

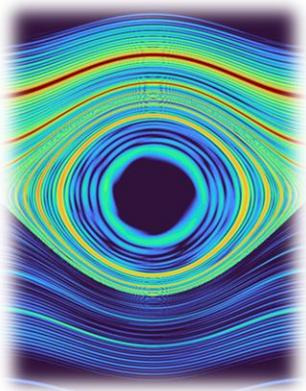
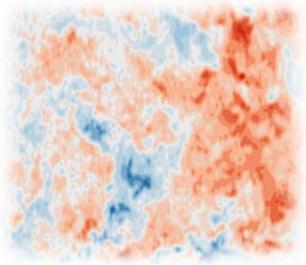
# Unitary Approximations of Koopman Operators

Matthew Colbrook

University of Cambridge

20/03/2024

C., "The mpEDMD Algorithm for Data-Driven Computations of Measure-Preserving Dynamical Systems," **SIAM Journal on Numerical Analysis**, 61(3), 2023.



# Motivation

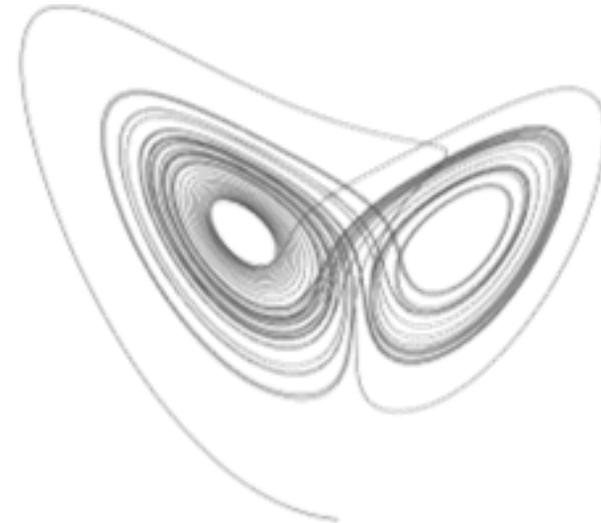
# Data-driven dynamical systems

State  $x \in \Omega \subseteq \mathbb{R}^d$ .

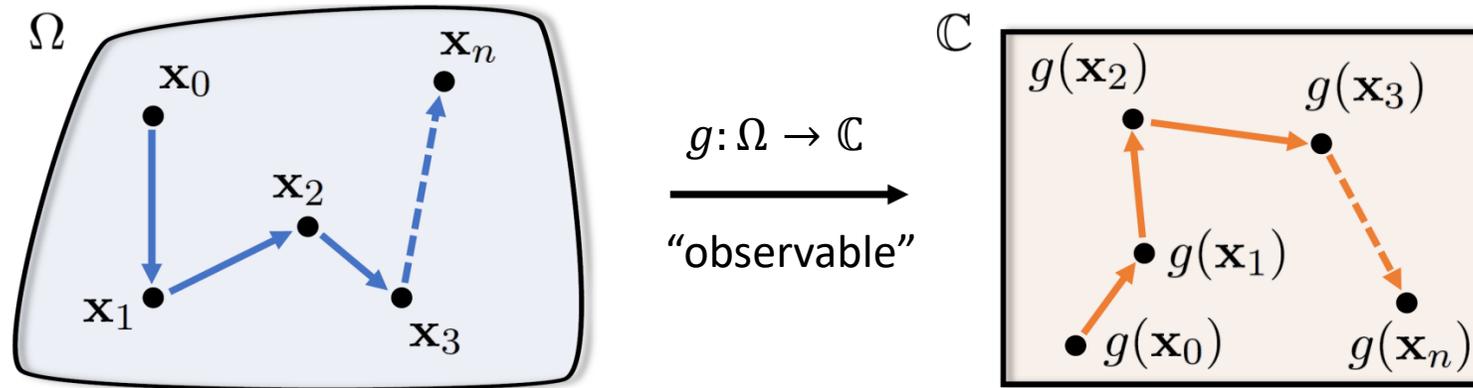
**Unknown** function  $F: \Omega \rightarrow \Omega$  governs dynamics:  $x_{n+1} = F(x_n)$

**Goal:** Learning from data  $\{x^{(m)}, y^{(m)} = F(x^{(m)})\}_{m=1}^M$ .

**Applications:** chemistry, climatology, control, electronics, epidemiology, finance, fluids, molecular dynamics, neuroscience, plasmas, robotics, video processing, etc.

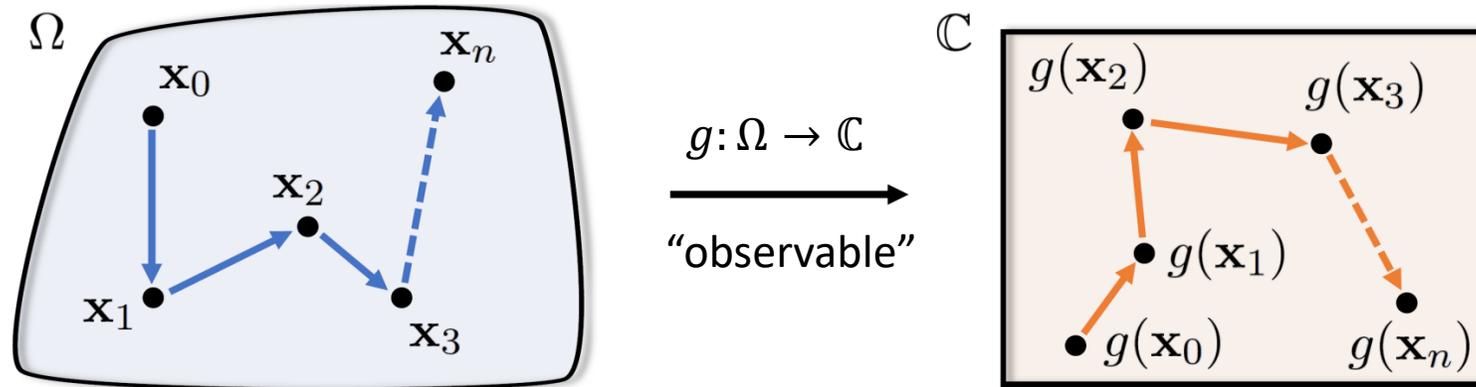


# Koopman Operator $\mathcal{K}$ : A global linearization



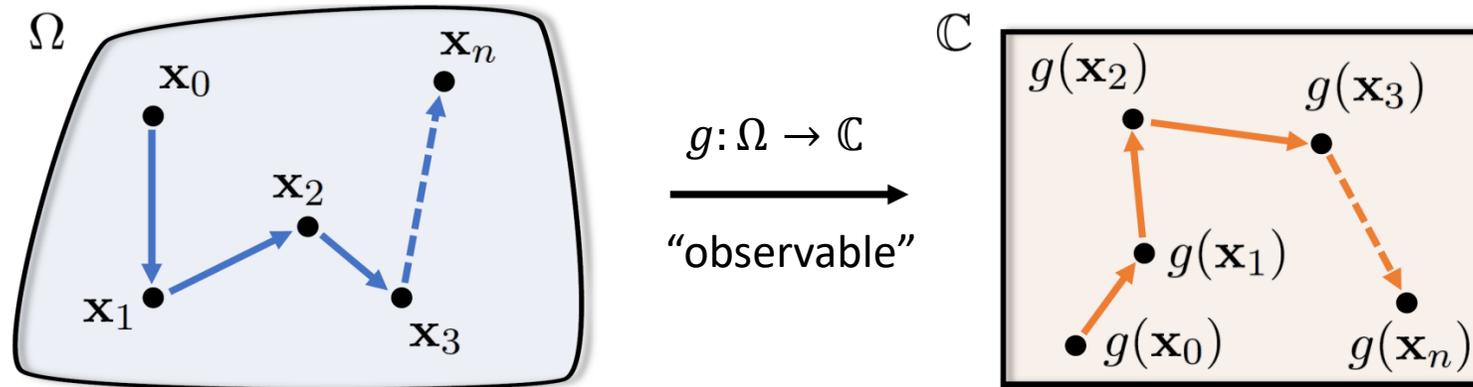
- Koopman, "Hamiltonian systems and transformation in Hilbert space," *Proc. Natl. Acad. Sci. USA*, 1931.
- Koopman, v. Neumann, "Dynamical systems of continuous spectra," *Proc. Natl. Acad. Sci. USA*, 1932.

# Koopman Operator $\mathcal{K}$ : A global linearization

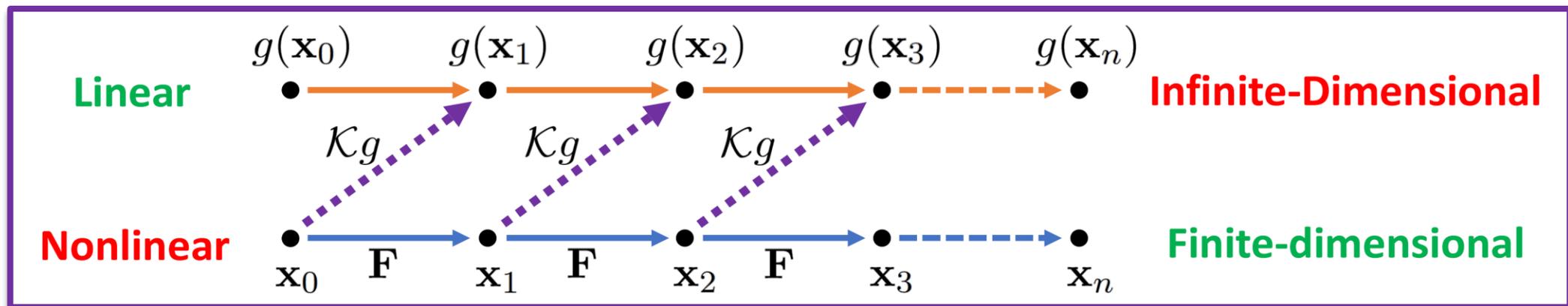


- $\mathcal{K}$  acts on functions  $g: \Omega \rightarrow \mathbb{C}$ ,  $[\mathcal{K}g](x) = g(F(x))$ .
- Function space:  $g \in L^2(\Omega, \omega)$ , positive measure  $\omega$ , inner product  $\langle \cdot, \cdot \rangle$ .

# Koopman Operator $\mathcal{K}$ : A global linearization

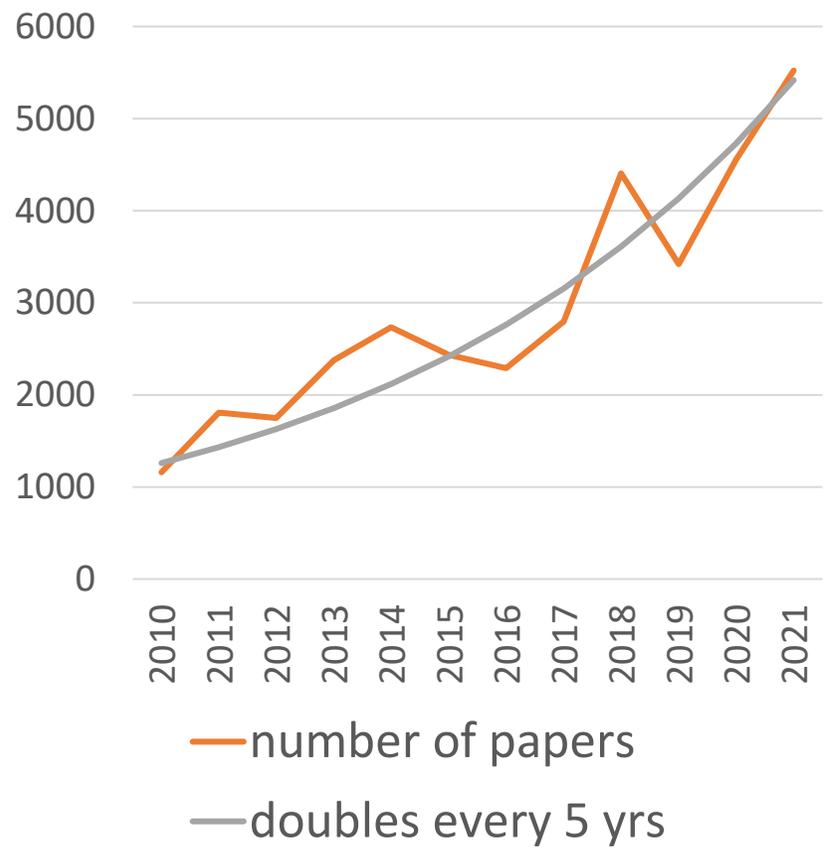


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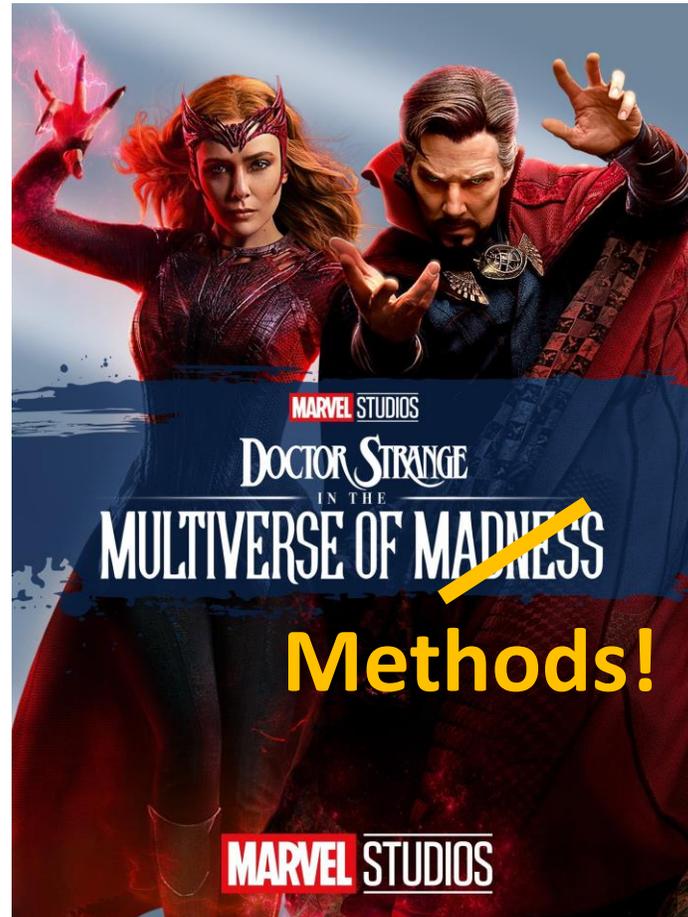
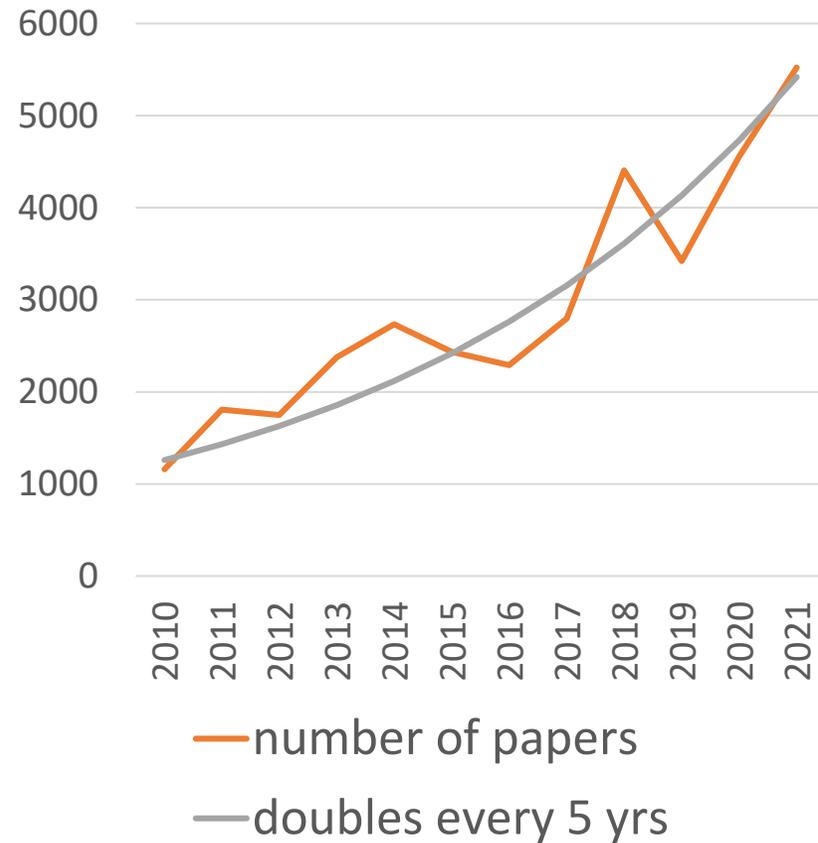


- Koopman, "Hamiltonian systems and transformation in Hilbert space," *Proc. Natl. Acad. Sci. USA*, 1931.
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## New Papers on “Koopman Operators”

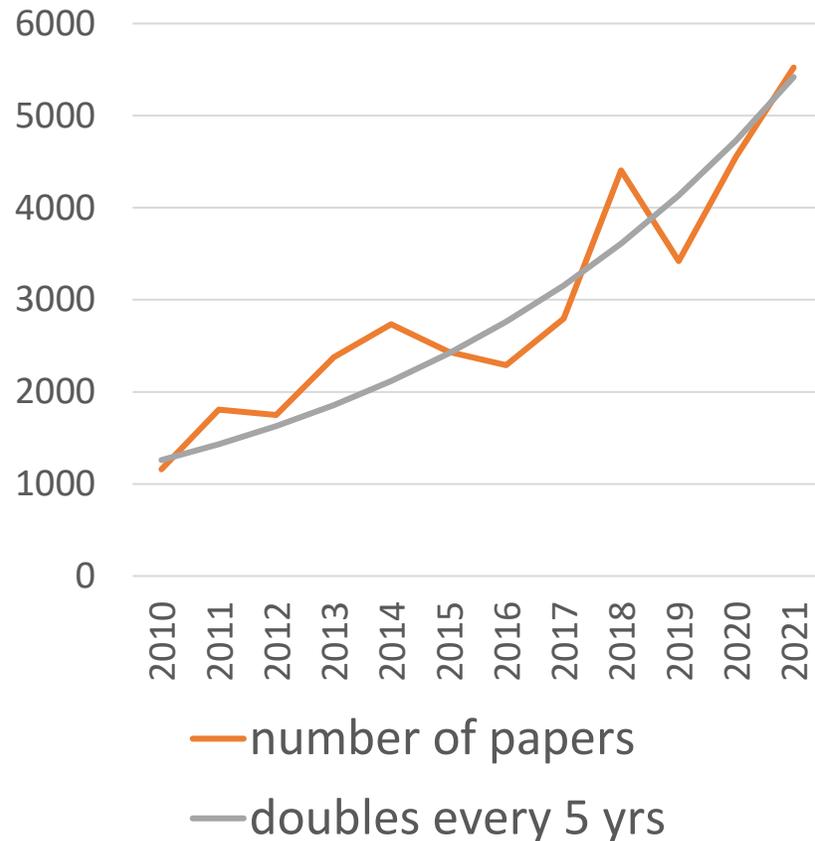


## New Papers on “Koopman Operators”



- C., “The Multiverse of Dynamic Mode Decomposition Algorithms,” **Handbook of Numerical Analysis, 2024.**

## New Papers on “Koopman Operators”



Koopman operators are  
classical in ergodic theory.



Graduate Texts  
in Mathematics

Peter Walters

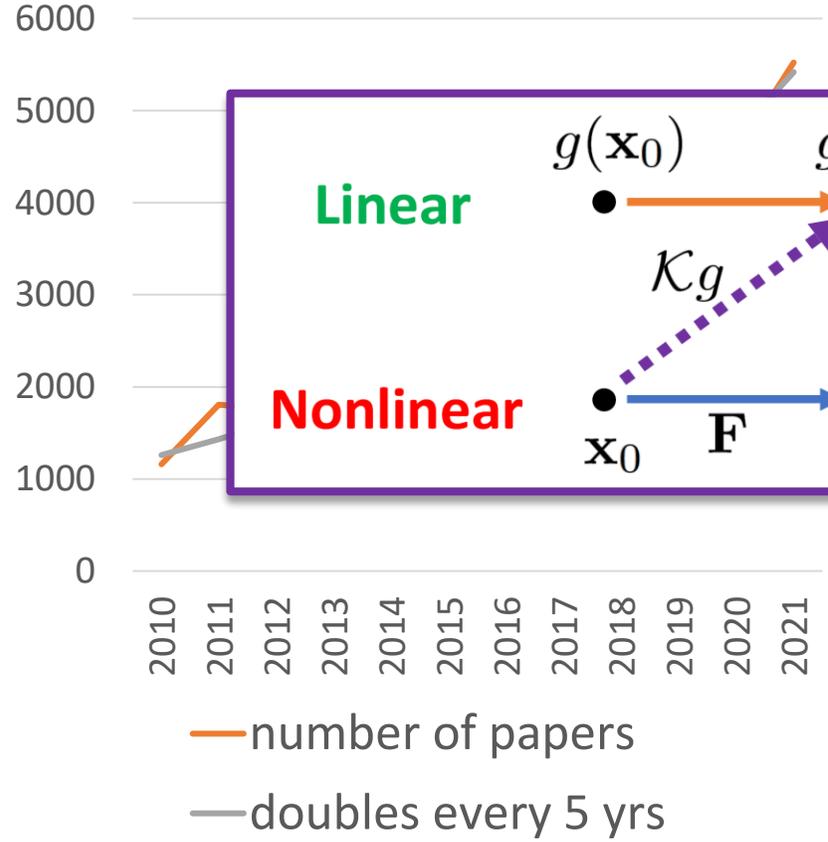
An Introduction  
to Ergodic Theory

Springer

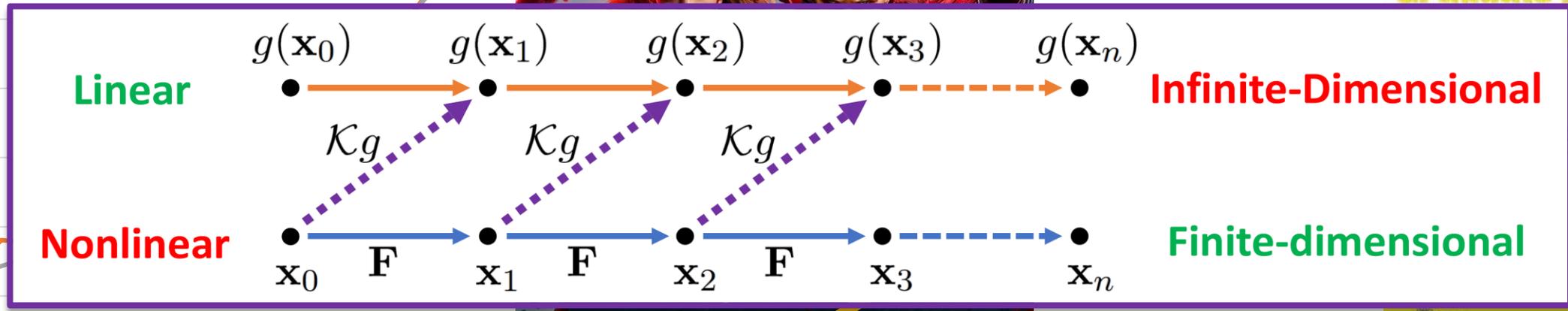
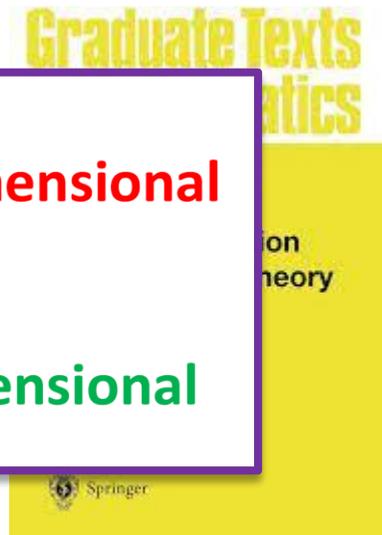
Why all this sudden interest?

- C., “The Multiverse of Dynamic Mode Decomposition Algorithms,” Handbook of Numerical Analysis, 2024.

### New Papers on "Koopman Operators"



Koopman operators are classical in ergodic theory.



## Methods!

Why all this sudden interest?  
 Data-driven  
 Deal with nonlinearity...

# Linear is much easier?

- Suppose  $\Omega = \mathbb{R}^d$ ,  $F(x) = Ax$ ,  $A \in \mathbb{R}^{d \times d}$ ,  $A = V\Lambda V^{-1}$ .

- Set  $\xi = V^{-1}x$ ,

$$\xi_n = V^{-1}x_n = V^{-1}A^n x_0 = \Lambda^n V^{-1}x_0 = \Lambda^n \xi_0$$

Trivial dynamics!



- For  $w^T A = \lambda w$ , set  $g(x) = w^T x$ ,

$$[\mathcal{K}g](x) = w^T Ax = \lambda g(x)$$

**Eigenfunction**

$$[\mathcal{K}g^n](x) = (w^T Ax)^n = \lambda^n g^n(x)$$

$$x_{n+1} = F(x_n)$$

$$[\mathcal{K}g](x) = g(F(x))$$

**Much more general (non-linear and even chaotic  $F$ ) ...**

# Koopman mode decomposition

$$x_{n+1} = F(x_n)$$

$$[\mathcal{K}g](x) = g(F(x))$$

$$g(x) = \sum_{\text{eigenvalues } \lambda_j} c_{\lambda_j} \varphi_{\lambda_j}(x) + \int_{-\pi}^{\pi} \phi_{\theta,g}(x) d\theta$$

eigenfunction of  $\mathcal{K}$       generalized eigenfunction of  $\mathcal{K}$

$$g(x_n) = [\mathcal{K}^n g](x_0) = \sum_{\text{eigenvalues } \lambda_j} c_{\lambda_j} \lambda_j^n \varphi_{\lambda_j}(x_0) + \int_{-\pi}^{\pi} e^{in\theta} \phi_{\theta,g}(x_0) d\theta$$

**Encodes:** geometric features, invariant measures, transient behavior, long-time behavior, coherent structures, quasiperiodicity, etc.

**GOAL:** Data-driven approximation of  $\mathcal{K}$  and its spectral properties.

# Our setting – unitary evolution

$$[\mathcal{K}g](x) = g(F(x)), \quad g \in L^2(\Omega, \omega)$$

$$g(x_n) = [\mathcal{K}^n g](x_0)$$

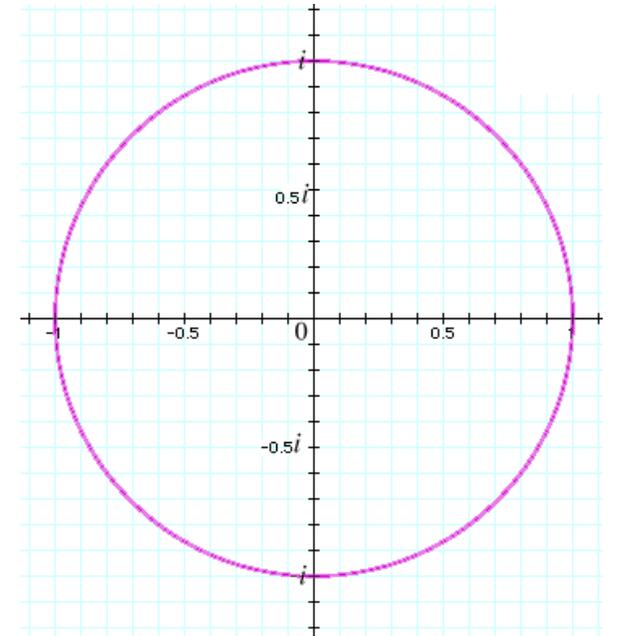
**Assume:** System is **measure-preserving** ( $F$  preserves  $\omega$ )

$$\Leftrightarrow \|\mathcal{K}g\| = \|g\| \text{ (isometry)}$$

$$\Leftrightarrow \mathcal{K}^* \mathcal{K} = I$$

$$\Rightarrow \text{Spec}(\mathcal{K}) \subseteq \{z: |z| \leq 1\}$$

(NB: consider unitary extensions of  $\mathcal{K}$  via Wold decomposition.)



Spectral measure  
(see later) on boundary

# Our setting – unitary evolution

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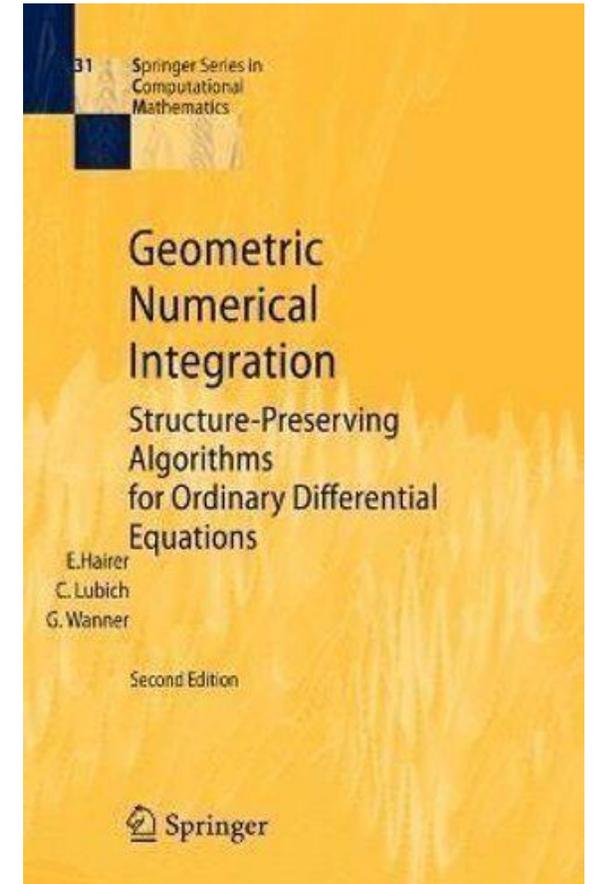
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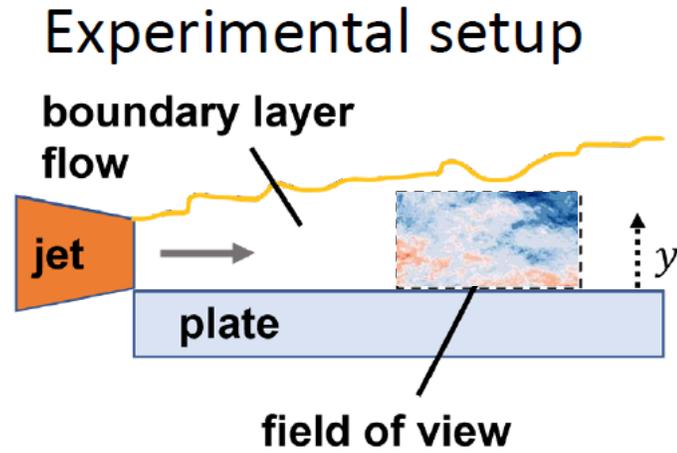
$$\Rightarrow \text{Spec}(\mathcal{K}) \subseteq \{z: |z| \leq 1\}$$

(NB: consider unitary extensions of  $\mathcal{K}$  via Wold decomposition.)

**WANT:** Approximation of  $\mathcal{K}$  that preserves  $\|\cdot\|$   
(e.g., stability, long-time behavior etc.)...



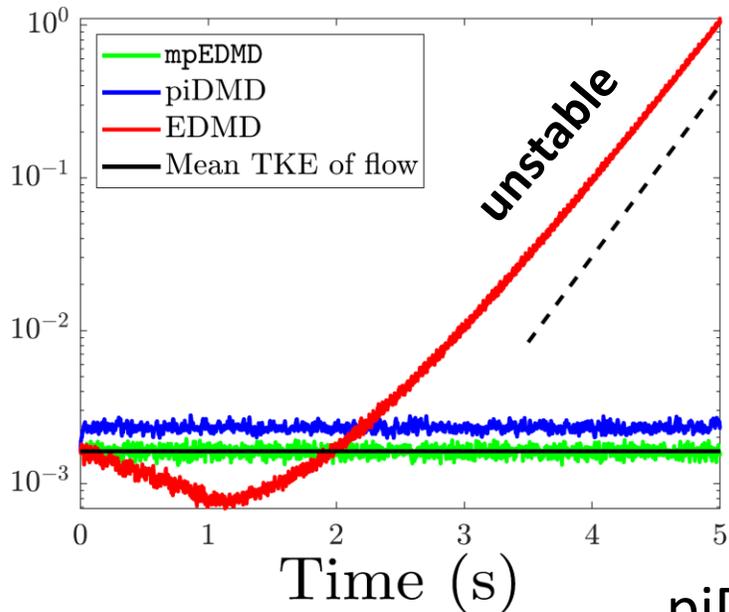
# Motivating example



- Reynolds number  $\approx 6.4 \times 10^4$
- Ambient dimension ( $d$ )  $\approx 100,000$  (velocity at measurement points)

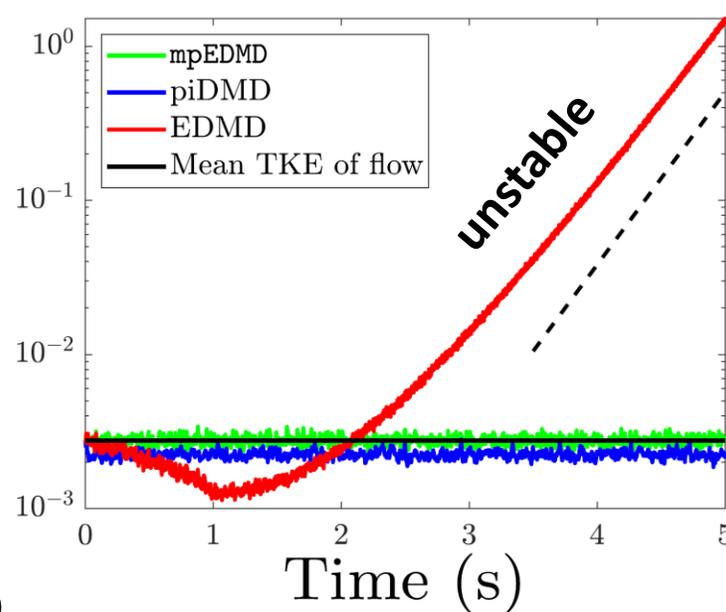
\*PIV data provided by Máté Szőke (Virginia Tech)

Turbulent K.E.  $y=5\text{mm}$



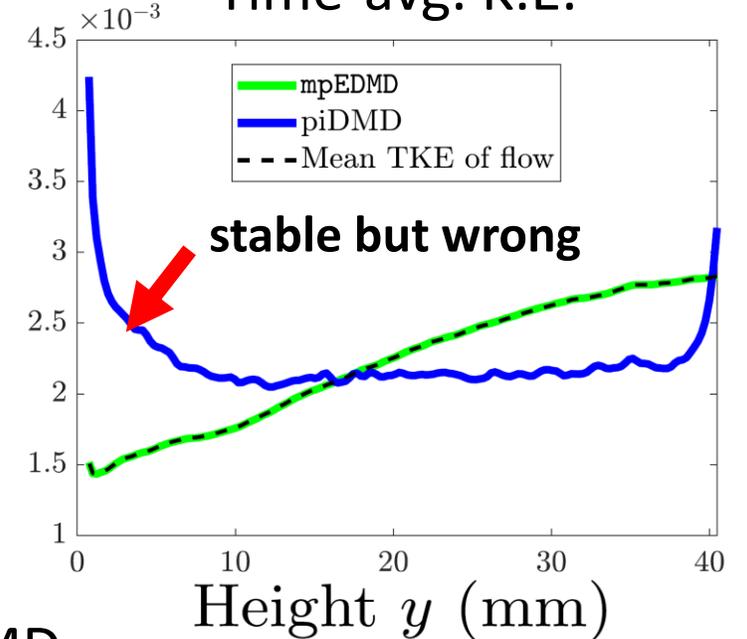
piDMD

Turbulent K.E.  $y=35\text{mm}$



EDMD

Time-avg. K.E.



• Baddoo, Herrmann, McKeon, Kutz, Brunton, "Physics-informed dynamic mode decomposition (piDMD)," preprint.

• Williams, Kevrekidis, Rowley "A data-driven approximation of the Koopman operator: Extending dynamic mode decomposition," *J. Nonlinear Sci.*, 2015.



# The most important slide

$$\begin{pmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & 0 & 1 \\ & & & 0 \end{pmatrix} \in \mathbb{C}^{N \times N}$$

polar  
decomposition



Circulant matrix

$$\begin{pmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & 0 & 1 \\ 1 & & & 0 \end{pmatrix} \in \mathbb{C}^{N \times N}$$

- Spectrum is  $\{0\}$ .
- Nilpotent evolution
- Spectrum is unstable.

- Spectrum converges to unit circle as  $N \rightarrow \infty$ .
- Unitary evolution.
- Spectrum is stable.

# The mpEDMD algorithm

# Extended Dynamic Mode Decomposition (EDMD)

Given dictionary  $\{\psi_1, \dots, \psi_N\}$  of functions  $\psi_j: \Omega \rightarrow \mathbb{C}$ ,

$$\{x^{(m)}, y^{(m)} = F(x^{(m)})\}_{m=1}^M$$

$$\langle \psi_k, \psi_j \rangle \approx \sum_{m=1}^M w_m \overline{\psi_j(x^{(m)})} \psi_k(x^{(m)}) = \left[ \underbrace{\begin{pmatrix} \psi_1(x^{(1)}) & \dots & \psi_N(x^{(1)}) \\ \vdots & \ddots & \vdots \\ \psi_1(x^{(M)}) & \dots & \psi_N(x^{(M)}) \end{pmatrix}}_{\Psi_X} \underbrace{\begin{pmatrix} w_1 & & \\ & \ddots & \\ & & w_M \end{pmatrix}}_W \underbrace{\begin{pmatrix} \psi_1(x^{(1)}) & \dots & \psi_N(x^{(1)}) \\ \vdots & \ddots & \vdots \\ \psi_1(x^{(M)}) & \dots & \psi_N(x^{(M)}) \end{pmatrix}}_{\Psi_X} \right]_{jk}$$

$$\langle \mathcal{K}\psi_k, \psi_j \rangle \approx \sum_{m=1}^M w_m \overline{\psi_j(x^{(m)})} \underbrace{\psi_k(y^{(m)})}_{[\mathcal{K}\psi_k](x^{(m)})} = \left[ \underbrace{\begin{pmatrix} \psi_1(x^{(1)}) & \dots & \psi_N(x^{(1)}) \\ \vdots & \ddots & \vdots \\ \psi_1(x^{(M)}) & \dots & \psi_N(x^{(M)}) \end{pmatrix}}_{\Psi_X} \underbrace{\begin{pmatrix} w_1 & & \\ & \ddots & \\ & & w_M \end{pmatrix}}_W \underbrace{\begin{pmatrix} \psi_1(y^{(1)}) & \dots & \psi_N(y^{(1)}) \\ \vdots & \ddots & \vdots \\ \psi_1(y^{(M)}) & \dots & \psi_N(y^{(M)}) \end{pmatrix}}_{\Psi_Y} \right]_{jk}$$

$$\mathcal{K} \longrightarrow \mathbb{K} = (\Psi_X^* W \Psi_X)^{-1} \Psi_X^* W \Psi_Y \in \mathbb{C}^{N \times N}$$

**Galerkin method!**

- Schmid, "Dynamic mode decomposition of numerical and experimental data," **J. Fluid Mech.**, 2010.
- Rowley, Mezić, Bagheri, Schlatter, Henningson, "Spectral analysis of nonlinear flows," **J. Fluid Mech.**, 2009.
- Kutz, Brunton, Brunton, Proctor, "Dynamic mode decomposition: data-driven modeling of complex systems," **SIAM**, 2016.
- Williams, Kevrekidis, Rowley "A data-driven approximation of the Koopman operator: Extending dynamic mode decomposition," **J. Nonlinear Sci.**, 2015.

feature map

## Least-squares route

$$\Psi(x) = [\psi_1(x) \quad \dots \quad \psi_N(x)], \quad g = \sum_{j=1}^N \mathbf{g}_j \psi_j = \Psi \mathbf{g} \in \text{span} \{\psi_1, \dots, \psi_N\}$$

$$\min_{\mathbb{K} \in \mathbb{C}^{N \times N}} \left\{ \int_{\Omega} \max_{\|\mathbf{g}\|_2=1} |[\mathcal{K}g](x) - \Psi(x)\mathbb{K}\mathbf{g}|^2 d\omega(x) = \int_{\Omega} \|\Psi(F(x)) - \Psi(x)\mathbb{K}\|_2^2 d\omega(x) \right\}$$

quadrature

$$\{x^{(m)}, y^{(m)} = F(x^{(m)})\}_{m=1}^M$$

$$\min_{\mathbb{K} \in \mathbb{C}^{N \times N}} \sum_{m=1}^M w_m \|\Psi(y^{(m)}) - \Psi(x^{(m)})\mathbb{K}\|_2^2$$

# A simple alteration

$$G = \Psi_X^* W \Psi_X, \quad G_{jk} \approx \langle \psi_k, \psi_j \rangle$$

Measure-preserving:  $\|\Psi \mathbf{g}\| = \|\Psi \mathbb{K} \mathbf{g}\|$ ,  $\|\Psi \mathbf{g}\|^2 \approx g^* G g$ ,  $\|\Psi \mathbb{K} \mathbf{g}\|^2 \approx g^* \mathbb{K}^* G \mathbb{K} g$

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$$\text{Enforce: } G = \mathbb{K}^* G \mathbb{K}$$

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$$G = \Psi_X^* W \Psi_X, \quad G_{jk} \approx \langle \psi_k, \psi_j \rangle$$

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Enforce:  $G = \mathbb{K}^* G \mathbb{K}$

quadrature

orthogonal  
Procrustes  
problem

$$\min_{\substack{\mathbb{K} \in \mathbb{C}^{N \times N} \\ G = \mathbb{K}^* G \mathbb{K}}} \sum_{m=1}^M w_m \left\| \Psi(\mathbf{y}^{(m)}) G^{-1/2} - \Psi(\mathbf{x}^{(m)}) \mathbb{K} G^{-1/2} \right\|_2^2$$

# The mpEDMD algorithm

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## Algorithm 4.1 The mpEDMD algorithm

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**Input:** Snapshot data  $\mathbf{X} \in \mathbb{C}^{d \times M}$  and  $\mathbf{Y} \in \mathbb{C}^{d \times M}$ , quadrature weights  $\{w_m\}_{m=1}^M$ , and a dictionary of functions  $\{\psi_j\}_{j=1}^N$ .

- 1: Compute the matrices  $\Psi_X$  and  $\Psi_Y$  and  $\mathbf{W} = \text{diag}(w_1, \dots, w_M)$ .
- 2: Compute an economy QR decomposition  $\mathbf{W}^{1/2} \Psi_X = \mathbf{Q}\mathbf{R}$ , where  $\mathbf{Q} \in \mathbb{C}^{M \times N}$ ,  $\mathbf{R} \in \mathbb{C}^{N \times N}$ .
- 3: Compute an SVD of  $(\mathbf{R}^{-1})^* \Psi_Y^* \mathbf{W}^{1/2} \mathbf{Q} = \mathbf{U}_1 \Sigma \mathbf{U}_2^*$ .
- 4: Compute the eigendecomposition  $\mathbf{U}_2 \mathbf{U}_1^* = \hat{\mathbf{V}} \Lambda \hat{\mathbf{V}}^*$  (via a Schur decomposition).
- 5: Compute  $\mathbb{K} = \mathbf{R}^{-1} \mathbf{U}_2 \mathbf{U}_1^* \mathbf{R}$  and  $\mathbf{V} = \mathbf{R}^{-1} \hat{\mathbf{V}}$ .

**Output:** Koopman matrix  $\mathbb{K}$  with eigenvectors  $\mathbf{V}$  and eigenvalues  $\Lambda$ .

---

$V_N = \text{span} \{\psi_1, \dots, \psi_N\}$   
 $\mathcal{P}_{V_N}: L^2(\Omega, \omega) \rightarrow V_N$   
 orthogonal projection

Some initial properties:

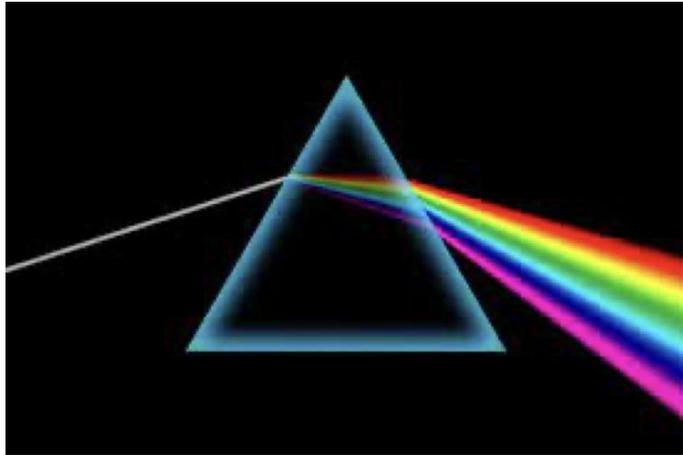
- As  $M \rightarrow \infty$ , EDMD:  $\mathcal{P}_{V_N} \mathcal{K} \mathcal{P}_{V_N}^*$ , mpEDMD: unitary part of polar decomp. of  $\mathcal{P}_{V_N} \mathcal{K} \mathcal{P}_{V_N}^*$ .
- Orthogonal Procrustes = constrained total least squares  $\implies$  better stability to noise!

# Convergence theory

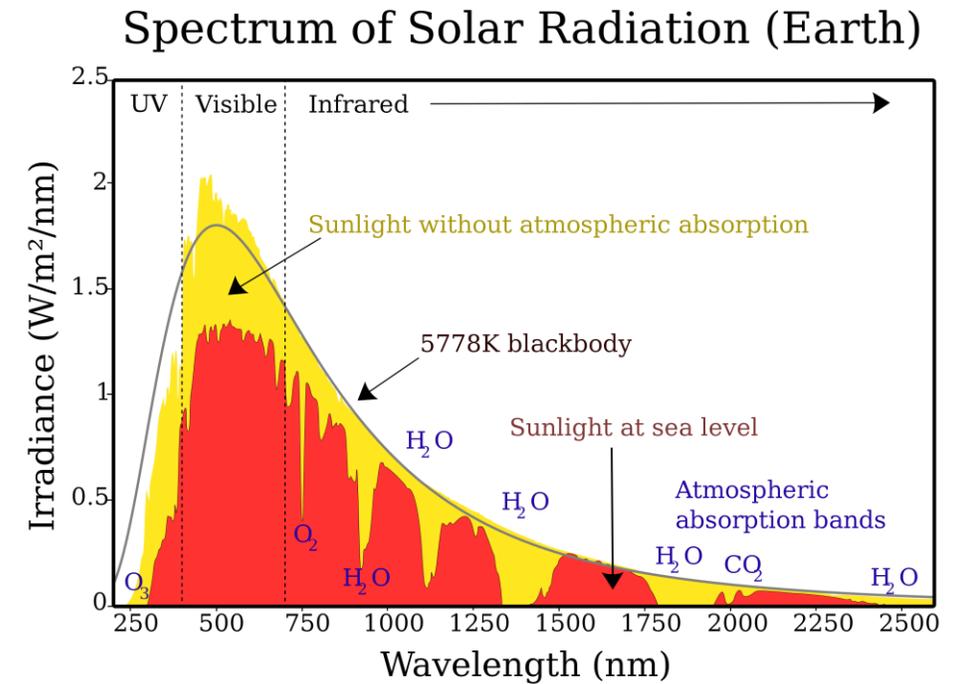
Key ingredient: unitary discretization.

# Spectral measures

White light contains a continuous spectra



Often interesting to look at the intensity of each wavelength



# Spectral measures $\rightarrow$ diagonalisation

- **Fin.-dim.:**  $B \in \mathbb{C}^{n \times n}$ ,  $B^*B = BB^*$ , orthonormal basis of e-vectors  $\{v_j\}_{j=1}^n$

$$v = \left[ \sum_{j=1}^n v_j v_j^* \right] v, \quad Bv = \left[ \sum_{j=1}^n \lambda_j v_j v_j^* \right] v, \quad \forall v \in \mathbb{C}^n$$

- **Inf.-dim.:** Normal Operator  $\mathcal{L}: \mathcal{D}(\mathcal{L}) \rightarrow \mathcal{H}$ . Typically, no basis of e-vectors!  
*Spectral theorem:* (projection-valued) spectral measure  $\mathcal{E}$

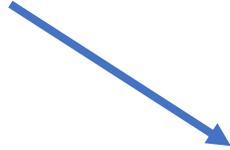
$$g = \left[ \int_{\text{Spec}(\mathcal{L})} 1 \, d\mathcal{E}(\lambda) \right] g, \quad \mathcal{L}g = \left[ \int_{\text{Spec}(\mathcal{L})} \lambda \, d\mathcal{E}(\lambda) \right] g, \quad \forall g \in \mathcal{H}$$

- **Spectral measures:**  $\mu_g(U) = \langle \mathcal{E}(U)g, g \rangle$  ( $\|g\| = 1$ ) probability measure.

# Simple way to understand spectral measures

moments

$\mu_g$  probability measures on  $\mathbb{T}$


$$\widehat{\mu}_g(n) = \frac{1}{2\pi} \int_{\mathbb{T}} \lambda^n d\mu_g(\lambda) = \frac{1}{2\pi} \langle \mathcal{K}^n g, g \rangle$$

$\lambda = \exp(i\theta)$  so Fourier coefficients in disguise.

Characterize forward-time dynamics and give back Koopman mode decomposition.

# Convergence of projection-valued measures

$$d\mathcal{E}_{N,M}(\lambda) = \sum_{j=1}^N v_j v_j^* G \delta(\lambda - \lambda_j) d\lambda$$

This assumption cannot be dropped in general!

**Theorem:** Suppose that the quadrature rule converges,  $\mathcal{K}$  is unitary,  $\lim_{N \rightarrow \infty} \text{dist}(h, V_N) = 0$  for any  $h \in L^2(\Omega, \omega)$ . Then for any continuous function  $\varphi: \mathbb{T} \rightarrow \mathbb{C}$ ,  $g \in L^2(\Omega, \omega)$  and  $\mathbf{g}_N \in \mathbb{C}^N$  with  $\lim_{N \rightarrow \infty} \|g - \Psi \mathbf{g}_N\| = 0$ ,

$$\lim_{N \rightarrow \infty} \limsup_{M \rightarrow \infty} \left\| \int_{\mathbb{T}} \varphi(\lambda) d\mathcal{E}(\lambda) g - \Psi \int_{\mathbb{T}} \varphi(\lambda) d\mathcal{E}_{N,M}(\lambda) \mathbf{g}_N \right\| = 0$$

$\mathbb{K}$ : mpEDMD matrix  
 $\lambda_j$ : eigenvalues of  $\mathbb{K}$   
 $v_j$ : eigenvectors of  $\mathbb{K}$   
 $V_N = \text{span} \{\psi_1, \dots, \psi_N\}$

Key ingredients:

- Strong convergence of Galerkin approximation.
- Polar decomposition  $\implies$  normal operators (allow Stone-Weierstrass).

# Convergence of scalar-valued measures

$$\mu_{\mathbf{g}}^{(N,M)}(U) = \mathbf{g}^* G \mathcal{E}_{N,M}(U) \mathbf{g} = \sum_{\lambda_j \in U} |\mathbf{v}_j^* G \mathbf{g}|^2$$

Captures weak convergence of measures

$$W_1(\mu, \nu) = \sup \left\{ \int_{\mathbb{T}} \varphi(\lambda) d(\mu - \nu)(\lambda) : \varphi \text{ Lipschitz } 1 \right\}$$

**Theorem:** Suppose quad. rule converges,  $\lim_{N \rightarrow \infty} \text{dist}(h, V_N) = 0$  for any  $h \in L^2(\Omega, \omega)$ . Then for  $g \in L^2(\Omega, \omega)$  and  $\mathbf{g}_N \in \mathbb{C}^N$  with  $\lim_{N \rightarrow \infty} \|g - \Psi \mathbf{g}_N\| = 0$ ,

$$\lim_{N \rightarrow \infty} \limsup_{M \rightarrow \infty} W_1(\mu_g, \mu_{\mathbf{g}}^{(N,M)}) = 0.$$

If  $V_N = \{g, \mathcal{K}g, \dots, \mathcal{K}^{N-1}g\}$  and  $g = \Psi \mathbf{g}$ , then

$$\limsup_{M \rightarrow \infty} W_1(\mu_g, \mu_{\mathbf{g}}^{(N,M)}) \lesssim \frac{\log(N)}{N}.$$

Matching autocorrelations!

$\mathbb{K}$ : mpEDMD matrix  
 $\lambda_j$ : eigenvalues of  $\mathbb{K}$   
 $\mathbf{v}_j$ : eigenvectors of  $\mathbb{K}$   
 $V_N = \text{span}\{\psi_1, \dots, \psi_N\}$

# Approximate all the spectrum

$$\text{Spec}_{\text{ap}}(\mathcal{K}) = \left\{ \lambda: \exists u_n, \|u_n\| = 1, \lim_{n \rightarrow \infty} \|(\mathcal{K} - \lambda)u_n\| = 0 \right\} = \text{Spec}(\mathcal{K}) \cap \mathbb{T}$$

(This is all the spectrum if  $\mathcal{K}$  unitary.)

**Theorem:** Suppose quad. rule converges,  $\lim_{N \rightarrow \infty} \text{dist}(h, V_N) = 0$  for any  $h \in L^2(\Omega, \omega)$ . Then

$$\lim_{N \rightarrow \infty} \limsup_{M \rightarrow \infty} \sup_{\lambda \in \text{Spec}_{\text{ap}}(\mathcal{K})} \text{dist}(\lambda, \text{Spec}(\mathbb{K})) = 0.$$

$\mathbb{K}$ : mpEDMD matrix

$\lambda_j$ : eigenvalues of  $\mathbb{K}$

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$V_N = \text{span} \{\psi_1, \dots, \psi_N\}$

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$$\lim_{N \rightarrow \infty} \limsup_{M \rightarrow \infty} \sup_{\lambda \in \text{Spec}_{\text{ap}}(\mathcal{K})} \text{dist}(\lambda, \text{Spec}(\mathbb{K})) = 0.$$

**Are there spurious eigenvalues?**

$\mathbb{K}$ : mpEDMD matrix

$\lambda_j$ : eigenvalues of  $\mathbb{K}$

$v_j$ : eigenvectors of  $\mathbb{K}$

$V_N = \text{span} \{\psi_1, \dots, \psi_N\}$

# Residuals $\Rightarrow$ avoid spurious eigenvalues!

$$G = \Psi_X^* W \Psi_X, A = \Psi_X^* W \Psi_Y$$

$$\begin{aligned} \|(\mathcal{K} - \lambda)\Psi \mathbf{g}\|^2 &= \langle (\mathcal{K} - \lambda)\Psi \mathbf{g}, (\mathcal{K} - \lambda)\Psi \mathbf{g} \rangle \\ &= \lim_{M \rightarrow \infty} \mathbf{g}^* \left[ (1 + |\lambda|^2)G - \bar{\lambda}A - \lambda A^* \right] \mathbf{g} \end{aligned} \quad \curvearrowright \quad \boxed{\mathcal{K}^* \mathcal{K} = I}$$

**Suitable conditions**  $\Rightarrow \lim_{N \rightarrow \infty} \min_{\mathbf{g} \in V_N} \|(\mathcal{K} - \lambda)\Psi \mathbf{g}\| / \|\mathbf{g}\| = \text{dist}(\lambda, \text{Spec}_{\text{ap}}(\mathcal{K}))$

## Two methods:

- Clean up procedure for tolerance  $\varepsilon$ .

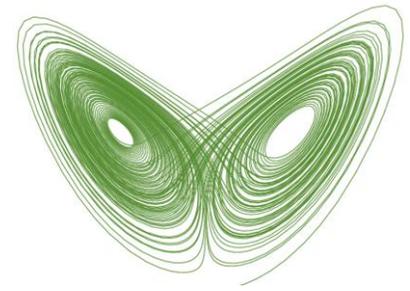
$$\boxed{\text{Spec}_{\text{ap}}(\mathcal{K}) = \left\{ \lambda: \exists u_n, \|u_n\| = 1, \lim_{n \rightarrow \infty} \|(\mathcal{K} - \lambda)u_n\| = 0 \right\}}$$

- Local minimization algorithm converges to  $\text{Spec}_{\text{ap}}(\mathcal{K})$ . Generalizes to general  $\mathcal{K}$ .

- 
- C., Townsend, "Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems," **CPAM**, 2024.
  - C., Ayton, Szóke, "Residual Dynamic Mode Decomposition," **J. Fluid Mech.**, 2023.

# Numerical examples

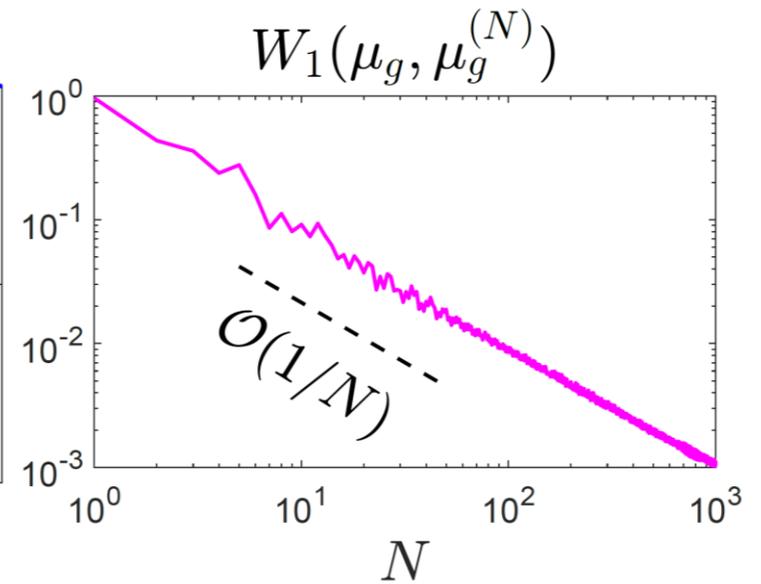
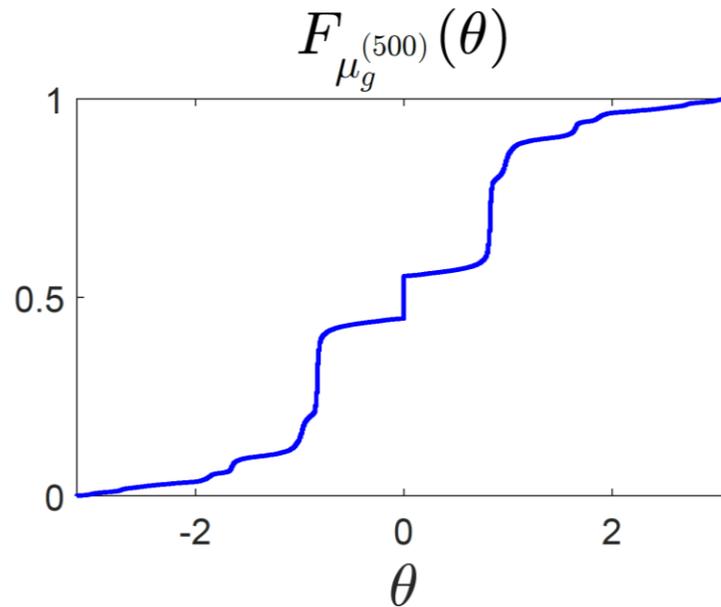
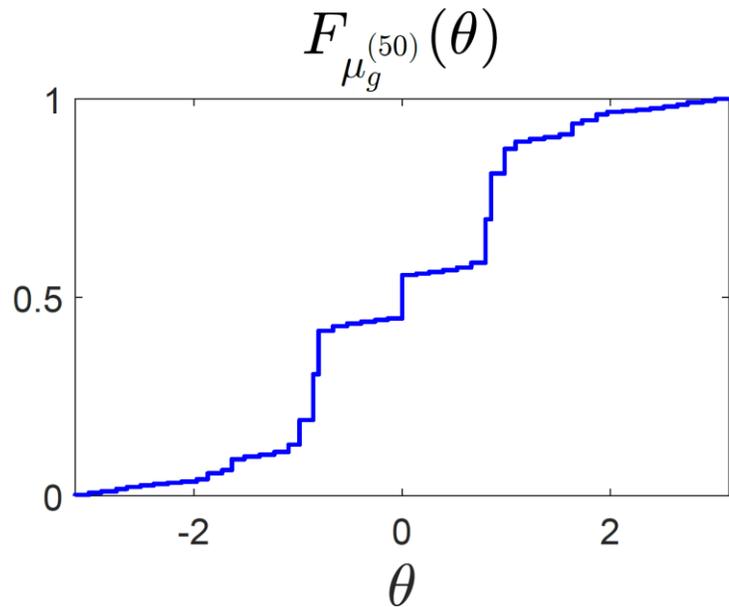
# Lorenz system



$$\dot{x}_1 = 10(x_2 - x_1), \quad \dot{x}_2 = x_1(28 - x_3) - x_2, \quad \dot{x}_3 = x_1x_2 - 8/3 x_3, \quad \Delta_t = 0.1$$

$$g(x_1, x_2, x_3) = c \tanh((x_1x_2 - 3x_3)/5), \quad V_N = \text{span}\{g, \mathcal{K}g, \dots, \mathcal{K}^{N-1}g\}$$

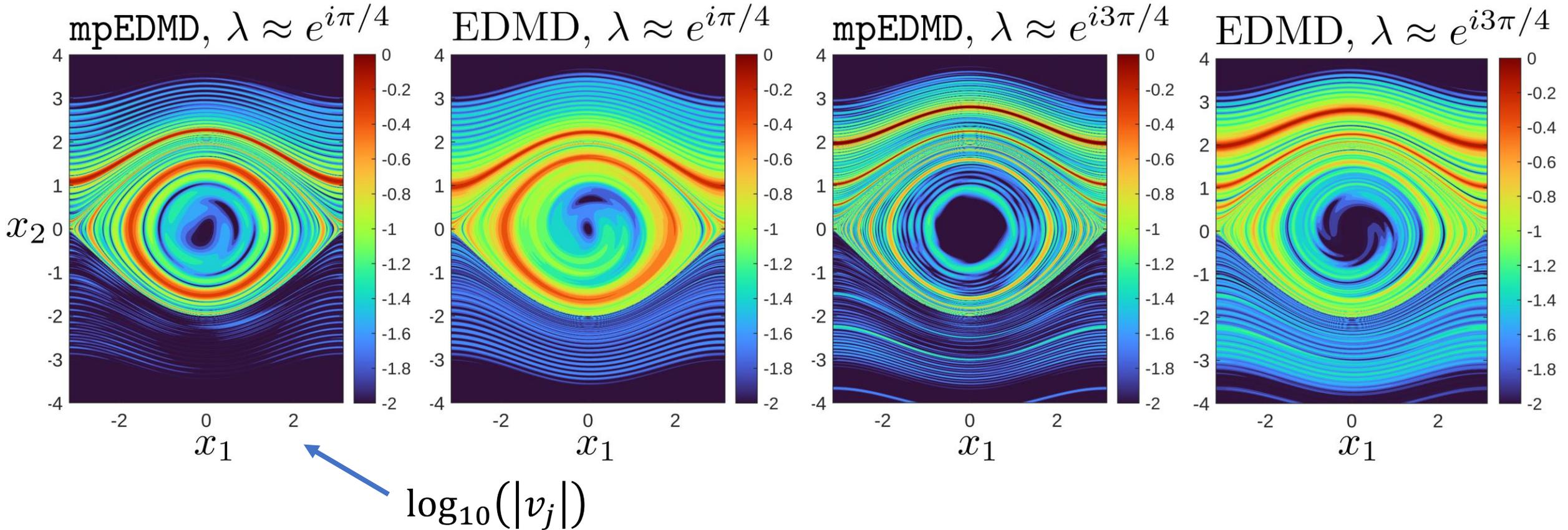
$$\text{Cdf: } F_\mu(\theta) = \mu(\{\exp(it) : -\pi \leq t \leq \theta\})$$



# Nonlinear pendulum

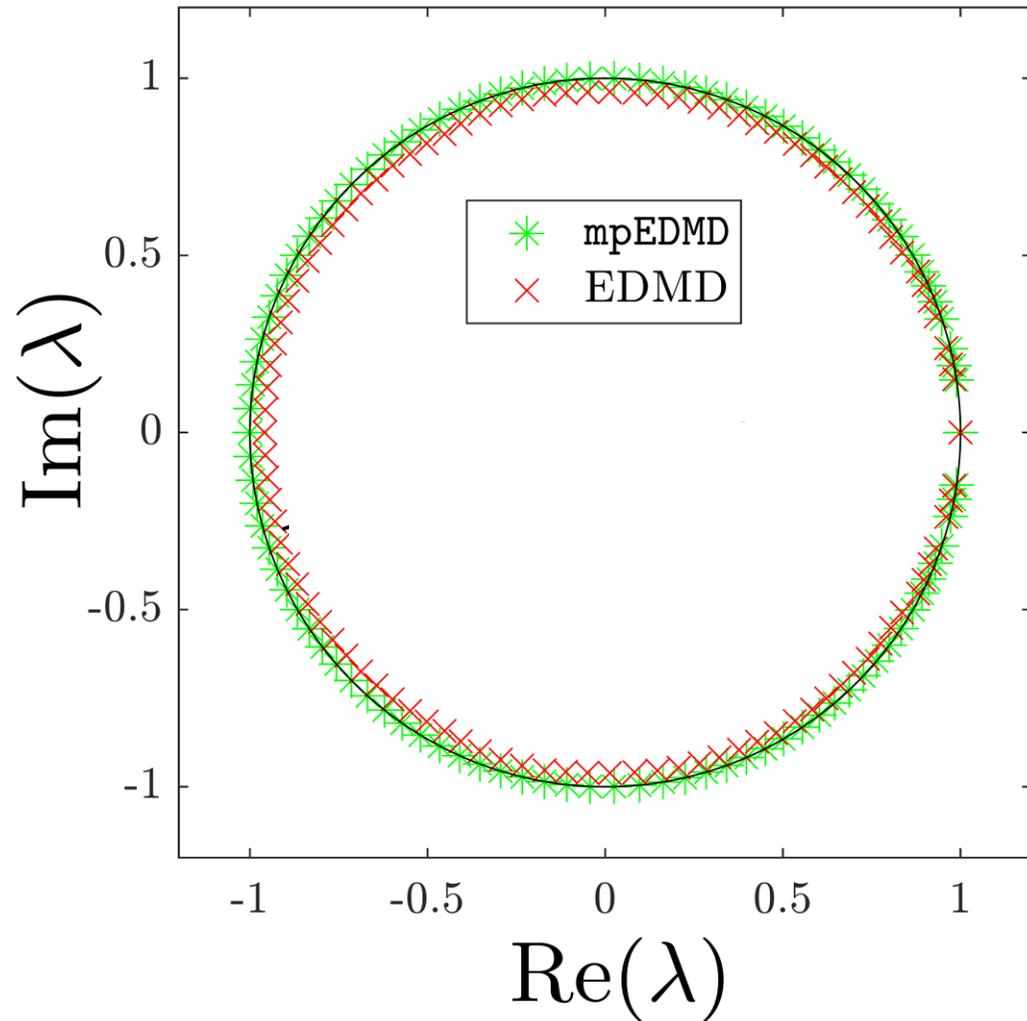
$$\dot{x}_1 = x_2, \quad \dot{x}_2 = -\sin(x_1), \quad \Omega = [-\pi, \pi]_{\text{per}} \times \mathbb{R}, \quad \Delta_t = 0.5$$

$$g(x) = \exp(ix_1) x_2 \exp(-x_2^2/2), \quad V_N = \text{span}\{g, \mathcal{K}g, \dots, \mathcal{K}^{99}g\}$$

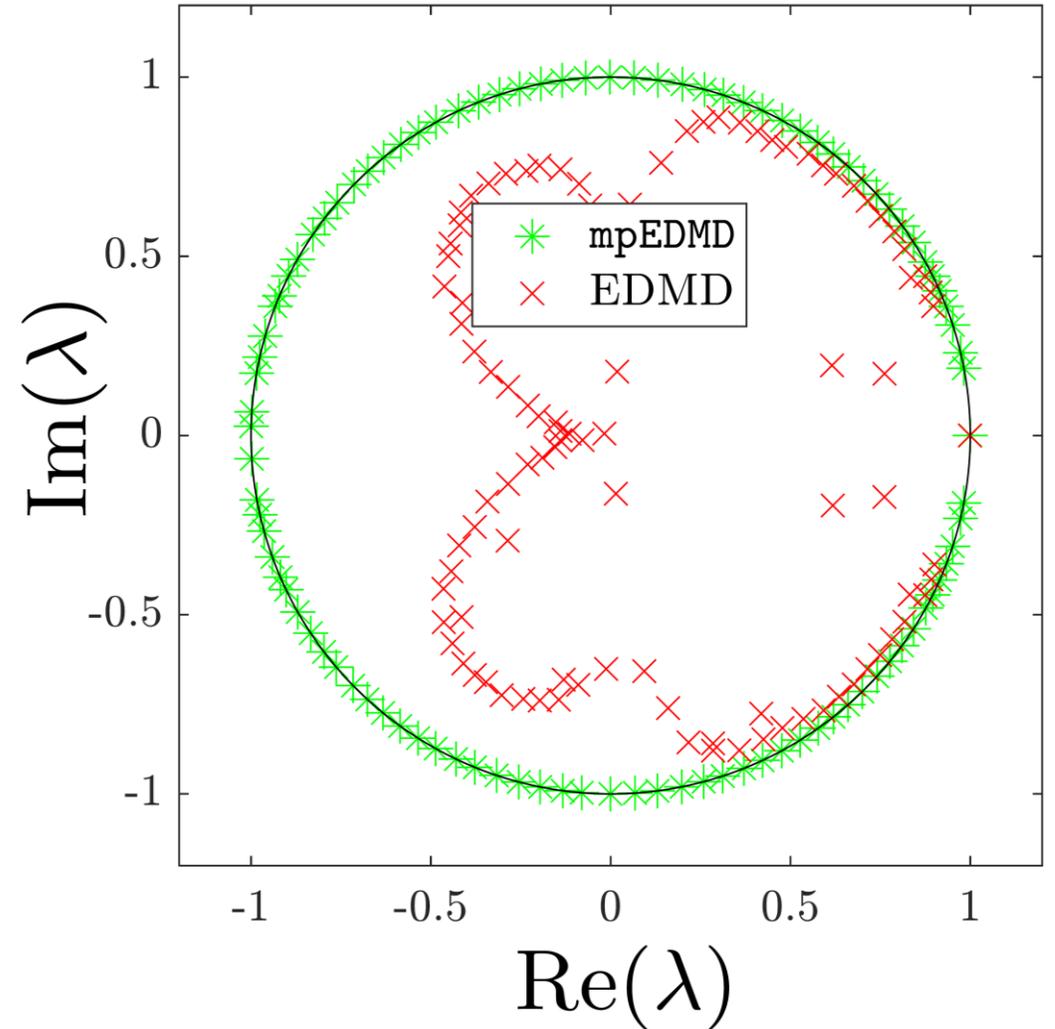


# Nonlinear pendulum

Noise free

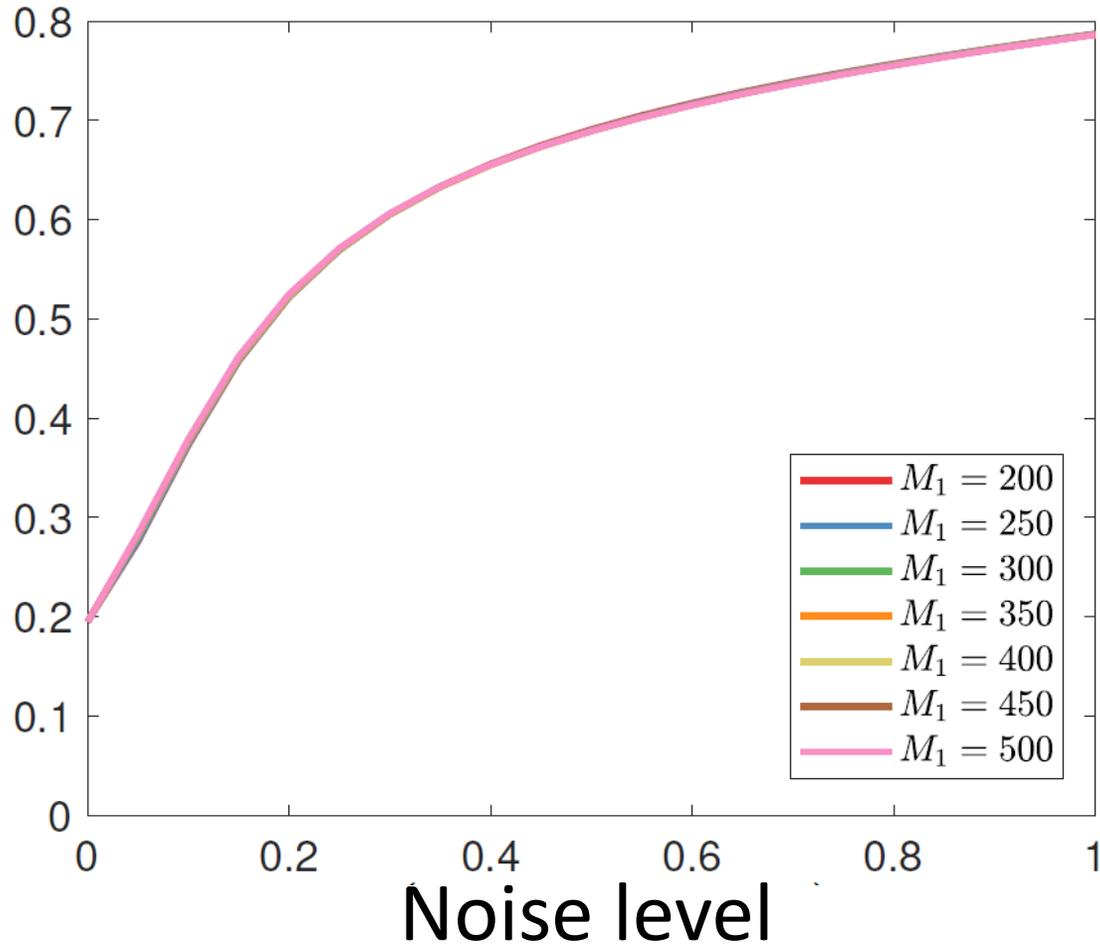


10% Gauss. noise for  $\Psi_X, \Psi_Y$

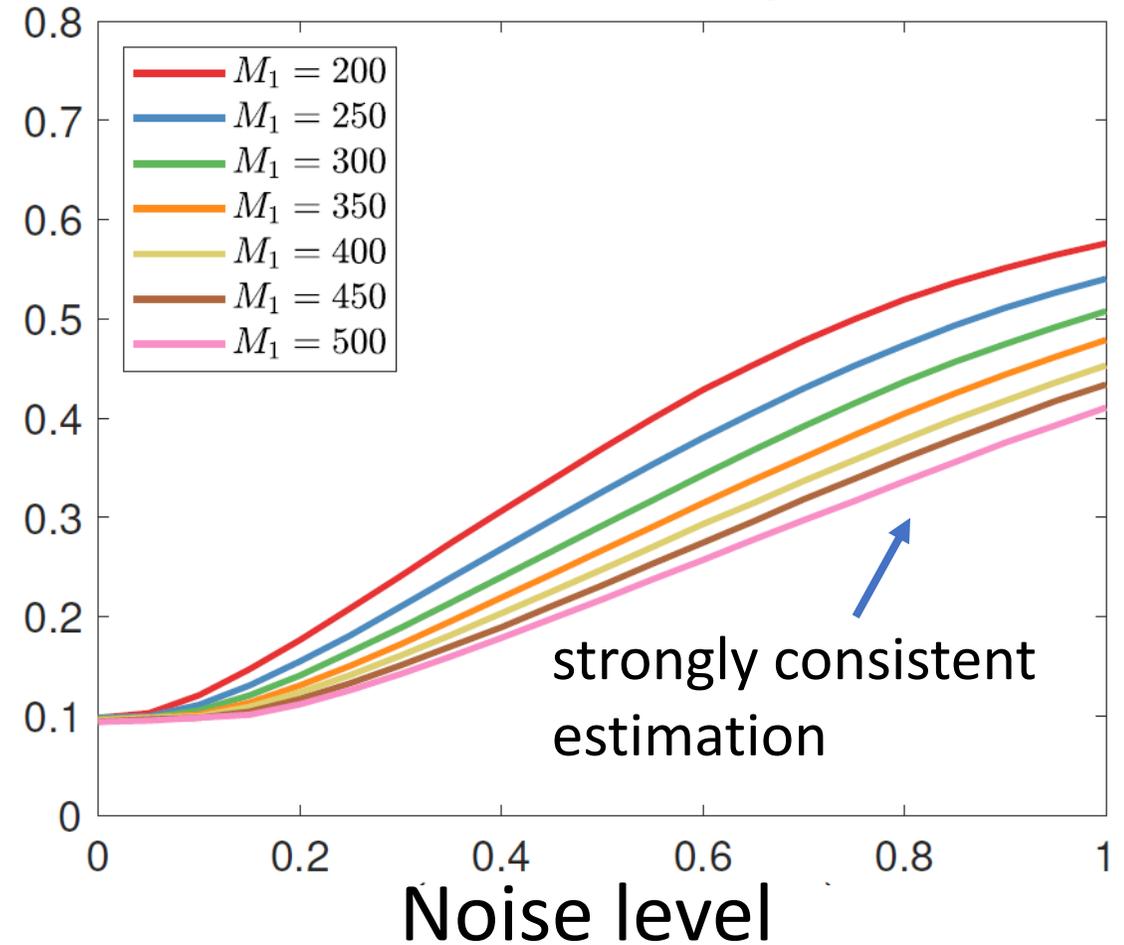


# Robustness to noise: Gauss. noise for $\Psi_X, \Psi_Y$

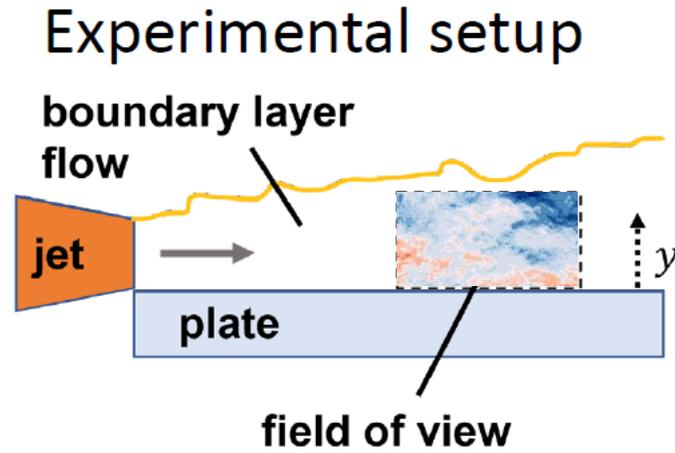
## Mean residual (EDMD)



## Mean residual (mpEDMD)



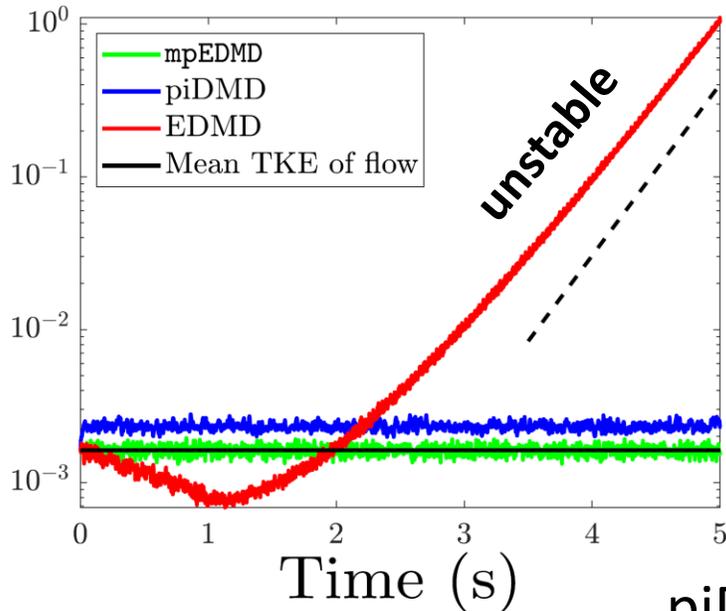
# Motivating example



- Reynolds number  $\approx 6.4 \times 10^4$
- Ambient dimension ( $d$ )  $\approx 100,000$  (velocity at measurement points)

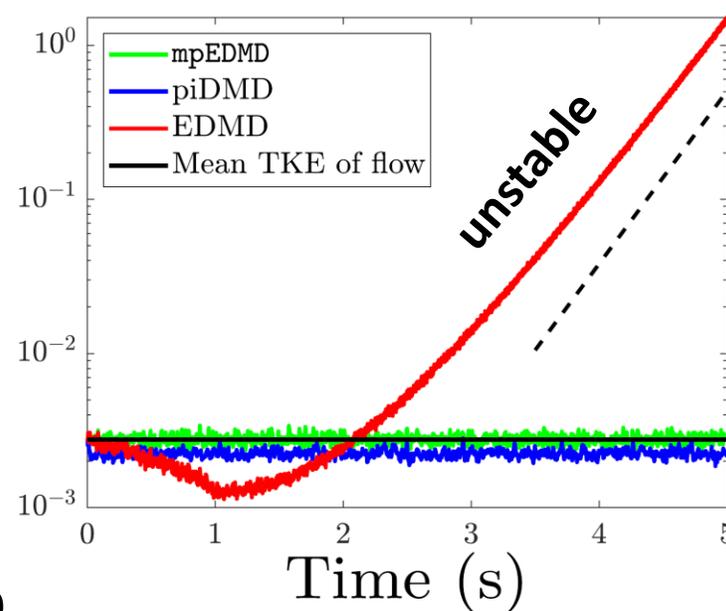
\*PIV data provided by Máté Szőke (Virginia Tech)

Turbulent K.E.  $y=5\text{mm}$



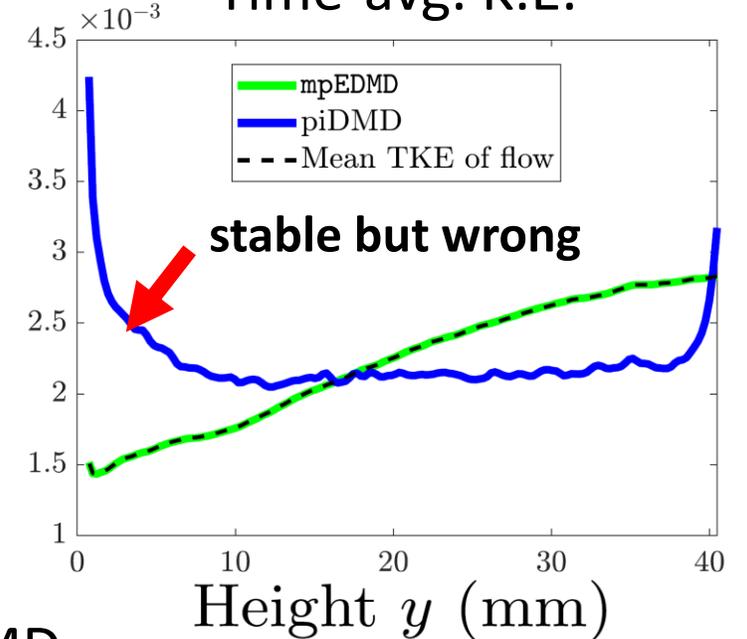
piDMD

Turbulent K.E.  $y=35\text{mm}$



EDMD

Time-avg. K.E.



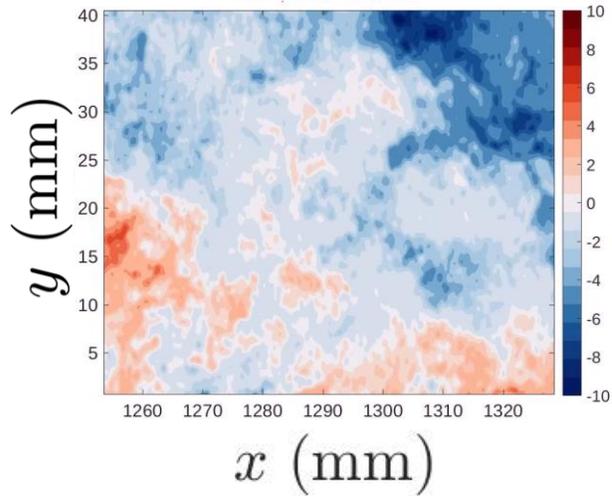
• Baddoo, Herrmann, McKeon, Kutz, Brunton, "Physics-informed dynamic mode decomposition (piDMD)," preprint.

• Williams, Kevrekidis, Rowley "A data-driven approximation of the Koopman operator: Extending dynamic mode decomposition," *J. Nonlinear Sci.*, 2015.

# Turbulence statistics

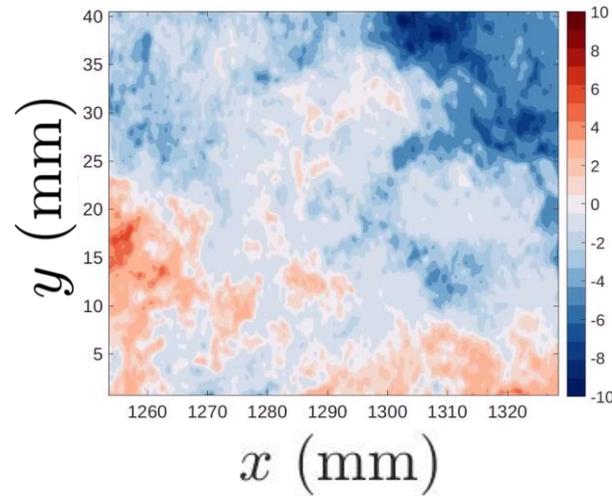
Flow

time=0.001000



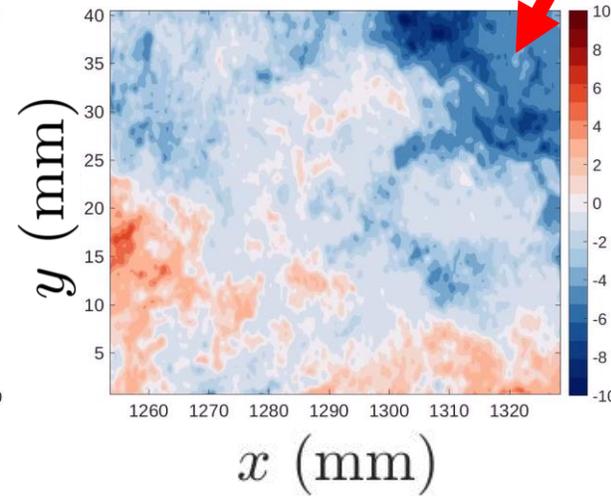
mpEDMD

time=0.001000



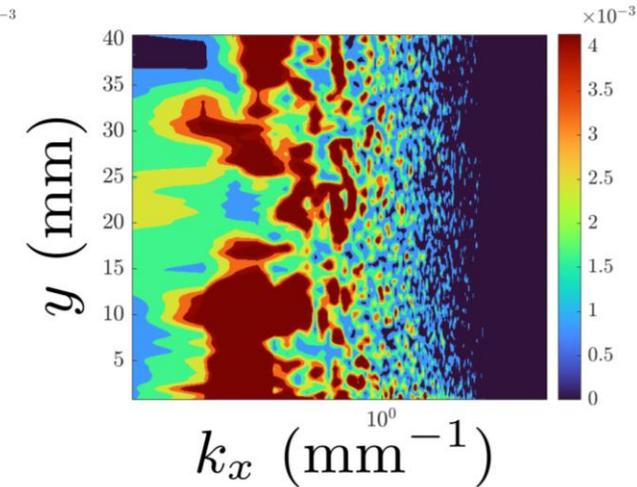
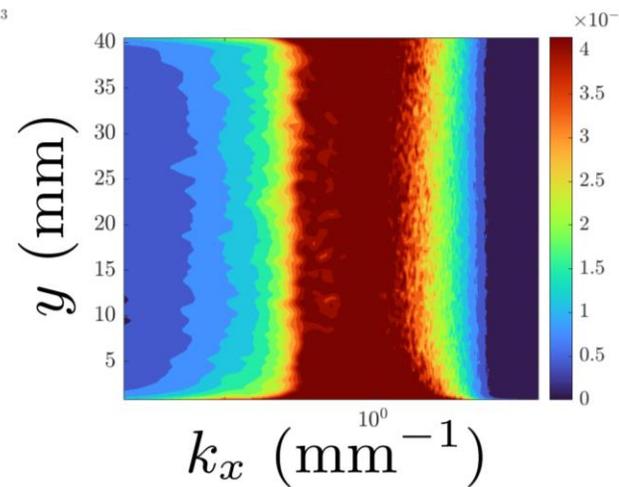
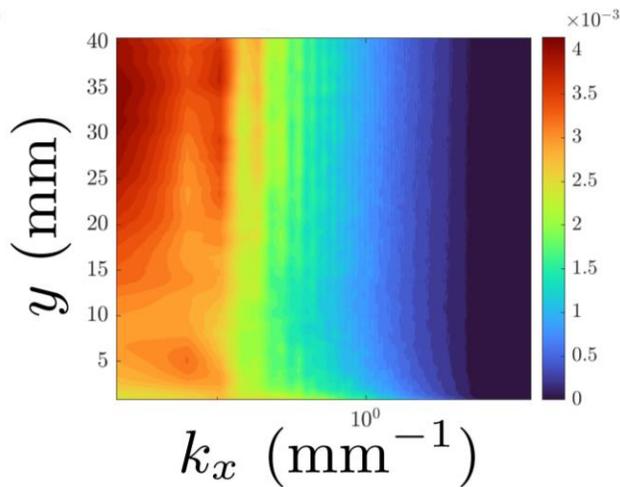
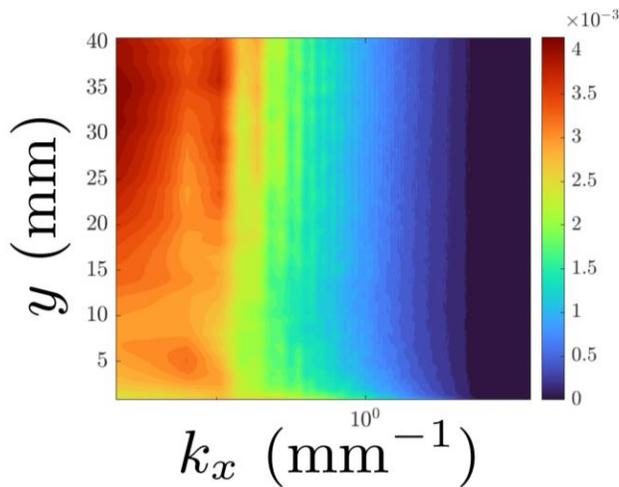
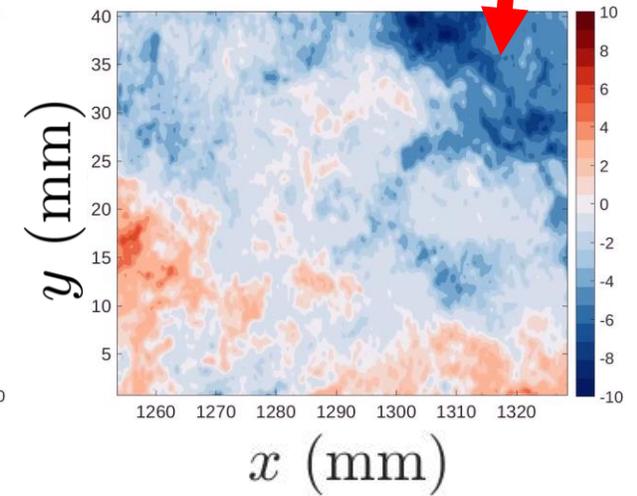
piDMD

time=0.001000



EDMD

time=0.001000



## Summary: *Polar decompositions + DMD*

- Convergence of spectral measures, spectra, Koopman mode decomposition.
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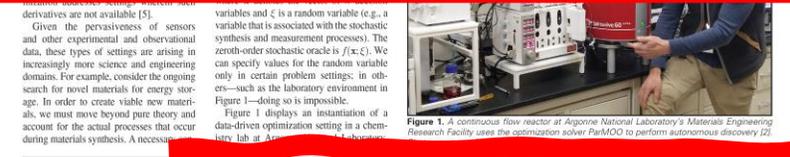
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*See Optimization on page 3*

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The classical, geometric way to analyze such systems—which dates back to the seminal work of Henri Poincaré—is based on the local analysis of fixed points, periodic orbits, stable or unstable manifolds, and so forth. Although Poincaré's framework has revolutionized our understanding of dynamical systems, this approach has at least two challenges in many modern applications: (i) Obtaining a global understanding of the nonlinear dynamics and (ii) handling systems that are either too complex to analyze or offer incomplete information about the evolution (i.e., unknown, high-dimensional, and highly nonlinear  $F$ ).

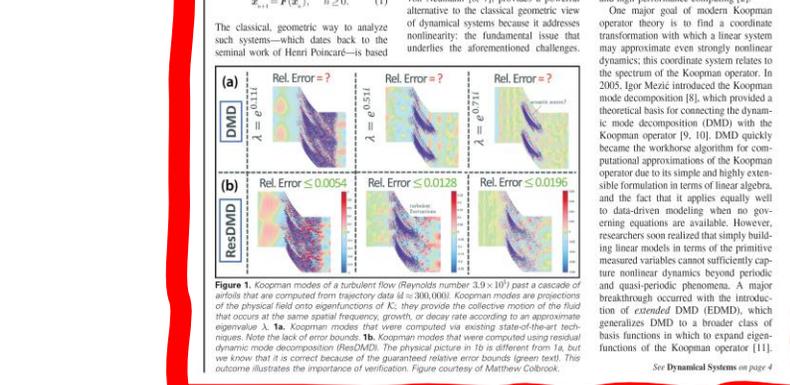
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We lift the nonlinear system (1) into an infinite-dimensional space of observable functions  $g: \Omega \rightarrow \mathbb{C}$  via a Koopman operator  $K$ :

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The evolution dynamics thus become linear, allowing us to utilize generic solution techniques that are based on spectral decompositions. In recent decades, Koopman operators have captivated researchers because of emerging data-driven and numerical implementations that coincide with the rise of machine learning and high-performance computing [2].

One major goal of modern Koopman operator theory is to find a coordinate transformation with which a linear system may approximate even strongly nonlinear dynamics; this coordinate system relates to the spectrum of the Koopman operator. In 2005, Igor Mezic introduced the Koopman mode decomposition [8], which provided a theoretical basis for connecting the dynamic mode decomposition (DMD) with the Koopman operator [9, 10]. DMD quickly became the workhorse algorithm for computational approximations of the Koopman operator due to its simple and highly extensible formulation in terms of linear algebra, and the fact that it applies equally well to data-driven modeling when no governing equations are available. However, researchers soon realized that simply building linear models in terms of the primitive measured variables cannot sufficiently capture nonlinear dynamics beyond periodic and quasi-periodic phenomena. A major breakthrough occurred with the introduction of *extended* DMD (EDMD), which generalizes DMD to a broader class of basis functions in which to expand eigenfunctions of the Koopman operator [11].

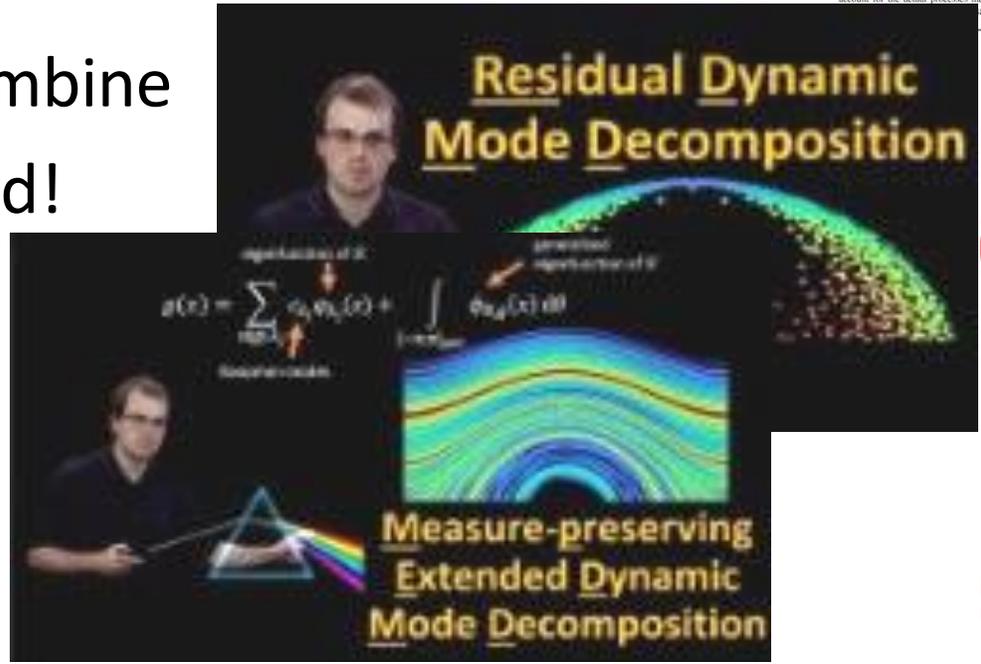


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Short video summaries available on YouTube



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We can compactly express this type of optimization problem as

$$\min_{\mathbf{x} \in \mathcal{B}_r} \mathbb{E}_\zeta [f(\mathbf{x}; \zeta)],$$

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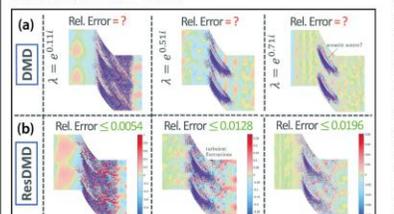


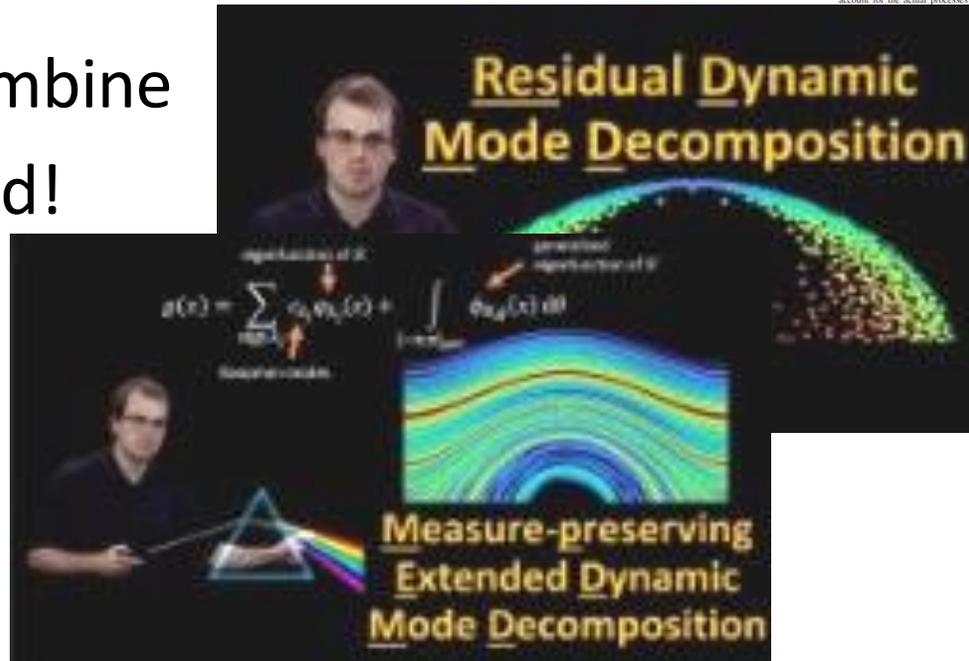
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See Dynamical Systems on page 4

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Ongoing: Further structure preserving Koopman methods



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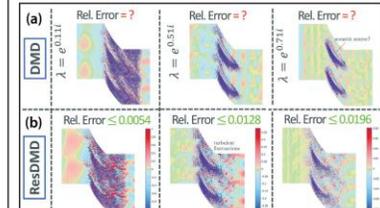


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