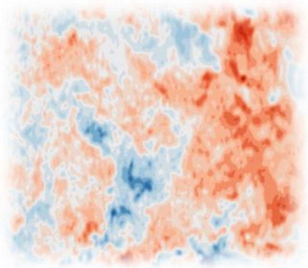
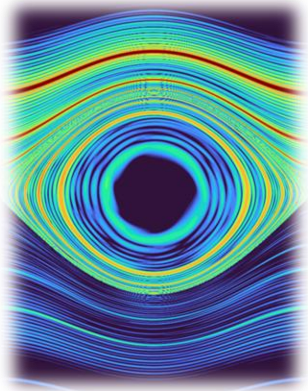




Learning unitary Koopman operators from trajectory data

Matthew Colbrook

University of Cambridge

26/02/2025

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

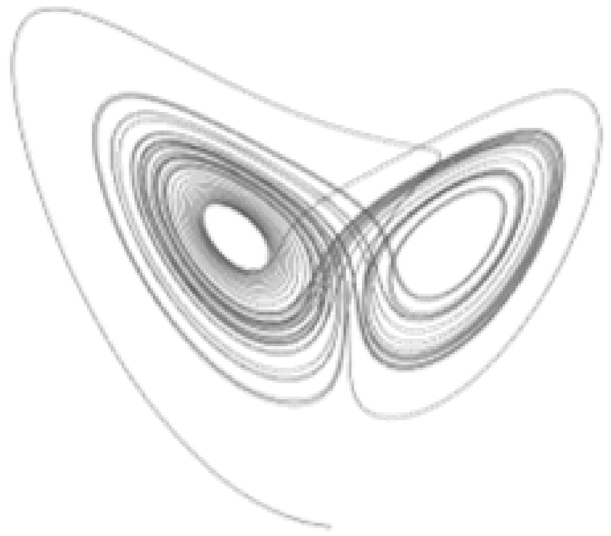
Data-driven dynamical systems

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

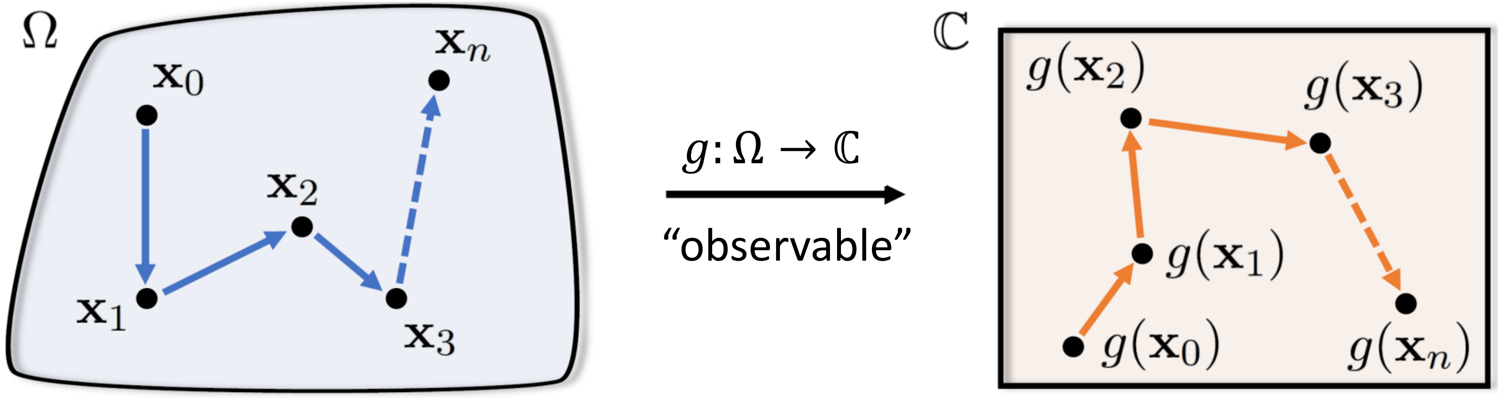
Unknown function $F: \Omega \to \Omega$ governs dynamics: $x_{n+1} = F(x_n)$.

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

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

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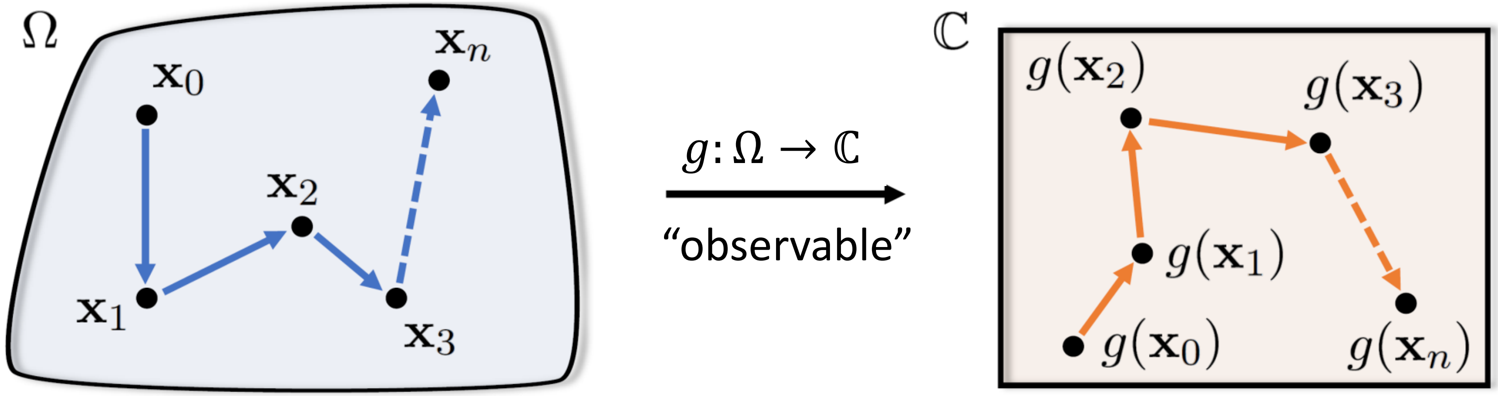

- $\mathcal{K}$ acts on functions $g:\Omega \to \mathbb{C}$, $[\mathcal{K}g](x) = g(F(x))$.
- Function space: $g \in L^2(\Omega,\omega)$, positive measure ω, inner product $\langle\cdot,\cdot\rangle$.

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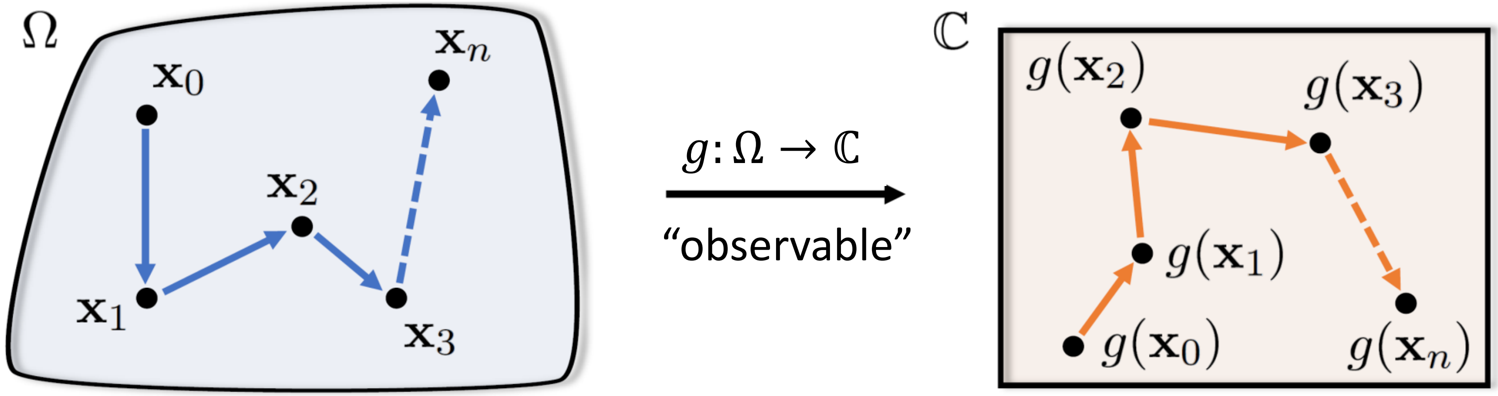

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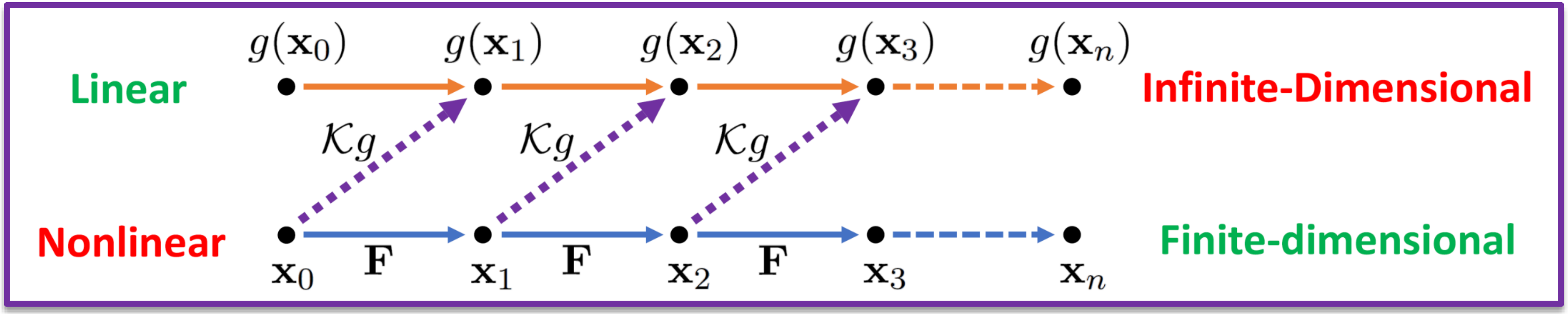

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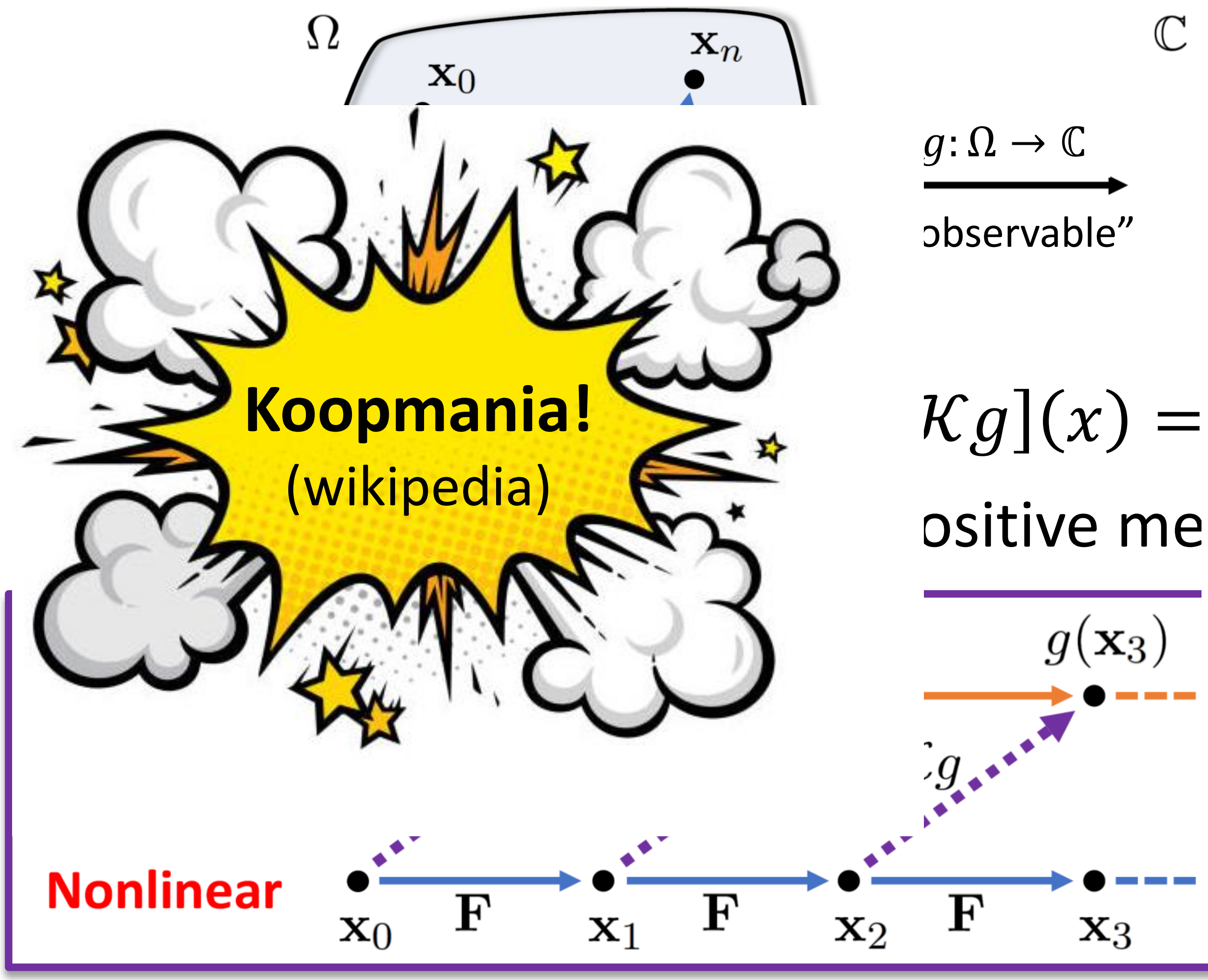

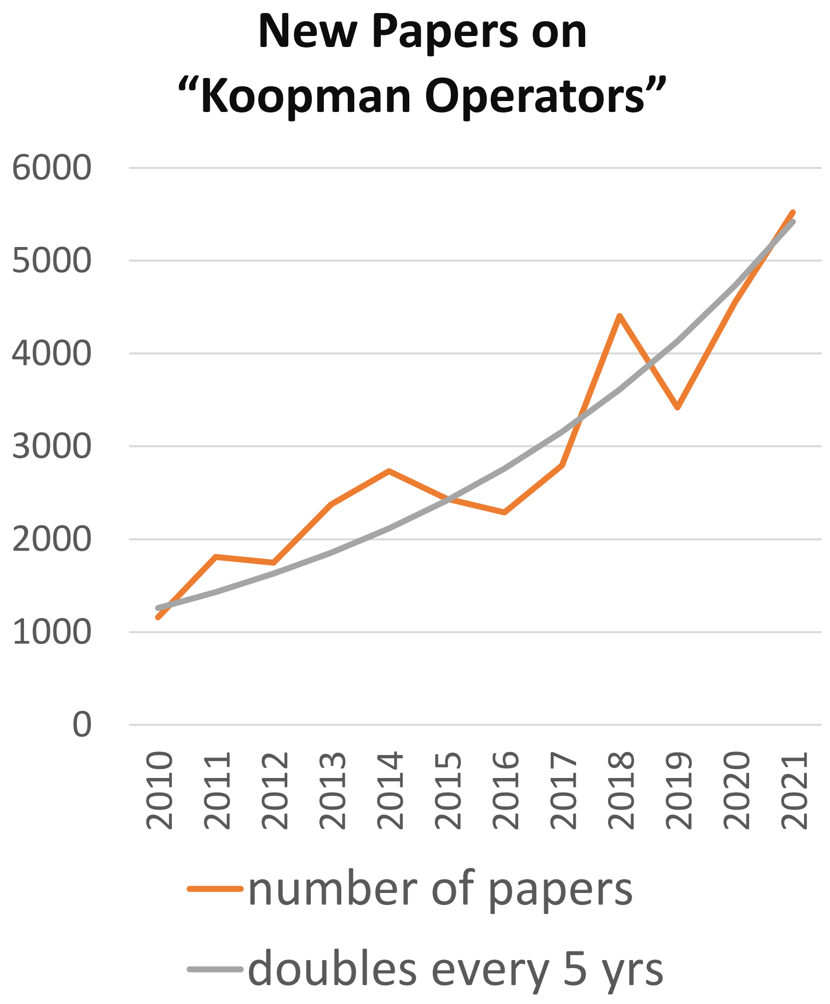

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Koopman mode decomposition

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

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

eigenfunction of $\mathcal{K}$

generalized eigenfunction of $\mathcal{K}$

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

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

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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Our setting – unitary evolution

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

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

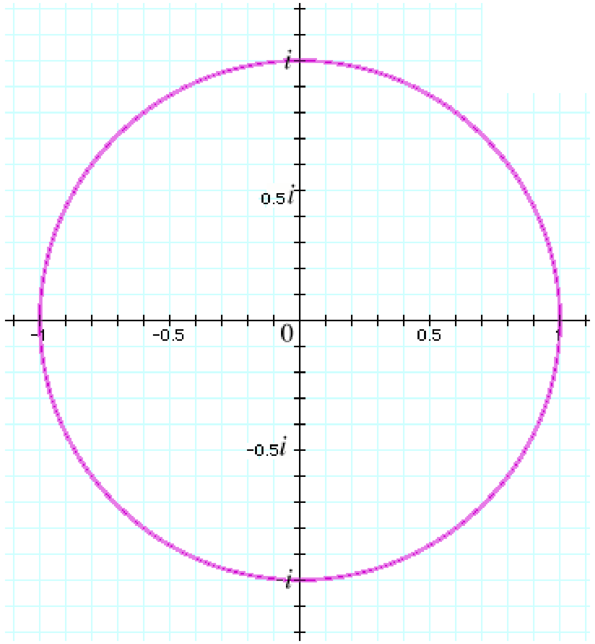
Assume: System is **measure-preserving** (F preserves ω)

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

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

$$\Longrightarrow \mathrm{Spec}(\mathcal{K}) \subseteq \{z : |z| \leq 1\}$$

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



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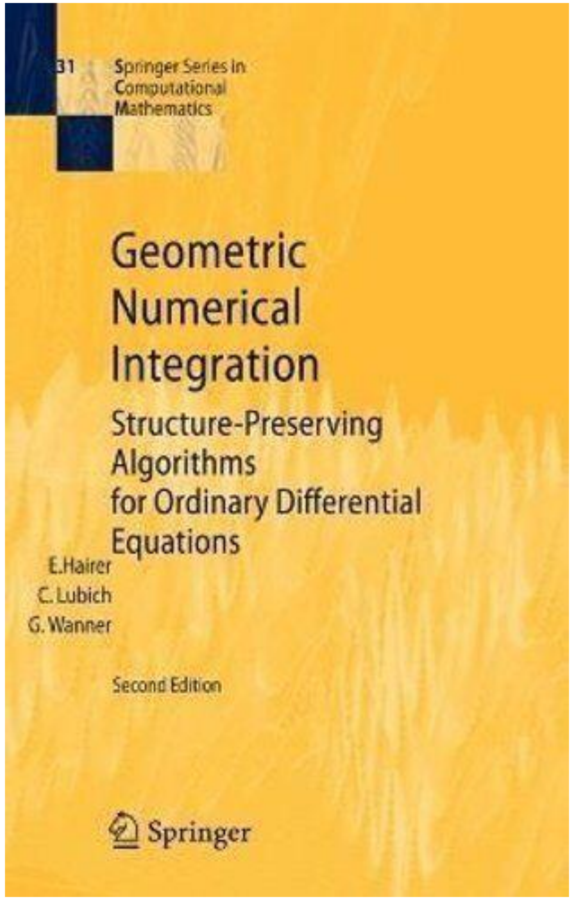

WANT: Approximation of $\mathcal{K}$ that preserves $\|\cdot\|$
(e.g., stability, long-time behavior etc.)...

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

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

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

Two-way infinite

truncate /discretize $\longrightarrow$

Jordan block!

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

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

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

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

The most important slide

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

polar decomposition $\longrightarrow$

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)

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

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

quadrature

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

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

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

- 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

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

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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 $\mathcal{P}_{V_N}\mathcal{K}\mathcal{P}_{V_N}^*$.

Spectral measures → diagonalisation

- **Finite dimensions:** Unitary $B \in \mathbb{C}^{n\times n}$, 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 e-vectors!
  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

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

$$\underset{\text{Fourier coefficients}}{\widehat{\mu_g}(n)} = \int_{\mathbb{T}} \underbrace{\lambda^n \, \mathrm{d}\mu_g(\lambda)}_{\text{moments}} = \underbrace{\langle \mathcal{K}^n g, g \rangle}_{\text{correlations}}$$

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 $\lim_{N\to\infty} \|g - \Psi\mathbf{g}_N\| = 0$,

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

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

Matching autocorrelations!

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

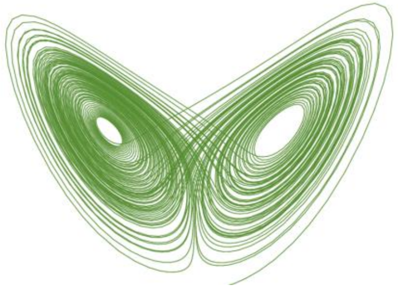
$\mathbb{K}$: mpEDMD matrix
λ_j: eigenvalues of $\mathbb{K}$
v_j: eigenvectors of $\mathbb{K}$
$V_N = \mathrm{span}\{\psi_1, \ldots, \psi_N\}$

Further convergence

- Projection-valued measures (e.g., functional calculus, L^2 forecasting).
- Koopman mode decomposition.
- Spectrum.
- Generalized eigenfunctions (but that's another story!)

Key ingredient: **unitary** discretization.

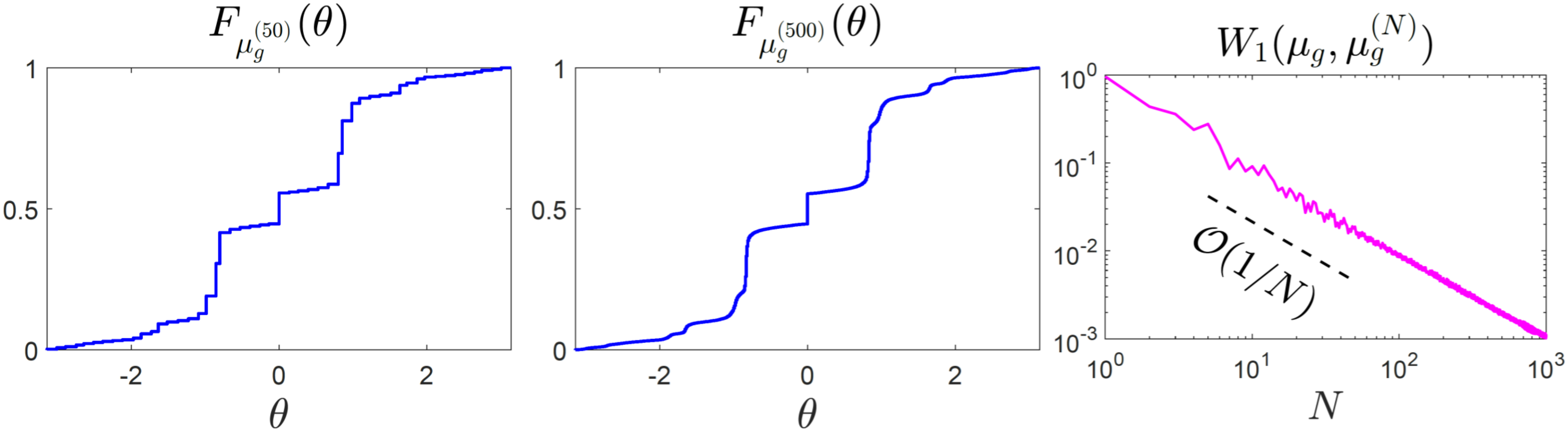
Lorenz system



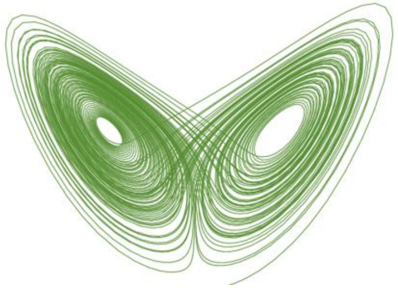
$$\dot{x}_1 = 10(x_2 - x_1), \qquad \dot{x}_2 = x_1(28 - x_3) - x_2, \qquad \dot{x}_3 = x_1 x_2 - 8/3\, x_3, \qquad \Delta_t = 0.1$$

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

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



Lorenz system



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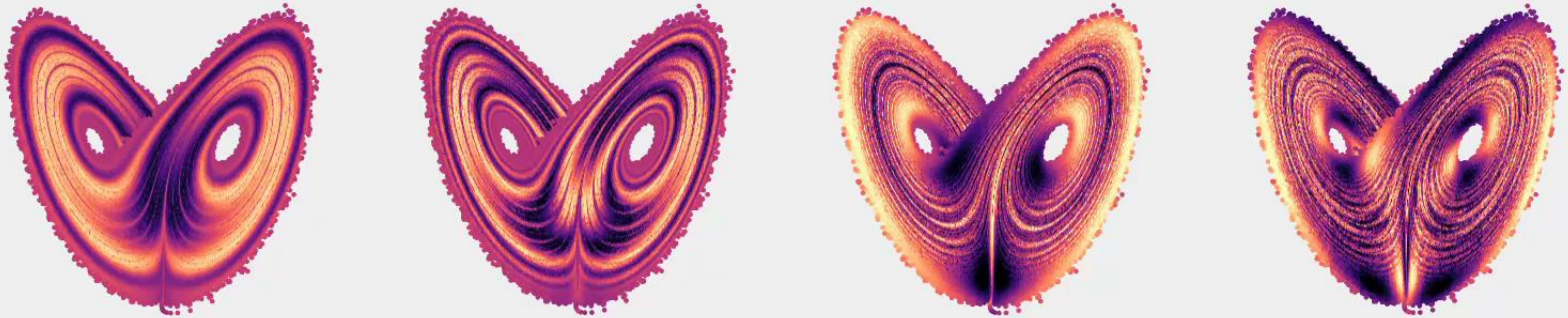
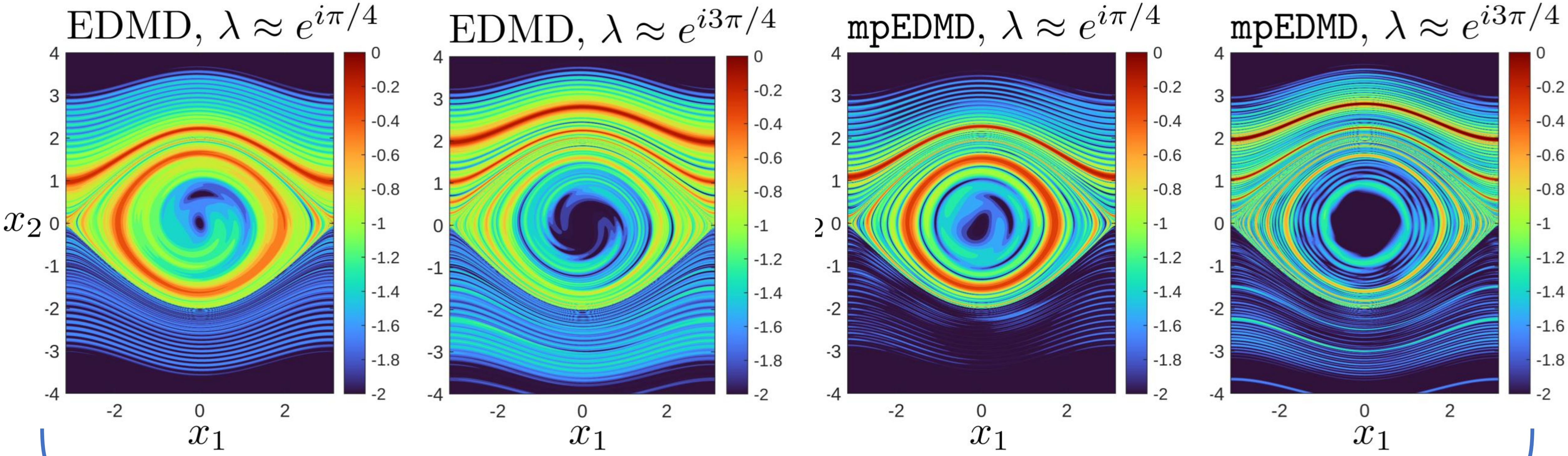
Coherent features!



Nonlinear pendulum

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

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



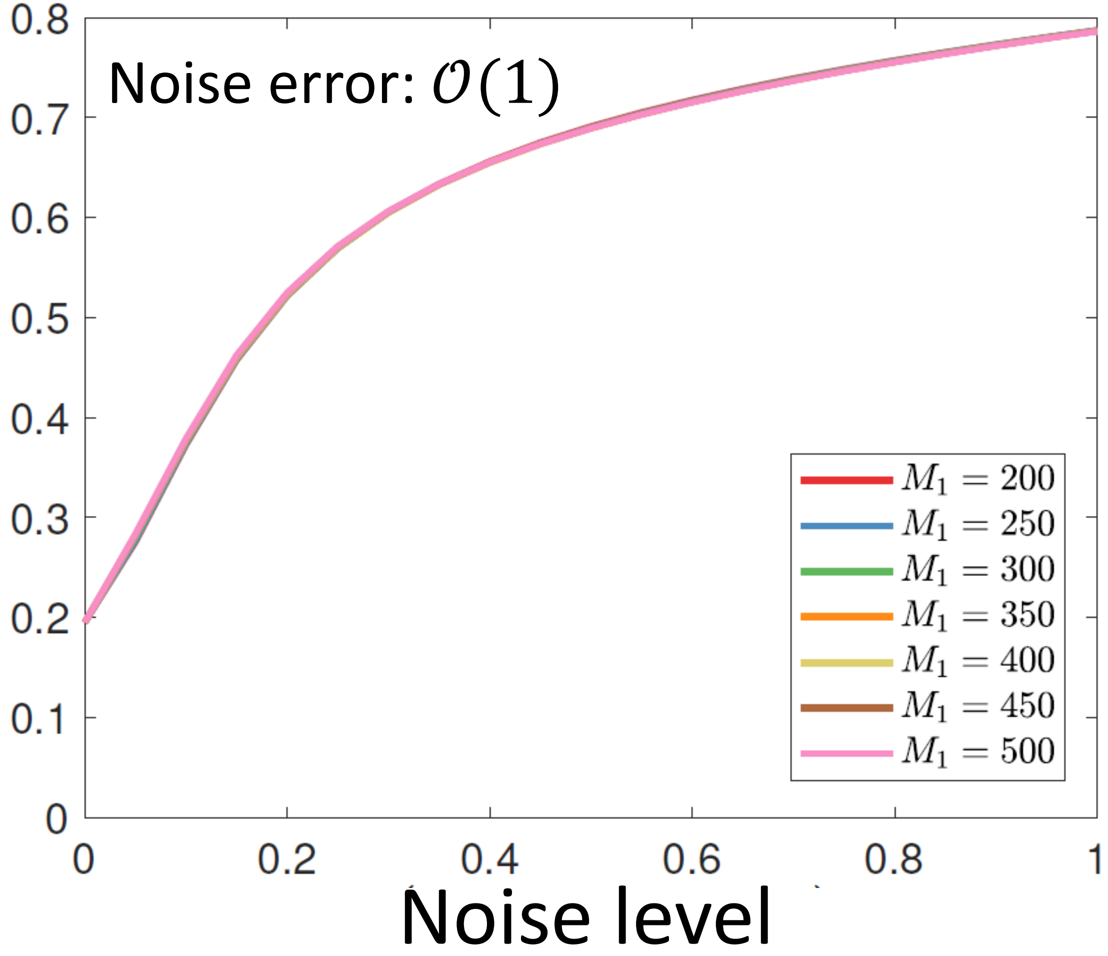
Dissipation, low accuracy

$\log_{10}(|v_j|)$

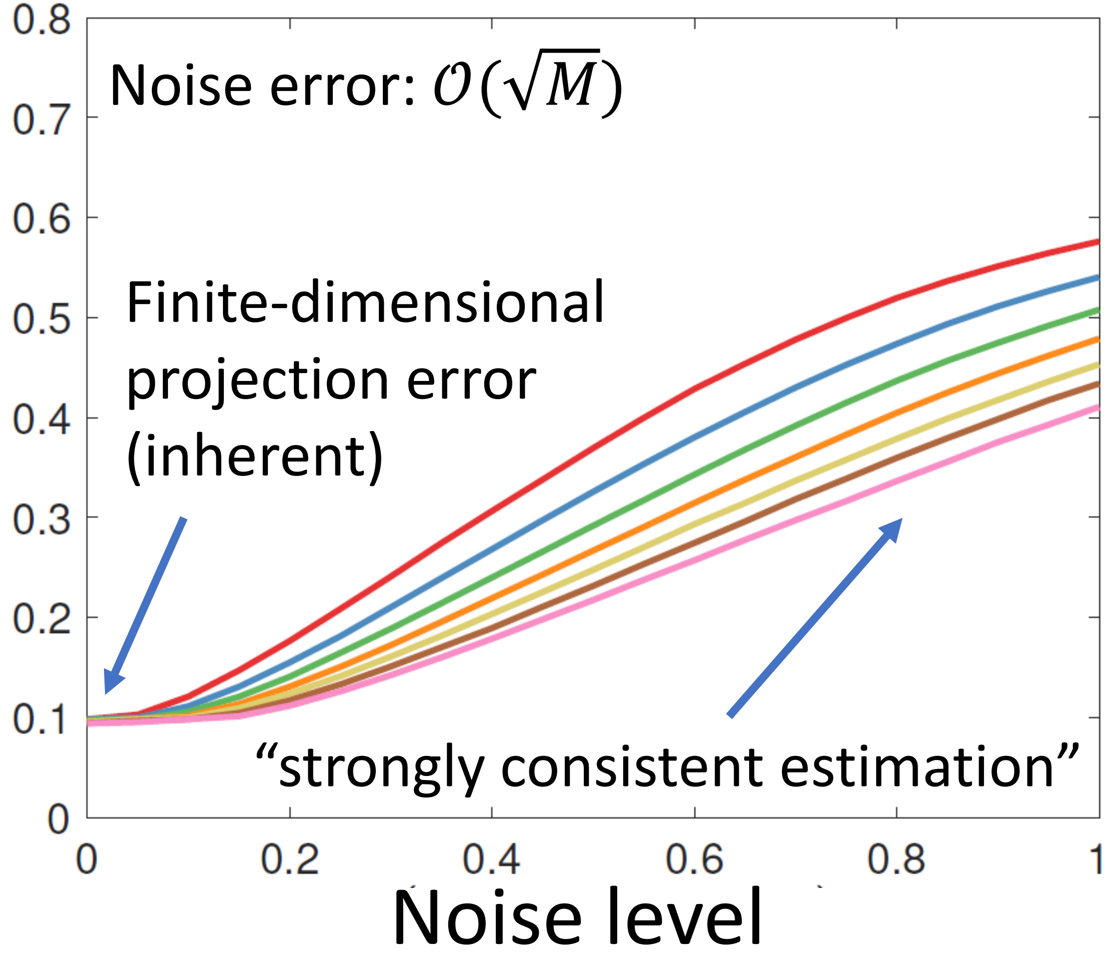
Conservative, high accuracy

Robustness to noise: Gauss. noise for Ψ_X, Ψ_Y

Mean inf. dim. residual (EDMD)

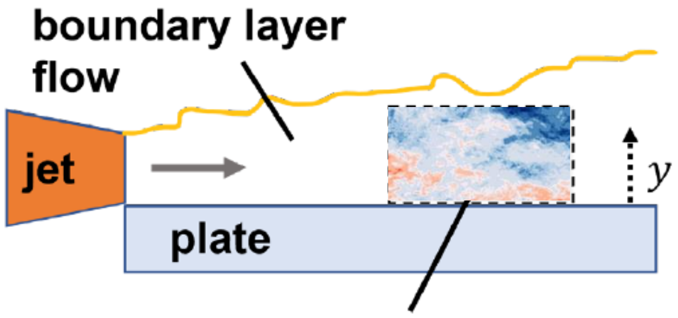


Mean inf. dim. residual (mpEDMD)



Turbulence (real data)

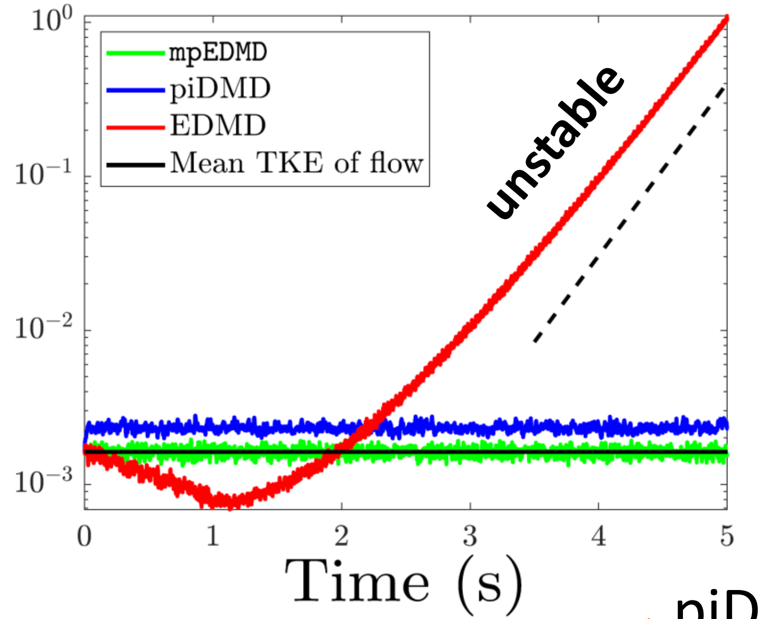
Experimental setup



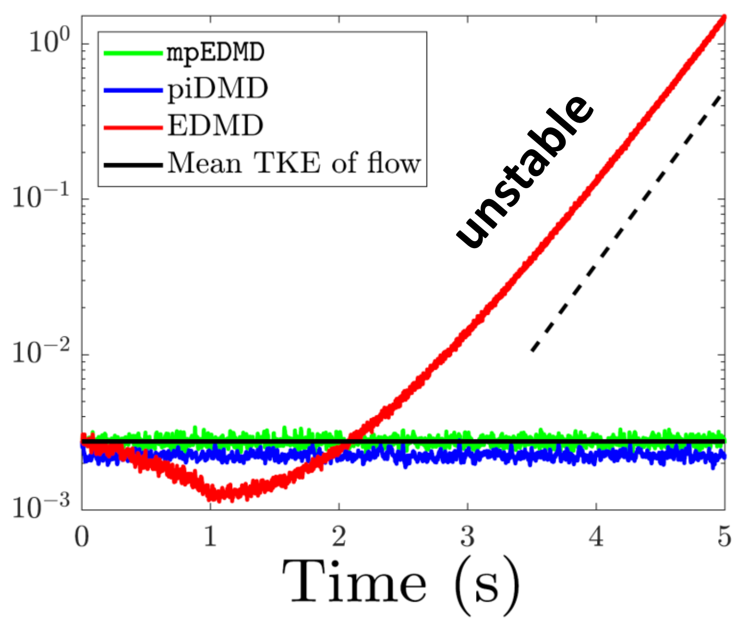
- Reynolds number $\approx 6.4 \times 10^4$
- Ambient dimension (d) $\approx 100{,}000$ (velocity at measurement points)

*PIV data provided by Máté Szőke (Virginia Tech)

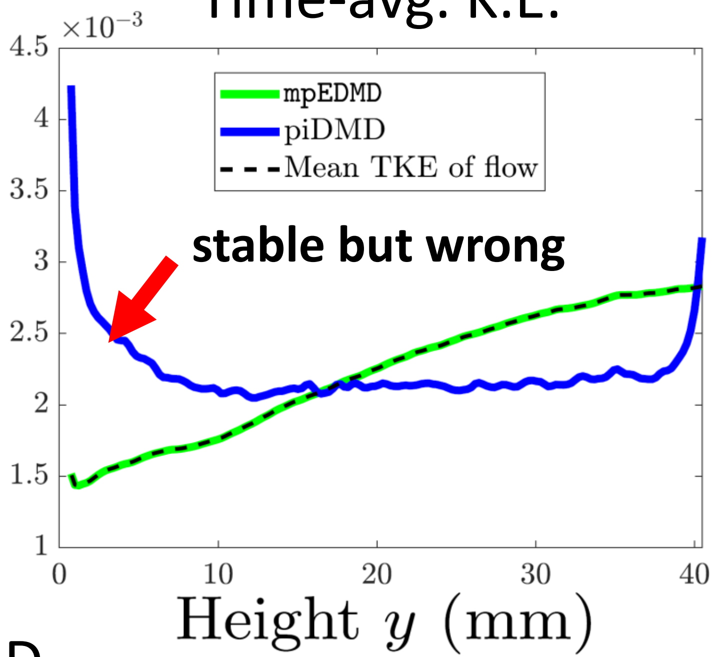
Turbulent K.E. y=5mm



Turbulent K.E. y=35mm



Time-avg. K.E.

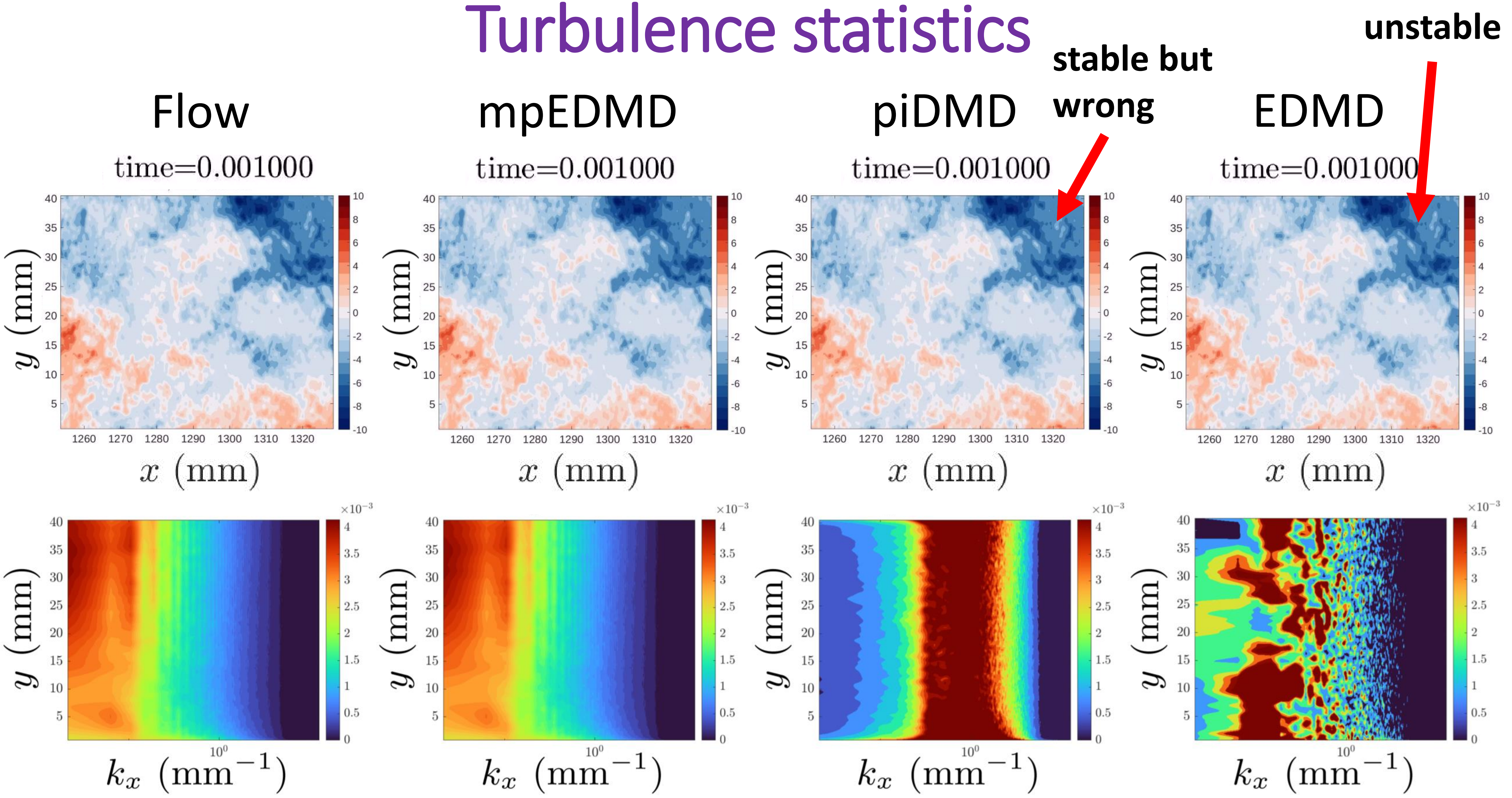


piDMD

EDMD

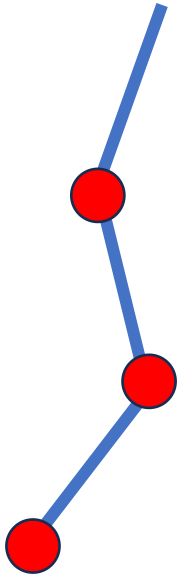
- Baddoo, Herrmann, McKeon, Kutz, Brunton, *"Physics-informed dynamic mode decomposition (piDMD),"* preprint.
- Williams, Kevrekidis, Rowley *"A data-driven approximation of the Koopman operator: Extending dynamic mode decomposition,"* **J. Nonlinear Sci.**, 2015.

Turbulence statistics



Future work (with Davide)

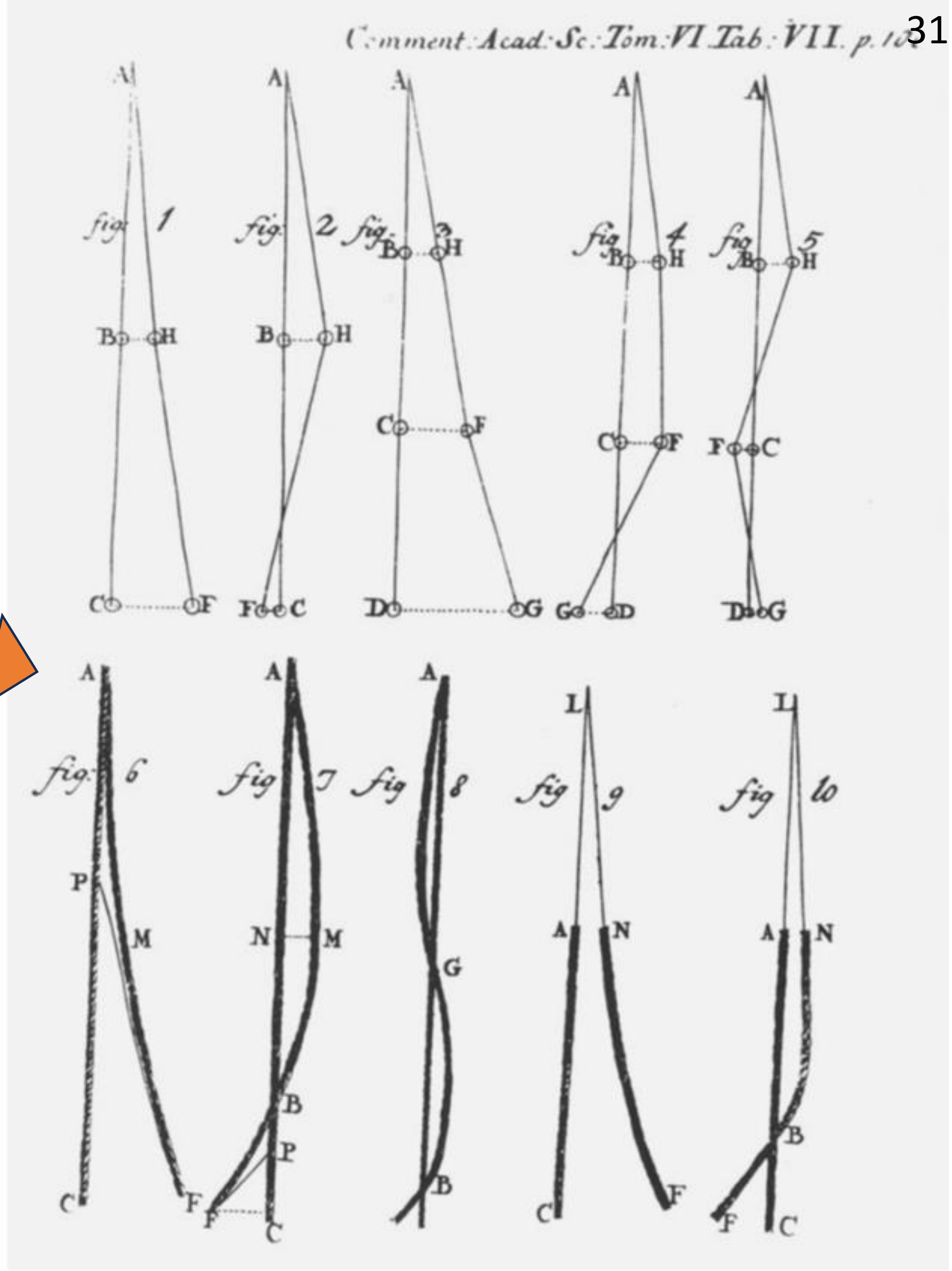
Earliest published image of an eigenvector from Daniel Bernoulli's 1733 masterpiece "Theoremata de oscillationibus corporum filo flexili connexorum et catenae verticaliter suspensae".



n pendula

Does it help collecting data using geometric integrators?

What happens as $n \to \infty$?



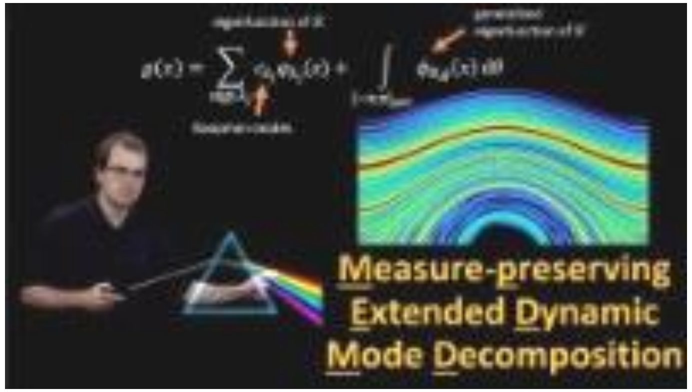
Summary: Geometric integration for EDMD

- 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.
- Simple, flexible: easy to combine with any DMD-type method!

OPPORTUNITY: further structure-preservation (e.g., learning symmetries)

Shameless plug: read more in upcoming CUP book, "Infinite-Dimensional Spectral Computations"

Short video summaries available on YouTube



https://github.com/MColbrook/Measure-preserving-Extended-Dynamic-Mode-Decomposition

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