Data-driven characterization and control of complex systems

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IPAM, 2017-10-02

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Nathan Kutz

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Josh Proctor

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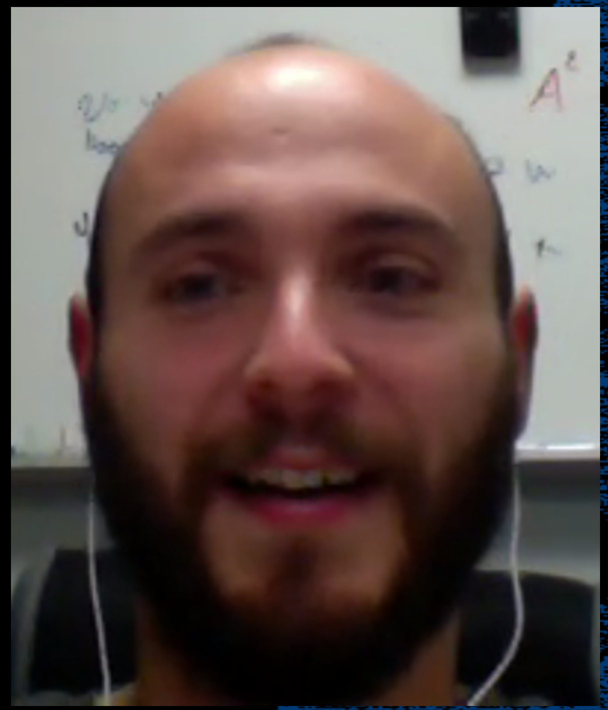
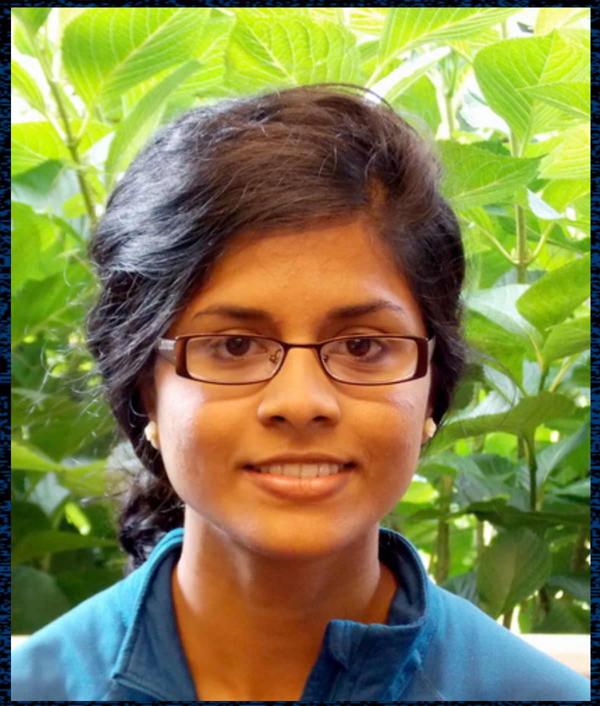
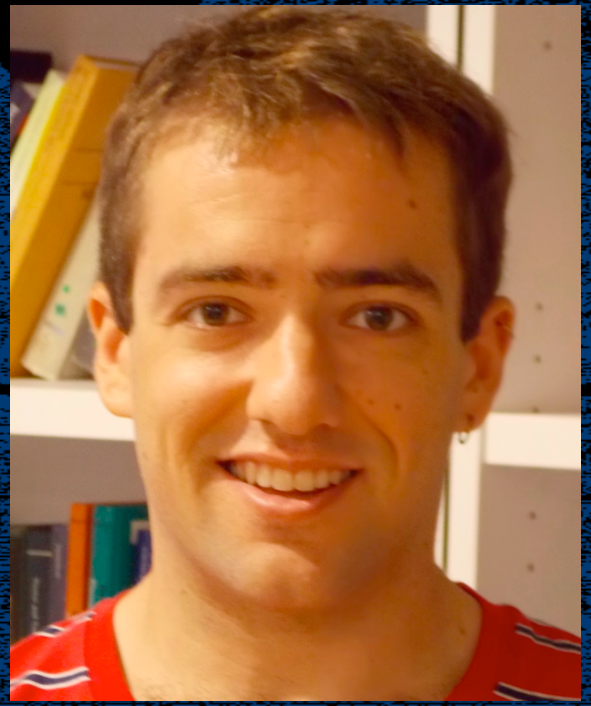


Eurika Kaiser

Niall Mangan



Krithika Manohar



Sam Rudy

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Open Problems, Key Challenges, Emerging Techniques

Open Problem: Often **equations are unknown**, or are only partially known
Key Challenges: Combinatorially large search space for candidate models
Emerging Techniques: Machine learning, sparse (parsimonious) methods

Open Problem: **Nonlinear** dynamics still poorly understood
Key Challenges: Topologically complex, no closed form (Poincare)
Emerging Techniques: Koopman spectral analysis (linear embeddings)

Open Problem: Optimal **nonlinear control** and estimation
Key Challenges: Finding intrinsic coordinates (Koopman eigenfunctions)
Emerging Techniques: Uncertainty quantification and robust control

Open Problem: **Chaos**, transients, intermittent, and uncertain phenomena
Key Challenges: Limitations of topological and operator perspectives
Emerging Techniques: Time delay embeddings facilitate linear regression

Open Problem: Optimal sensing for problems with **multi scale physics**
Key Challenges: Largely heuristic, brute-force, lack of basic principles
Emerging Techniques: Compressed sensing, library learning

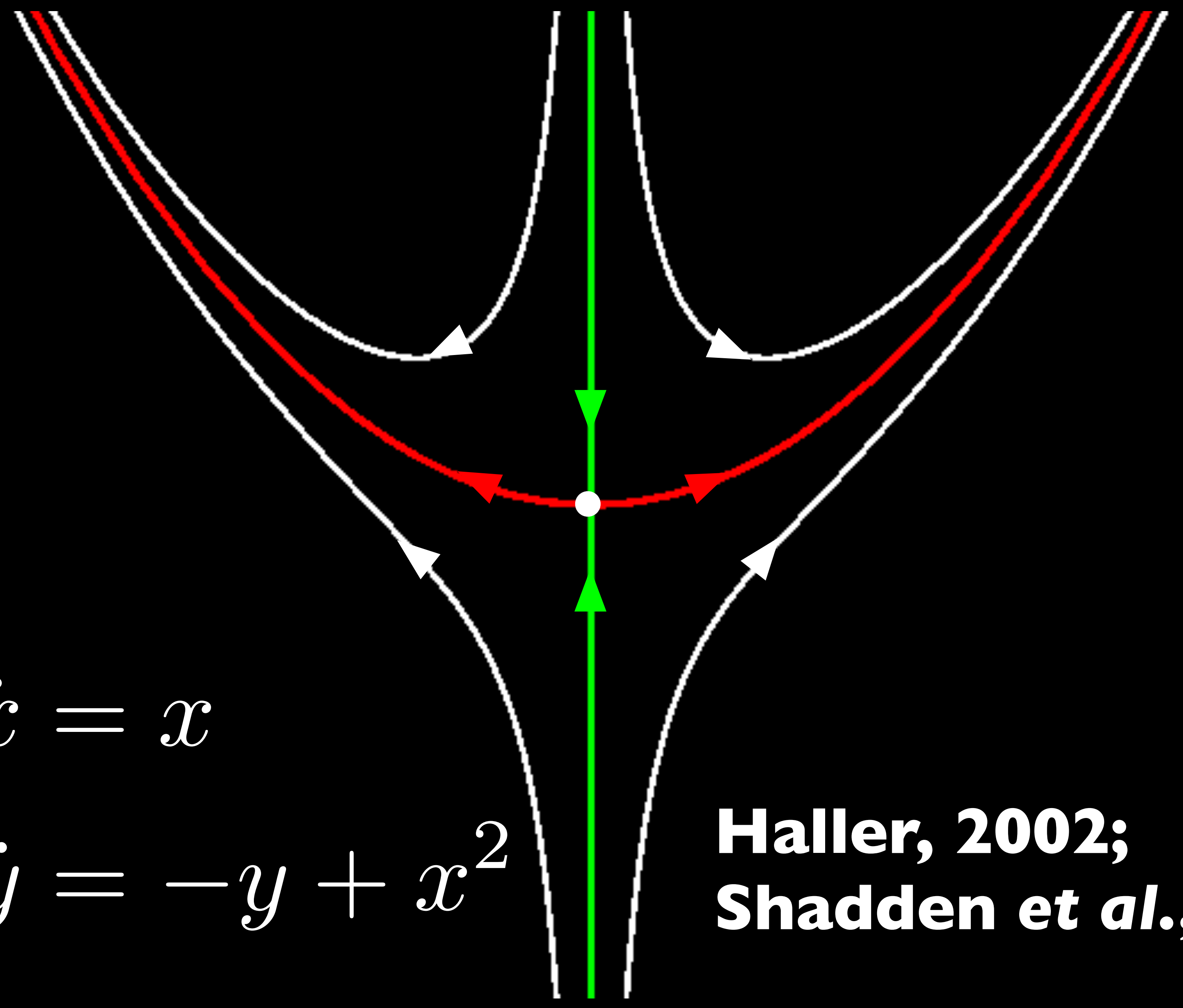
Dynamical Systems: Poincare and Geometry

Dynamics

$$\frac{d}{dt}\mathbf{x} = \mathbf{f}(\mathbf{x}), \quad \Rightarrow \quad \mathbf{F}_t(\mathbf{x}(t_0)) = \mathbf{x}(t_0 + t) = \mathbf{x}(t_0) + \int_{t_0}^{t_0+t} \mathbf{f}(\mathbf{x}(\tau))\, d\tau.$$

$$\Rightarrow \quad \mathbf{x}_{k+1} = \mathbf{F}_t(\mathbf{x}_k),$$

Discrete-time update

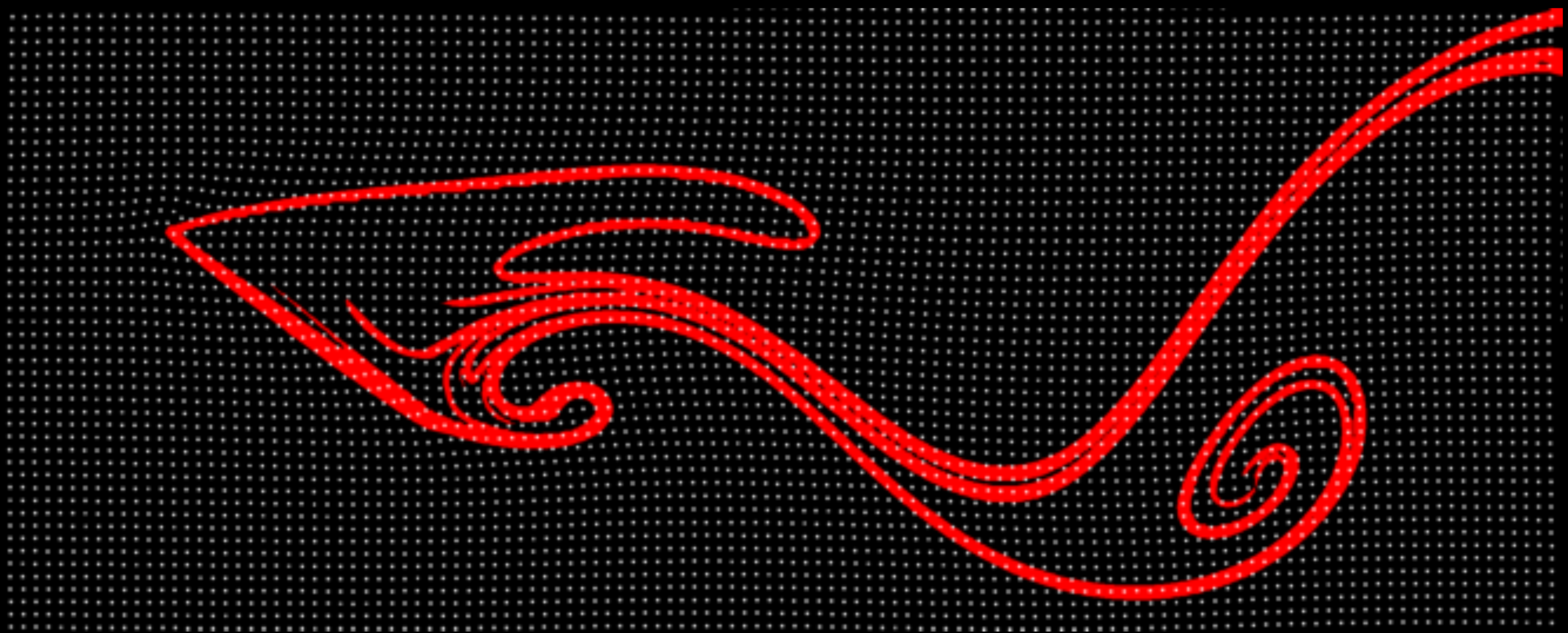


$$\dot{x} = x$$

$$\dot{y} = -y + x^2$$

Haller, 2002;
Shadden *et al.*, 2005

Finite-time Lyapunov exponents (FTLE)



Dynamical Systems: Koopman and Operators

Dynamics

$$\frac{d}{dt}\mathbf{x} = \mathbf{f}(\mathbf{x}), \quad \Rightarrow \quad \mathbf{F}_t(\mathbf{x}(t_0)) = \mathbf{x}(t_0+t) = \mathbf{x}(t_0) + \int_{t_0}^{t_0+t} \mathbf{f}(\mathbf{x}(\tau))\, d\tau.$$

$$\Rightarrow \quad \mathbf{x}_{k+1} = \mathbf{F}_t(\mathbf{x}_k),$$ Discrete-time update

Koopman operator

$$\mathcal{K}_t g = g \circ \mathbf{F}_t \quad \Rightarrow \quad \mathcal{K}_t g(\mathbf{x}_k) = g(\mathbf{F}_t(\mathbf{x}_k)) = g(\mathbf{x}_{k+1}).$$

$$\Rightarrow \quad g(\mathbf{x}_{k+1}) = \mathcal{K}_t g(\mathbf{x}_k).$$ Discrete-time update

Koopman invariant subspace:

$$g = \sum_{k=1}^{\infty} \alpha_k y_k.$$

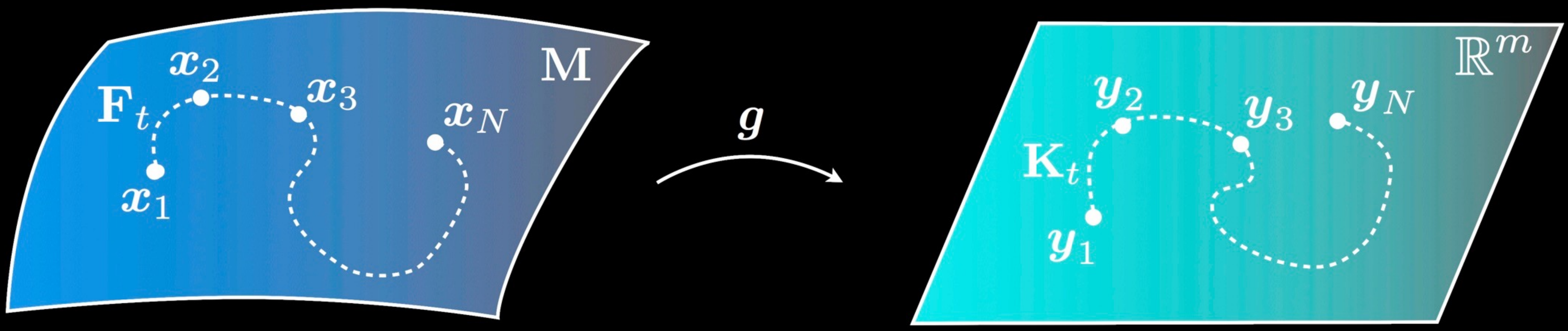
$$g = \alpha_1 y_{s_1} + \alpha_2 y_{s_2} + \cdots + \alpha_m y_{s_m},$$

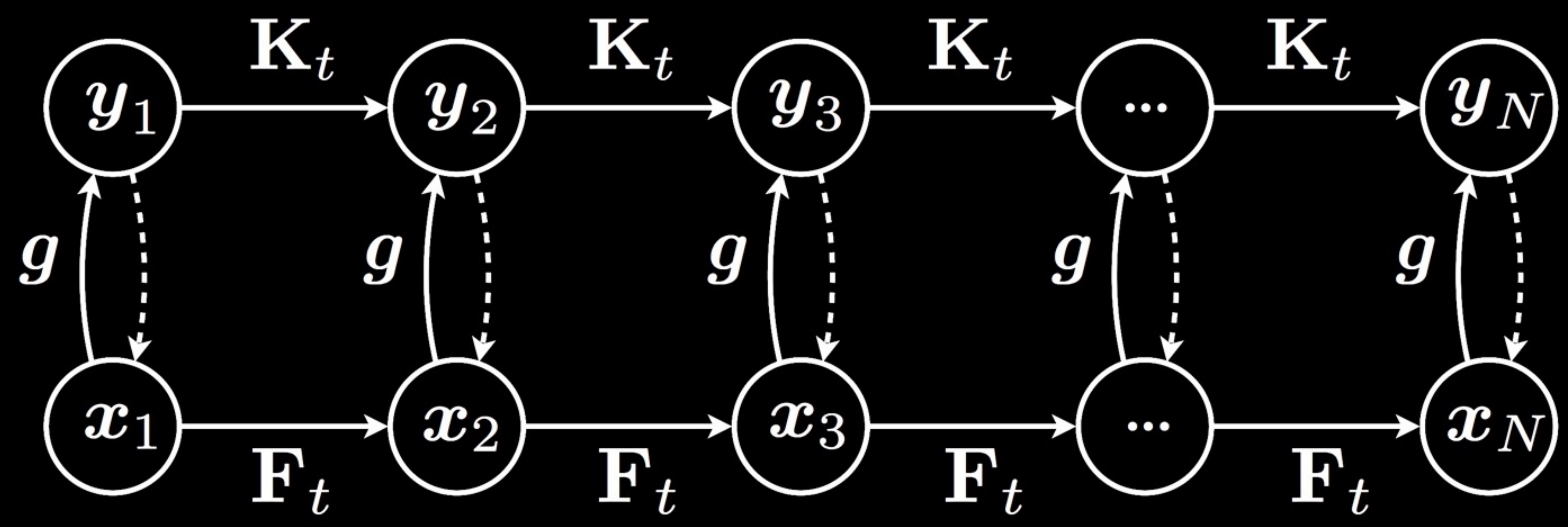
$$\mathcal{K} g = \beta_1 y_{s_1} + \beta_2 y_{s_2} + \cdots + \beta_m y_{s_m}.$$

Koopman operator $\mathcal{K}$ is infinite dimensional and *linear*

Koopman, *PNAS* 1931.
Mezic, *Nonlinear Dynamics* 2005.
Mezic, *ARFM* 2013.
Williams, Kevrekidis, Rowley, *JNS* 2015.

Dynamical Systems: Koopman and Operators





$\mathbf{F}_t : \boldsymbol{x}_k \mapsto \boldsymbol{x}_{k+1}$

$\boldsymbol{g} : \boldsymbol{x}_k \mapsto \boldsymbol{y}_k$

$\mathbf{K}_t : \boldsymbol{y}_k \mapsto \boldsymbol{y}_{k+1}$

Koopman invariant subspace:

$$g = \sum_{k=1}^{\infty} \alpha_k y_k.$$

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Williams, Kevrekidis, Rowley, *JNS* 2015.

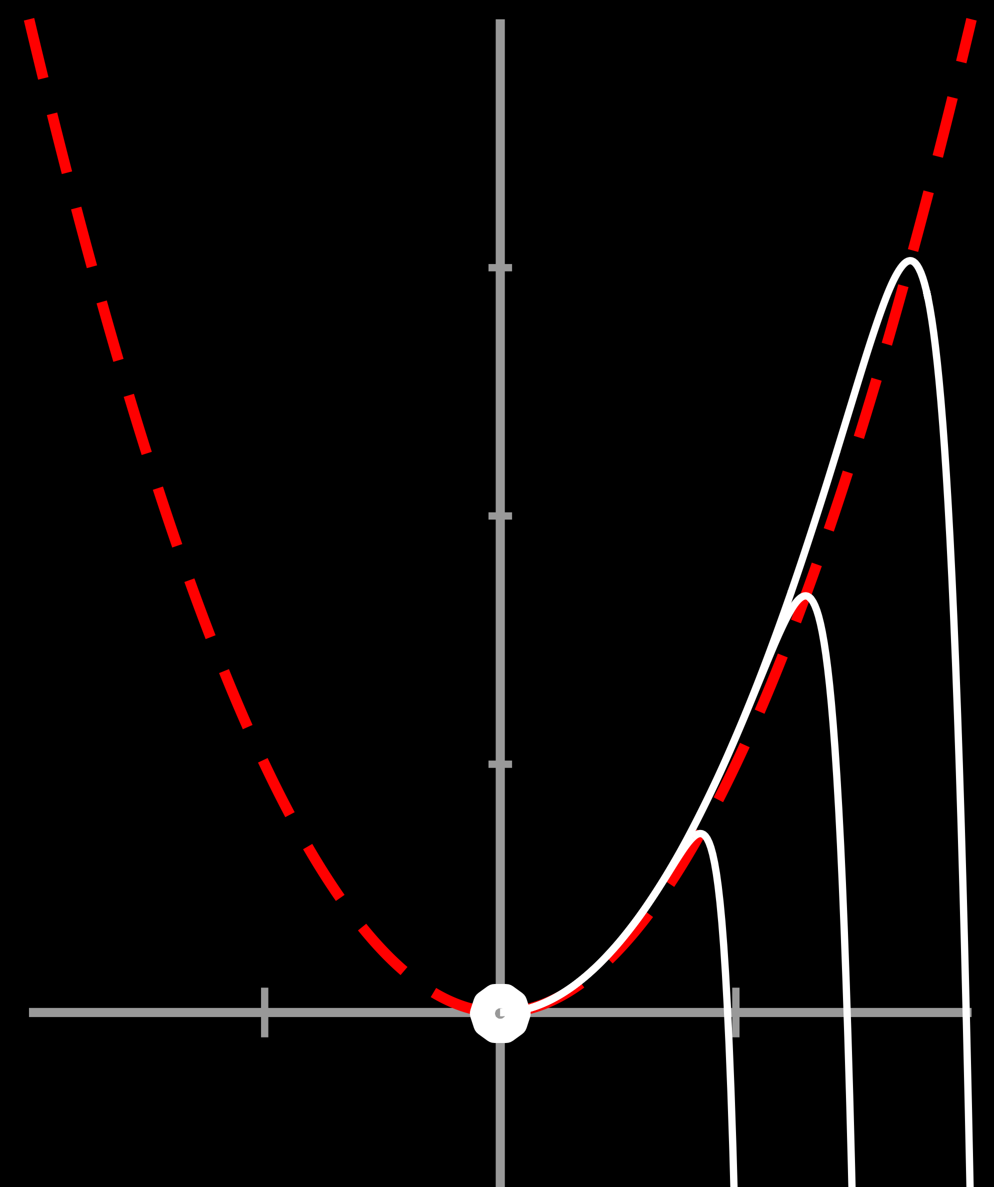
Example: Koopman Linear Embedding

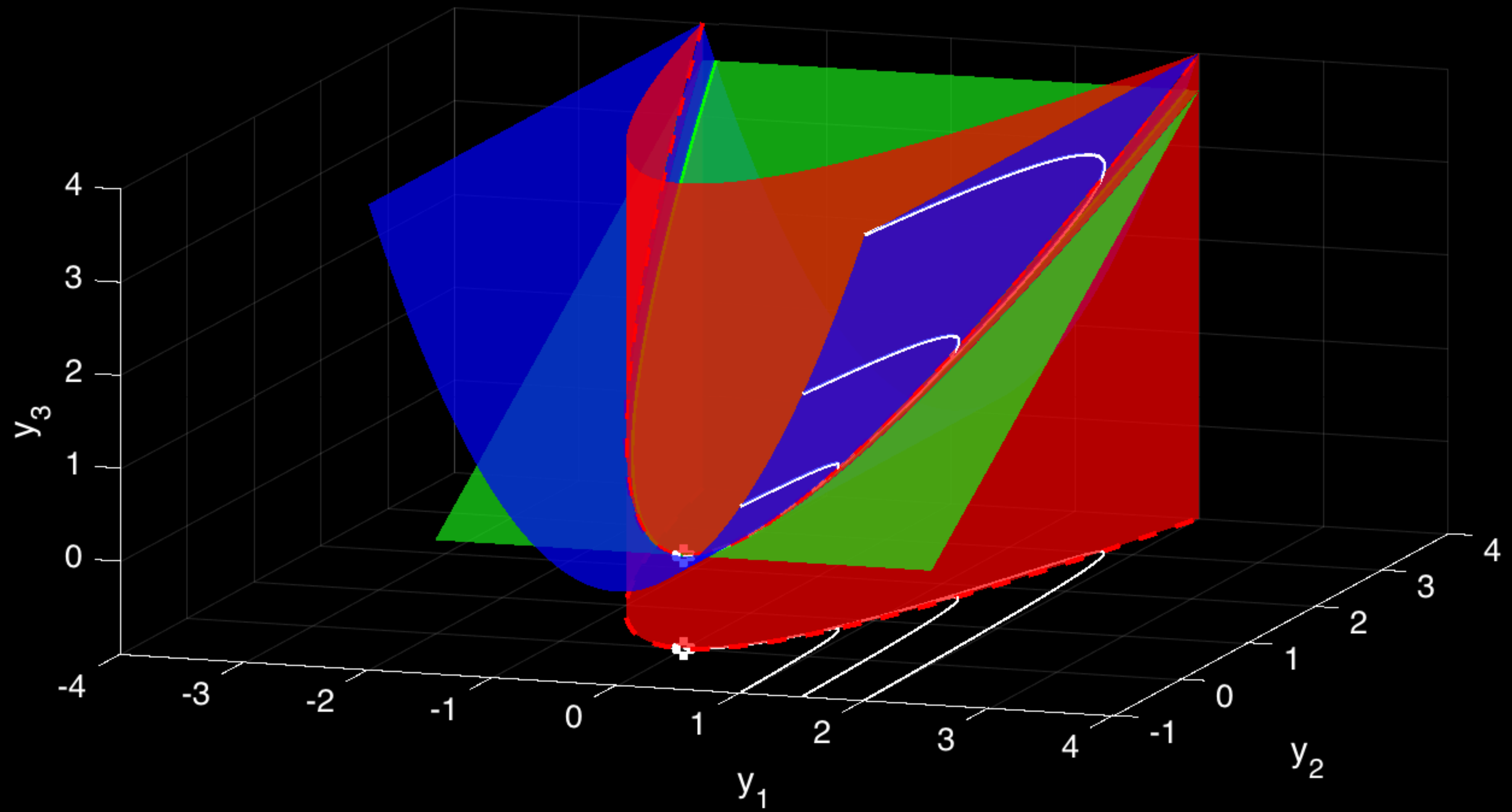
Nonlinear dynamics:

$$\dot{x}_1 = \mu x_1$$
$$\dot{x}_2 = \lambda(x_2 - x_1^2)$$

Koopman linear system:

$$\frac{d}{dt}\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} \mu & 0 & 0 \\ 0 & \lambda & -\lambda \\ 0 & 0 & 2\mu \end{bmatrix}\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \quad \text{for} \quad \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ x_1^2 \end{bmatrix}$$





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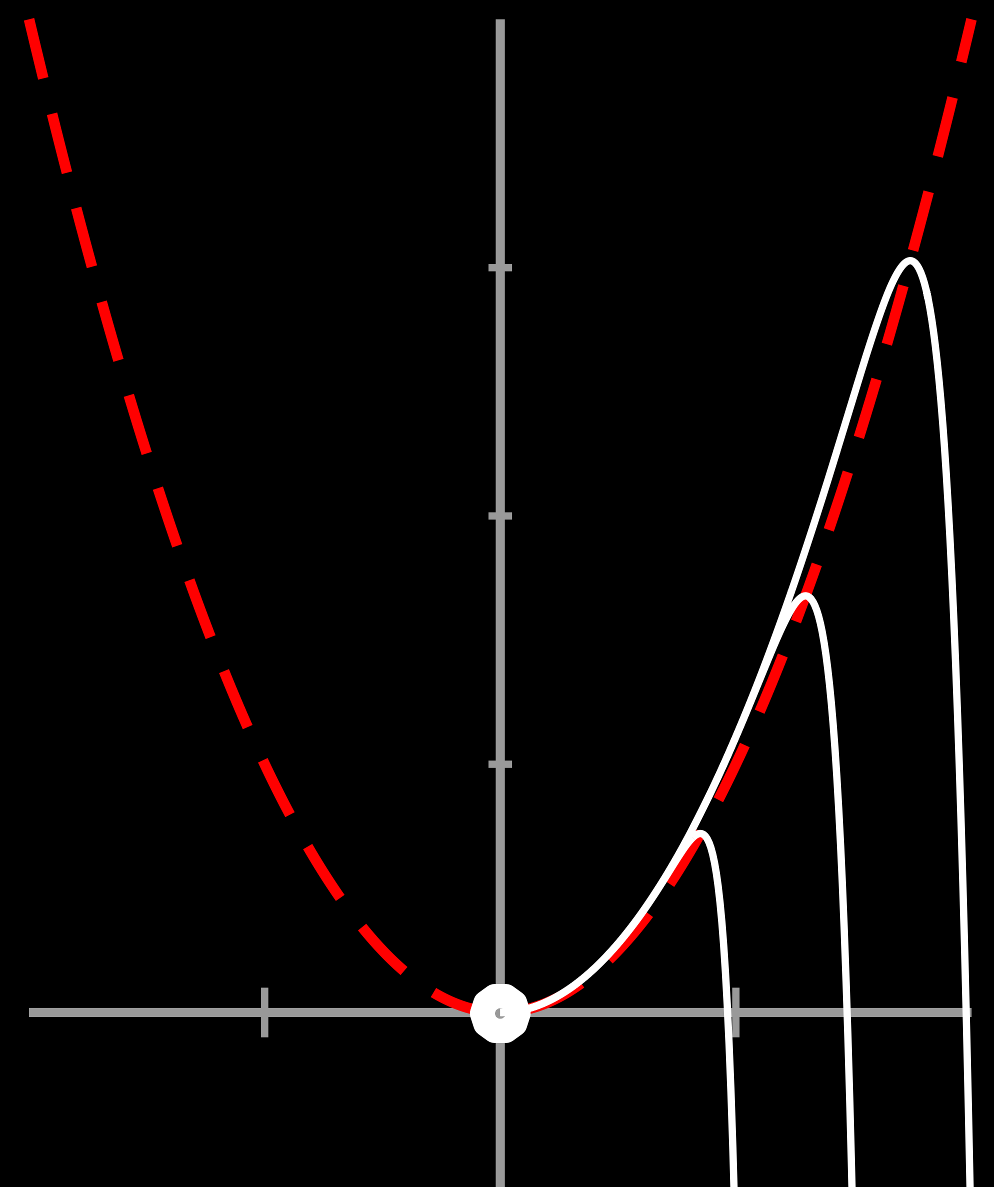
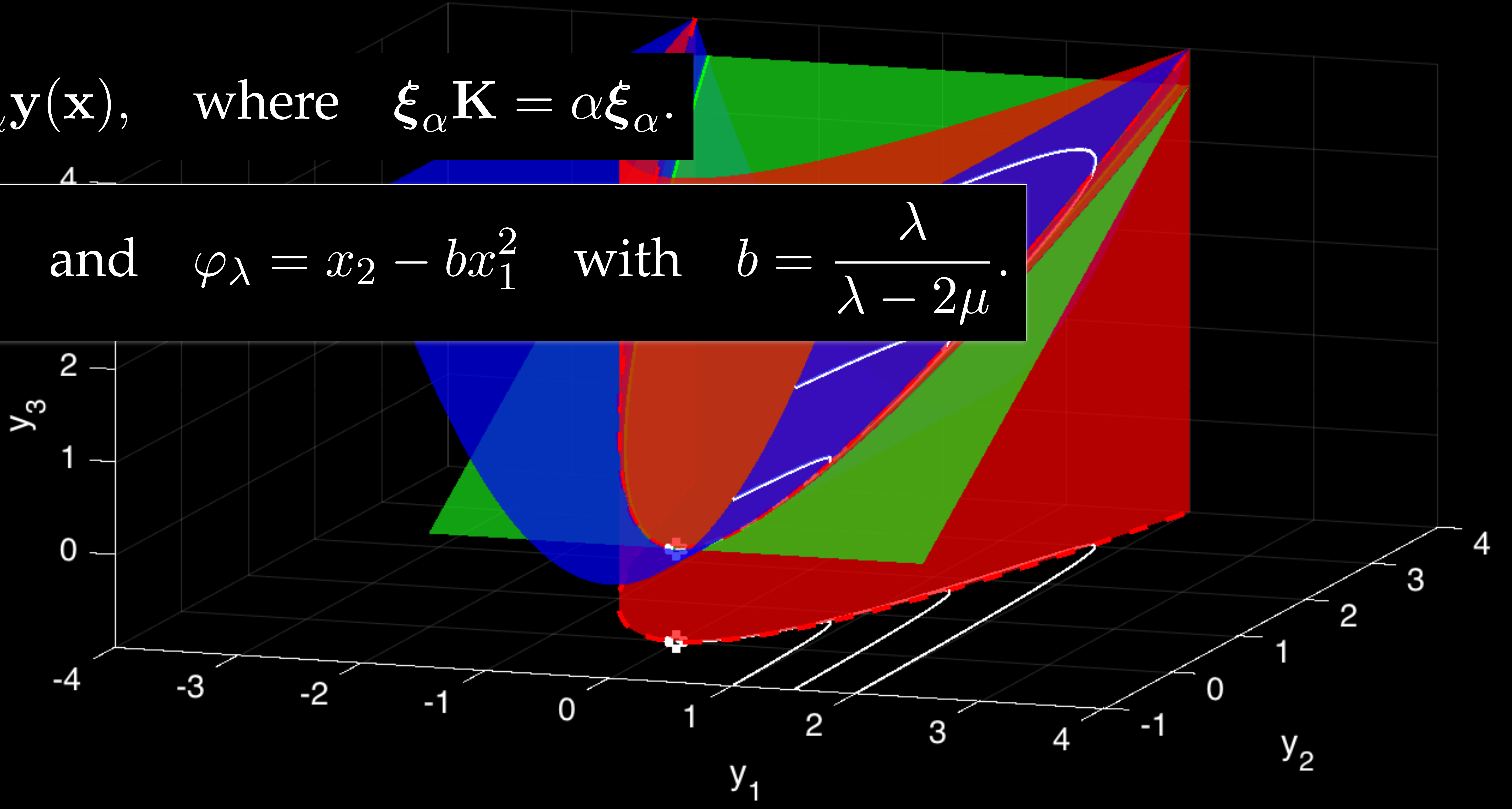
Eigen-observables: $\varphi_\alpha(\mathbf{x}) = \boldsymbol{\xi}_\alpha \mathbf{y}(\mathbf{x}), \quad \text{where} \quad \boldsymbol{\xi}_\alpha \mathbf{K} = \alpha \boldsymbol{\xi}_\alpha.$

$$\varphi_\mu = x_1, \quad \text{and} \quad \varphi_\lambda = x_2 - b x_1^2 \quad \text{with} \quad b = \frac{\lambda}{\lambda - 2\mu}.$$





Koopman Operator Optimal Control

Dynamics with inputs:

$$\frac{d}{dt}\begin{bmatrix}x_1\\x_2\end{bmatrix} = \begin{bmatrix}\mu & 0\\0 & \lambda\end{bmatrix}\begin{bmatrix}x_1\\x_2\end{bmatrix} + \begin{bmatrix}0\\-\lambda x_1^2\end{bmatrix} + \begin{bmatrix}0\\1\end{bmatrix}u,$$

Koopman linear system with inputs:

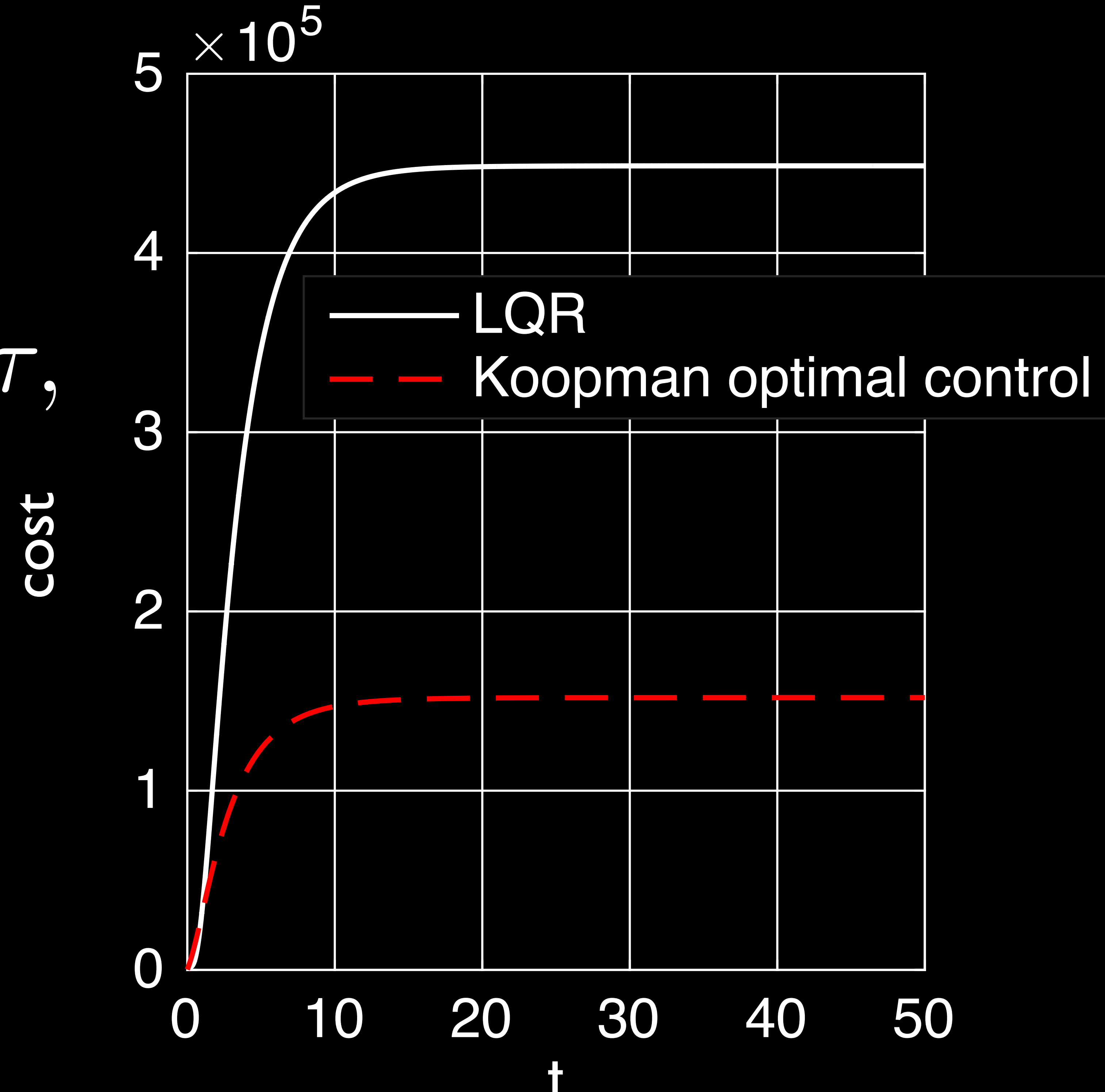
$$\frac{d}{dt}\begin{bmatrix}y_1\\y_2\\y_3\end{bmatrix} = \begin{bmatrix}\mu & 0 & 0\\0 & \lambda & -\lambda\\0 & 0 & 2\mu\end{bmatrix}\begin{bmatrix}y_1\\y_2\\y_3\end{bmatrix} + \begin{bmatrix}0\\1\\0\end{bmatrix}u.$$

LQR Cost function:

$$J = \int_0^\infty \mathbf{x}^T(\tau)\mathbf{Q}\mathbf{x}(\tau) + \mathbf{u}(\tau)^T\mathbf{R}\mathbf{u}(\tau)\,d\tau,$$

Nonlinear optimal controller:

$$u = -\begin{bmatrix}\tilde{K}_1 & \tilde{K}_2\end{bmatrix}\begin{bmatrix}x_1\\x_2\end{bmatrix} - \tilde{K}_3 x_1^2.$$



Data

Sparse
Multi-scale

Nonlinear
Dynamics

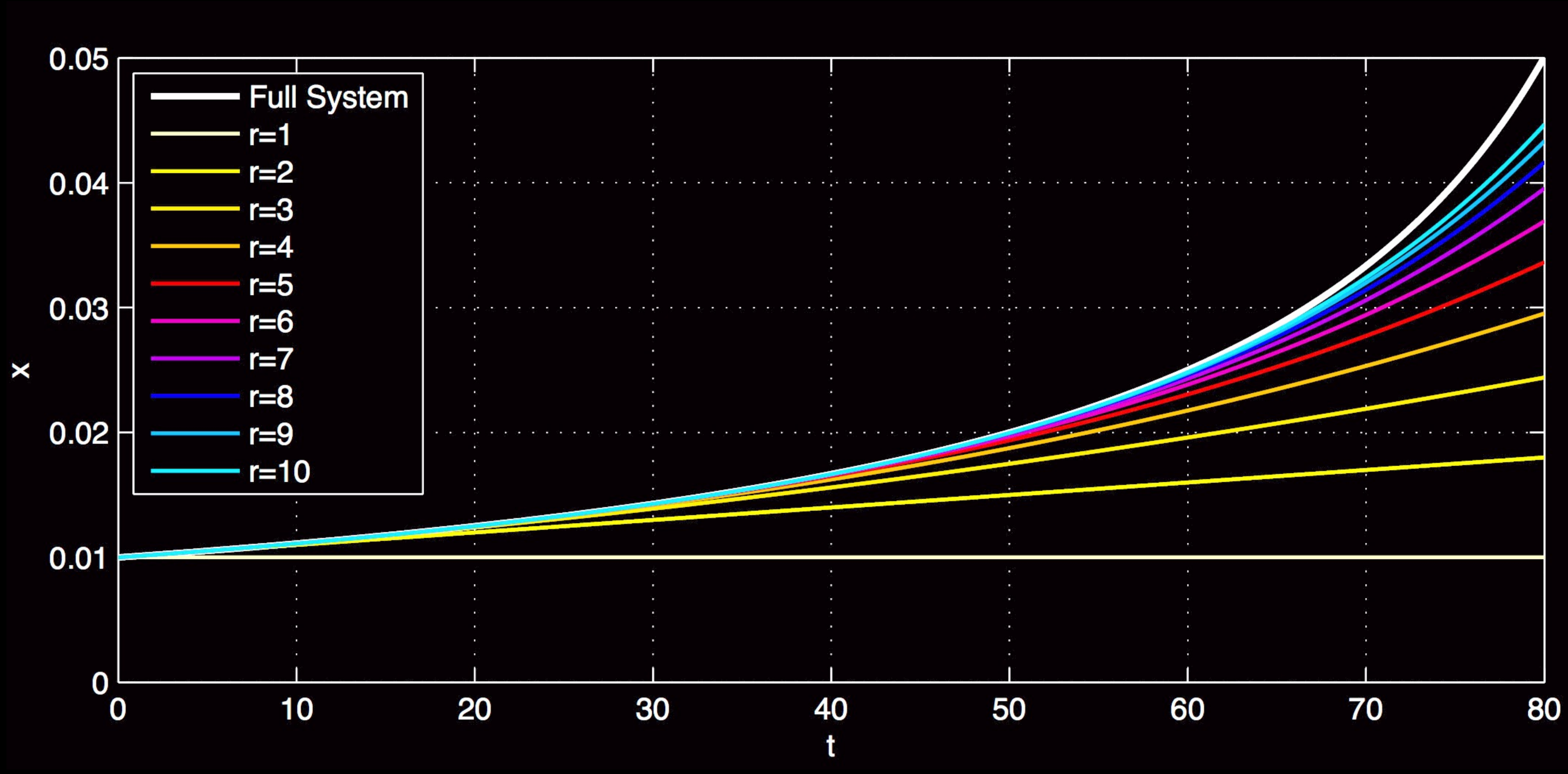
Koopman
Invariant
Subspace

Koopman Operator
Optimal Control

Nonlinear
Optimal
Control

Dynamical Systems: Koopman and Operators

$$\frac{d}{dt}x = x^2 \quad \Rightarrow \quad \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} x \\ x^2 \end{bmatrix}$$



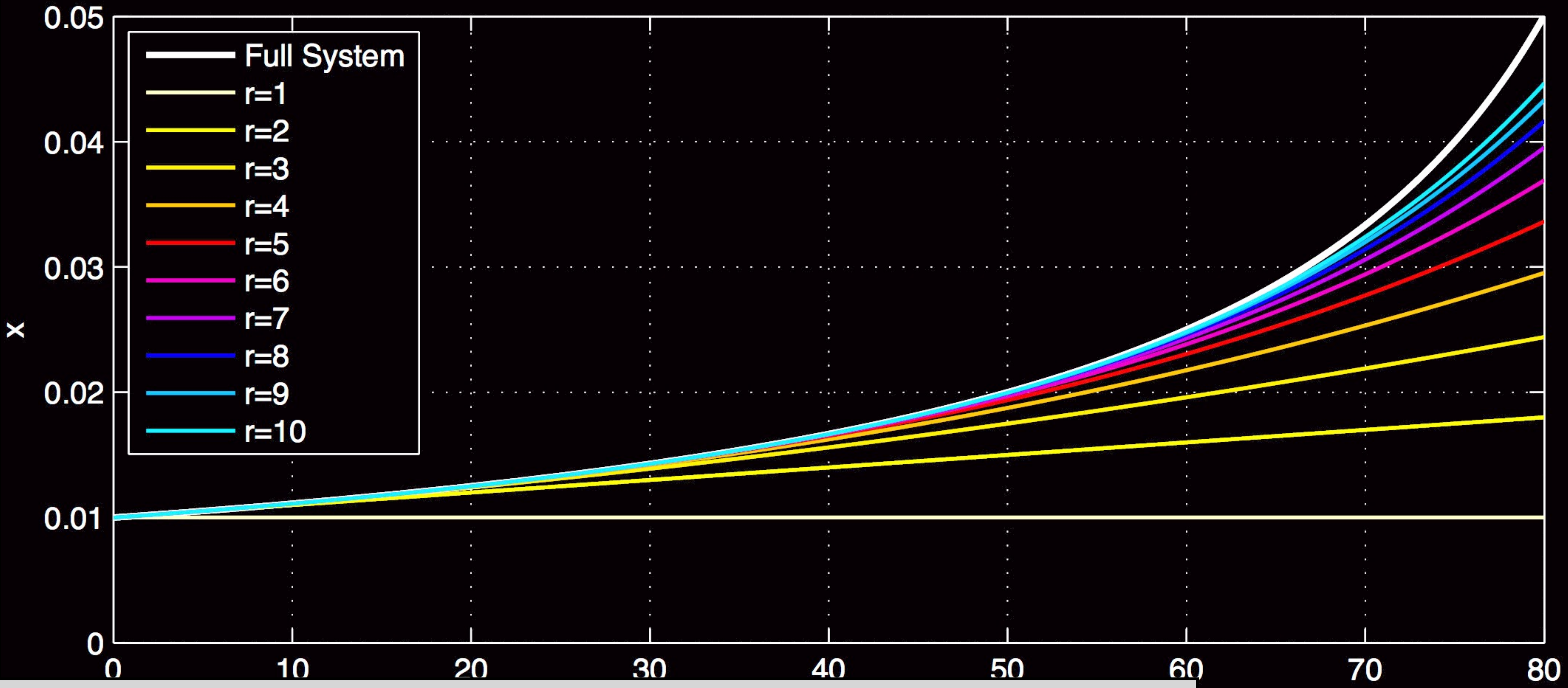
$$\Rightarrow \quad \frac{d}{dt}y_2 = 2x\dot{x} = 2x^3$$

$$\Rightarrow \quad \frac{d}{dt}\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ \vdots \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 2 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 3 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 4 & \cdots \\ 0 & 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ \vdots \end{bmatrix} \quad \text{where} \quad \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ \vdots \end{bmatrix} = \begin{bmatrix} x \\ x^2 \\ x^3 \\ x^4 \\ x^5 \\ \vdots \end{bmatrix}.$$

Dynamical Systems: Koopman and Operators

$$\frac{d}{dt}x = x^2 \quad \Rightarrow \quad \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} x \\ x^2 \end{bmatrix}$$

$$\Rightarrow \quad \frac{d}{dt}y_2 = 2x\dot{x} = 2x^3$$



$$\varphi(x) = e^{-1/x} \quad \Longrightarrow \quad \frac{d}{dt}\varphi(x) = x^{-2}e^{-1/x}\dot{x} = \varphi(x).$$

$$\Rightarrow \quad \frac{d}{dt}\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ \vdots \end{bmatrix} = \begin{bmatrix} 0 & & & & & \\ 0 & 0 & 2 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 3 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 4 & \cdots \\ 0 & 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ \vdots \end{bmatrix} \quad \text{where} \quad \begin{bmatrix} \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ \vdots \end{bmatrix} = \begin{bmatrix} \\ x^2 \\ x^3 \\ x^4 \\ x^5 \\ \vdots \end{bmatrix}.$$

Koopman Eigenfunctions Define Invariant Subspaces

Linear dynamics in eigenfunction coordinates

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

Nonlinear dynamics in original coordinates

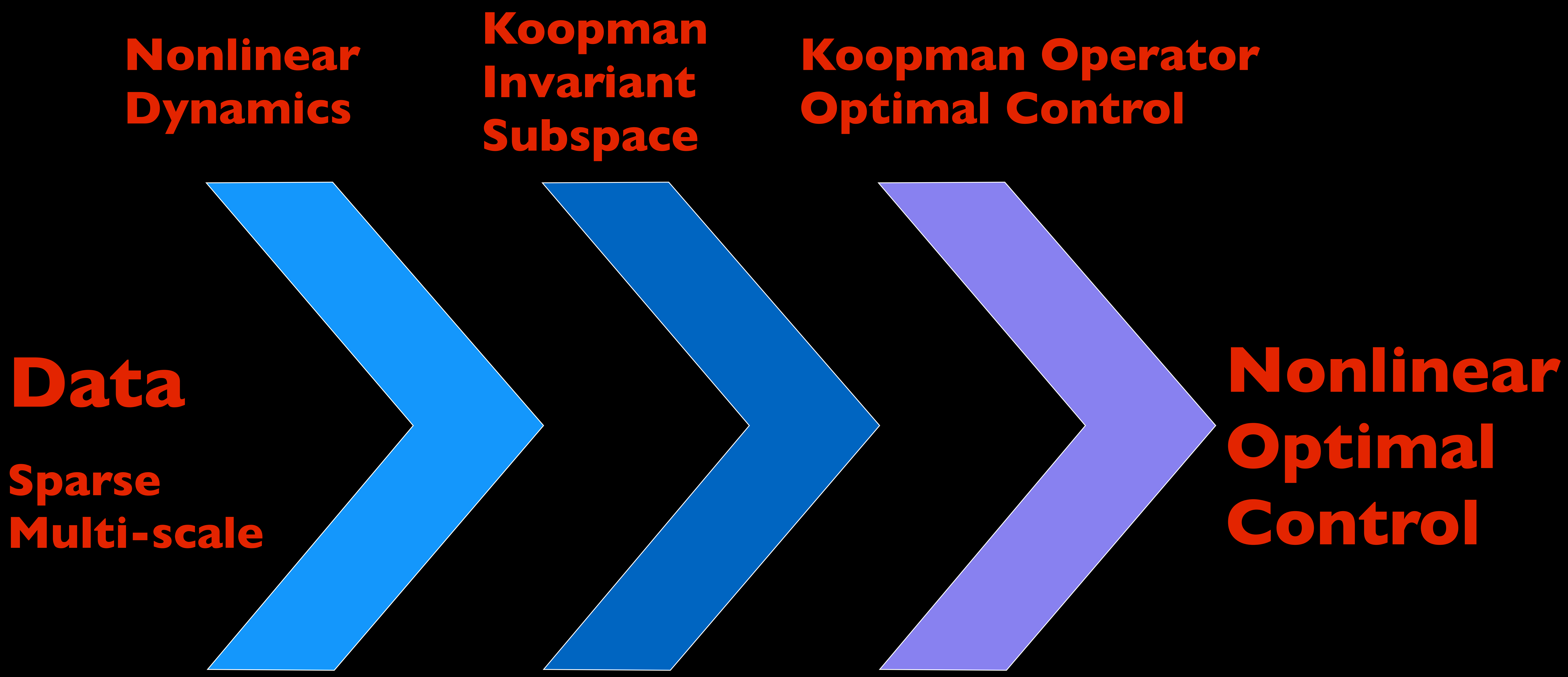
$$\frac{d}{dt}\mathbf{x} = \mathbf{f}(\mathbf{x})$$

$$\frac{d}{dt}\varphi(\mathbf{x}) = \nabla\varphi(\mathbf{x}) \cdot \mathbf{f}(\mathbf{x}) \implies \boxed{\nabla\varphi(\mathbf{x}) \cdot \mathbf{f}(\mathbf{x}) = \lambda\varphi(\mathbf{x})}$$

PDE for Koopman Eigenfunctions!

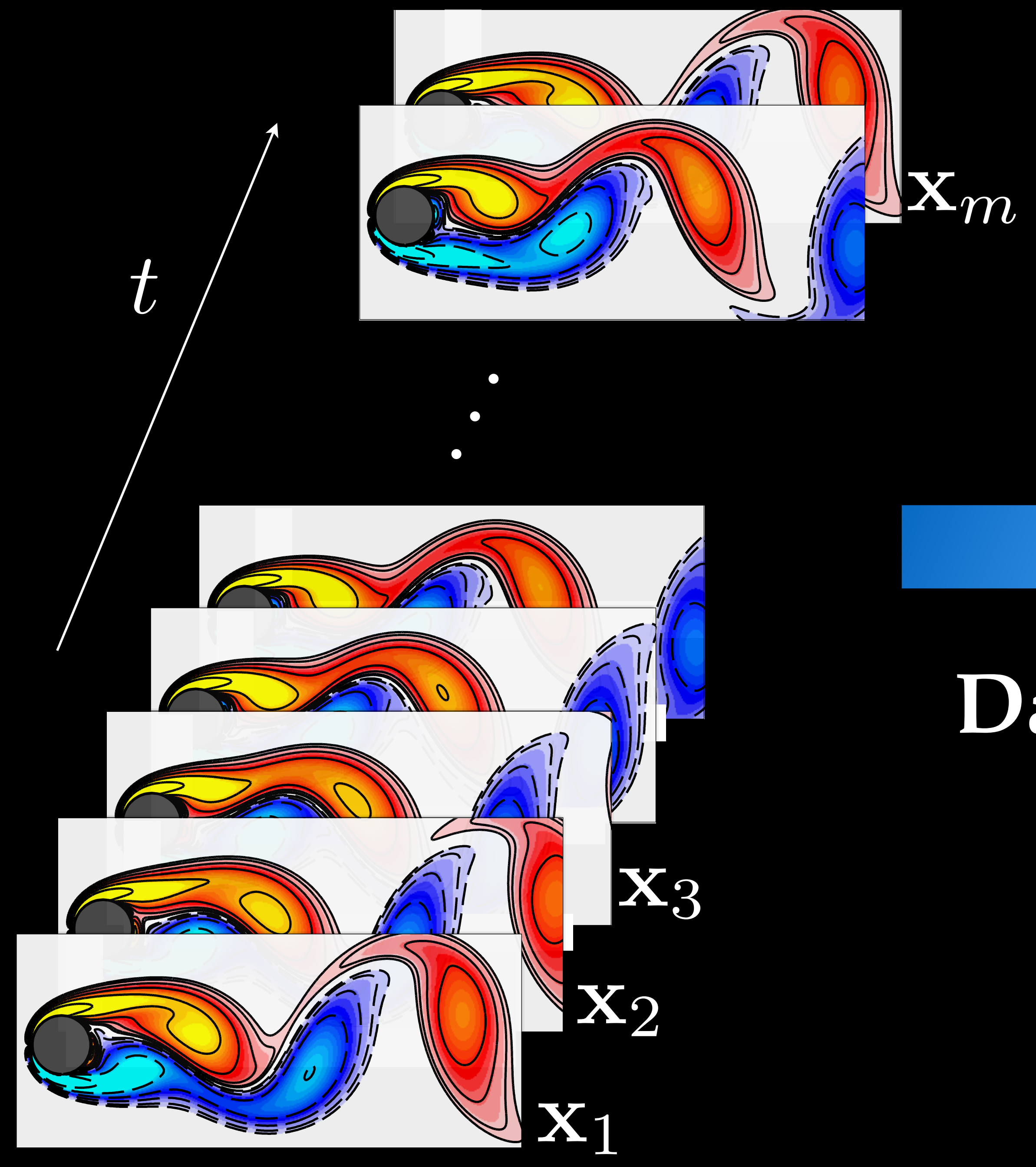
$$\frac{d}{dt}x = x^2$$

$$\varphi(x) = e^{-1/x} \implies \frac{d}{dt}\varphi(x) = x^{-2}e^{-1/x}\dot{x} = \varphi(x).$$


Data
Sparse
Multi-scale
Nonlinear
Dynamics
Koopman
Invariant
Subspace
Koopman Operator
Optimal Control
Nonlinear
Optimal
Control

Dynamic Mode Decomposition (DMD)

1. Collect Data



Data

2. Organize into Matrices

$$\mathbf{X} = \begin{bmatrix} | & | & & | \\ \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_{m-1} \\ | & | & & | \end{bmatrix}$$

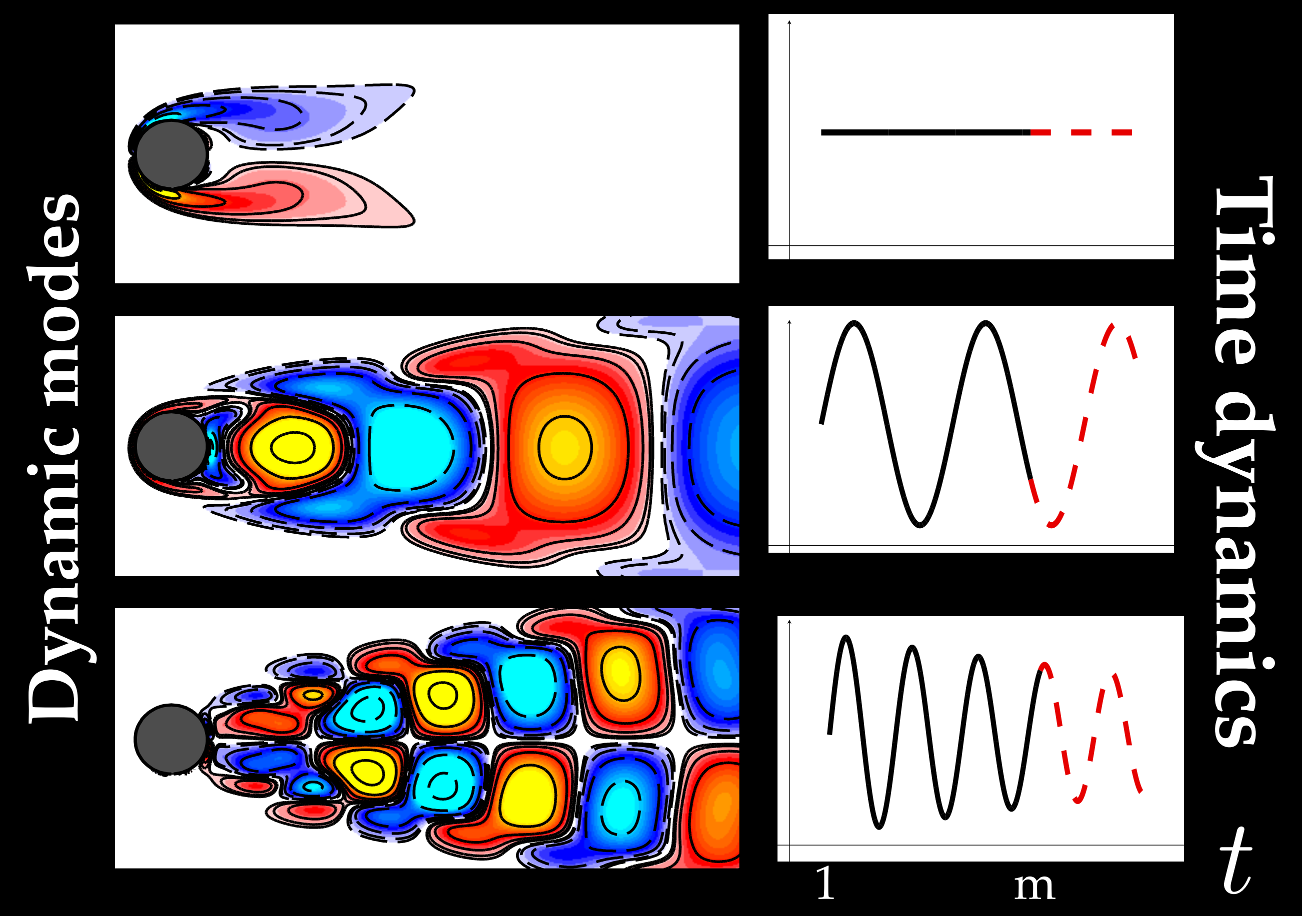
$$\mathbf{X}' = \begin{bmatrix} | & | & & | \\ \mathbf{x}_2 & \mathbf{x}_3 & \cdots & \mathbf{x}_m \\ | & | & & | \end{bmatrix}$$

$$\mathbf{A} = \mathbf{X}'\mathbf{X}^{\dagger}$$

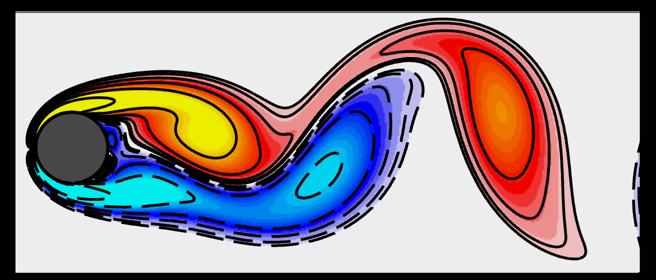
Regression

3. DMD

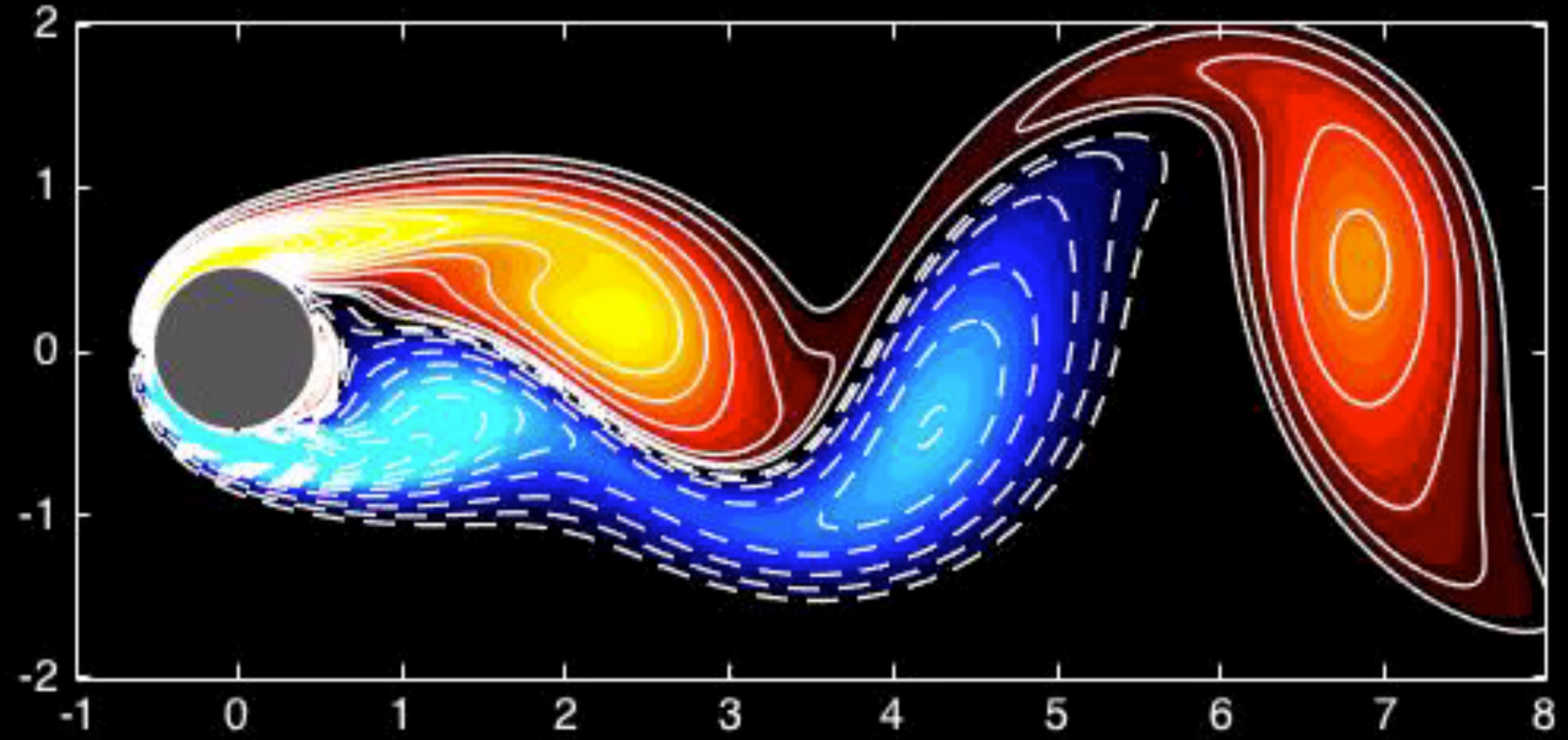
a) Diagnostics



b) Future state prediction

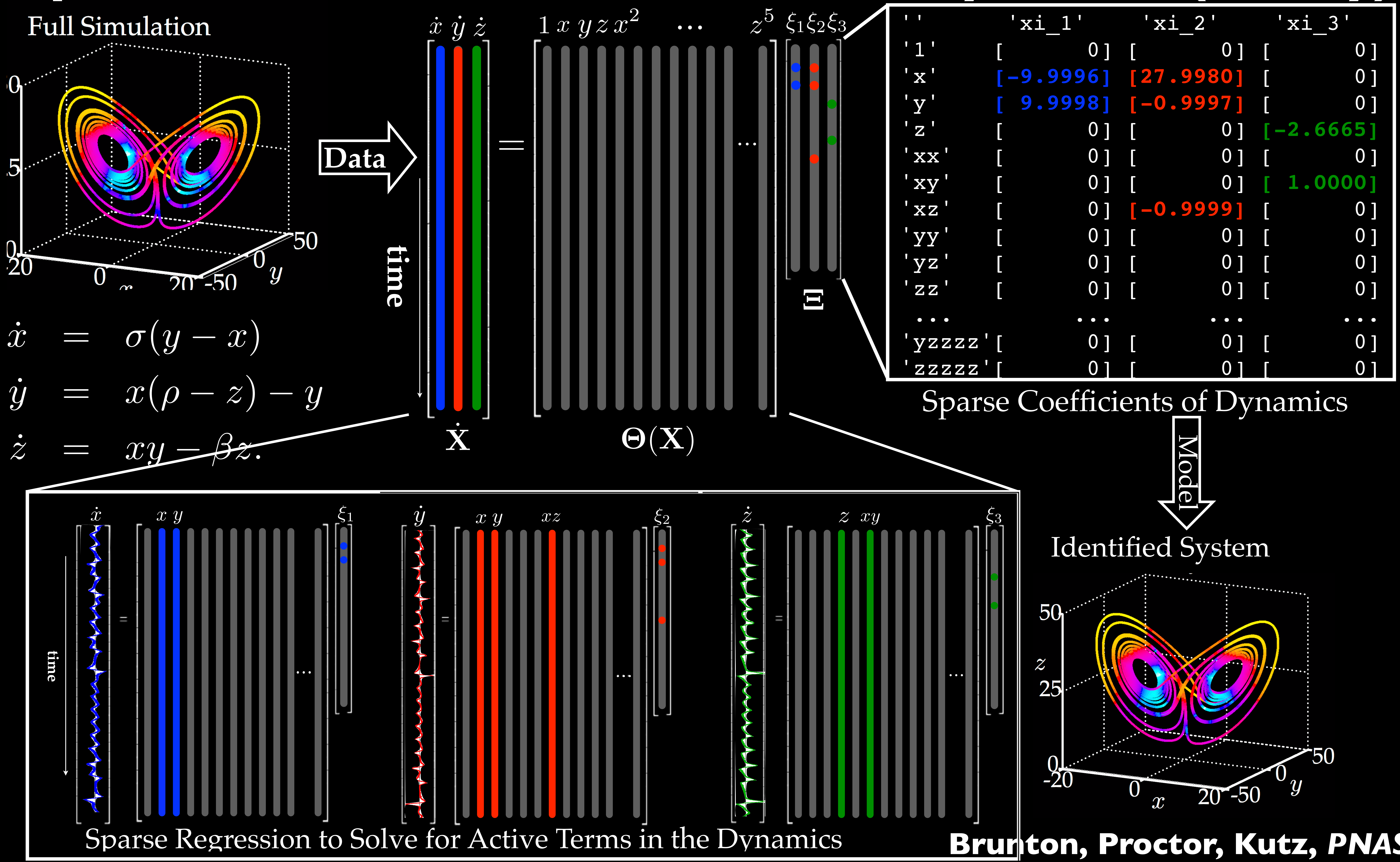


$$\mathbf{x}_{k+1} = \mathbf{A}\mathbf{x}_k$$



Schmid, *JFM* 2010.
Rowley, Mezic, Bagheri, Schlatter, Henningson, *JFM* 2009.
Tu, Rowley, Luchtenburg, Brunton, Kutz, *JCD* 2014.
Kutz, Brunton, Brunton, Proctor, *SIAM* 2016.
Klus, Nuske, Koltai, Wu, Kevrekidis, Schutte, Noe, *arXiv* 2017

Sparse Identification of Nonlinear Dynamics (SINDy)

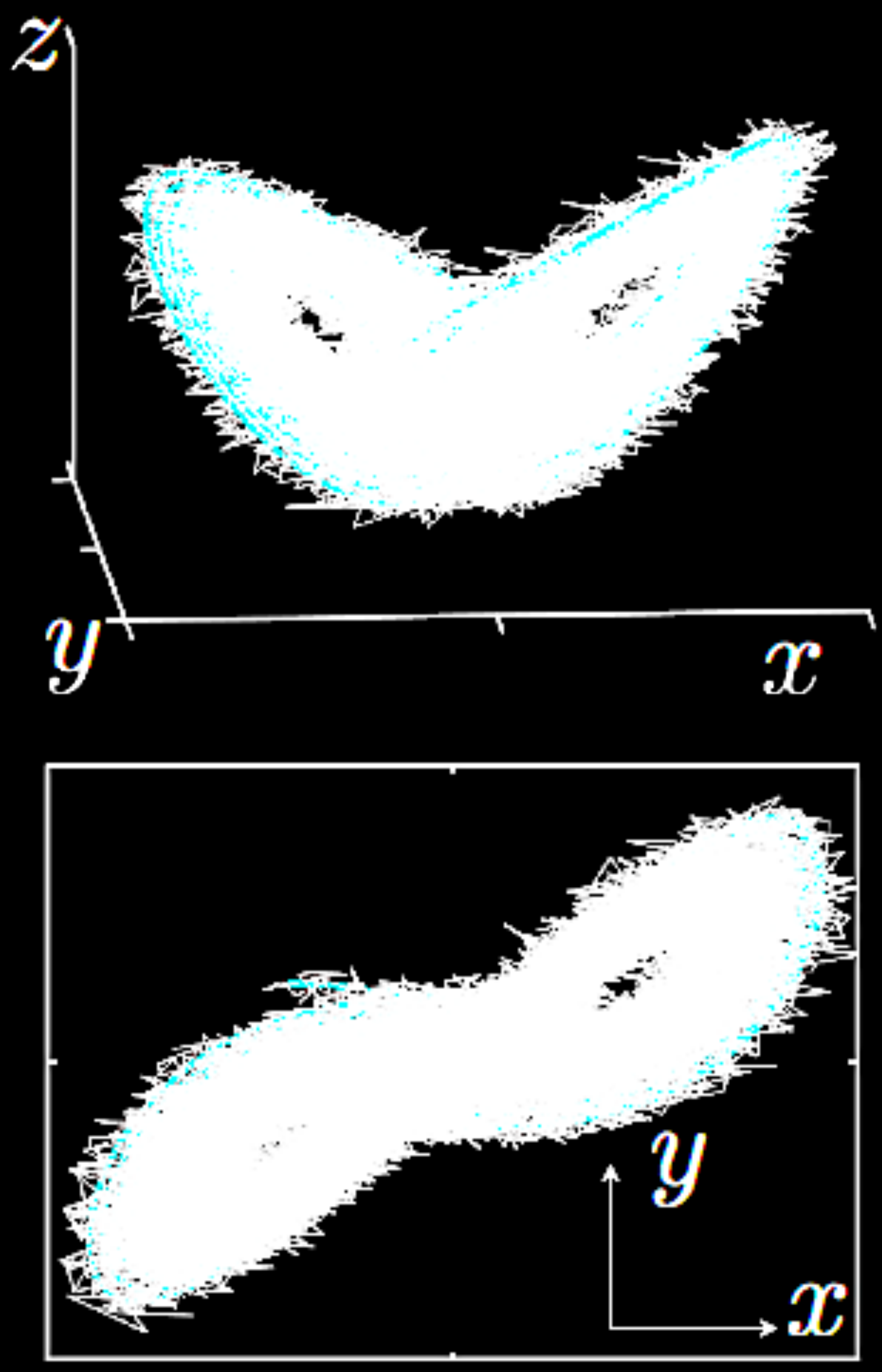


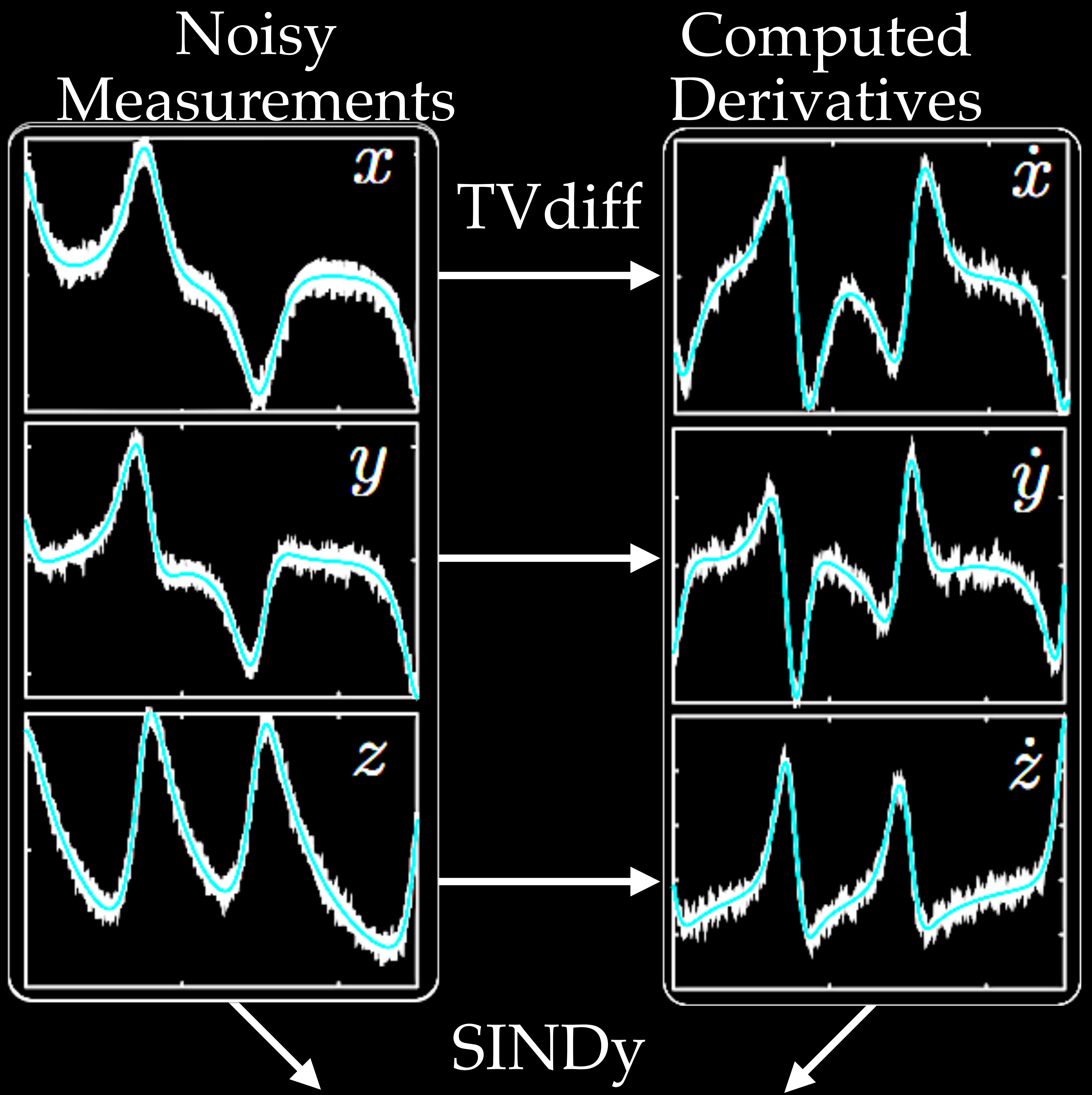
''	'xi_1'	'xi_2'	'xi_3'
'1'	[0]	[0]	[0]
'x'	[-9.9996]	[27.9980]	[0]
'y'	[9.9998]	[-0.9997]	[0]
'z'	[0]	[0]	[-2.6665]
'xx'	[0]	[0]	[0]
'xy'	[0]	[0]	[1.0000]
'xz'	[0]	[-0.9999]	[0]
'yy'	[0]	[0]	[0]
'yz'	[0]	[0]	[0]
'zz'	[0]	[0]	[0]
...	...	...	...
'yzzzz'	[0]	[0]	[0]
'zzzzz'	[0]	[0]	[0]

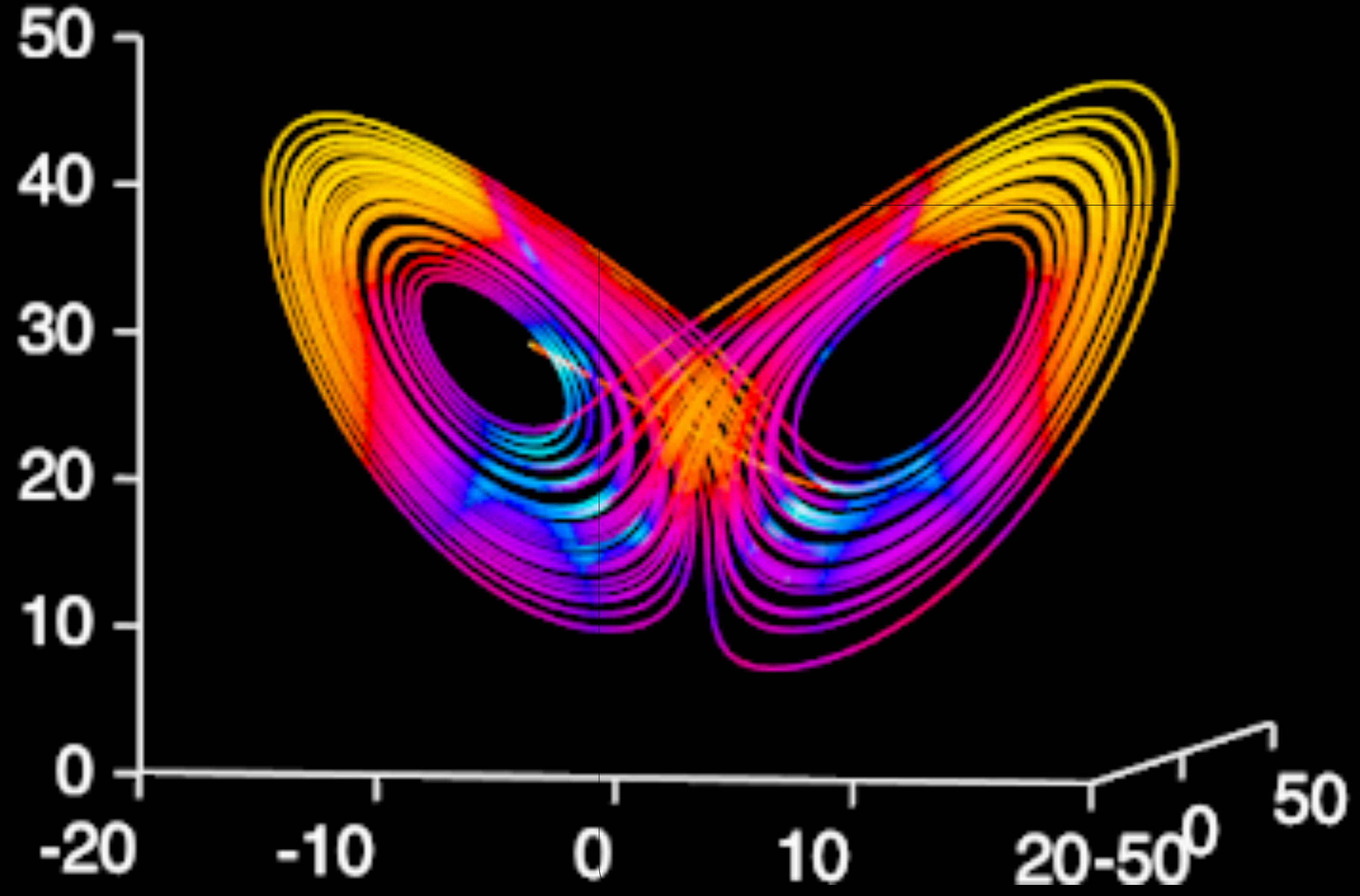
Brunton, Proctor, Kutz, *PNAS* 2016.

SINDy: Noisy State Measurements

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

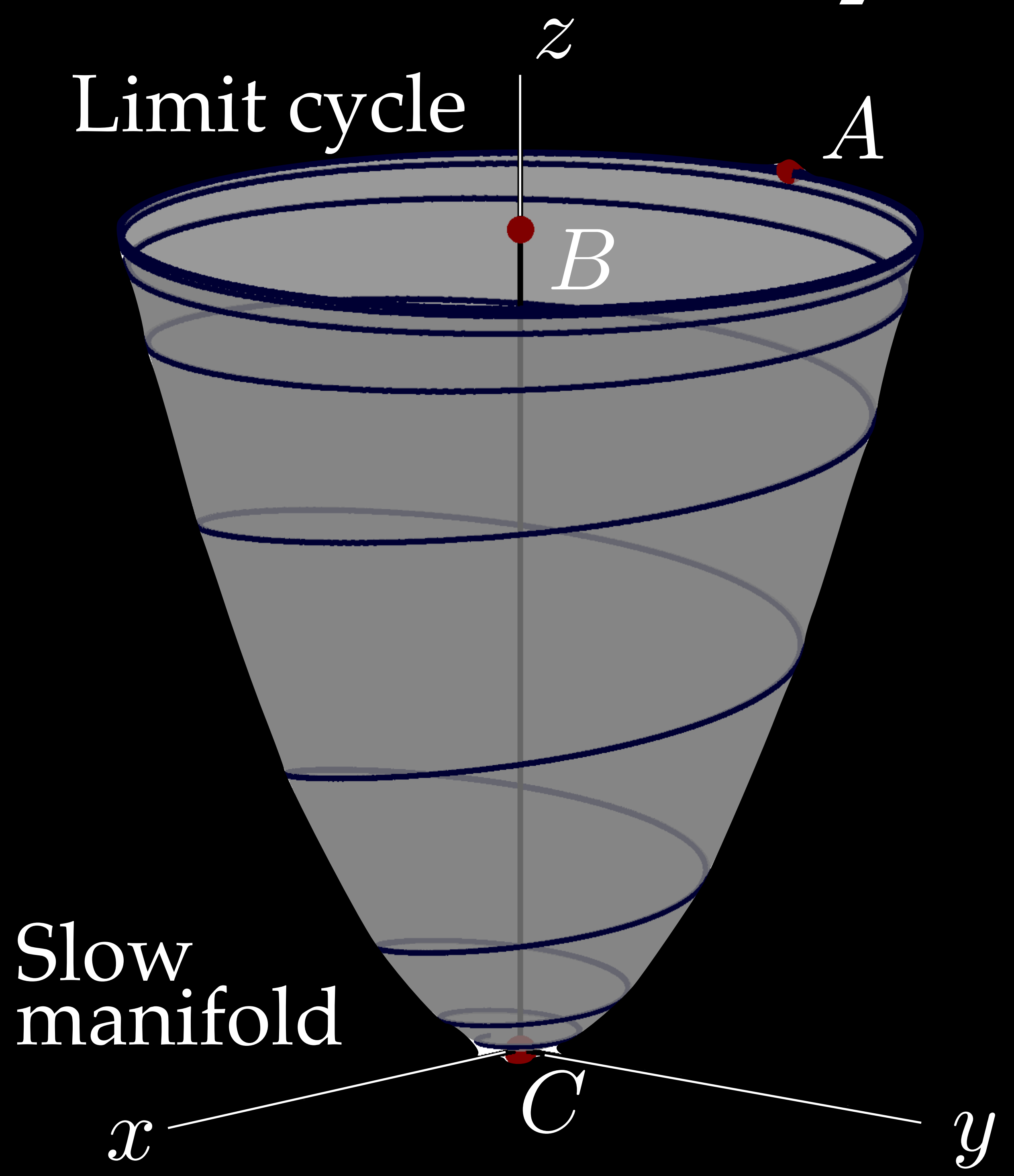




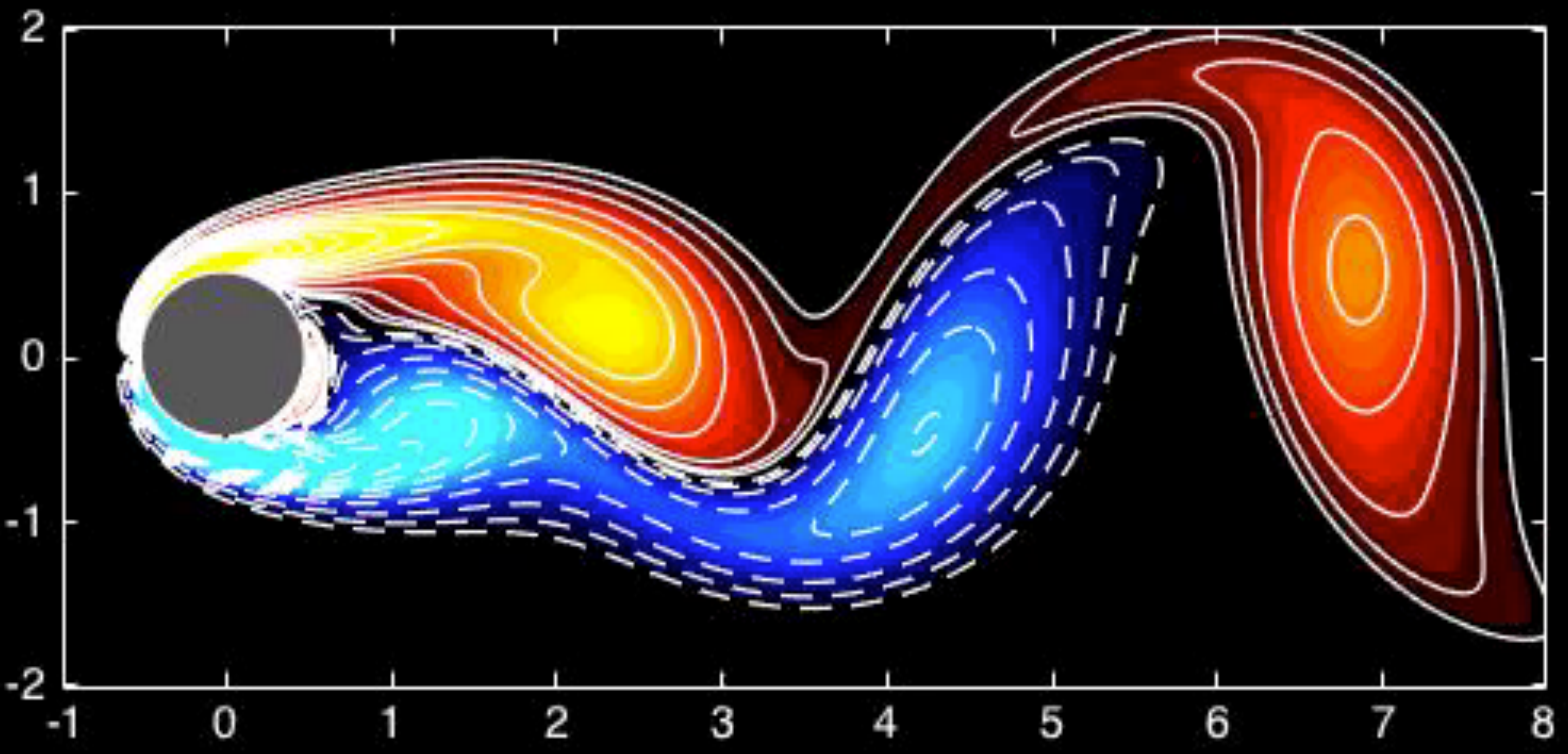


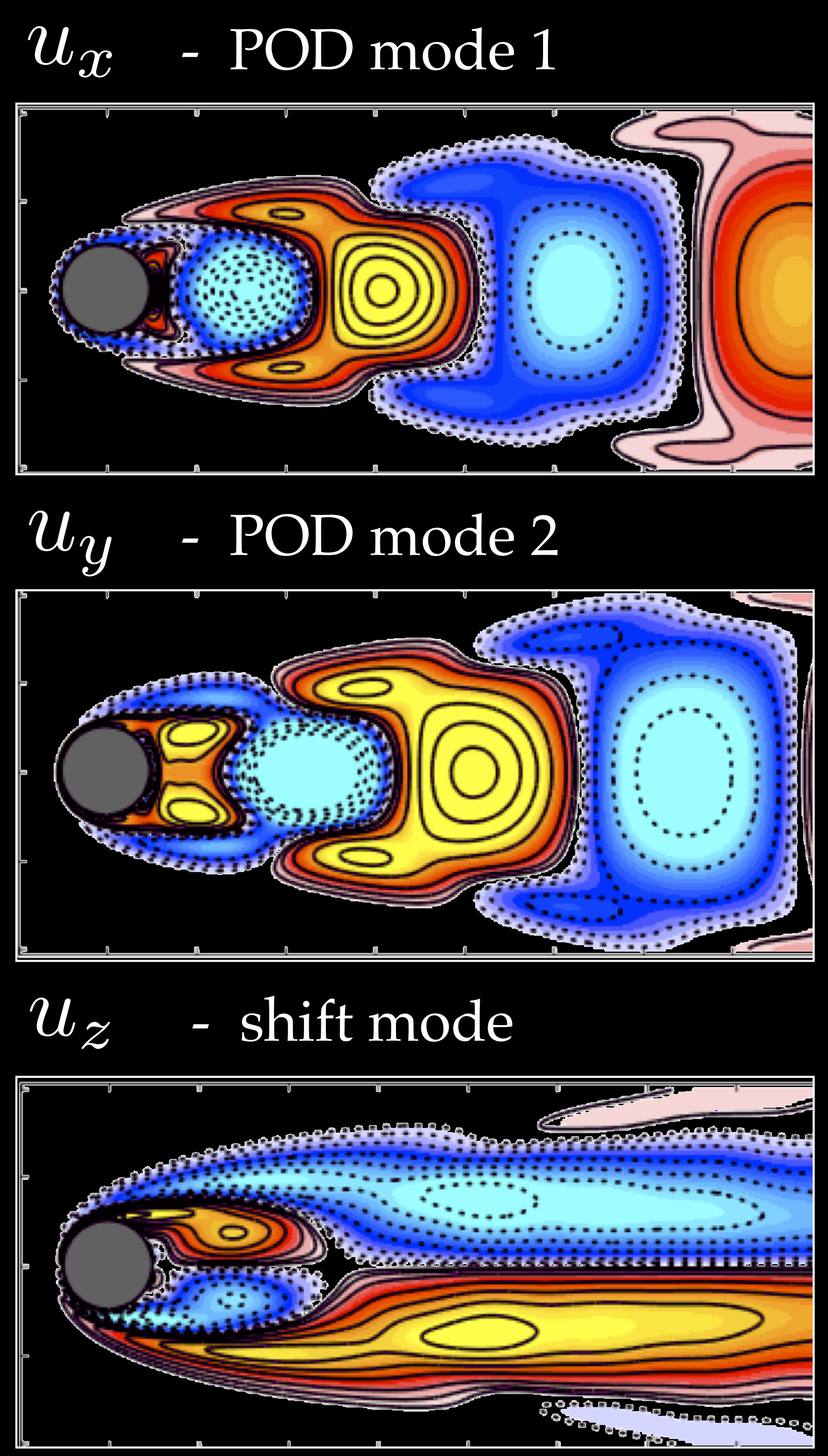
	'xi_1'	'xi_2'	'xi_3'
'x'	[-9.9614]	[27.5343]	[0]
'y'	[9.9796]	[-0.8038]	[0]
'z'	[0]	[0]	[-2.6647]
'xx'	[0]	[0]	[0]
'xy'	[0]	[0]	[1.0003]
'xz'	[0]	[-0.9900]	[0]

SINDy: Vortex Shedding Past a Cylinder



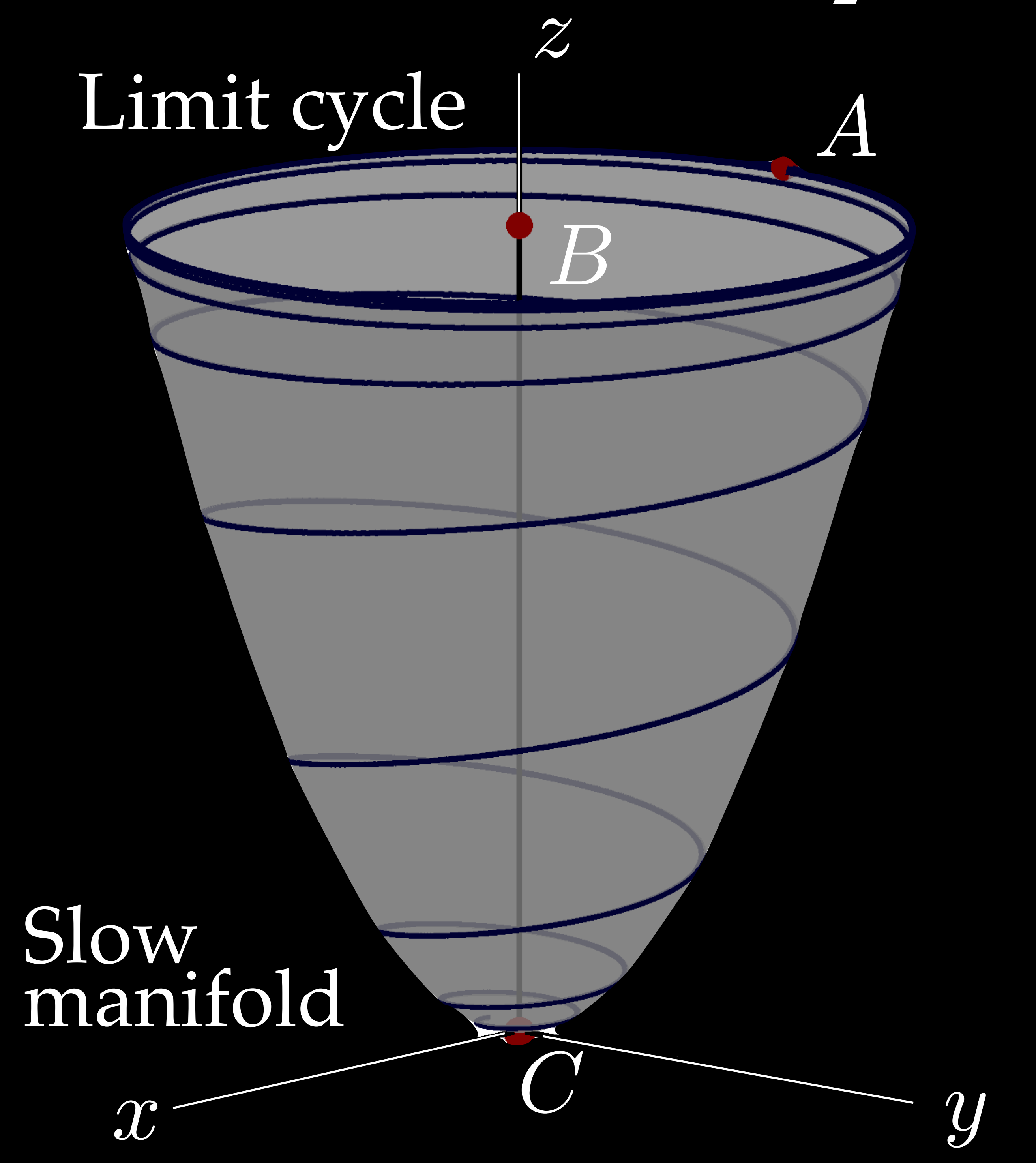
$$\begin{aligned}\dot{x} &= \mu x - \omega y + Axz\\ \dot{y} &= \omega x + \mu y + Ayz\\ \dot{z} &= -\lambda(z - x^2 - y^2).\end{aligned}$$



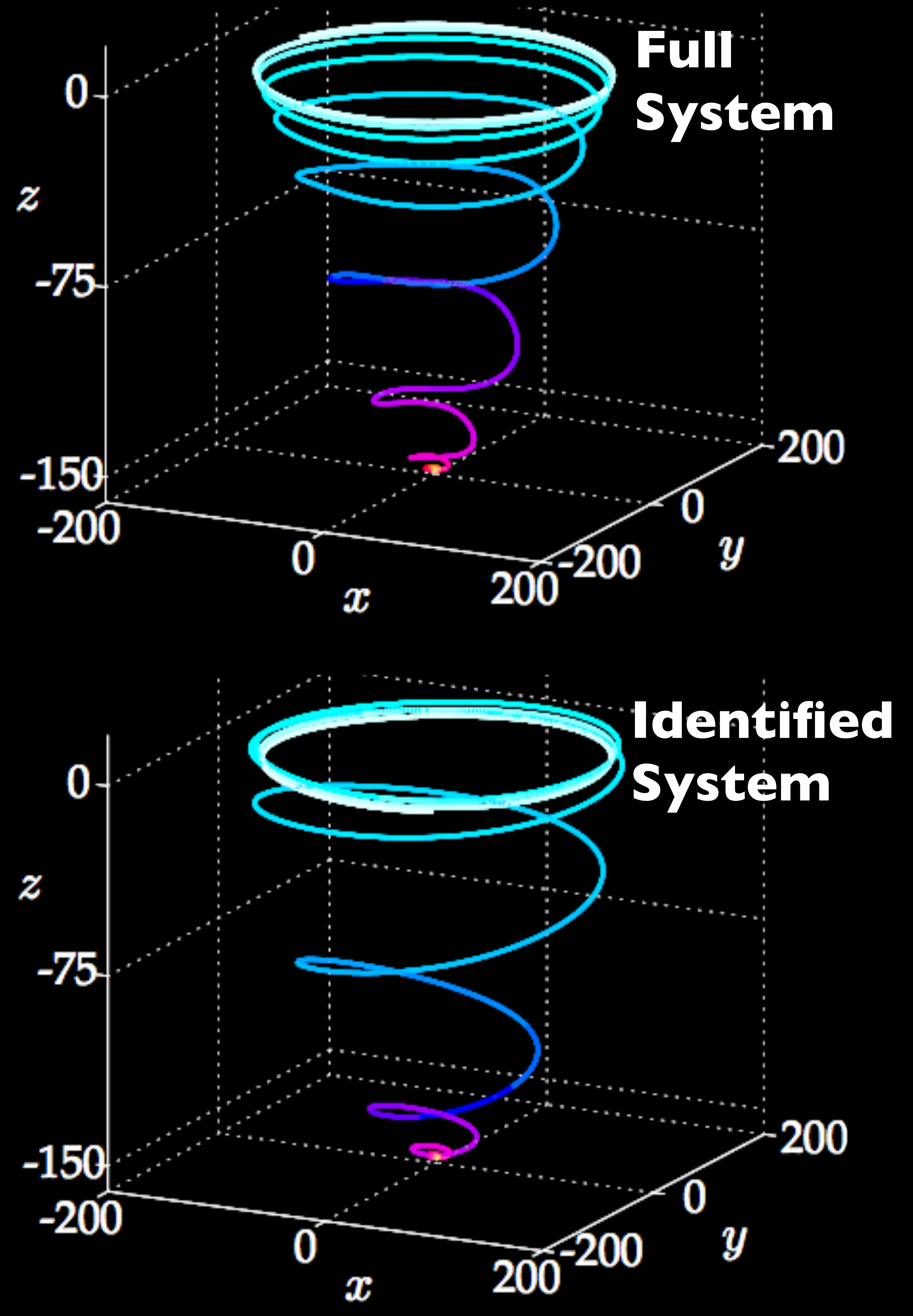


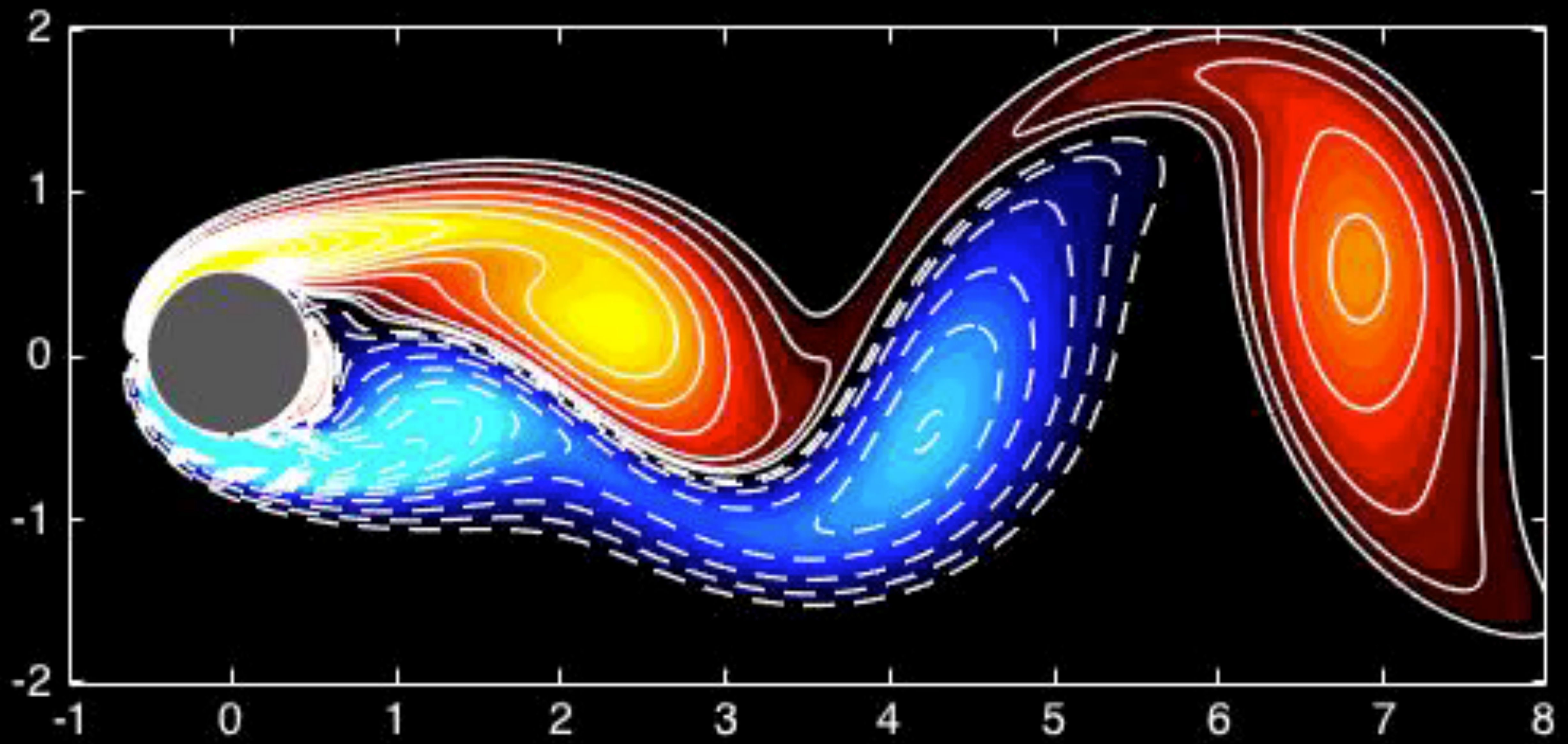
Ruelle and Takens, 1971
Zebib, 1987 and Jackson, 1987
Noack *et al.*, JFM 2003.

SINDy: Vortex Shedding Past a Cylinder



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

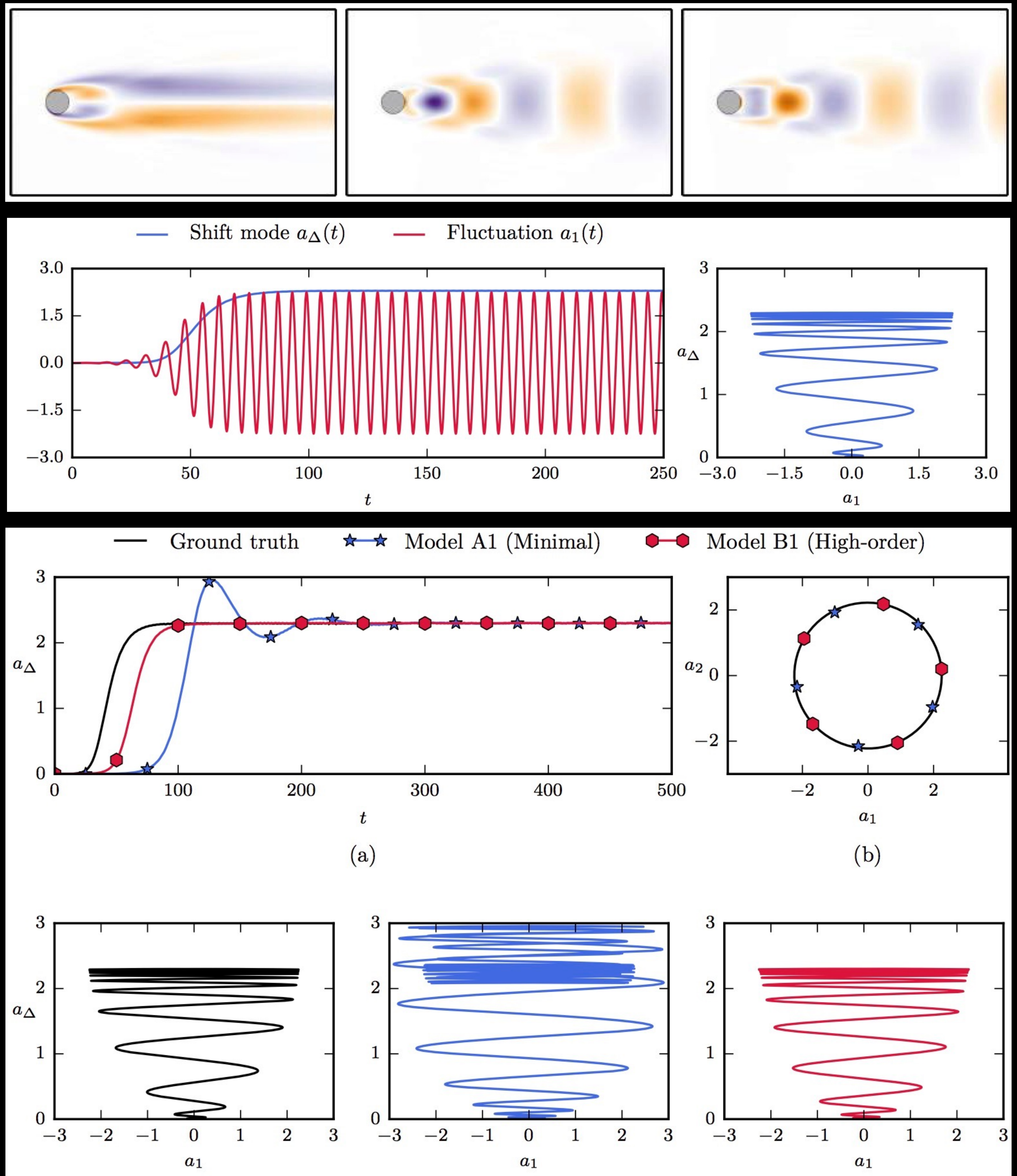


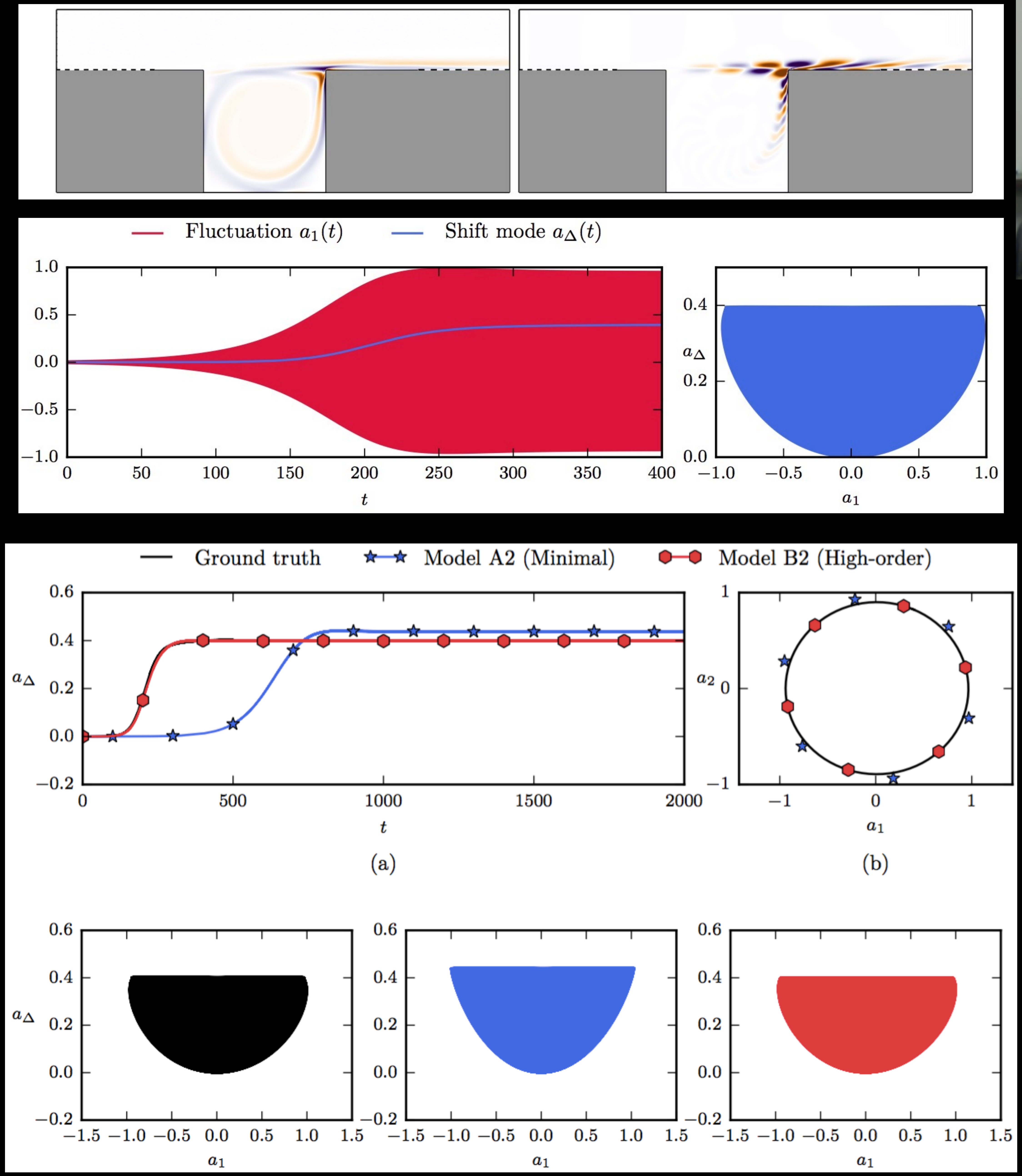


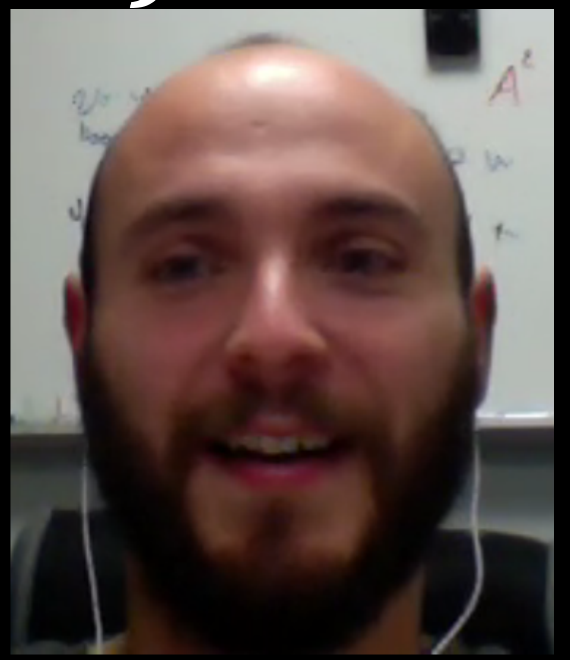
Ruelle and Takens, 1971
Zebib, 1987 and Jackson, 1987
Noack *et al.*, JFM 2003.
Brunton, Proctor, Kutz, PNAS 2016.

Constrained Sparse Galerkin Regression

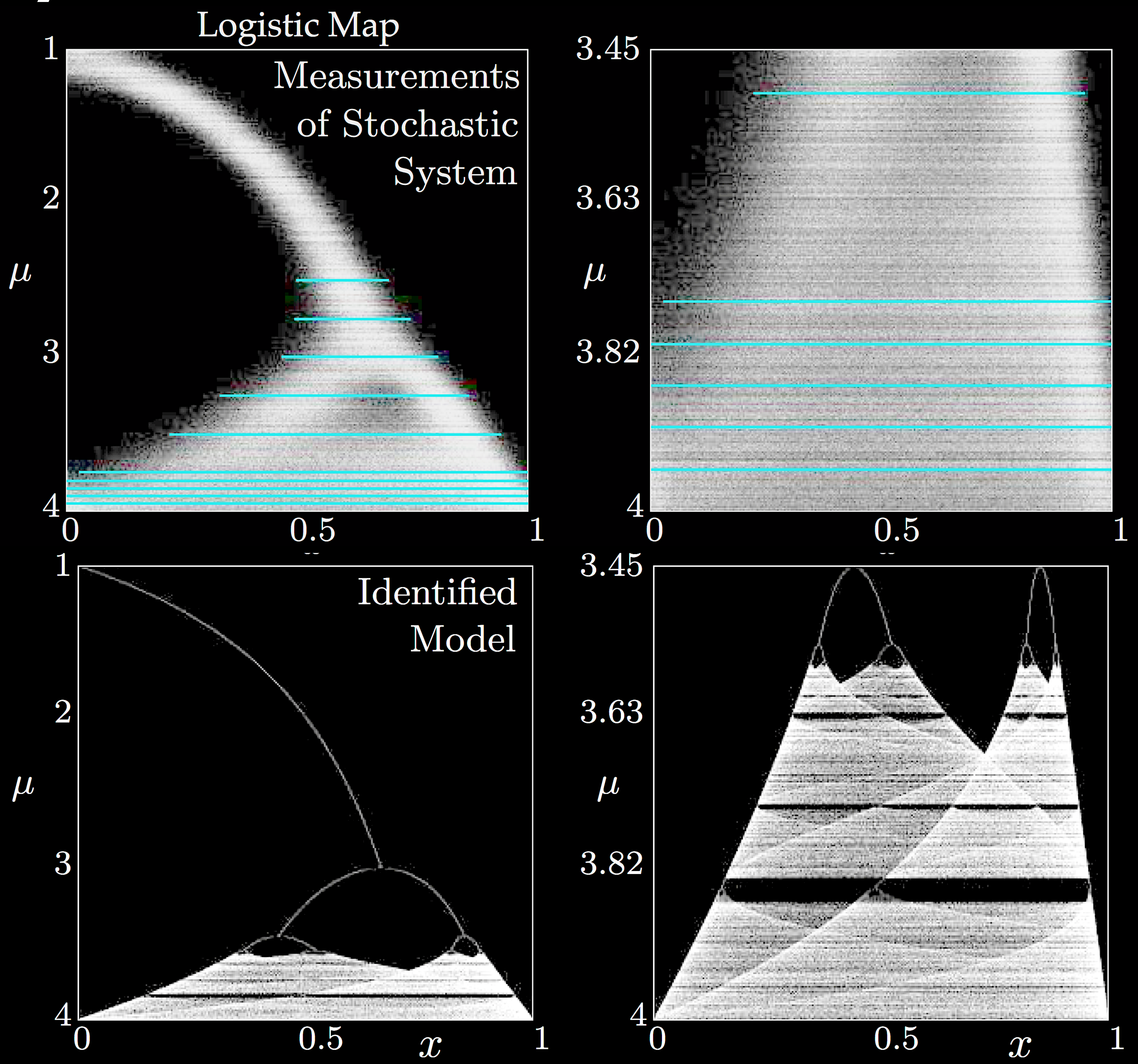
J-C Loiseau, SLB
To appear in JFM, 2017







SINDy: Bifurcation Parameters and Forcing



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

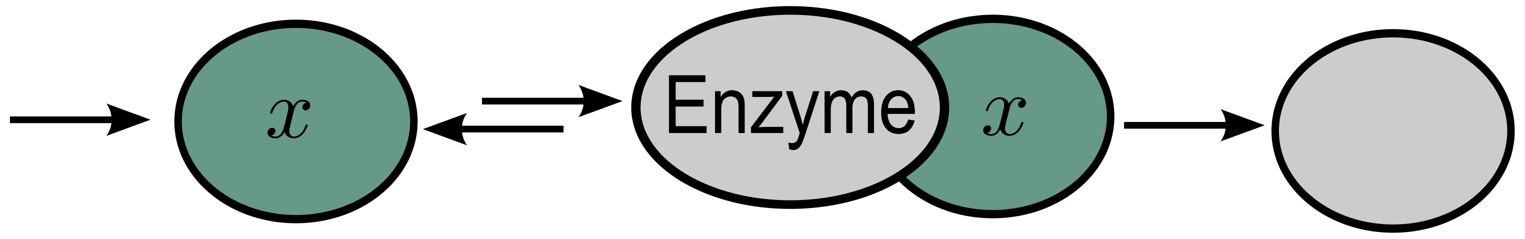
$$\boxed{\begin{aligned} \dot{\mathbf{x}} &= \mathbf{f}(\mathbf{x};\mu) \\ \dot{\mu} &= 0. \end{aligned}}$$

Brunton, Proctor, Kutz, *PNAS* 2016.

SINDy: Rational Function Nonlinearity

Mangan, SLB, Proctor, Kutz

IEEE Trans. Mol. Bio Multi-Scale Comm.



$$\dot{x} = 0.6 - \frac{1.5x}{0.3 + x}$$

1) Build function library from data $\mathbf{x}(\mathbf{t}), \dot{x}_k(\mathbf{t})$ such that $\boldsymbol{\Theta}(\mathbf{X}, \dot{x}_k)\boldsymbol{\xi} = \mathbf{0}$

2) Calculate $\mathbf{N} = null(\boldsymbol{\Theta})$

3) Alternating Directions Method: find $\boldsymbol{\alpha}$ such that $\boldsymbol{\xi}$ is sparse

4) Assemble inferred model

Including Information Theory for Model Selection

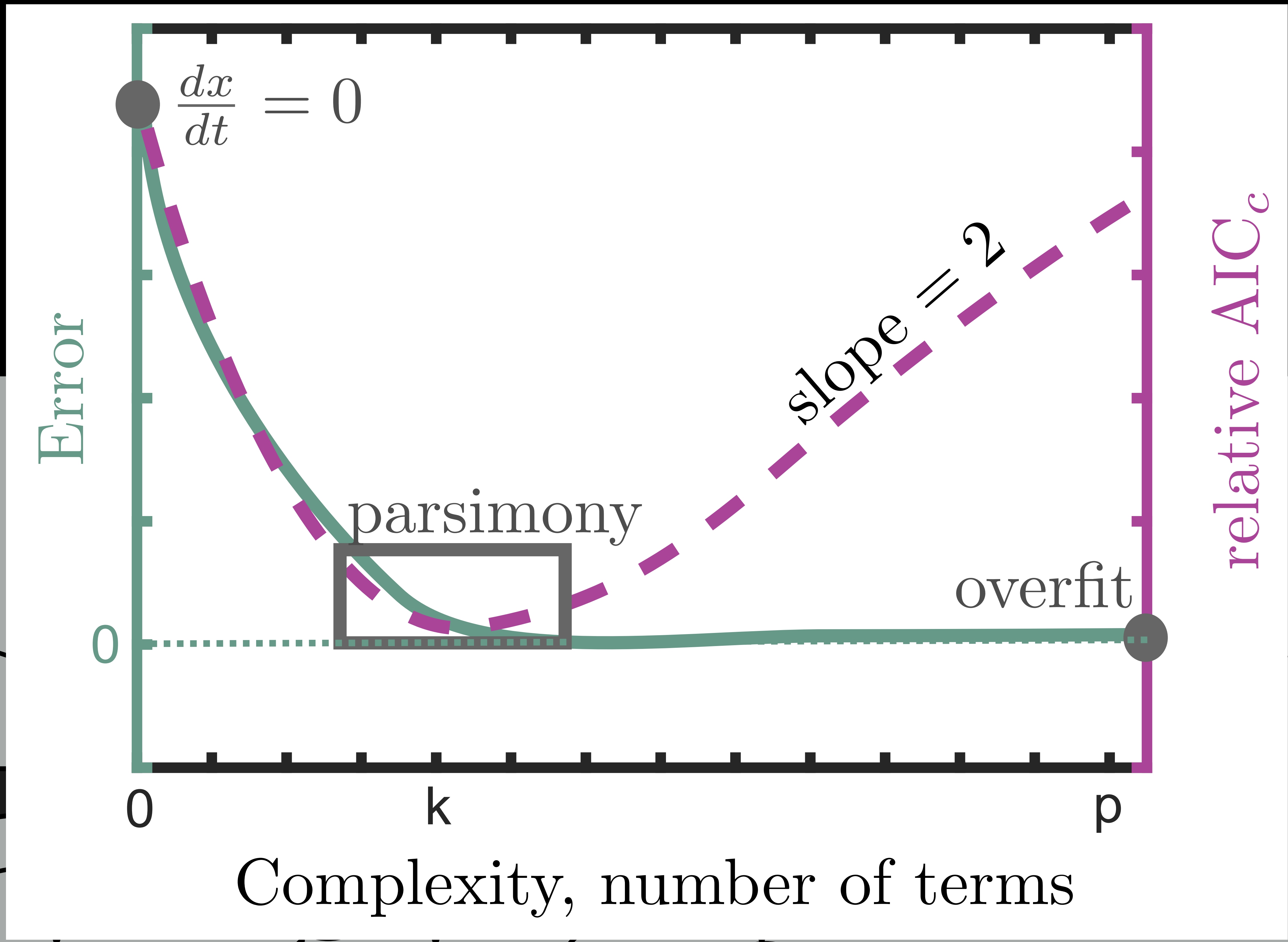
Proceedings of the Royal Society A

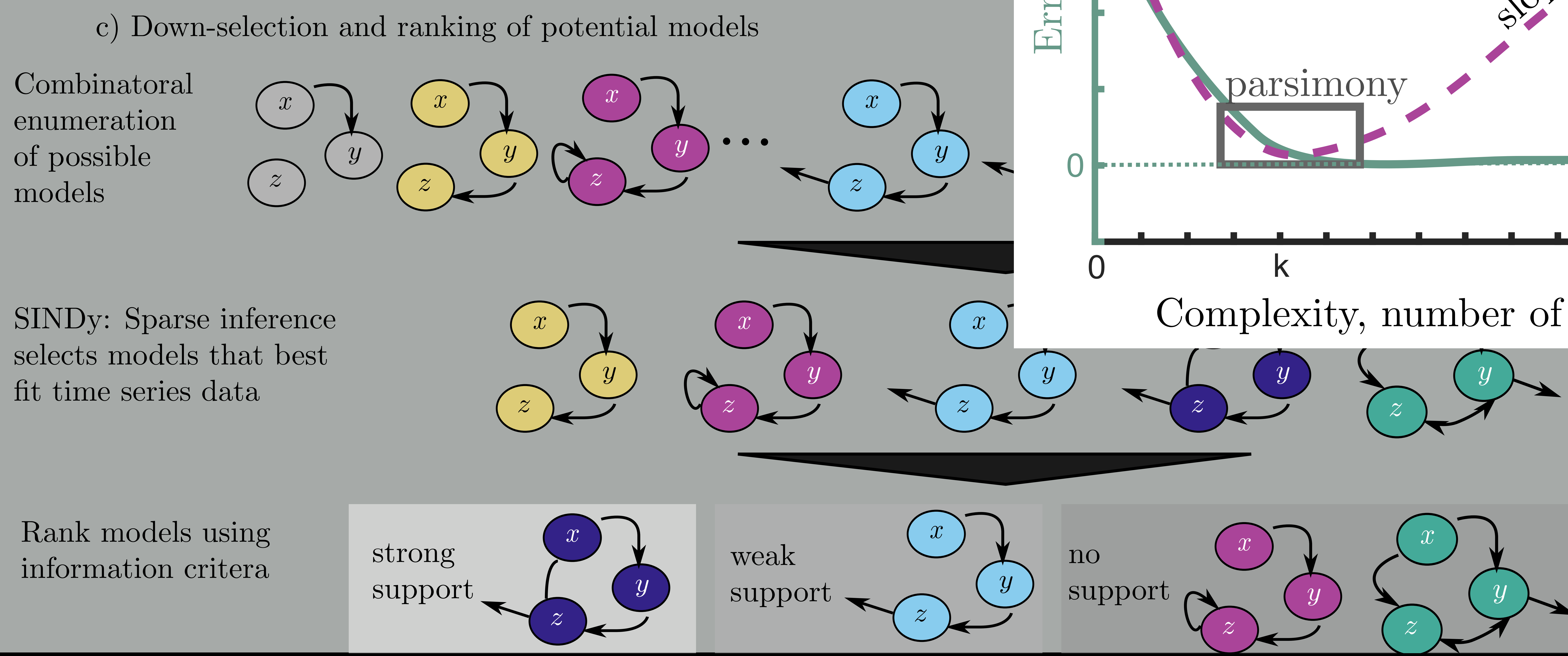
Mangan, Kutz, SLB, Proctor

Including Information Theory for Model Selection

Proceedings of the Royal Society A

Mangan, Kutz, SLB, Proctor





SINDy: Partial Differential Equations

Rudy, SLB, Proctor, Kutz
Science Advances, 2017

Open Problems, Key Challenges, Emerging Techniques

Open Problem: Often **equations are unknown**, or are only partially known
Key Challenges: Combinatorially large search space for candidate models
Emerging Techniques: Machine learning, sparse (parsimonious) methods

Open Problem: **Nonlinear** dynamics still poorly understood
Key Challenges: Topologically complex, no closed form (Poincare)
Emerging Techniques: Koopman spectral analysis (linear embeddings)

Open Problem: Optimal **nonlinear control** and estimation
Key Challenges: Finding intrinsic coordinates (Koopman eigenfunctions)
Emerging Techniques: Uncertainty quantification and robust control

Data → Dynamics

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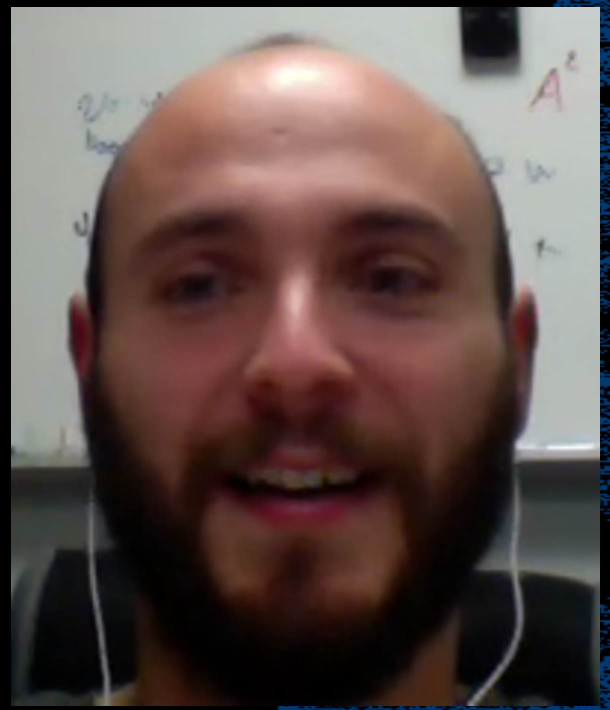
Bing Brunton

Josh Proctor

J.-C. Loiseau



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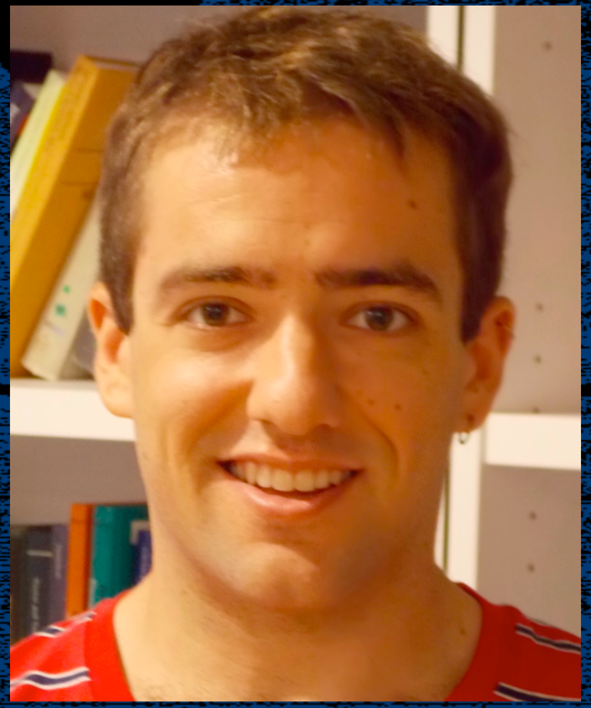

Sam Rudy

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