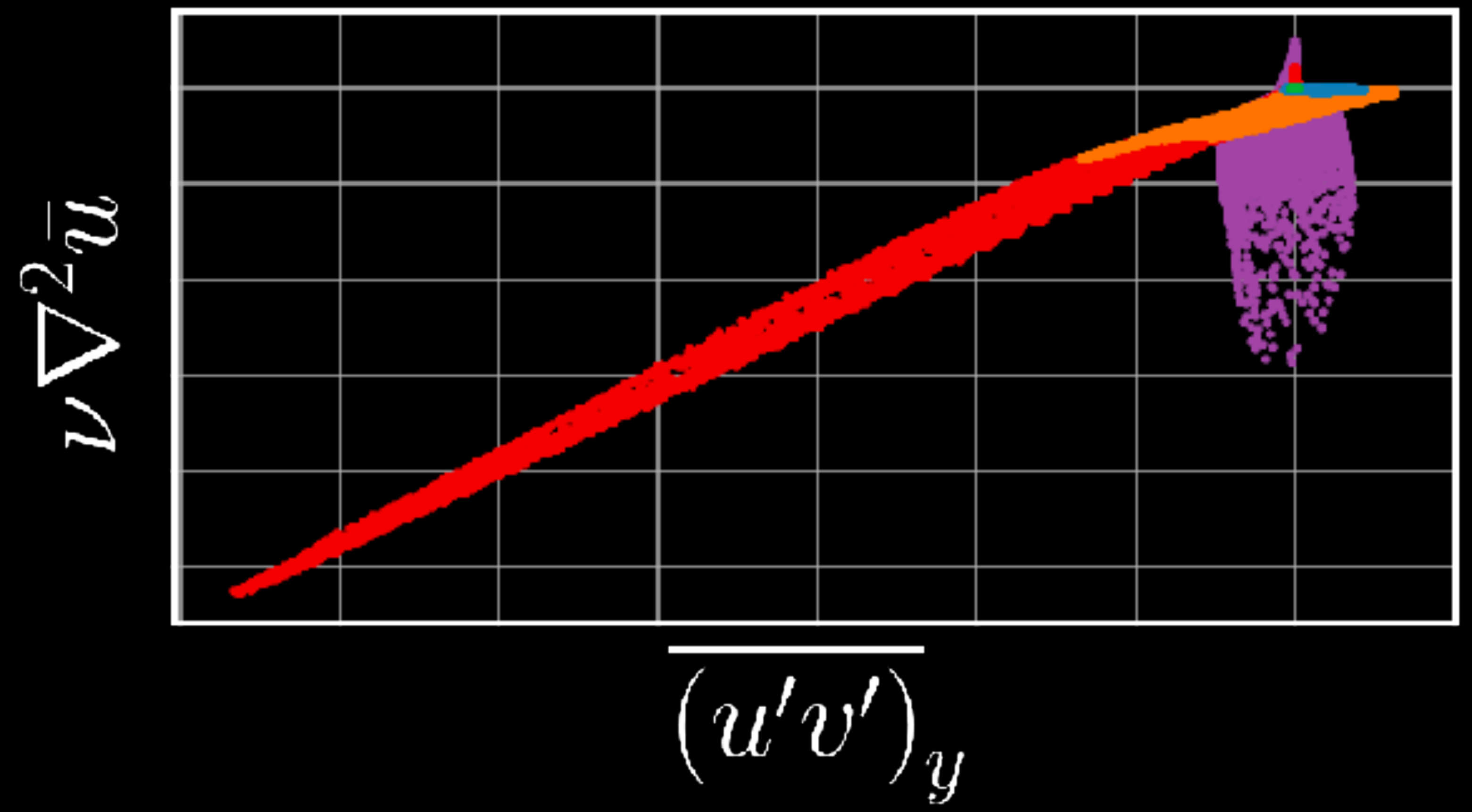


Callaham, Koch, Brunton, Kutz, SLB, *To appear Nat Comm 2021*

Equation space representation

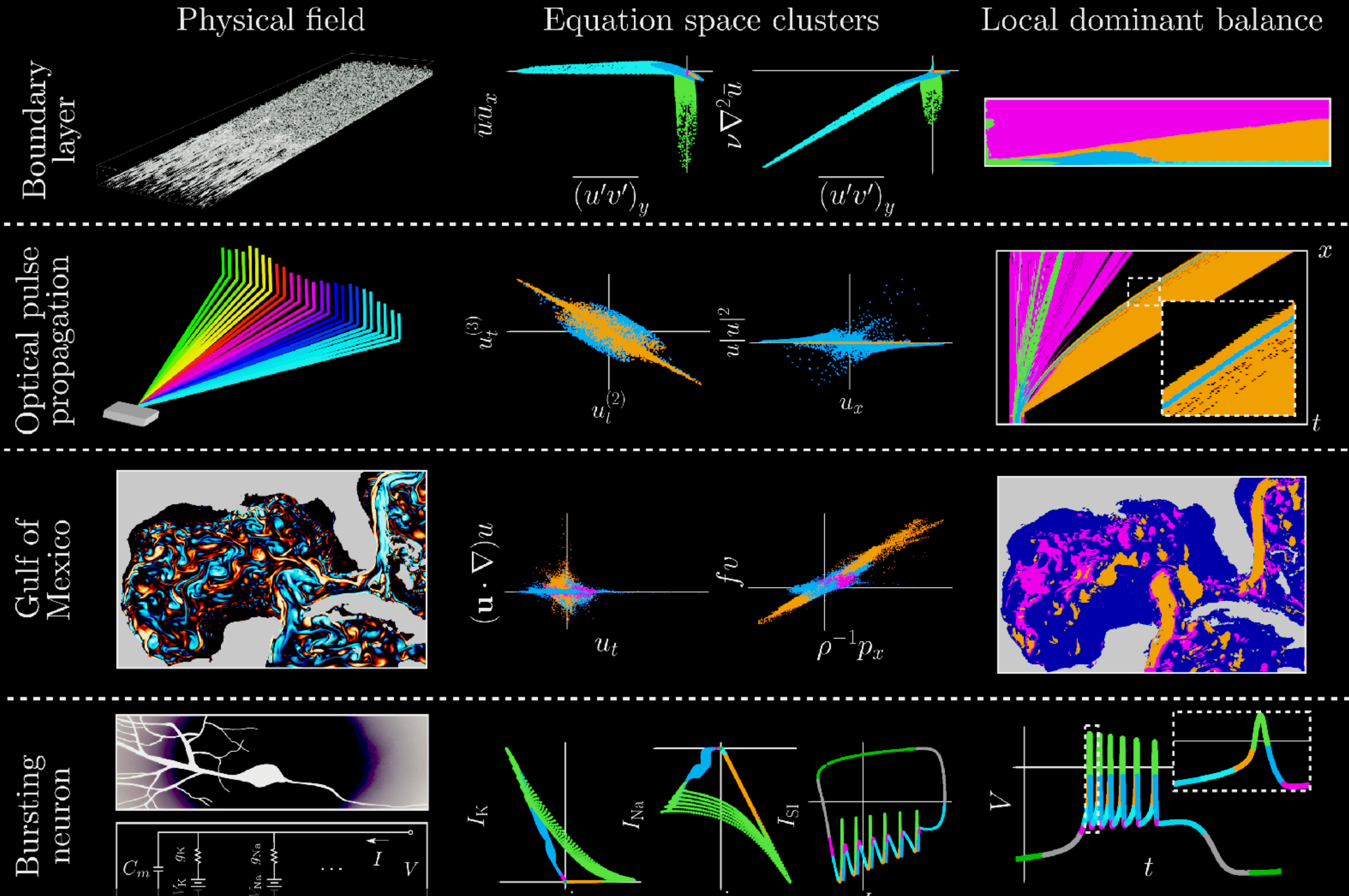






- Clustering (GMM)
- Subspace identification (Sparse PCA)
- Interpretable balance laws

Callaham, Koch, Brunton, Kutz, SLB, *To appear Nat Comm 2021*



Callaham, Koch, Brunton, Kutz, SLB, *To appear Nat Comm 2021*

There is a need for INTERPRETABLE and GENERALIZABLE Machine Learning

$F = ma$

There is a need for INTERPRETABLE and GENERALIZABLE Machine Learning

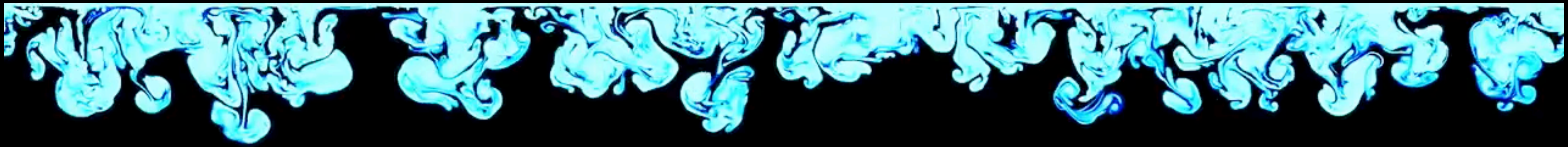
EVERYTHING SHOULD BE MADE
AS SIMPLE AS POSSIBLE,
BUT NOT SIMPLER.

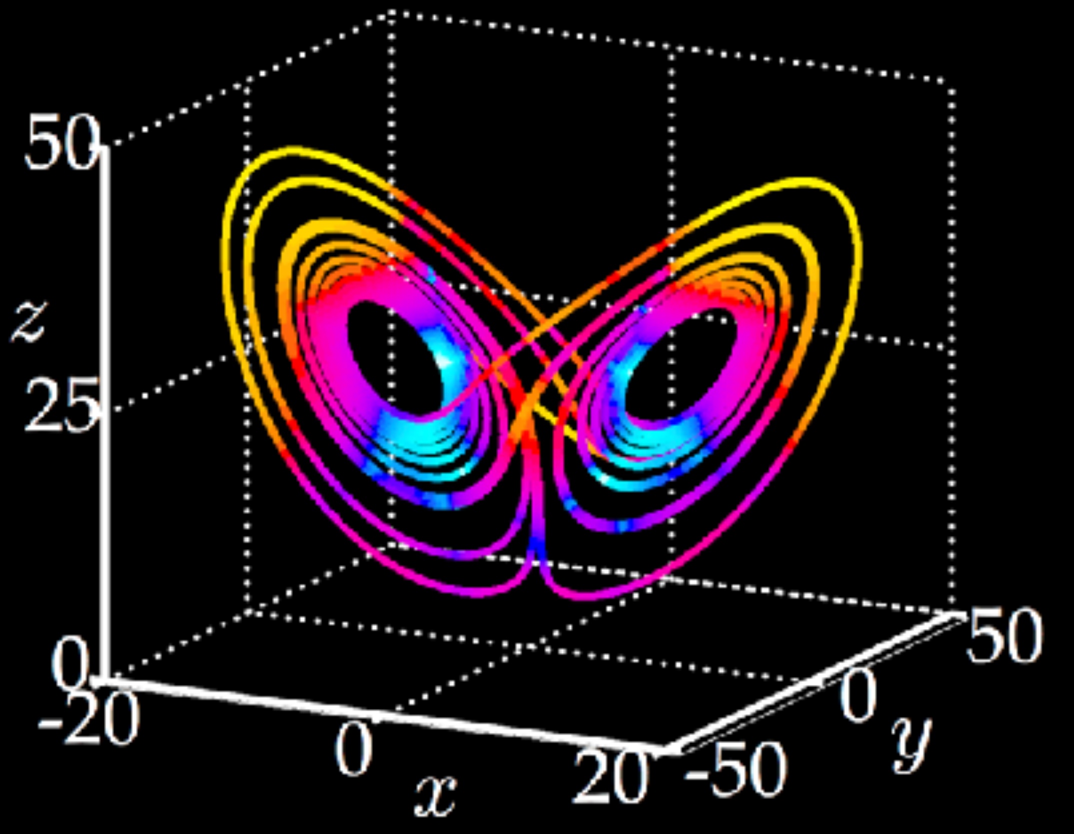
Albert Einstein

There is a need for INTERPRETABLE and GENERALIZABLE Machine Learning

- LOW-DIMENSIONAL
- SPARSE

Chaotic Thermal Convection



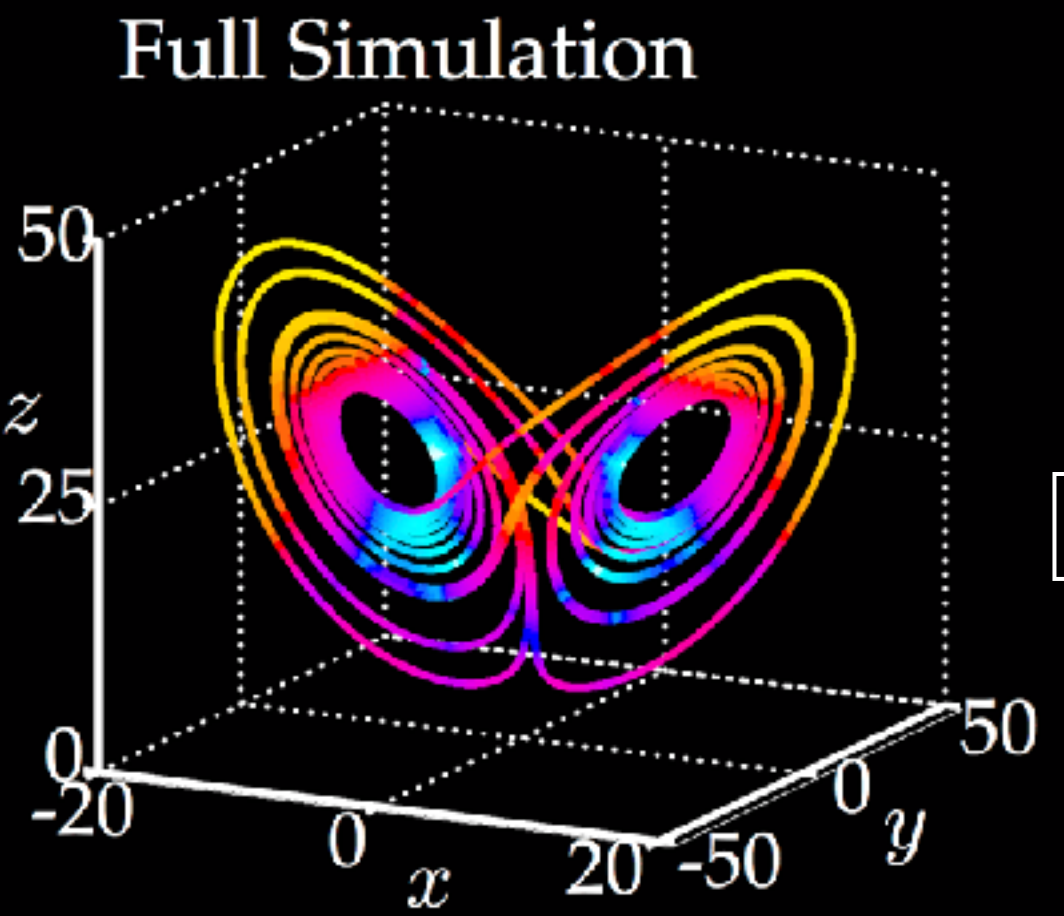


$$\dot{x} = \sigma(y - x)$$
$$\dot{y} = x(\rho - z) - y$$
$$\dot{z} = xy - \beta z.$$

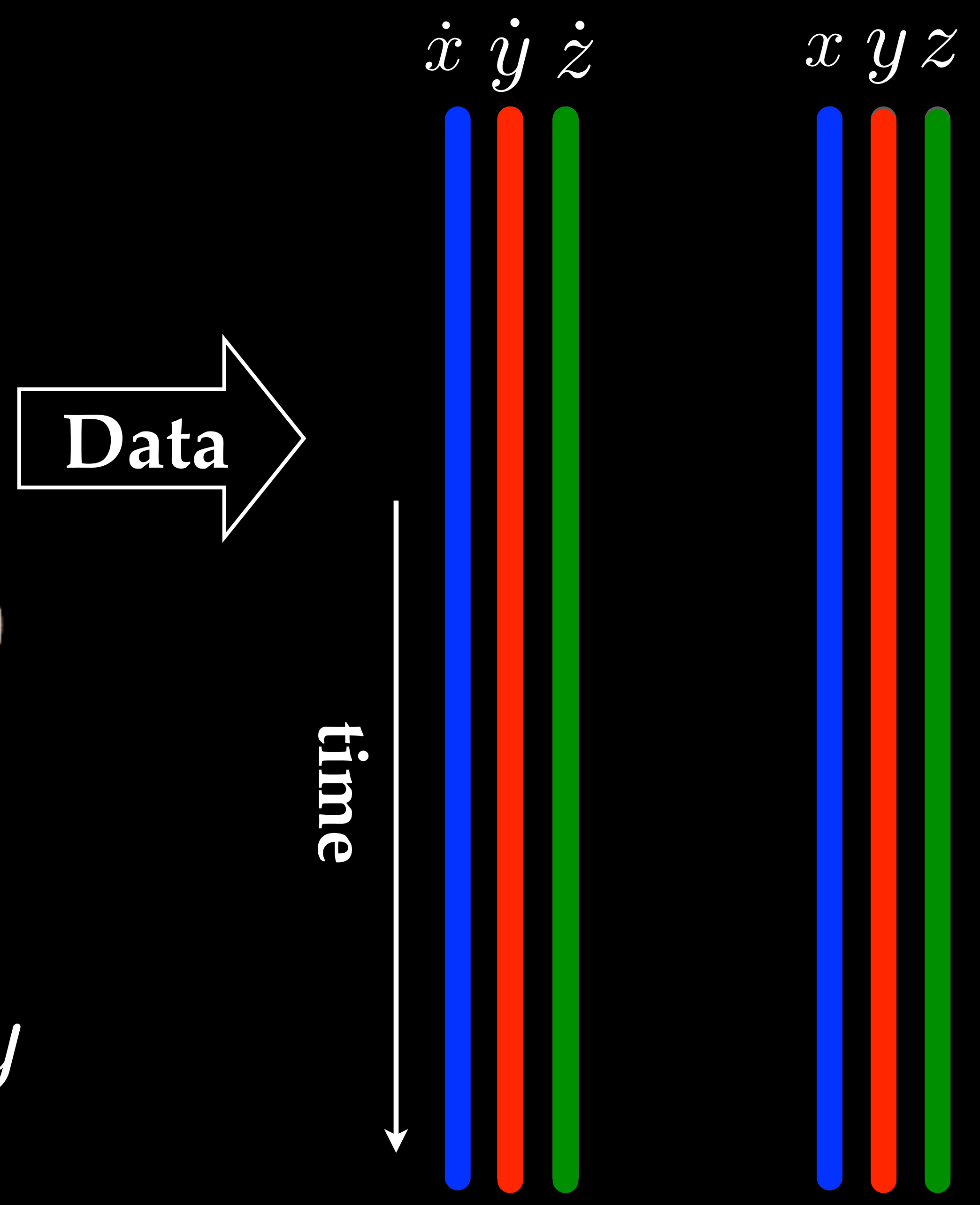
YouTube: turbulenceteam

Lorenz, Fetter, Hamilton, 1963

Sparse Identification of Nonlinear Dynamics (SINDy)

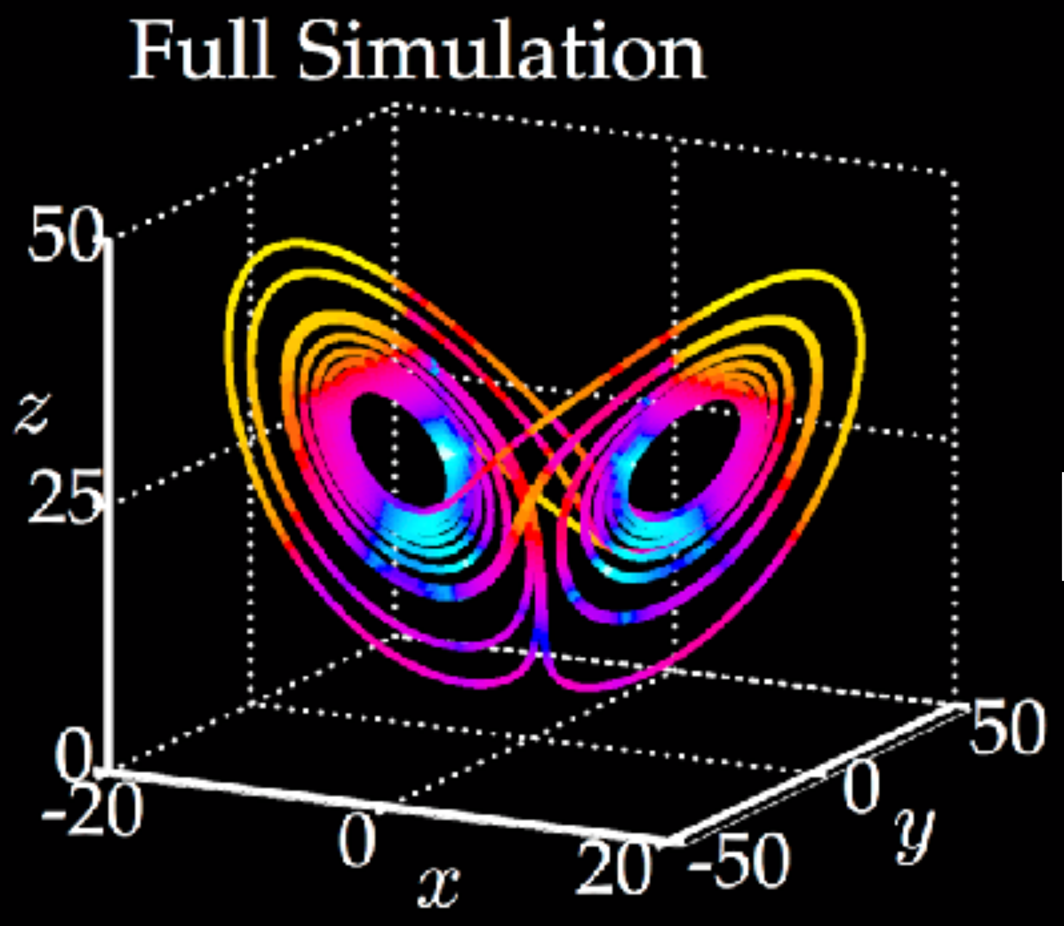


$$\dot{x} = \sigma(y - x)$$
$$\dot{y} = x(\rho - z) - y$$
$$\dot{z} = xy - \beta z.$$

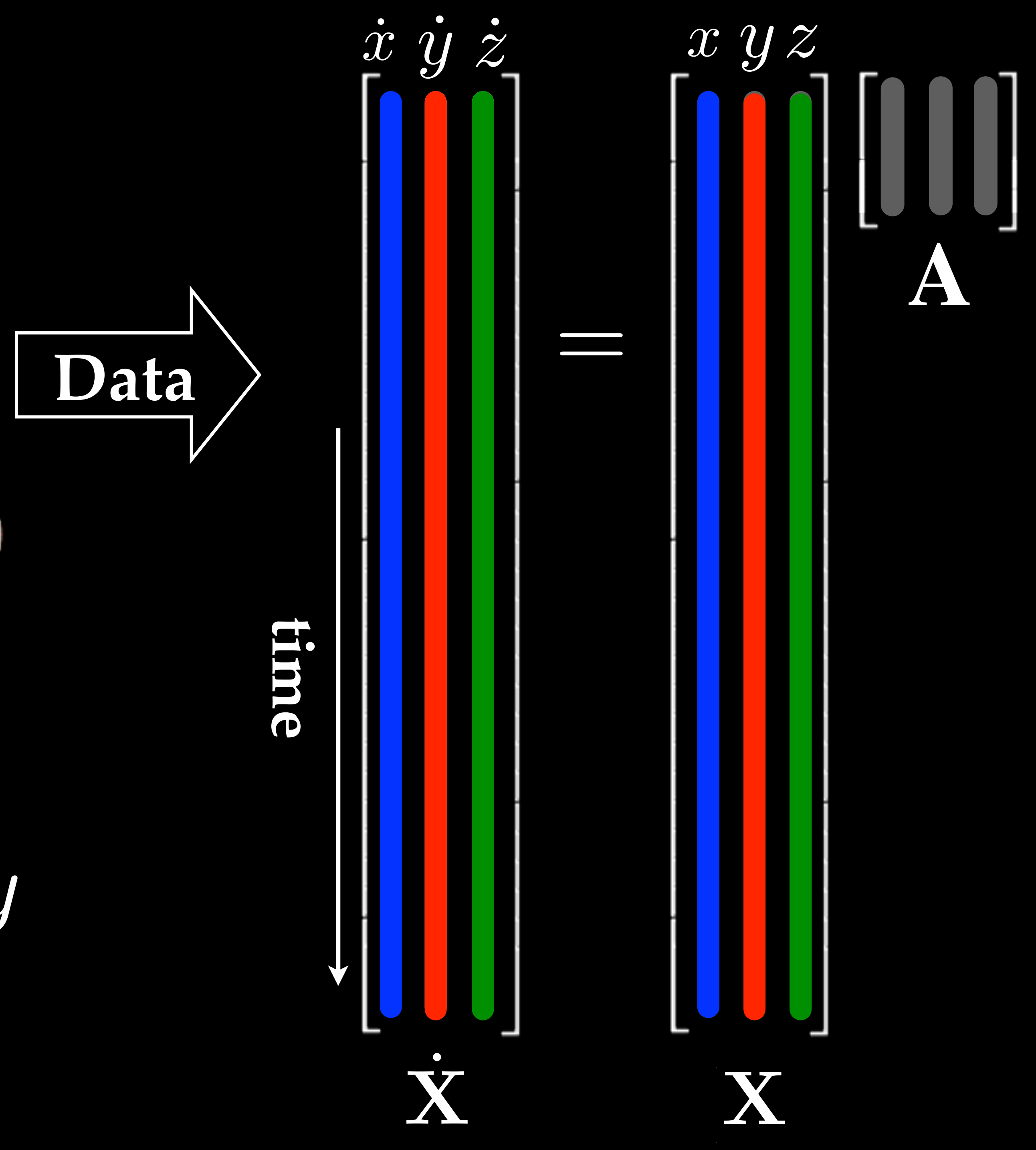


SLB, Proctor, Kutz, *PNAS* 2016.

Sparse Identification of Nonlinear Dynamics (SINDy)



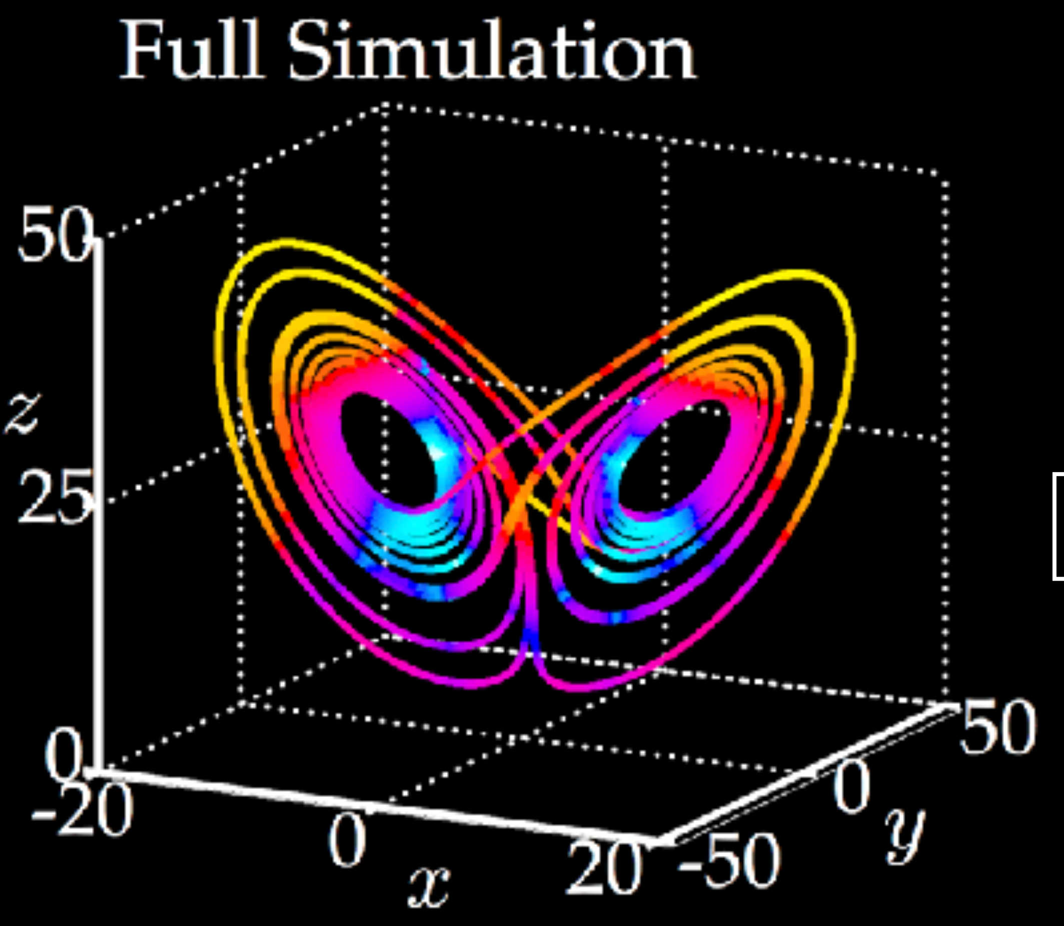
$$\dot{x} = \sigma(y - x)$$
$$\dot{y} = x(\rho - z) - y$$
$$\dot{z} = xy - \beta z.$$



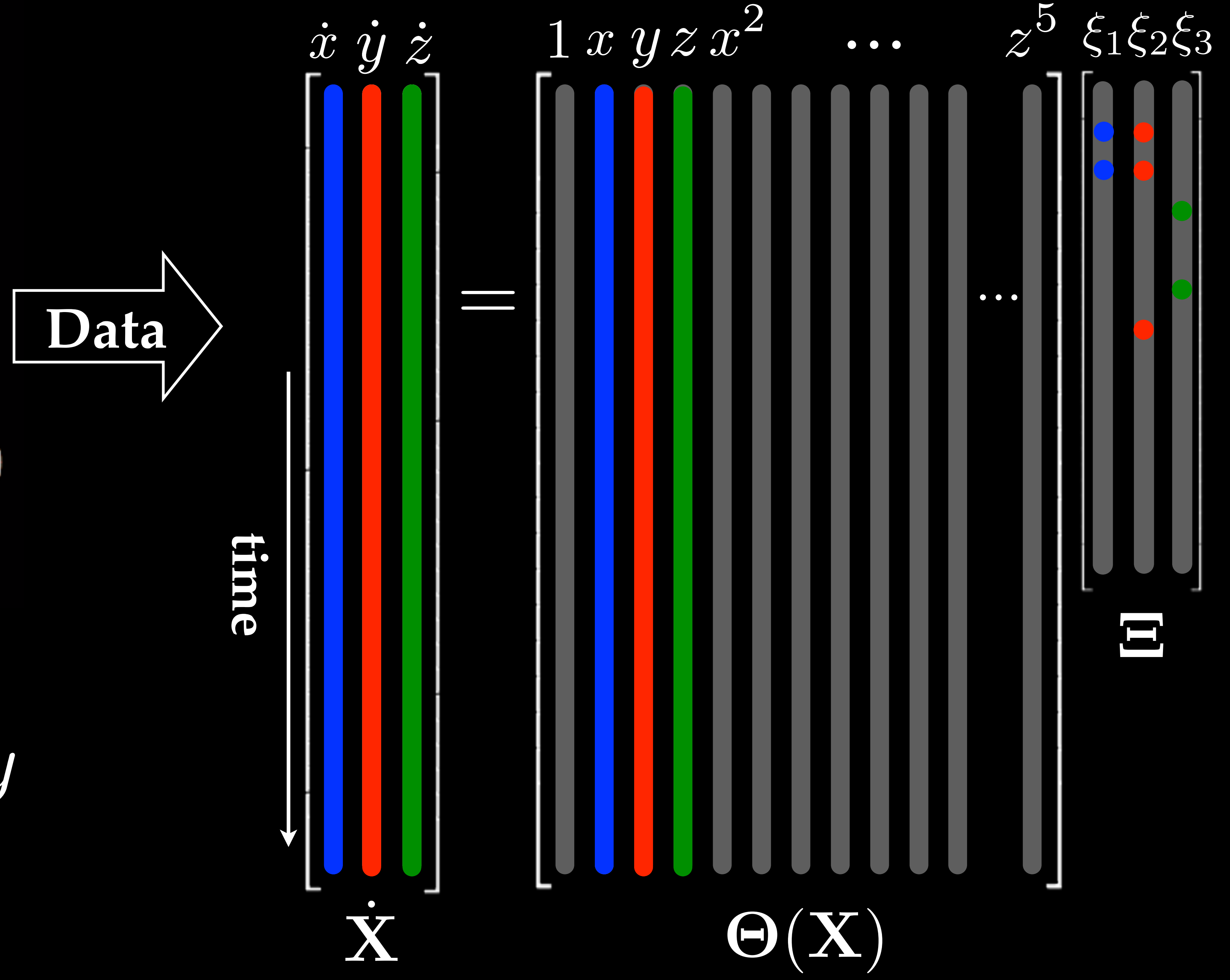
DMD

SLB, Proctor, Kutz, *PNAS* 2016.

Sparse Identification of Nonlinear Dynamics (SINDy)

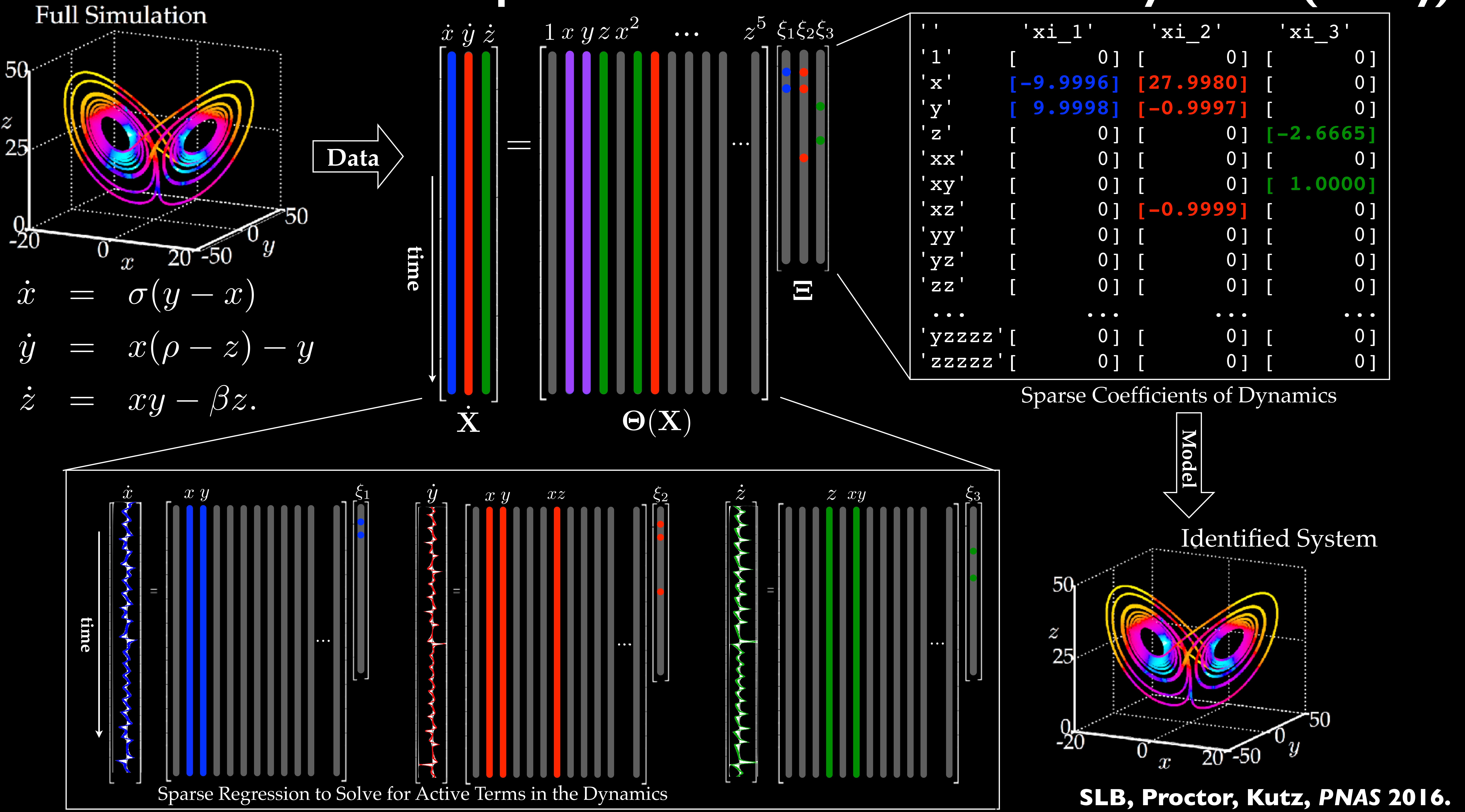


$$\dot{x} = \sigma(y - x)$$
$$\dot{y} = x(\rho - z) - y$$
$$\dot{z} = xy - \beta z.$$



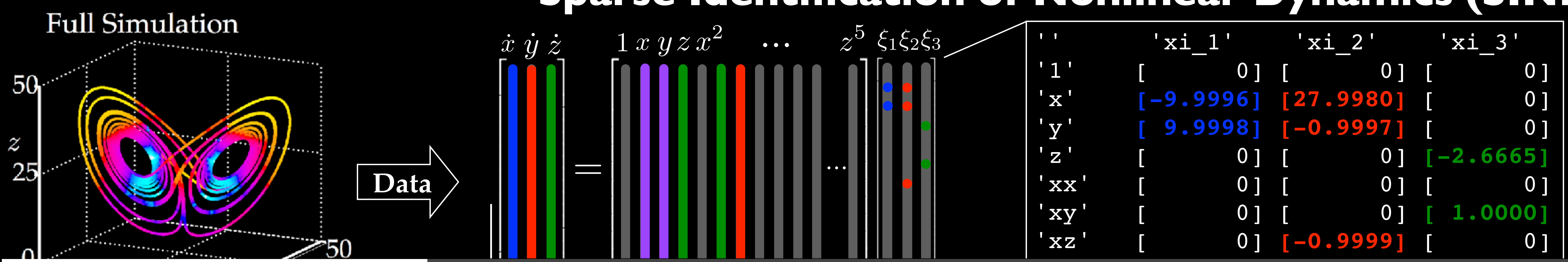
SLB, Proctor, Kutz, *PNAS* 2016.

Sparse Identification of Nonlinear Dynamics (SINDy)



SLB, Proctor, Kutz, *PNAS* 2016.

Sparse Identification of Nonlinear Dynamics (SINDy)

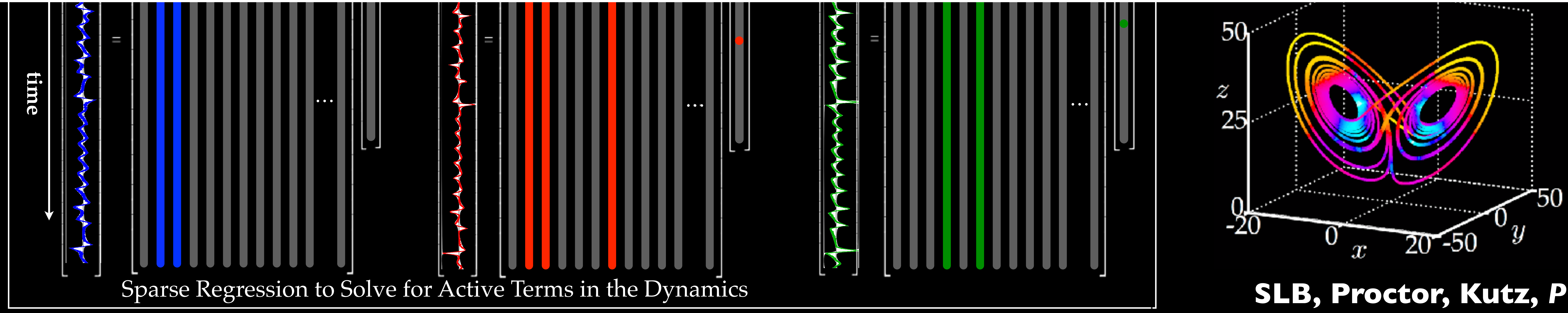


PySINDy

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).

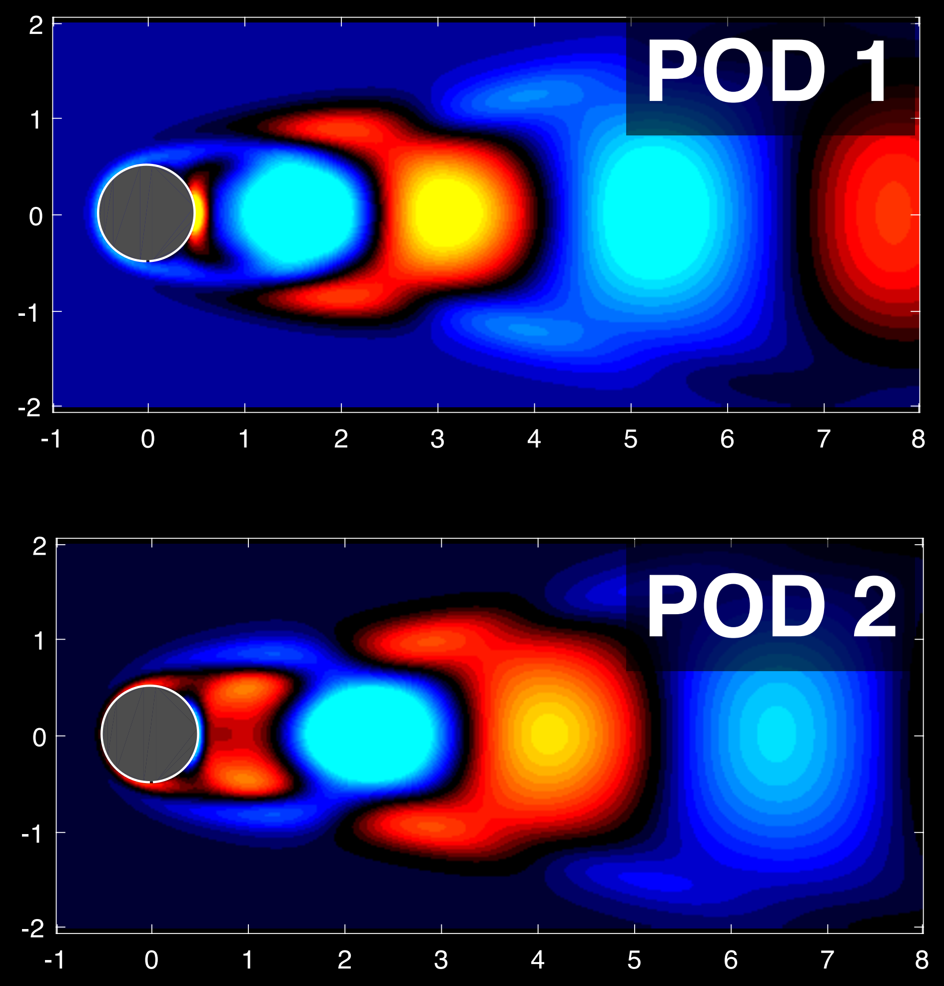


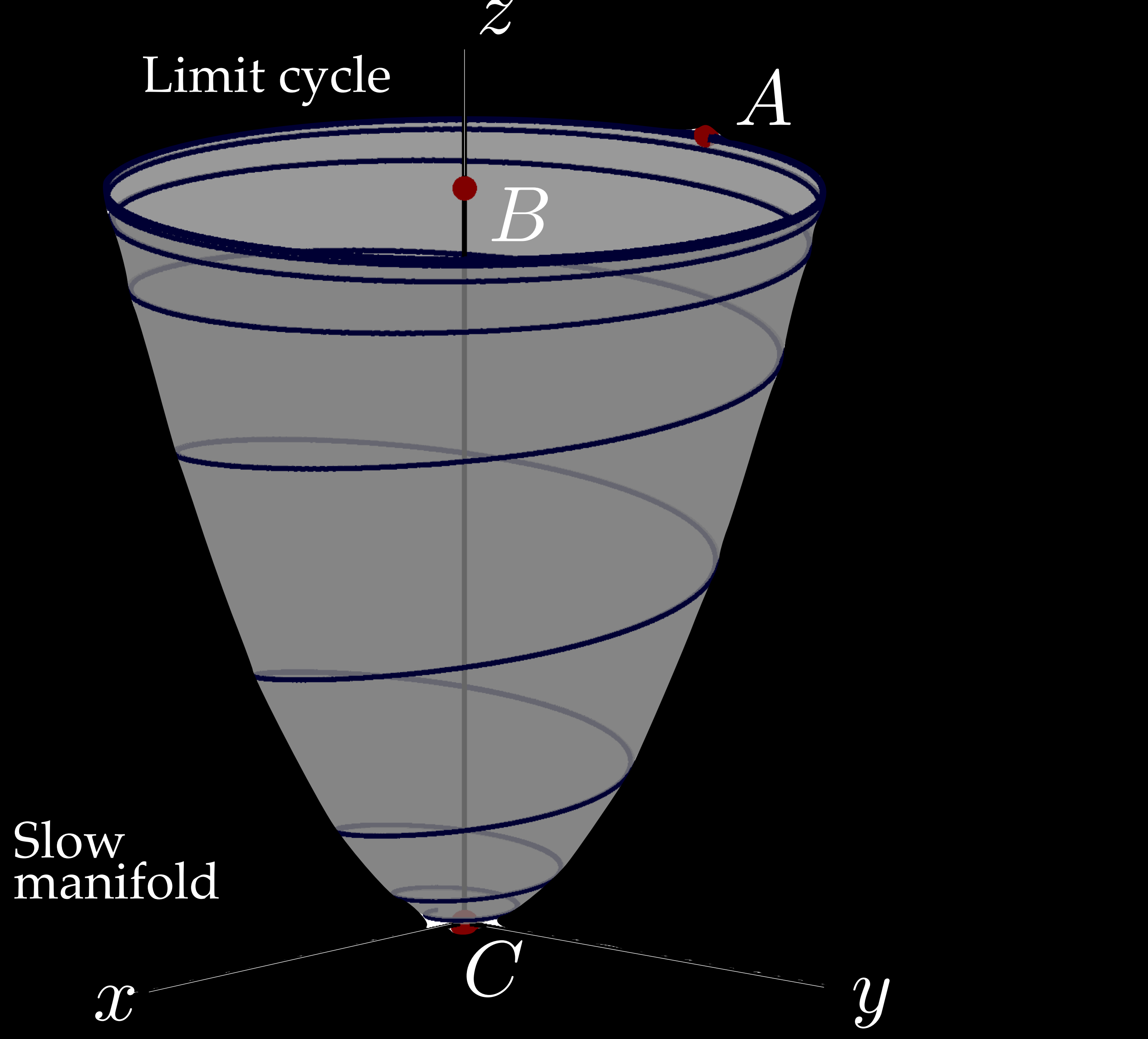
SLB, Proctor, Kutz, *PNAS* 2016.

PDEs

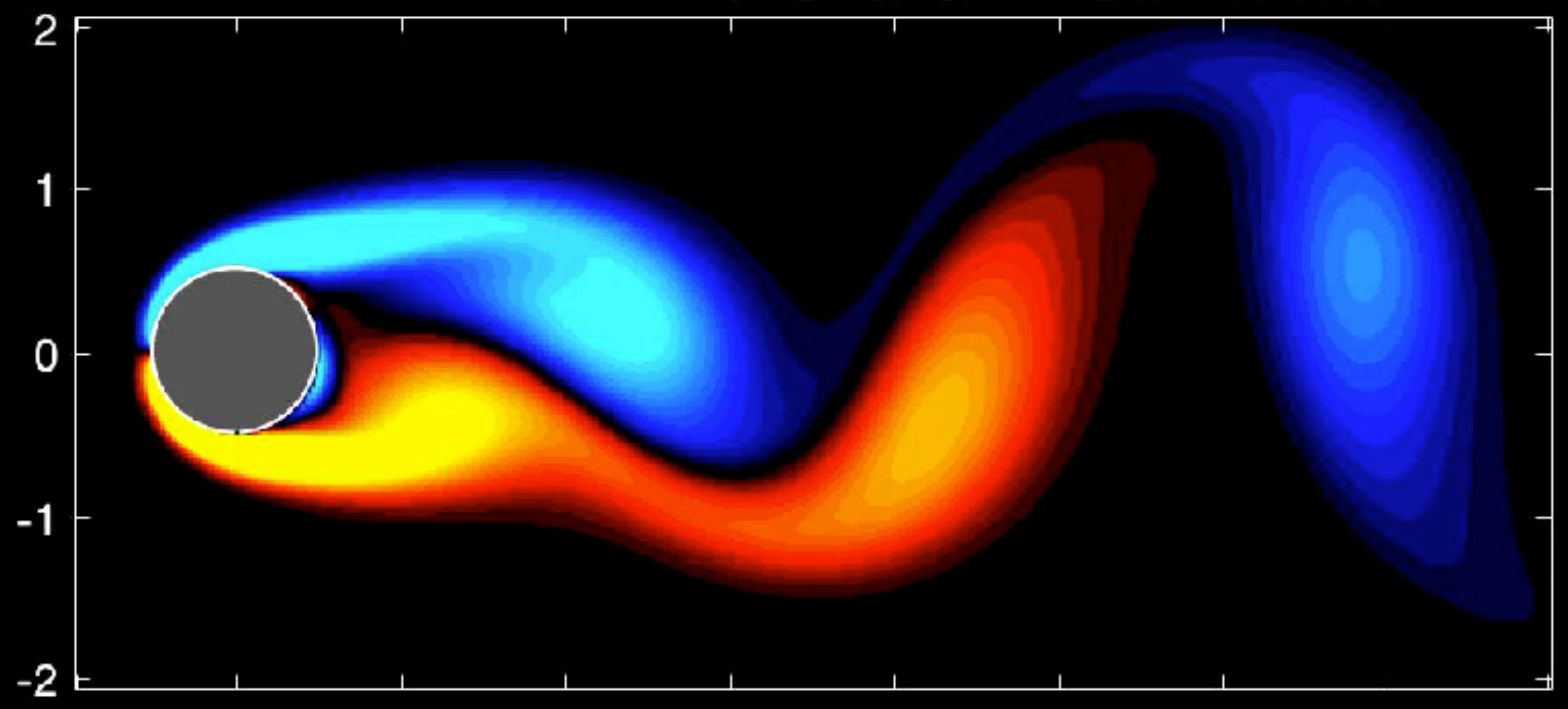
Rudy, SLB, Proctor, Kutz
***Science Advances*, 2017**

REDUCED ORDER MODELS





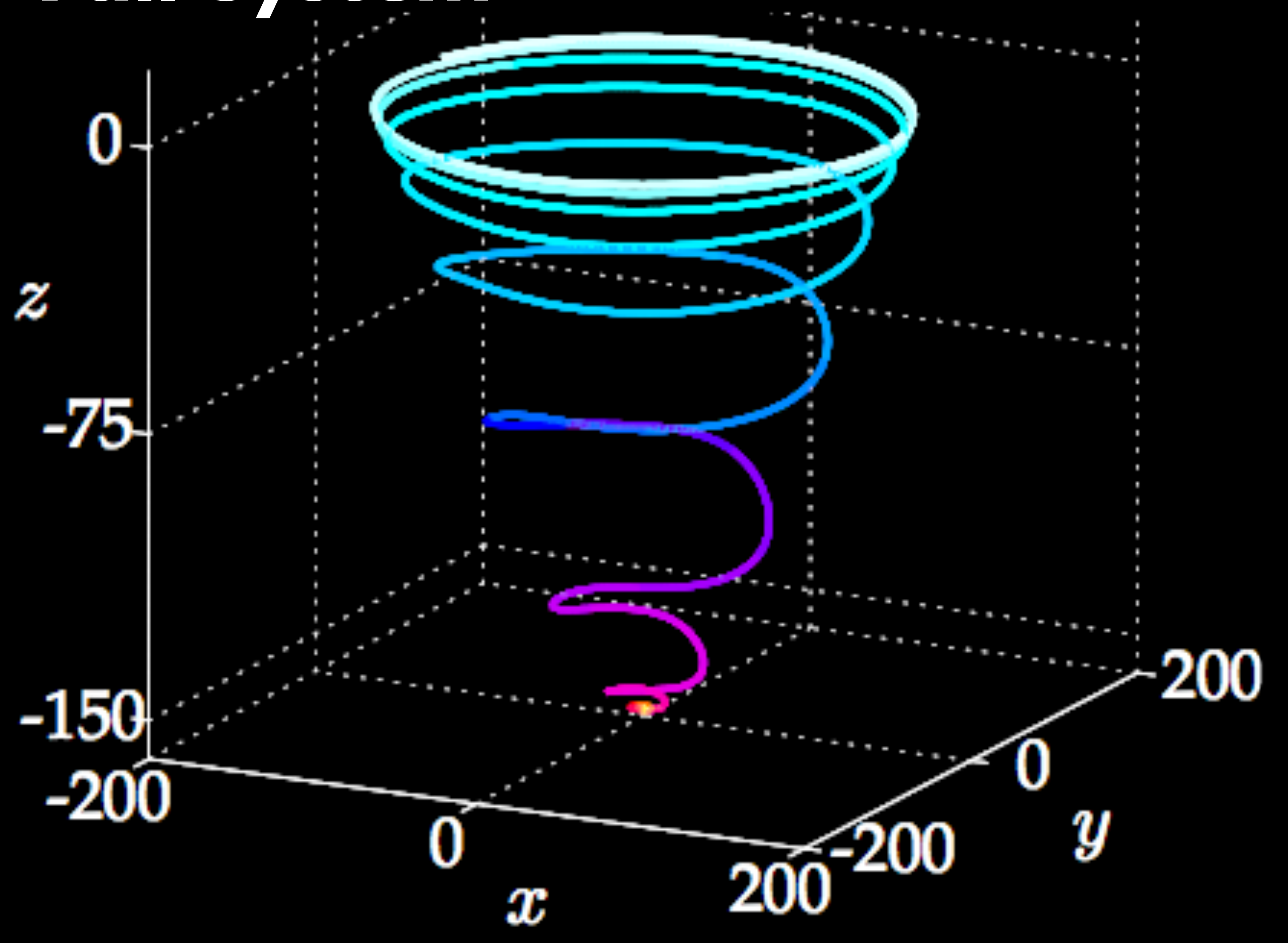
$$\begin{aligned} \dot{x} &= \mu x - \omega y + Axz \\ \dot{y} &= \omega x + \mu y + Ayz \\ \dot{z} &= -\lambda(z - x^2 - y^2). \end{aligned}$$



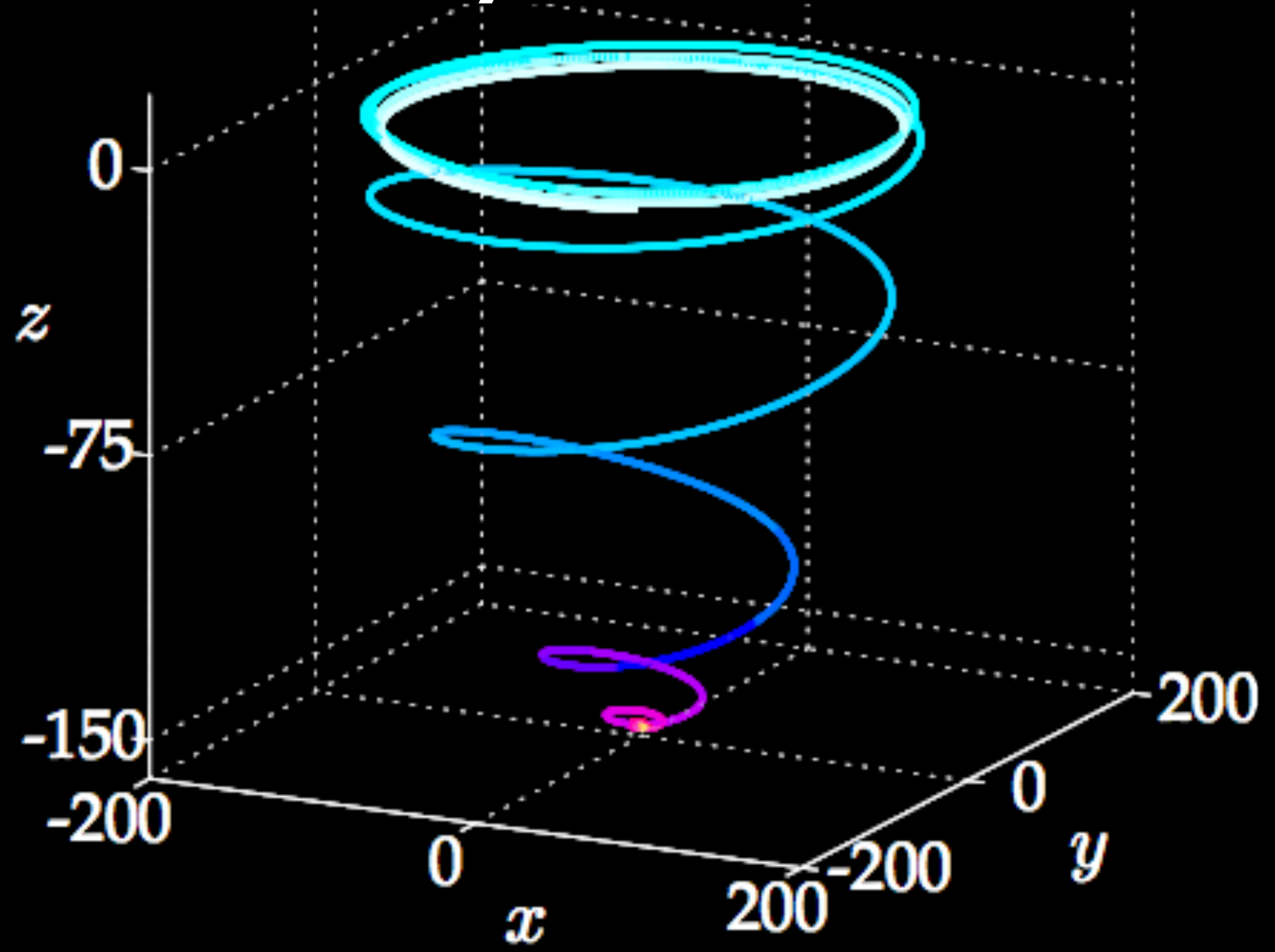
Noack *et al.*, JFM 2003.

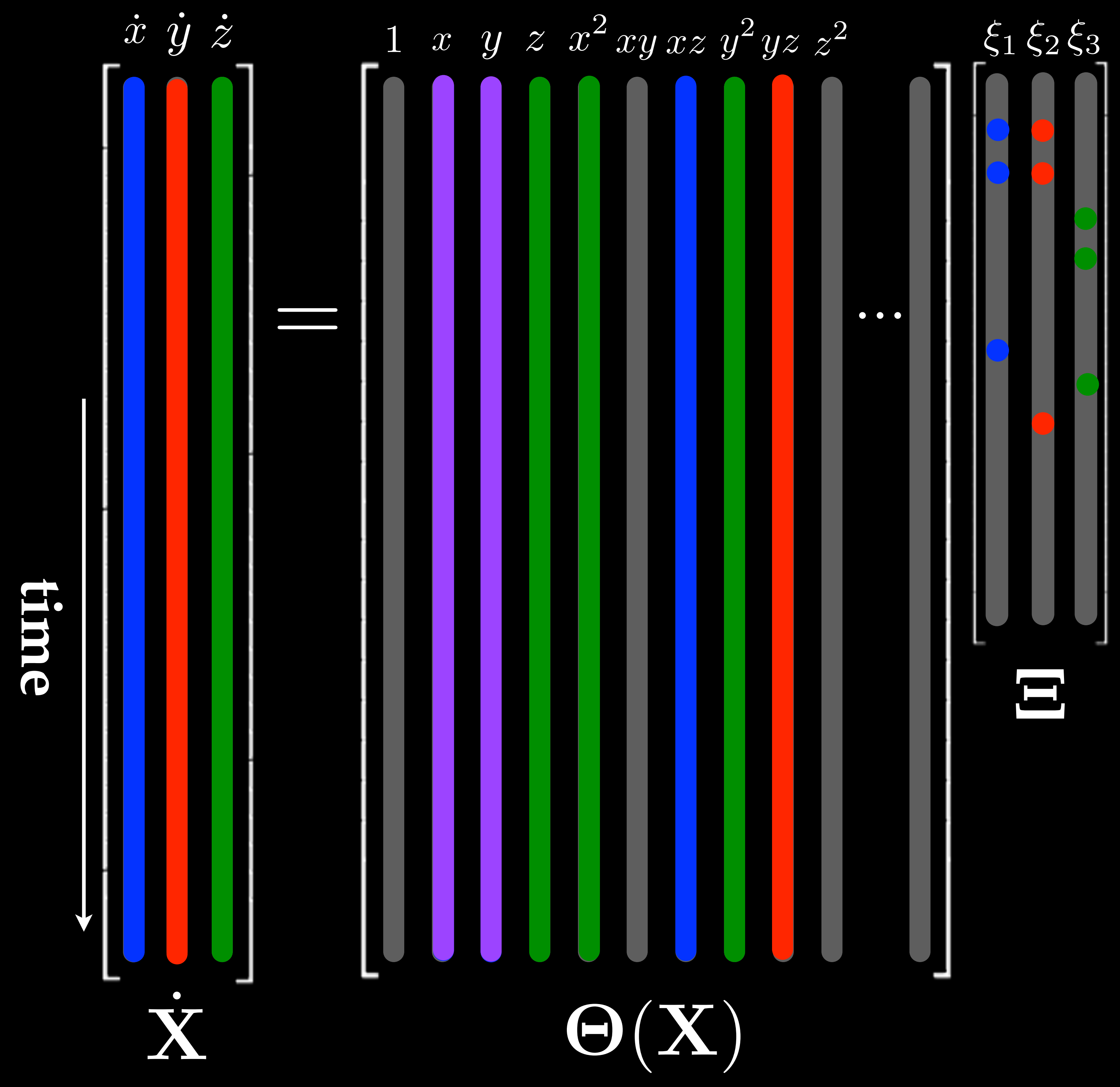
Sparse Identification of Nonlinear Dynamics (SINDy)

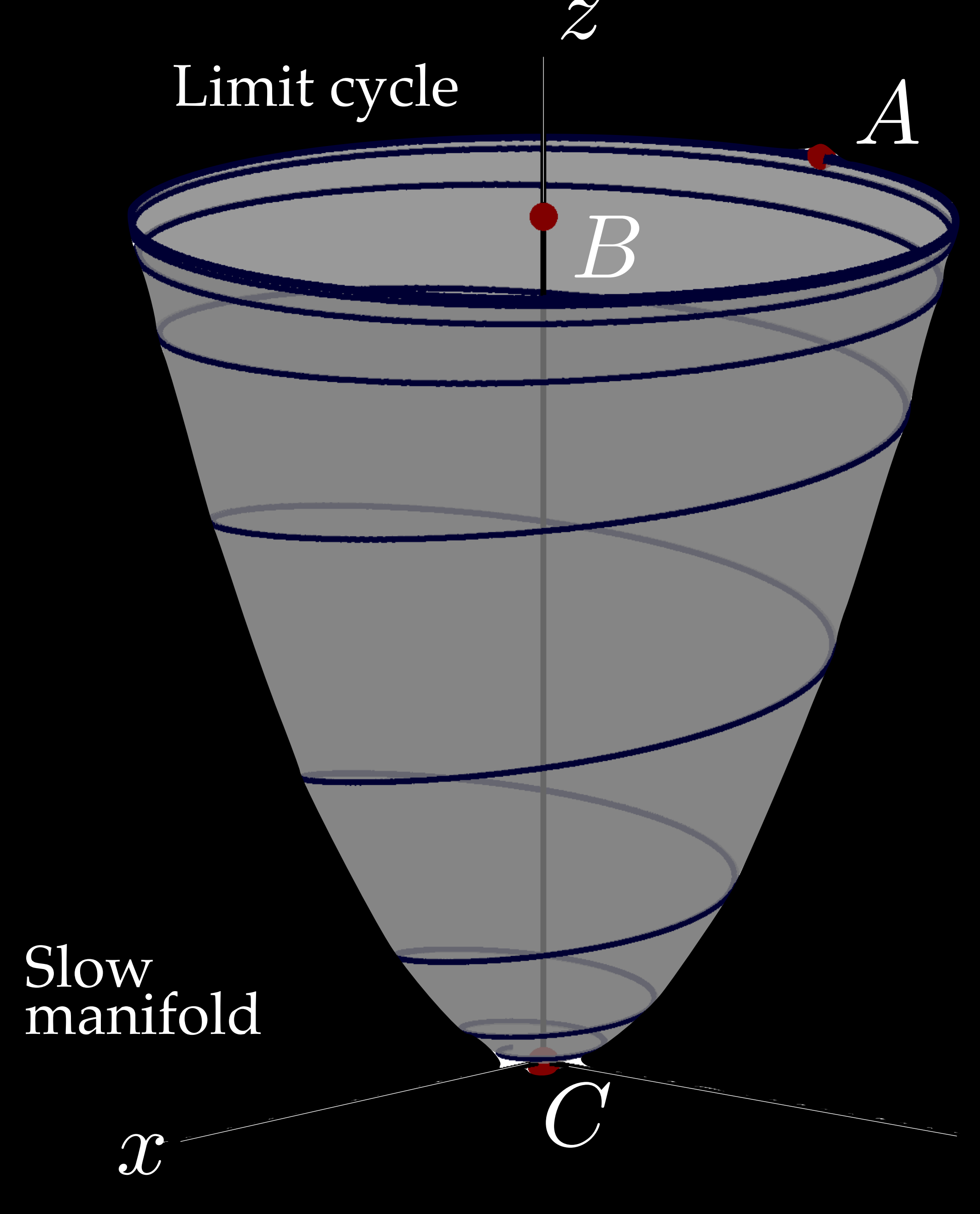
Full System



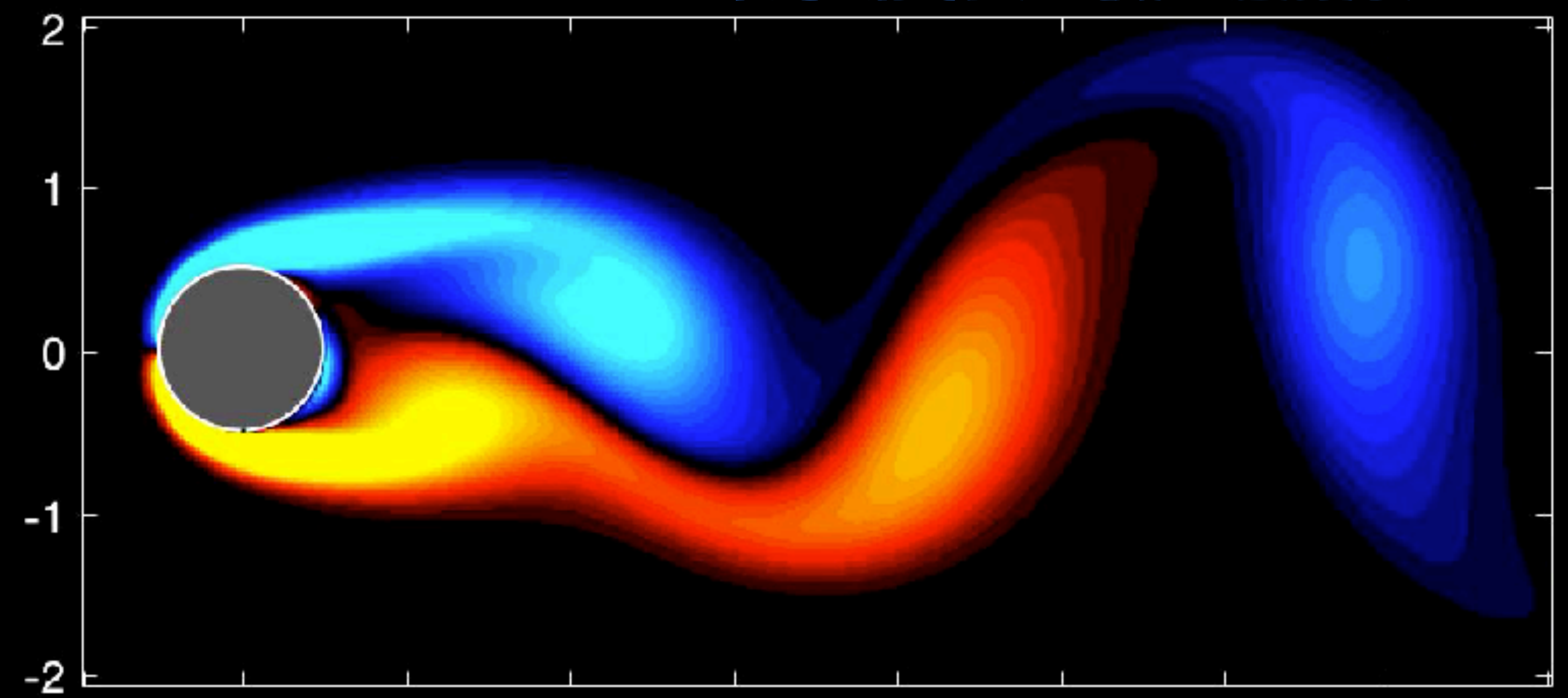
Identified System





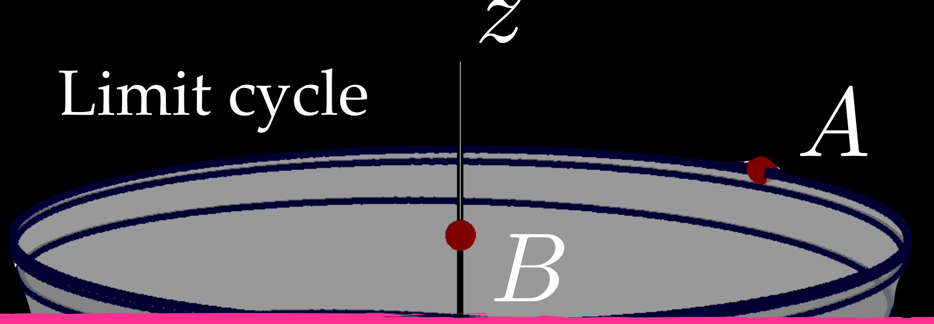


$$\begin{aligned}
\dot{x} &= \mu x - \omega y + Axz \\
\dot{y} &= \omega x + \mu y + Ayz \\
\dot{z} &= -\lambda(z - x^2 - y^2).
\end{aligned}$$

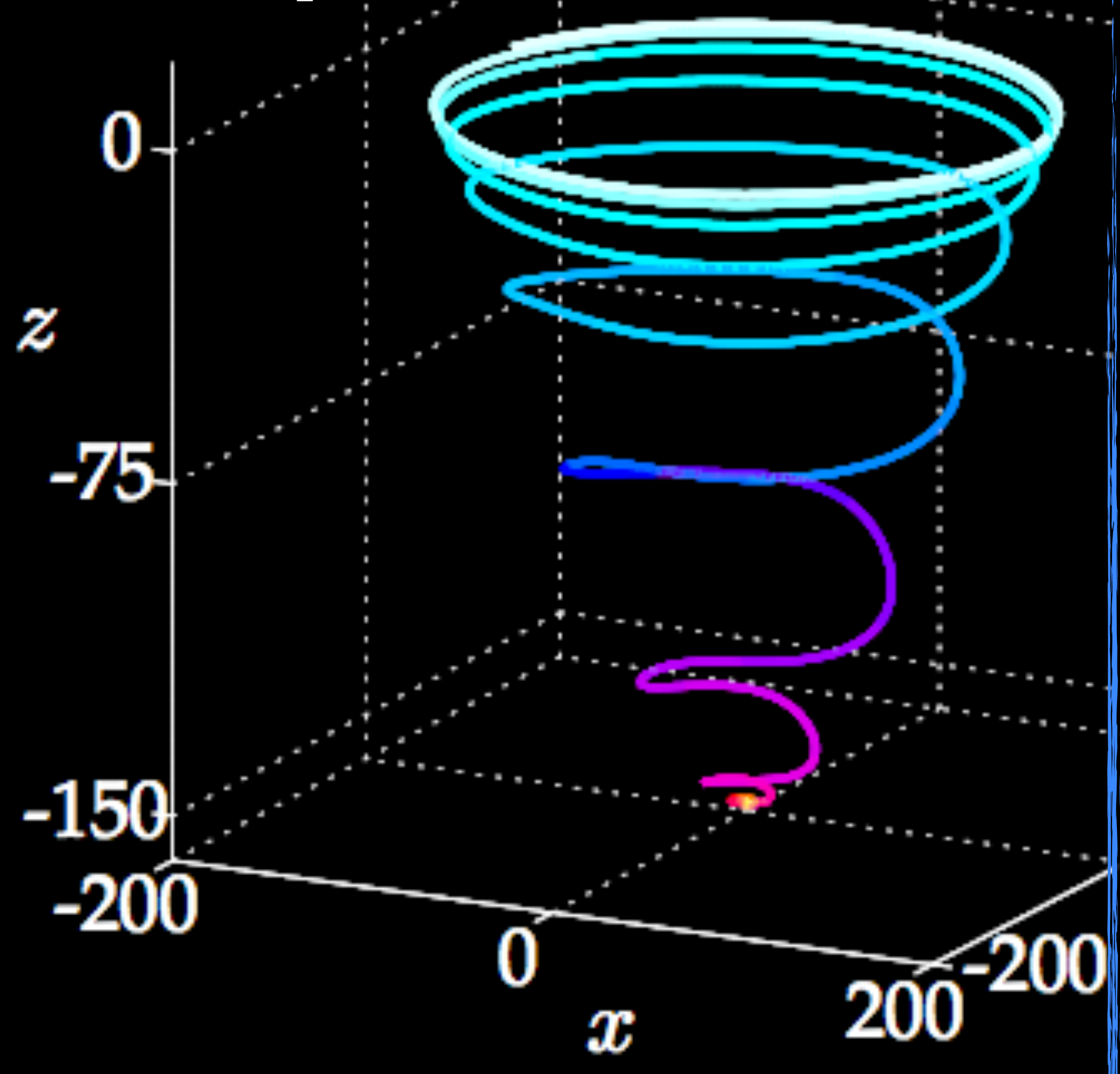


SLB, Proctor, Kutz, *PNAS* 2016.
Loiseau & SLB, *JFM* 838, 2018

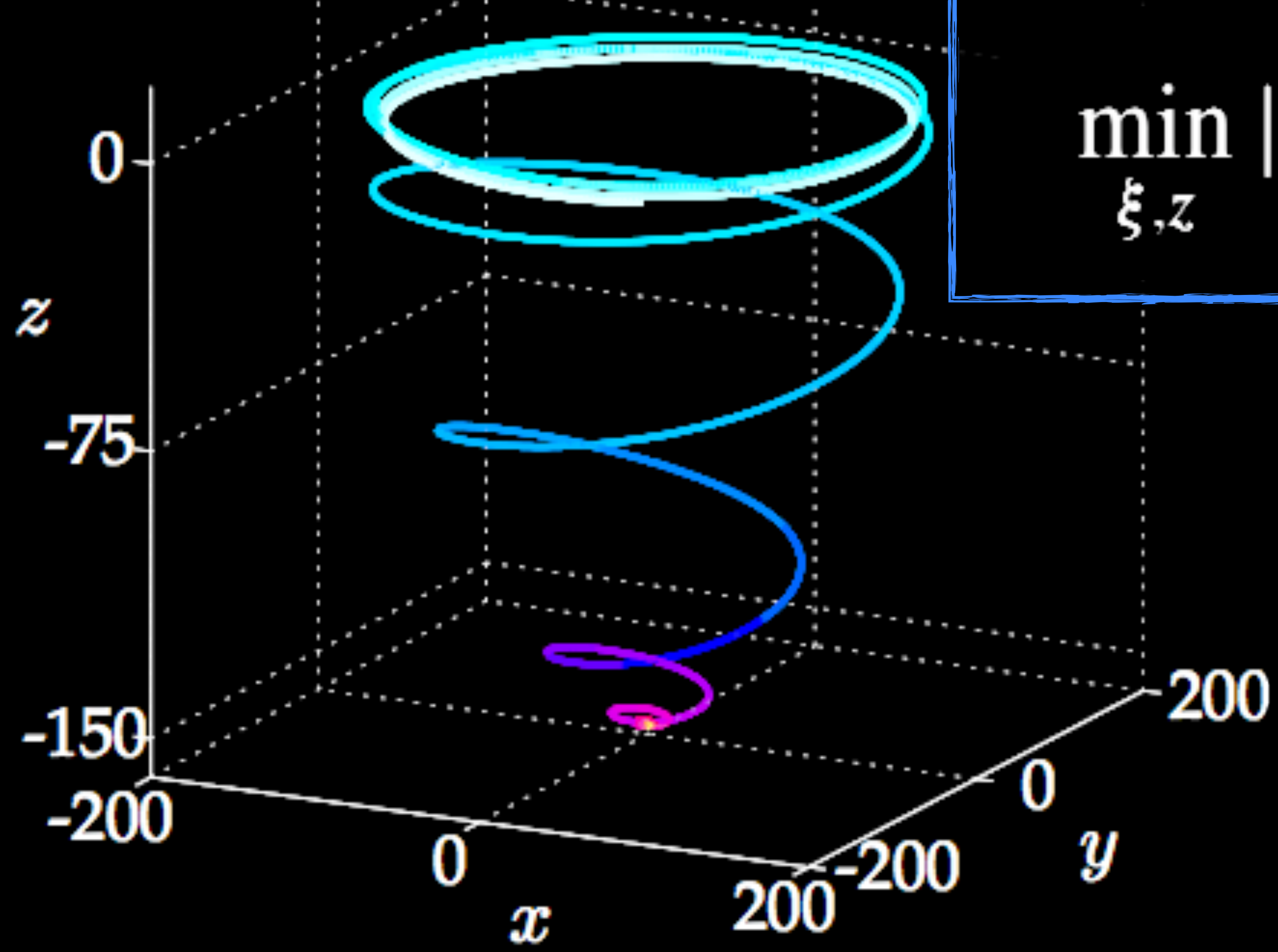
Sparse Identification of Nonlinear Dynamics (SINDy)



Full System



Identified System



Innovation 1: Enforcing known constraints

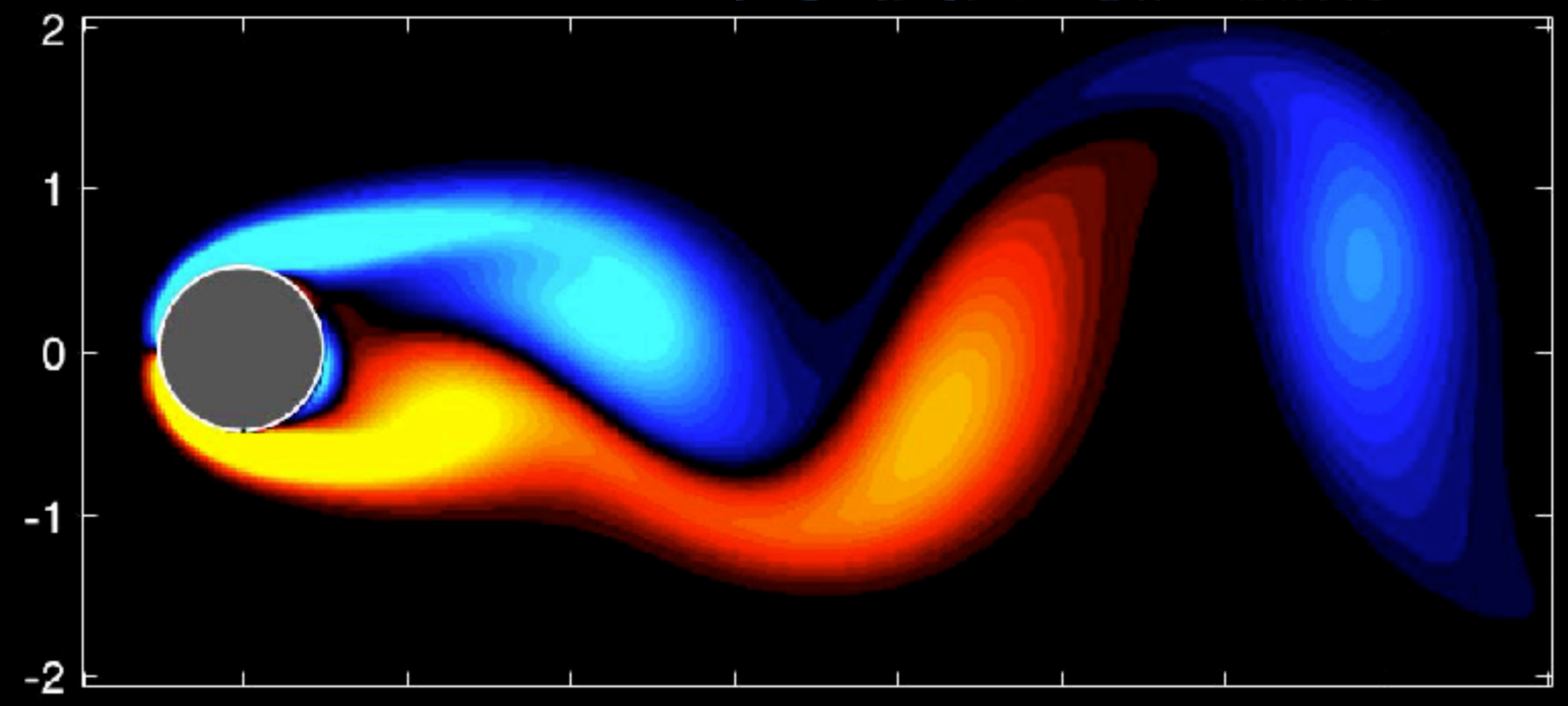
- Skew-symmetric quadratic nonlinearities to enforce energy conservation
- Improved stability

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

Innovation 2: Higher-order Nonlinearities

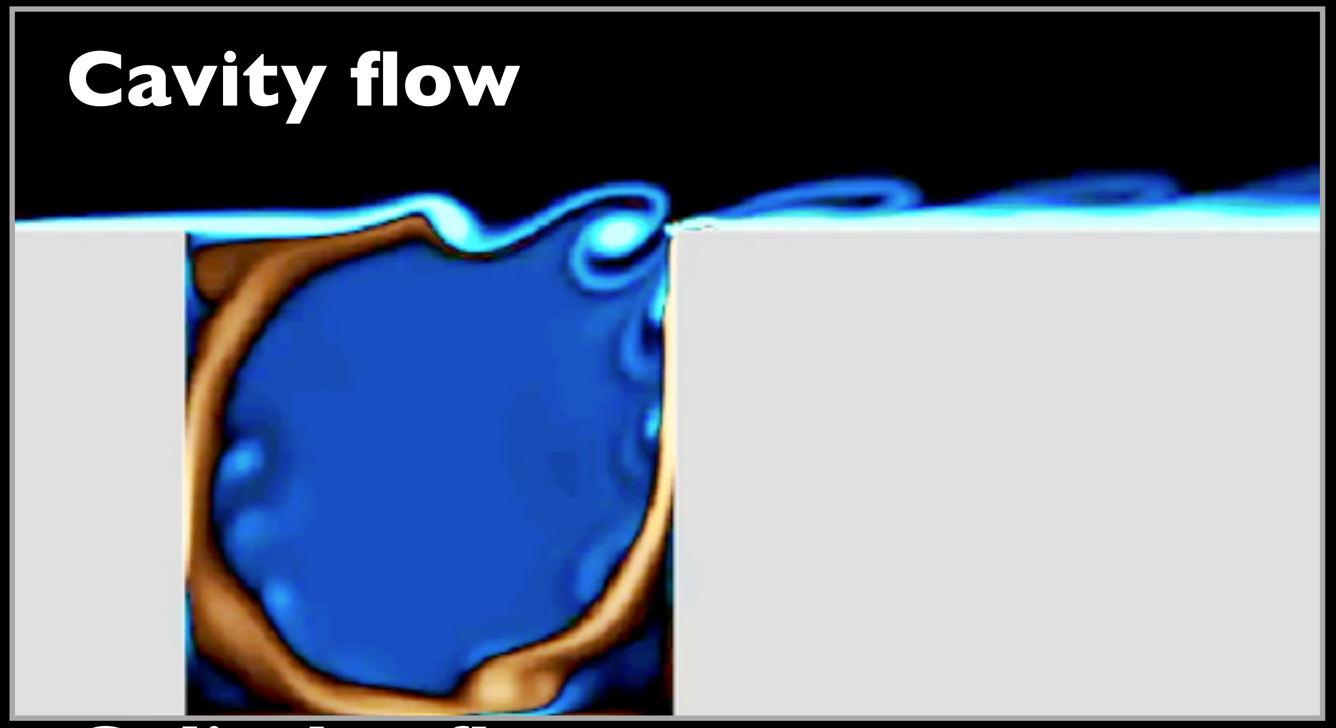
- Cubic, Quintic, Septic terms approximate truncated terms in Galerkin expansion

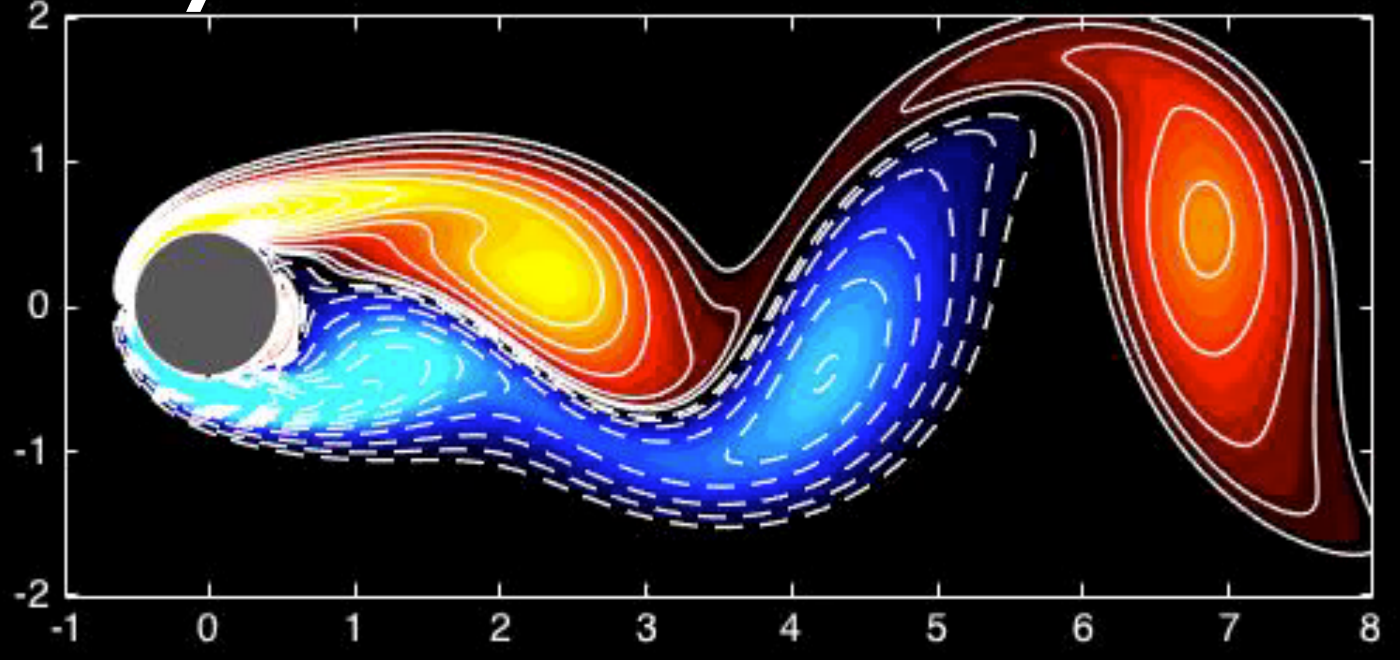
$$\begin{aligned} \dot{x} &= \mu x - \omega y + Axz \\ \dot{y} &= \omega x + \mu y + Ayz \\ \dot{z} &= -\lambda(z - x^2 - y^2). \end{aligned}$$

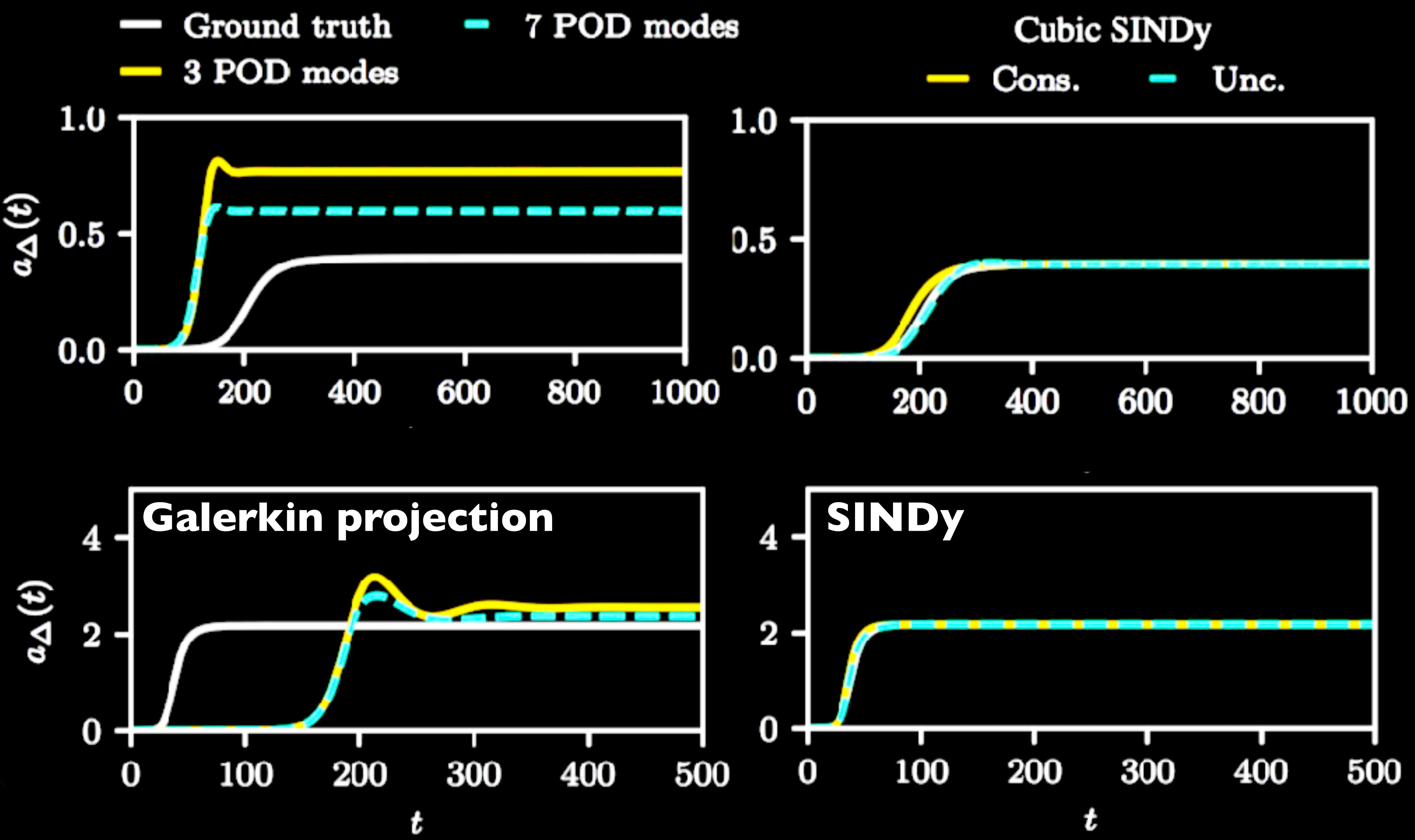


SLB, Proctor, Kutz, *PNAS* 2016.
Loiseau & SLB, *JFM* 838, 2018

Constrained Sparse Galerkin Regression





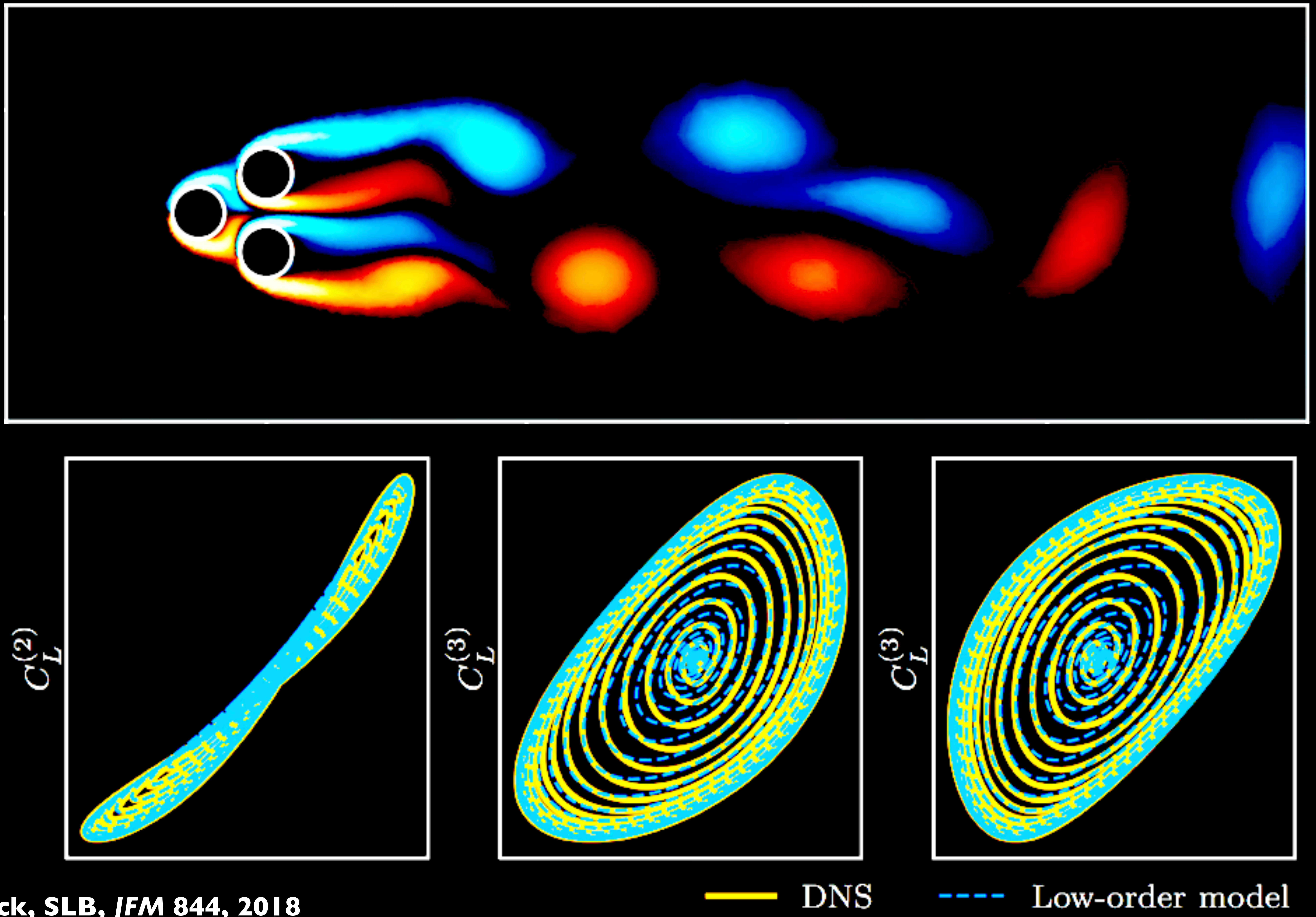


$$\ddot{x} - \underbrace{\left(0.2 - 0.24x^2 - 0.15\dot{x}^2\right)}_{k(x,\dot{x})}\dot{x} + 1.26x = 0$$

Spring-Mass Damper with Nonlinear Damping!

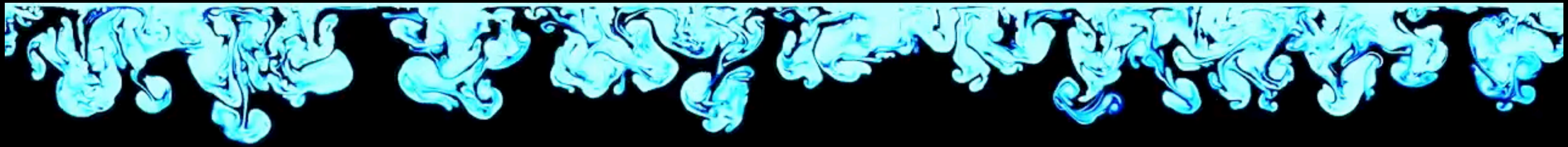
Loiseau & SLB, *JFM* 838, 2018

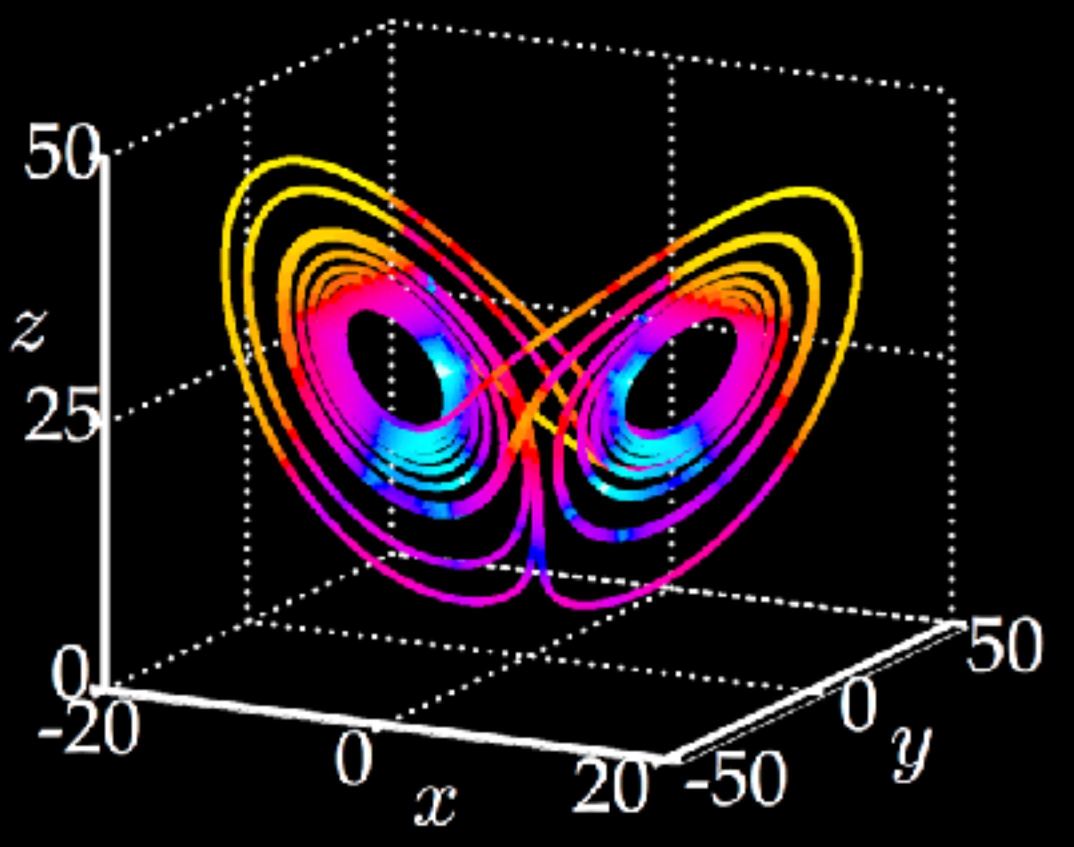
More Complex Flow: Fluidic Pinball



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

CHAOTIC THERMAL CONVECTION



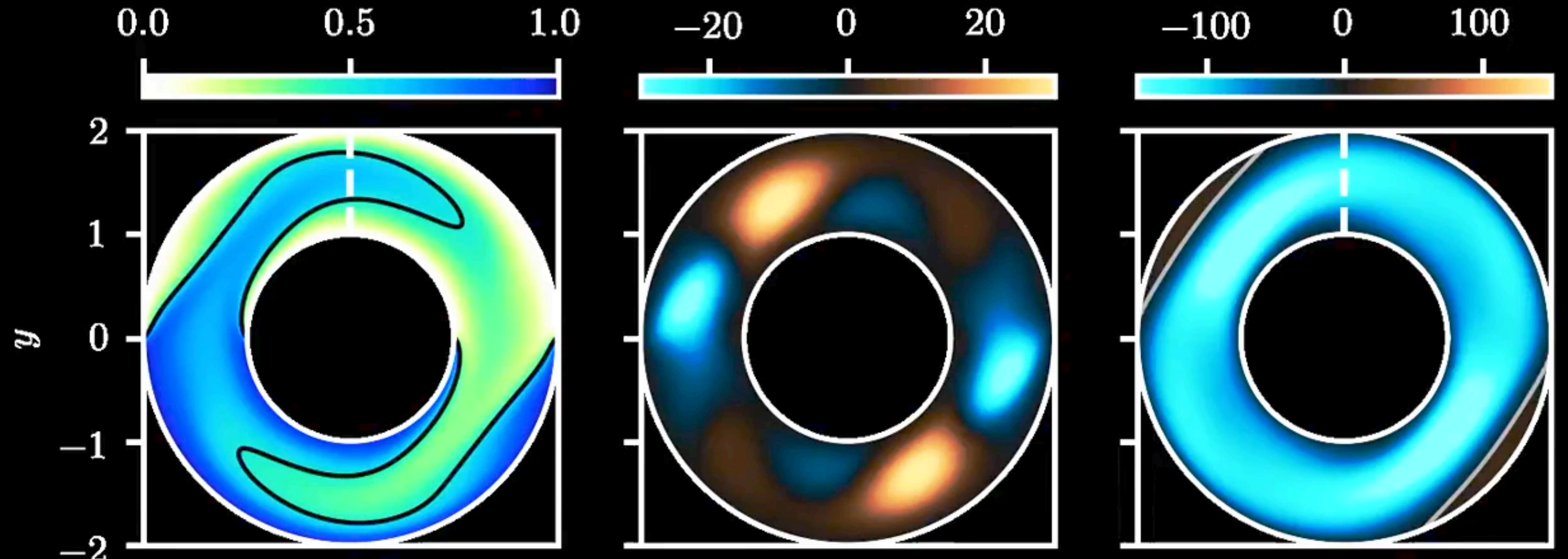


$$
\begin{aligned}
\dot{x} &= \sigma(y - x) \\
\dot{y} &= x(\rho - z) - y \\
\dot{z} &= xy - \beta z.
\end{aligned}
$$

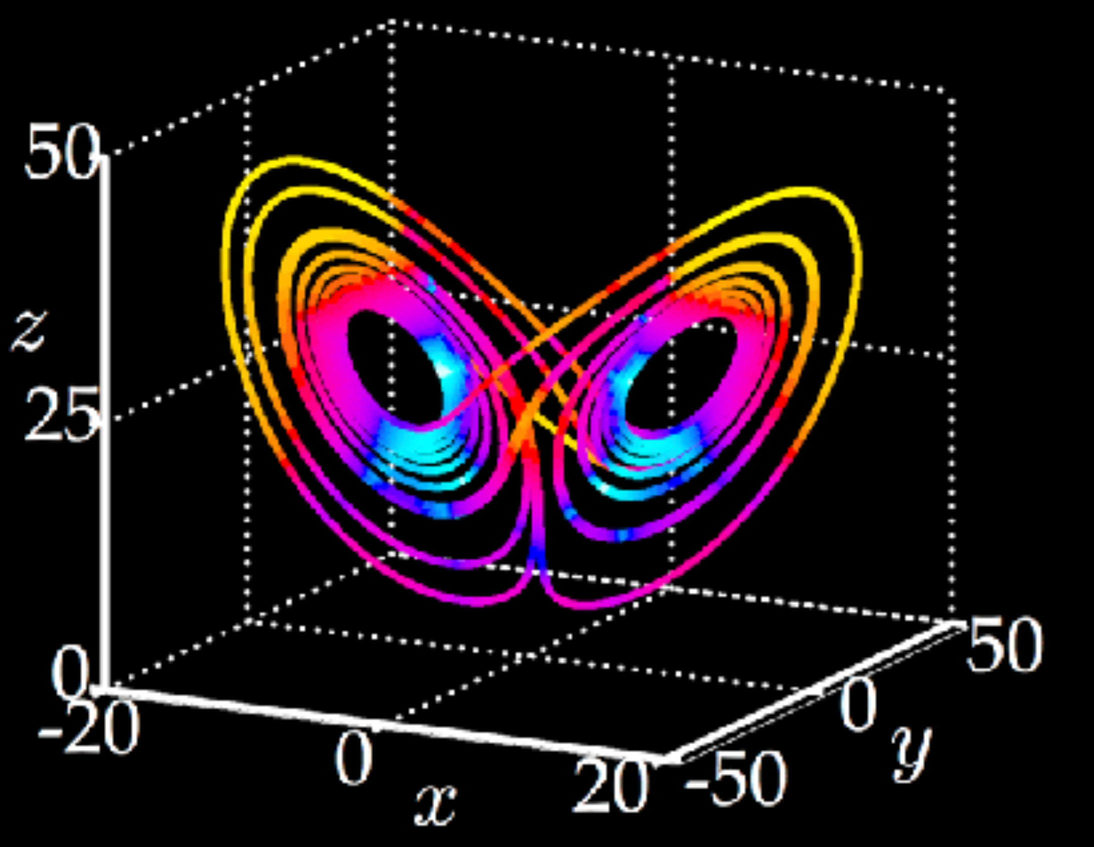
YouTube: turbulenceteam

Lorenz, Fetter, Hamilton, 1963

CHAOTIC THERMAL CONVECTION



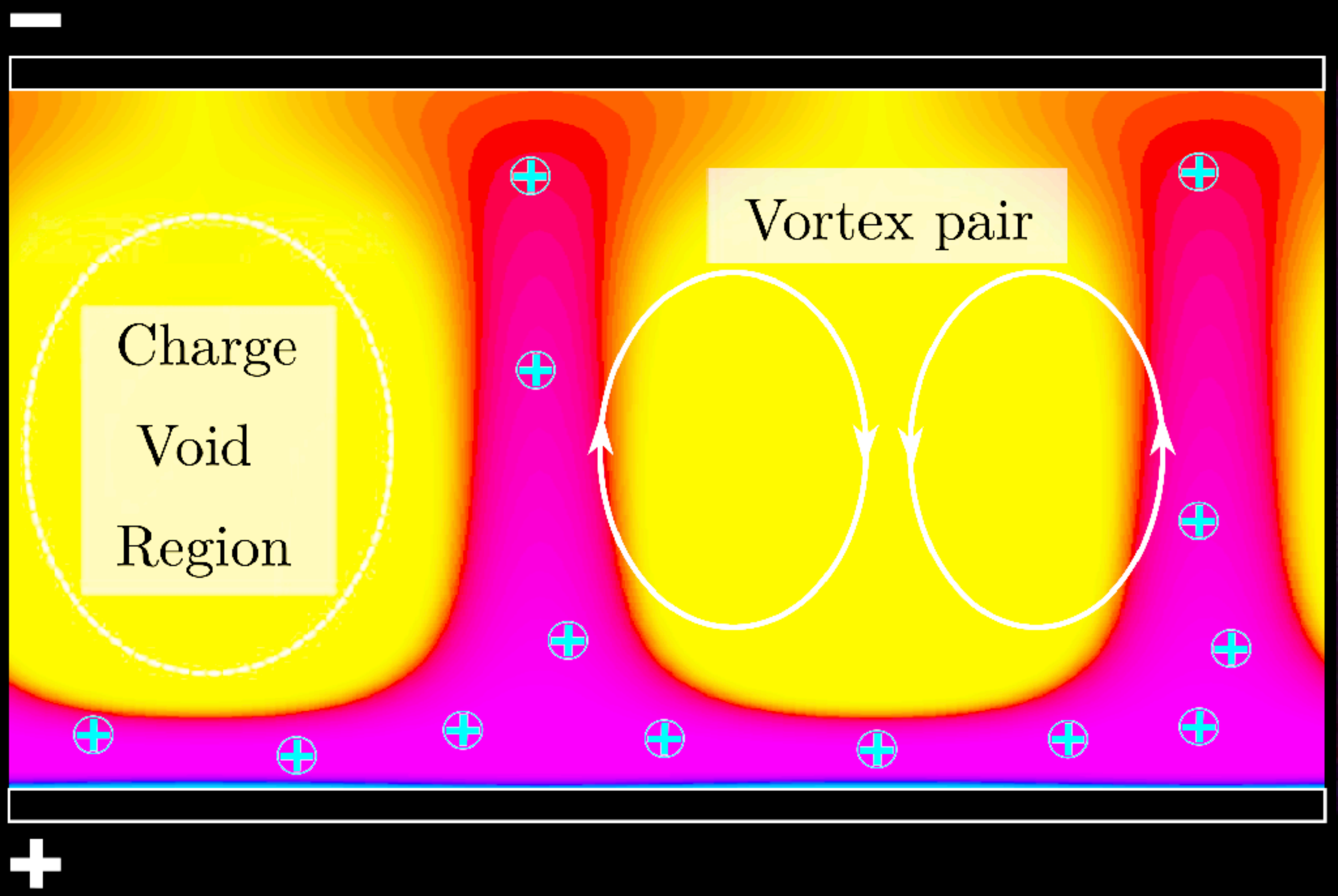
(a) Temperature (b) Radial velocity (c) Azimuthal velocity



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

JC Loiseau, *TCFD* 2020

CHAOTIC ELECTROCONVECTION



Three way coupling:

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

$$\nabla \cdot \mathbf{u}^* = 0$$

$$\rho \frac{D\mathbf{u}^*}{Dt^*} = -\nabla P^* + \mu \nabla^2 \mathbf{u}^* - \rho_c^* \nabla \phi^*$$

$$\frac{\partial \rho_c^*}{\partial t^*} = -\nabla \cdot [(\mathbf{u}^* - \mu_b \nabla \phi^*)\rho_c^* - D_c \nabla \rho_c^*]$$

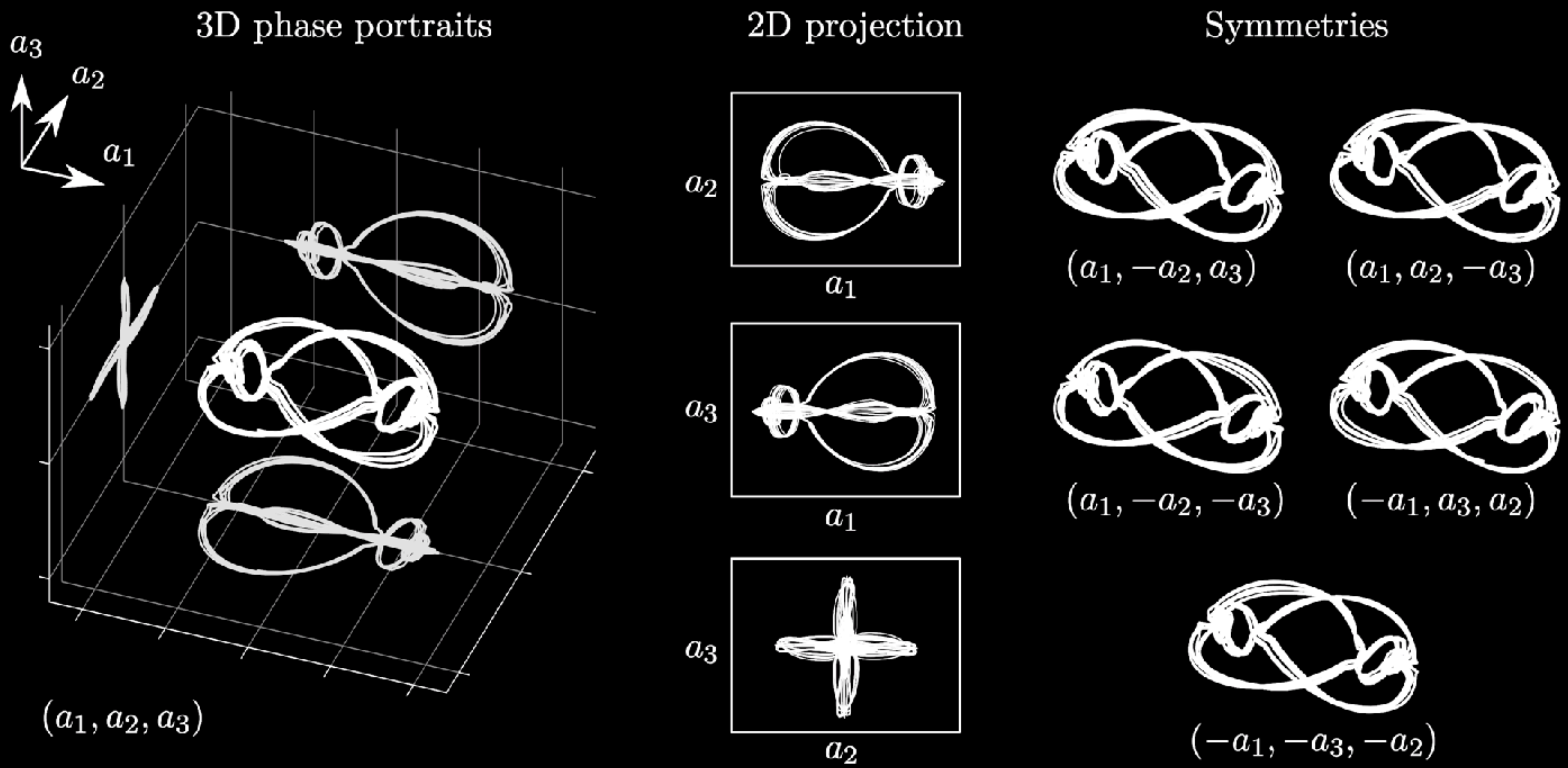
$$\nabla^2 \phi^* = -\frac{\rho_c^*}{\epsilon}$$

Guan, SLB, Novosselov, *arXiv 2020*

Chaotic Electroconvection

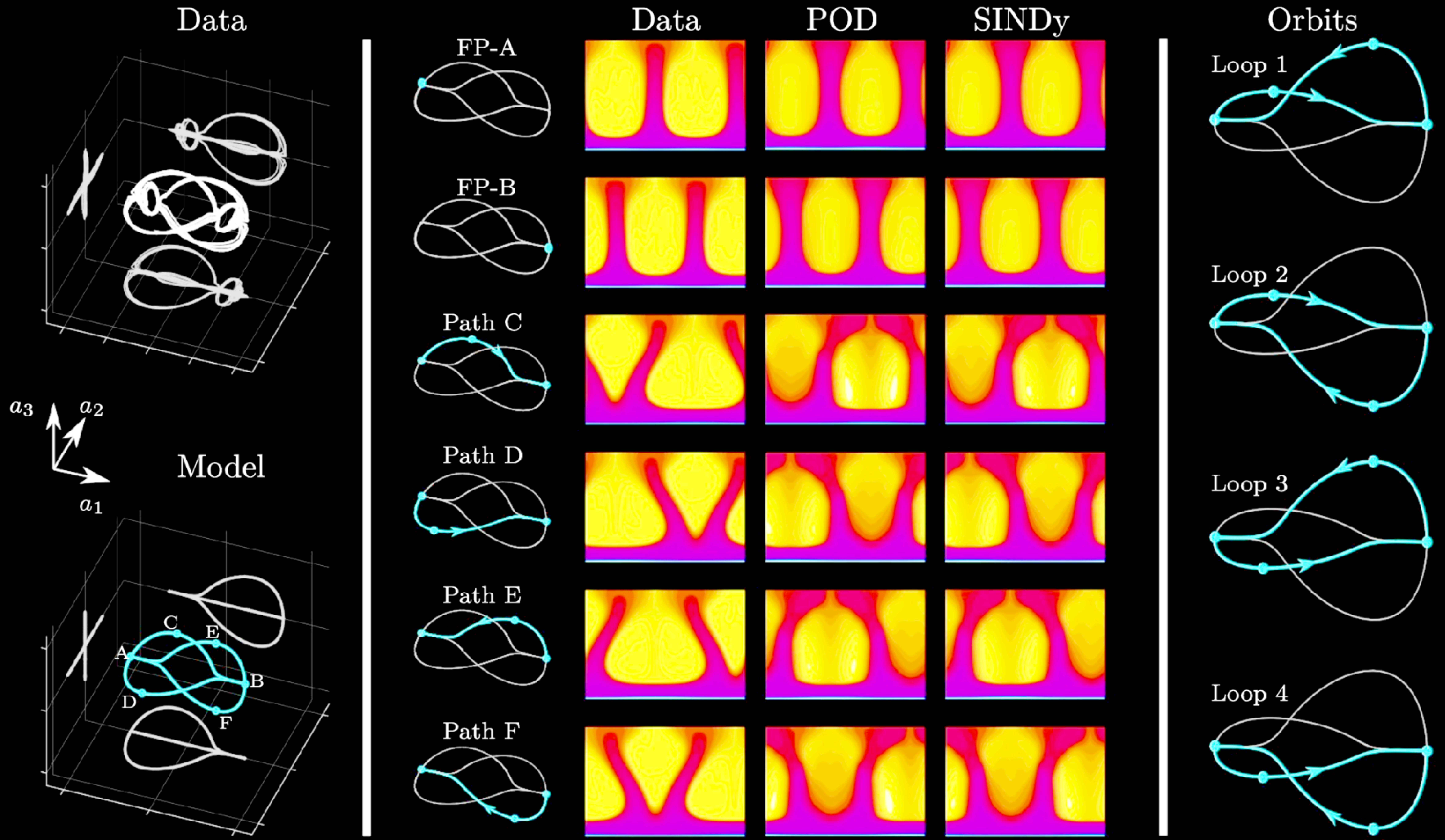
Guan, SLB, Novosselov, *arXiv 2020*

Symmetry in the Data



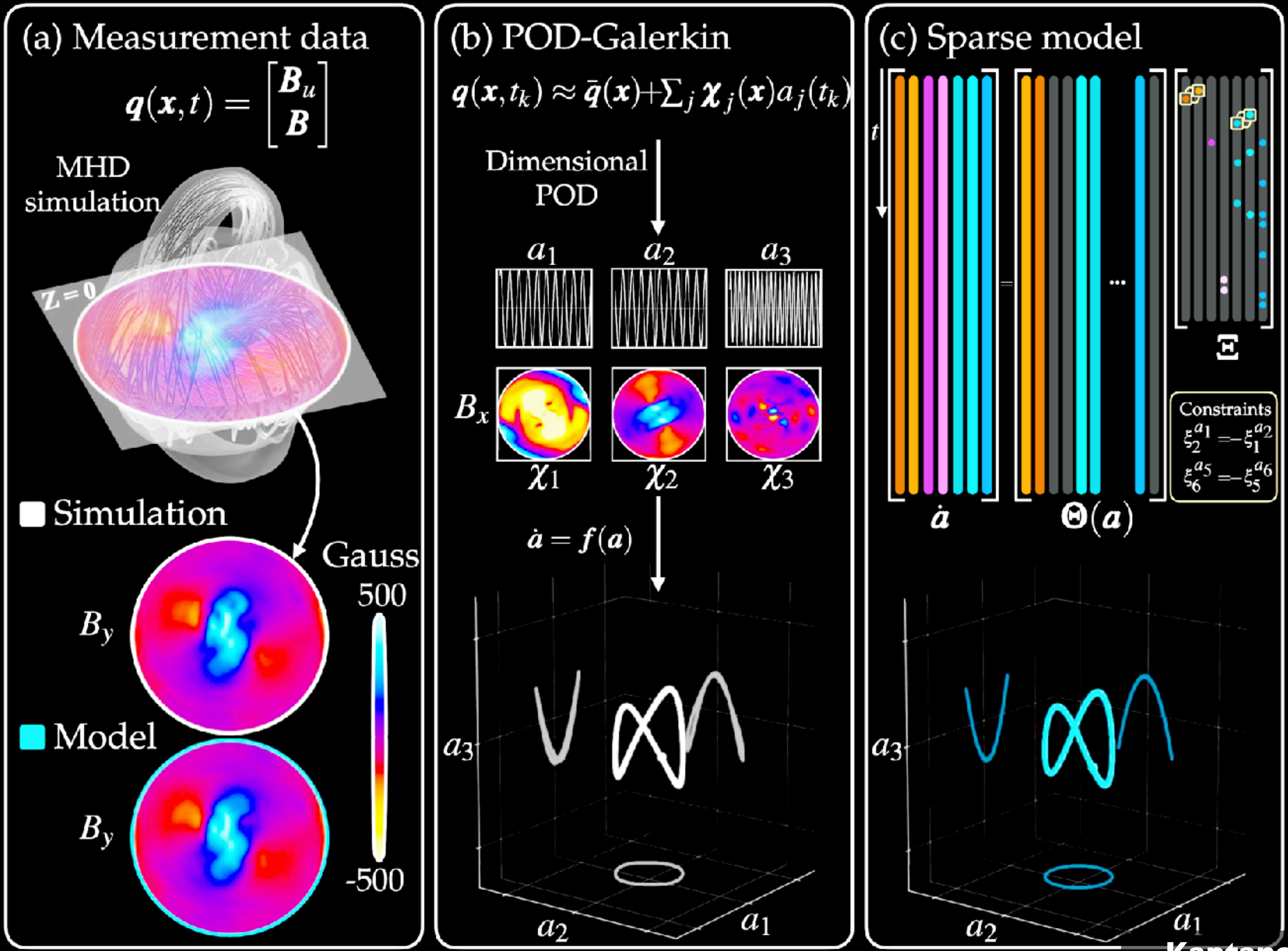
	a_1	a_2	a_3	a_1^2	a_1a_2	a_1a_3	a_2^2	a_2a_3	a_3^2	a_1^3	$a_1^2a_2$	$a_1^2a_3$	$a_1a_2^2$	$a_1a_2a_3$	$a_1a_3^2$	a_2^3	$a_2^2a_3$	$a_2a_3^2$	a_3^3
$\dot{a}_1$	ξ_1						ξ_2		$-\xi_2$	ξ_3			ξ_4		ξ_4				
$\dot{a}_2$		ξ_5			$-\xi_2$						ξ_6					ξ_7		ξ_8	
$\dot{a}_3$			ξ_5			ξ_2						ξ_6					ξ_8		ξ_7

Guan, SLB, Novosselov, *arXiv 2020*



Guan, SLB, Novosselov, *arXiv 2020*

MAGNETOHYDRODYNAMICS (MHD)



Kaptanoglu, Morgan, Hansen, SLB, *arXiv 2020*

Langevin Regression

Describes evolution of trajectories

Langevin equation

$$\dot{x} = f(x) + \sigma(x)w(t)$$

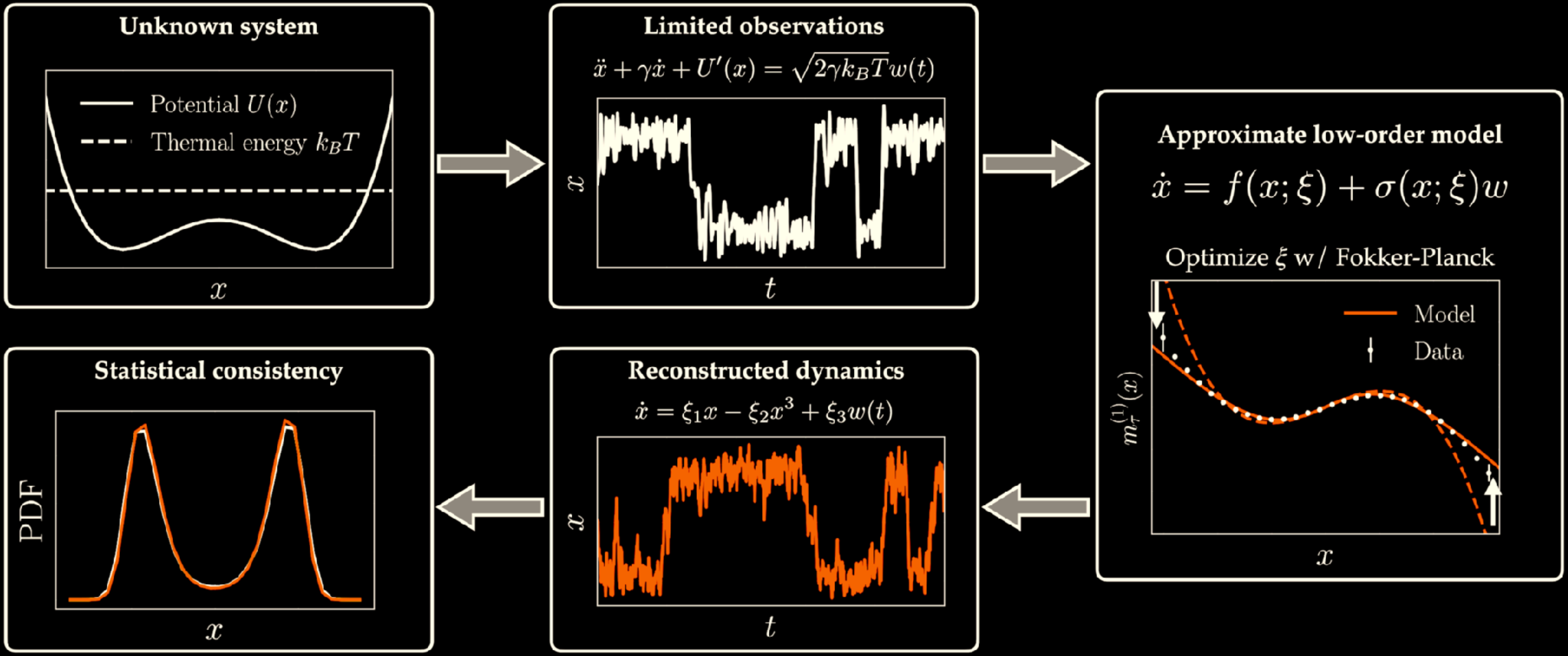
Describes evolution of distributions

Fokker-Planck equation

$$\frac{\partial p}{\partial t} = -\nabla \cdot (fp) + \nabla^2 \left(\frac{\sigma^2 p}{2} \right)$$

Callaham, Loiseau, Rigas, SLB, arXiv:2009.01006 2020

LANGEVIN REGRESSION

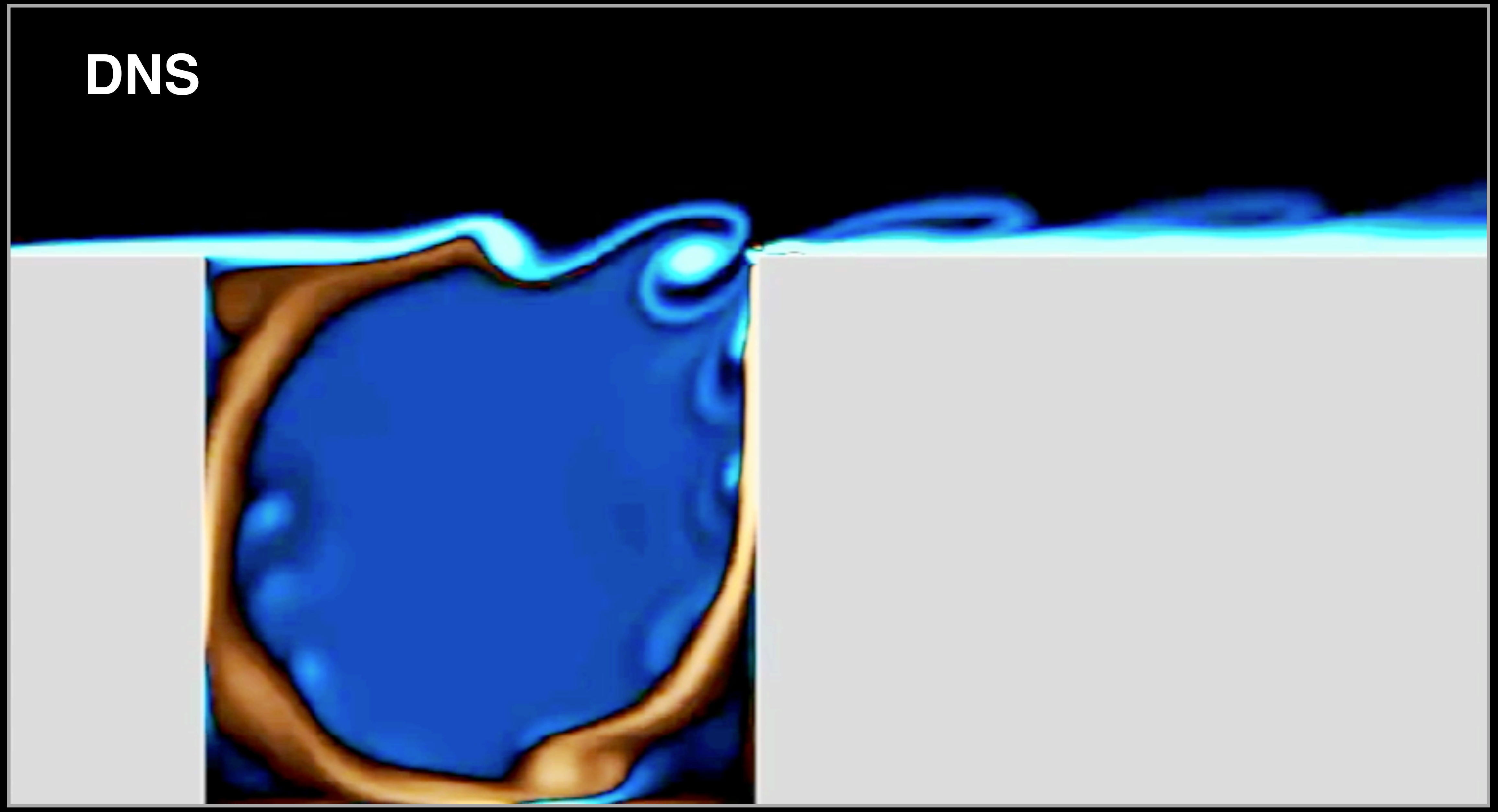


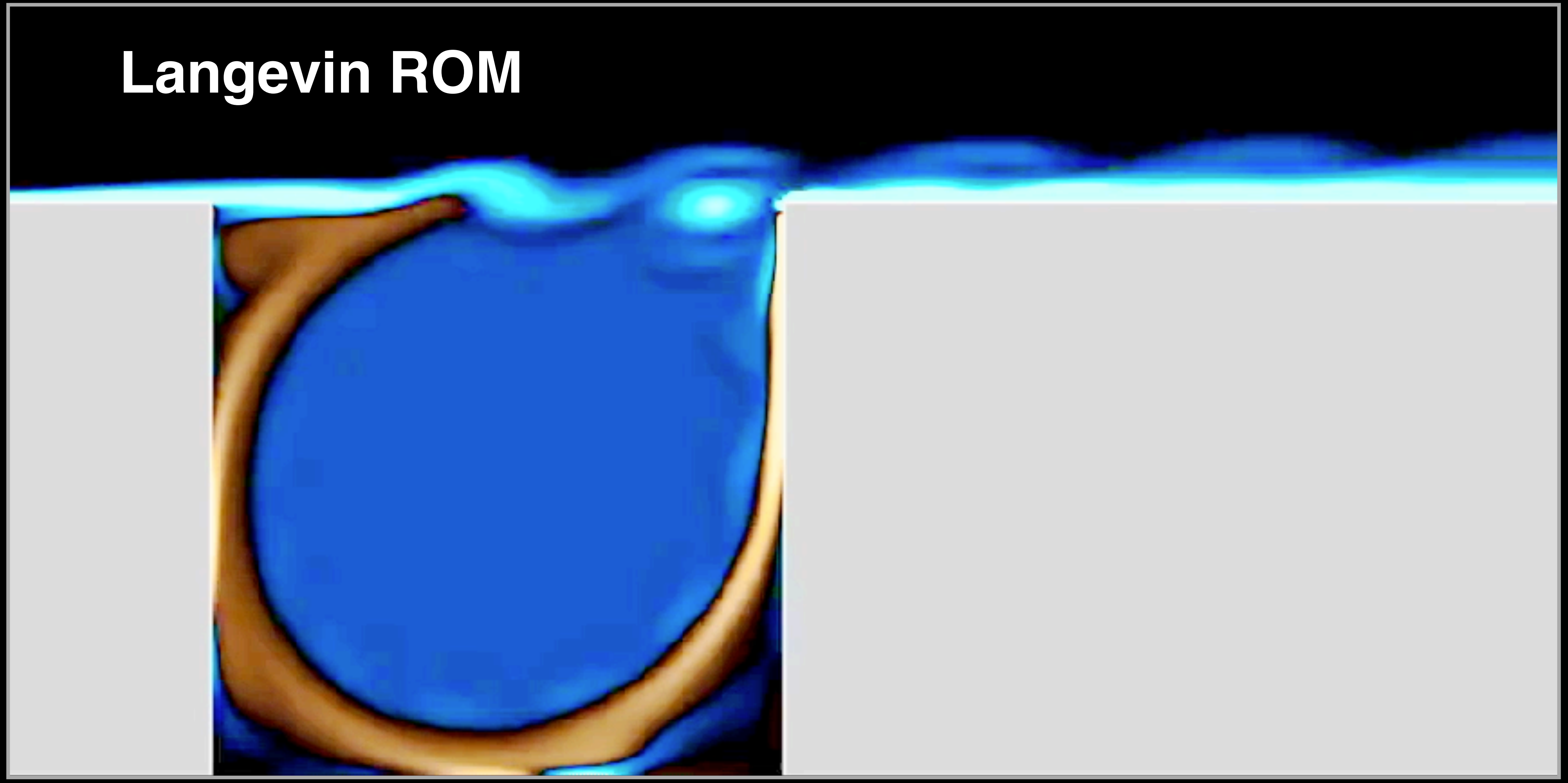
Callaham, Loiseau, Rigas, SLB, arXiv:2009.01006 2020

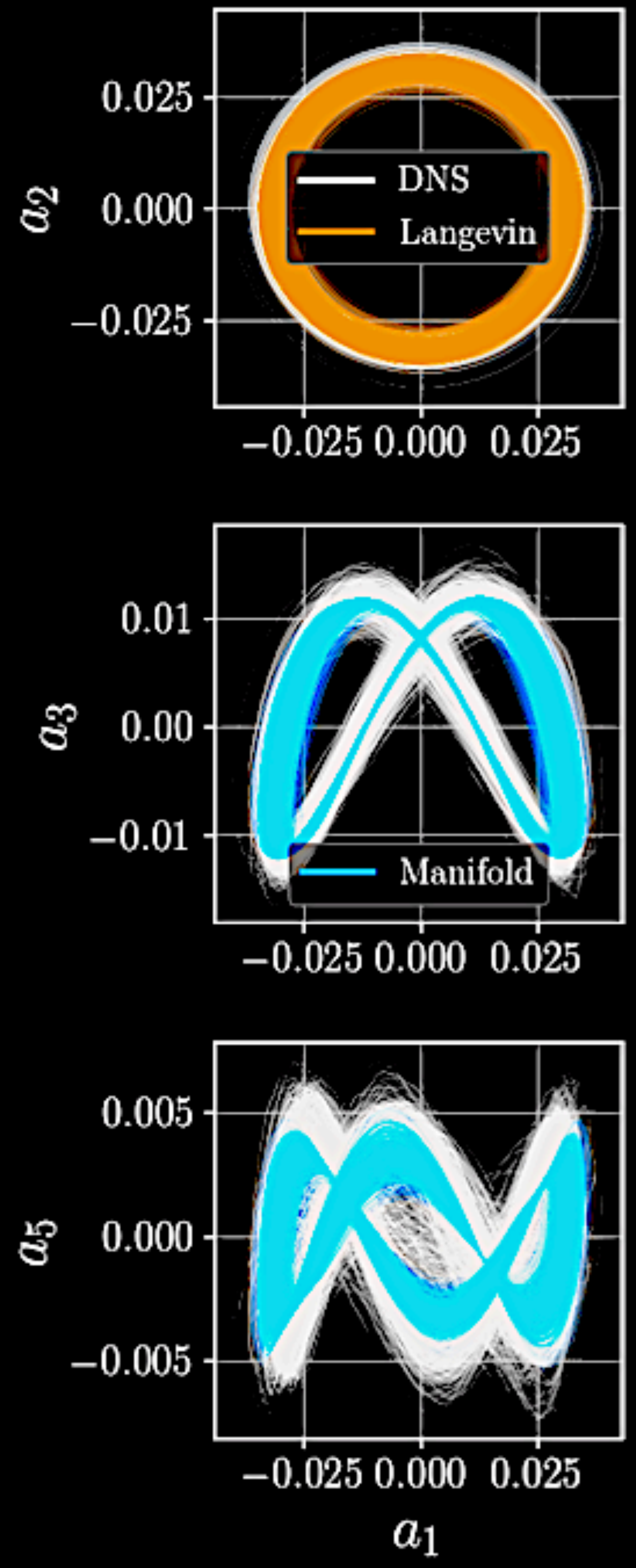
Langevin Regression

Callaham, Loiseau, Rigas, SLB, arXiv:2009.01006 2020

Stochastic Cavity Model








QUESTIONS