measure-preserving Extended Dynamic Mode Decomposition: Structure-preserving Koopmanism

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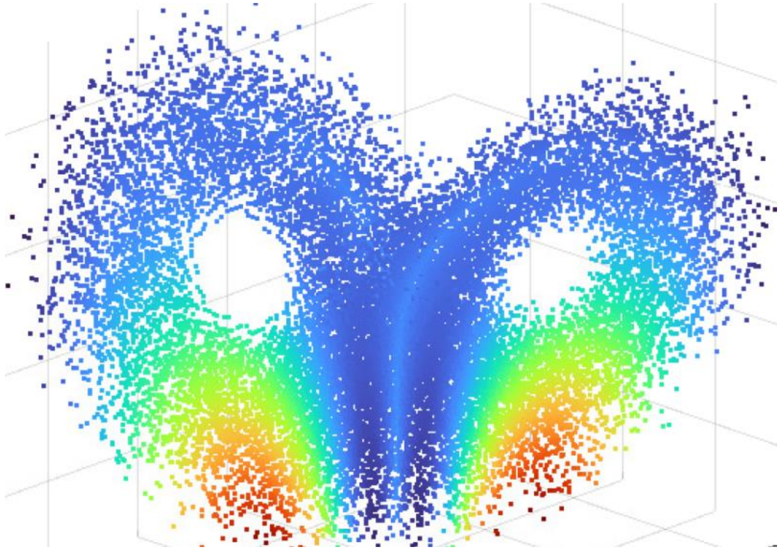
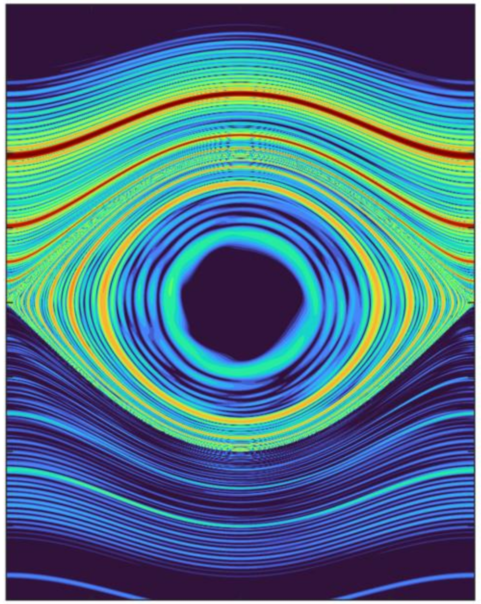
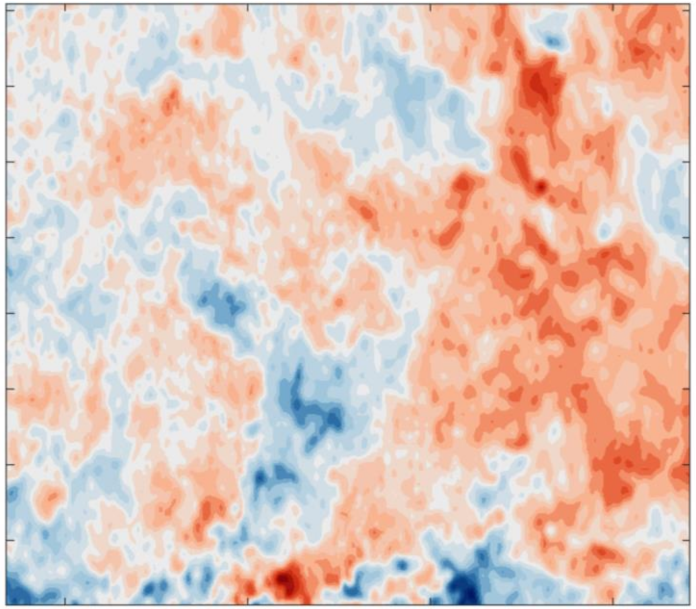






Data-driven dynamical systems

- State $x \in \Omega \subseteq \mathbb{R}^d$, ***unknown*** function $F: \Omega \rightarrow \Omega$ governs dynamics

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

- **Given:** Trajectory data $\left\{x^{(m)}, y^{(m)} = F\left(x^{(m)}\right)\right\}_{m=1}^{M}$
- **Koopman operator** $\mathcal{K}$ acts on <u>functions</u> $g: \Omega \rightarrow \mathbb{C}$

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

- $\mathcal{K}$ is ***linear*** but acts on an ***infinite-dimensional*** space.
- Work in $L^2(\Omega, \omega)$ for positive measure ω, with inner product $\langle\cdot,\cdot\rangle$.

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

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

Setting

Typical approach: $\mathcal{K} \longrightarrow \mathbb{K} \in \mathbb{C}^{N \times N}$

Challenges:

1) **Spectral pollution:** Approximate spurious modes $\lambda \notin \mathrm{Spec}(\mathcal{K})$.

2) **Spectral invisibility:** Miss parts of $\mathrm{Spec}(\mathcal{K})$.

3) **Continuous spectra.**

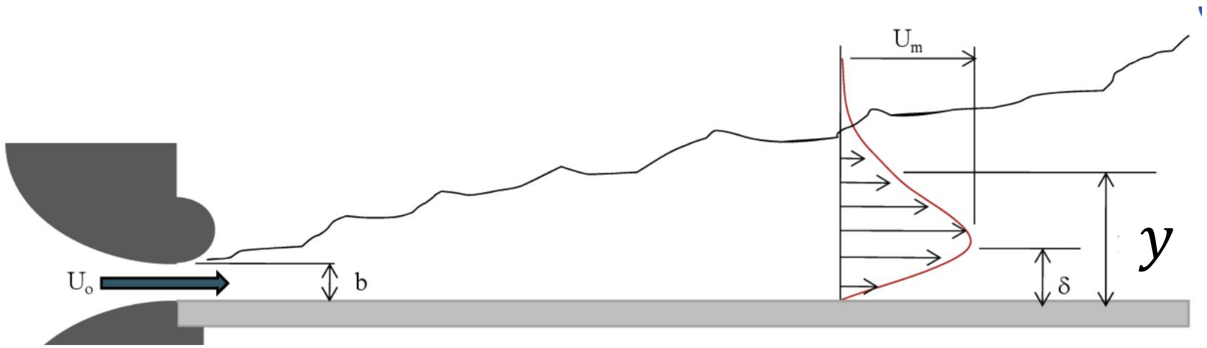
Assume: System is **measure-preserving**

$$\Leftrightarrow \mathcal{K}^*\mathcal{K} = I \text{ (isometry)}$$ (we consider unitary extensions)

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

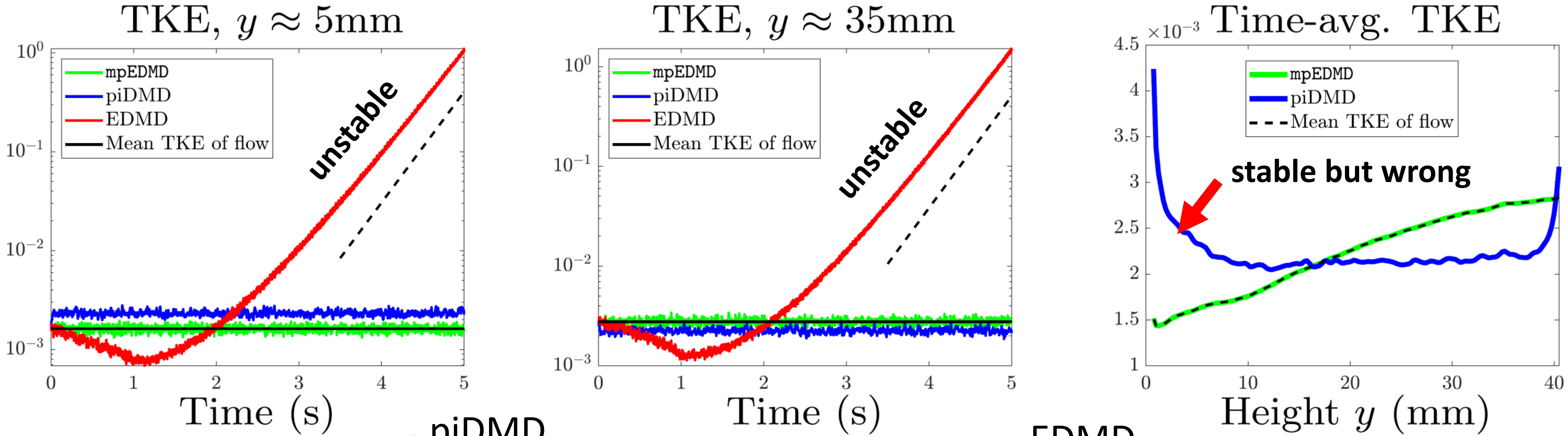
WANT: Method preserves measure (e.g., stability, long-time behavior etc.)...

Motivating example



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

*Raw measurements provided by Máté Szőke (Virginia Tech)



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.

Extended Dynamic Mode Decomposition (EDMD)

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

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

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

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

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

- 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.

Another interpretation

$$\Psi(x) = [\psi_1(x) \;\; \dots \;\; \psi_N(x)], \qquad g = \sum_{j=1}^{N} \mathbf{g}_j \psi_j = \Psi\mathbf{g}, \qquad \mathcal{K}g = \Psi\mathbb{K}\mathbf{g} + R(g,\cdot)$$

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

$\downarrow$ quadrature

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

A simple idea

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

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

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

quadrature

orthogonal Procrustes problem

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

The mpEDMD algorithm

Algorithm: `mpEDMD` for approximating spectral properties of $\mathcal{K}$.

Input: Snapshot data $\{\boldsymbol{x}^{(m)}, \boldsymbol{y}^{(m)} = F(\boldsymbol{x}^{(m)})\}_{m=1}^{M}$, quadrature weights $\{w_m\}_{m=1}^{M}$, and a dictionary of functions $\{\psi_j\}_{j=1}^{N}$.

1: Compute $G = \Psi_X^* W \Psi_X$ and $A = \Psi_X^* W \Psi_Y$
2: Compute an SVD of $G^{-1/2} A^* G^{-1/2} = U_1 \Sigma U_2^*$
3: Compute the eigendecomposition $U_2 U_1^* = \hat{V} \Lambda \hat{V}^*$
4: Compute $\mathbb{K} = G^{-1/2} U_2 U_1^* G^{1/2}$ and $V = G^{-1/2} \hat{V}$

Output: Koopman matrix $\mathbb{K}$, with eigenvectors V and eigenvalues Λ.

In a nutshell: *Galerkin meets polar decomposition*.

(This also allows us to prove numerical stability.)

Relation to previous approaches

- **Physics-informed DMD:** Similar approach but doesn't use nonlinear observables or matrix G. Hence in general, not measure-preserving.

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

- **Periodic approximations via partitioning of state-space (e.g., on tori):** Can be considered a particular case of mpEDMD, related to Ulam's method.

  Govindarajan, Mohr, Chandrasekaran, Mezić, *"On the approximation of Koopman spectra for measure preserving transformations,"* **SIAM J. Appl. Dyn. Syst.**, 2019.

- **Compact regularizations of the skew-adjoint generator:** Measure-preserving method in continuous time through RKHS.

  Das, Giannakis, Slawinska, *"Reproducing kernel Hilbert space compactification of unitary evolution groups,"* **Appl. Comput. Harm. Anal.**, 2021.

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Spectral measures → diagonalisation

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

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

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

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

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

Convergence of projection-valued measure

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

This assumption cannot be dropped in general!

Theorem: Suppose that the quadrature rule converges, $\mathcal{K}$ is unitary, $\lim_{N\to\infty}\operatorname{dist}(h,V_N)=0$ for any $h\in L^2(\Omega,\omega)$. Then for any Lipschitz test function ξ, $g\in L^2(\Omega,\omega)$ and $\boldsymbol{g}_N\in\mathbb{C}^N$ with $\lim_{N\to\infty}\|g-\Psi\boldsymbol{g}_N\|=0$,

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

Key ingredients:

- Strong convergence of Galerkin approximation.
- Discretization by normal operators.

$\mathbb{K}$: mpEDMD matrix

λ_j: eigenvalues of $\mathbb{K}$

v_j: eigenvectors of $\mathbb{K}$

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

Convergence of scalar-valued measure

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

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

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

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

Matching autocorrelations!

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

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

Avoid spectral invisibility!

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

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What about spectral pollution?

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

Residuals ⇒ avoid spectral pollution!

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

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

Suitable conditions $\Longrightarrow \lim_{N\to\infty} \min_{g\in V_N} \|(\mathcal{K}-\lambda)\Psi \boldsymbol{g}\| / \|g\| = \mathrm{dist}(\lambda, \mathrm{Spec}_{\mathrm{ap}}(\mathcal{K}))$

Two methods:

- Clean up procedure for tolerance ε.
- Local minimization algorithm converges to $\mathrm{Spec}_{\mathrm{ap}}(\mathcal{K})$.

- C., T., *"Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems,"* preprint.
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Residuals ⇒ avoid spectral pollution!

Executive summary of **ResDMD**: (considers **<u>inf-dim</u>** residuals)

- Rigorous convergence for spectra and pseudospectra of general Koopman operators from snapshot data.
- Error bounds ⟹ aposteri verification of spectral quantities, Koopman mode decompositions, and learned dictionaries.
- Deals with spectral measures of general measure-preserving systems with explicit high-order convergence.

Suitable

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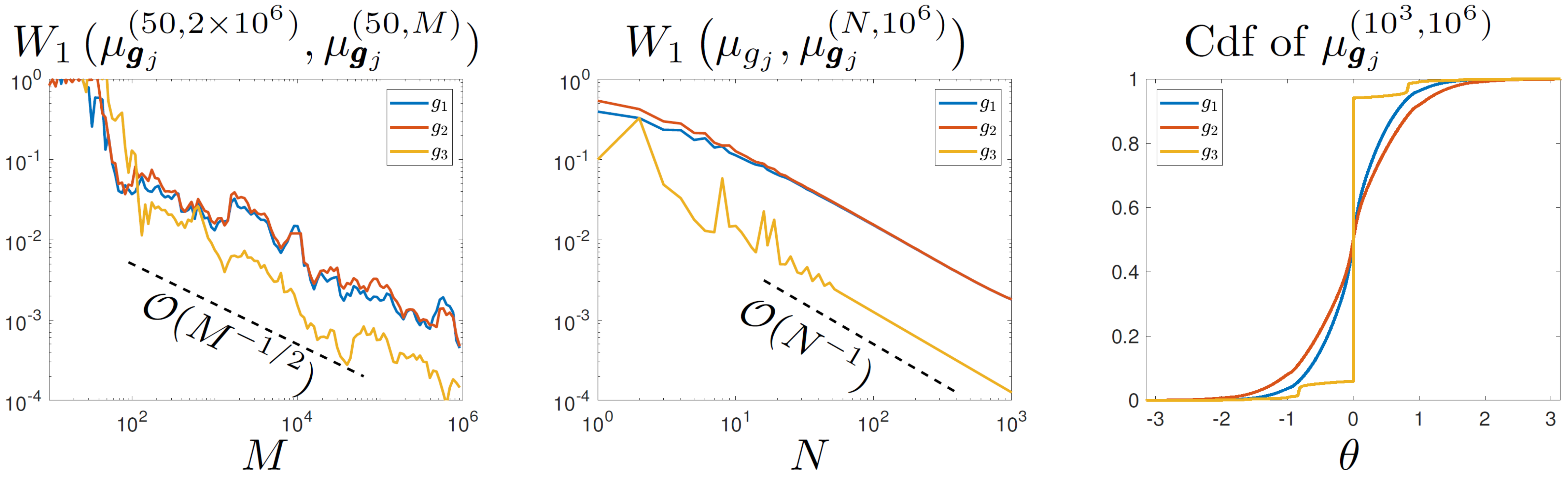
Lorenz system: scalar-valued spec meas

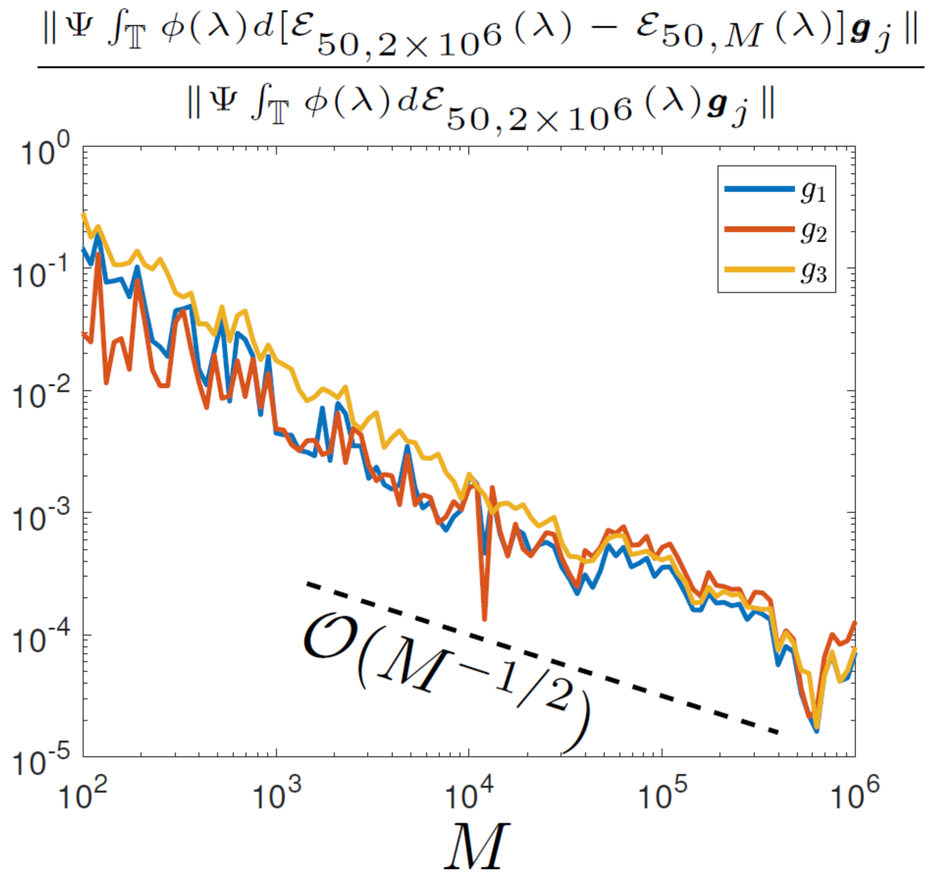
$$\dot{x}_1 = 10(x_2 - x_1), \quad \dot{x}_2 = x_1(28 - x_3) - x_2, \quad \dot{x}_3 = x_1 x_2 - 8/3\, x_3, \quad \Delta_t = 0.1$$

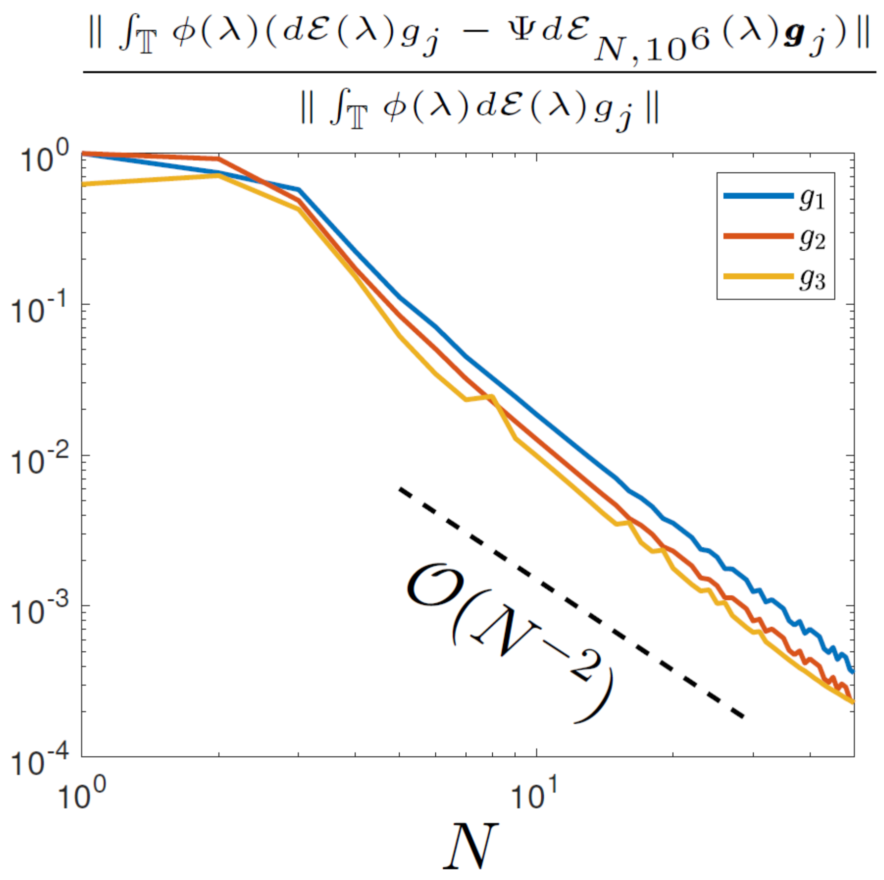
$$g_j = c_j[x]_j, \quad V_N = \mathrm{span}\{g_j, \mathcal{K}g_j, \dots, \mathcal{K}^{N-1}g_j\}$$



Lorenz system: projection-valued spec meas

$$V_N = \text{span}\{g_1, g_2, g_3, \mathcal{K}g_1, \mathcal{K}g_2, \mathcal{K}g_3, \dots, \mathcal{K}^{q-1}g_1, \mathcal{K}^{q-1}g_2, \mathcal{K}^{q-1}g_3\}$$
$$\phi(\lambda) = (1-\lambda)^2 \log(1-\lambda)$$





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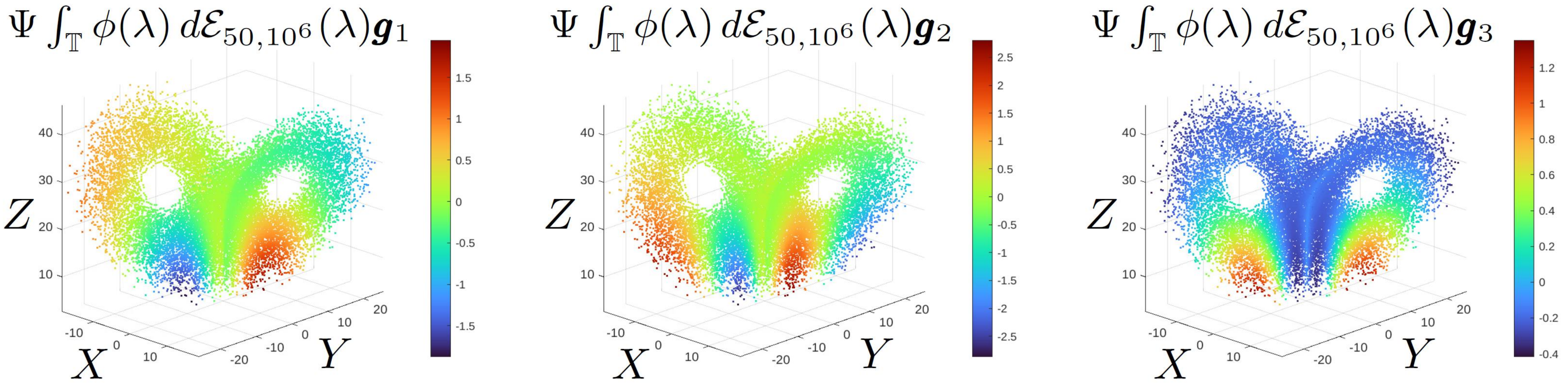
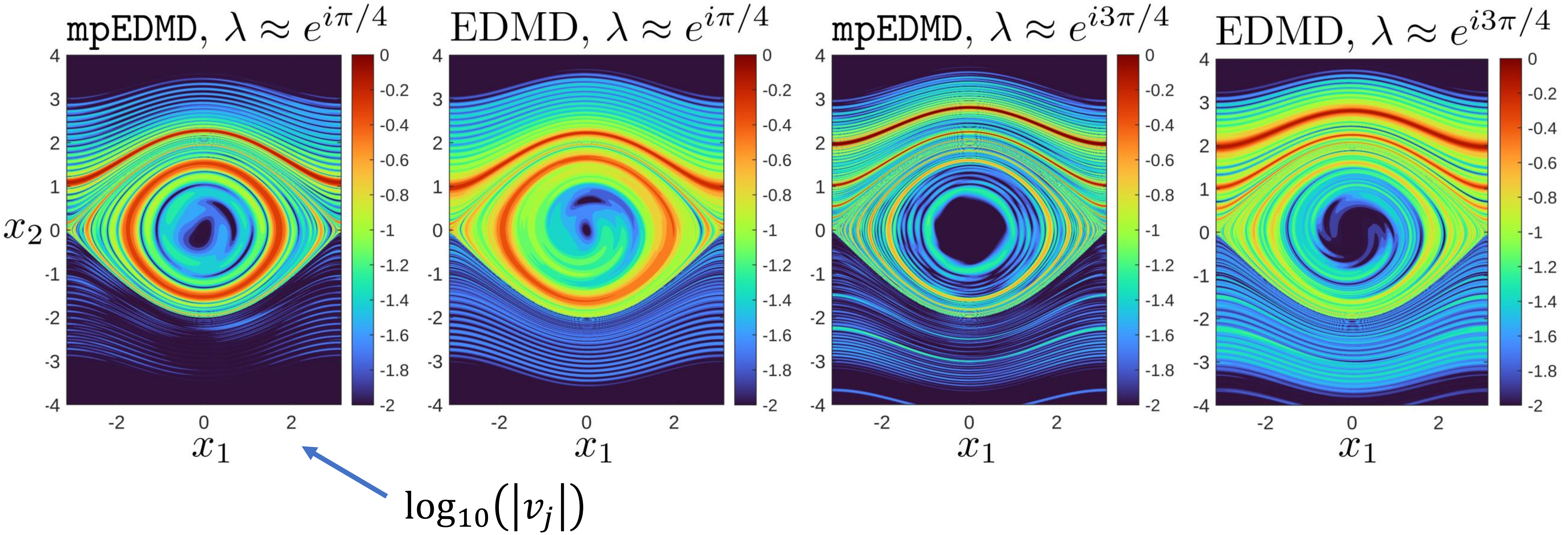


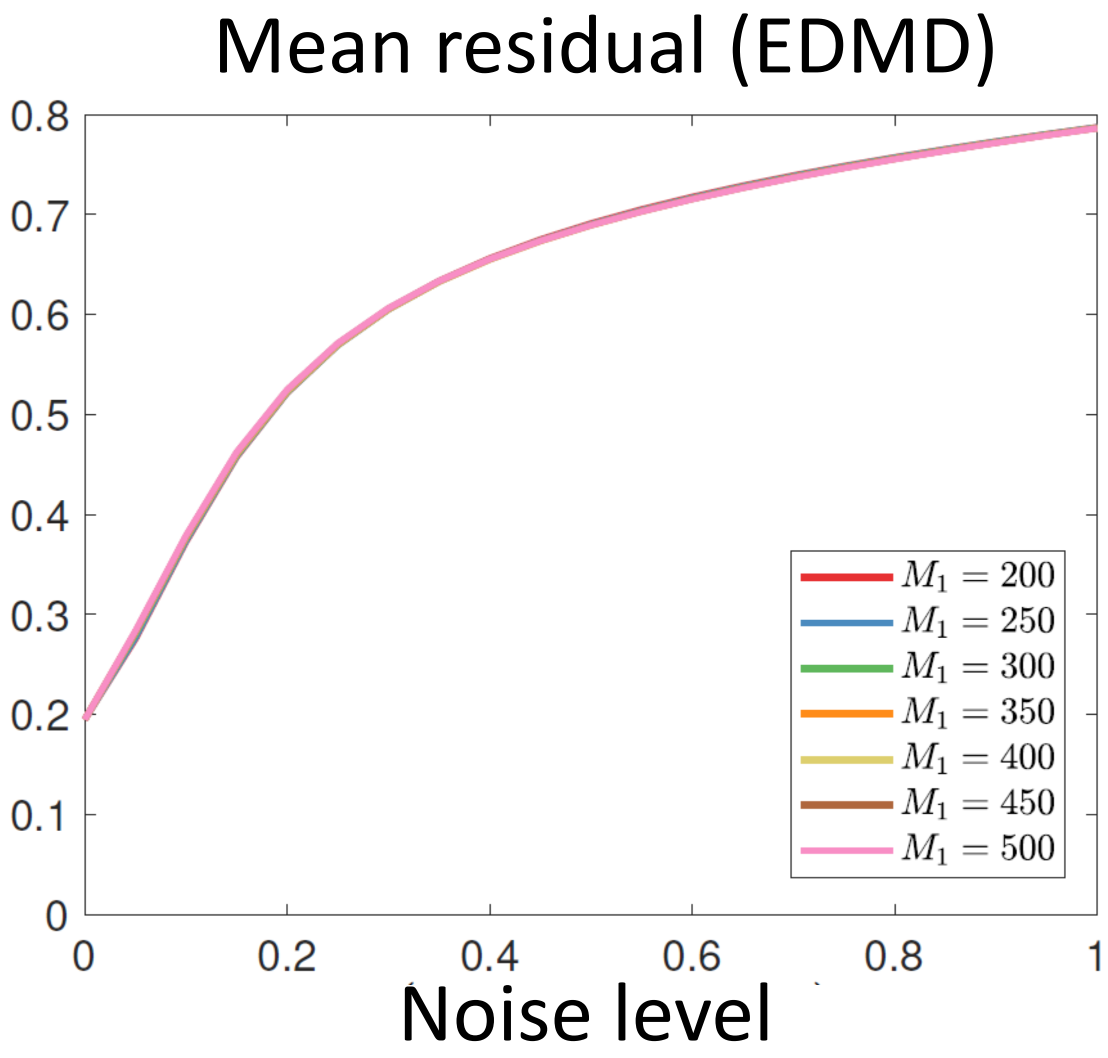
Nonlinear pendulum

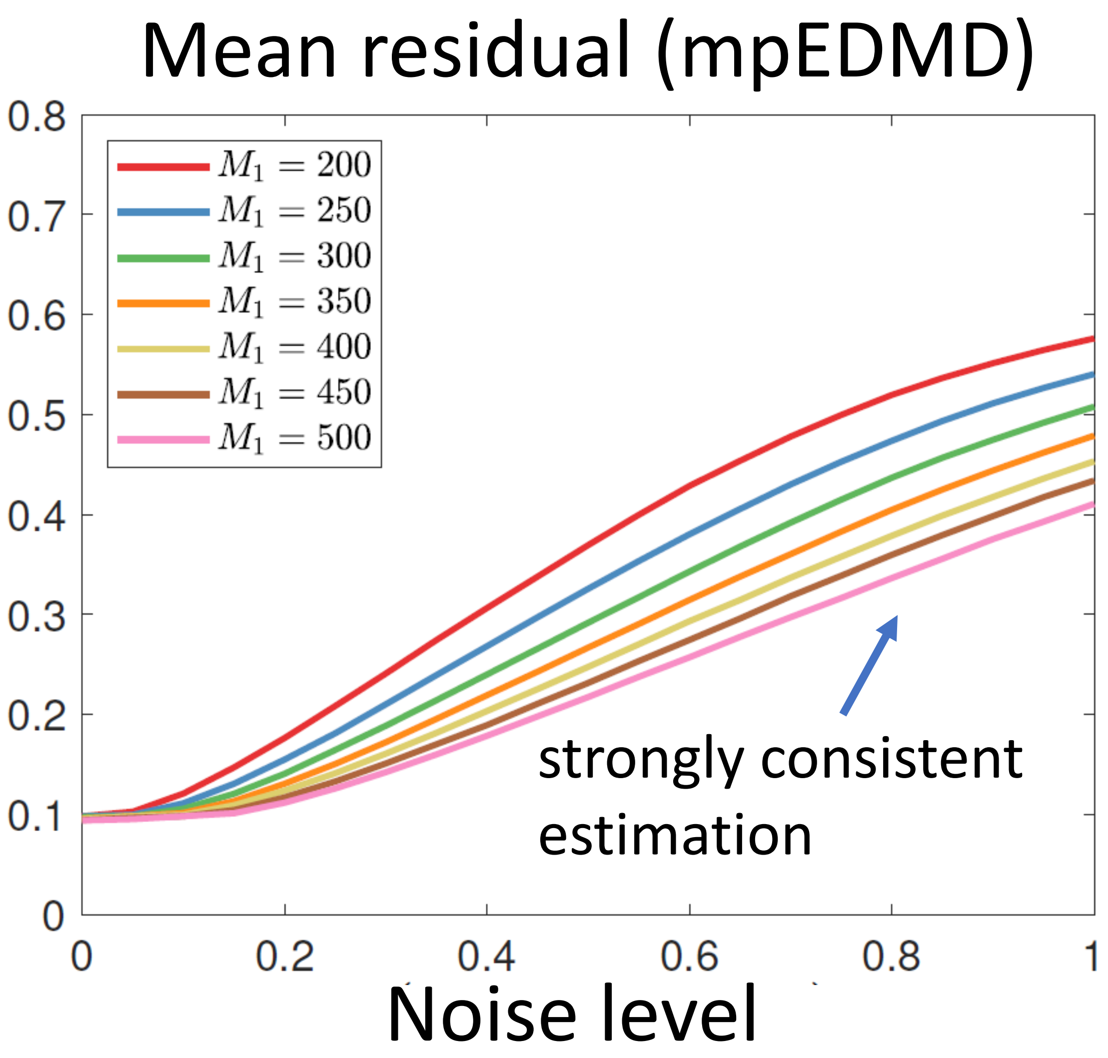
$$\dot{x}_1 = x_2, \qquad \dot{x}_2 = -\sin(x_1), \qquad \Omega = [-\pi, \pi]_{\mathrm{per}} \times \mathbb{R}, \qquad \Delta_t = 0.5$$

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

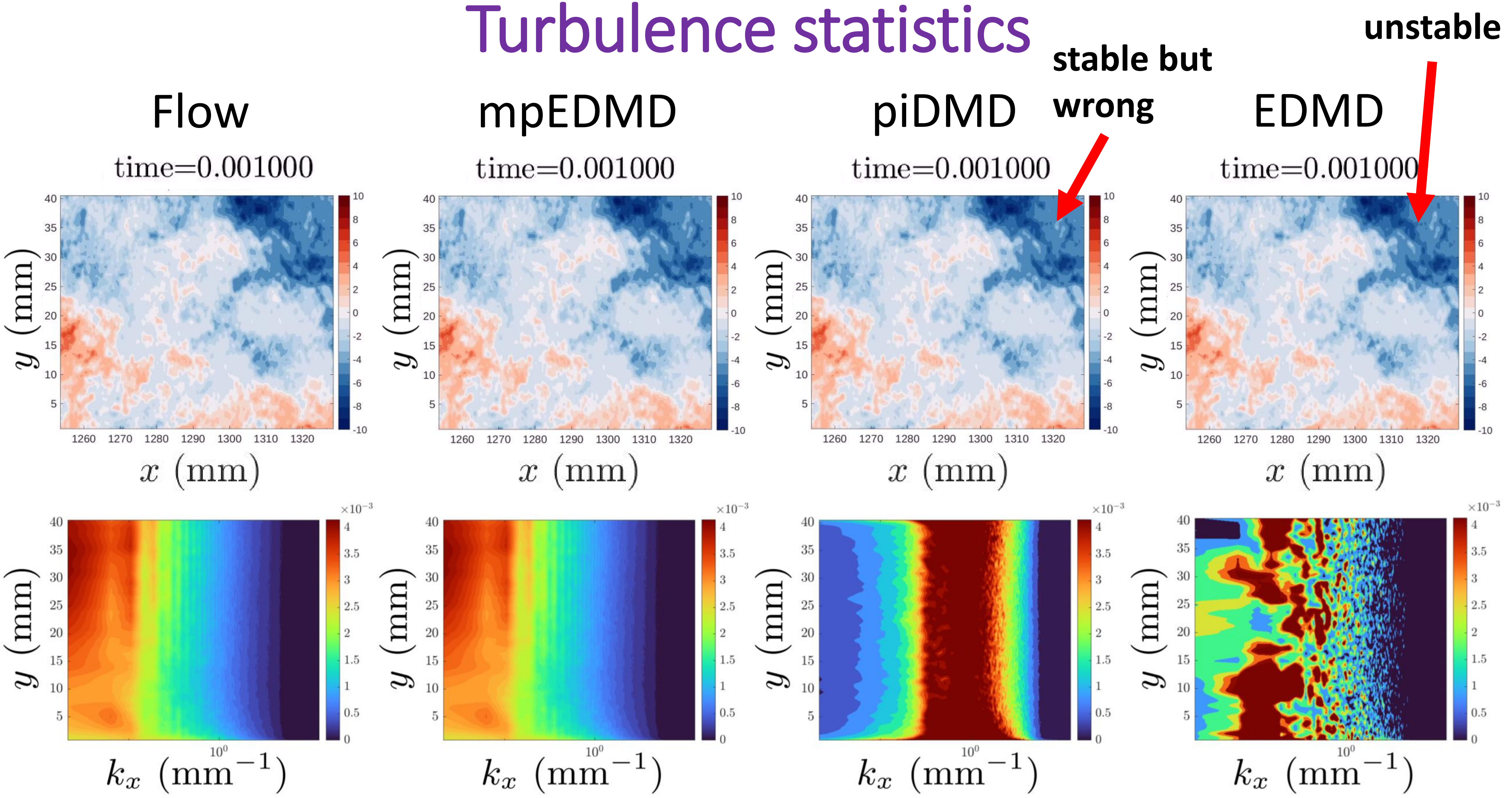


Robustness to noise: Gauss. noise for Ψ_X, Ψ_Y





Turbulence statistics



Summary: Structure-preserving Koopmanism for arbitrary measure-preserving systems.

- 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!

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

Summary

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Read more about these breakthroughs in SIAM News!

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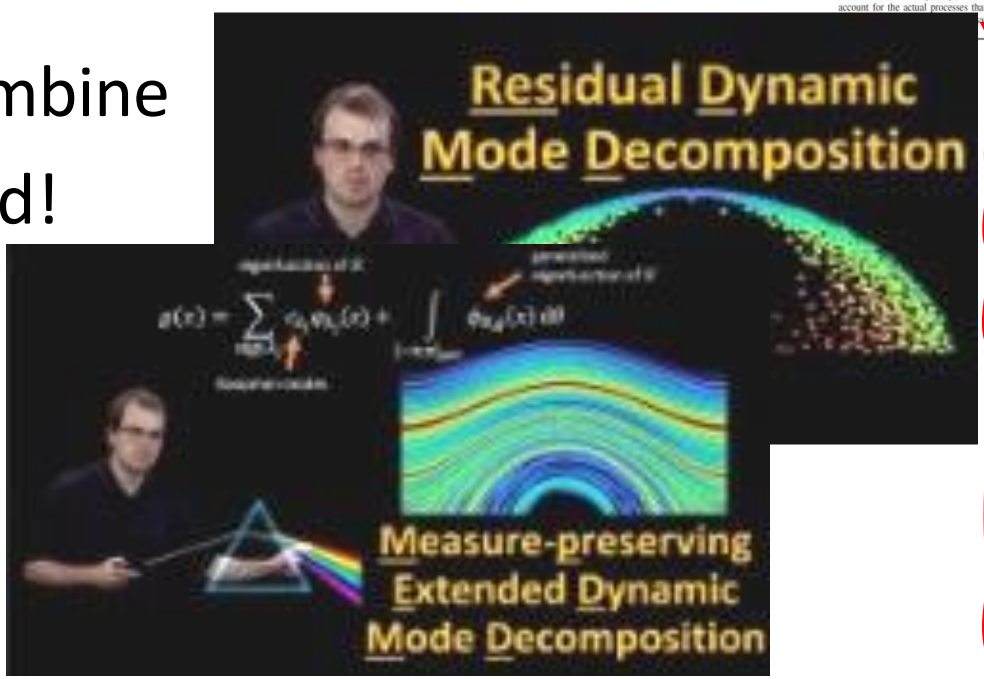
Volume 56/ Issue 1
January/February 2023

Optimization and Learning with Zeroth-order Stochastic Oracles

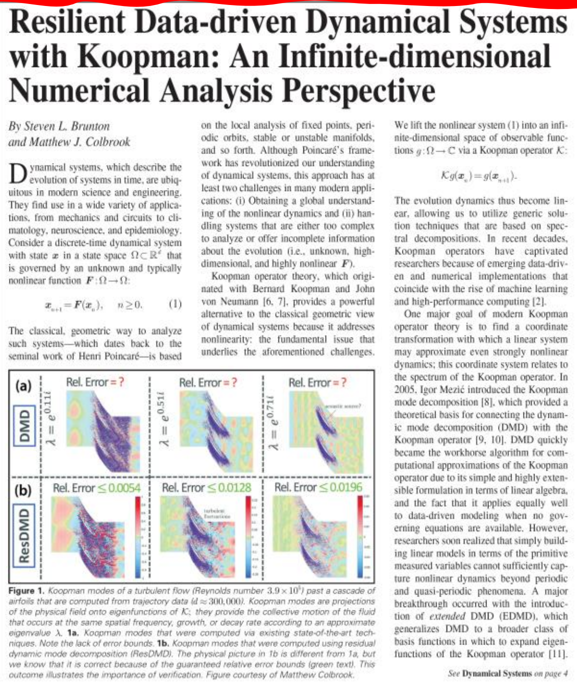
By Stefan M. Wild

Read more about these breakthroughs in SIAM News!



Short video summaries available on YouTube:

(Thank you Steve Brunton for letting me use your channel!)


Resilient Data-driven Dynamical Systems with Koopman: An Infinite-dimensional Numerical Analysis Perspective

By Steven L. Brunton and Matthew J. Colbrook

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References

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