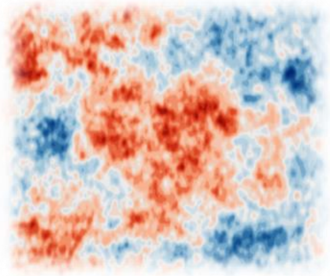
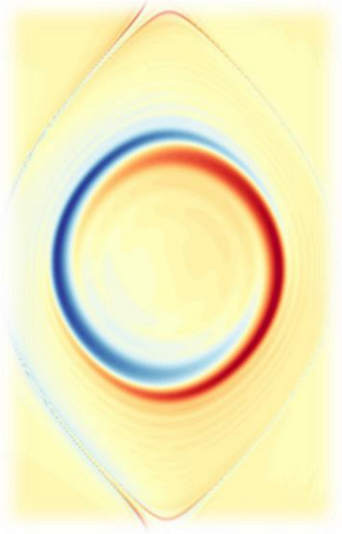
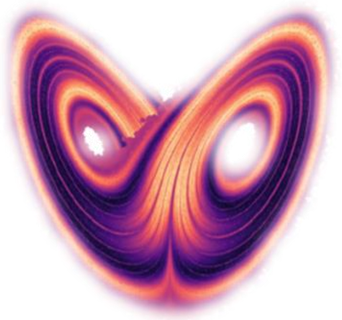






# Computing spectral properties of unitary Koopman Operators

Matthew Colbrook

University of Cambridge

10/06/2024

- C., Townsend, *“Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems”* **Communications on Pure and Applied Mathematics**, 2024.
- C., *"The mpEDMD Algorithm for Data-Driven Computations of Measure-Preserving Dynamical Systems,"* **SIAM Journal on Numerical Analysis**, 2023.
- C., Drysdale, Horning, *“Rigged Dynamic Mode Decomposition: Data-Driven Generalized Eigenfunction Decompositions for Koopman Operators”*, arxiv preprint.
- C., *“The Multiverse of Dynamic Mode Decomposition Algorithms,”* **Handbook of Numerical Analysis**, 2024.

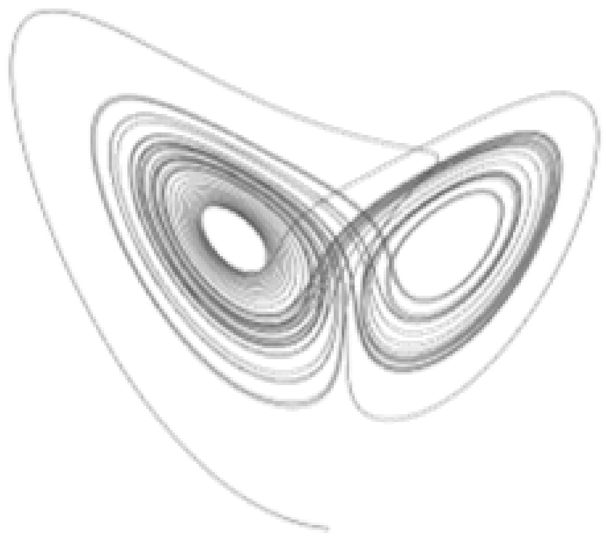
# Data-driven dynamical systems

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

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

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

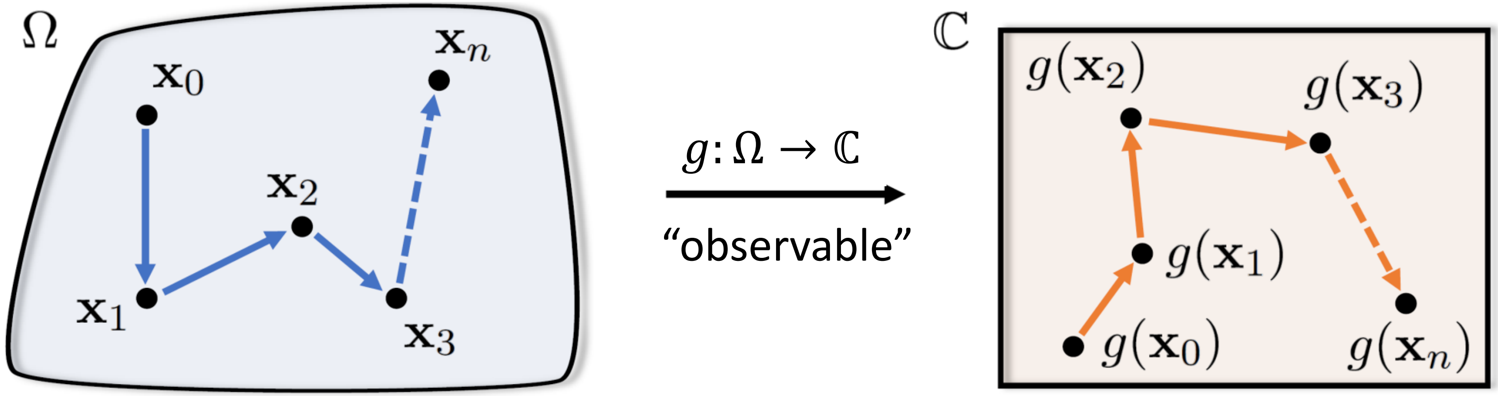
**Applications:** chemistry, climatology, control, electronics, epidemiology, finance, fluids, molecular dynamics, neuroscience, plasmas, robotics, video processing, etc.



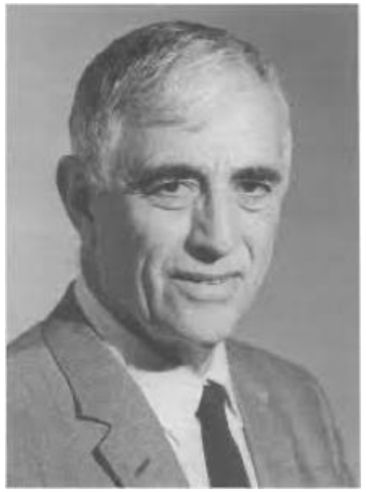
**Surveys:**


- Brunton, Budišić, Kaiser, Kutz, *"Modern Koopman theory for dynamical systems,"* SIAM Review, 2022.
- Budišić, Mohr, Mezić, *"Applied Koopmanism,"* Chaos, 2012.
- C., *"The Multiverse of Dynamic Mode Decomposition Algorithms,"* Handbook of Numerical Analysis, 2024.

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



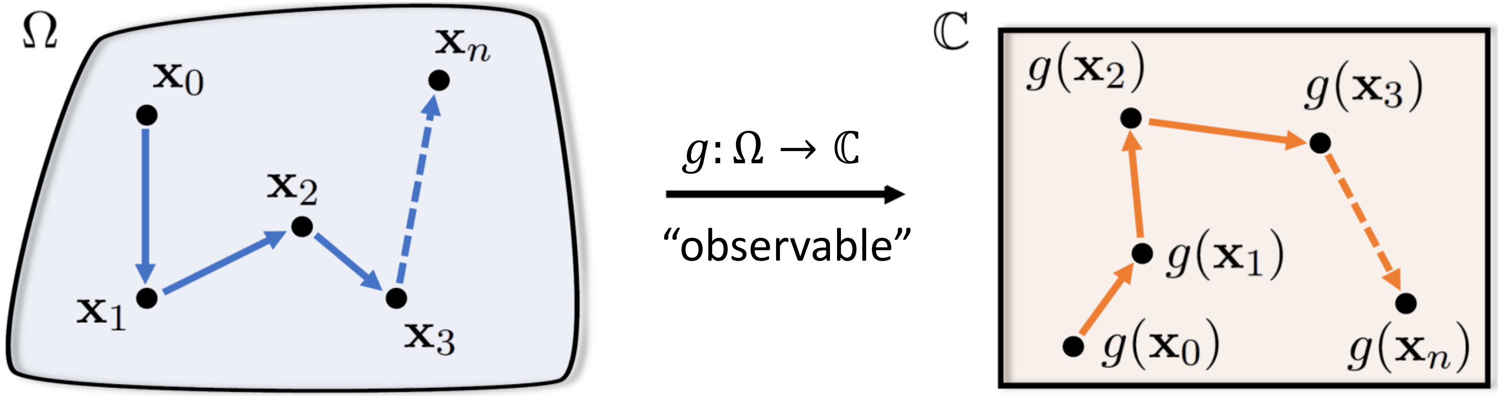

Koopman



von Neumann

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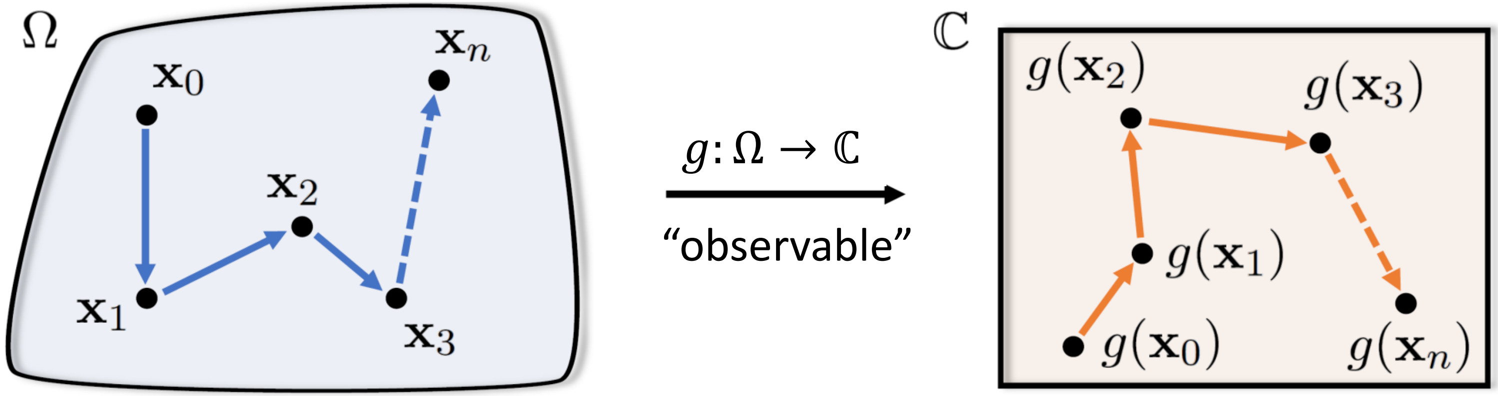


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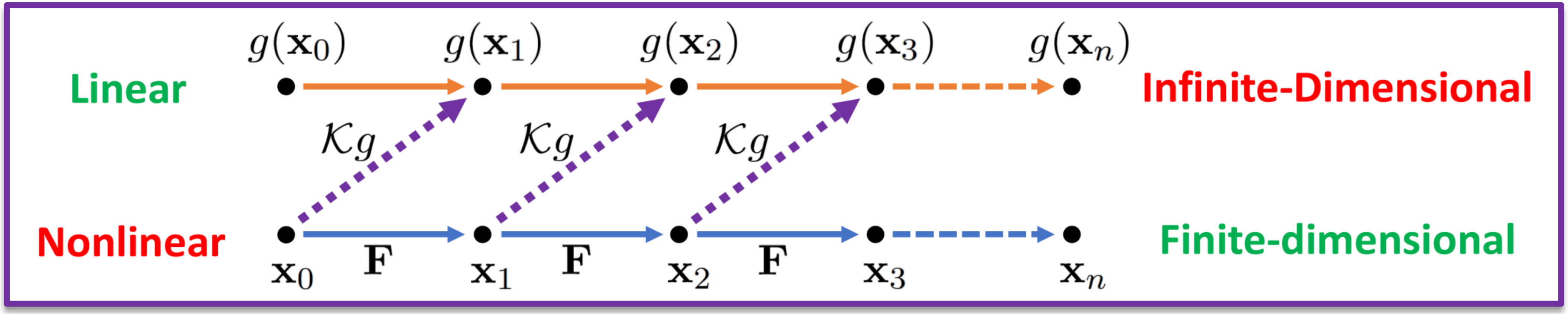



- Koopman, "*Hamiltonian systems and transformation in Hilbert space,*" **Proc. Natl. Acad. Sci. USA**, 1931.
- Koopman, v. Neumann, "*Dynamical systems of continuous spectra,*" **Proc. Natl. Acad. Sci. USA**, 1932.

# Koopman mode decomposition

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

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

eigenfunction of $\mathcal{K}$

continuous spectrum

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

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

**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.**


- Mezić, "*Spectral properties of dynamical systems, model reduction and decompositions,*" **Nonlinear Dynamics**, 2005.

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

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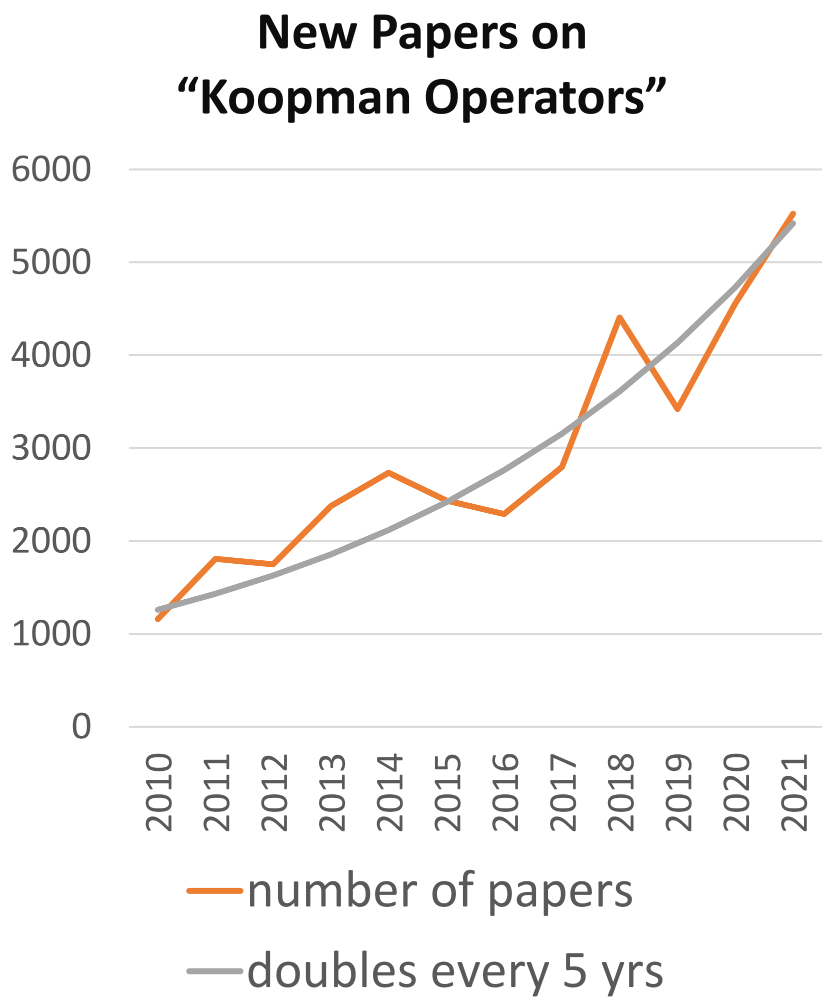
New Papers on
"Koopman Operators"
6000
5000
4000
3000
2000
1000
0
2010
2011
2012
2013
2014
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2019
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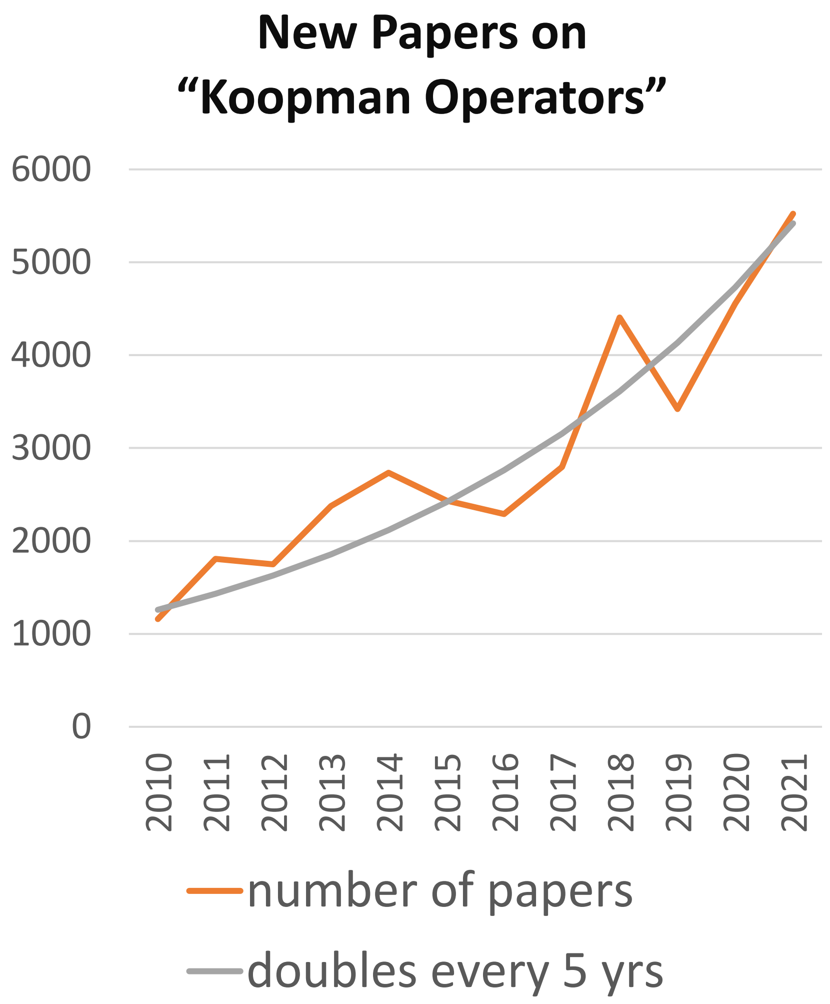
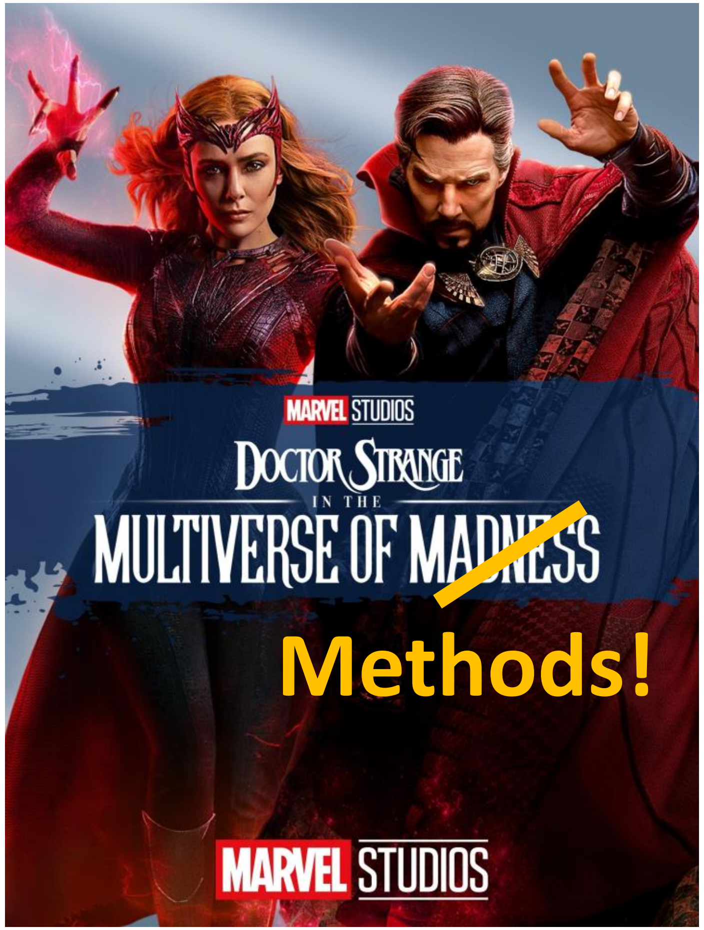
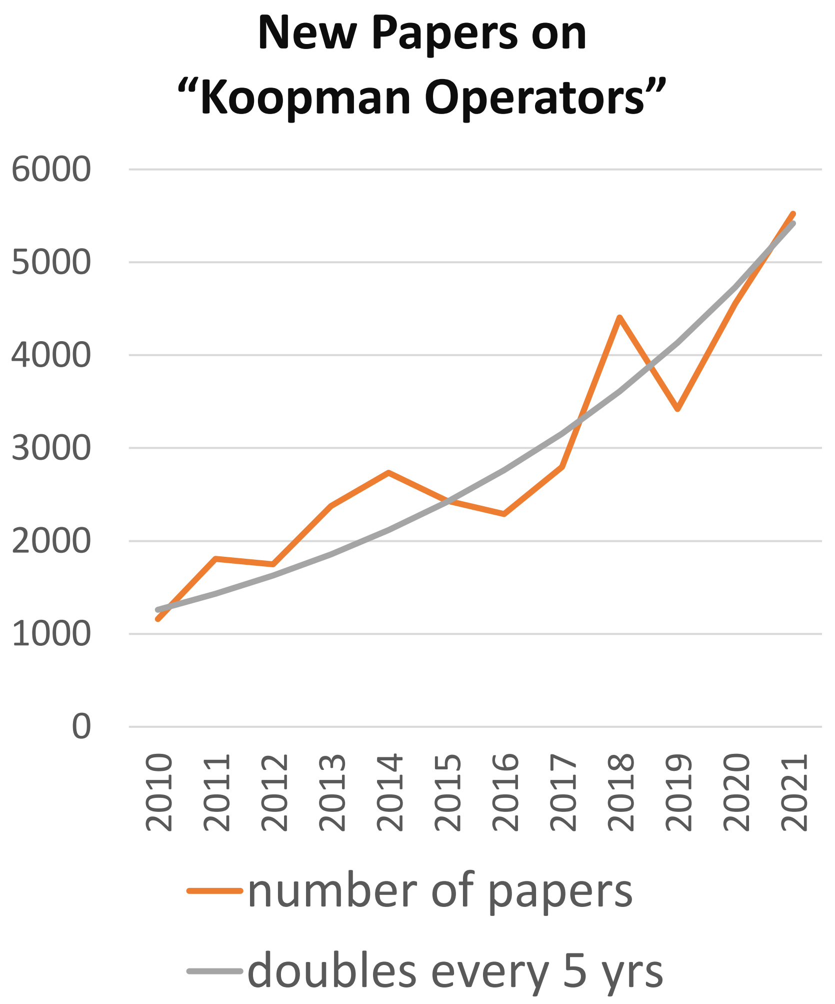
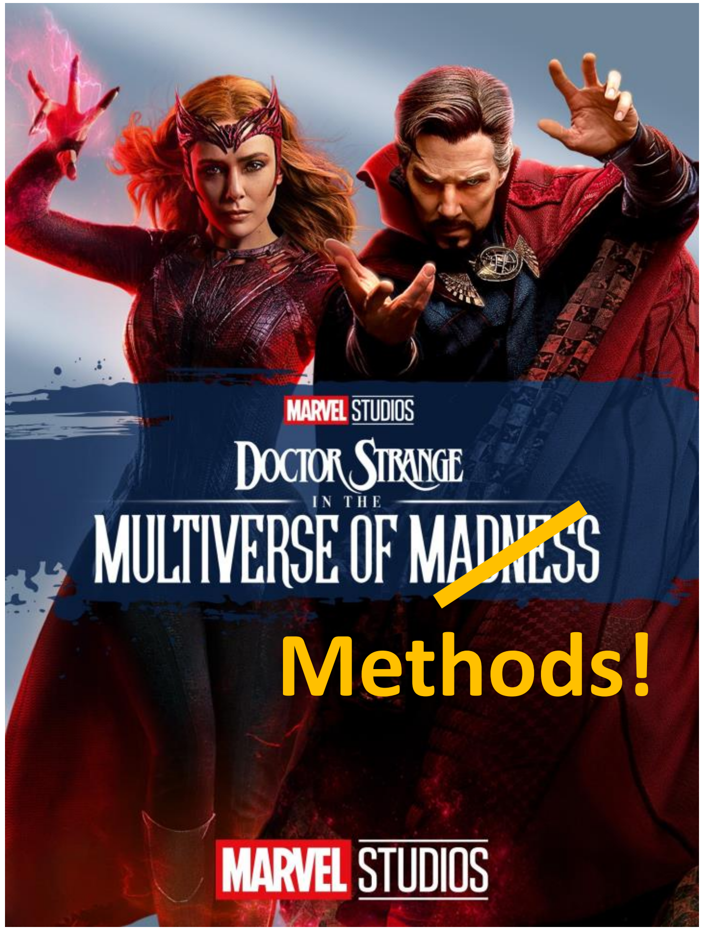
2021
number of papers
doubles every 5 yrs



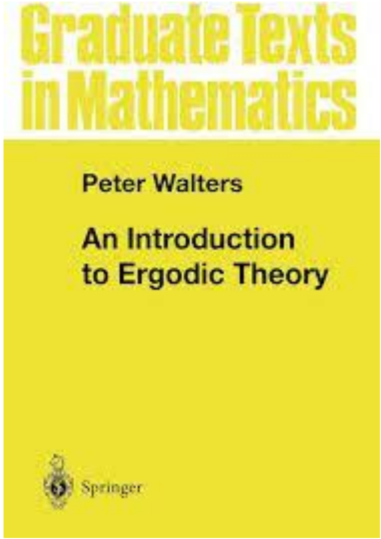




- C., *"The Multiverse of Dynamic Mode Decomposition Algorithms,"* **Handbook of Numerical Analysis**, 2024.



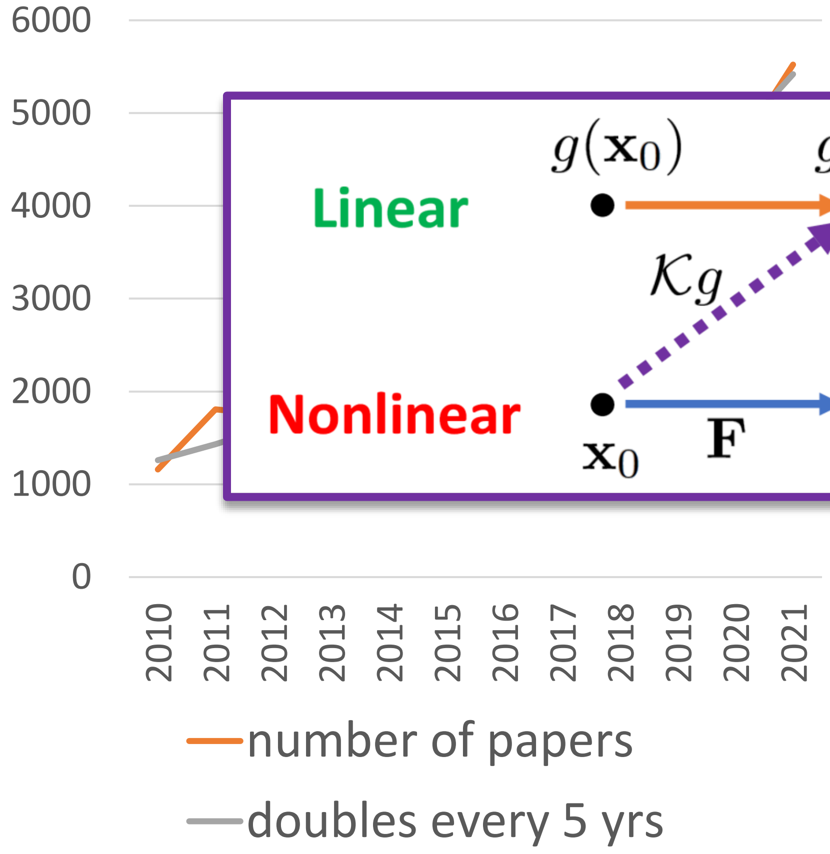

**Koopman operators are classical in ergodic theory.**

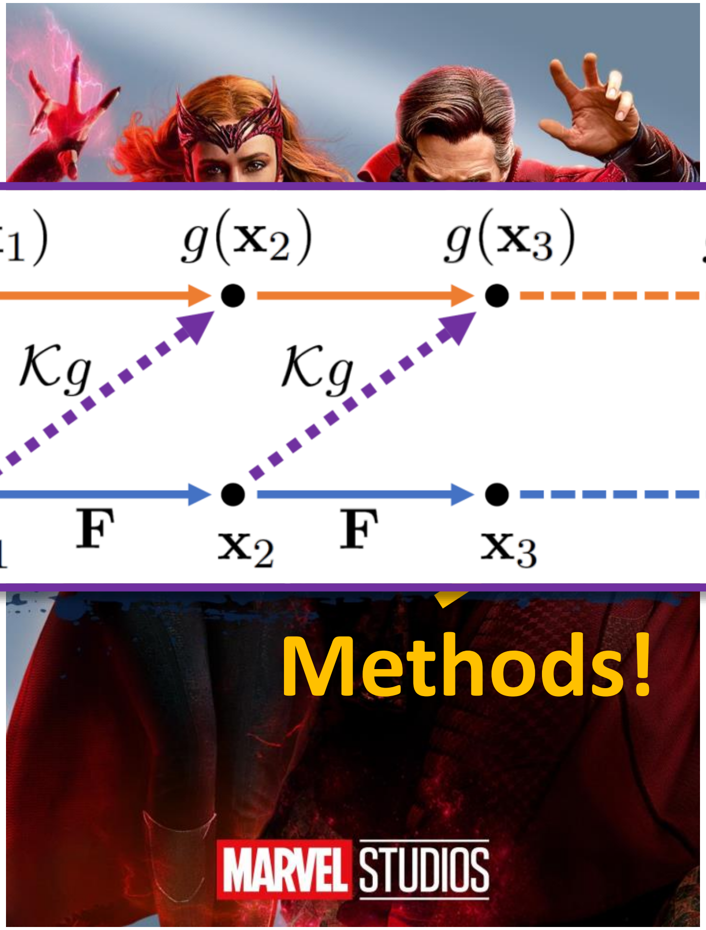


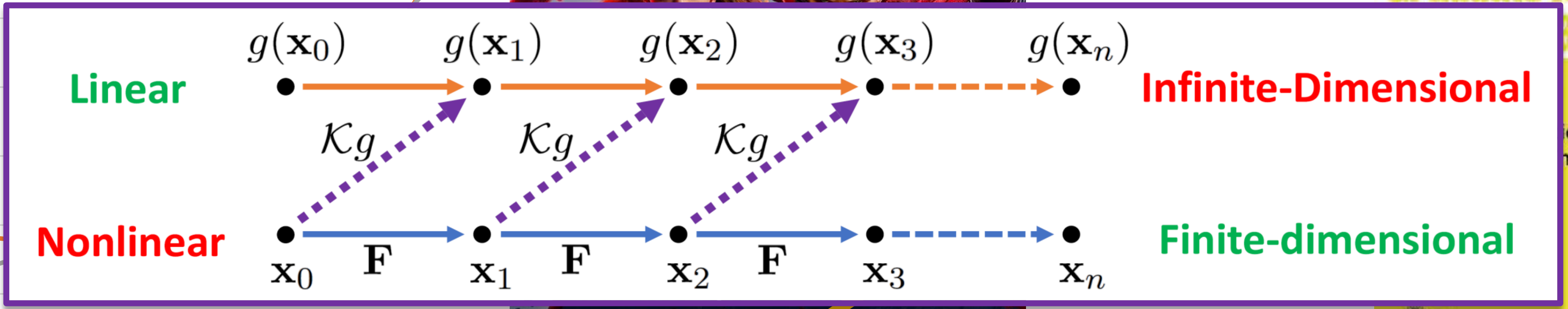

**Why all this sudden interest?**

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

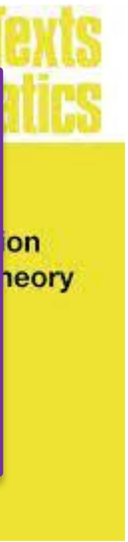
**New Papers on "Koopman Operators"**




**Koopman operators are classical in ergodic theory.**




**Why all this sudden interest?**

- **Data-driven**
- **Deal with nonlinearity**
- **Easy-to-use methods**

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

# Setting: Measure-preserving systems

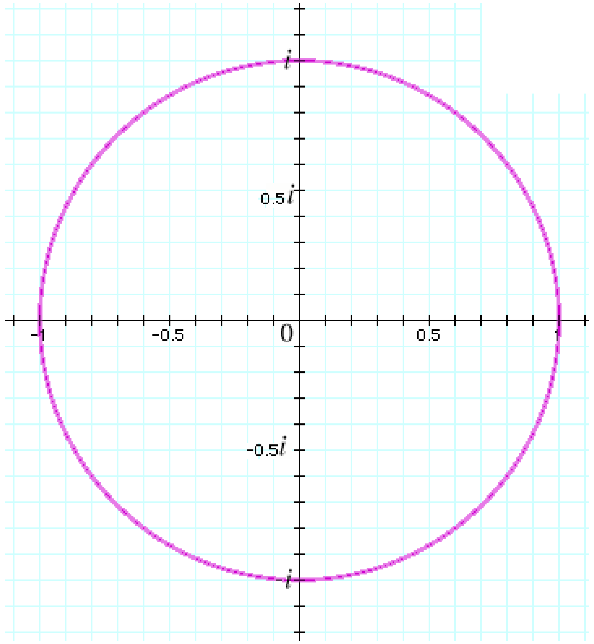
$$[\mathcal{K}g](x) = g(F(x)), \qquad g \in L^2(\Omega, \omega)$$

$F$ preserves $\omega \Leftrightarrow \|\mathcal{K}g\| = \|g\|$ (isometry)

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

$\Rightarrow \mathrm{Sp}(\mathcal{K}) \subseteq \{z: |z| \leq 1\}$

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




**First Problem:** We want our discretization to respect this property!

# Measure-preserving EDMD

*Building unitary discretizations…*

# Shift example (on $\ell^2(\mathbb{Z})$)

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

Two-way infinite

- Spectrum is unit circle.
- Spectrum is stable.
- Continuous spectra.
- Unitary evolution.

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


**Lots of Koopman operators are built up from operators like these!**

# How to fix a Jordan block

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

polar decomposition →

Circulant matrix

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

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

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

# Extended Dynamic Mode Decomposition (EDMD)

$$\Psi(x) = [\psi_1(x) \;\; \ldots \;\; \psi_N(x)], \qquad g = \sum_{j=1}^{N} \mathbf{g}_j \psi_j = \Psi \mathbf{g} \in \operatorname{span}\{\psi_1, \ldots, \psi_N\}$$

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

quadrature

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

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

$\mathbb{K}$: **Galerkin method** on $V_N = \operatorname{span}\{\psi_1, \ldots, \psi_N\}$


- 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.

# A simple alteration

$$G_{jk} = \sum_{m=1}^{M} w_m \overline{\psi_j(x^{(m)})} \psi_k(x^{(m)}) \approx \langle \psi_k, \psi_j \rangle$$

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

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

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

quadrature

**Orthogonal Procrustes problem**

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

# The mpEDMD algorithm

**Algorithm 4.1** The mpEDMD algorithm

**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 $\mathbf{\Psi}_X$ and $\mathbf{\Psi}_Y$ and $\mathbf{W} = \mathrm{diag}(w_1, \ldots, w_M)$.
2: Compute an economy QR decomposition $\mathbf{W}^{1/2}\mathbf{\Psi}_X = \mathbf{QR}$, where $\mathbf{Q} \in \mathbb{C}^{M\times N}$, $\mathbf{R} \in \mathbb{C}^{N\times N}$.
3: Compute an SVD of $(\mathbf{R}^{-1})^*\mathbf{\Psi}_Y^*\mathbf{W}^{1/2}\mathbf{Q} = \mathbf{U}_1\mathbf{\Sigma}\mathbf{U}_2^*$.
4: Compute the eigendecomposition $\mathbf{U}_2\mathbf{U}_1^* = \hat{\mathbf{V}}\mathbf{\Lambda}\hat{\mathbf{V}}^*$ (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 $\mathbf{\Lambda}$.

$V_N = \mathrm{span}\,\{\psi_1, \ldots, \psi_N\}$
$\mathcal{P}_{V_N}: L^2(\Omega, \omega) \to V_N$
orthogonal projection

As $M \to \infty$, **unitary part** of polar decomposition of $\mathcal{P}_{V_N}\mathcal{K}\mathcal{P}_{V_N}^*$.

**Convergence:** spectral measures (see later), Koopman mode decomposition,…


- C., *"The mpEDMD Algorithm for Data-Driven Computations of Measure-Preserving Dynamical Systems,"* **SINUM**, 2023.
- Code: https://github.com/MColbrook/Measure-preserving-Extended-Dynamic-Mode-Decomposition

# Spectral measures → diagonalisation

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

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

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- **Infinite dimensions:** Unitary $\mathcal{K}$. Typically, **no basis of eigenfunctions**!
  *Spectral theorem*: (projection-valued) spectral measure $\mathcal{E}$

$$g = \left[\int_{\mathrm{Spec}(\mathcal{K})} 1 \, \mathrm{d}\mathcal{E}(\lambda)\right] g, \qquad \mathcal{K}g = \left[\int_{\mathrm{Spec}(\mathcal{K})} \lambda \, \mathrm{d}\mathcal{E}(\lambda)\right] g, \qquad \forall g \in L^2(\Omega, \omega)$$

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

# Spectral measures → dynamics

$\mu_g$ probability measures on $\mathbb{T} = \{z \in \mathbb{C} : |z| = 1\}$

$$\widehat{\mu_g}(n) = \int_{\mathbb{T}} \lambda^n \, \mathrm{d}\mu_g(\lambda) = \langle \mathcal{K}^n g, g \rangle$$

Fourier coefficients

moments

correlations

Characterize forward-time dynamics ⇒ Koopman mode decomposition.

# Convergence of measures

$$\mu_{\mathbf{g}}^{(N,M)}(U) = \sum_{\lambda_j \in U} \left|v_j^* G\mathbf{g}\right|^2$$

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

Captures weak convergence of measures

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

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

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

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

**Matching autocorrelations!**

$\mathbb{K}$: mpEDMD matrix

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

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

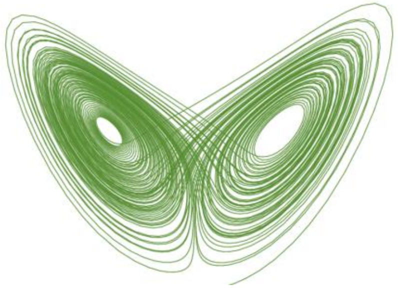
$V_N = \mathrm{span}\{\psi_1, \ldots, \psi_N\}$

# Further convergence

- Projection-valued measures (e.g., functional calculus, $L^2$ forecasting).
- Koopman mode decomposition.
- Spectrum.
- Resolvent (see later!)

Key ingredient: **unitary** discretization.

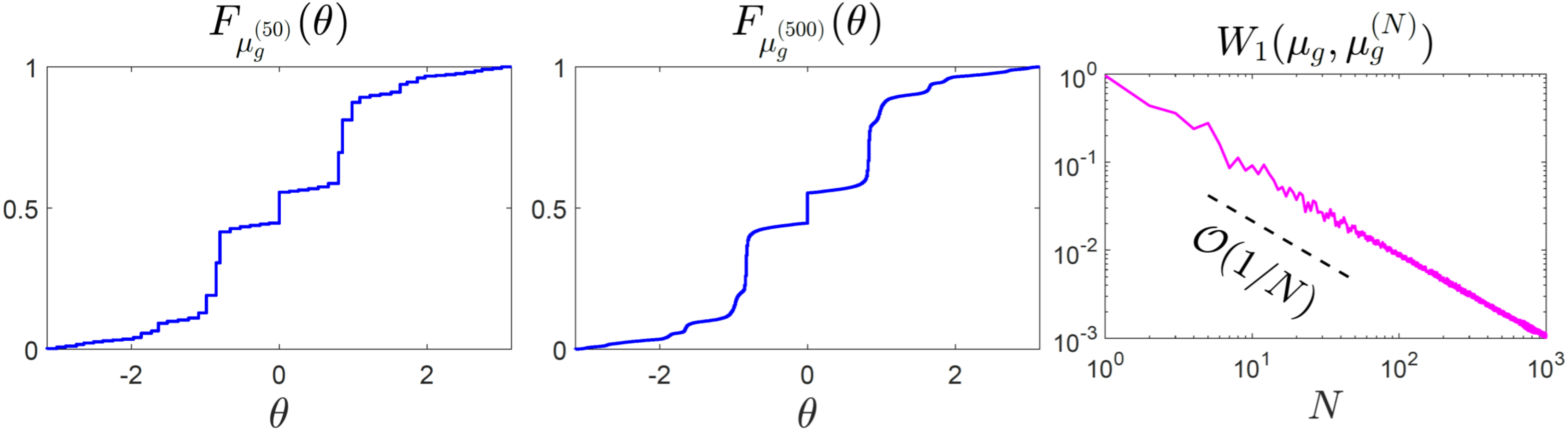
# Lorenz system



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

$$g(x_1, x_2, x_3) = c\,\tanh((x_1 x_2 - 3x_3)/5), \qquad V_N = \mathrm{span}\{g, \mathcal{K}g, \ldots, \mathcal{K}^{N-1}g\}$$

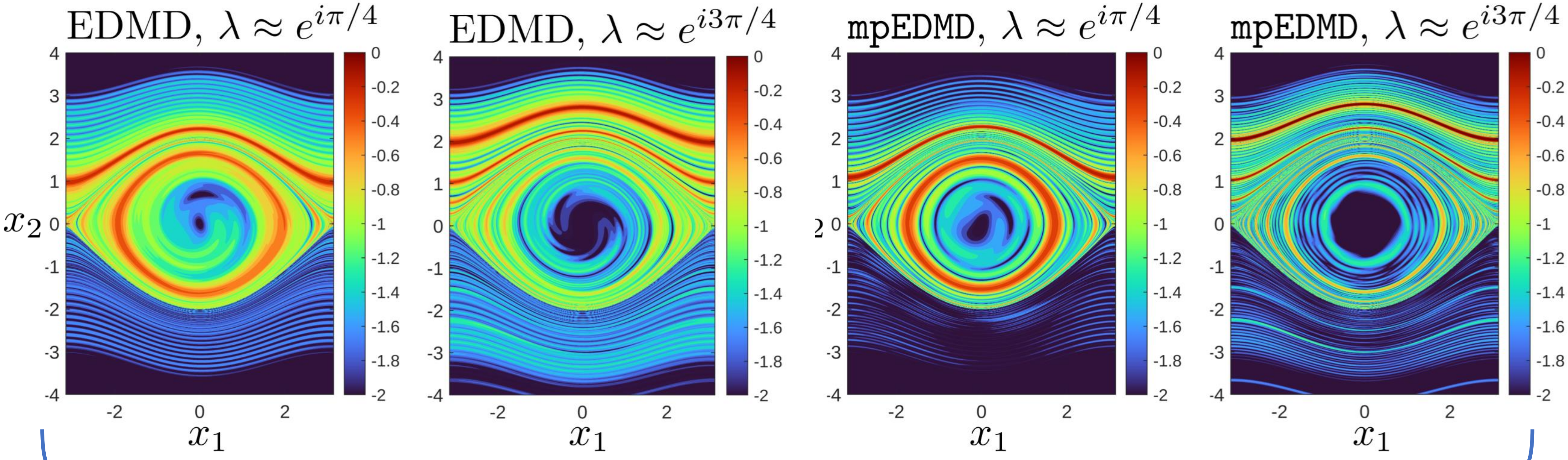
Cdf: $F_\mu(\theta) = \mu(\{\exp(it) : -\pi \le t \le \theta\})$



# Nonlinear pendulum

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

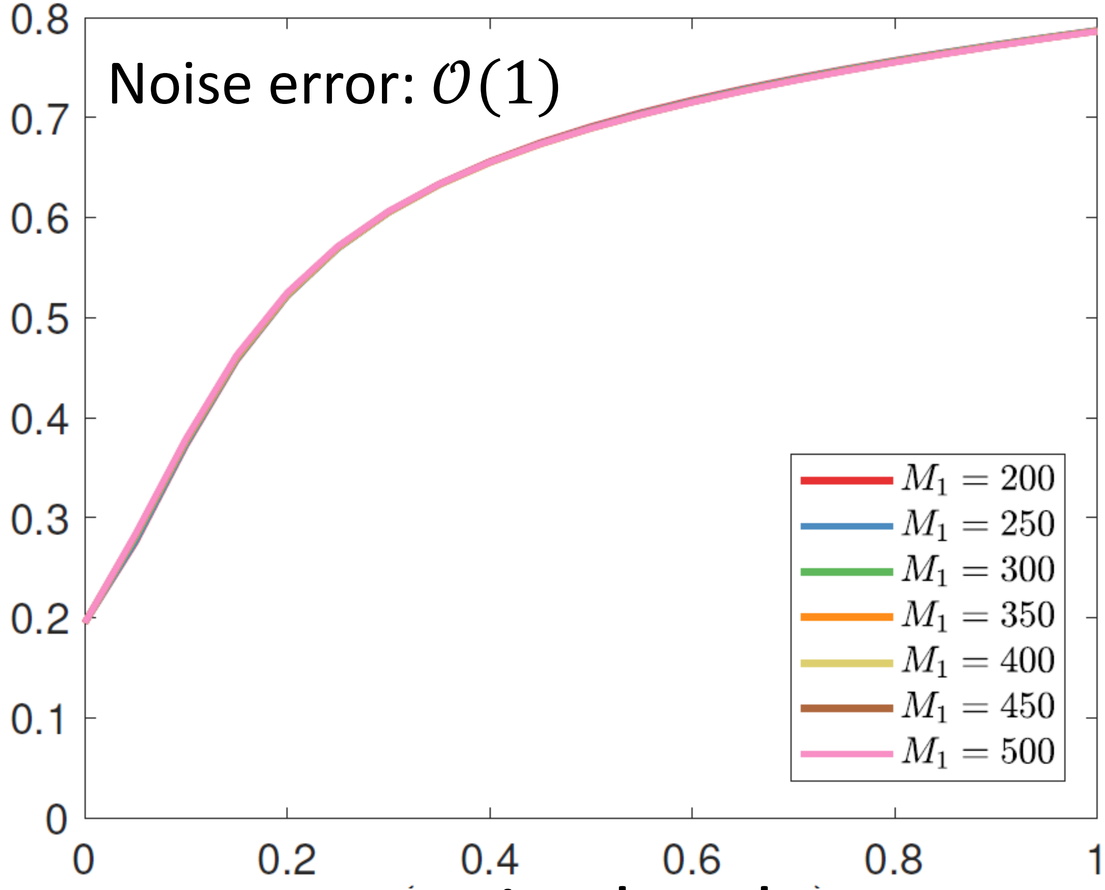
$$g(x) = \exp(ix_1)\, x_2 \exp(-x_2^2/2), \qquad V_N = \text{span}\{g, \mathcal{K}g, \dots, \mathcal{K}^{99}g\}$$




**Dissipation, low accuracy** $\log_{10}(|v_j|)$ **Conservative, high accuracy**

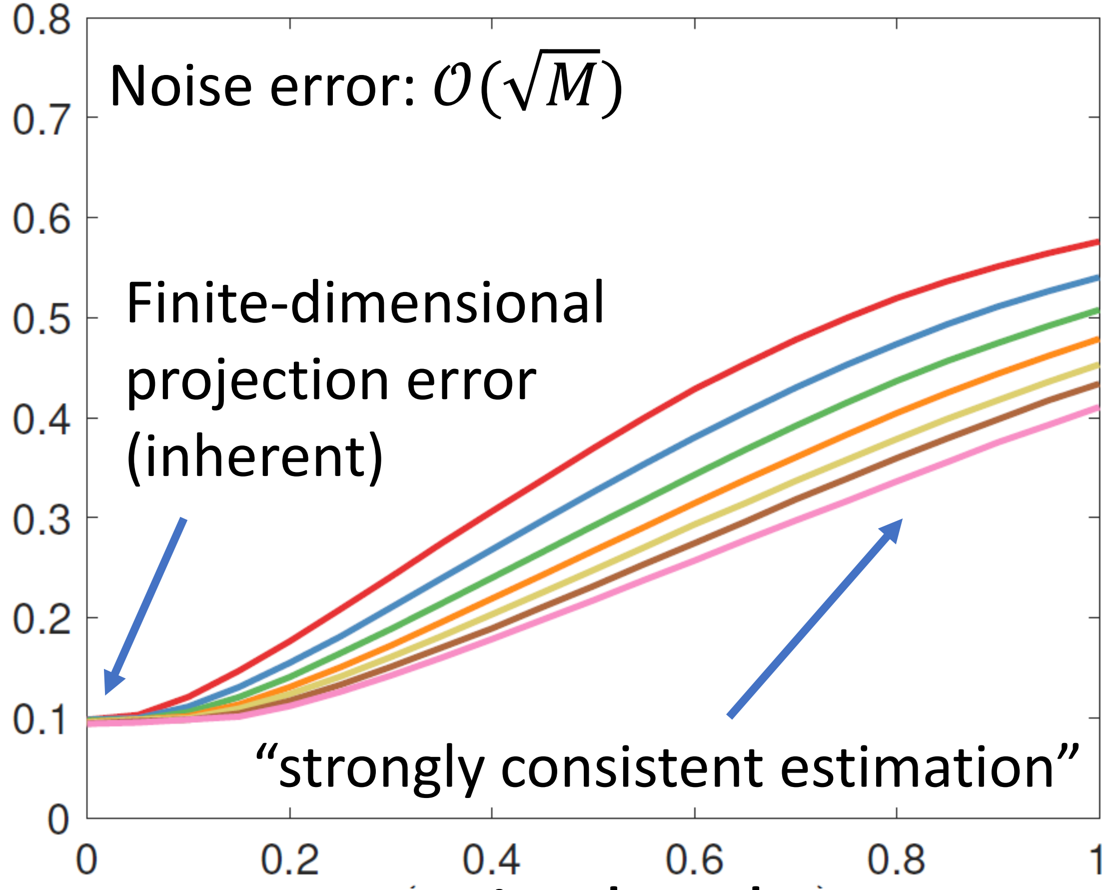
# Robustness to noise: Gauss. noise for $\Psi_X, \Psi_Y$

Mean inf. dim. residual (EDMD)




Noise level

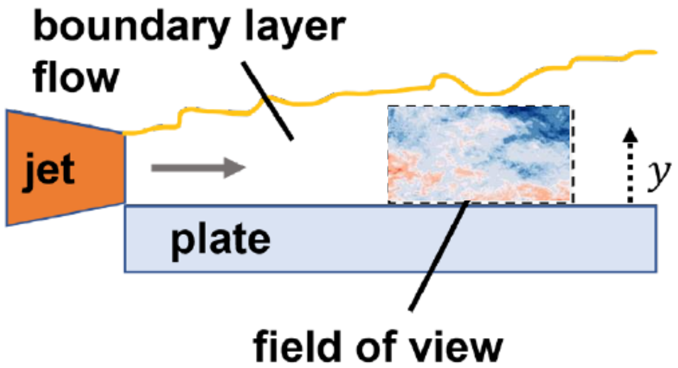
Mean inf. dim. residual (mpEDMD)




Noise level

# Turbulence (real data)

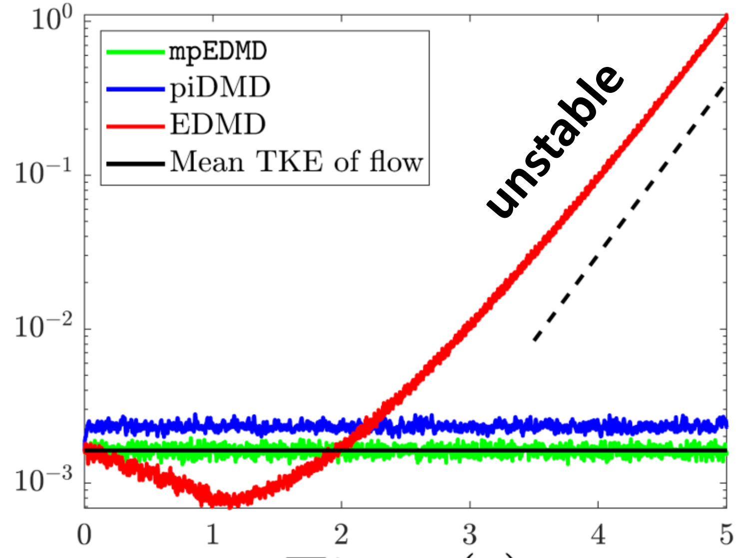
Experimental setup



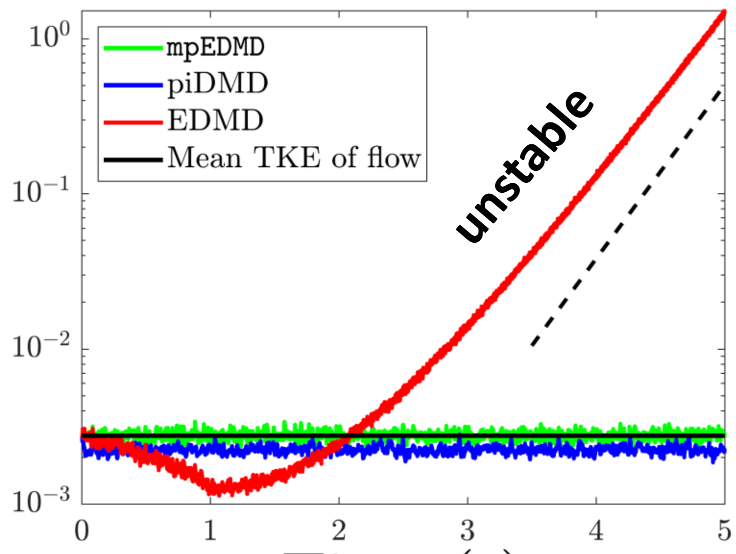

- Reynolds number $\approx 6.4 \times 10^4$
- Ambient dimension ($d$) $\approx$ 100,000 (velocity at measurement points)

*PIV data provided by Máté Szőke (Virginia Tech)

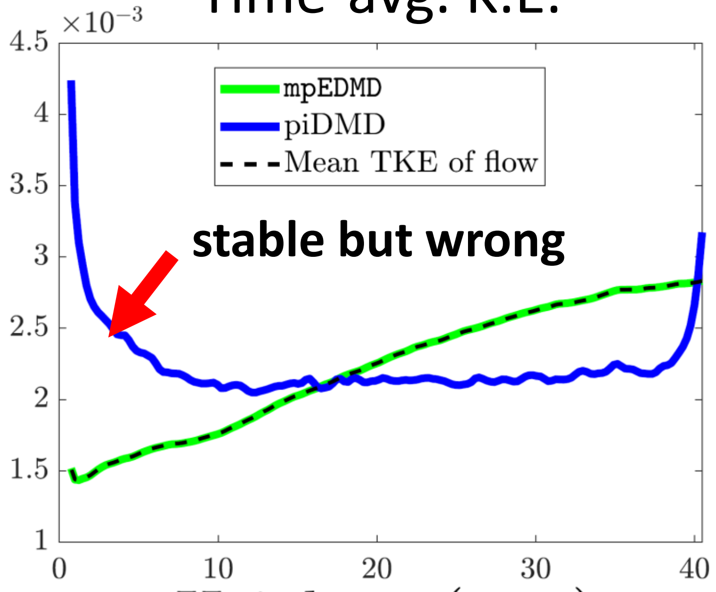
Turbulent K.E. y=5mm




Turbulent K.E. y=35mm




Time-avg. K.E.

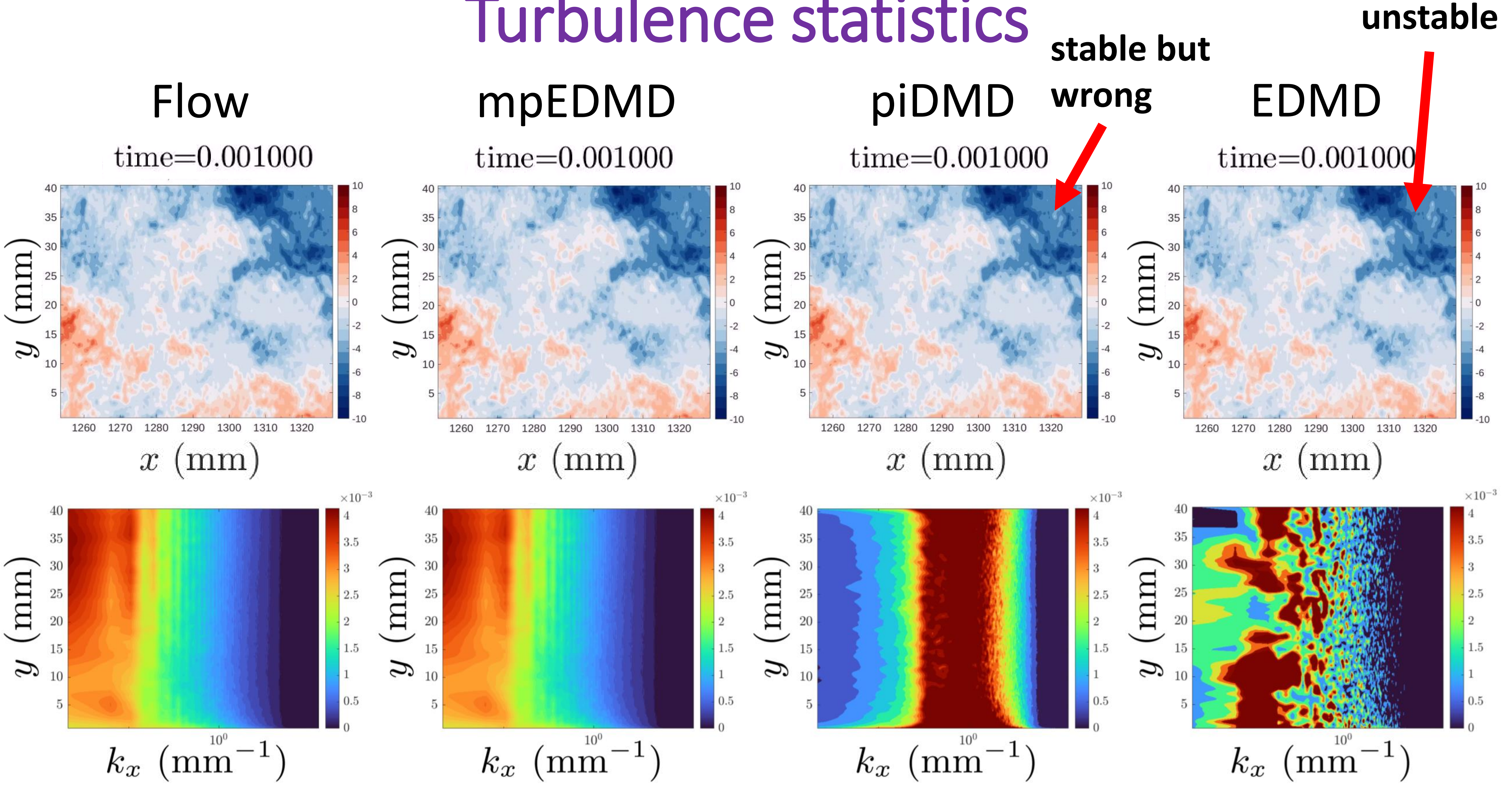



piDMD

EDMD


- 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



# Setting: Measure-preserving systems

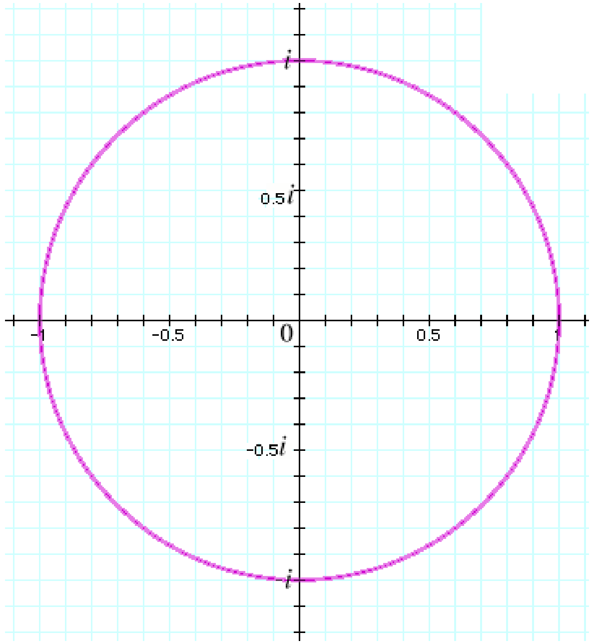
$$[\mathcal{K}g](x) = g\big(F(x)\big), \qquad g \in L^2(\Omega, \omega)$$

$F$ preserves $\omega \iff \|\mathcal{K}g\| = \|g\|$ (isometry)

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

$\implies \mathrm{Sp}(\mathcal{K}) \subseteq \{z: |z| \leq 1\}$

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




**Second Problem:** Often $\mathcal{K}$ doesn't have basis of eigenfunctions

(i.e., **continuous spectra**)

# Rigged DMD

*Dealing with continuous spectra…*

# Back to the shift!

$$e_j \to e_{j-1}$$

"Solve" $(U - zI)u_z = 0$

$$u_z = \sum_{j=-\infty}^{\infty} z^j e_j$$

$$U = \begin{pmatrix} \ddots & \ddots & & & & \\ & 0 & 1 & & & \\ & & 0 & 1 & & \\ & & & 0 & 1 & \\ & & & & 0 & \ddots \\ & & & & & \ddots \end{pmatrix}$$

Two-way infinite

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Doesn't live in $\ell^2(\mathbb{Z})$!!!

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Two-way infinite

Let $|z| = 1$, $\phi = \sum_{j=-\infty}^{\infty} \phi_j e_j$ where $\phi_j$ decay faster than any inverse polynomial.

Test functions

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$$\langle u_z, \phi \rangle = \sum_{j=-\infty}^{\infty} z^j \overline{\phi_j}, \qquad \langle U u_z, \phi \rangle = \langle u_z, U^* \phi \rangle = \sum_{j=-\infty}^{\infty} z^j \overline{\phi_{j-1}} = z \langle u_z, \phi \rangle$$

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Generalised eigenfunctions $u_z$ and generalised eigenvalues $\{z: |z| = 1\}$

# Another example: Nonlinear pendulum

$$\dot{x}_1 = x_2, \qquad \dot{x}_2 = -\sin(x_1)$$
$$\Omega = [-\pi, \pi]_{\text{per}} \times \mathbb{R},$$
$$\Delta_t = 1,$$
$$\omega = \text{ Lebesgue measure}$$

**Considered a challenge in Koopman theory!**

nature COMMUNICATIONS

ARTICLE

DOI: 10.1038/s41467-018-07210-0 OPEN

## Deep learning for universal linear embeddings of nonlinear dynamics

Bethany Lusch [1,2], J. Nathan Kutz[1] & Steven L. Brunton[1,2]

Identifying coordinate transformations that make strongly nonlinear dynamics approximately linear has the potential to enable nonlinear prediction, estimation, and control using linear theory. The Koopman operator is a leading data-driven embedding, and its eigenfunctions provide intrinsic coordinates that globally linearize the dynamics. However, identifying and representing these eigenfunctions has proven challenging. This work leverages deep learning to discover representations of Koopman eigenfunctions from data. Our network is parsimonious and interpretable by construction, embedding the dynamics on a low-dimensional

# Explicit diagonalization using Radon transform!

- Action-angle coordinates ($n$ degrees of freedom):

$$\dot{\mathbf{I}} = \mathbf{0}, \qquad \dot{\boldsymbol{\theta}} = \mathbf{I}, \qquad \Omega = \mathbb{R}^n \times [-\pi, \pi]_{\text{per}}^n$$

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- $g$ in Schwartz space,

$$g(\mathbf{I}, \boldsymbol{\theta}) = \sum_{\mathbf{k} \in \mathbb{Z}^n} \hat{g}_{\mathbf{k}}(\mathbf{I}) e^{i\mathbf{k}\cdot\boldsymbol{\theta}}, \qquad \hat{g}_{\mathbf{k}}(\mathbf{I}) = \frac{1}{(2\pi)^n} \int_{[-\pi,\pi]^n_{\mathrm{per}}} g(\mathbf{I}, \boldsymbol{\theta})\, e^{-i\mathbf{k}\cdot\boldsymbol{\theta}} \mathrm{d}\boldsymbol{\theta}$$

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$$\hat{g}_{\mathbf{k}}(\mathbf{I}) = \sum_{j=1}^{\infty} \sum_{m=-\infty}^{\infty} \int_{[-\pi,\pi]_{\mathrm{per}}} \left\langle {g_\theta^{(\mathbf{k},m,j)}}^* | g \right\rangle g_\theta^{(\mathbf{k},m,j)} \mathrm{d}\theta$$

$$g_\theta^{(\mathbf{k},m,j)} = \frac{1}{(2\pi)^n} \delta(\theta + 2\pi m - \Delta t \mathbf{k} \cdot \mathbf{I}) \psi_j^{(k)} e^{i\mathbf{k}\cdot\boldsymbol{\theta}}$$

Generalised eigenfunctions

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Generalised eigenfunctions

Plane wave

Supported on hyperplane

Orthonormal basis of hyperplane

# Gelfand's theorem → diagonalisation

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

$$v = \sum_{j=1}^{n} (v_j{}^* v) v_j, \qquad Bv = \sum_{j=1}^{n} \lambda_j (v_j{}^* v) v_j \qquad \forall v \in \mathbb{C}^n$$

- **Infinite dimensions:** Unitary $\mathcal{K}$. Typically, **no basis of eigenfunctions**!
  Some technical assumptions (can always be realized):

$$g = \int_{[-\pi,\pi]_{\mathrm{per}}} \langle g_\theta^* | g \rangle \, g_\theta \, \mathrm{d}\nu(\theta), \qquad \mathcal{K} g = \int_{[-\pi,\pi]_{\mathrm{per}}} e^{i\theta} \langle g_\theta^* | g \rangle \, g_\theta \, \mathrm{d}\nu(\theta)$$

$g \in S \subset L^2(\Omega, \omega)$

Koopman modes

generalized eigenfunctions
*distributions* $\in \mathcal{S}^*$

$e^{i\theta} = \lambda$

**Koopman Mode Decomposition**

# Rigged DMD: Smoothing

**Carathéodory function**:

$$F_g(z) = (\mathcal{K} + zI)(\mathcal{K} - zI)^{-1}g = \int_{[-\pi,\pi]_{\text{per}}} \frac{e^{i\theta} + z}{e^{i\theta} - z} \langle g_\theta^* | g \rangle \, g_\theta \, \mathrm{d}\nu(\theta)$$

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Let $r = 1 + \varepsilon > 1, \theta_0 \in [-\pi, \pi]_{\mathrm{per}}$,

$$\frac{1}{4\pi}\left[F_g\left(r^{-1}e^{i\theta_0}\right) - F_g\left(re^{i\theta_0}\right)\right]$$

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**Poisson kernel**

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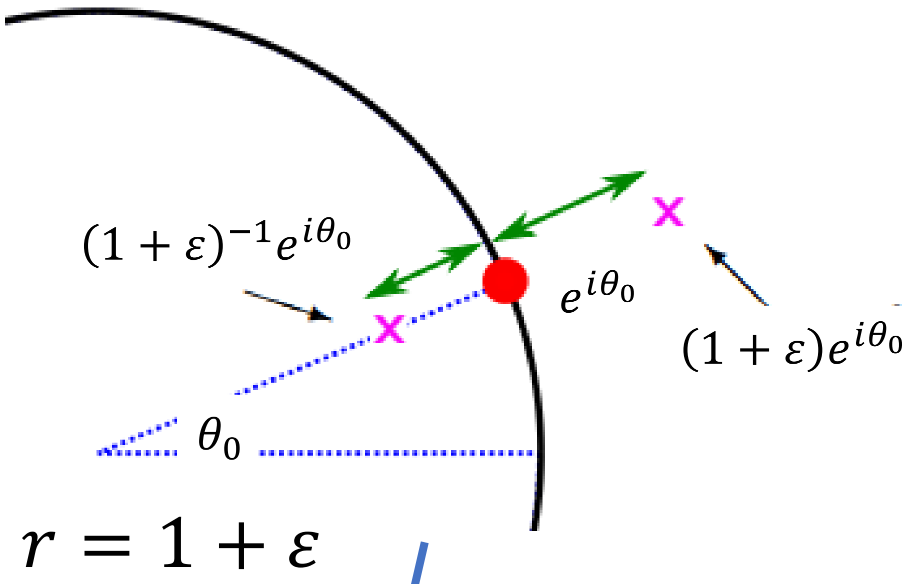
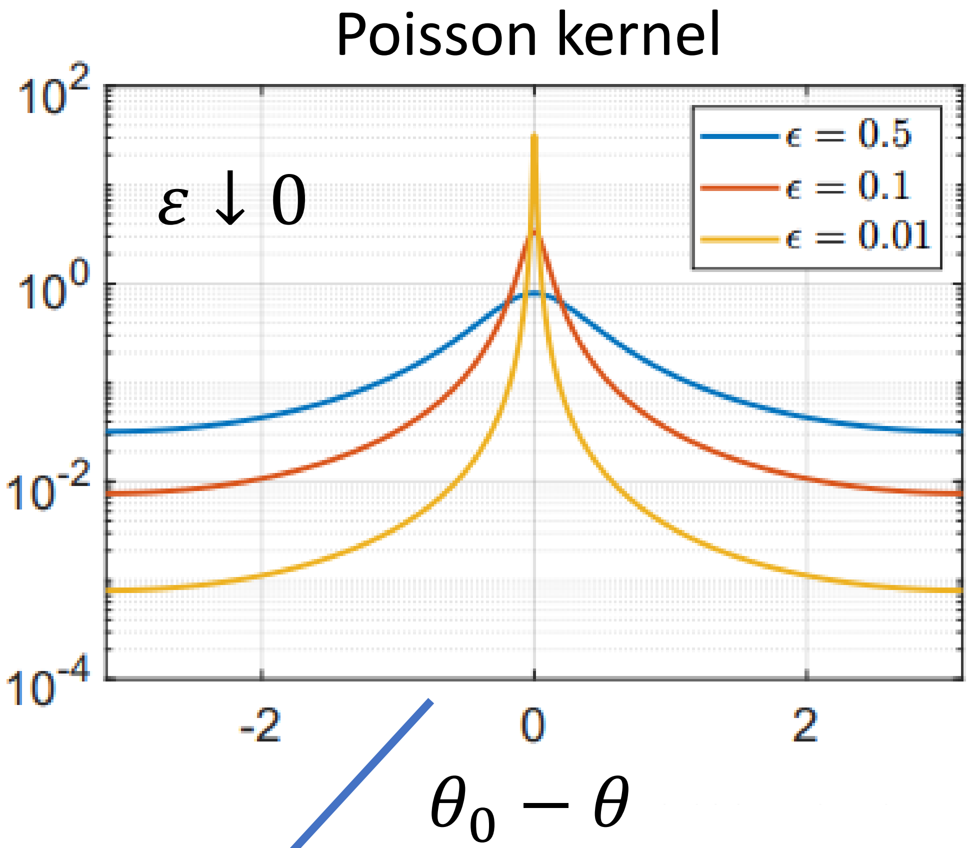
*Smoothed* generalized eigenfunction

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*Smoothed* generalized eigenfunction

# $F_g$ requires $(\mathcal{K} - zI)^{-1}$

**EDMD diverges:**

$$\begin{pmatrix} \ddots & \ddots & & & & \\ & 0 & 1 & & & \\ & & 0 & 1 & & \\ & & & 0 & 1 & \\ & & & & 0 & \ddots \\ & & & & & \ddots \end{pmatrix}$$

Two-way infinite

$$\mathbb{K}_{\text{EDMD}} = \begin{pmatrix} 0 & 1 & & & \\ & \ddots & \ddots & & \\ & & & 0 & 1 \\ & & & & 0 \end{pmatrix}$$

Acts on $\text{span}\{e_{-N}, \ldots, e_N\}$

E.g., if $|z| < 1$,

$$(\mathbb{K}_{\text{EDMD}} - zI)^{-1} e_0 = \sum_{j=1}^{N} \frac{-1}{z^j} e_{-j}$$

Exponential blowup as $N \to \infty$.

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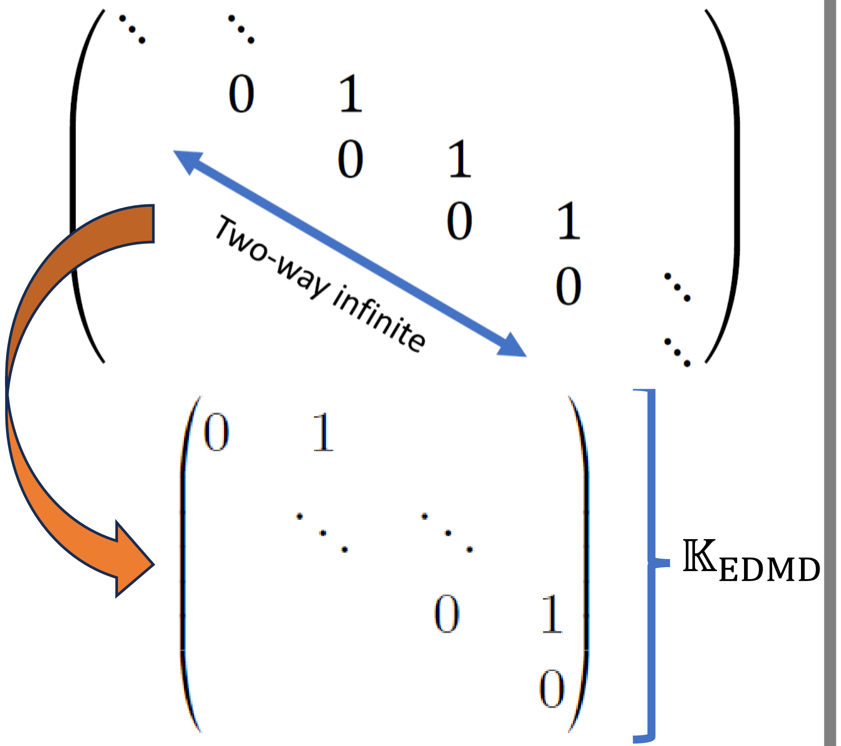


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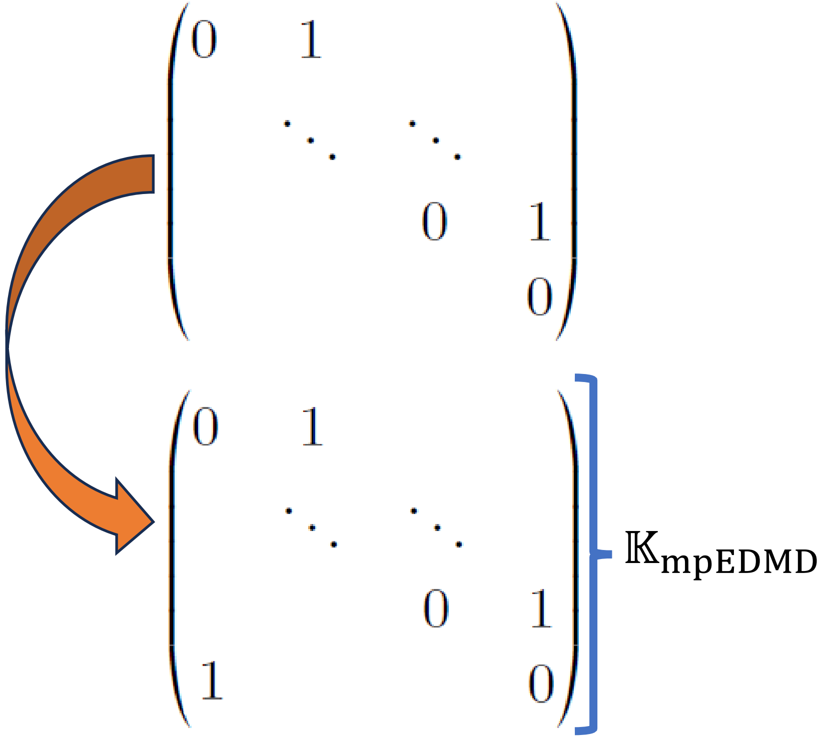


General method: unitary part of a **polar decomposition** of EDMD!

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General method: unitary part of a **polar decomposition** of EDMD!

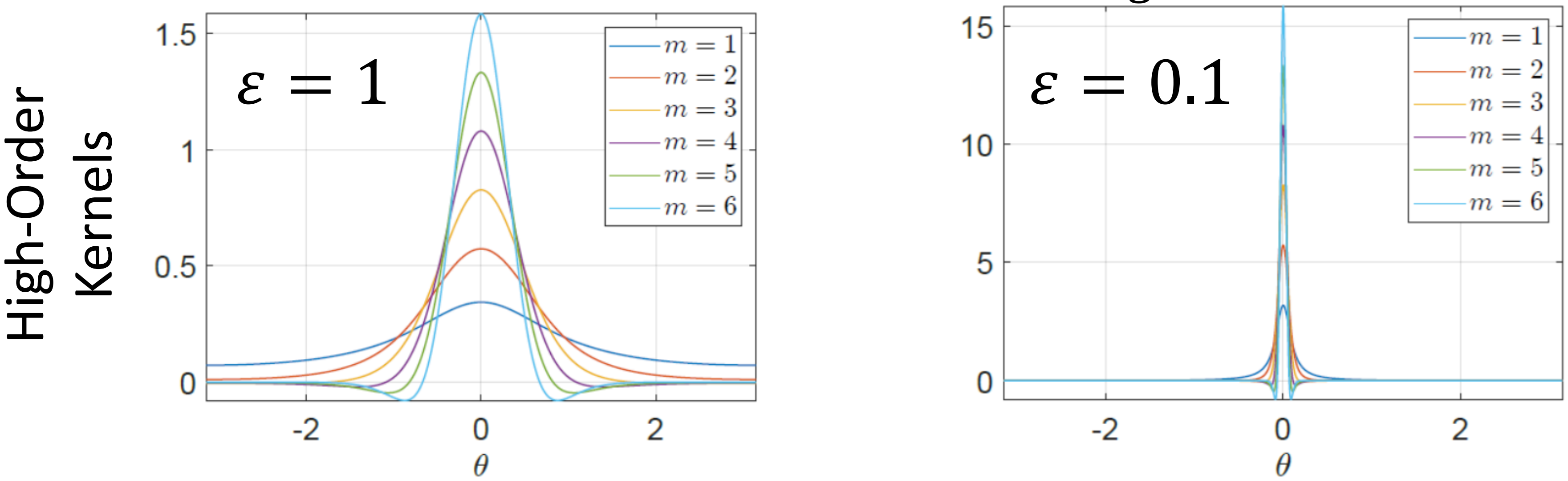
## Rigged DMD converges:

- For general $\mathcal{K}$: $(\mathbb{K}_{\mathrm{mpEDMD}} - zI)^{-1}\mathbf{g}$ converges to $(\mathcal{K} - zI)^{-1} g$ as $\lim_{N\to\infty} \lim_{M\to\infty}$
- Hence, Rigged DMD converges as $\lim_{\varepsilon \downarrow 0} \lim_{N\to\infty} \lim_{M\to\infty}$
- ResDMD allows us to select $\varepsilon = \varepsilon(N)$ adaptively (convergence in **2 limits**)

# Better smoothing kernels as $\varepsilon \downarrow 0$

- Poisson kernel: **slow** convergence $\mathcal{O}(\varepsilon \log(1/\varepsilon))$.
- Construct high-order *rational* kernels using $F_g(z)$.

Smaller $\varepsilon$ requires more data



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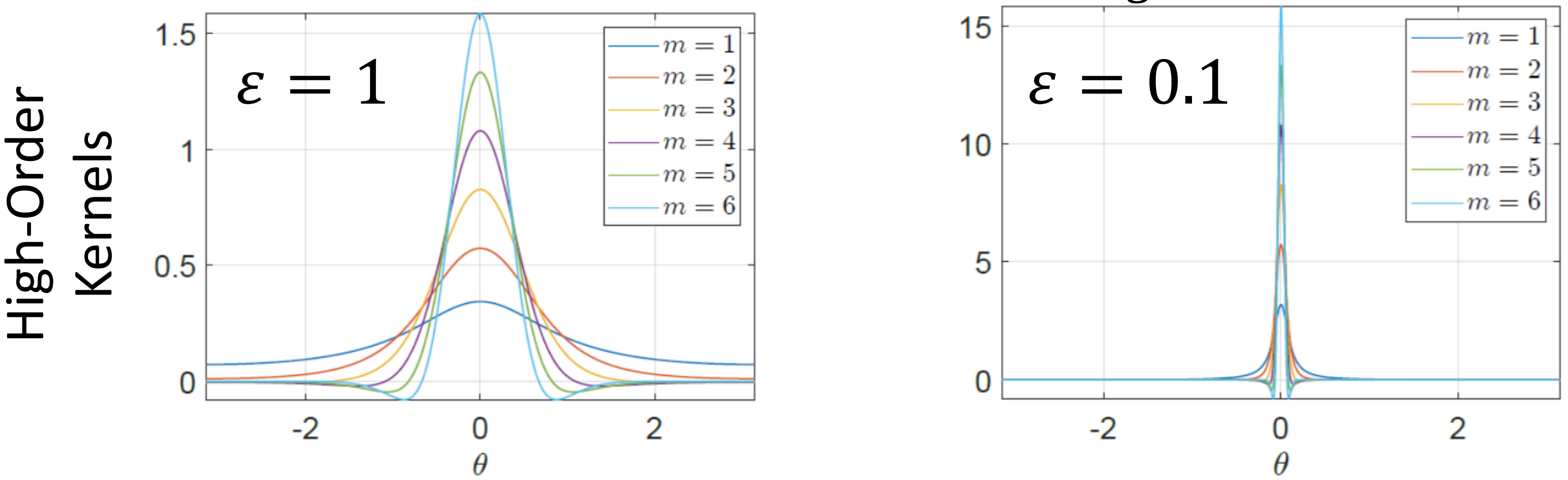
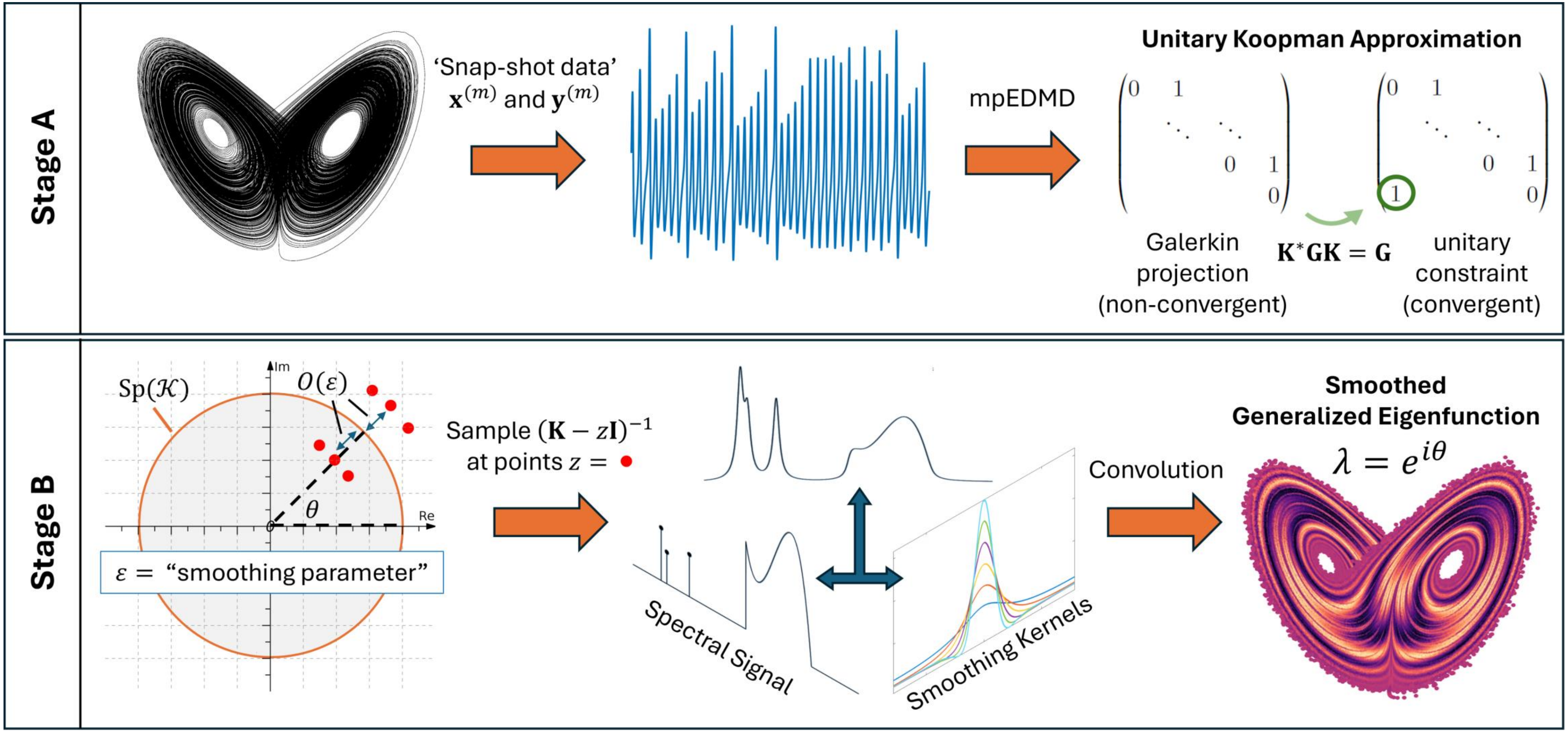



**Theorem**: Suppose quadrature rule converges & $\lim_{N\to\infty} \mathrm{dist}(h, V_N) = 0$ for any $h \in L^2(\Omega, \omega)$. Choosing $N = N(\varepsilon)$, **fast** $\mathcal{O}(\varepsilon^m \log(1/\varepsilon))$ convergence for:

- Generalized eigenfunctions (topology of $\mathcal{S}^*$).
- Spectral measures: pointwise, $L^p$, weak,…
- Forecasting (i.e., iterating Koopman mode decomposition), coherency etc.

# Rigged DMD

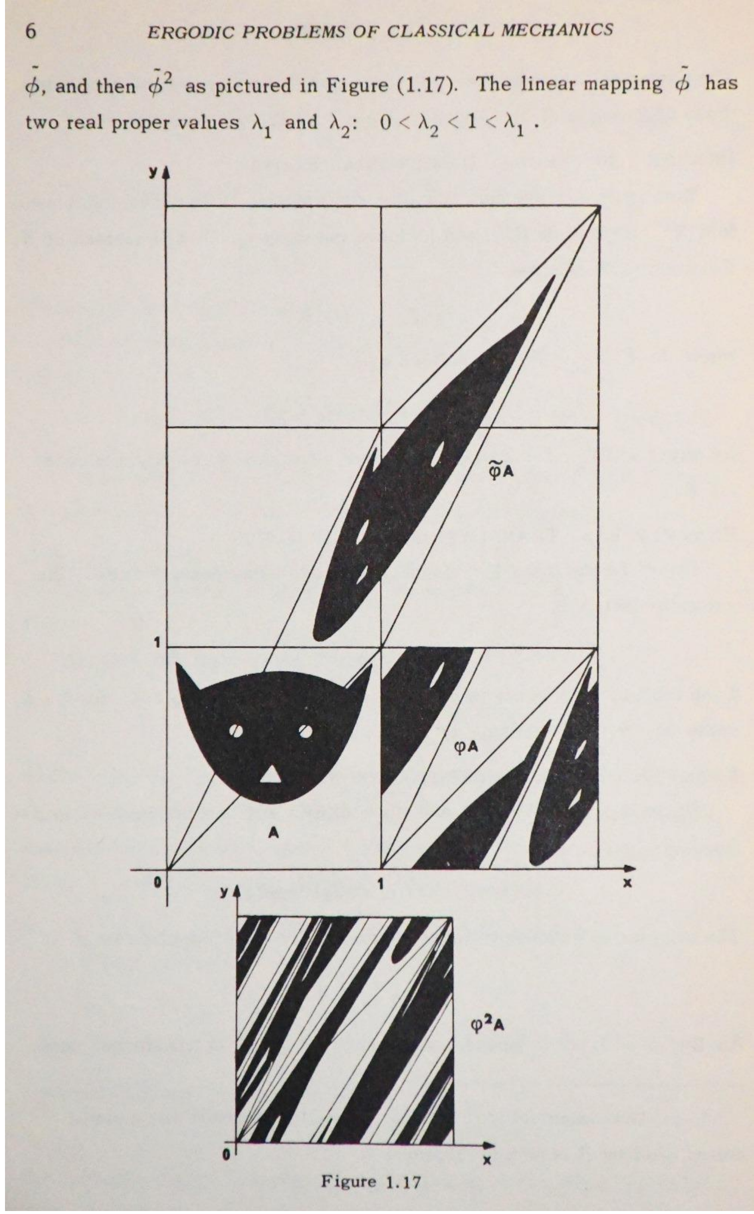



- C., Drysdale, Horning, *"Rigged Dynamic Mode Decomposition: Data-Driven Generalized Eigenfunction Decompositions for Koopman Operators"*, arxiv preprint.
- Code*:* https://github.com/MColbrook/Rigged-Dynamic-Mode-Decomposition

# Example: Arnold's cat map

$F(x, y) = (2x + y, x + y) \mod 2\pi$

$\Omega = [-\pi, \pi]^2_{\text{per}}, \quad \omega =$ Lebesgue measure


6 ERGODIC PROBLEMS OF CLASSICAL MECHANICS

$\bar{\phi}$, and then $\bar{\phi}^2$ as pictured in Figure (1.17). The linear mapping $\bar{\phi}$ has two real proper values $\lambda_1$ and $\lambda_2$: $0 < \lambda_2 < 1 < \lambda_1$ .



Figure 1.17

Arnold's "Ergodic Problems of Classical Mechanics"

# Example: Arnold's cat map

*Experimental details*

Length-one trajectories, $M = 50 \times 50, N = 500$

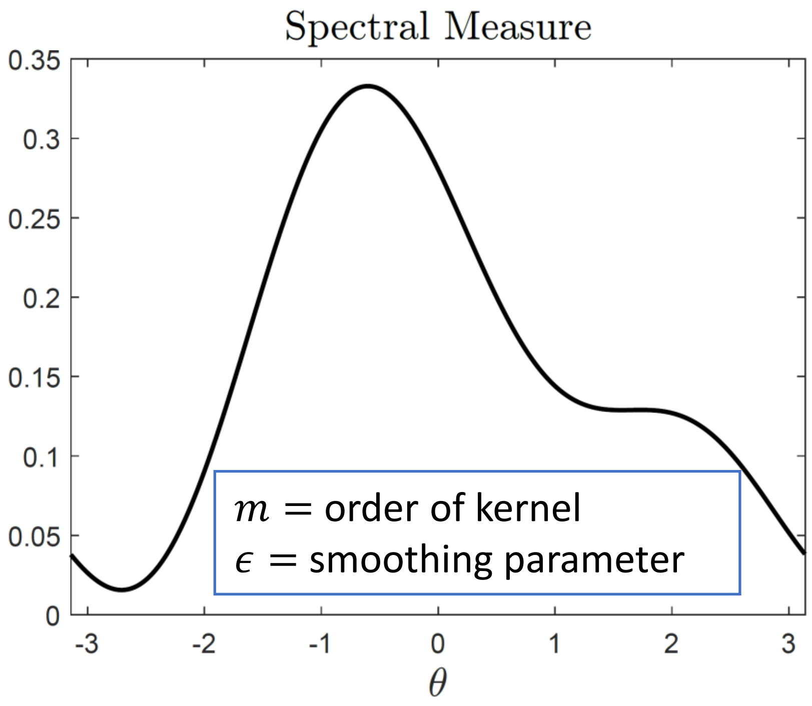
$g(x,y) = \sin(x) + \frac{1}{2}\sin(2x+y) + \frac{i}{4}\sin(5x+3y)$

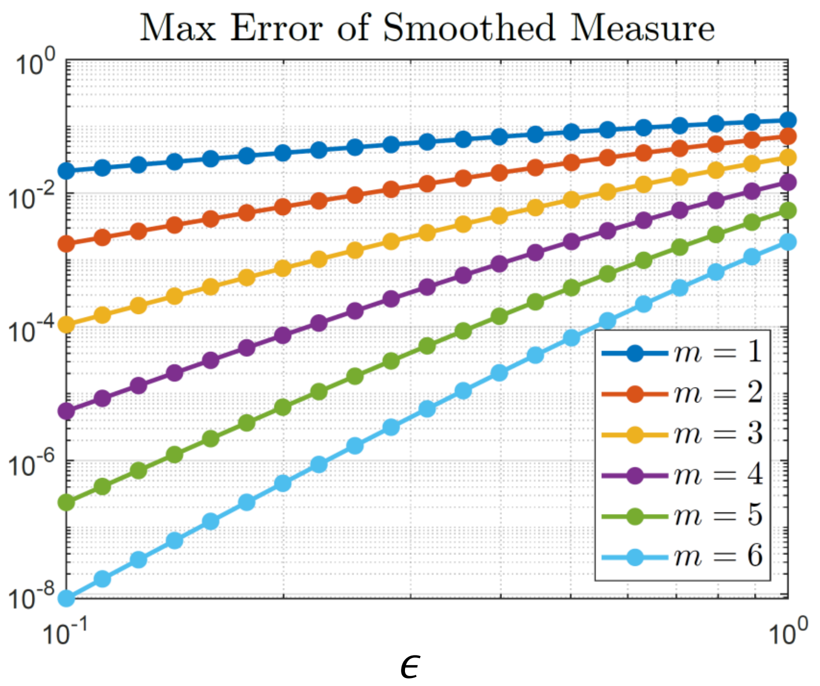
Krylov subspace: $V_N = \{g, \mathcal{K}g, \ldots, \mathcal{K}^{N-1}g\}$

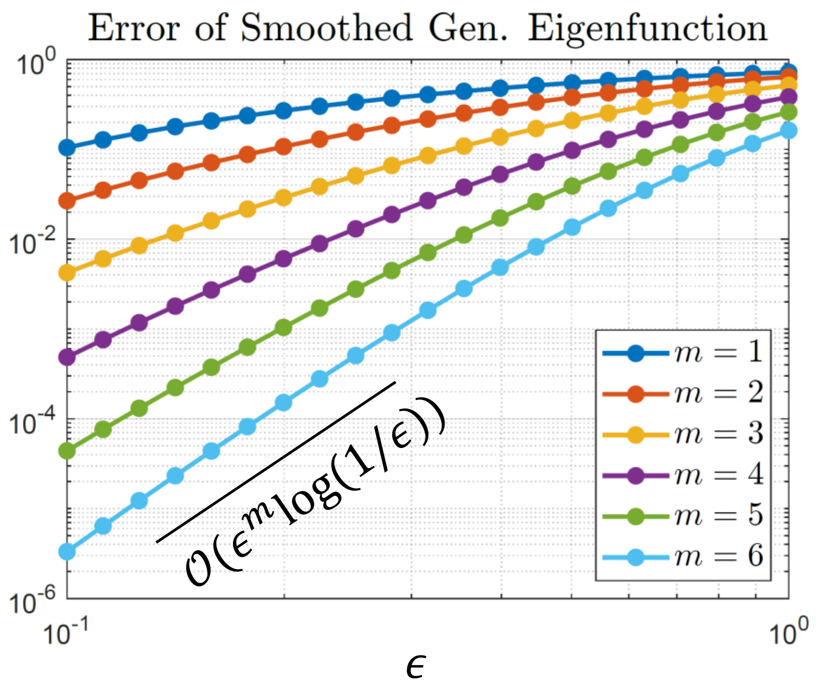
$F(x,y) = (2x+y, x+y) \mod 2\pi$

$\Omega = [-\pi,\pi]^2_{\text{per}}, \quad \omega =$ Lebesgue measure

**Explicit formula:** $g_\theta$ become more oscillatory as $\epsilon \downarrow 0$ (non-decaying Fourier series)

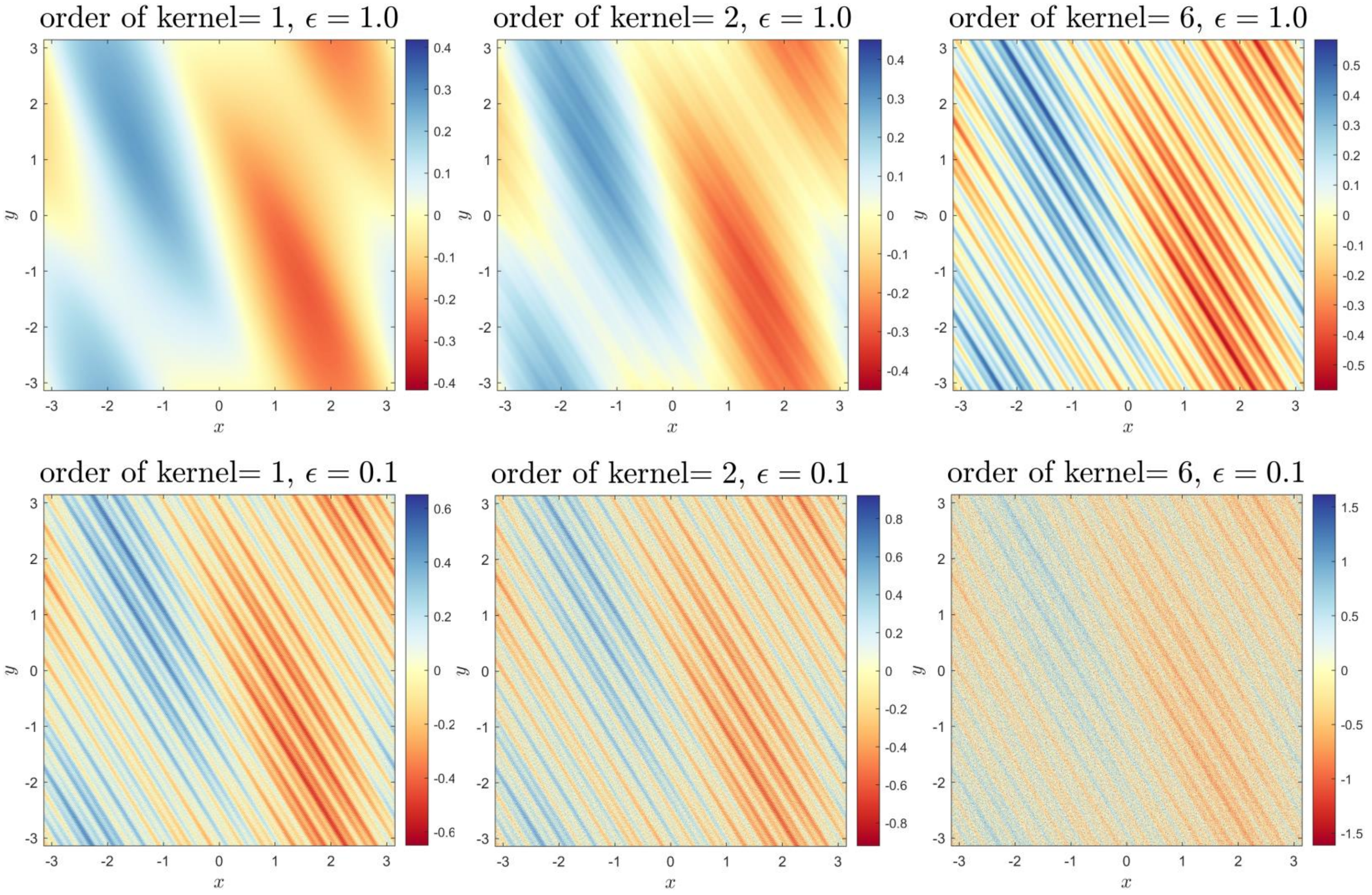


Higher kernel order (accuracy)

Higher resolution ($\varepsilon \downarrow 0$)



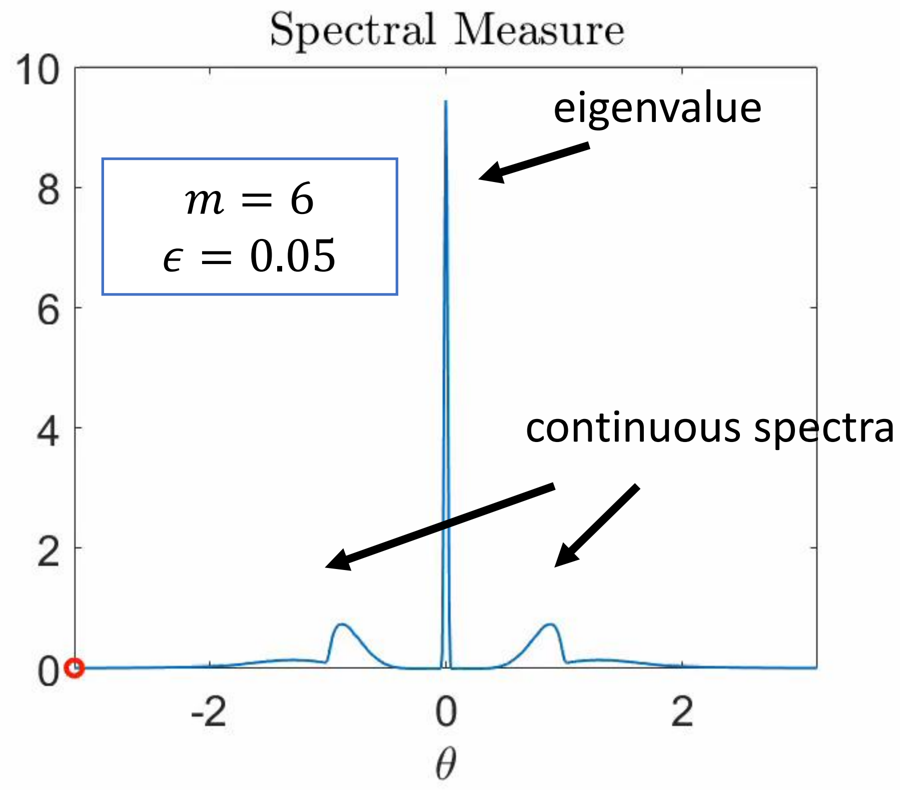

Increased oscillations of generalized eigenfunction

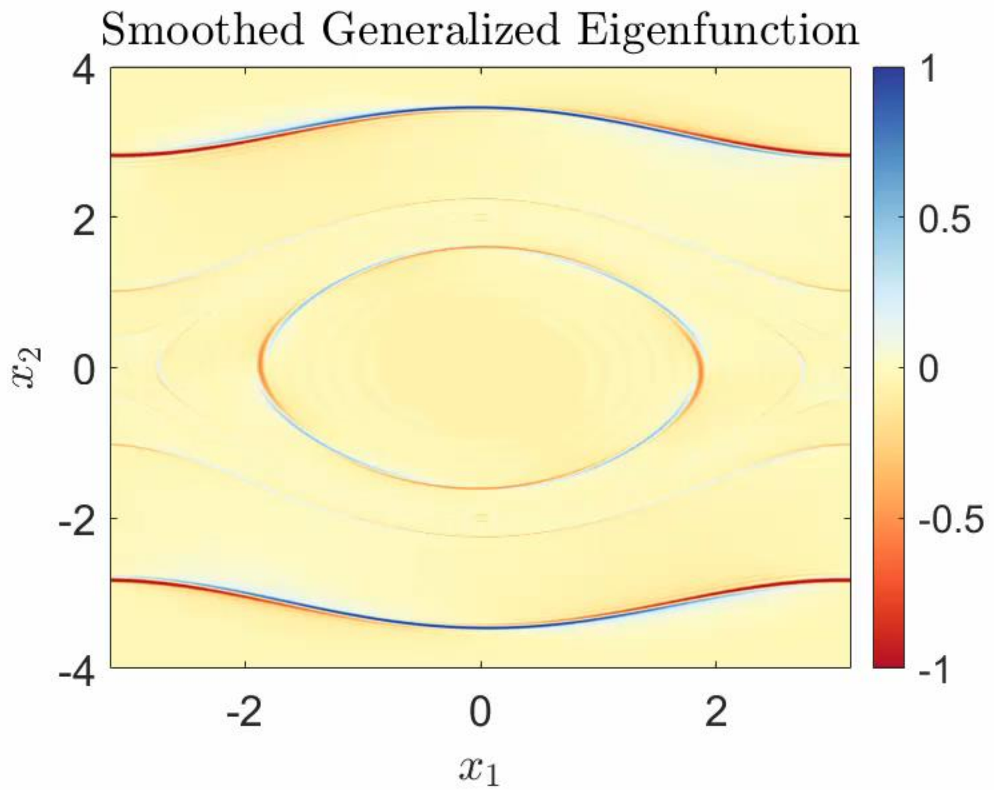
# Example: Nonlinear pendulum

*Experimental Details*
Length-one trajectories over grid
$M = 500 \times 500, N = 300$
$g(x_1, x_2) = \exp(ix_1)/\cosh(x_2)$
Krylov subspace: $V_N = \{g, \mathcal{K}g, \ldots, \mathcal{K}^{N-1}g\}$

$\dot{x}_1 = x_2,\ \dot{x}_2 = -\sin(x_1),\qquad \Omega = [-\pi, \pi]_{\text{per}} \times \mathbb{R},\qquad \Delta_t = 1,\qquad \omega =$ Lebesgue measure

**Explicit formula:** $g_\theta$ become plane waves concentrated on unions of lines of constant energy as $\epsilon \downarrow 0$.



# Interlude: Can we always find an $\mathcal{S}$?

- If $\mathcal{K}$ is represented by an infinite matrix with finitely many non-zero entries in each column, can build $\mathcal{S}$ using weighted sequence spaces.
- Always possible using time-delay embedding:

$$\{\text{Unions (different } g\text{) of spaces } \mathrm{span}\{g, \mathcal{K}g, \dots, \mathcal{K}^{N-1}g, \dots\}\} \subset \mathcal{S}$$

- Generalises shift example but in coefficient space w.r.t. Krylov subspaces.

# Interlude: Can we always find an $\mathcal{S}$?

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- Always possible using time-delay embedding:

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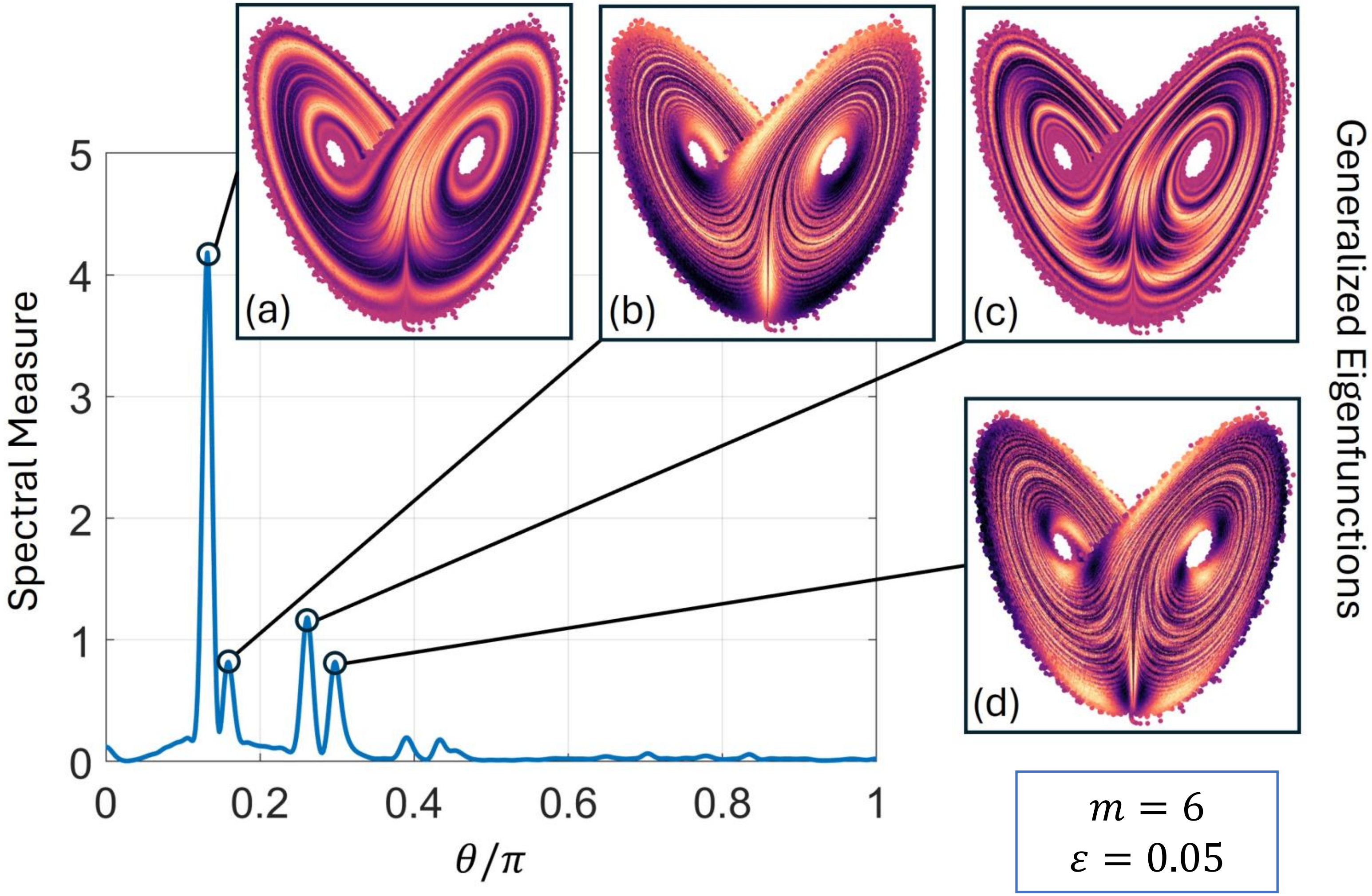
- Generalises shift example but in coefficient space w.r.t. Krylov subspaces.

Let’s do this for Lorenz…

# Example: Lorenz system

$\dot{x}_1 = 10(x_2 - x_1),\ \dot{x}_2 = x_1(28 - x_3) - x_2,\ \dot{x}_3 = x_1x_2 - 8/3\,x_3, \quad \Delta_t = 0.05, \ \ \Omega = \text{attractor},\ \ \omega = \text{SRB measure}$




$m = 6$
$\varepsilon = 0.05$

No formula for
generalized eigenfunctions!!

*Experimental Details*

Single trajectory (ergodic system)

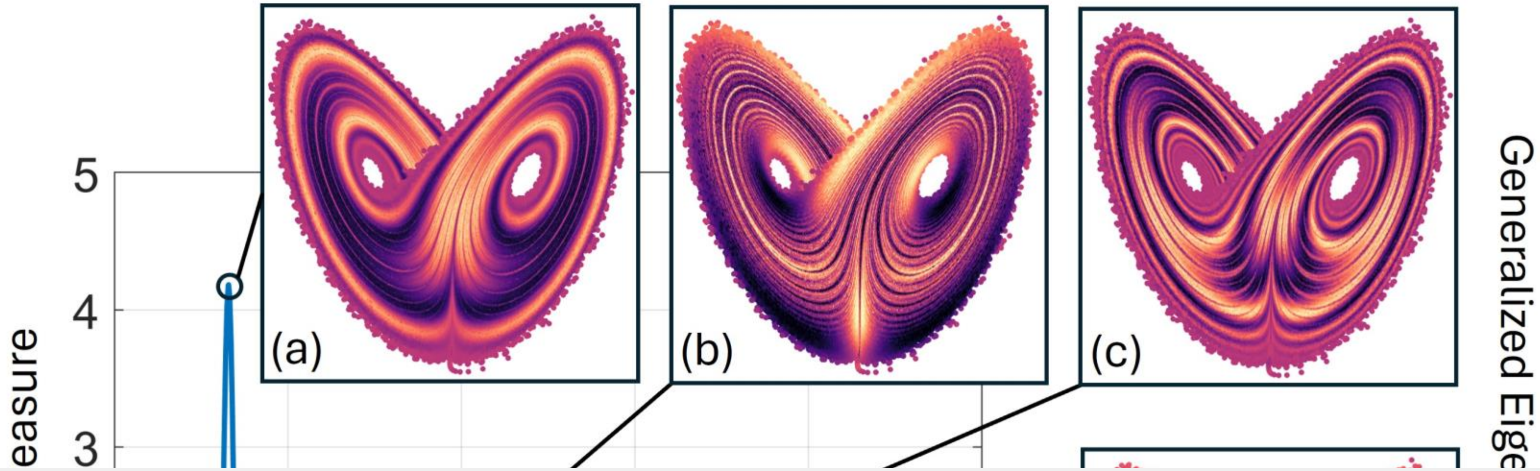
$M = 10000, N = 1000$

$$g(x_1, x_2, x_3) = \tanh\left(\frac{x_1x_2 - 5x_3}{10}\right) - c$$

Krylov subspace: $V_N = \{g, \mathcal{K}g, \dots, \mathcal{K}^{N-1}g\}$

# Example: Lorenz system

$\dot{x}_1 = 10(x_2 - x_1),\ \dot{x}_2 = x_1(28 - x_3) - x_2,\ \dot{x}_3 = x_1 x_2 - 8/3\, x_3, \quad \Delta_t = 0.05, \ \ \Omega = \text{attractor},\ \ \omega = \text{SRB measure}$




No formula for
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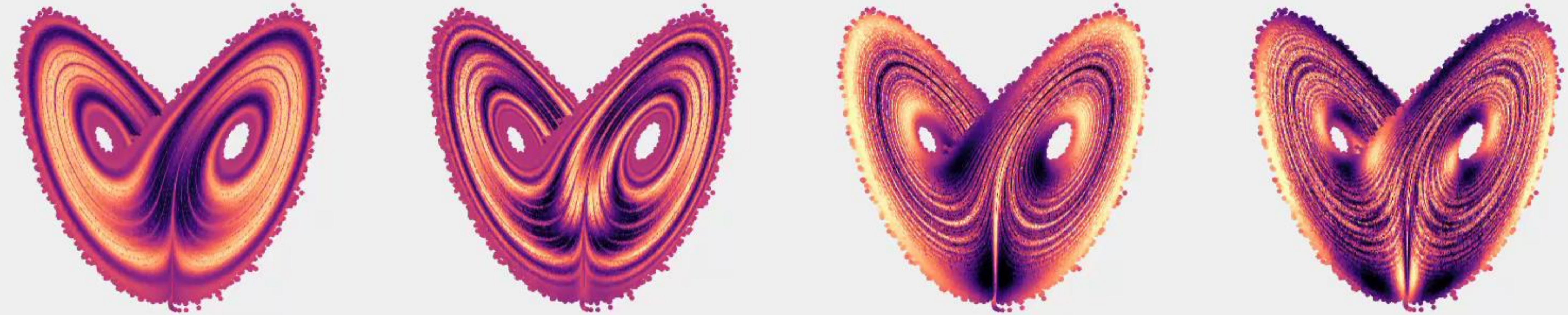
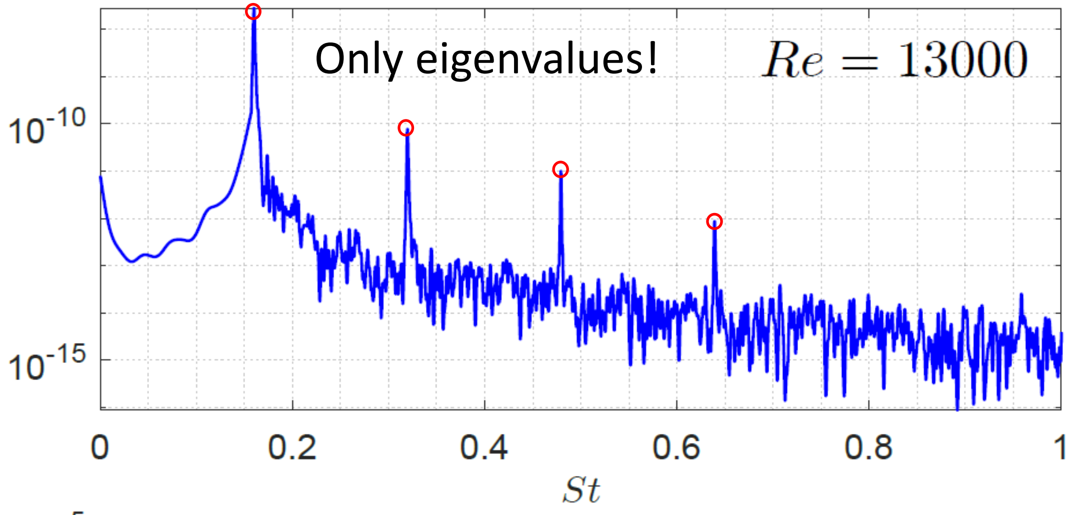
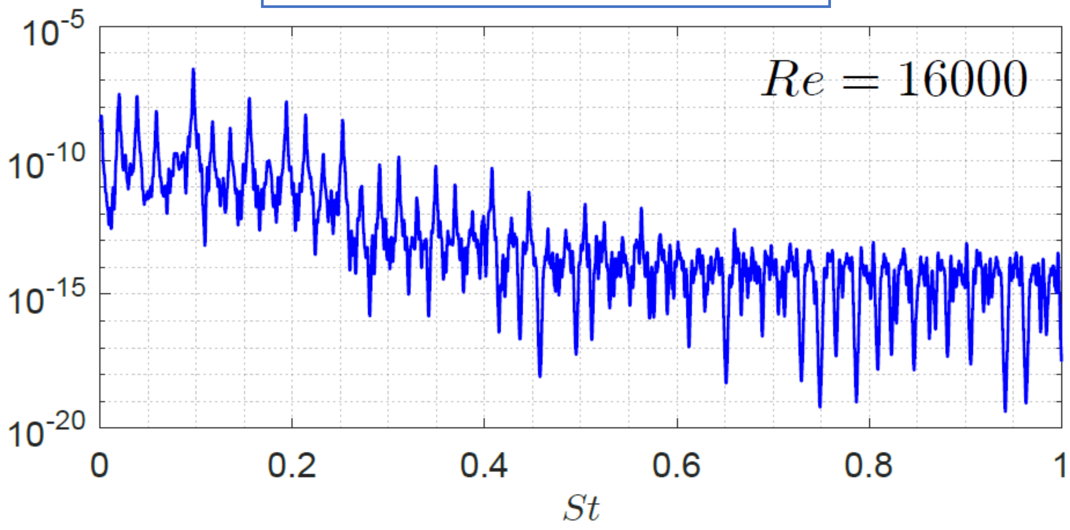
*Experimental Details*

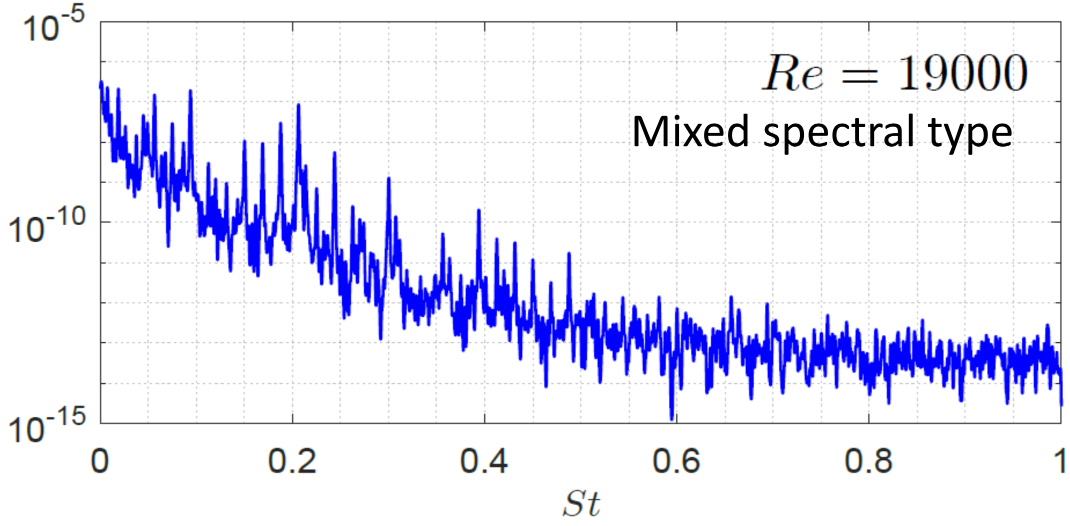


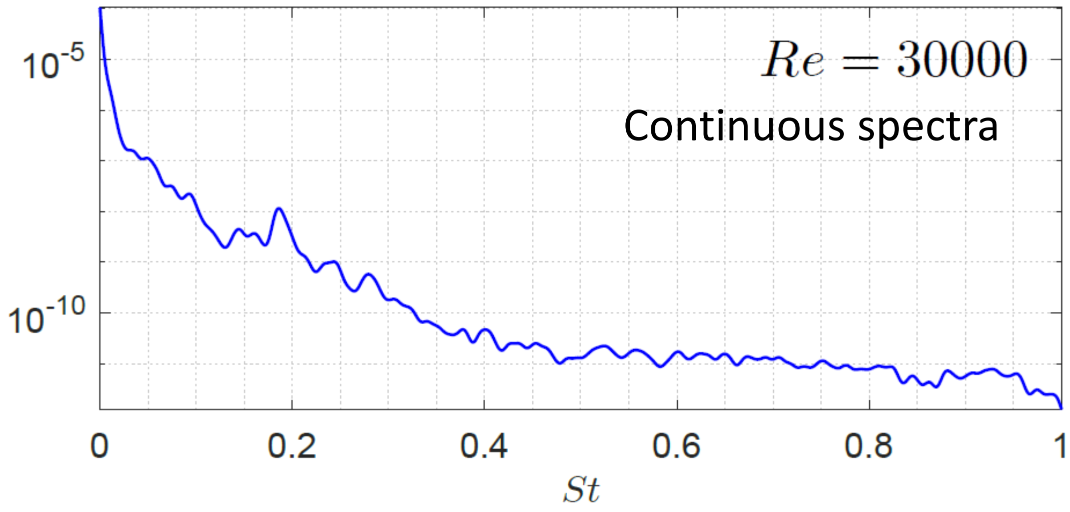
# Example: Noisy cavity flow (spectral measures)

Single trajectory
$M = 10000, N$ varies
Basis: POD modes
20% Gaussian noise
*Raw measurements provided
Arbabi and Mezić (PRF 2017)



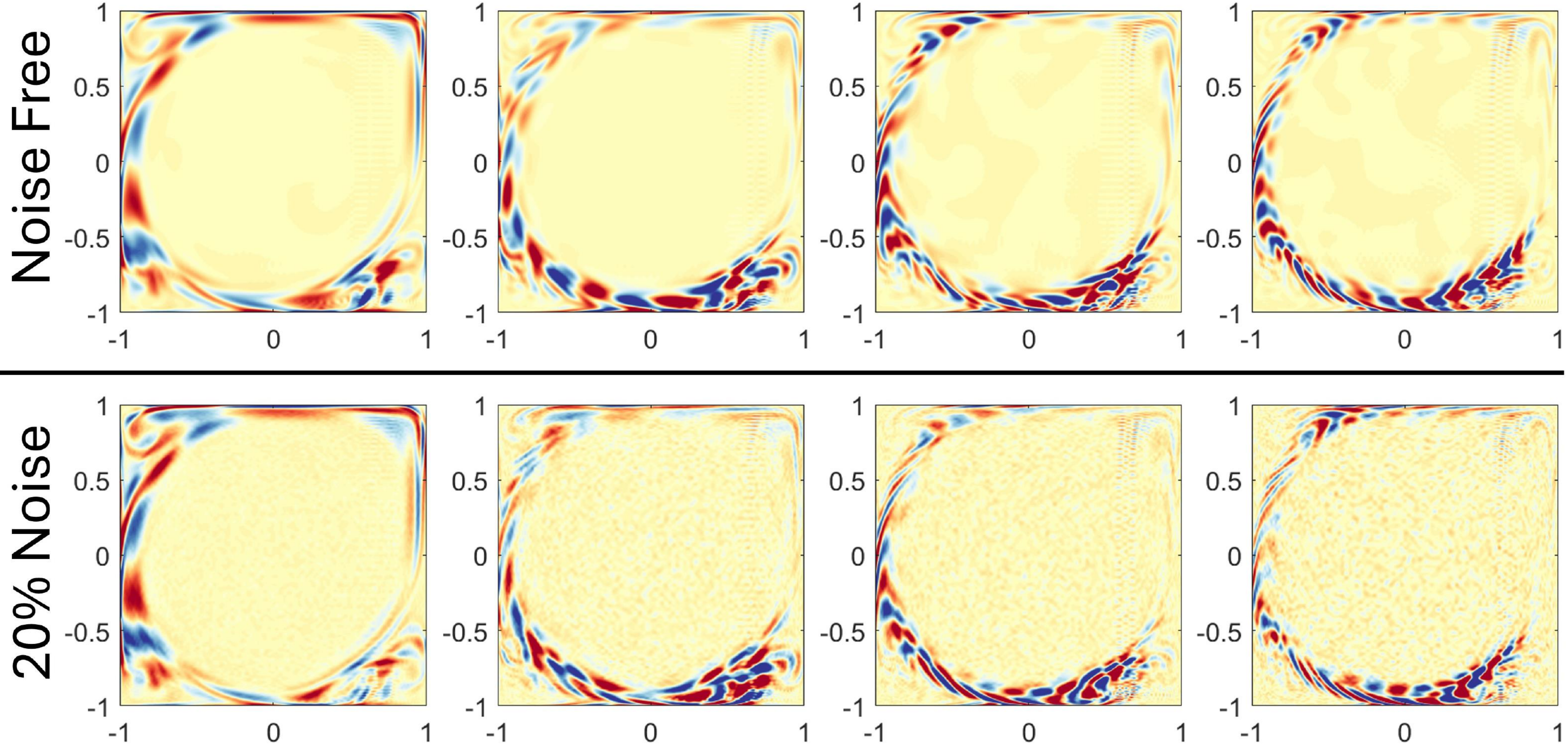



# Example: Noisy cavity flow (generalized Koopman modes)

Re=30000
Deep in the continuous spectrum!!!



# Summary

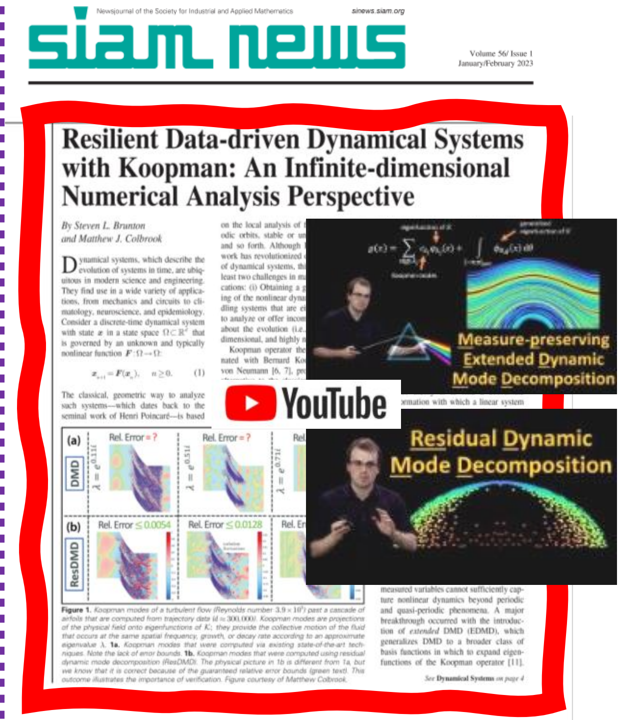
**Practical + dictionary agnostic + theoretical guarantees**

- **mpEDMD**
  - EDMD + enforcing measure-preserving (polar decomposition of Galerkin)
  - Convergence of spectral measures, spectra, Koopman mode decomposition.
  - Long-time stability, improved qualitative behavior, increased stability to noise.
- **Rigged DMD**
  - Continuous spectra and generalized eigenfunctions.
  - Smoothing kernels + resolvent (using mpEDMD).
  - High-order convergence.

**Future work**
- Use in control
- What about other function spaces? E.g., RKHS

[General (non-measure-preserving) systems: ResDMD]

**Brief Summaries**



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