Data-driven discovery and control of complex systems: uncovering interpretable and generalizable models

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Nathan Kutz

Josh Proctor

Bing Brunton

J-Ch. Loiseau

Bernd Noack

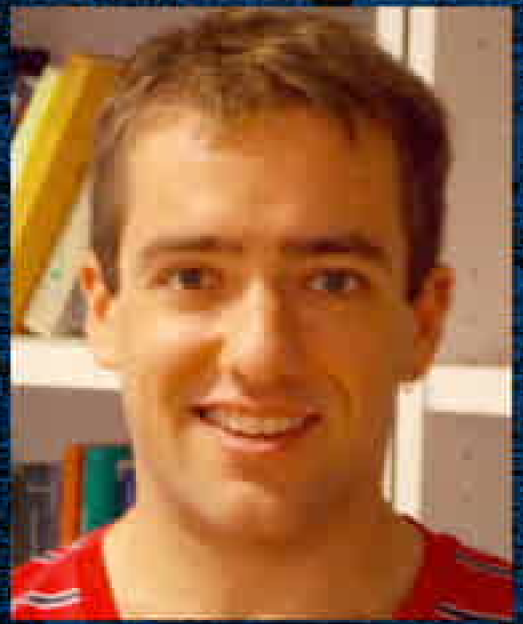
Eurika Kaiser

Niall Mangan

Bethany Lusch

Krithika Manohar

Sam Rudy



Kathleen Champion

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NVIDIA

magic leap

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Often equations are unknown or are only partially known:

- Model discovery with machine learning & sparse optimization

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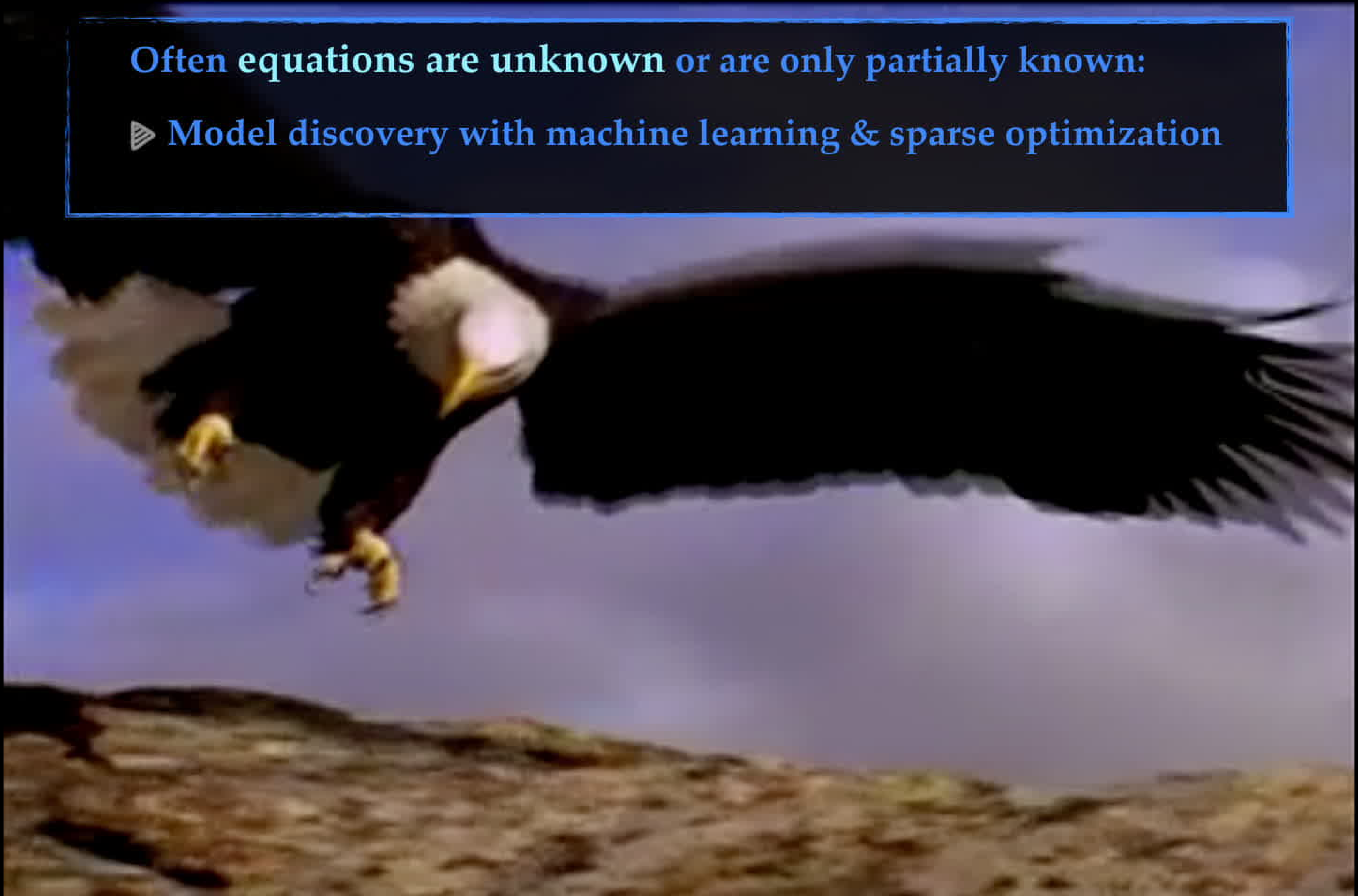

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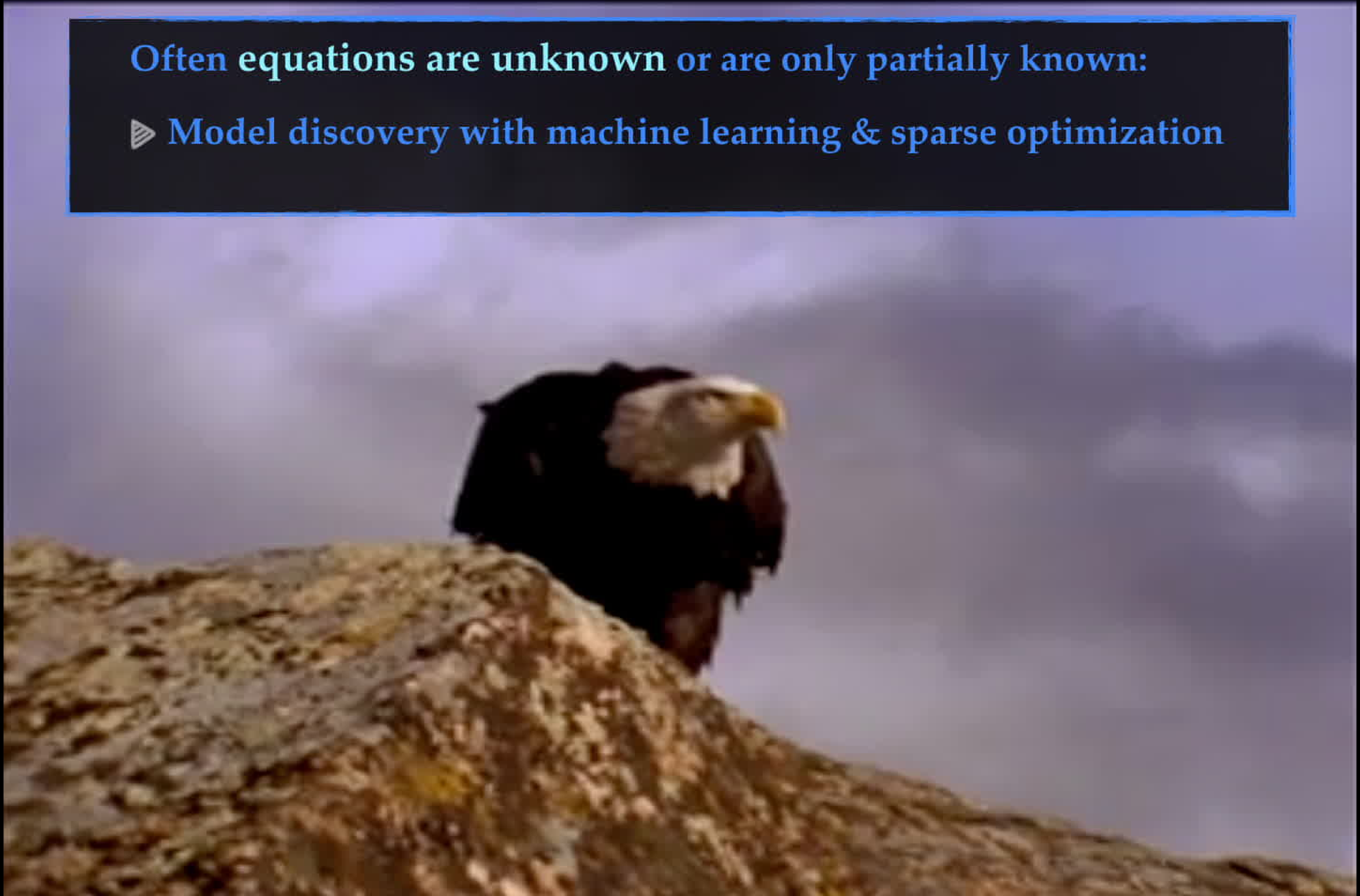


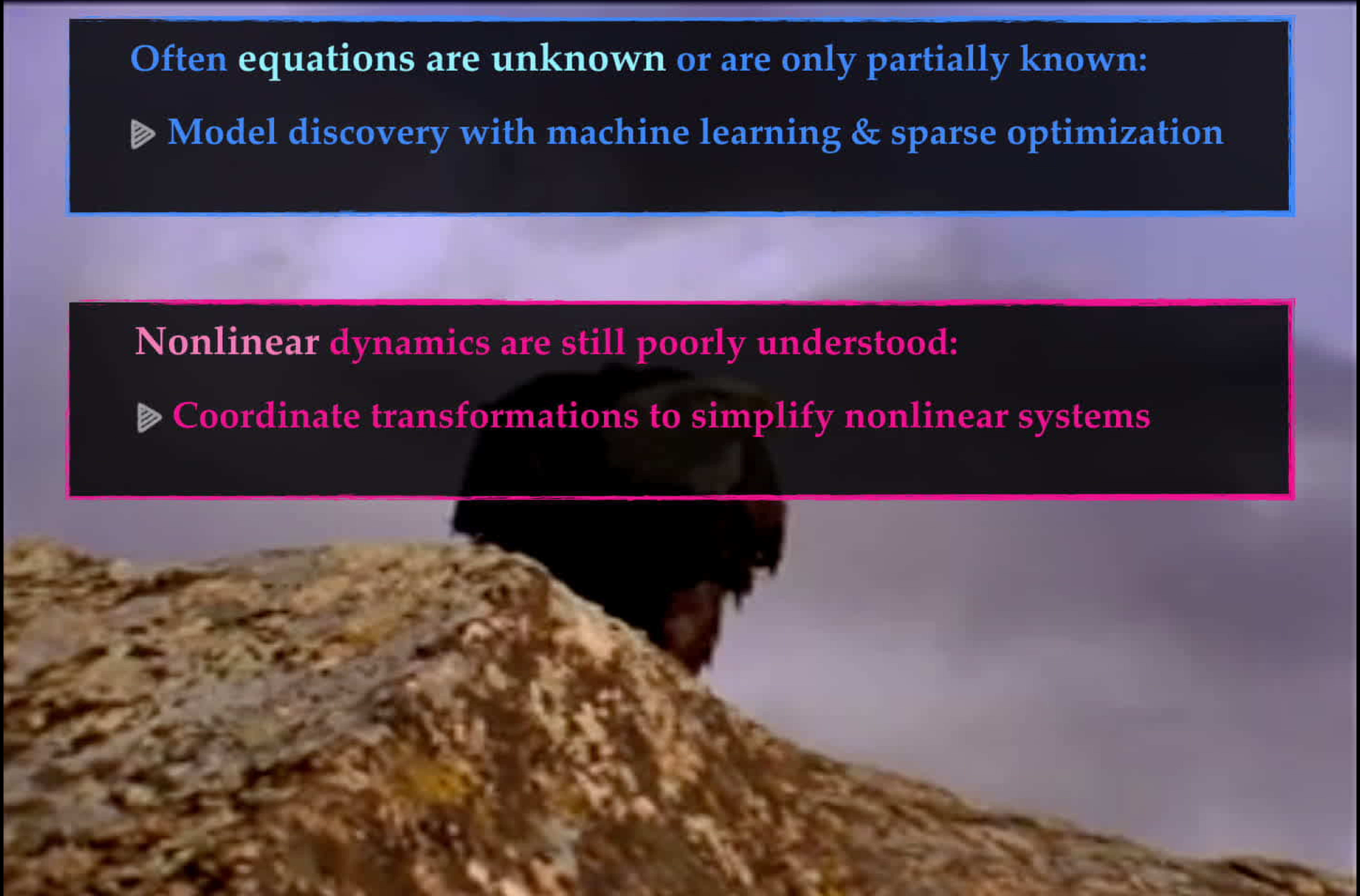
Data-driven discovery and control of complex systems: uncovering interpretable and generalizable models

Often **equations are unknown** or are only partially known:

- Model discovery with machine learning & sparse optimization

Nonlinear dynamics are still poorly understood:

- Coordinate transformations to simplify nonlinear systems



Data-driven discovery and control of complex systems: uncovering interpretable and generalizable models

Often **equations are unknown** or are only partially known:

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Our approach:

- Learn physics from data: interpretable and generalizable
- Respect known, or partially known, physics
- The existence of patterns facilitate sparse (few) measurements
- Machine learning is high-dimensional optimization with data

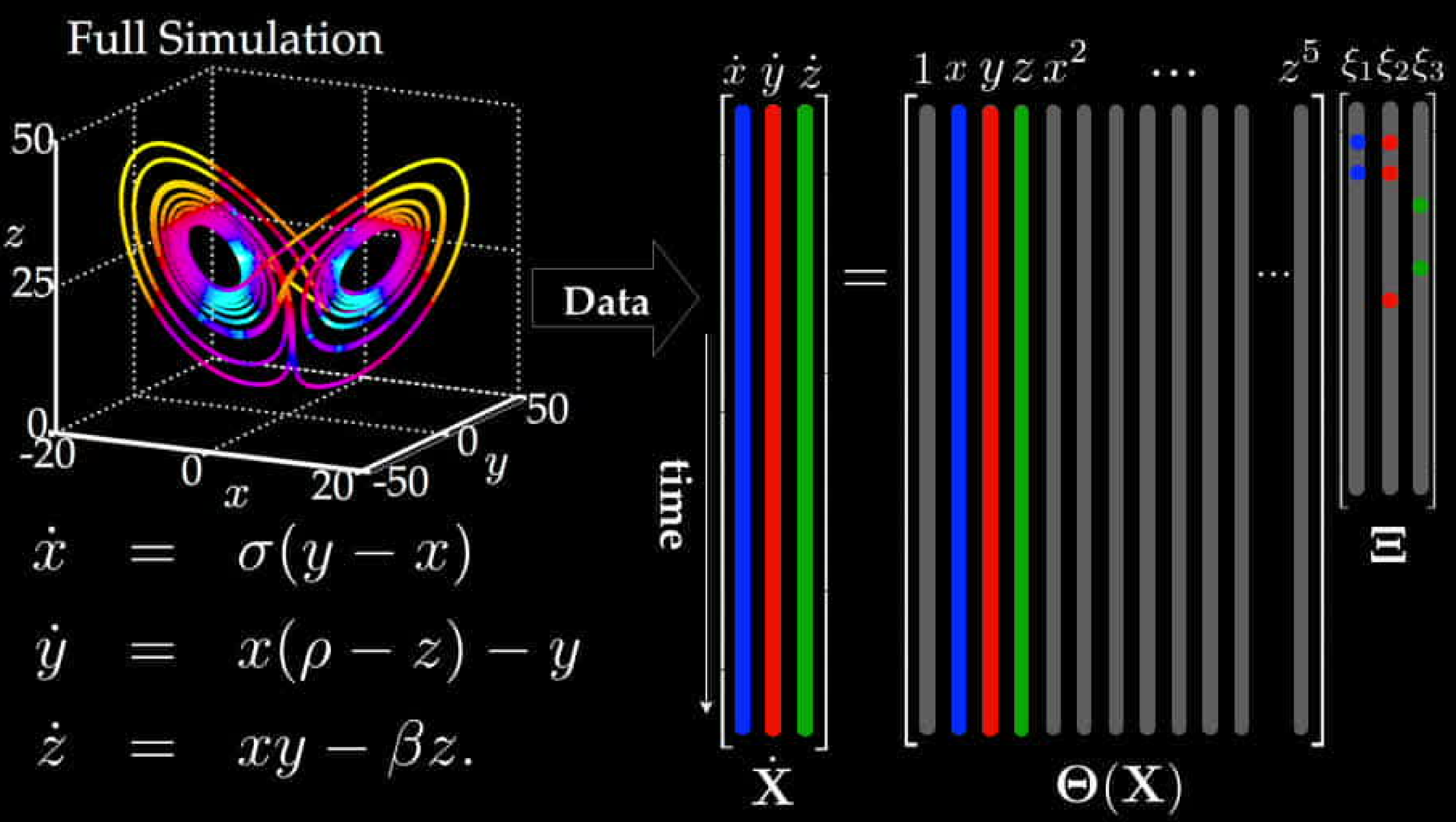
MODEL DISCOVERY

Lots of great work:

Gonzalez-Garcia, Rico-Martinez, Kevrekidis, *Comp. Chem. Eng.* 1998
Yao and Bollt, *Physica D*, 2007
Bongard and Lipson, *PNAS* 2007
Schmidt and Lipson, *Science* 2009
Wang, Yang, Lai, Kovanis, Grebogi, *PRL* 2011
Bright, Lin, Kutz, *Phys. Fluids*, 2013
Schaeffer, Caflisch, Hauck, Osher, *PNAS* 2013
Noe, et al., Molecular dynamics, 2013-2016
Schaeffer, *PRSA*, 2017
Schaeffer, Tran, Ward, *SIAP*, 2018
Raissi, Perdikaris, Karniadakis, *JCP* 2019
… and many more!!!

Sparsity/parsimony in dynamics

Sparse Identification of Nonlinear Dynamics (SINDy)



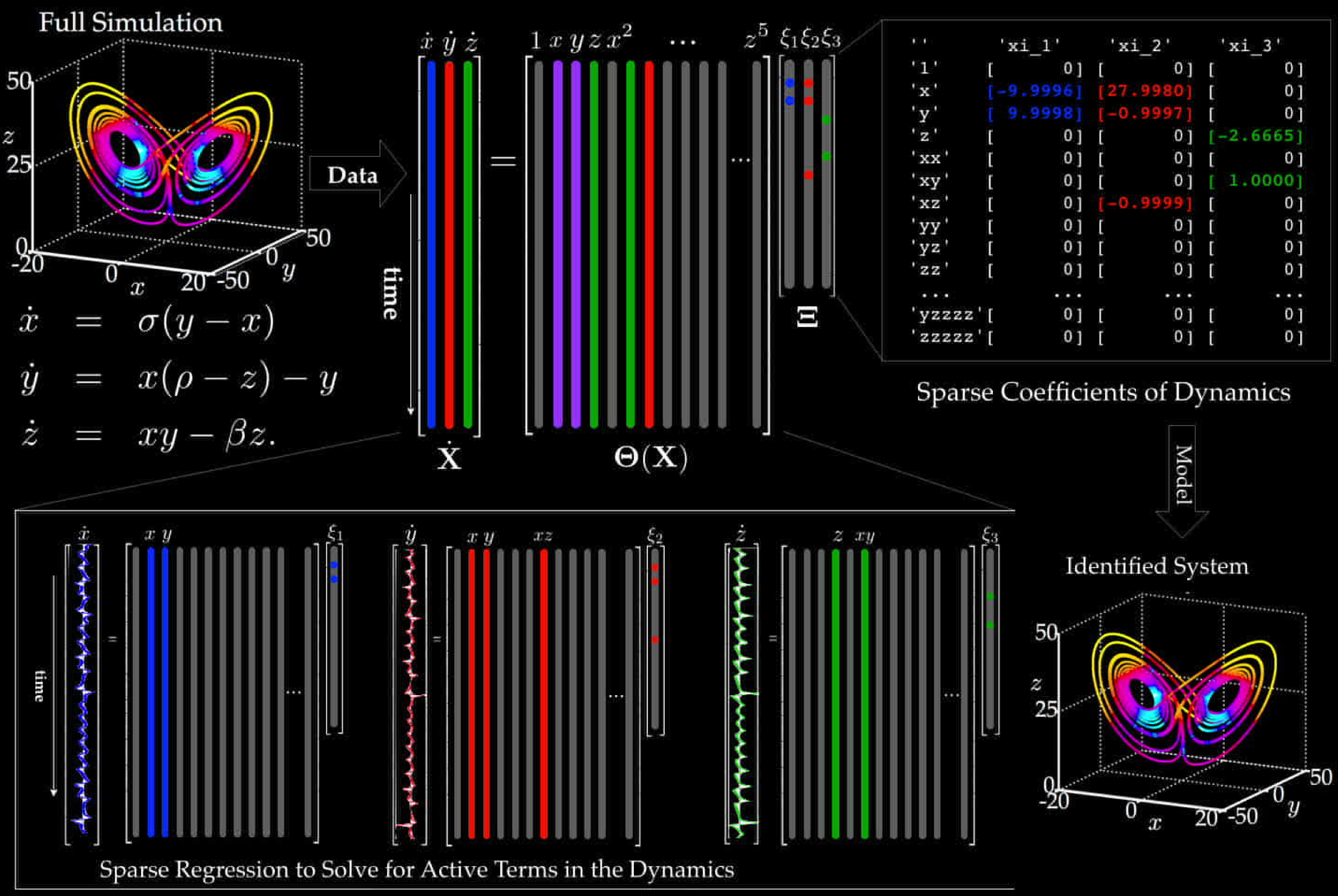
$$\begin{aligned}\dot{x} &= \sigma(y - x)\\ \dot{y} &= x(\rho - z) - y\\ \dot{z} &= xy - \beta z.\end{aligned}$$

Nathan Kutz

Josh Proctor

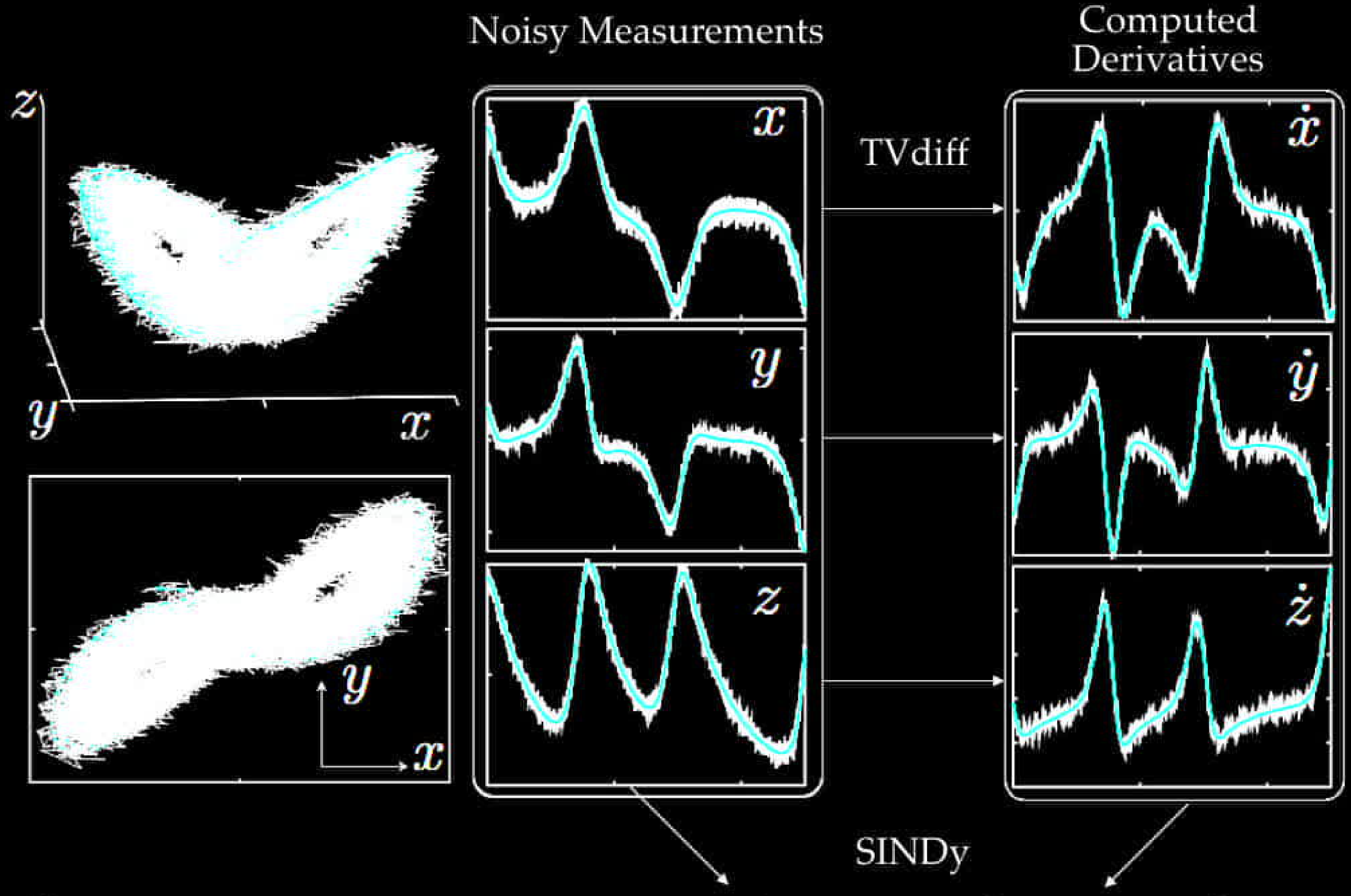
SLB, Proctor, Kutz, *PNAS* 2016.

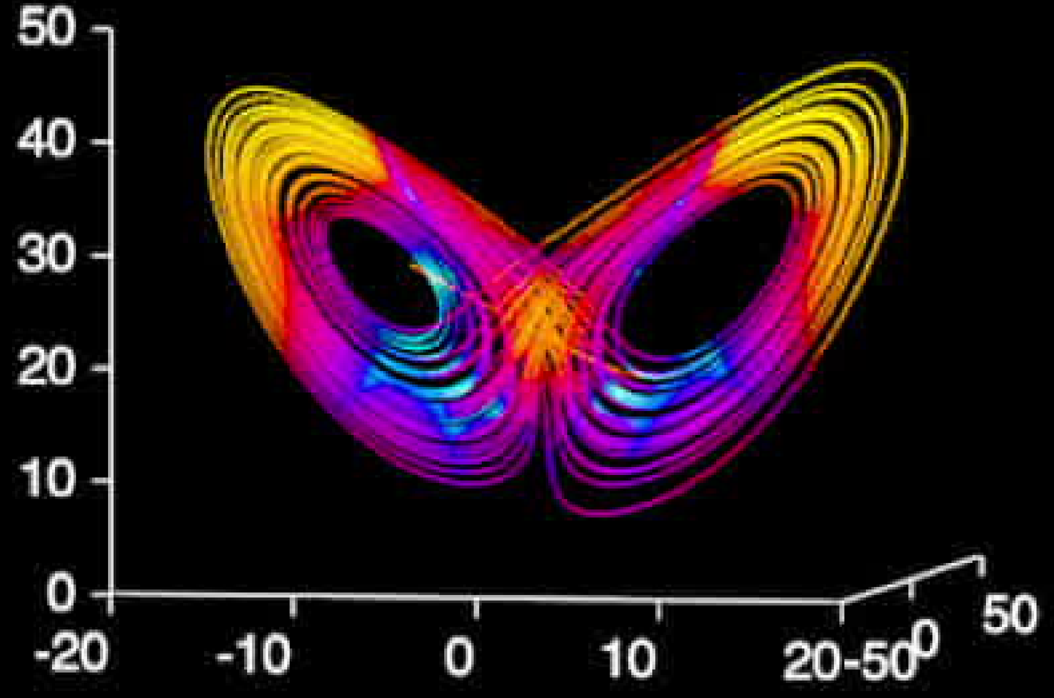
Sparse Identification of Nonlinear Dynamics (SINDy)



SLB, Proctor, Kutz, *PNAS* 2016.

SINDy: Noisy State Measurements



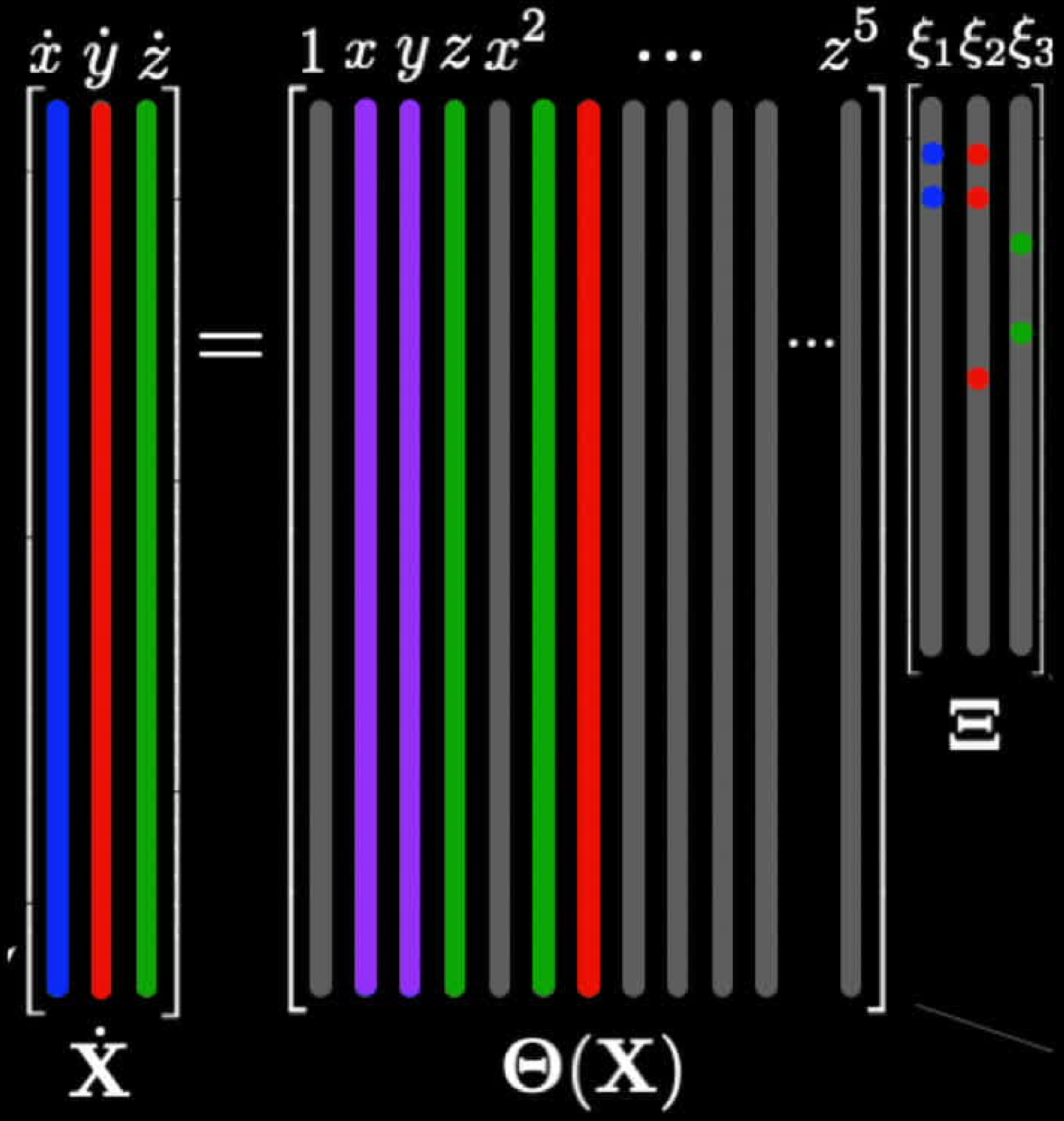


	'xi_1'	'xi_2'	'xi_3'
'x'	[-9.9614]	[27.5343]	[0]
'y'	[9.9796]	[-0.8038]	[0]
'z'	[0]	[0]	[-2.6647]
'xx'	[0]	[0]	[0]
'xy'	[0]	[0]	[1.0003]
'xz'	[0]	[-0.9900]	[0]

Rudin, Osher, Fatemi, *Physica D*, 1992.
Brunton, Proctor, Kutz, *PNAS* 2016.

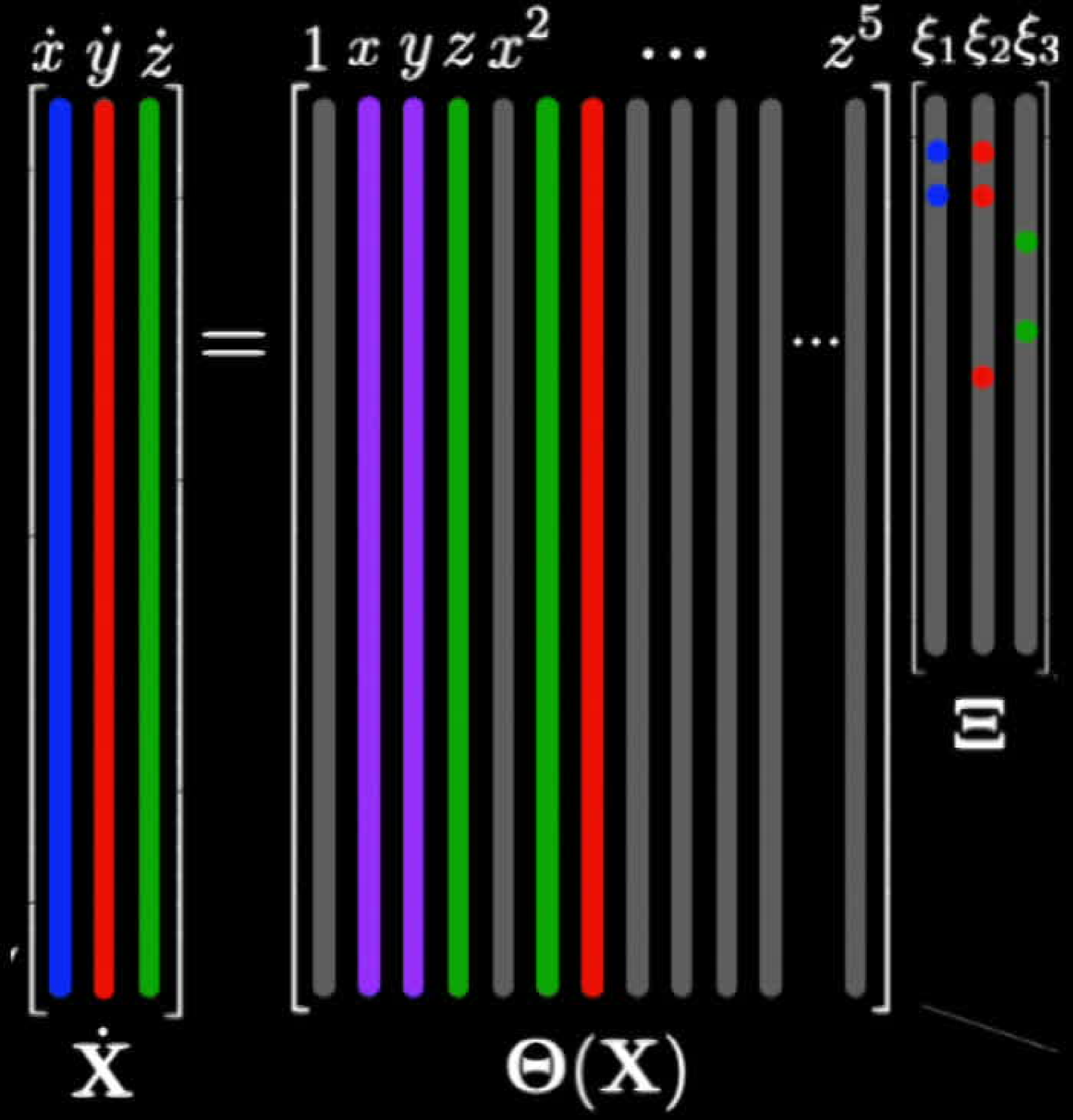
Parsimonious modeling

$$\|\dot{\mathbf{X}} - \Theta(\mathbf{X})\Xi\| + \lambda\|\Xi\|_0$$



Parsimonious modeling

$$\|\dot{\mathbf{X}} - \boldsymbol{\Theta}(\mathbf{X})\boldsymbol{\Xi}\| + \lambda\|\boldsymbol{\Xi}\|_0$$



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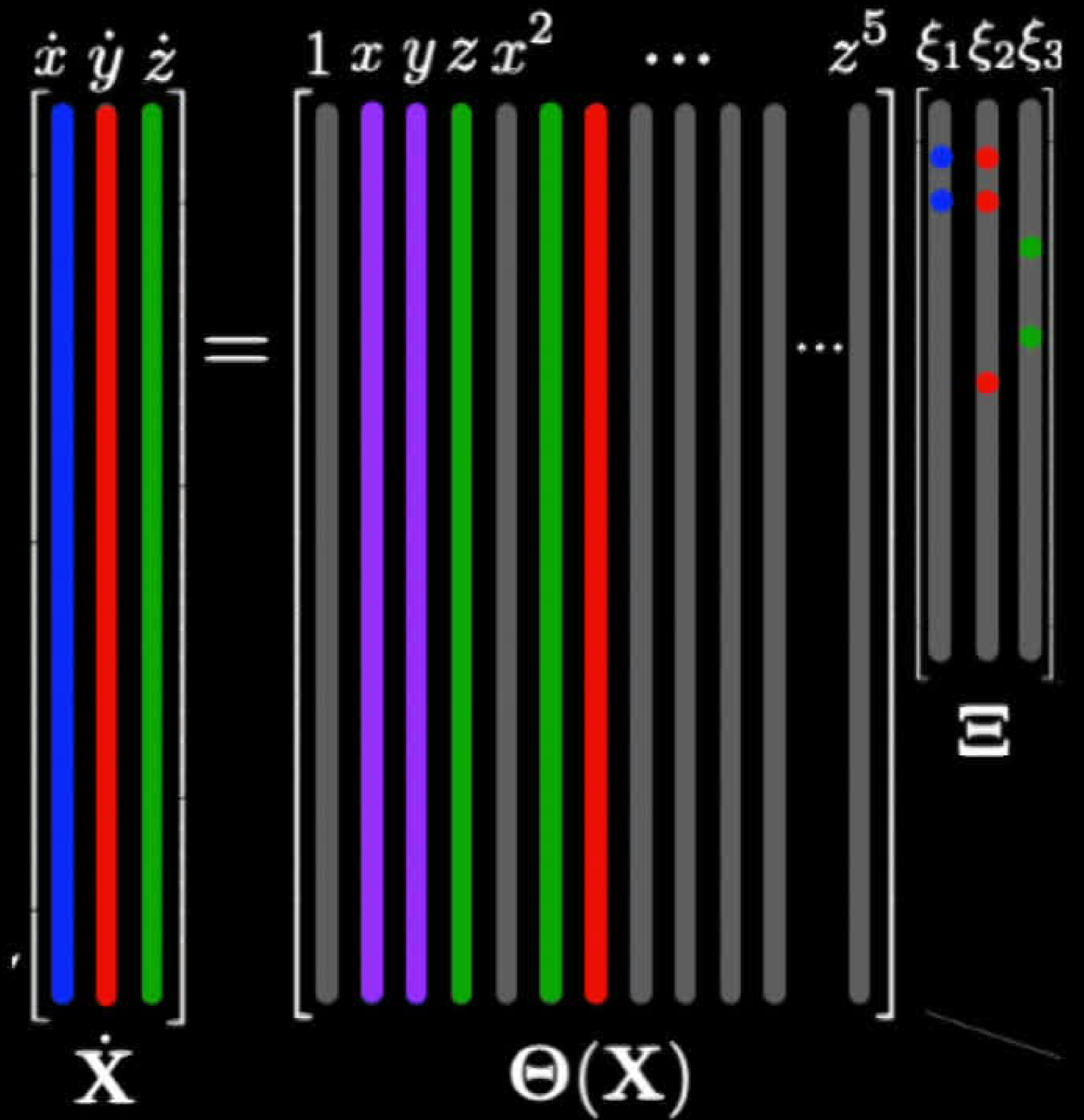

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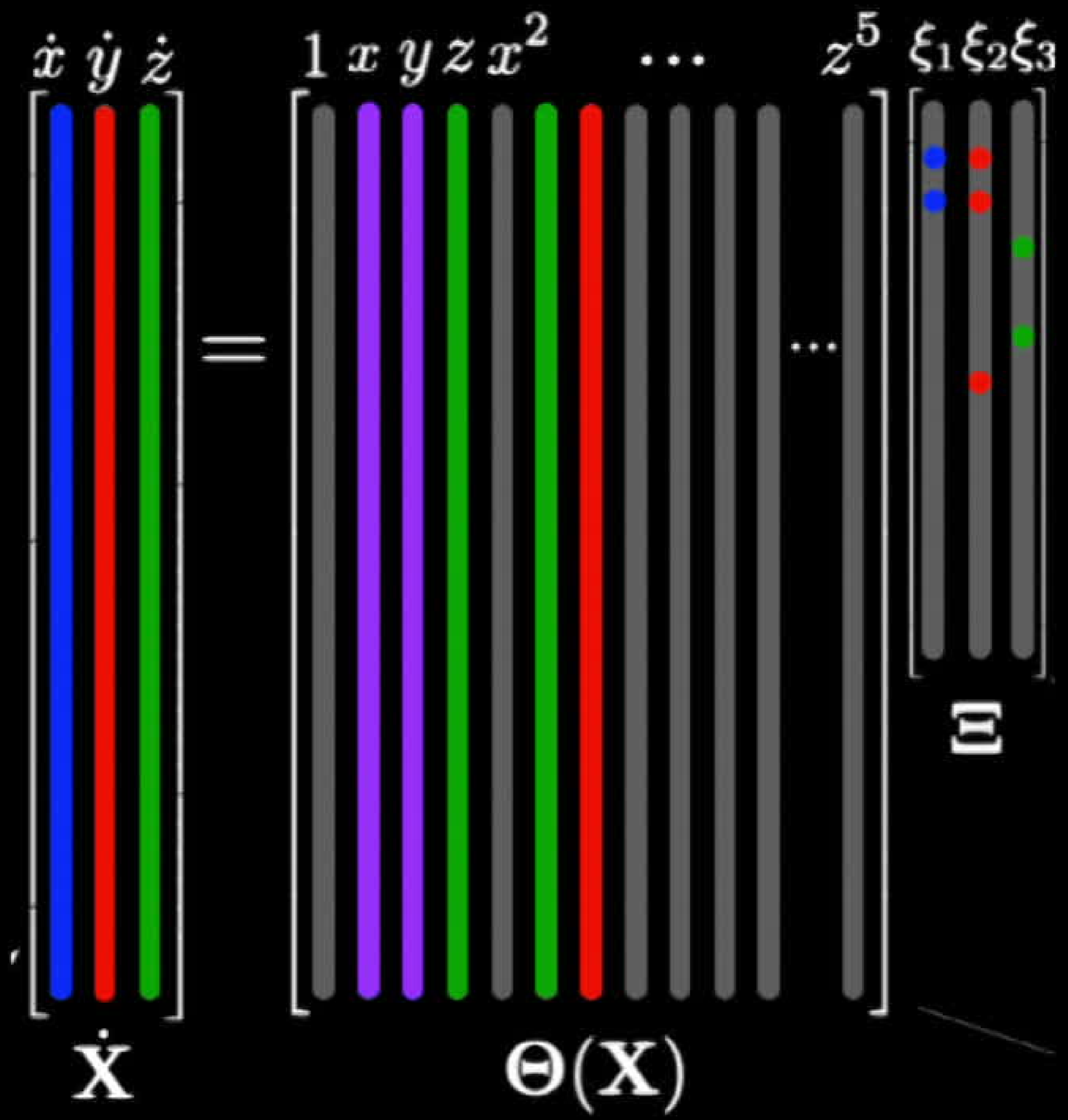

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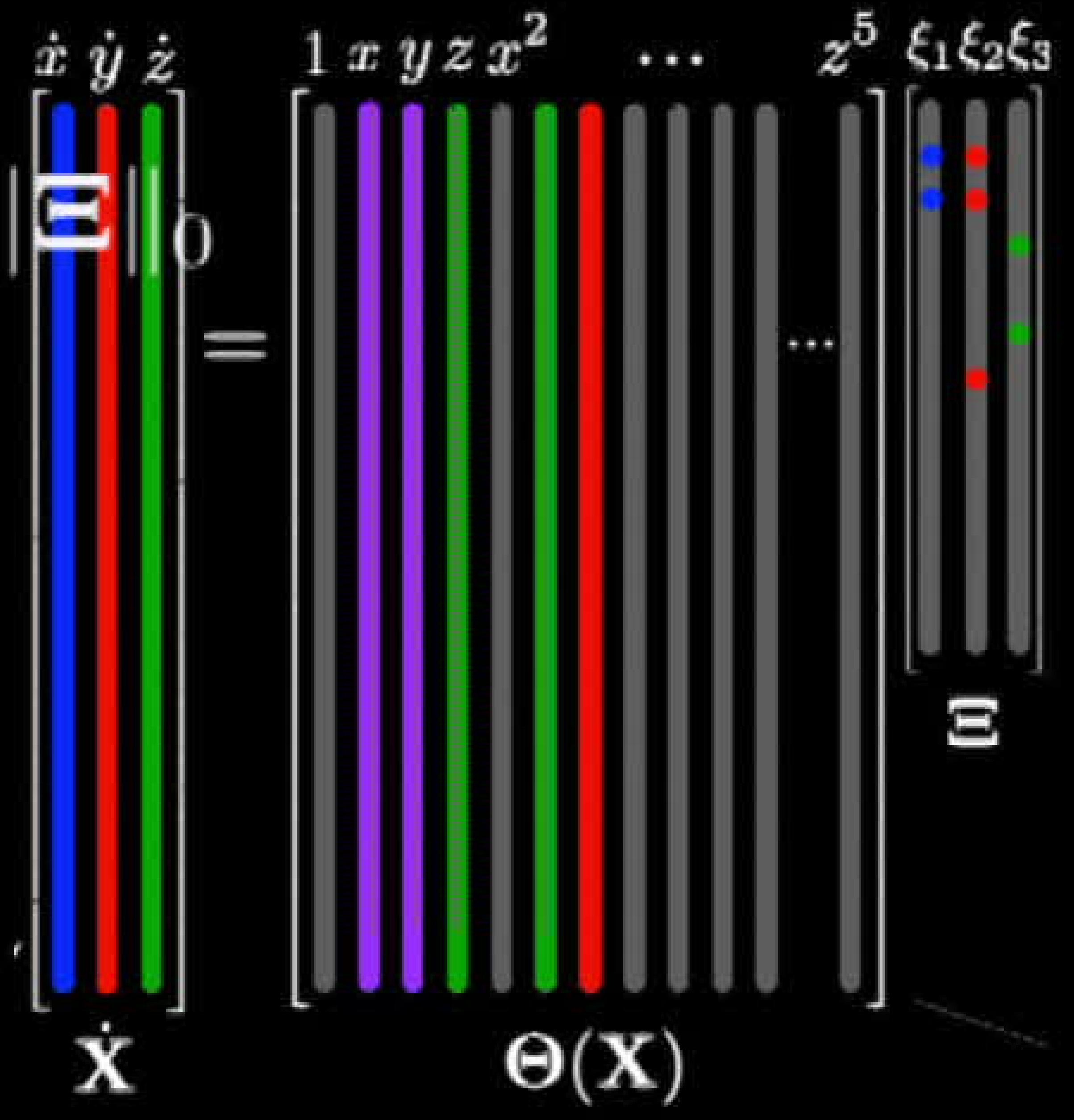
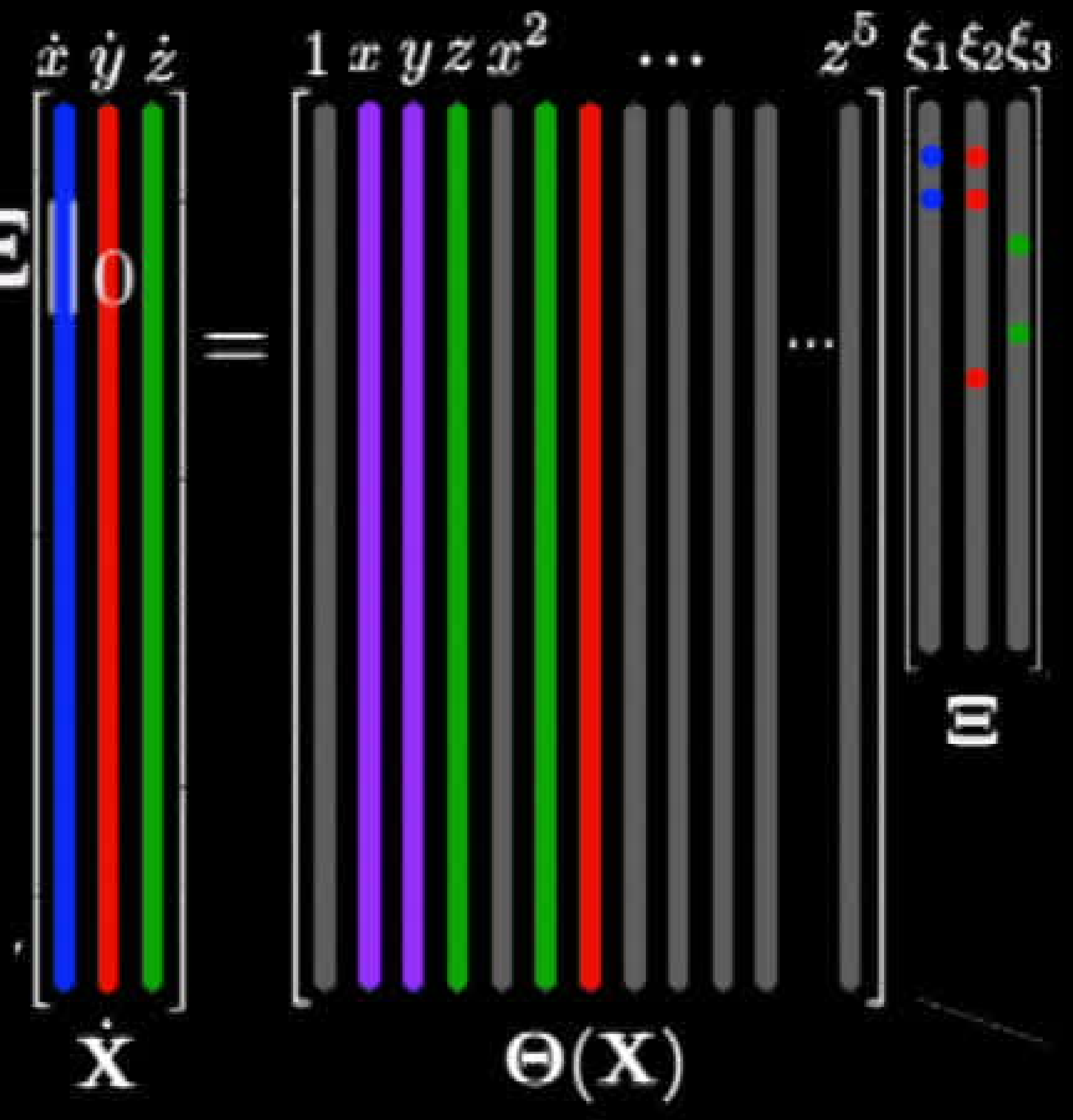


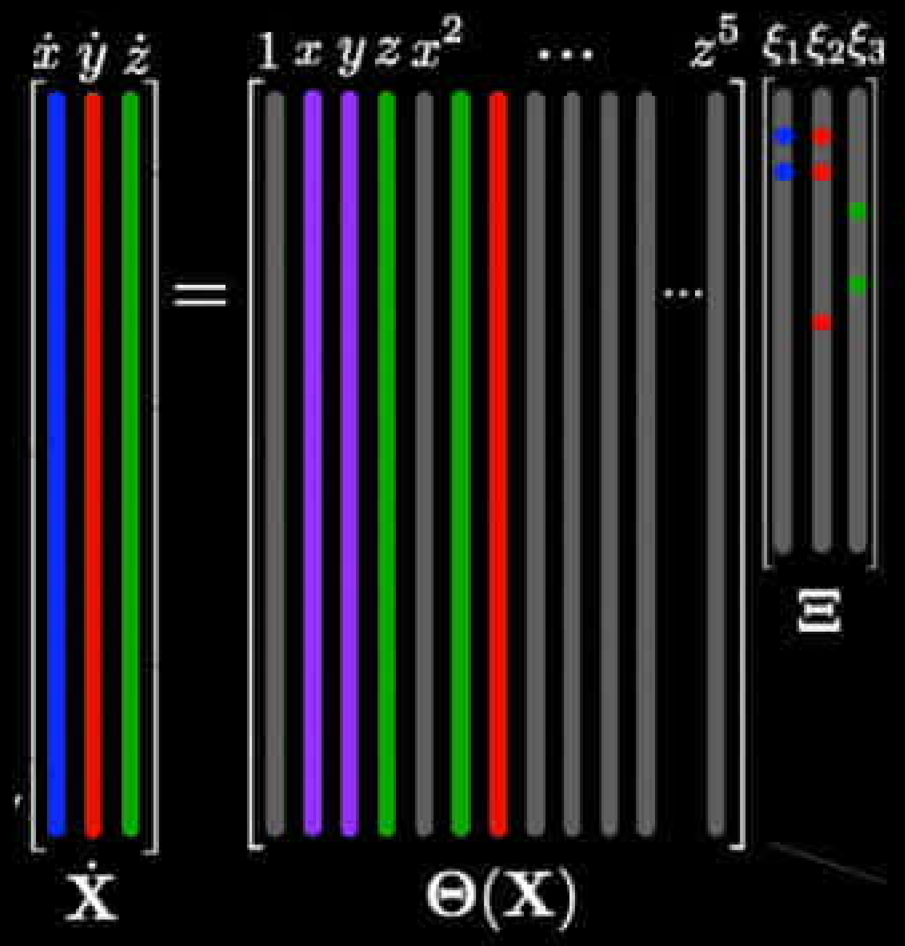
Parsimonious modeling

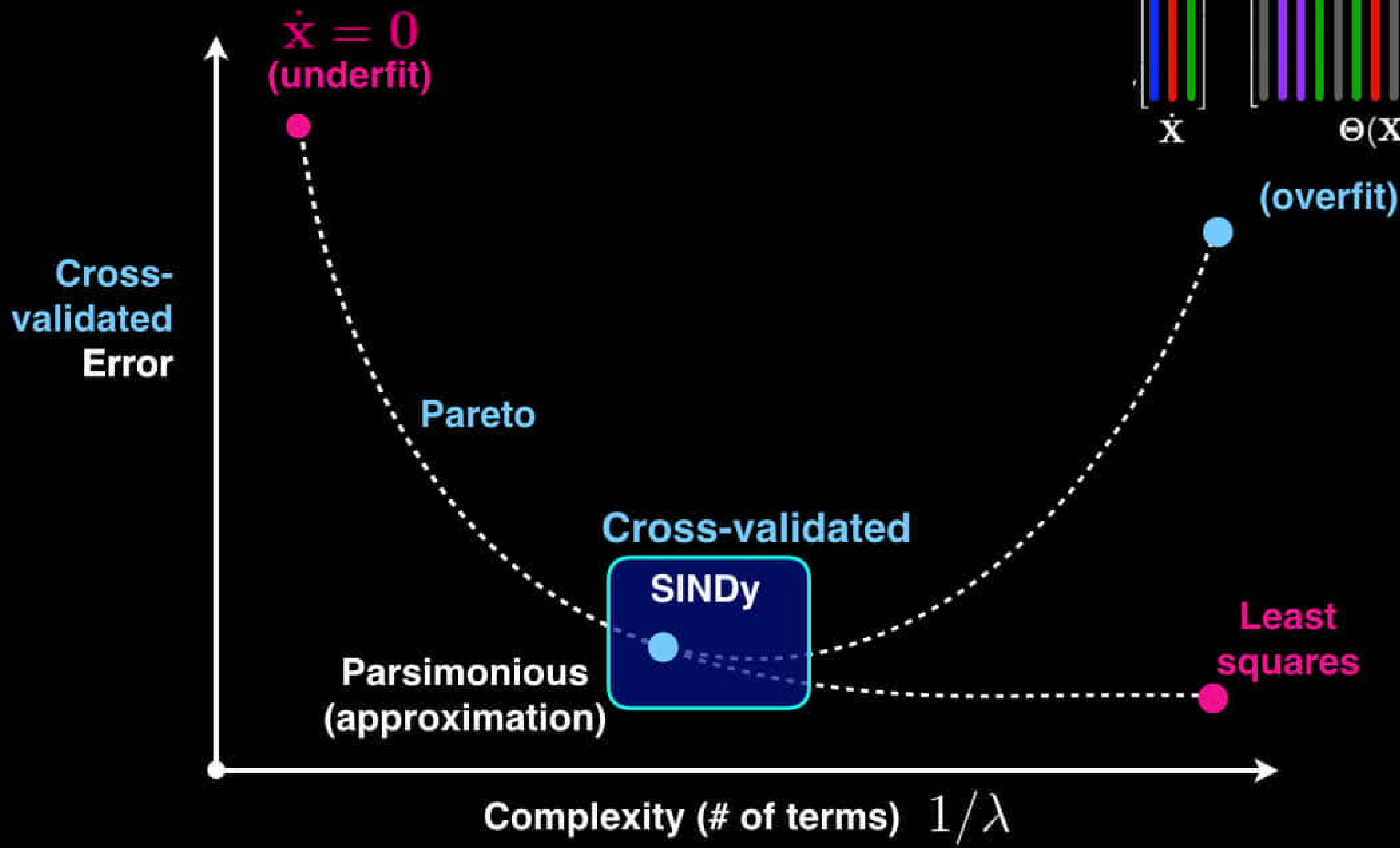
$$\|\dot{\mathbf{X}} - \Theta(\mathbf{X})\Xi\| + \lambda\|\Xi\|_0$$



Parsimonious modeling

$$\|\dot{\mathbf{X}} - \Theta(\mathbf{X})\Xi\| + \lambda\|\Xi\|_0$$



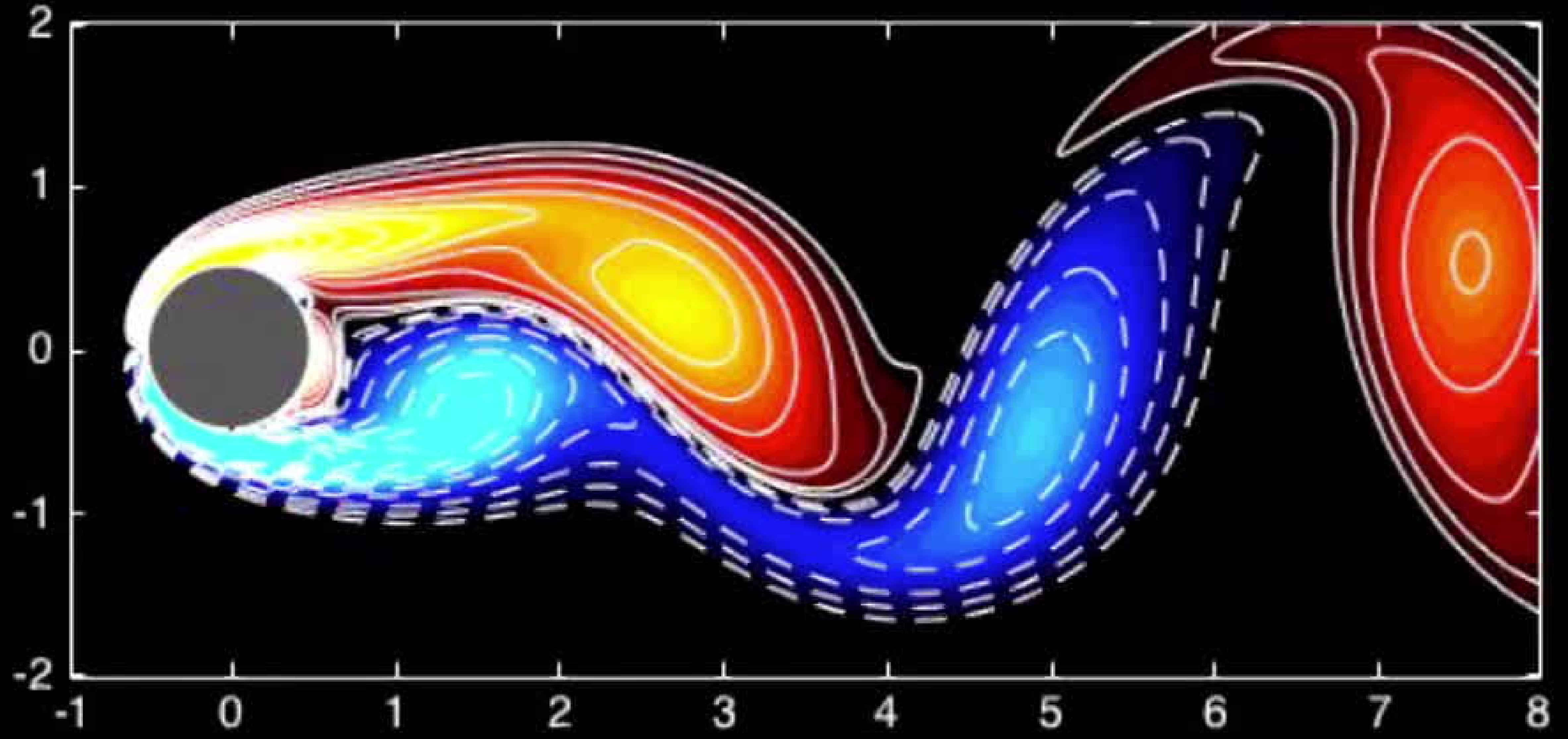


Optimization (SR3): Zheng, Askham, SLB, Kutz, Aravkin *IEEE Access*, 2019
Model selection: Mangan, SLB, Kutz, Proctor, *PRSA 2017*

Bongard and Lipson, *PNAS* 2007
Schmidt and Lipson, *Science* 2009
Nuske, Noe, et al., 2013-16

FLUIDS

SINDy: Vortex Shedding Past a Cylinder



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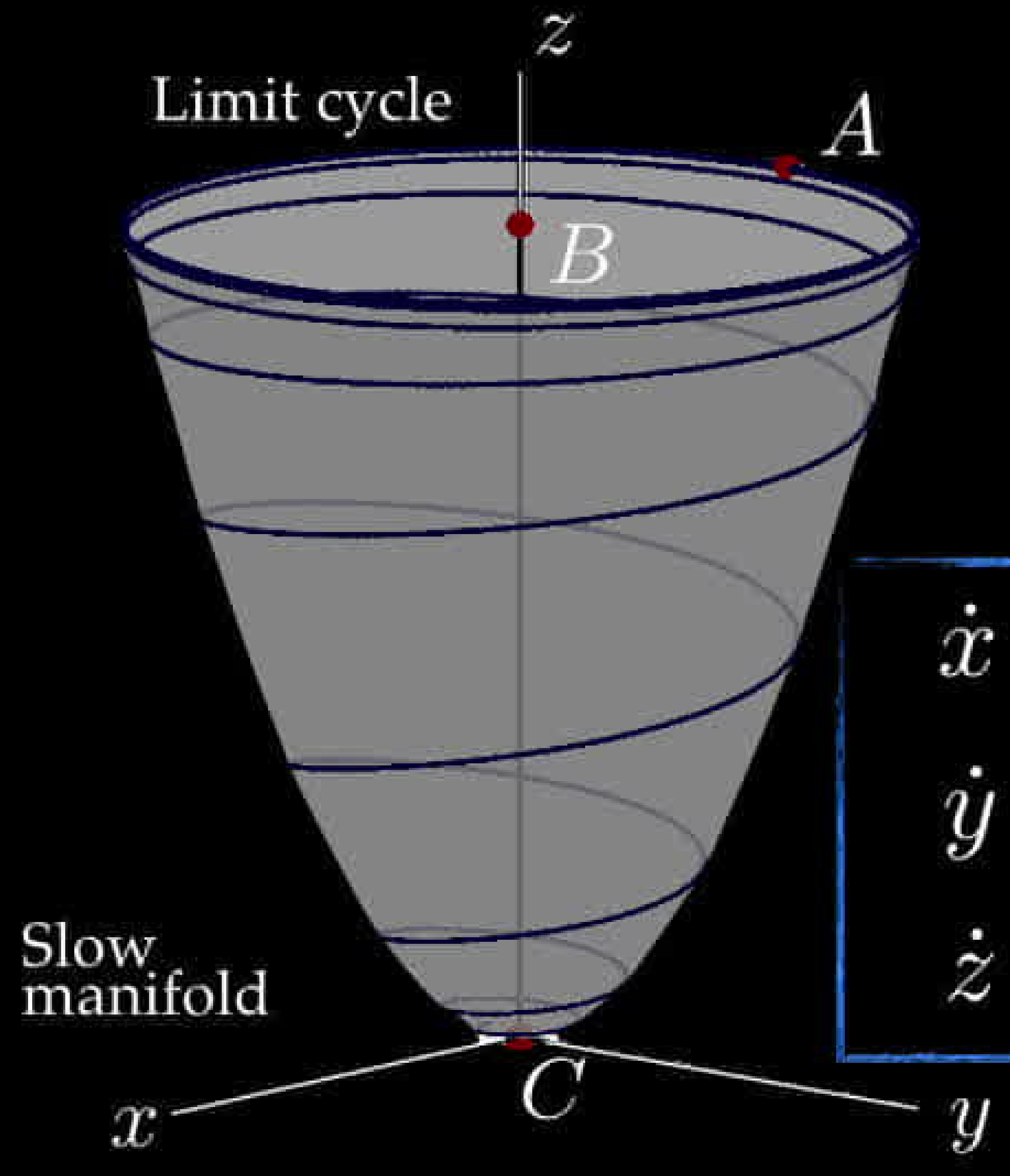
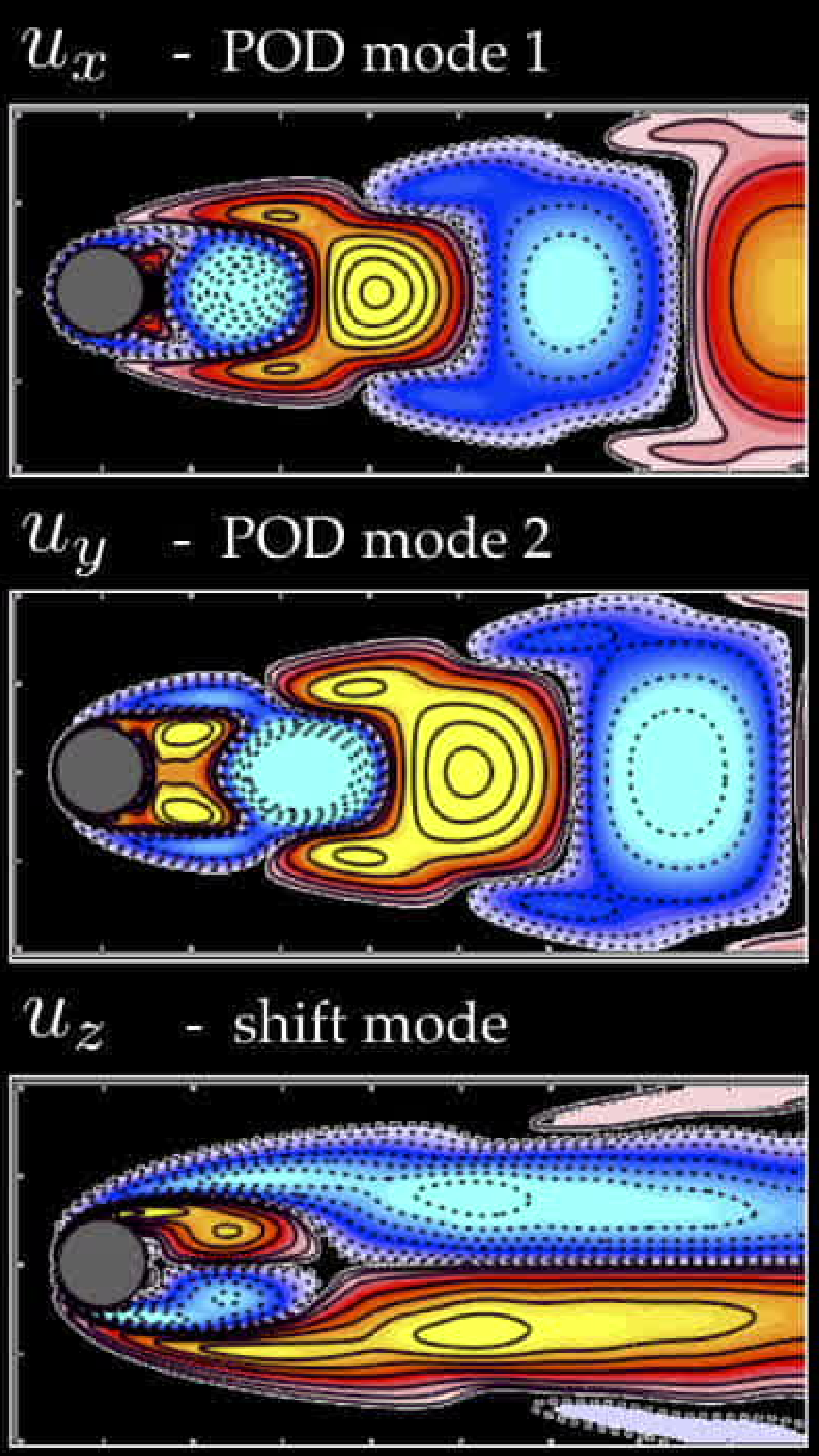
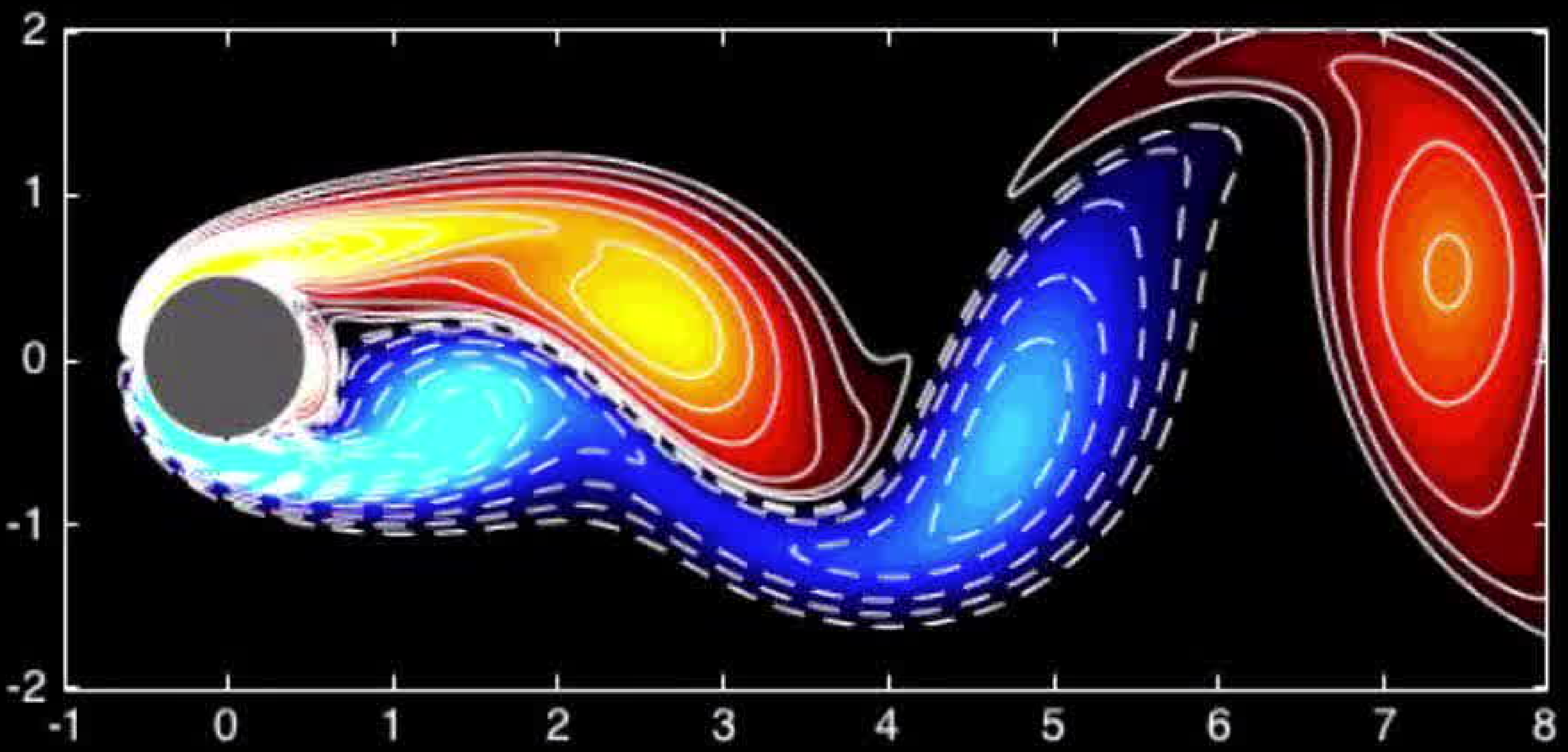


$$
\begin{aligned}
\dot{x} &= \mu x - \omega y + Axz \\
\dot{y} &= \omega x + \mu y + Ayz \\
\dot{z} &= -\lambda(z - x^2 - y^2).
\end{aligned}
$$





Ruelle and Takens, 1971
Zebib, 1987 and Jackson, 1987
Noack *et al.*, JFM 2003.

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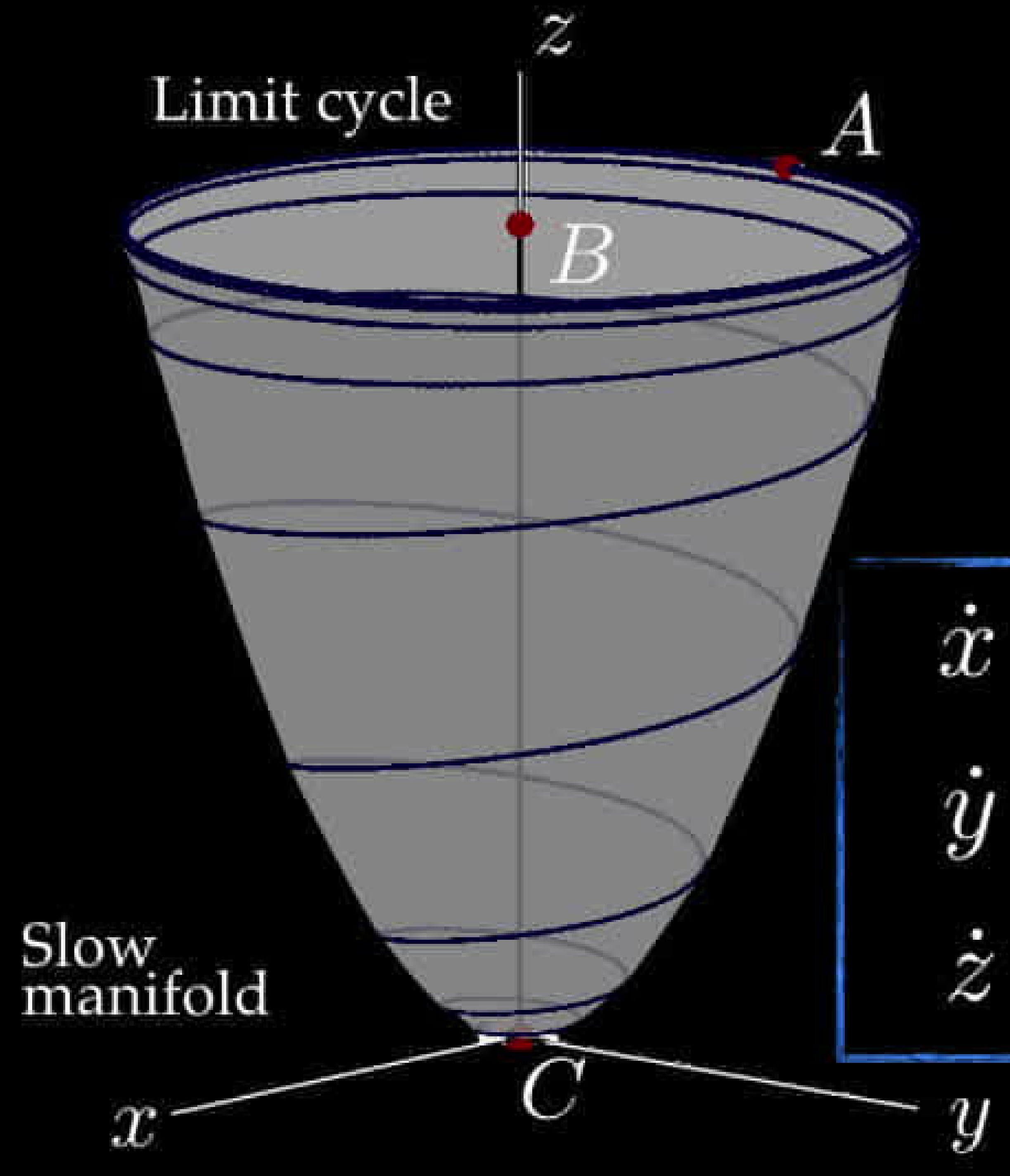

$$\dot{x} = \mu x - \omega y + Axz$$
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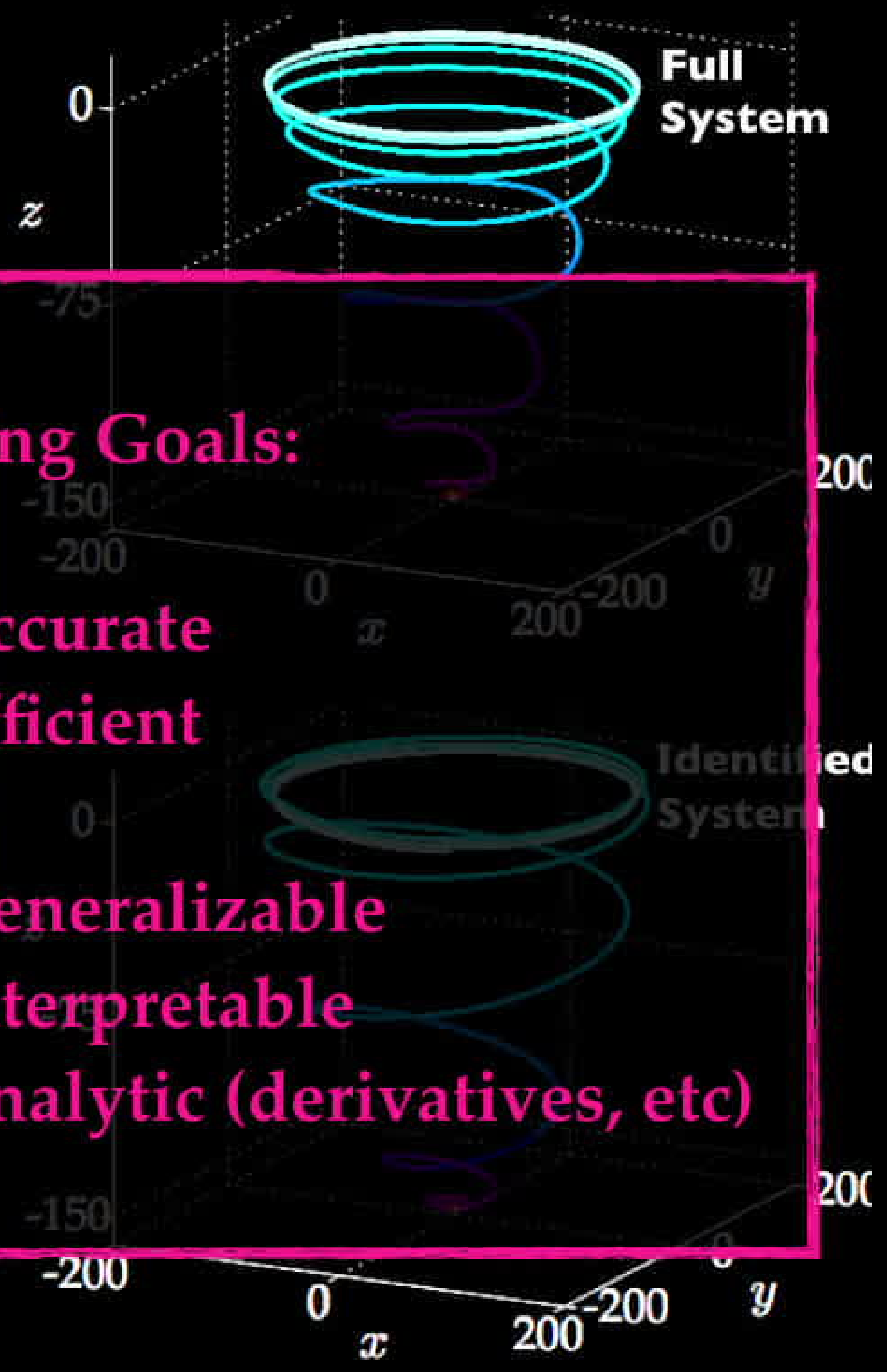
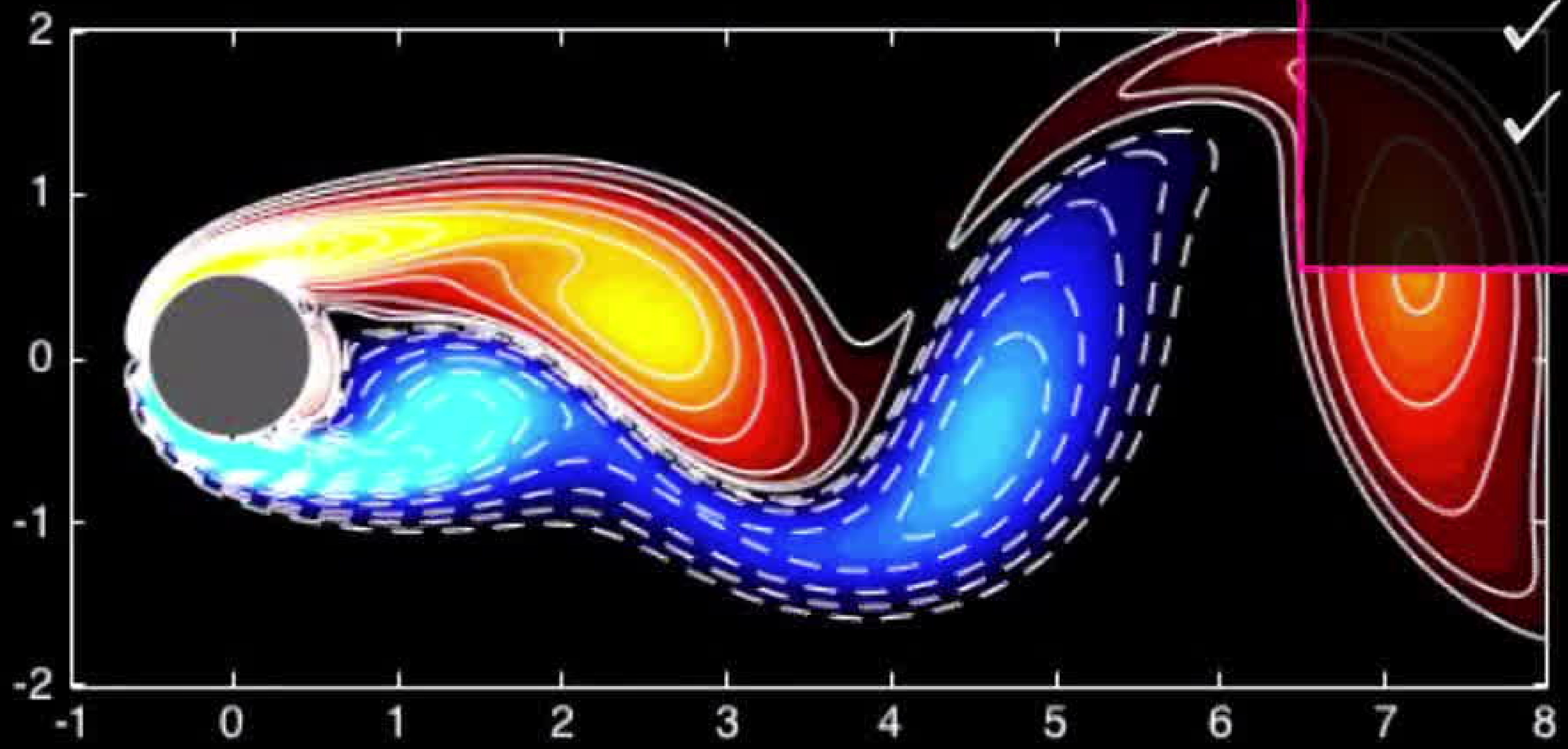


Modeling Goals:

- ✓ Accurate
- ✓ Efficient
- ✓ Generalizable
- ✓ Interpretable
- ✓ Analytic (derivatives, etc)



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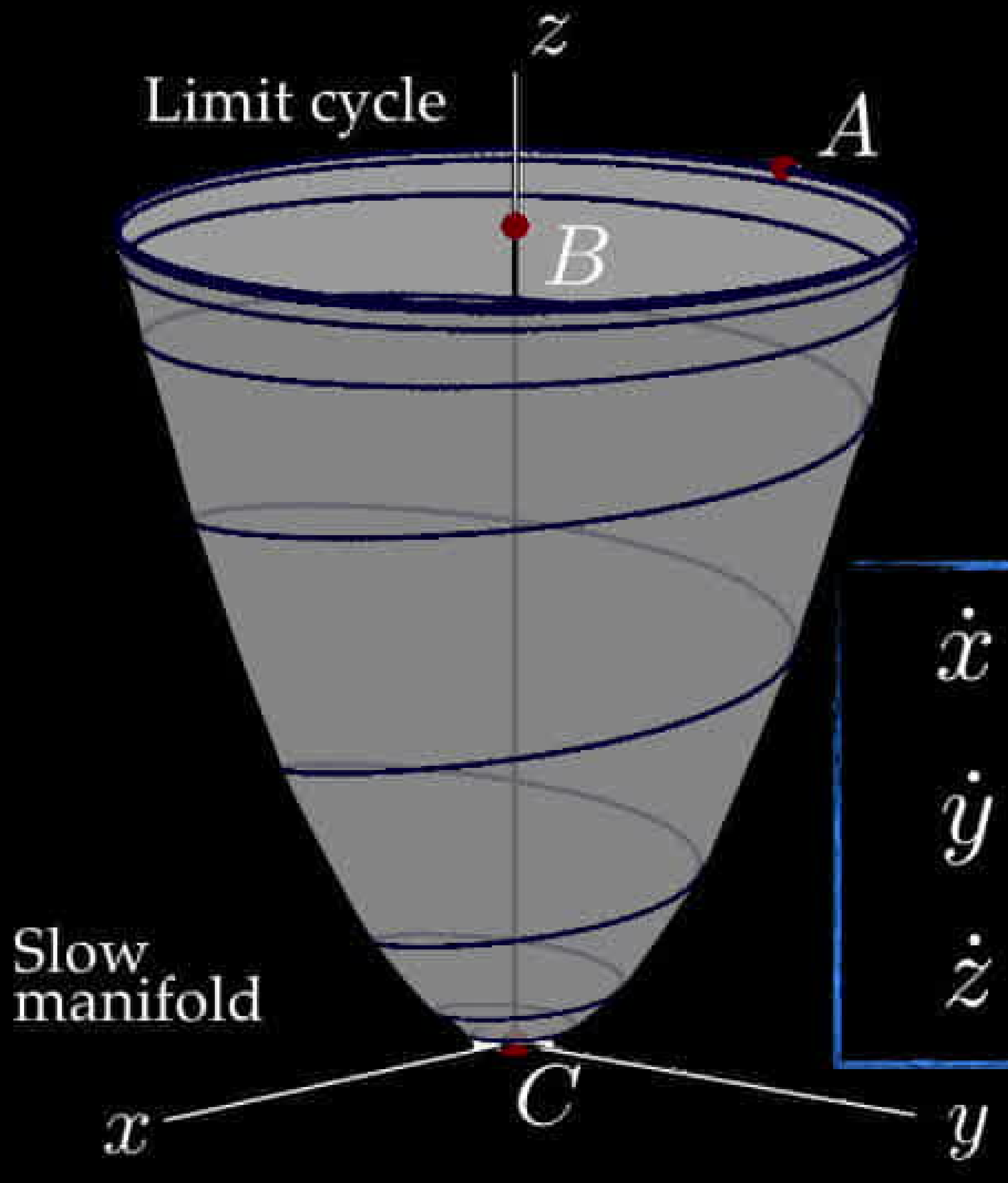
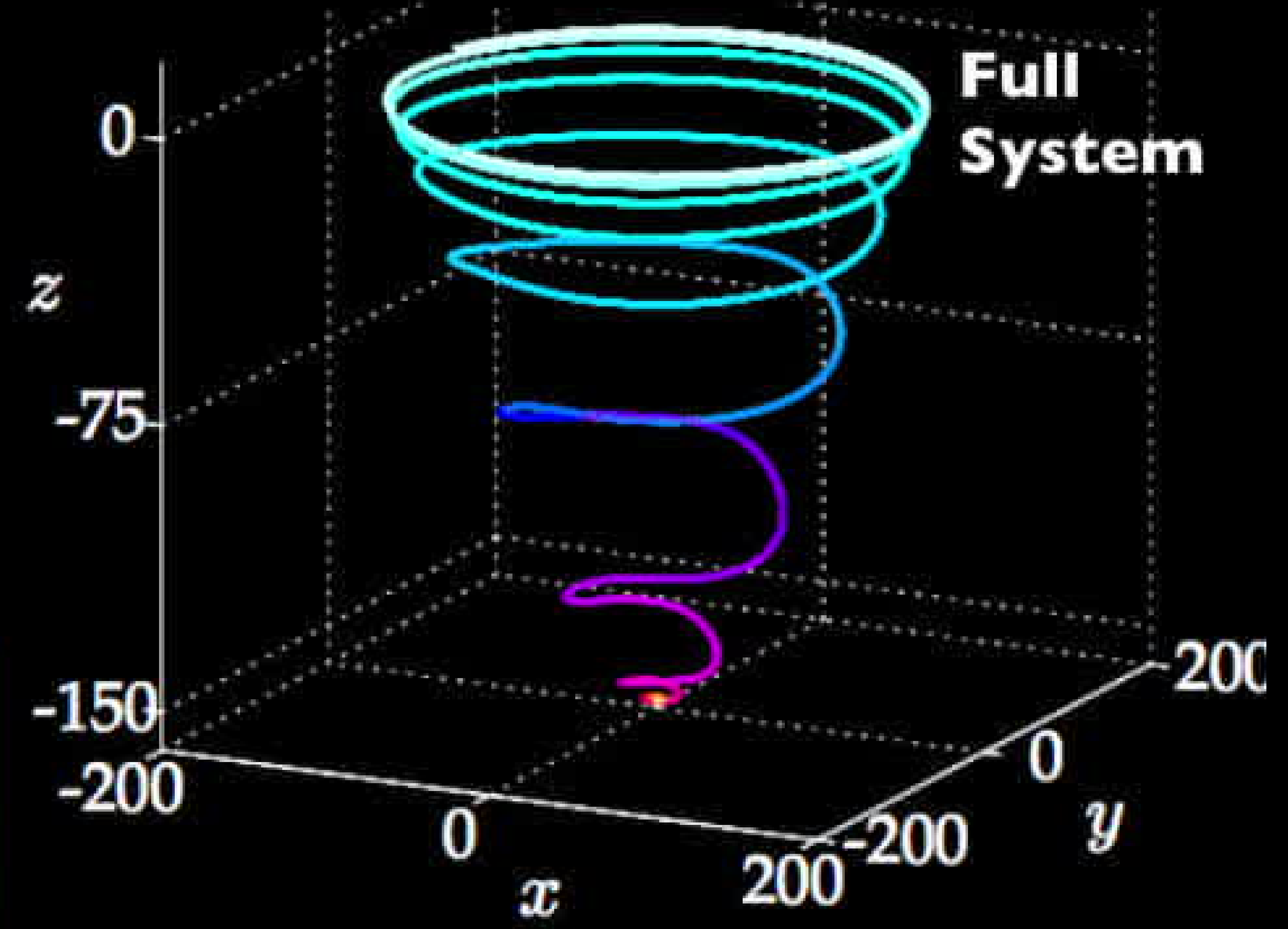
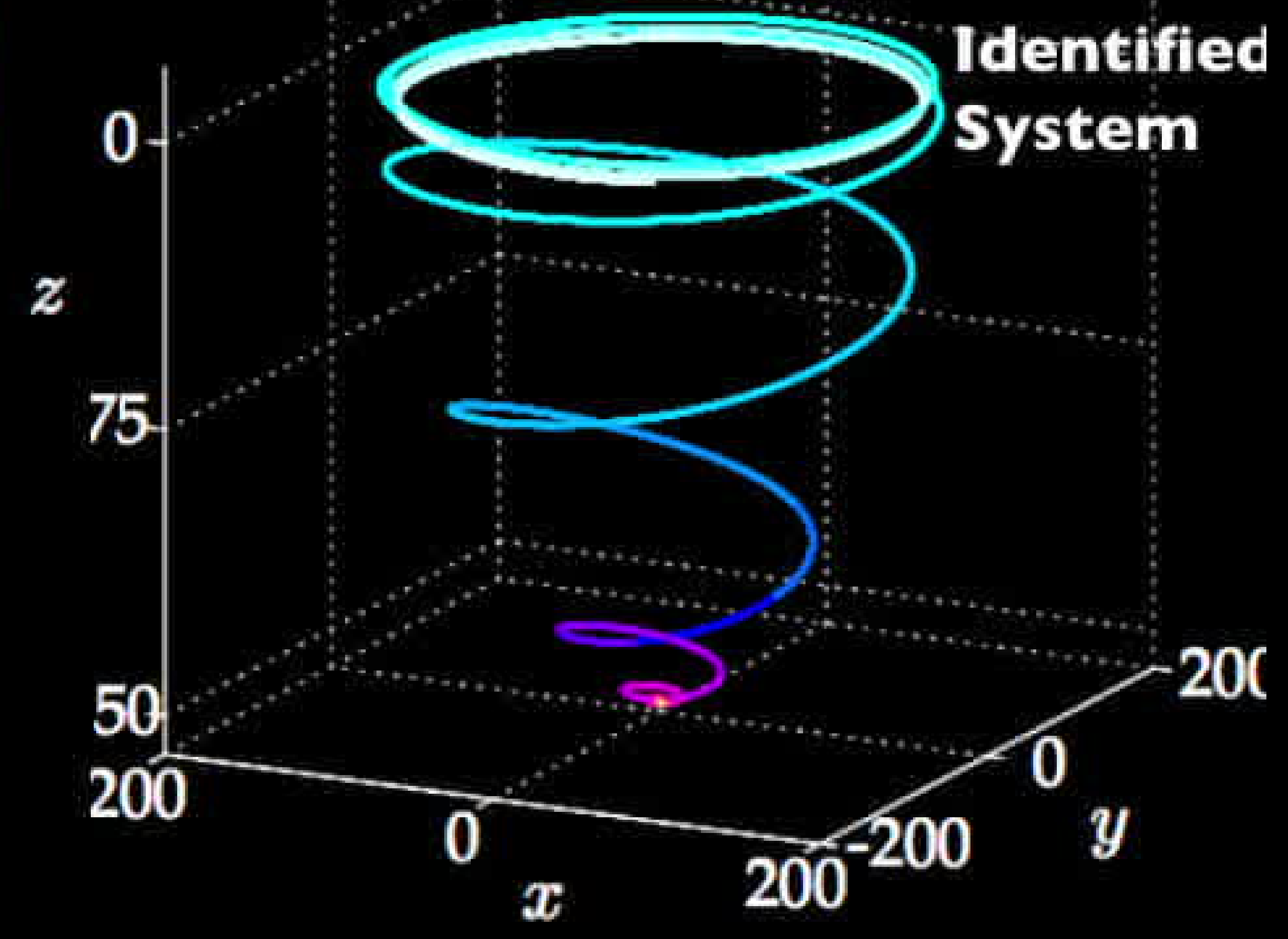
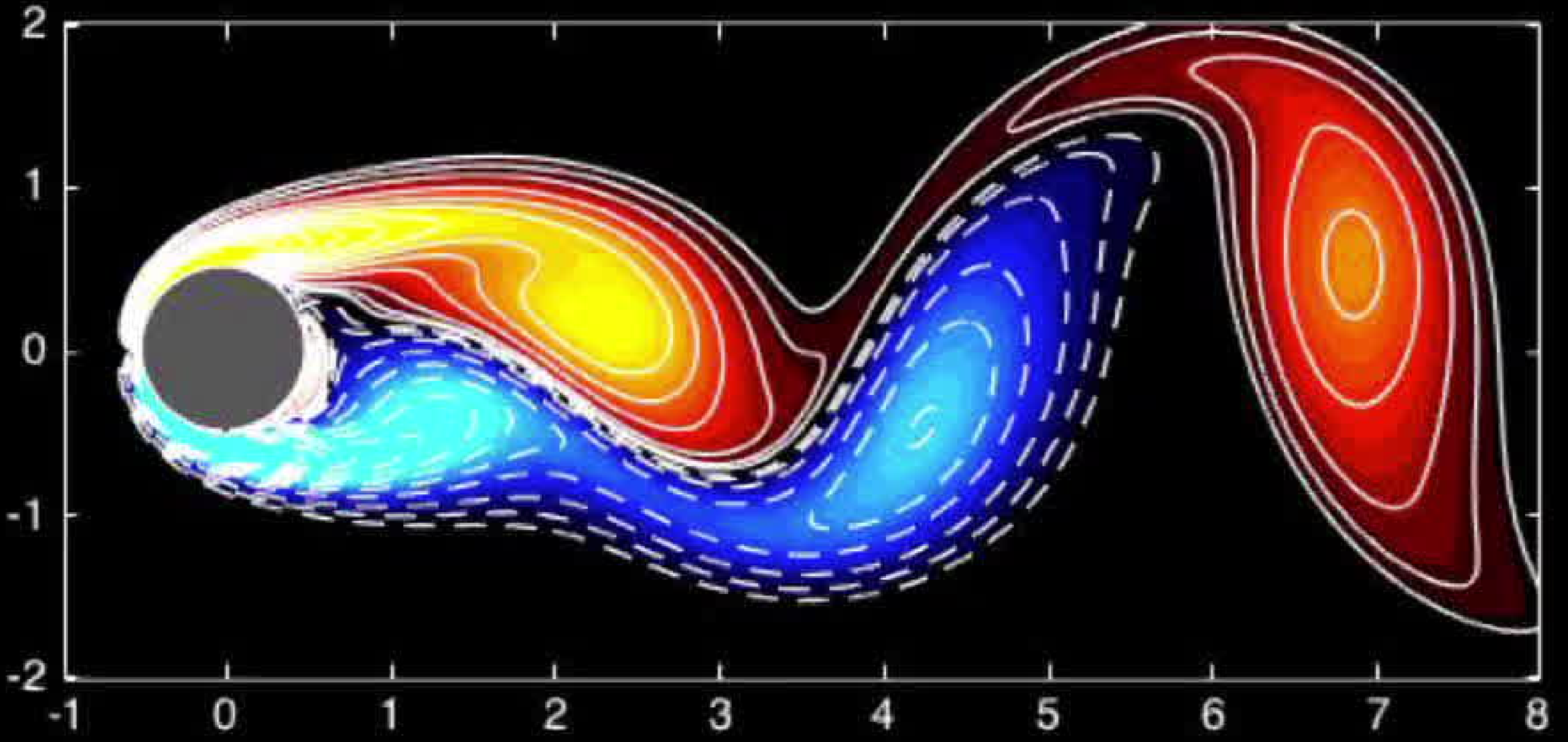


$$\begin{aligned}\dot{x} &= \mu x - \omega y + Axz\\ \dot{y} &= \omega x + \mu y + Ayz\\ \dot{z} &= -\lambda(z - x^2 - y^2).\end{aligned}$$







Ruelle and Takens, 1971
Zebib, 1987 and Jackson, 1987
Noack *et al.*, JFM 2003.
SLB, Proctor, Kutz, PNAS 2016.

Constrained Sparse Galerkin Regression

Innovation 1: Enforcing known constraints

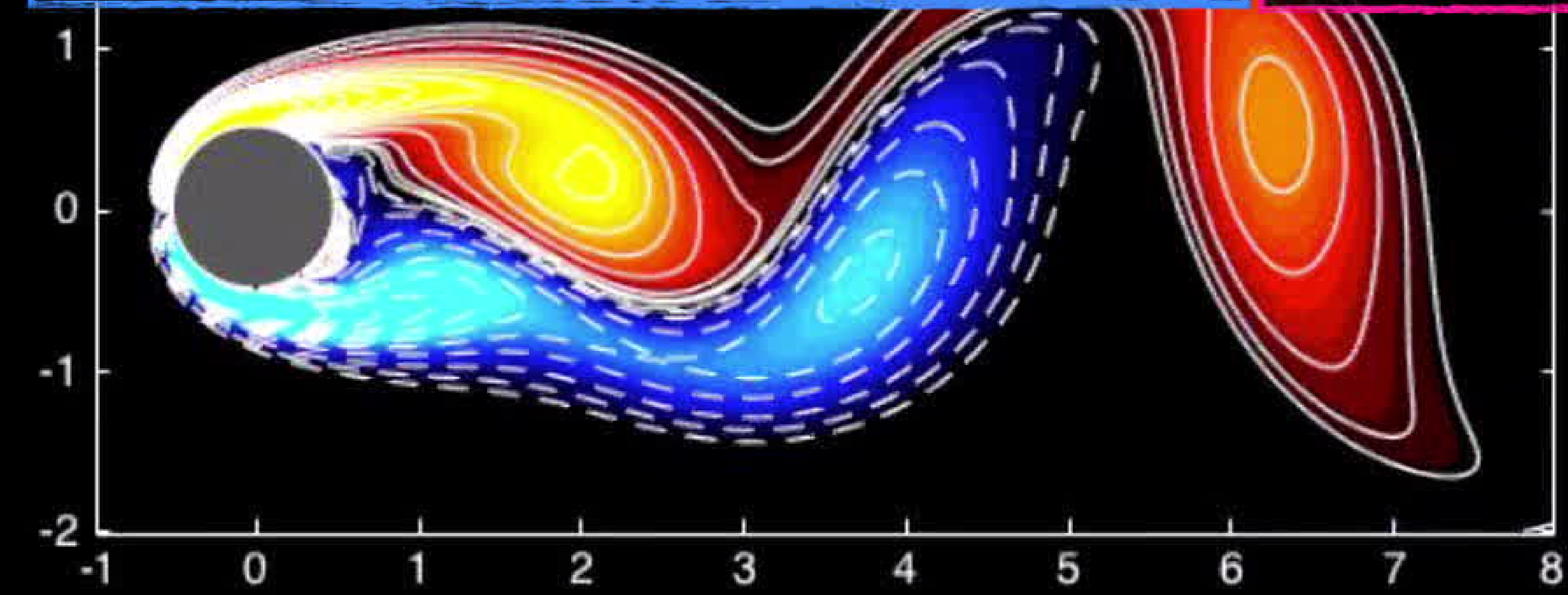
- Skew-symmetric quadratic nonlinearities to enforce energy conservation
- Improved stability

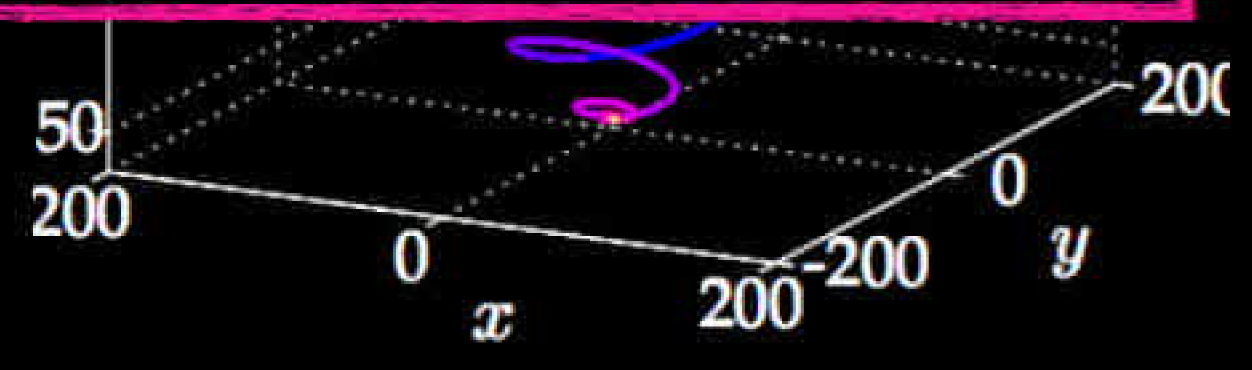
$$\min_{\xi, z} \|\Theta(X)\Xi - \dot{X}\|_2^2 + z^T(C\xi - d)$$

Innovation 2: Higher-order Nonlinearities

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

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

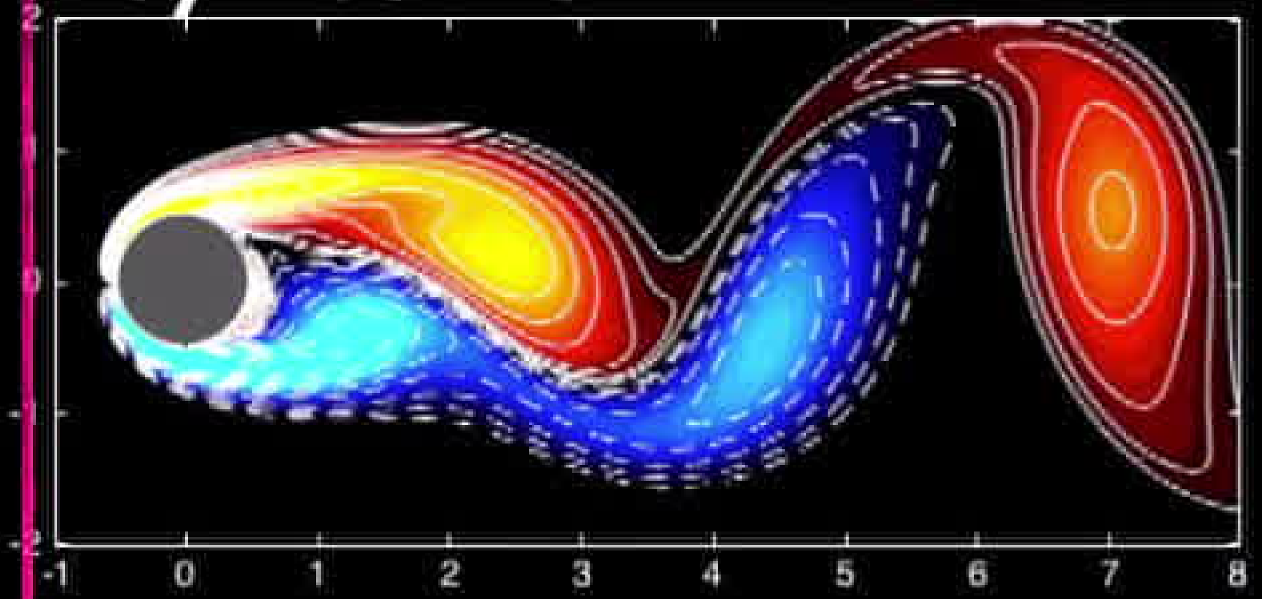


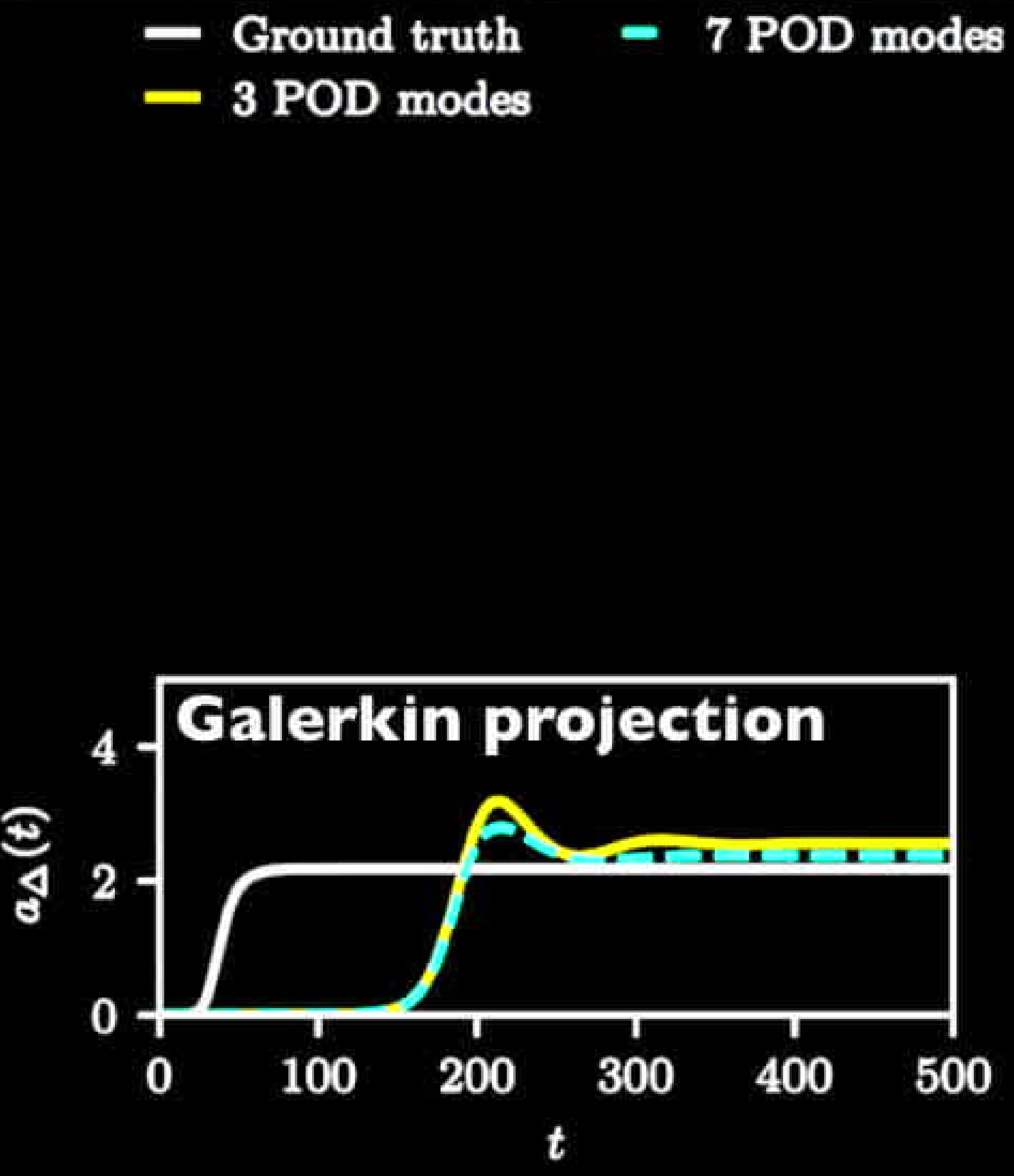


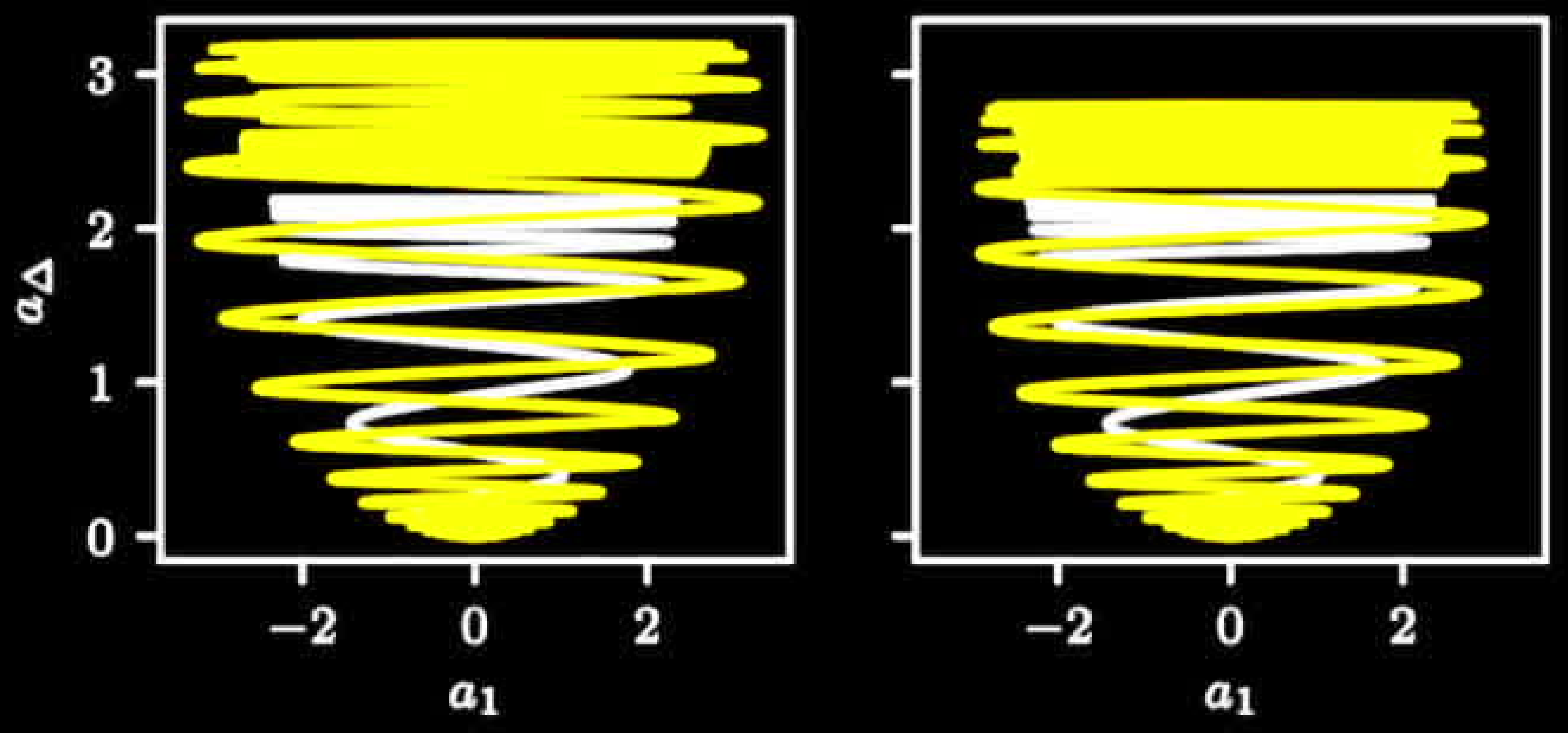
Loiseau & SLB, *JFM* 838, 2018

Constrained Sparse Galerkin Regression

Cylinder flow



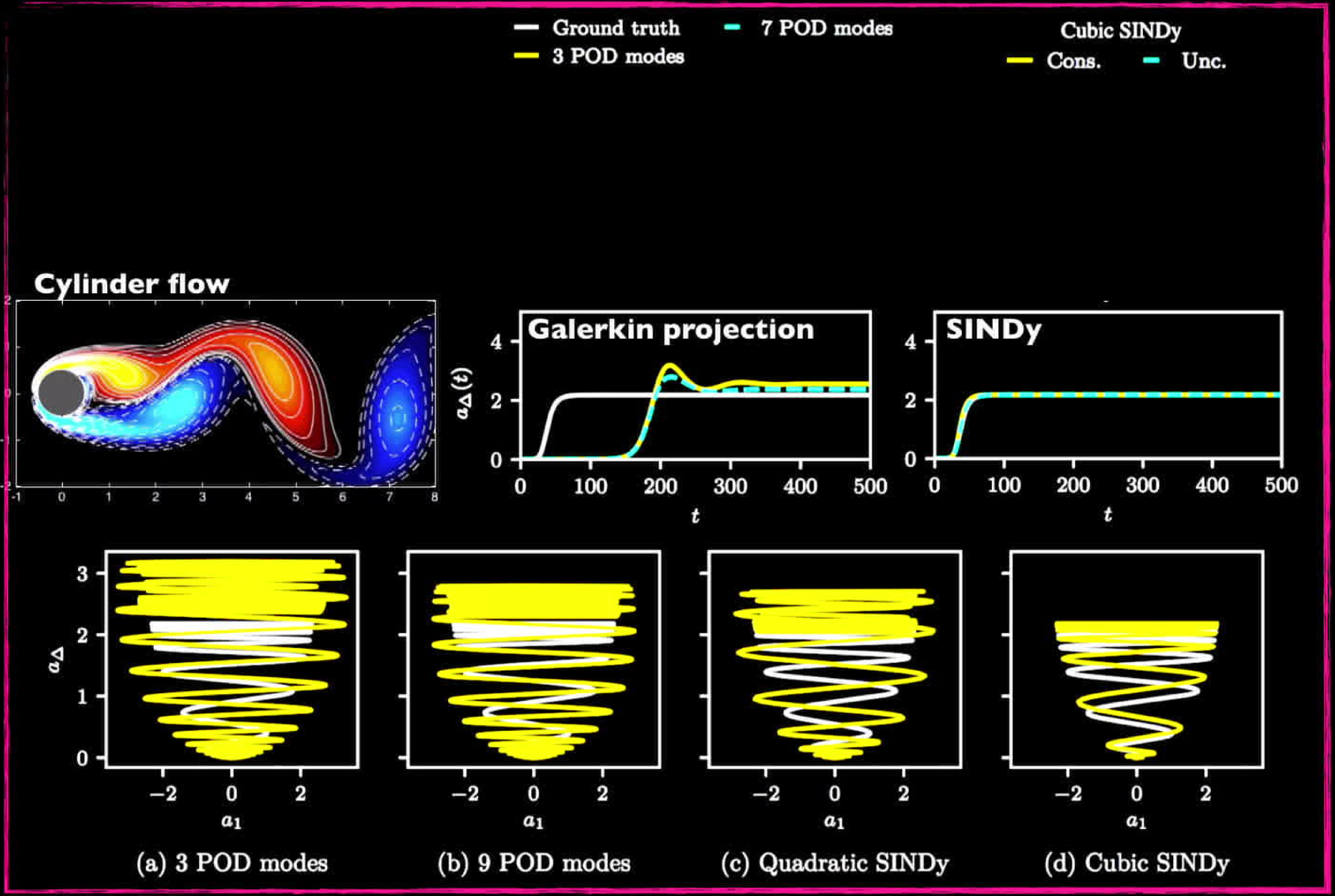




(a) 3 POD modes (b) 9 POD modes

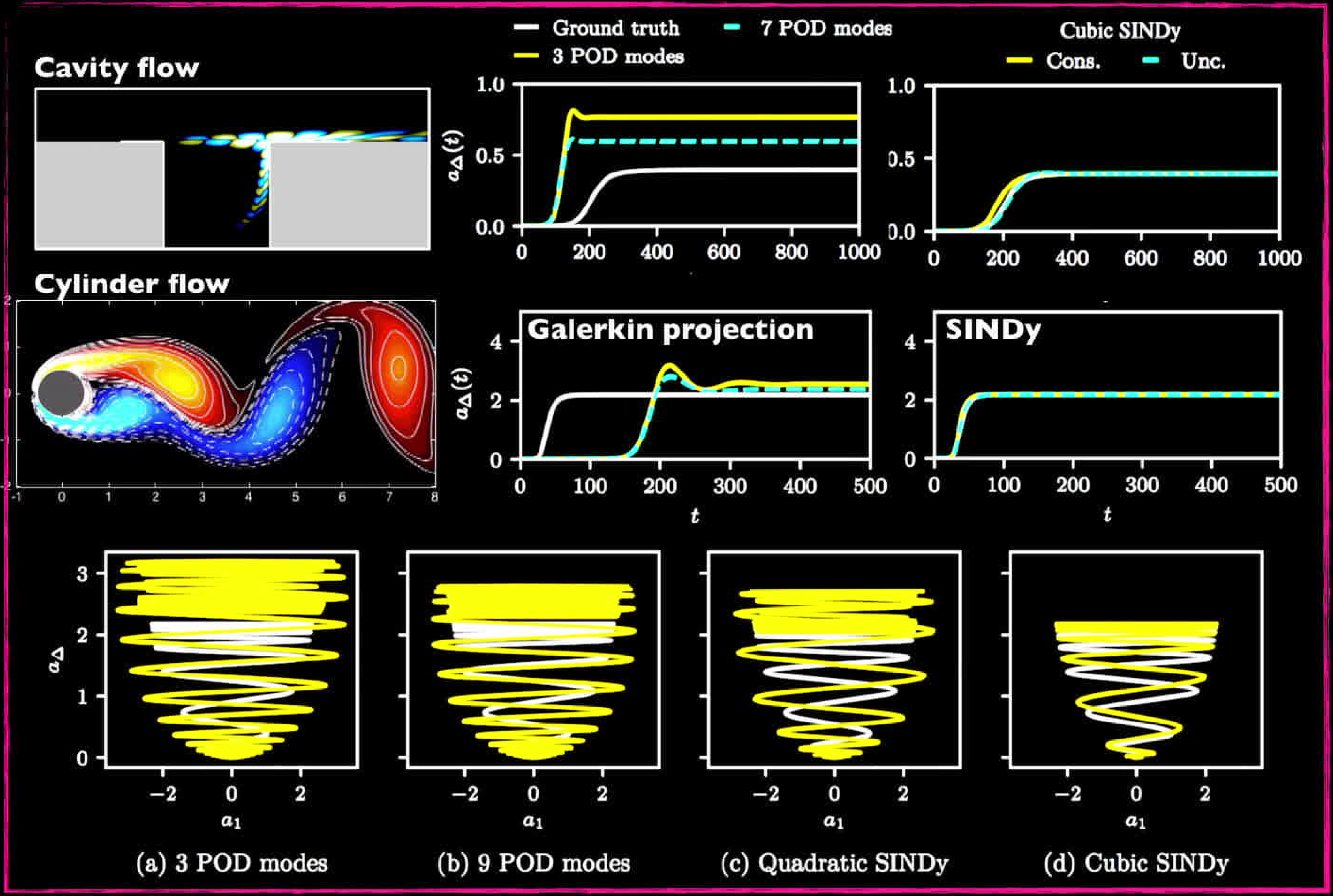
Loiseau & SLB, *JFM* 838, 2018

Constrained Sparse Galerkin Regression



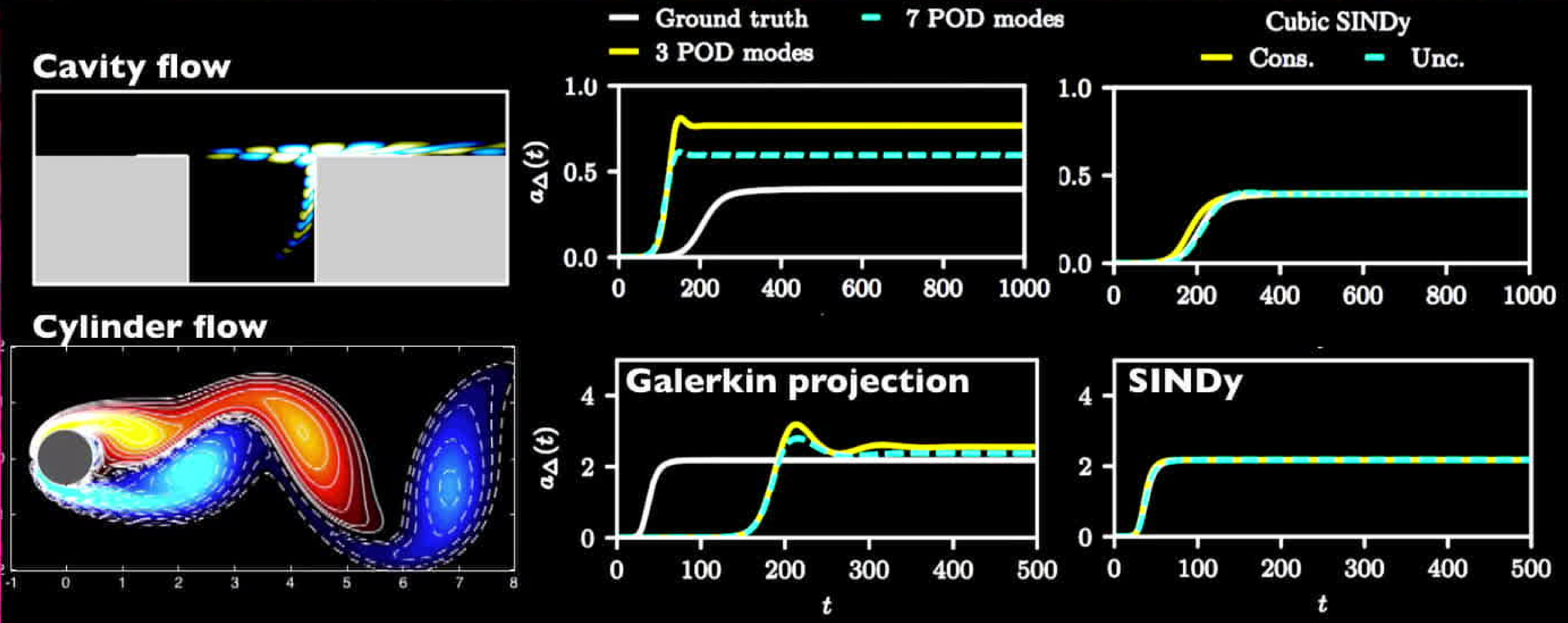
Loiseau & SLB, *JFM* 838, 2018

Constrained Sparse Galerkin Regression



Loiseau & SLB, *JFM* 838, 2018

Constrained Sparse Galerkin Regression

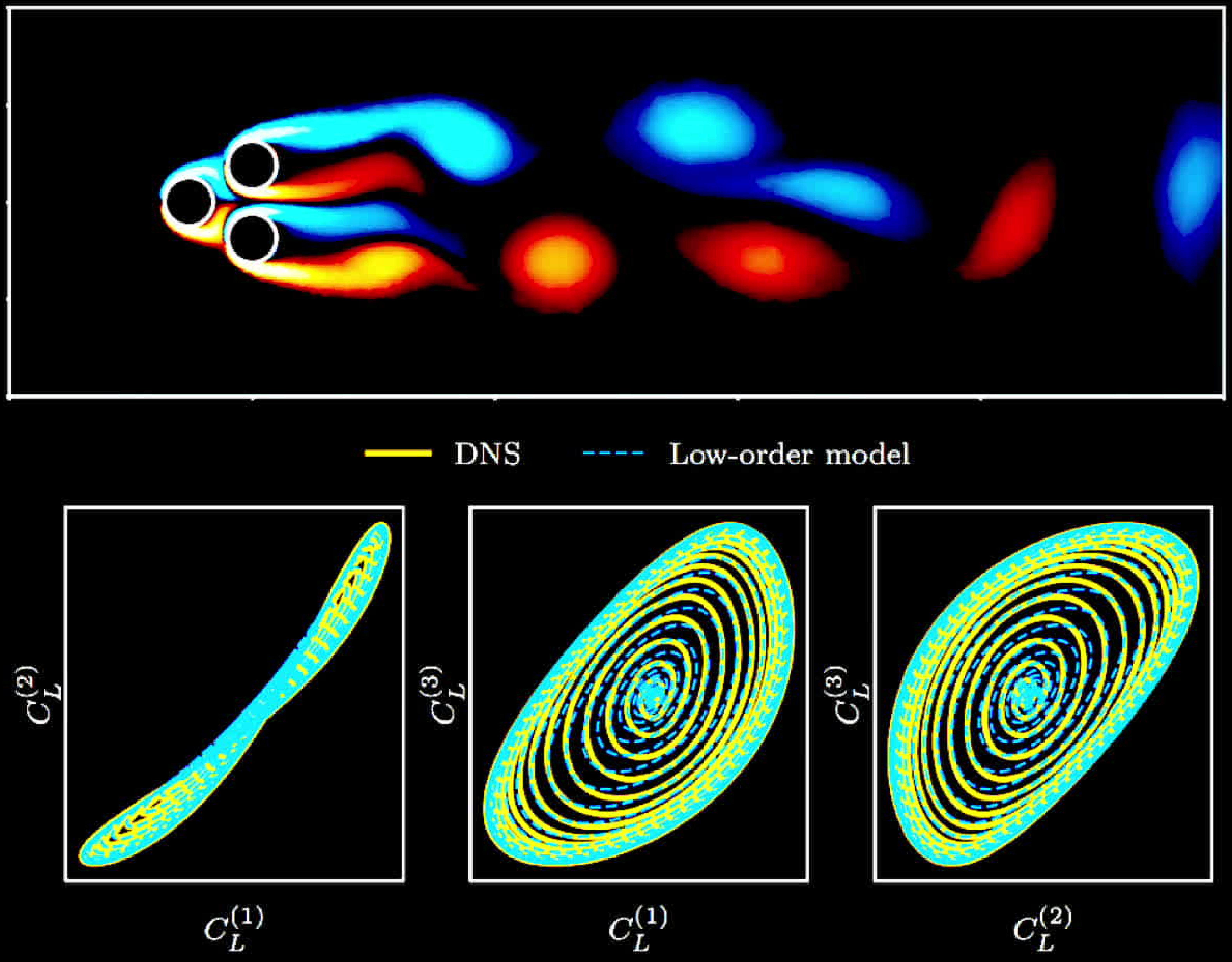


$$\ddot{x} - \underbrace{\left(0.2 - 0.24x^2 - 0.15\dot{x}^2\right)}_{k(x,\dot{x})}\dot{x} + 1.26x = 0$$

Spring-Mass Damper with Nonlinear Damping!

Loiseau & SLB, *JFM* 838, 2018

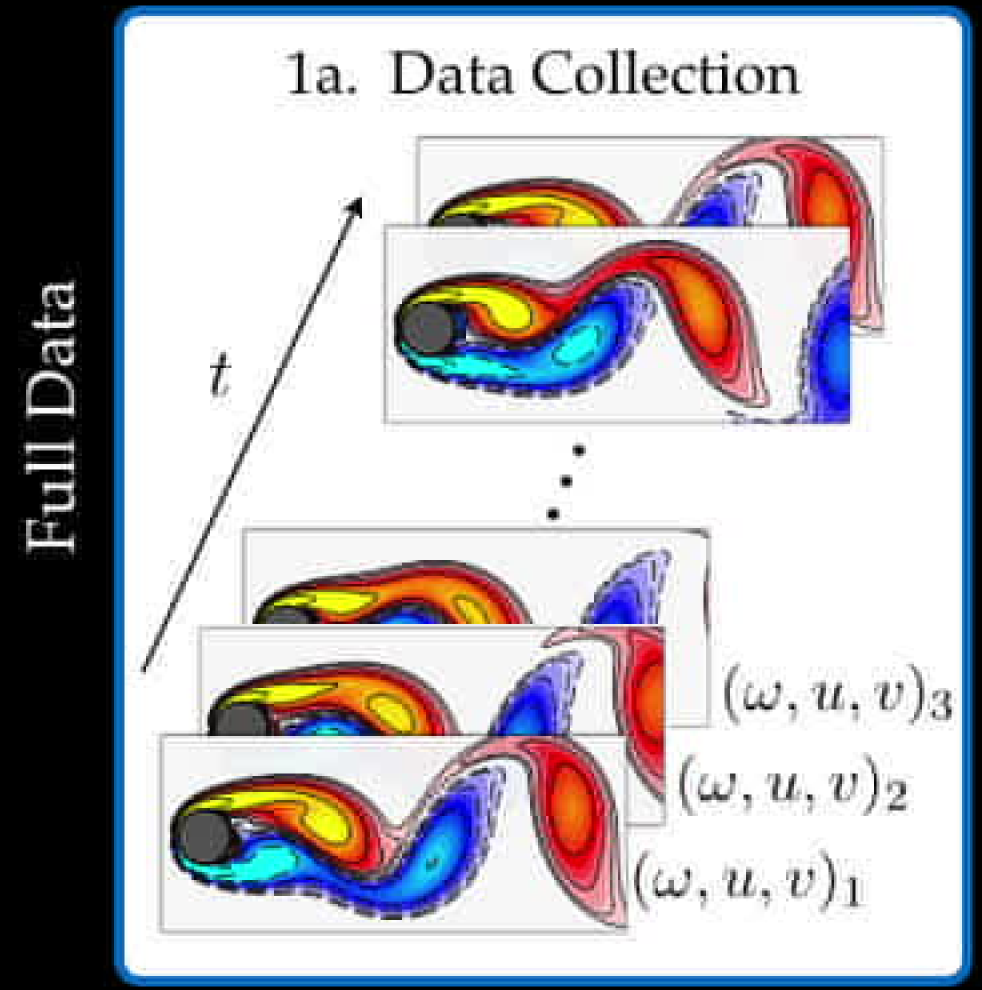
More Complex Flow: Fluidic Pinball



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

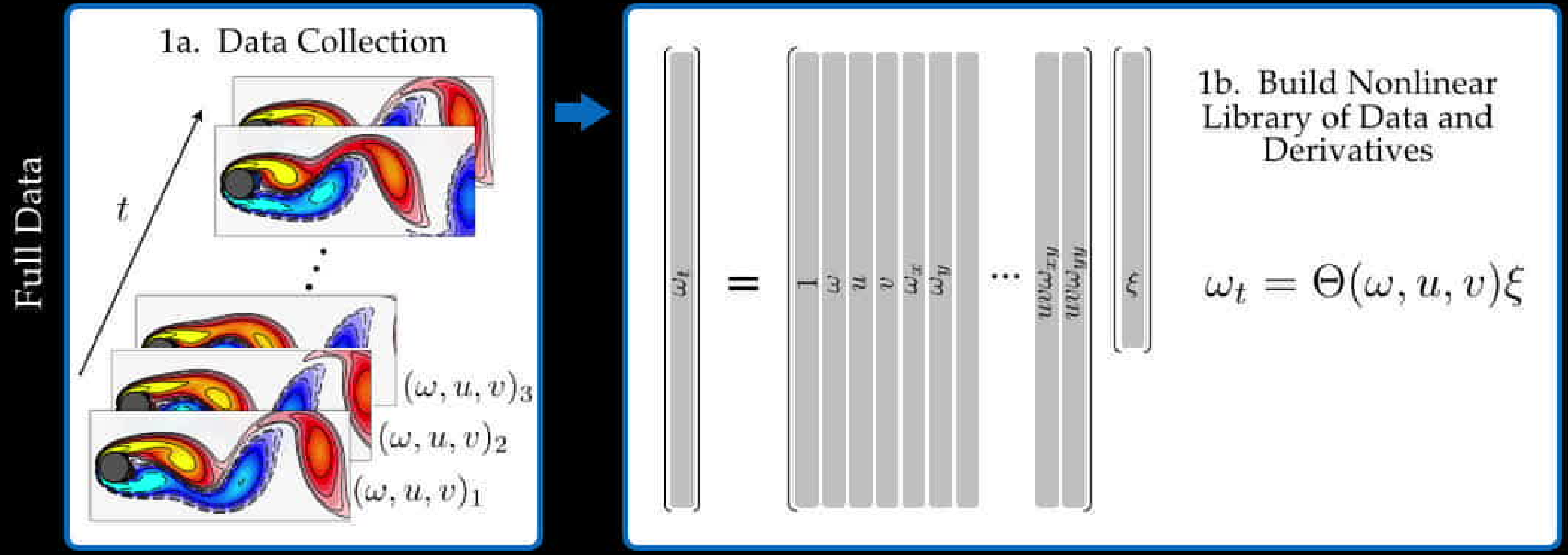
PDES

SINDy: Partial Differential Equations



Rudy, Brunton, Proctor, Kutz
Science Advances, 2017

SINDy: Partial Differential Equations



Rudy, Brunton, Proctor, Kutz
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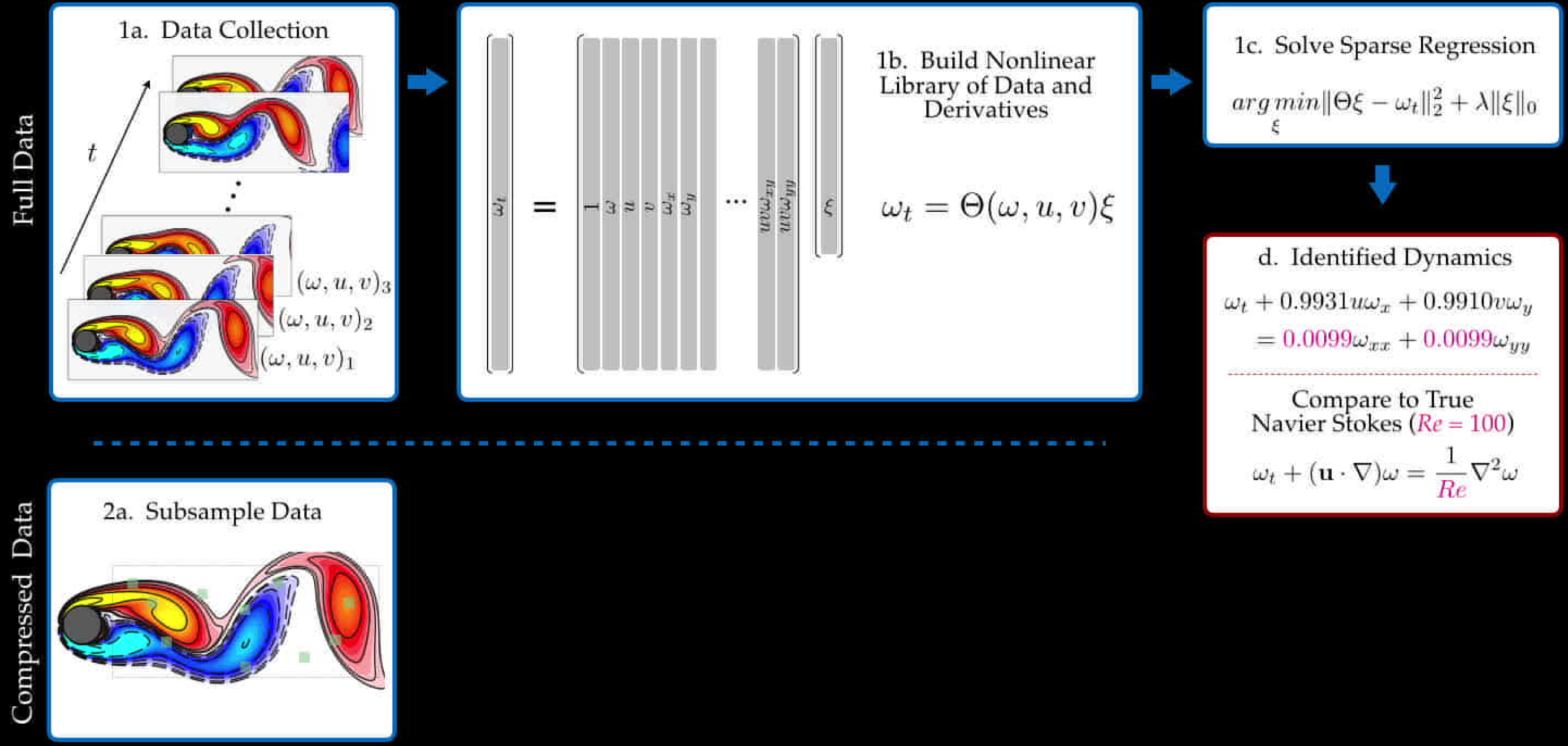
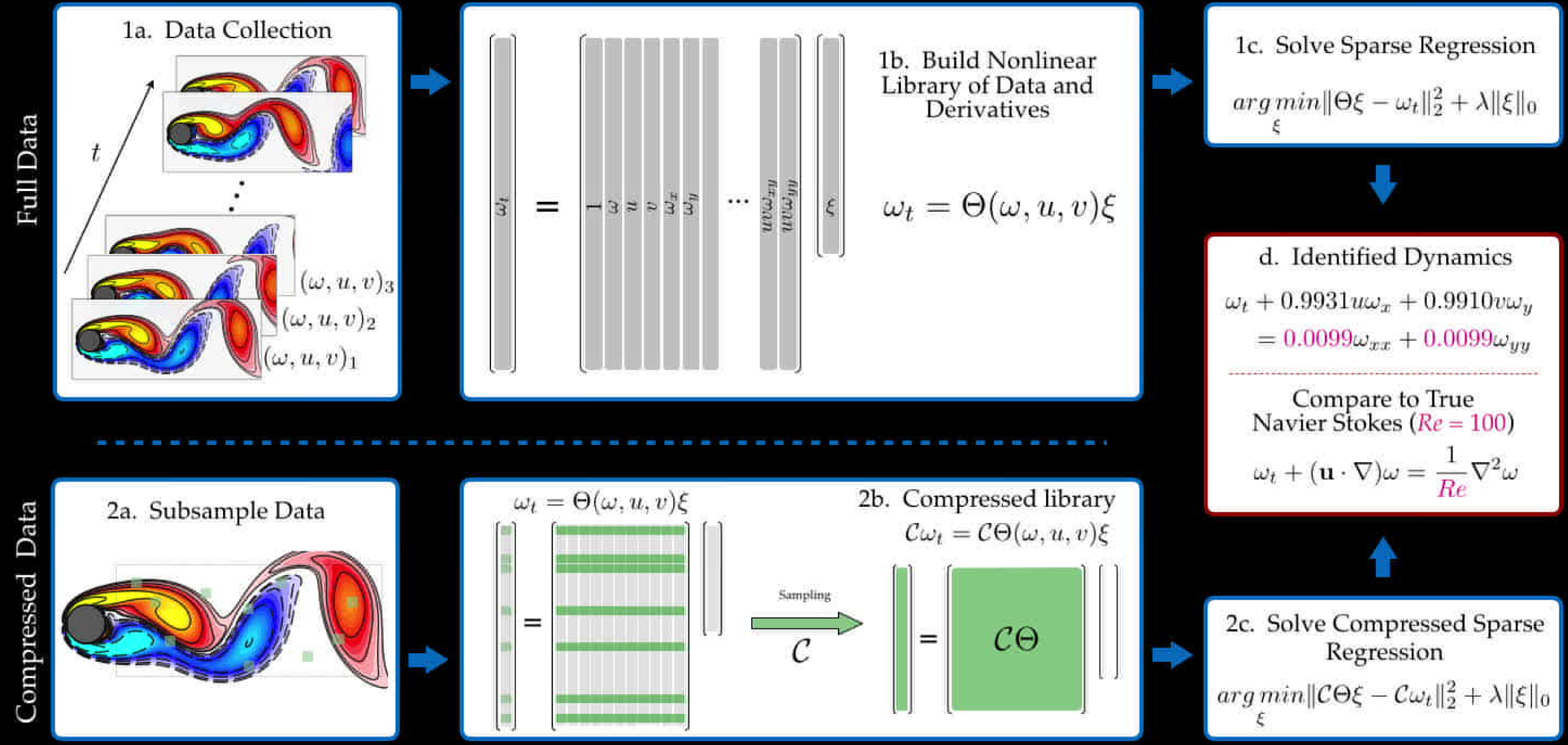
SINDy: Partial Differential Equations



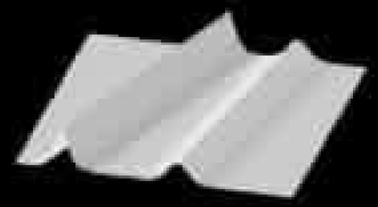
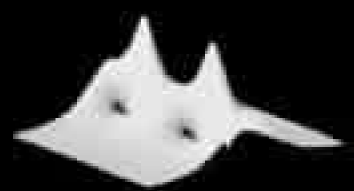
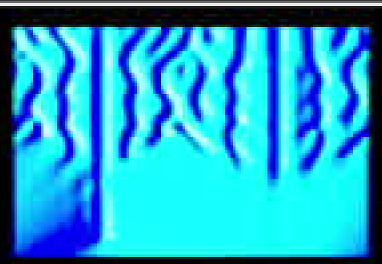
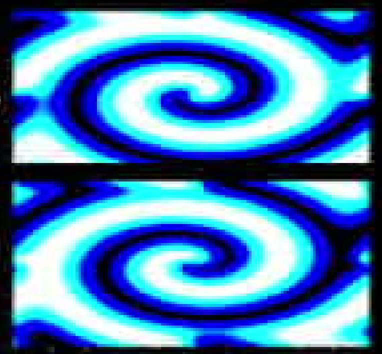
Rudy, Brunton, Proctor, Kutz
***Science Advances*, 2017**

SINDy: Partial Differential Equations



Rudy, Brunton, Proctor, Kutz
Science Advances, 2017

SINDy: Partial Differential Equations

PDE	Form	Error (no noise, noise)
 KdV	$u_t + 6uu_x + u_{xxx} = 0$	1%±0.2%, 7%±5%
 Burgers	$u_t + uu_x - \epsilon u_{xx} = 0$	0.15%±0.06%, 0.8%±0.6%
 Schrödinger	$iu_t + \frac{1}{2}u_{xx} - \frac{x^2}{2}u = 0$	0.25%±0.01%, 10%±7%
 NLS	$iu_t + \frac{1}{2}u_{xx} + \lvert u\rvert^2 u = 0$	0.05%±0.01%, 3%±1%
 KS	$u_t + uu_x + u_{xx} + u_{xxxx} = 0$	1.3%±1.3%, 52%±1.4%
u v  Reaction Diffusion	$u_t = 0.1\nabla^2 u + \lambda(A)u - \omega(A)v$ $v_t = 0.1\nabla^2 v + \omega(A)u + \lambda(A)v$ $A^2 = u^2 + v^2, \omega = -\beta A^2, \lambda = 1 - A^2$	0.02% ± 0.01%, 3.8% ± 2.4%
 Navier Stokes	$\omega_t + (\mathbf{u}\cdot\nabla)\omega = \frac{1}{Re}\nabla^2\omega$	1% ± 0.2% , 7% ± 6%

Rudy, Brunton, Proctor, Kutz
Science Advances, 2017

SUMMARY

High-Level Goals:

- Model discovery
- Good coordinates
- Big data to smart data

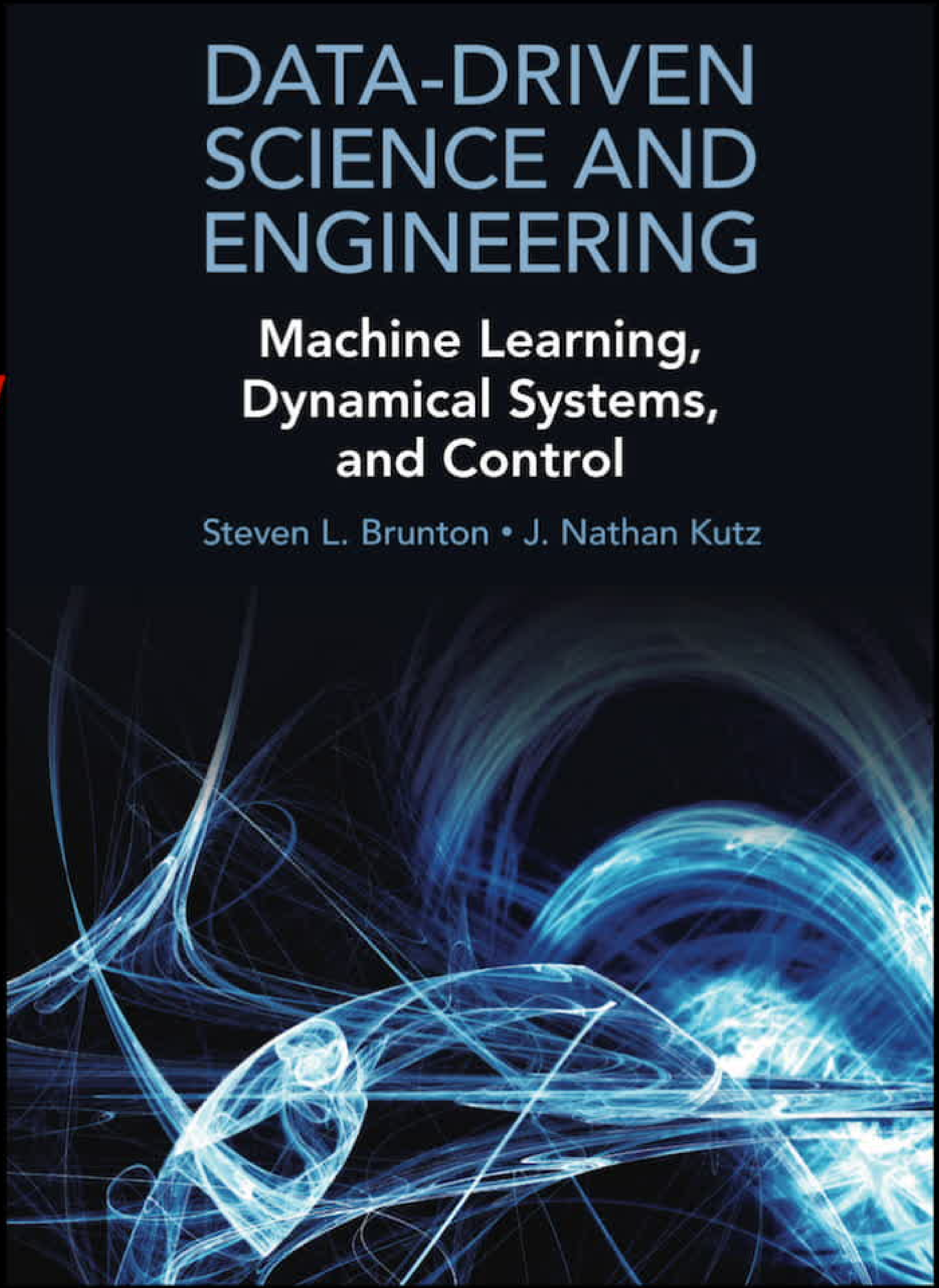
- Limited data/computation
- Not black-box

Modeling Goals:

- Accurate
- Efficient

- Generalizable
- Interpretable
- Analytic (derivatives, etc)

NEW BOOK



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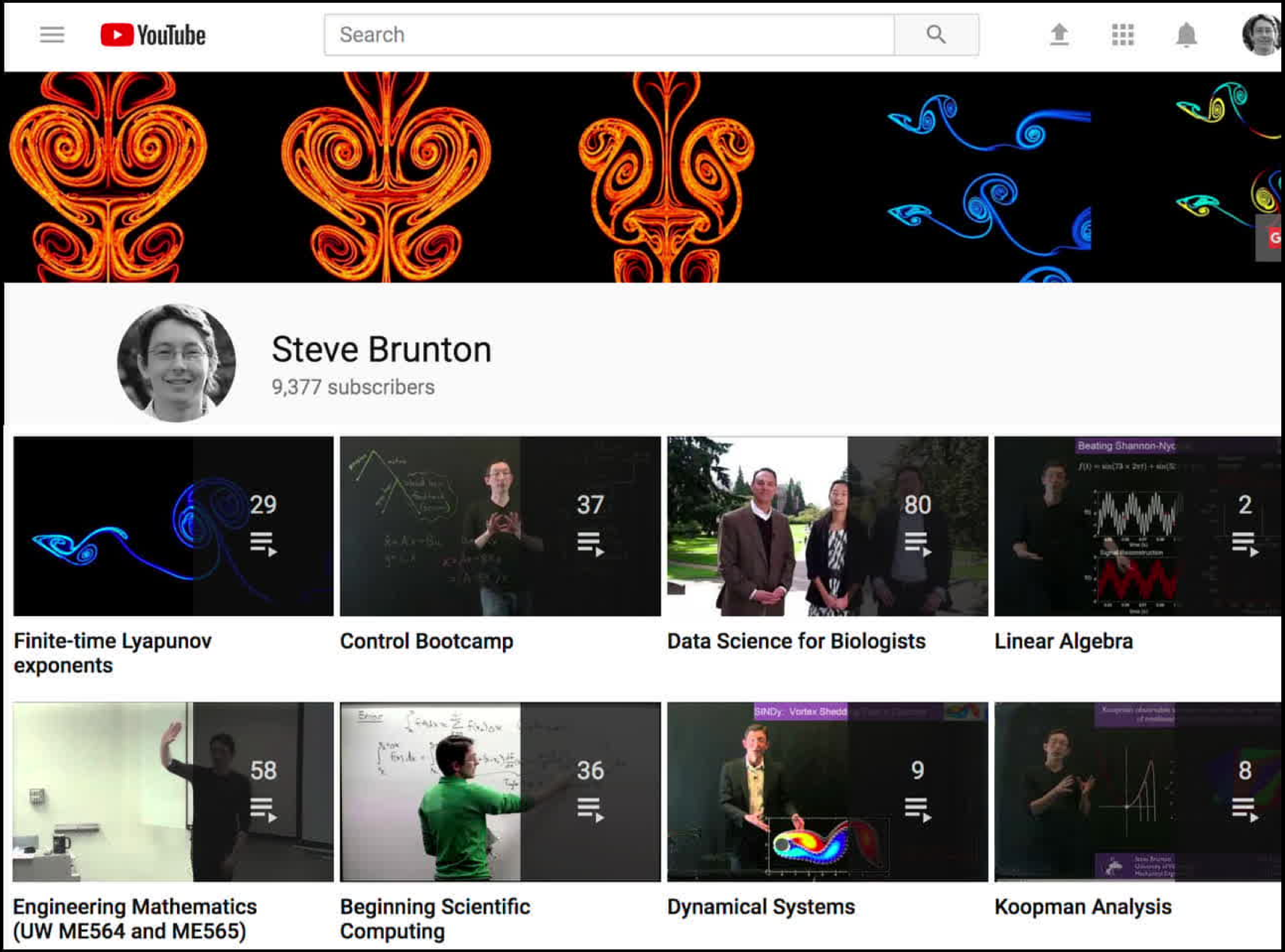
VIDEOS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Control Bootcamp
80
Data Science for Biologists
Beating Shannon-Nyq
2
Linear Algebra
58
Engineering Mathematics (UW ME564 and ME565)
36
Beginning Scientific Computing
SINDy: Vortex Shedd
9
Dynamical Systems
8
Koopman Analysis

QUESTIONS?

QUESTIONS?

QUESTIONS?

QUESTIONS?

QUESTIONS?

QUESTIONS?

QUESTIONS?