Reduced-order models in fluid mechanics

Clancy Rowley

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Outline

- Balanced POD
  - Approximate balanced truncation using empirical Gramians
  - Example: linearized channel flow

- Dynamic Mode Decomposition (DMD)
  - Overview of DMD
  - Nonlinear systems and the Koopman operator
  - Extended DMD for nonlinear systems
  - Ergodic theory: separating structure from randomness

Approximate balanced truncation using snapshots

- Linear time-invariant system

$$\dot{x} = Ax + Bu$$
$$y = Cx$$

- Gramians

$$W_c = \int_0^\infty e^{At} B B^T e^{A^T t} dt \qquad W_o = \int_0^\infty e^{A^T t} C^T C e^{At} dt$$

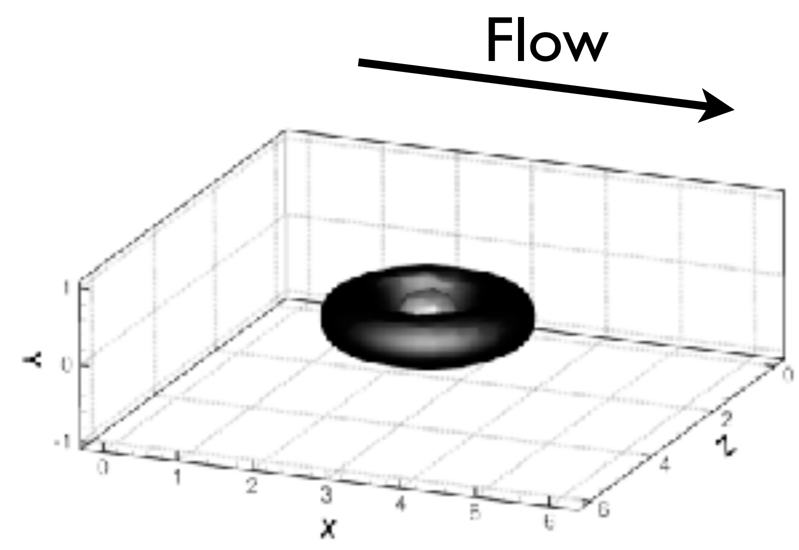
  - Instead of solving Lyapunov equations, approximate the Gramians by quadrature, from snapshots of the impulse response $x(t_k) = e^{At_k} B$ and adjoint impulse response $z(t_k) = e^{A^T t_k} C^T$

- Balanced POD
  - This procedure looks a lot like POD, but get two sets of modes that are bi-orthogonal, and one does a Petrov-Galerkin projection instead of a Galerkin projection

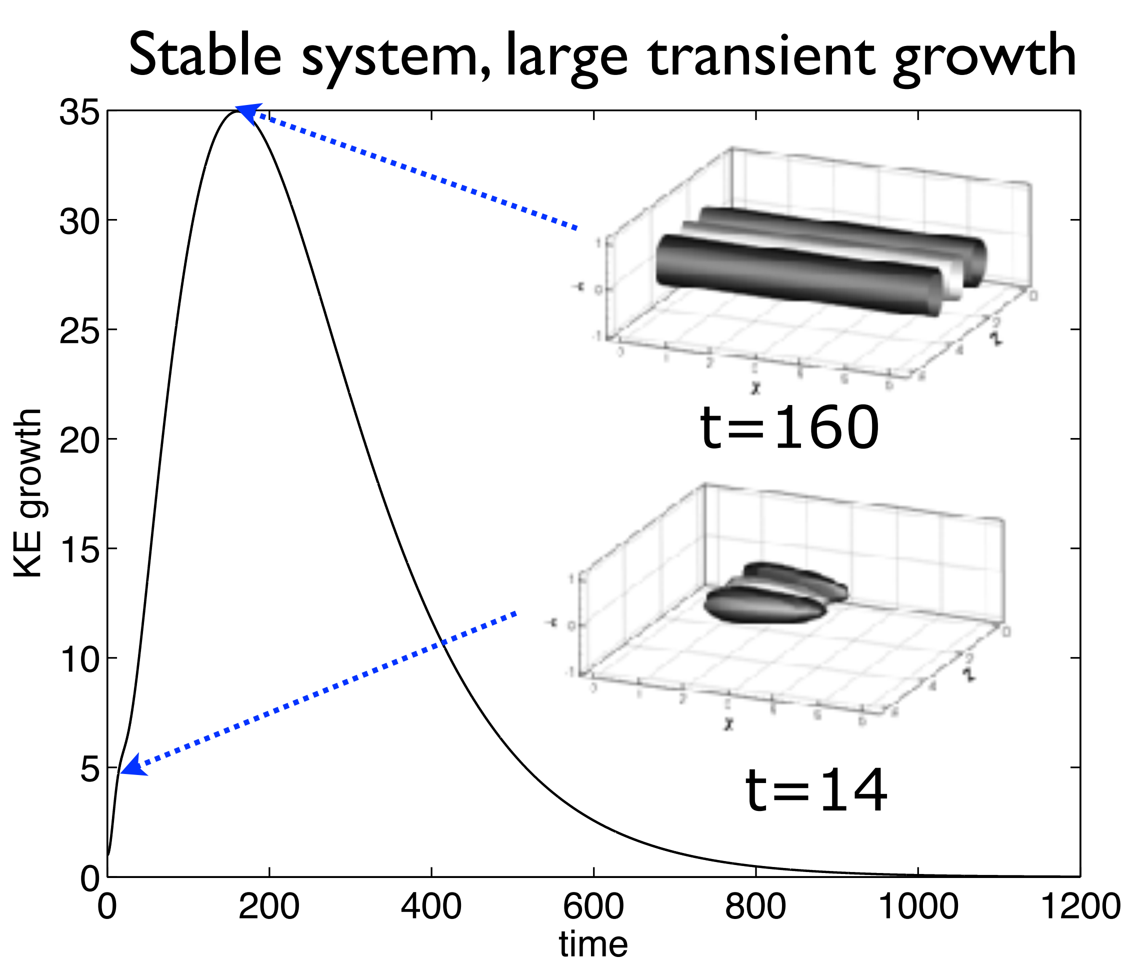
Moore, IEEE TAC, 1981
Rowley, *Int J. Bifurcation & Chaos*, 2005

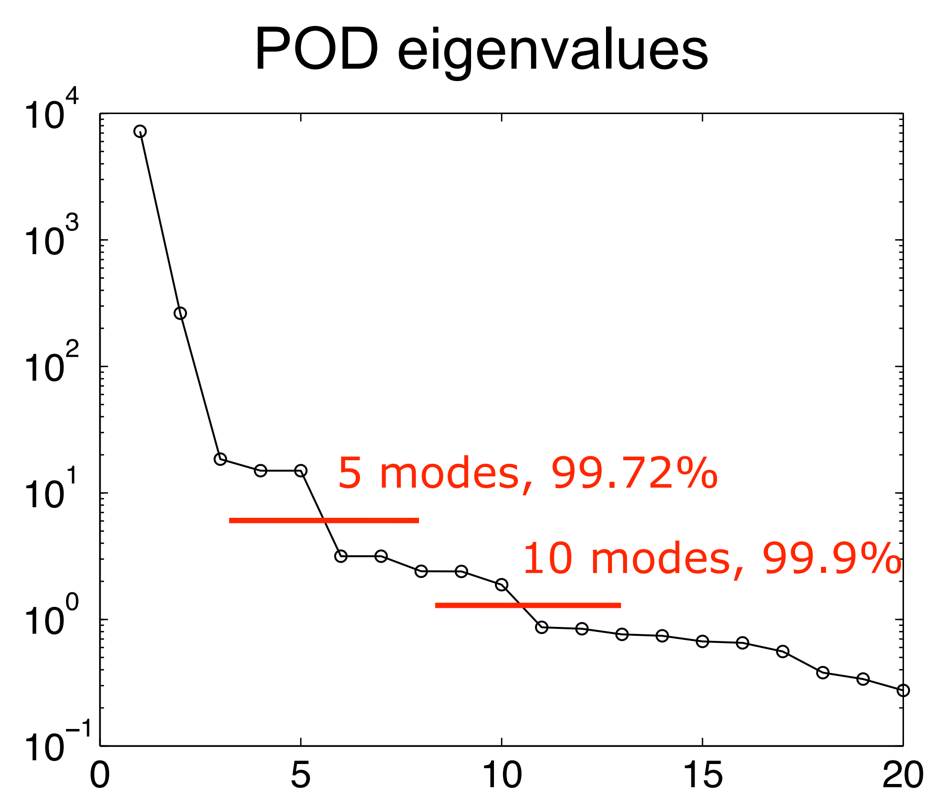
Example: Linearized channel flow

- Example: linearized channel flow in a periodic box
  - Consider linear development of small perturbations
  - Stable system, but large transient growth (non-normal)
- Approach
  - DNS, Re = 2000, 32 x 65 x 32 grid, 133,120 states
  - Try to capture linear dynamics with a reduced-order model



initial perturbation
(vertical velocity)

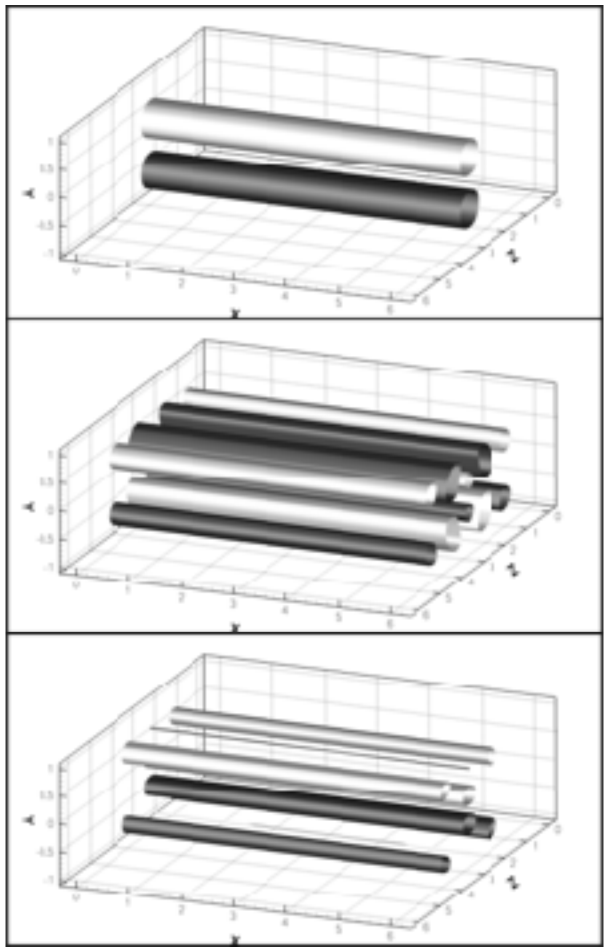




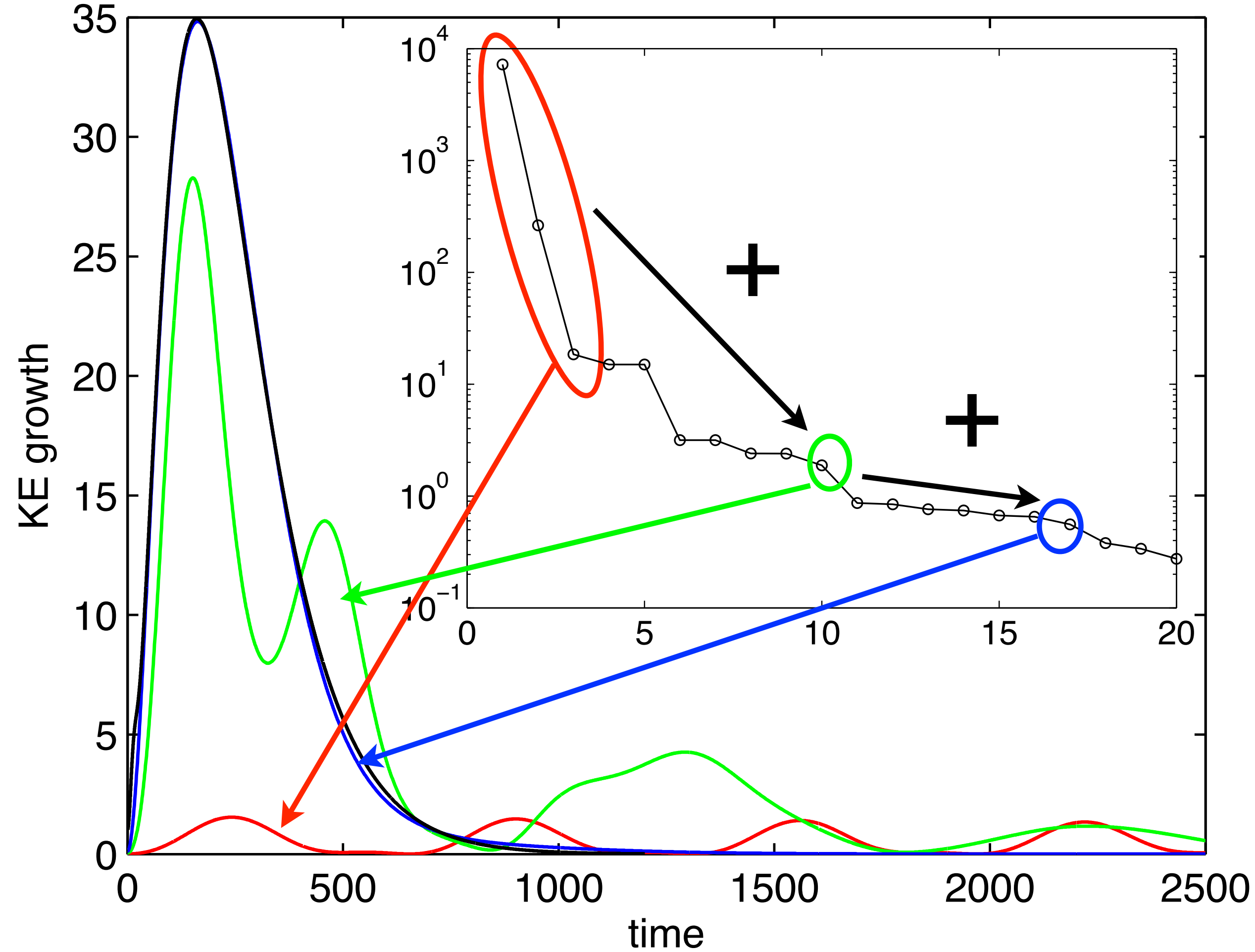
Ilak & Rowley, *Physics of Fluids*, 2008

POD model performance

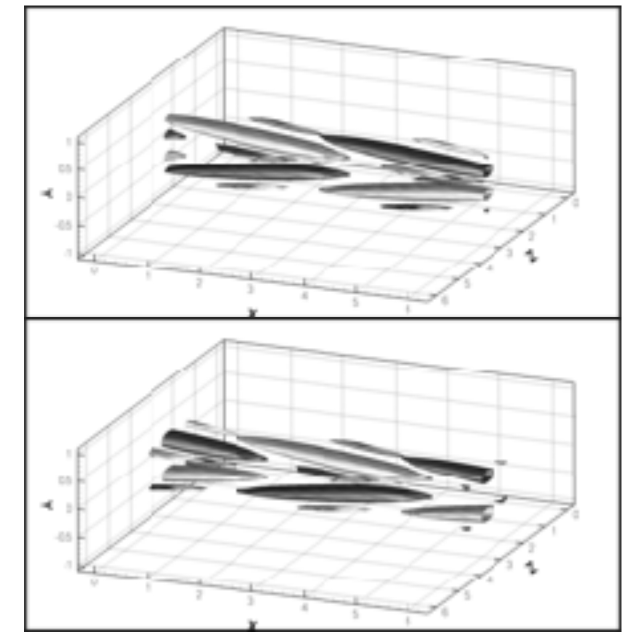
POD modes 1-3



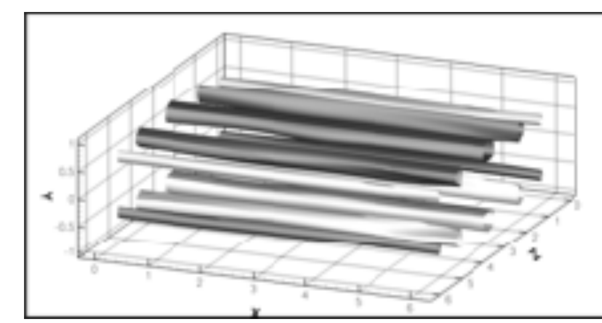
Standard POD



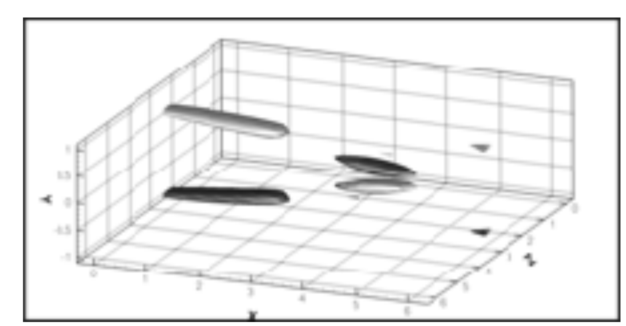
POD modes 4-5



POD mode 10



POD mode 17



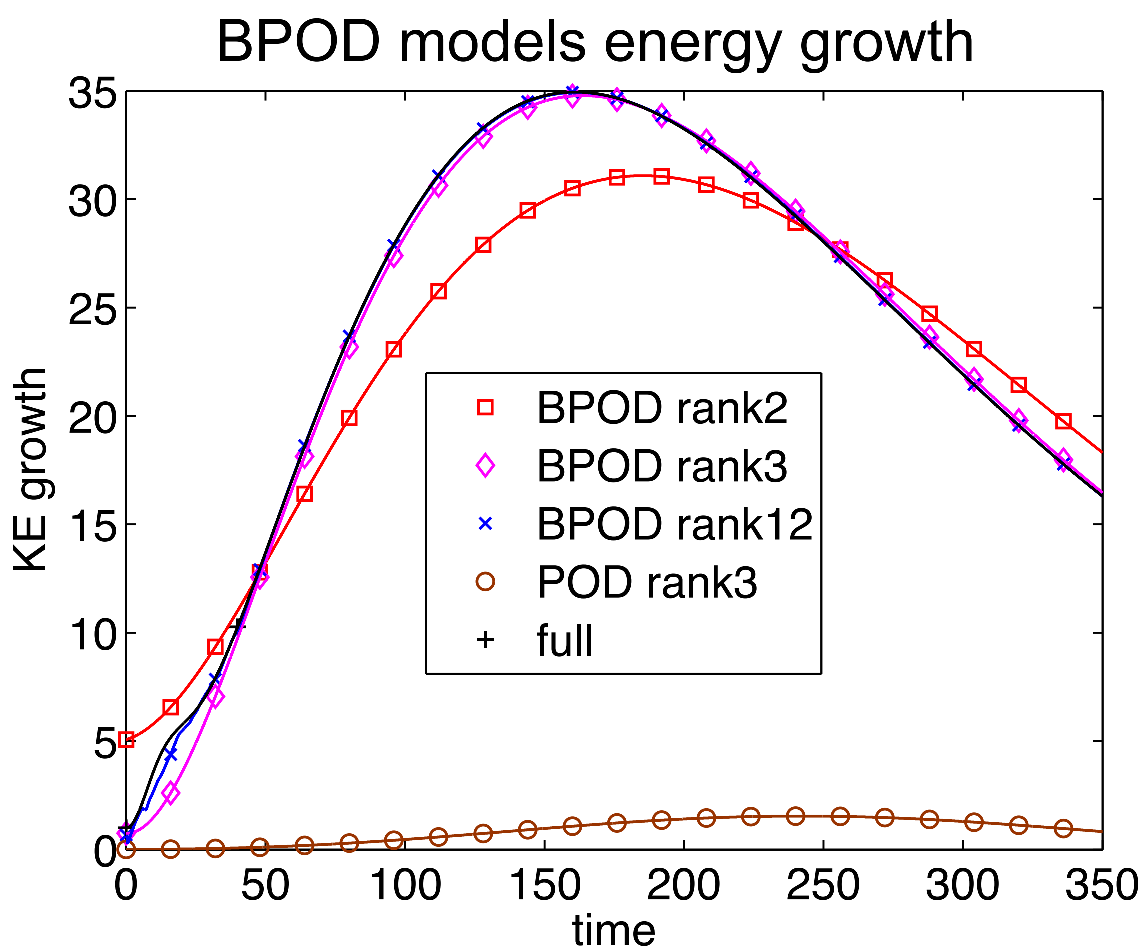
- 5-order model with modes 1,2,3,10,17 much better than 5-mode model with modes 1–5.

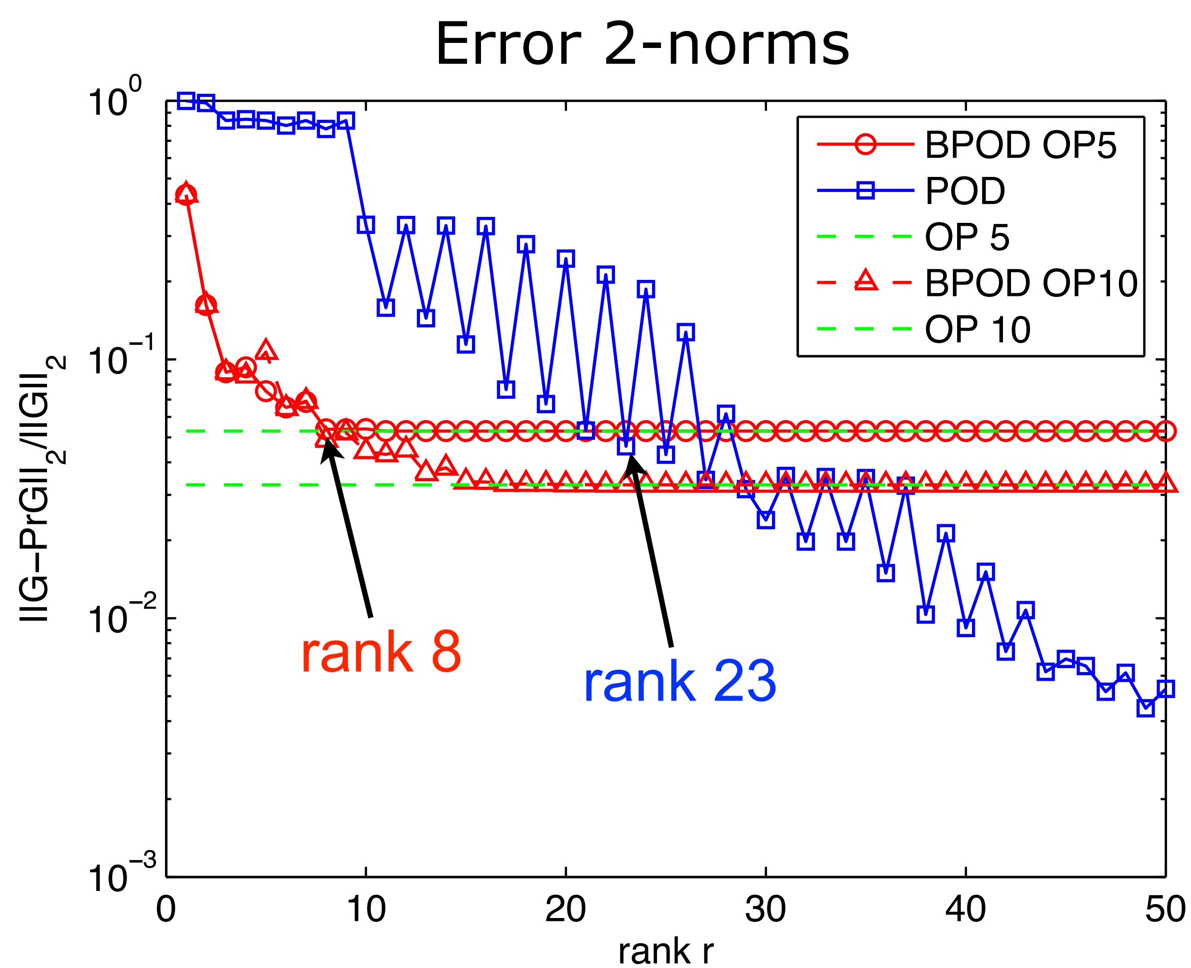
Conclusion: some low-energy POD modes are very important for the system dynamics. Can't naively use just the most energetic ones.

Balancing energy and sensitivity

- What went wrong?
  - The most energetic states are not always the most important
  - Some states that have small energy can nevertheless have a large influence on the flow
- This corresponds to controllability/observability
  - The most controllable states have large energy
  - The most observable states have large sensitivity
- Balanced truncation strikes a balance between these
  - Determine a change of coordinates in which the most controllable states are also the most observable states
  - Balanced POD is an approximation of balanced truncation that is tractable for high-dimensional systems

Balanced POD models are more accurate

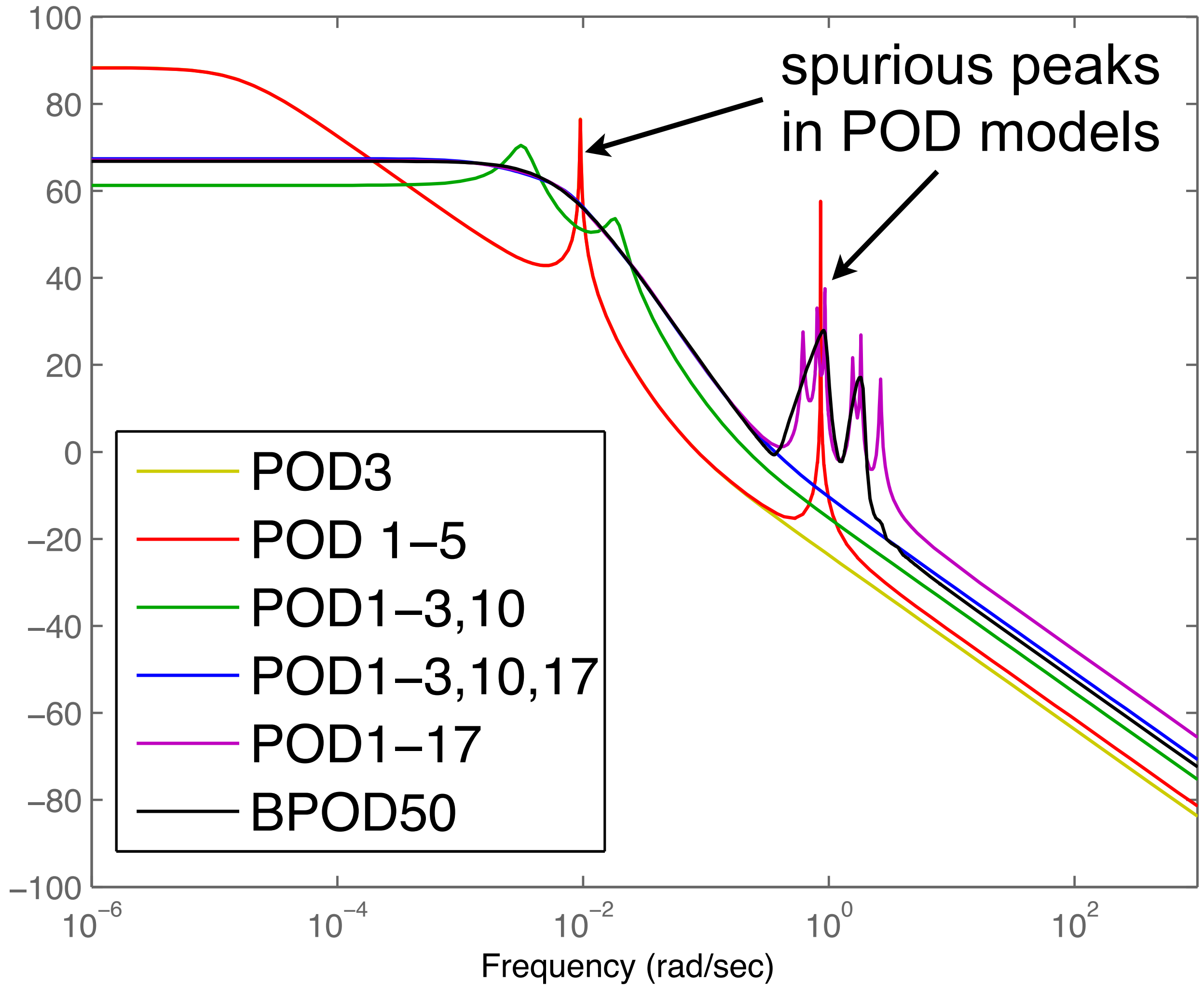




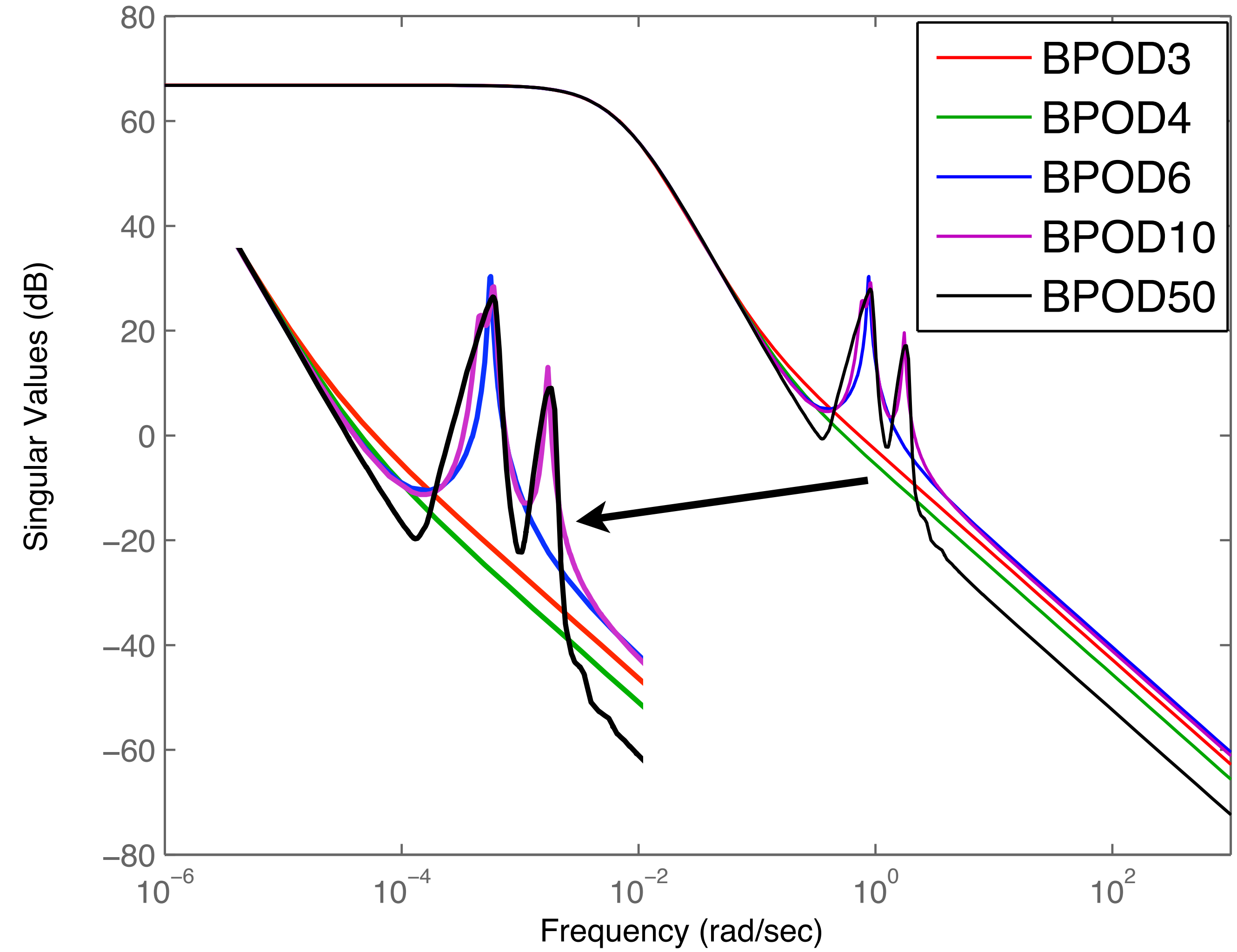
- Three-mode BPOD model excellent at capturing the energy growth
- Rank 8 BPOD model sufficient to correctly capture the dynamics of the first five POD modes, compared to at least 23 POD modes
- Explanation: BPOD weights modes by their observability, or dynamical importance, not just energy

Balanced POD models are less fragile

POD singular value Bode plot



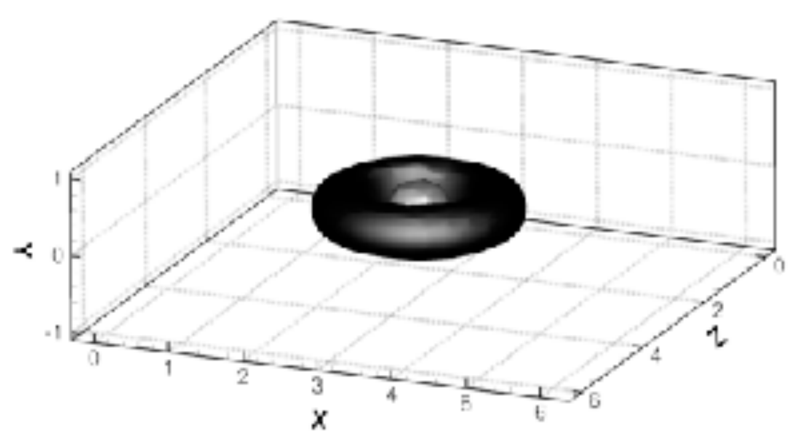
BPOD singular value Bode plot



- POD poorly captures low-pass behavior, spurious peaks
- BPOD models more "robust" than POD (no spurious lightly-damped modes)

Conclusions

- POD can perform poorly, even for a linear system for which 5 modes capture 99% of the energy
- This bad behavior is typical for non-normal systems with large transient energy growth (common in shear flows)
- Reason: low-energy modes can be strongly observable (have a large effect on dynamics)
- Models that balance controllability and observability perform well



Rowley and Dawson. Model Reduction for Flow Analysis and Control. *Annual Reviews of Fluid Mechanics* 49:387–417, 2017

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Dynamic Mode Decomposition

- Dynamic Mode Decomposition (DMD) defined by an algorithm:
  - Collect snapshots of data $\mathbf{x}_0, \mathbf{x}_1, \mathbf{x}_2, \ldots$
  - Assume the data are linearly related:

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

  - Use Krylov-subspace algorithm to approximate eigenvalues and eigenvectors of A (without ever determining A explicitly: know $\mathbf{x}_0, A\mathbf{x}_0, \ldots, A^{n-1}\mathbf{x}_0$)
  - Eigenvectors of A are called "DMD modes"

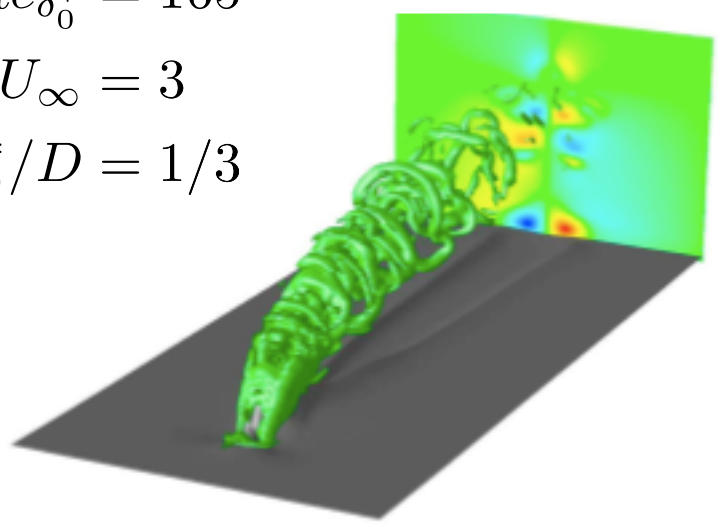
- Hitch: typically the dynamics are nonlinear, and the linear assumption does not hold

P. Schmid, APS 2008; JFM, 2010

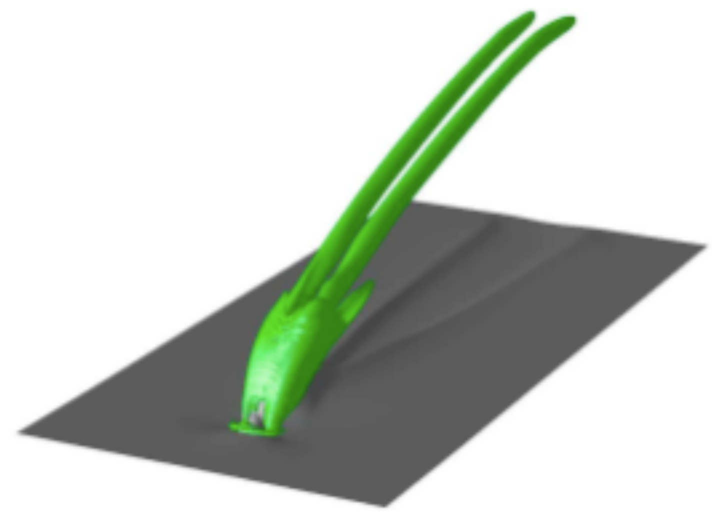
Example: jet in crossflow

- Linearize a jet in crossflow about an unstable equilibrium

$$Re_{\delta_0^*} = 165$$
$$V_{\text{jet}}/U_\infty = 3$$
$$\delta_0^*/D = 1/3$$



Instantaneous snapshot



Unstable equilibrium

- Compute global modes, compare frequencies with observed frequencies in shear layer and near-wall fluctuations

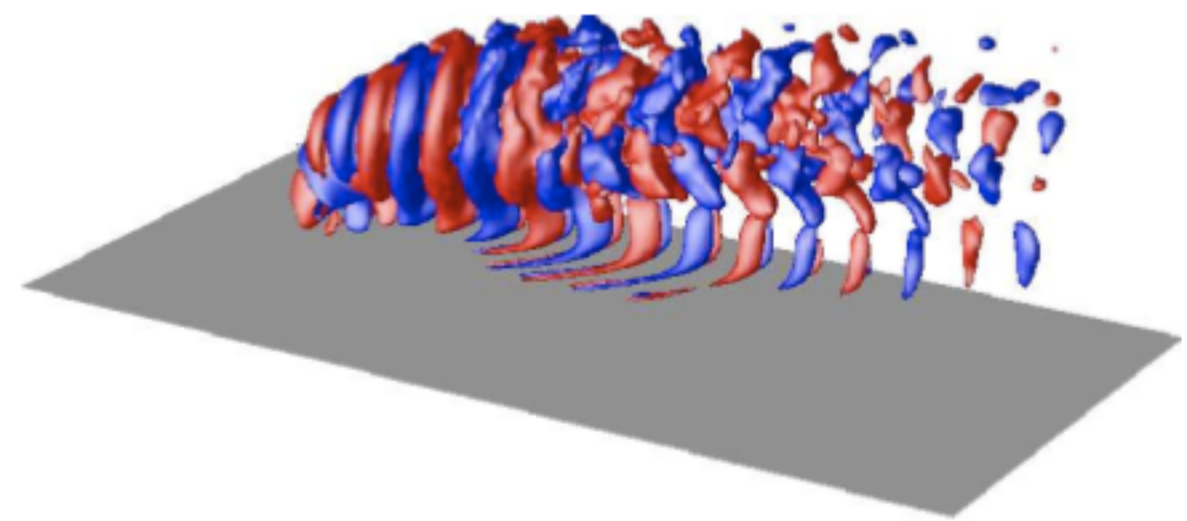
	Observed	Global mode
Shear layer	St = 0.141	St = 0.169
Near wall	St = 0.0174	St = 0.043

Frequency mismatch

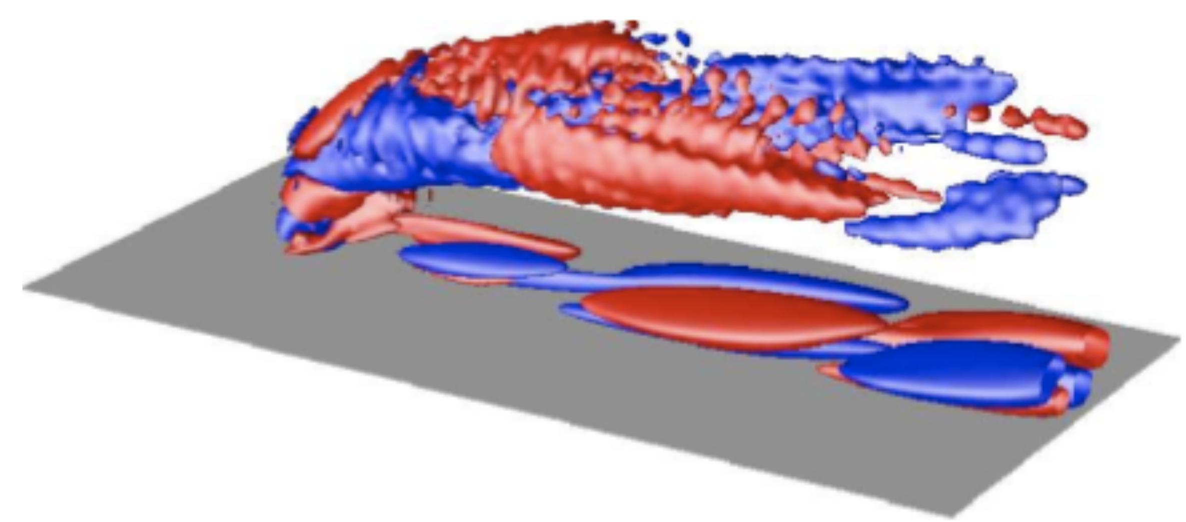
[Bagheri, Schlatter, Schmid, Henningson, JFM 2009]

Dynamic Mode Decomposition for jet in crossflow

- DMD modes capture relevant structures and frequencies
  - High-frequency mode captures structures in the shear layer
  - Low-frequency mode captures near-wall structures associated with horseshoe vortex



St = 0.141

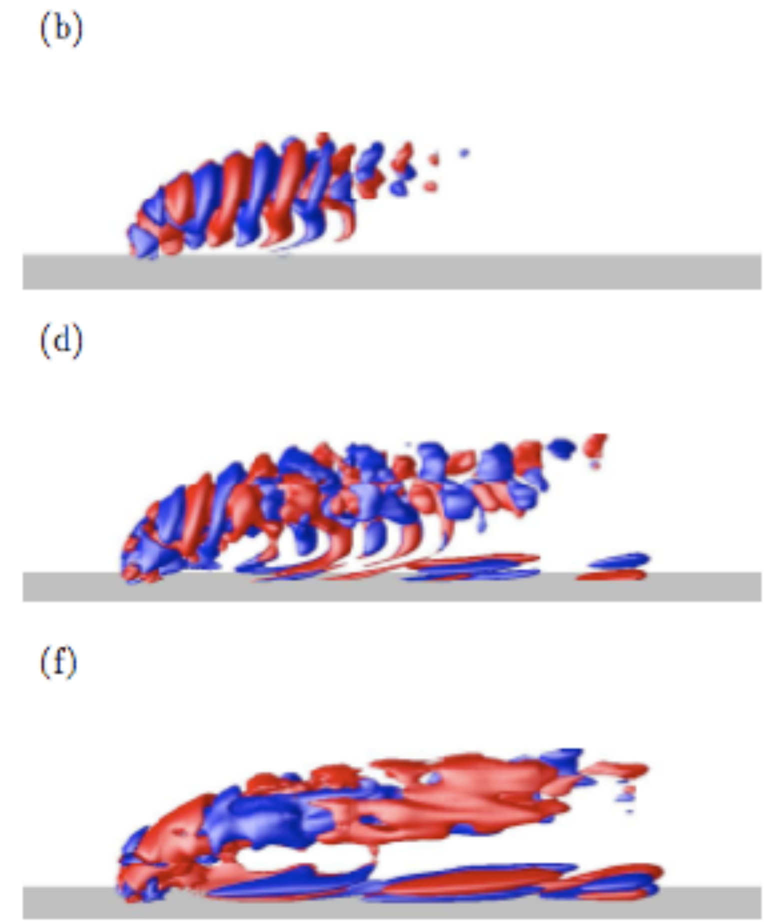


St = 0.017

Rowley, Mezic, Bagheri, Schlatter, and Henningson, JFM, 2009

Comparison with Proper Orthogonal Decomposition

- POD modes
  - Show similar spatial structures to DMD modes
  - Time coefficients of POD modes contain multiple frequencies
  - DMD mode coefficients contain, by construction, a single frequency



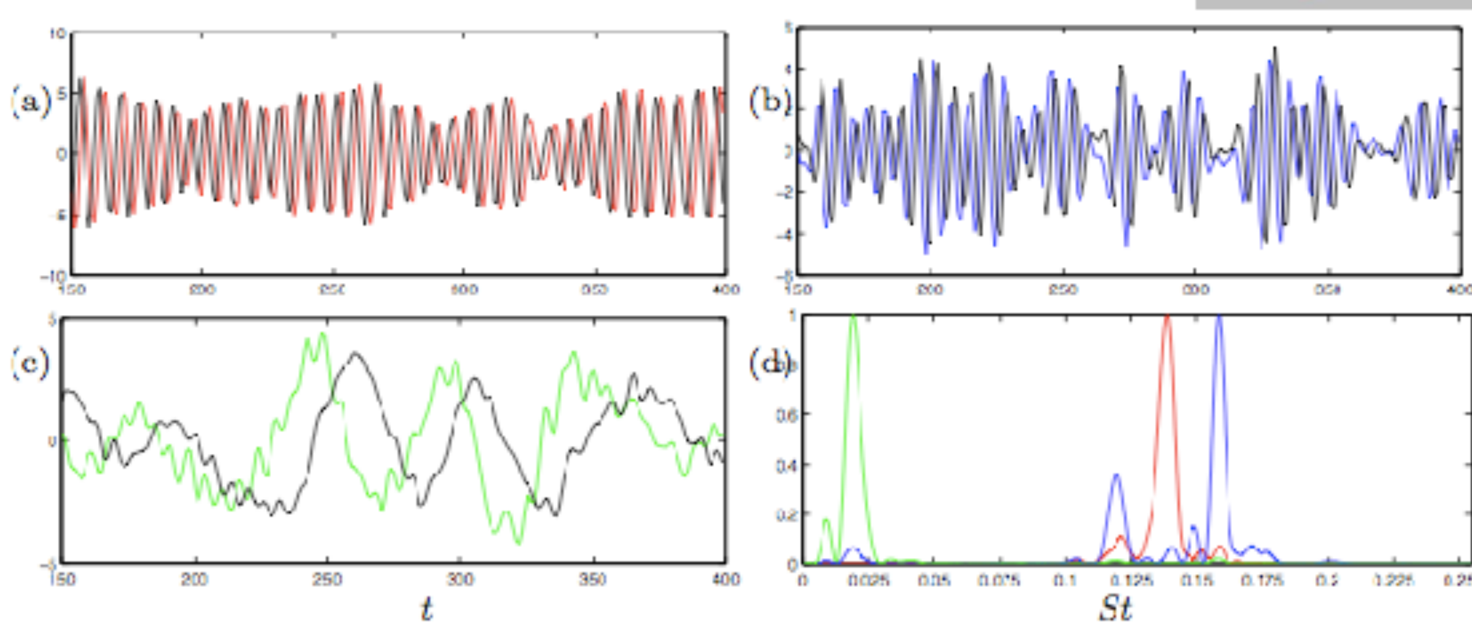


FIGURE 19. The temporal behavior of POD modes are show in terms of the POD coefficients. (a) POD coefficients of the first pair, (b) second pair and (c) third pair of modes. The power spectrum of the signals in (a,b,c) is shown with the same color.

Why did that work?

- The linearization did not capture the right behavior
- The DMD modes did capture the right frequencies, and the structures look physically reasonable
- But DMD was based on the assumption the flow was linear!
- This worked because there was a linear system that fit the observed behavior (oscillations at a few frequencies)
- Can DMD say anything about truly nonlinear systems?
- To answer this, we look at something called the Koopman operator

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Koopman operator

- The Koopman operator
  - Infinite-dimensional linear operator that completely describes the behavior of a nonlinear system
  - Idea: trade nonlinearity for increased system dimension
- Two key features
  - Eigenfunctions of the Koopman operator determine coordinates in which a system is linear
  - Eigenfunctions separate structure from randomness
- (Extended) DMD
  - provides an algorithm for approximating Koopman eigenvalues/ eigenfunctions

Koopman operator and eigenfunctions

- Consider a nonlinear system (discrete time)

$$x_{k+1} = T(x_k) \qquad\qquad x_k \in X$$

- The Koopman operator U acts on functions of x:

$$U : L^2(X) \to L^2(X)$$

$$Uf(x) = f(T(x))$$

- It is linear:

$$U(\alpha f + \beta g)(x) = \alpha U f(x) + \beta U g(x)$$

- Suppose U has an eigenfunction $U\varphi = \lambda\varphi$ and let $z = \varphi(x)$
- Then z evolves linearly:

$$z_{k+1} = \varphi(x_{k+1}) = \varphi(T(x_k)) = U\varphi(x_k) = \lambda\varphi(x_k) = \lambda z_k$$

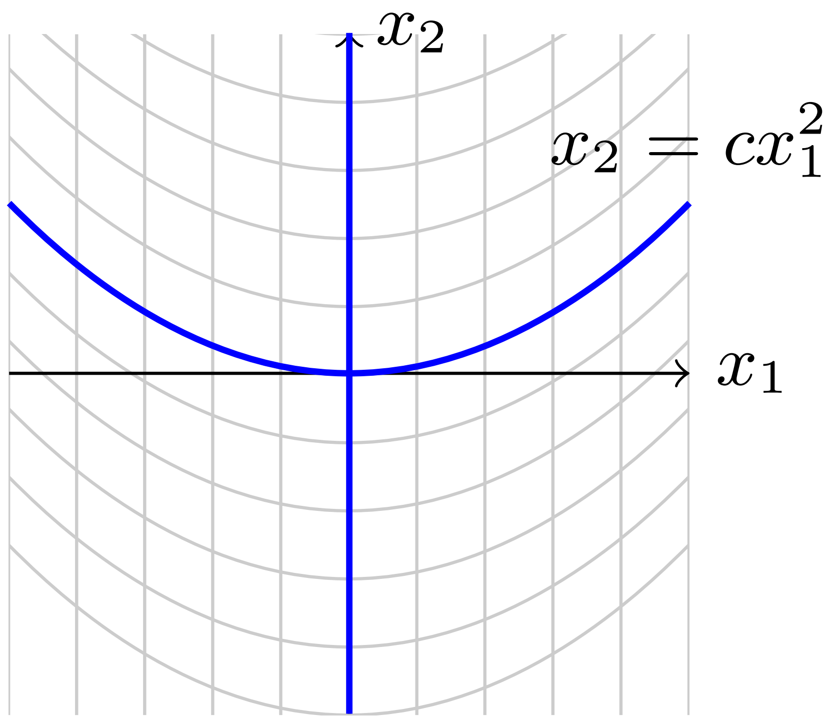
Koopman, PNAS, 1931
Cornfeld, Sinai, Fomin, *Ergodic Theory*, 1982

Example: two-dimensional map

Consider the map

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \mapsto \begin{bmatrix} \lambda x_1 \\ \mu x_2 + (\lambda^2 - \mu) c x_1^2 \end{bmatrix}$$

This system has an equilibrium at the origin, and invariant manifolds given by $x_1 = 0$ and $x_2 = cx_1^2$



Koopman eigenvalues are $\lambda,\ \mu$ with eigenfunctions

$$\varphi_\lambda(\mathbf{x}) = x_1$$

$$\varphi_\mu(\mathbf{x}) = x_2 - cx_1^2$$

In the coordinates $(z_1, z_2) = (x_1, x_2 - cx_1^2)$, the dynamics are linear:

$$\begin{bmatrix} z_1 \\ z_2 \end{bmatrix} \mapsto \begin{bmatrix} \lambda z_1 \\ \mu z_2 \end{bmatrix}$$

Tu, Rowley, et al, JCD, 2014
Rowley & Dawson, ARFM, 2017

Koopman eigenfunctions from data: Extended DMD

- Approximate the Koopman operator directly
- For Extended DMD, the user supplies:
  - A set of observables $\psi_j \in L^2(X)$ (basis functions)
  - Values of the observables at sample points $\mathbf{x}_k$ and $T(\mathbf{x}_k)$
- May be viewed as a projection of the Koopman operator onto a subspace spanned by the observables ψ_j

$$X = \begin{bmatrix} \psi_1(\mathbf{x}_1) & \cdots & \psi_1(\mathbf{x}_n) \\ \vdots & & \vdots \\ \psi_m(\mathbf{x}_1) & \cdots & \psi_m(\mathbf{x}_n) \end{bmatrix} \qquad X^\# = \begin{bmatrix} \psi_1(T(\mathbf{x}_1)) & \cdots & \psi_1(T(\mathbf{x}_n)) \\ \vdots & & \vdots \\ \psi_m(T(\mathbf{x}_1)) & \cdots & \psi_m(T(\mathbf{x}_n)) \end{bmatrix}$$

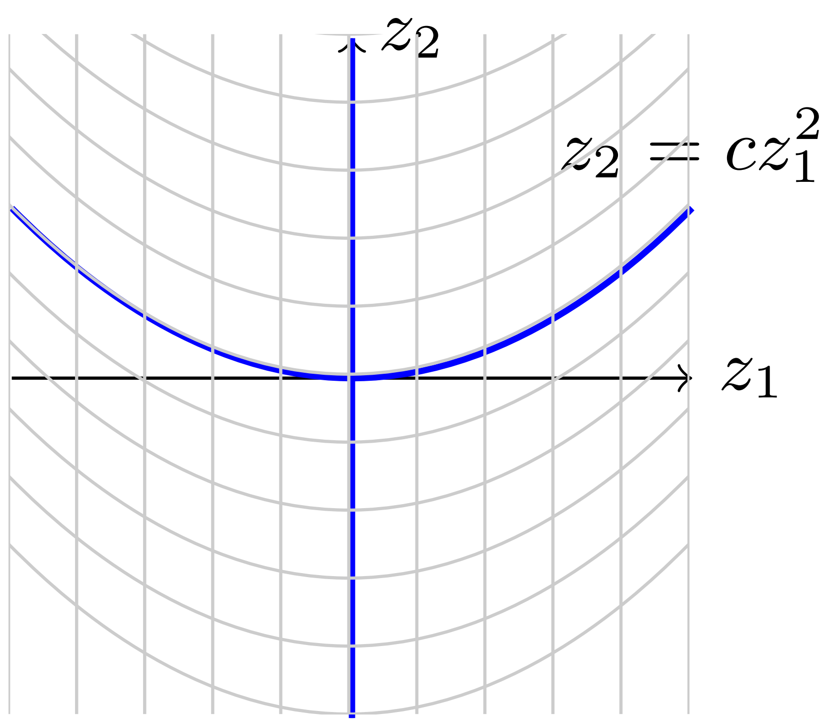
  - Let $A = X^\# X^+$. Then A is a projection of U onto subspace spanned by $\{\psi_j\}$
  - Note: if the observables are the components of the state, this is regular DMD

Comparing DMD and EDMD

Recall our 2D example:

$$\begin{bmatrix} z_1 \\ z_2 \end{bmatrix} \mapsto \begin{bmatrix} \lambda z_1 \\ \mu z_2 + (\lambda^2 - \mu) c z_1^2 \end{bmatrix}$$

This system has an equilibrium at the origin, and invariant manifolds given by $z_1 = 0$ and $z_2 = c z_1^2$



Koopman eigenvalues are $\lambda, \ \mu$ with eigenfunctions

$$\varphi_\lambda(\mathbf{z}) = z_1$$
$$\varphi_\mu(\mathbf{z}) = z_2 - c z_1^2$$

In addition, φ_λ^k is an eigenfunction with eigenvalue λ^k, the product $\varphi_\lambda \varphi_\mu$ is an eigenfunction with eigenvalue $\lambda\mu$, etc.

Comparing DMD and EDMD

- Apply DMD to this example, with initial states z given by (1,1), (5,5), (–1,1), (–5,5), with $\lambda = 0.9$, $\mu = 0.5$
  - Case 1: observable $\psi(\mathbf{z}) = (z_1, z_2)$
    If c = 0, so that the system is linear, then DMD eigenvalues are 0.9 and 0.5: good!

    If c = 1, however, then DMD eigenvalues are 0.9 and 2.002. These do not correspond to Koopman eigenvalues, and one might even presume the equilibrium is *unstable*!

  - Case 2: observable $\psi(\mathbf{z}) = (z_1, z_2, z_1^2)$
    The EDMD eigenvalues are 0.9, 0.5, and 0.81 = 0.9^2, which agree with the Koopman eigenvalues.

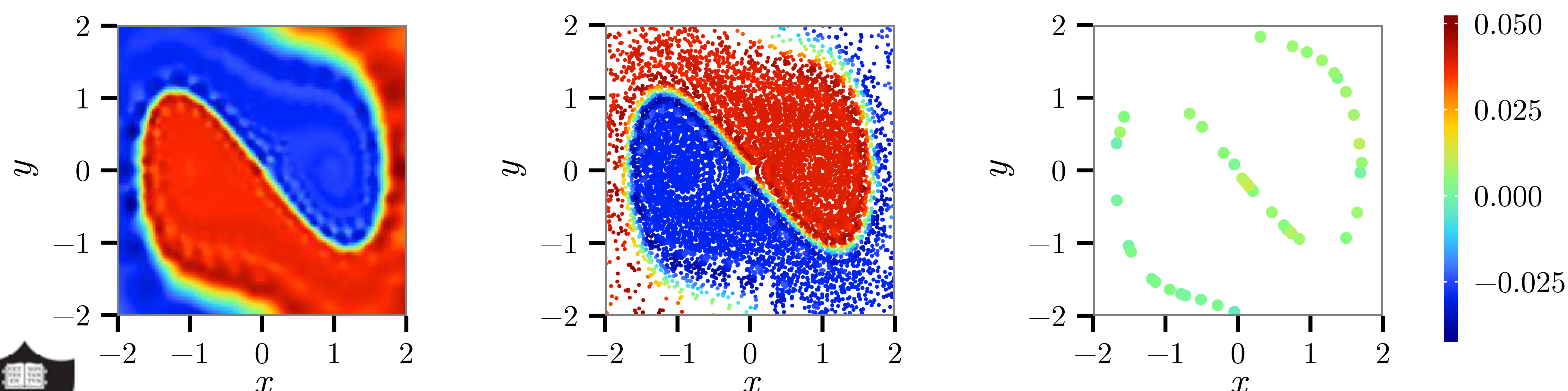
Main point: for a nonlinear system, DMD can give erroneous results. Need a richer set of "observables."

Example: a nonlinear ODE

- Consider the Duffing equation

$$\ddot{x} + \delta\dot{x} + x(x^2 - 1) = 0$$

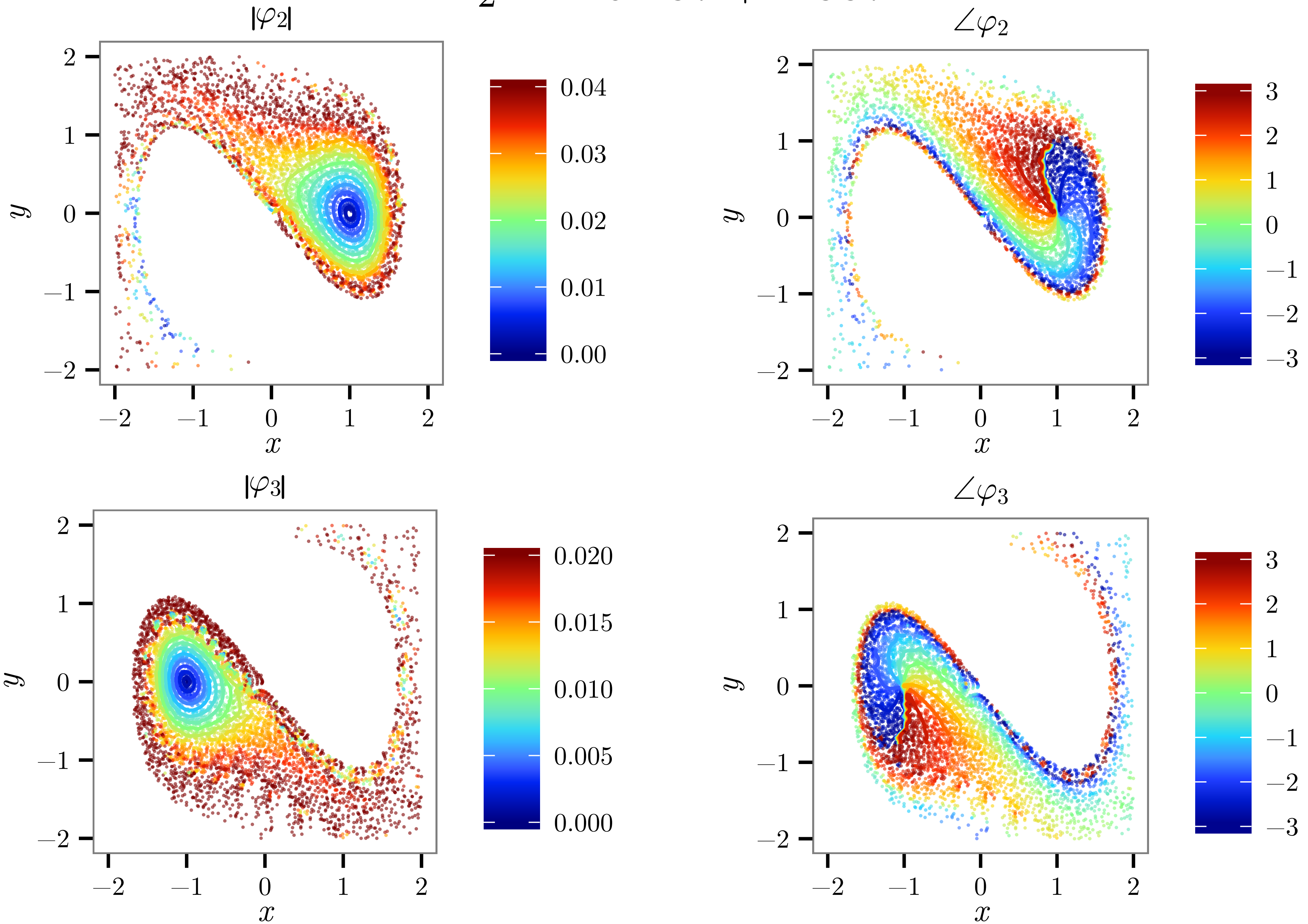
- Compute EDMD
  - δ = 0.5, 10^3 trajectories with 11 samples each
  - Basis functions: 1000 radial basis functions (thin plate splines)
- $\lambda_0 = -10^{-14}$ eigenfunction is the constant function
- $\lambda_1 = -10^{-3}$ eigenfunction reveals basins of attraction



Dynamics in each basin

- Eigenfunctions determine coordinates in which dynamics in each basin are linear

$$\lambda_2 = -0.237 + 1.387i$$



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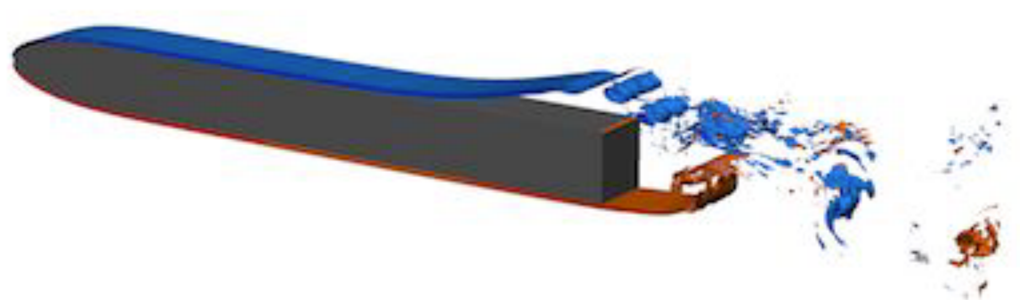
Structure vs. randomness

- Many physical problems exhibit some "structure" amidst apparent "randomness":
  - For instance, small-scale turbulence on top of a regular vortex shedding



- There is little hope of a low-order model capturing details of the "randomness"
- Goal: determine a low-order model for the "structured" part, ignore the "random" part.

Crash course in ergodic theory

- The Koopman operator provides a way to separate "structure" from "randomness"
- Look at maps $x \mapsto T(x)$ $x \in [0,1]$
- Two examples:

$$T(x) = x + \alpha \pmod 1$$

$$T(x) = 2x \pmod 1$$

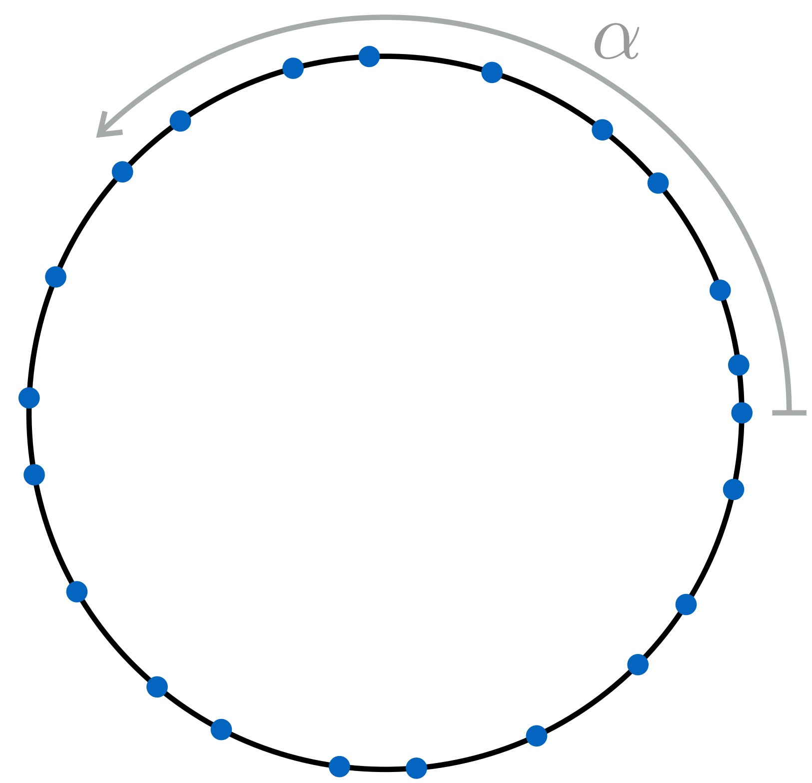
Rotation on the circle

- Consider the map

$$x \mapsto T(x) \qquad x \in [0,1]$$

$$\boxed{T(x) = x + \alpha \pmod 1}$$

α irrational



- Identify $[0,1]$ with the unit circle:

$$x \mapsto e^{2\pi i x}$$

- The system is ergodic:
  - The only invariant sets are sets of full measure (or zero measure)
- The dynamics are simple and "structured"

Expanding map on the circle

- Now consider the map

$$T(x) = 2x \pmod 1$$

  - Fixed point at $x = 0$
  - Some points go to the fixed point:

$$\frac{1}{8} \mapsto \frac{1}{4} \mapsto \frac{1}{2} \mapsto 0$$

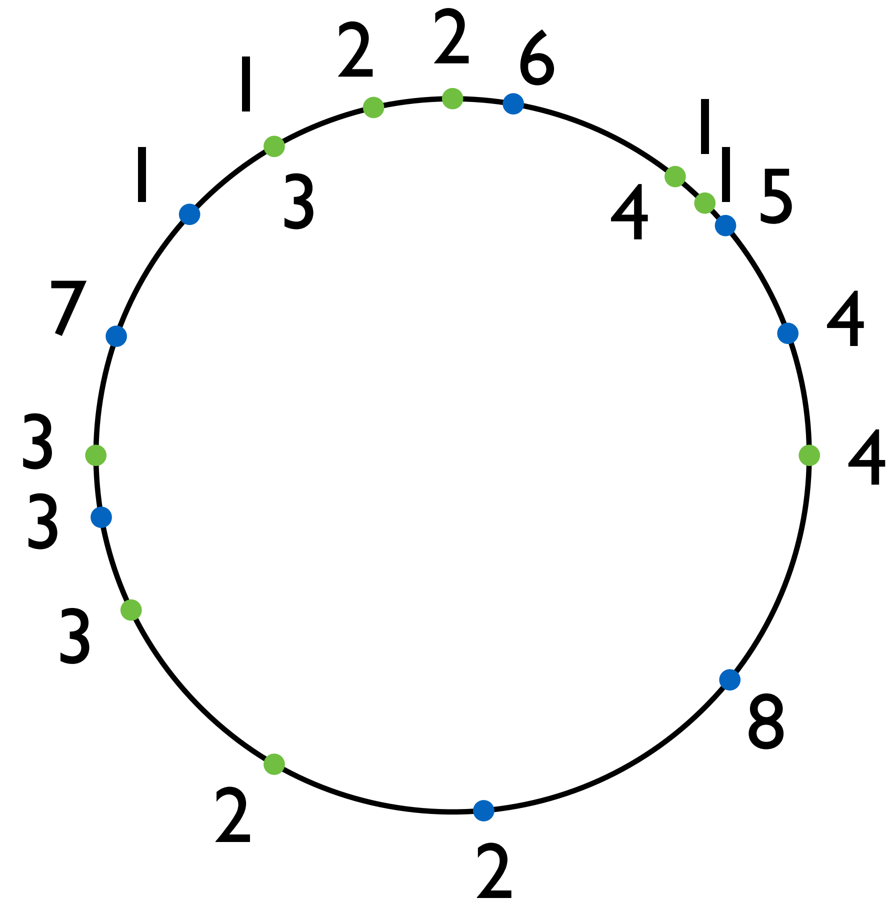
  - Period 2 orbit:

$$\frac{1}{3} \mapsto \frac{2}{3} \mapsto \frac{1}{3} \mapsto \cdots$$

  - Period 3 orbit:

$$\frac{1}{7} \mapsto \frac{2}{7} \mapsto \frac{4}{7} \mapsto \frac{1}{7} \cdots$$

  - Any irrational number: dense orbit



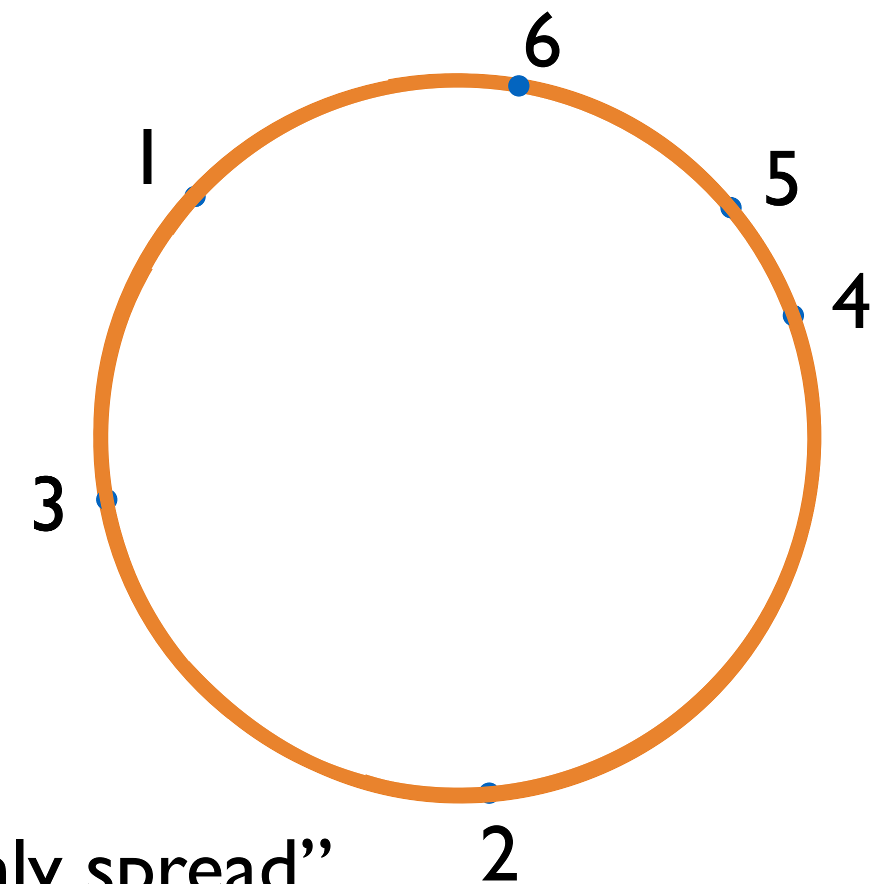
- This map is also ergodic
(the only invariant sets have measure zero or one)
  - However, the dynamics are not at all "structured"

Expanding map on the circle

- Now consider the map

$$\boxed{T(x) = 2x \pmod 1}$$

- The map is ergodic
  - The only invariant sets have measure zero or one
- The map is also "mixing"
  - Any subset of finite measure is "evenly spread" around the circle
- Has all the hallmarks of chaos
  - Countably infinite number of periodic orbits, all unstable
  - A dense orbit
  - Nearby points spread exponentially
  - Symbolic dynamics: T corresponds to shifting the decimal to the right in the binary expansion of x: e.g., $x = 0.01101010000100\ldots$



Back to the Koopman operator

- Koopman operator U acts on functions $f \in L^2([0,1])$

$$Uf(x) = f(T(x))$$

- Ergodicity and mixing are spectral properties of U:
  - T is ergodic iff any function f that satisfies $Uf = f$ is a constant (a.e.)
  - T is (weak) mixing iff U has no eigenfunctions besides constants
- First example: $T(x) = x + \alpha \pmod 1$
  - U has an eigenfunction $\varphi(x) = e^{2\pi i x}$ with eigenvalue $e^{2\pi i \alpha}$

$$(U\varphi)(x) = \varphi(T(x)) = e^{2\pi i(x+\alpha)} = e^{2\pi i \alpha}\varphi(x)$$

  - Dynamics are "structured"
- Second example: $T(x) = 2x \pmod 1$
  - U has no eigenfunctions besides the constant function
  - The dynamics are purely "chaotic": there is no structure

Use EDMD to approximate structured dynamics

- Plan:
  - Use EDMD to approximate the Koopman operator from data
  - Eigenvalues and corresponding eigenfunctions indicate "structured" components of dynamics
  - Question: what will happen to the continuous spectrum? Will we be able to tell the difference between "true" eigenvalues and spurious ones?

Use EDMD to separate structure from randomness

- Example: system with mixed spectrum

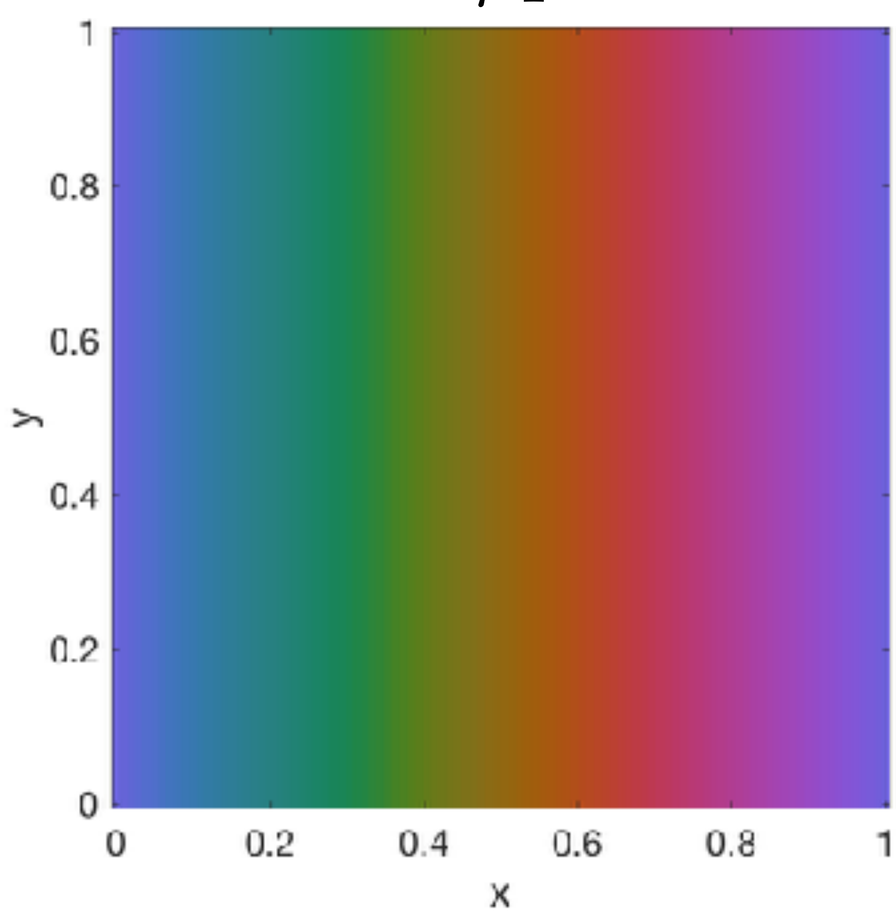
$$T(x, y) = (x + \alpha, 3y) \quad (\text{mod } 1)$$

  - x-coordinate is "structured", y-coordinate is "mixing"
  - Eigenfunctions $\varphi_k(x, y) = e^{2\pi i k x}$ eigenvalues $e^{2\pi i k \alpha}$ $k \in \mathbb{Z}$

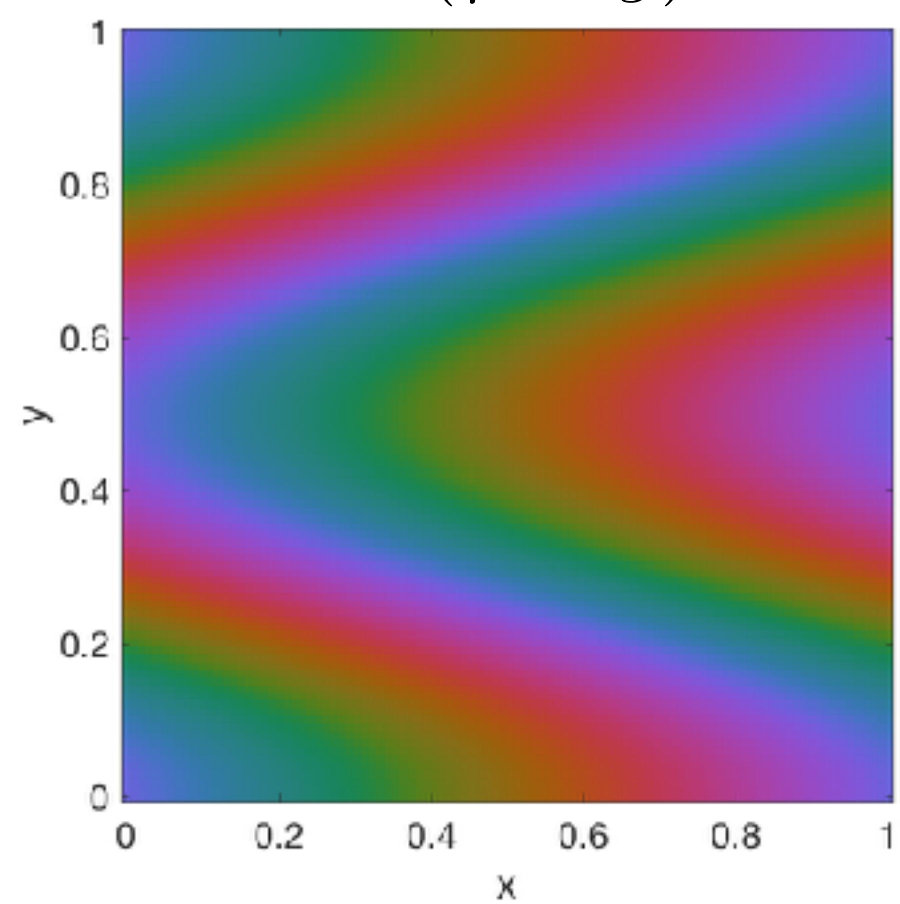
- Nonlinear coordinate change to make more interesting

$$\tilde{T} = g^{-1} T g \qquad g(x, y) = (x + \tfrac{1}{2}(1 + \cos 2\pi y), y)$$

$\angle \varphi_1$

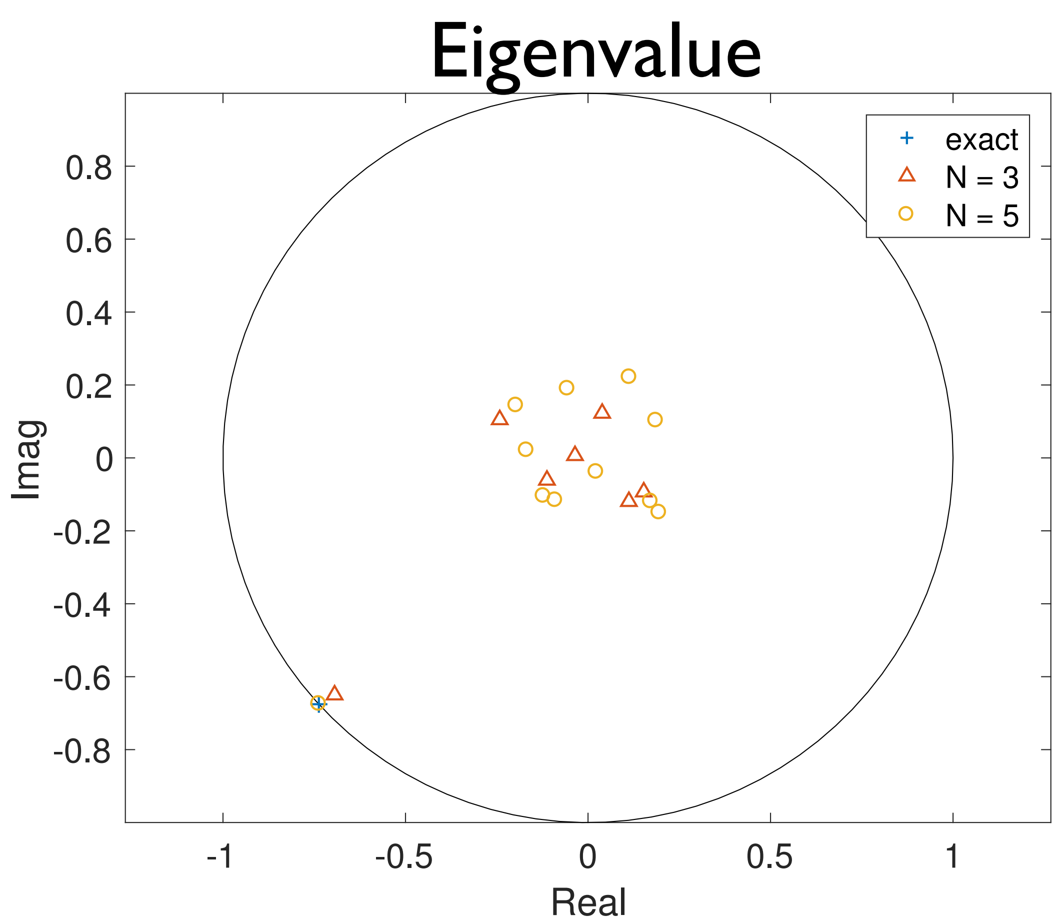


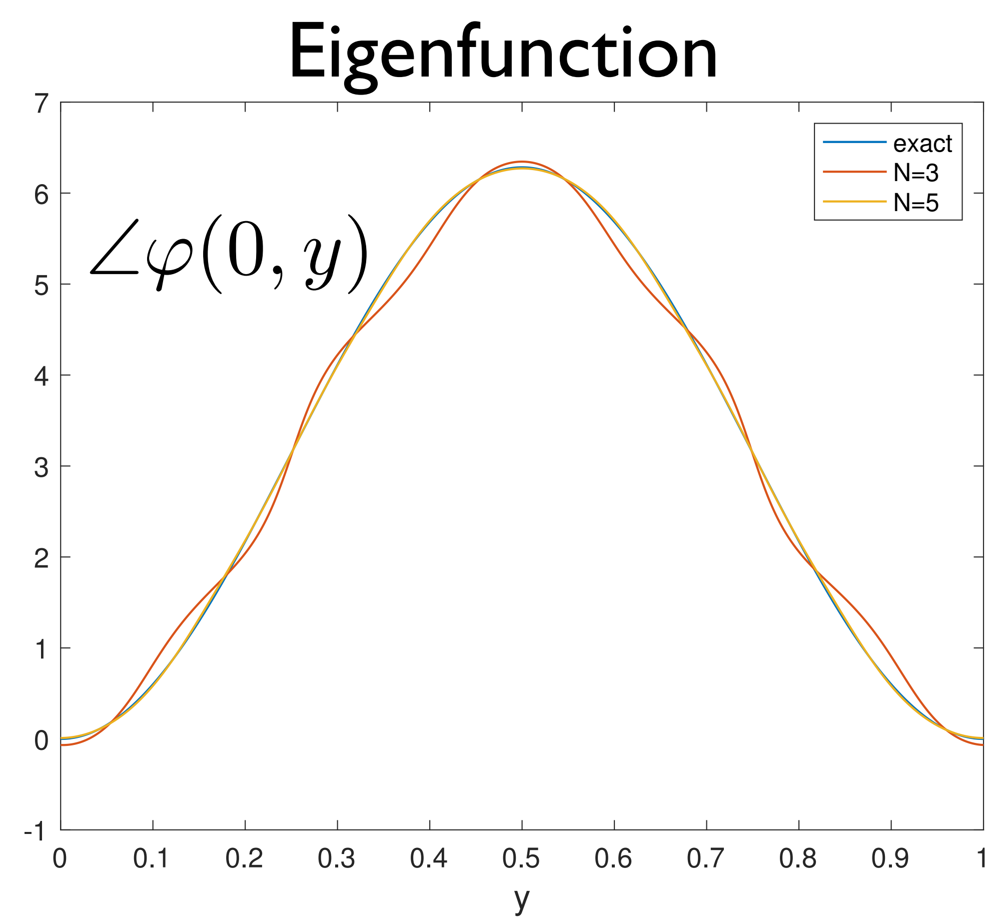
$\angle(\varphi_1 \circ g)$



EDMD results

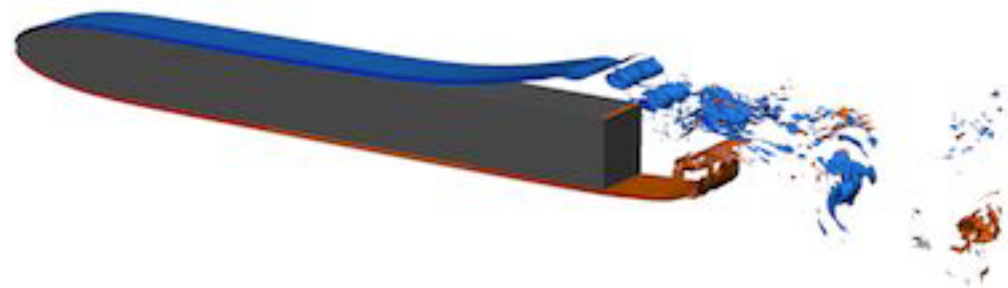
- Apply EDMD to this example
  - Fourier basis functions $\left\{e^{2\pi i(x+jy)}\right\}_{j=-N}^{N}$
  - Sample 1000 random points
- The "true" eigenvalue clearly stands out
  - The eigenvalue and eigenfunction are close to the correct value for N = 3, and nearly identical for N = 5.



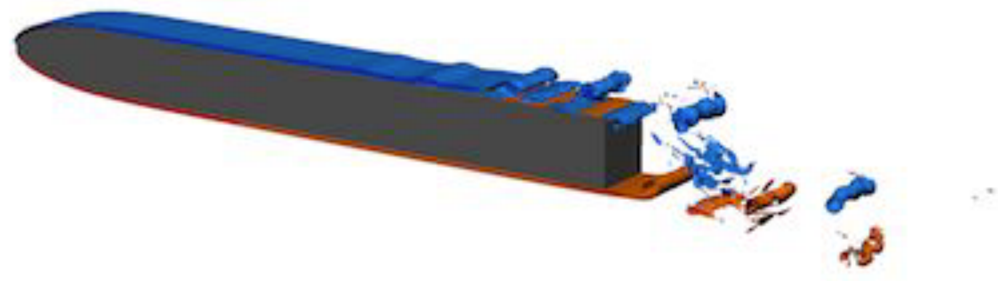


Apply DMD to separated flow past a flat plate

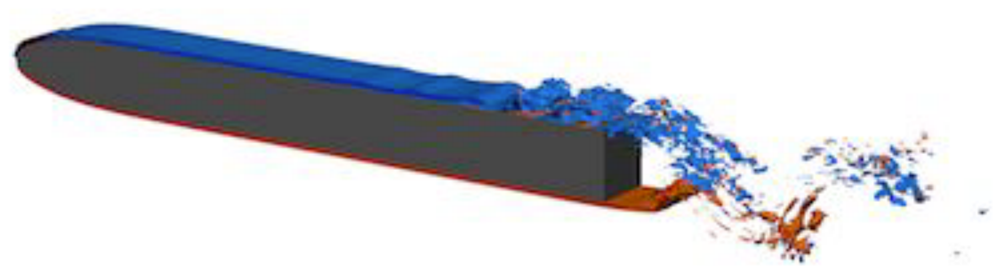
- No forcing



- Forcing at $f^+ = 4.7$

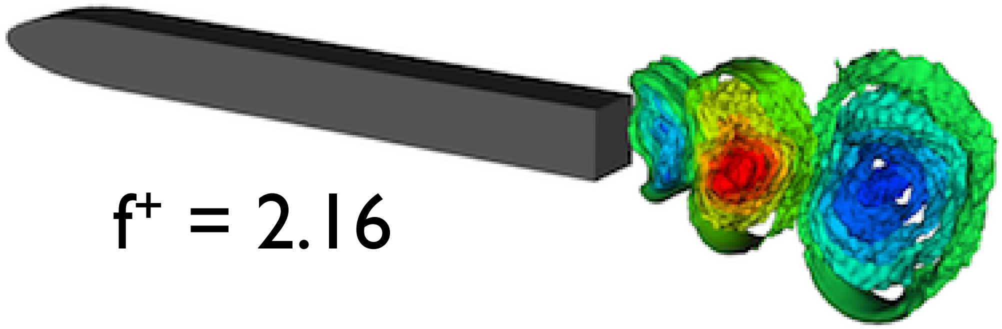


- Forcing at $f^+ = 6.4$

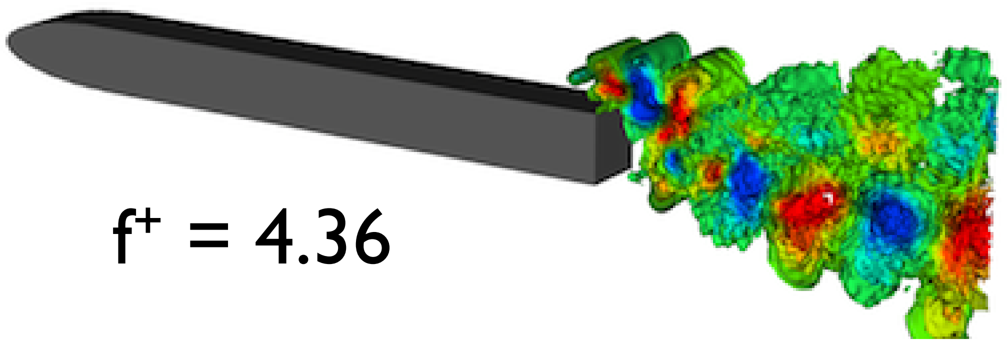


DMD modes in flow past a flat plate

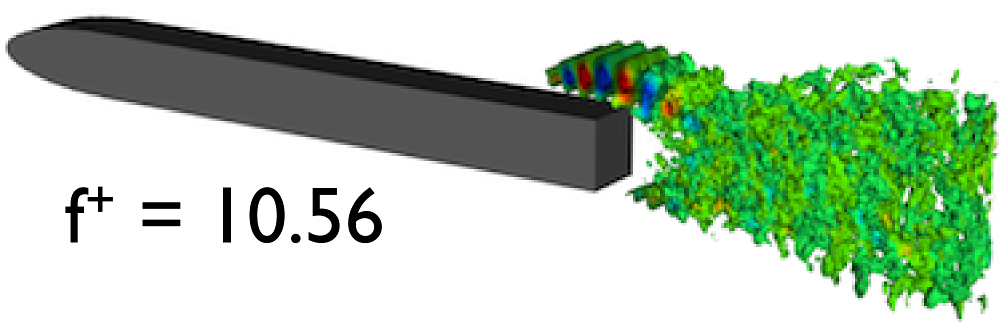
No forcing



$f^+ = 2.16$

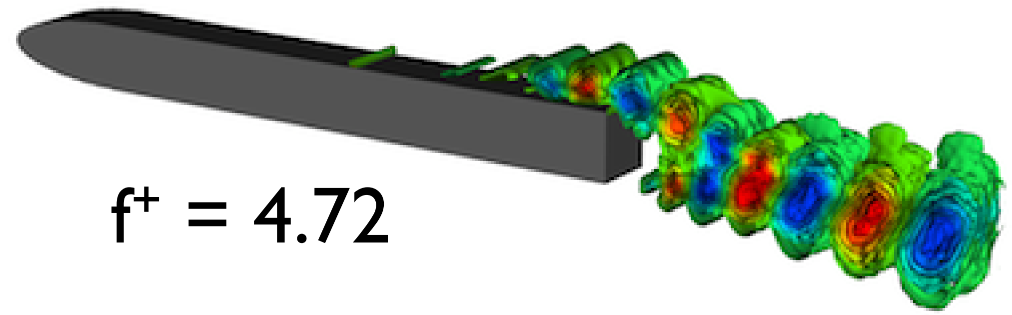


$f^+ = 4.36$

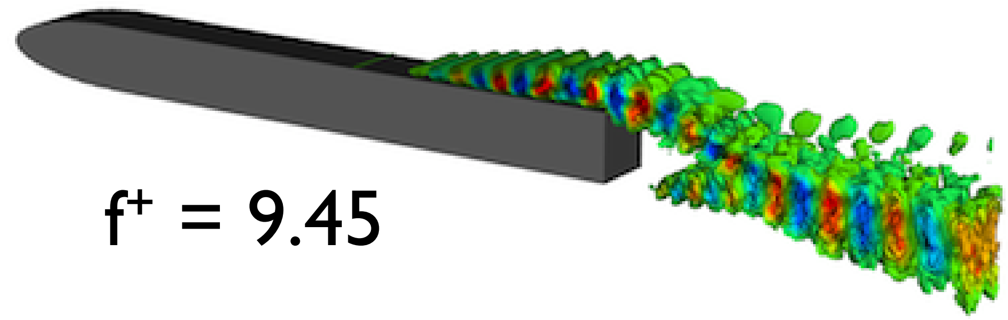


$f^+ = 10.56$

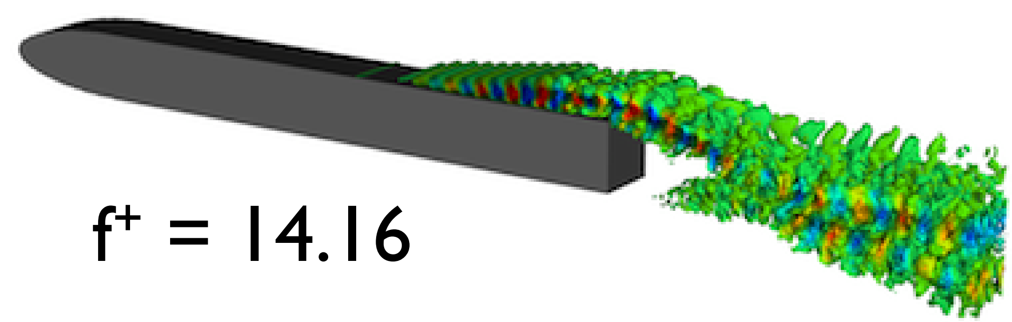
Forcing at $f^+ = 4.7$



$f^+ = 4.72$



$f^+ = 9.45$



$f^+ = 14.16$

Conclusions

- Balanced models
  - Many shear flows are non-normal: large transient energy growth.
  - For these systems, POD typically performs poorly; balanced models perform well
- Dynamic mode decomposition
  - Fit linear dynamics to data
  - For nonlinear systems, extended DMD approximates the Koopman operator
  - Eigenfunctions of the Koopman operator determine coordinates in which a system is linear, and can separate structured from random components
- Many unanswered questions
  - How to choose good basis functions (observables) for EDMD?
  - How to distinguish "true" eigenvalues from "spurious" ones?
  - High-dimensional nonlinear systems?

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