Koopman operators and a programme on the foundations of infinite-dimensional spectral computations

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C., Townsend, "*Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems*"

C., Ayton, Szőke, "*Residual Dynamic Mode Decomposition: Robust and verified Koopmanism*"

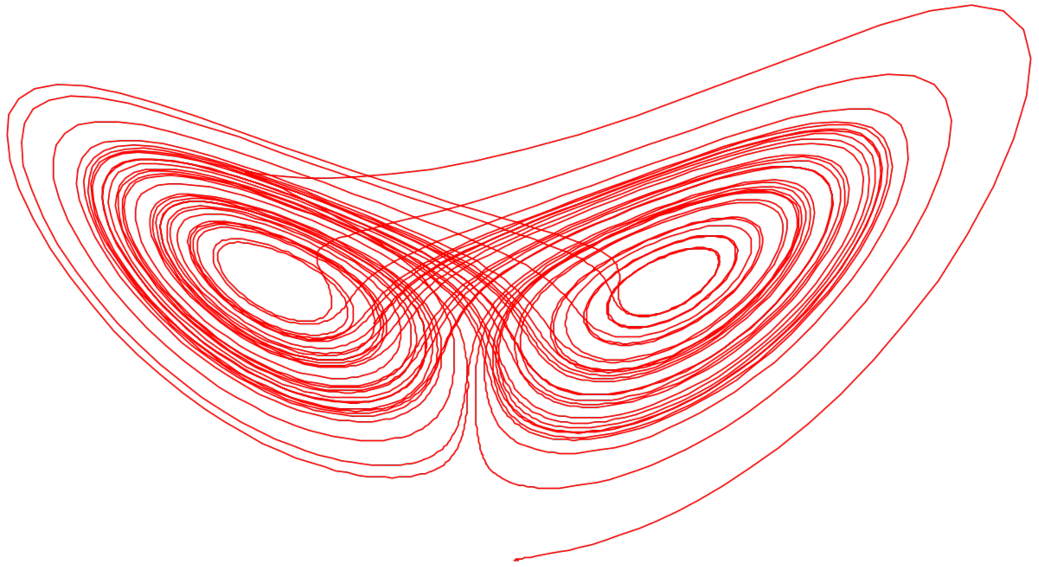
http://www.damtp.cam.ac.uk/user/mjc249/home.html: slides, papers, and code

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:** Learn about system from data $\left\{x^{(m)}, y^{(m)} = F(x^{(m)})\right\}_{m=1}^{M}$
  - E.g., **data from** trajectories, experimental measurements, simulations, …
  - E.g., **used for** forecasting, control, design, understanding, …
- **Applications:** chemistry, climatology, electronics, epidemiology, finance, fluids, molecular dynamics, neuroscience, plasmas, robotics, video processing, …



Data-driven dynamical systems

- **Carleman linearisation:** Carleman, *"Application de la théorie des équations intégrales linéaires aux systèmes d'équations différentielles non linéaires,"* Acta Mathematica, 1932.
- **Filtering:** Kalman, *"A new approach to linear filtering and prediction problems,"* Journal of Basic Engineering, 1960.
- **Ulam's method:** Ulam, *"A Collection of Mathematical Problems,"* IP, 1960.
- **Model order reduction:** Benner, Gugercin, Willcox, *"A survey of projection-based model reduction methods for parametric dynamical systems,"* SIAM Review, 2015.
- **Sparse identification of $\boldsymbol{F}$:** Brunton, Proctor, Kutz, *"Discovering governing equations from data by sparse identification of nonlinear dynamical systems,"* Proceedings of the National Academy of Sciences, 2016.
- **Kernel analog forecasting:** Burov, Giannakis, Manohar, Stuart, *"Kernel analog forecasting: Multiscale test problems,"* Multiscale Modeling & Simulation, 2021.
- **Deep learning:** Lu, Jin, Pang, Zhang, Karniadakis, *"Learning nonlinear operators via DeepONet based on the universal approximation theorem of operators,"* Nature Machine Intelligence, 2021.
- **Machine learning:** Schmidt, Lipson, *"Distilling free-form natural laws from experimental data,"* Science, 2009.

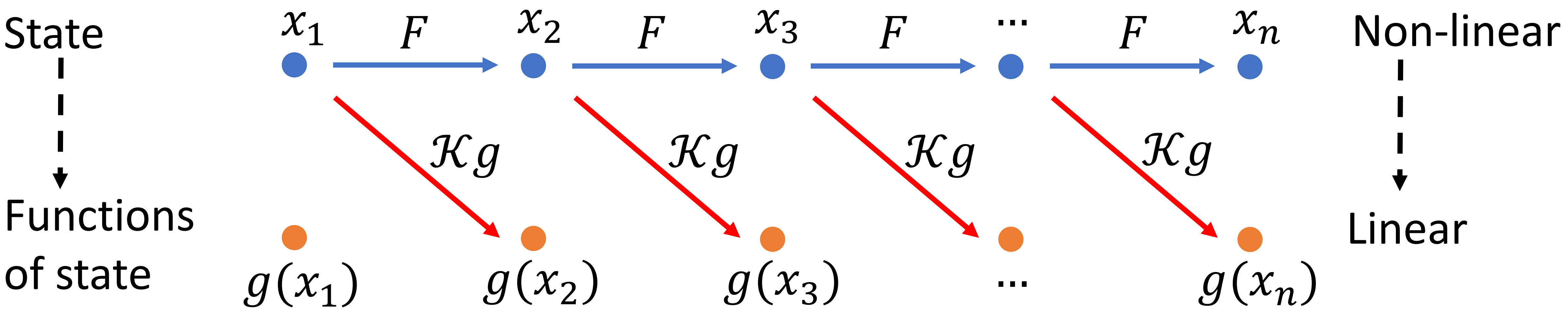
Can we develop general verified methods?

Operator viewpoint

- **Koopman operator** $\mathcal{K}$ acts on <u>functions</u> $g: \Omega \to \mathbb{C}$

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

- $\mathcal{K}$ is ***linear*** but acts on an ***infinite-dimensional*** space.



- Work in $L^2(\Omega, \omega)$ for positive measure ω, with inner product $\langle\cdot,\cdot\rangle$.

- Koopman, *"Hamiltonian systems and transformation in Hilbert space,"* **Proceedings of the National Academy of Sciences**, 1931.
- Koopman, v. Neumann, *"Dynamical systems of continuous spectra,"* **Proceedings of the National Academy of Sciences**, 1932.

Why is linear (much) easier?

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

Dynamics become trivial!

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

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

- Let $w^{\mathrm{T}}A = \lambda w$, set $\varphi(x) = w^{\mathrm{T}}x$,

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

Eigenfunction

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

Koopman mode decomposition

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

eigenfunction of $\mathcal{K}$

generalised eigenfunction of $\mathcal{K}$

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

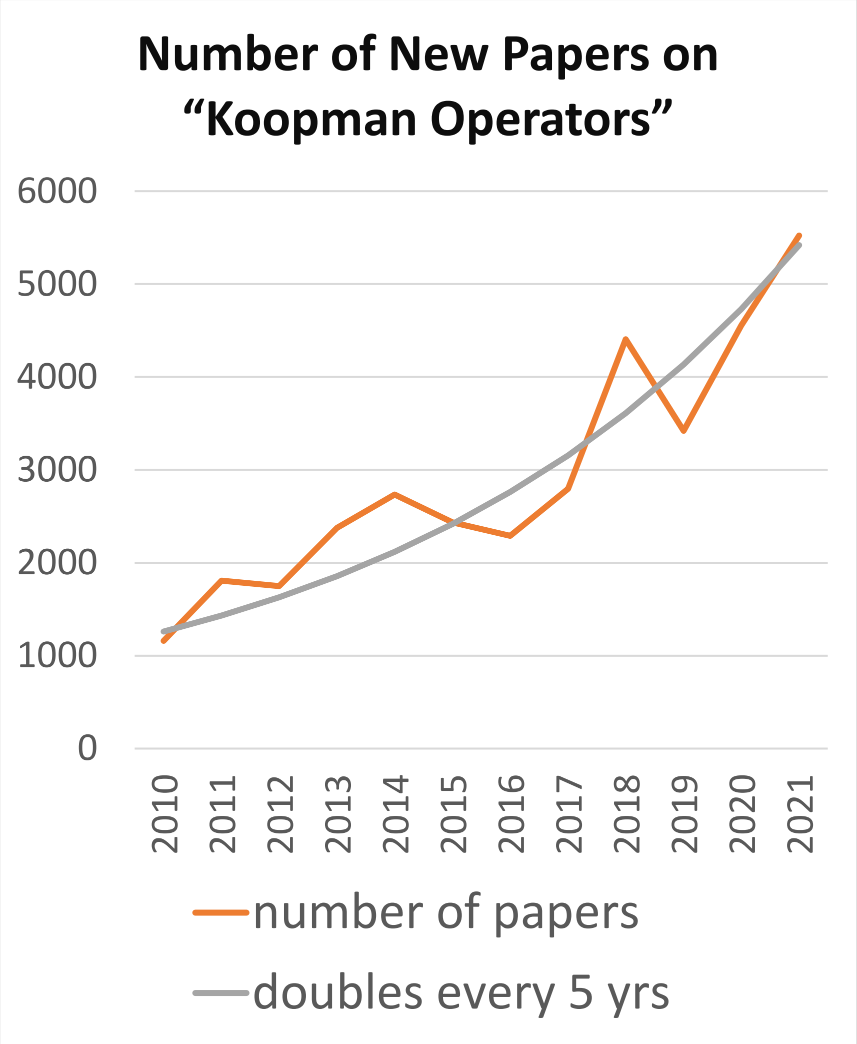
$$g(x_n) = [\mathcal{K}^n g](x_0) = \sum_{\text{eigenvalues } \lambda_j} c_{\lambda_j} {\lambda_j}^n \varphi_{\lambda_j}(x_0) + \int_{-\pi}^{\pi} e^{in\theta} \phi_{\theta,g}(x_0)\, \mathrm{d}\theta$$

Encodes: geometric features, invariant measures, transient behaviour, long-time behaviour, 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.

Koopmania*: a revolution in the big data era



≈35,000 papers over last decade.

Very little on convergence guarantees or verification.

Why is this lacking?

Dealing with infinite dimensions is notoriously hard …

**Wikipedia*: “its wild surge in popularity is sometimes jokingly called ‘Koopmania’”

Can we compute spectral properties in inf. dim.?

$$\mathcal{K} \text{ "="} \begin{pmatrix} k_{11} & k_{12} & \cdots \\ k_{21} & k_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}, \qquad \mathcal{K}\left(\sum_{l=1}^{\infty} g_l \psi_l\right) = \sum_{j=1}^{\infty}\left(\sum\nolimits_{l=1}^{\infty} k_{jl} g_l\right)\psi_j$$

basis expansion of $g: \Omega \to \mathbb{C}$

Finite-dimensional	$\Longrightarrow$	**Infinite-dimensional**
Eigenvalues of $B \in \mathbb{C}^{n\times n}$	$\Longrightarrow$	Spectrum, $\mathrm{Spec}(\mathcal{K})$
$\{\lambda_j \in \mathbb{C}: \det(B - \lambda_j I) = 0\}$	$\Longrightarrow$	$\{\lambda \in \mathbb{C}: \mathcal{K} - \lambda I \text{ is not invertible}\}$

"Most operators that arise in practice are not presented in a representation in which they are ***diagonalized****, and it is often very hard to locate even a single point in the spectrum. Thus, one often has to settle for numerical approximations [...] Unfortunately, there is a dearth of literature on this basic problem and, so far as we have been able to tell,* ***there are no proven [general] techniques****."* W. Arveson, Berkeley (1994)

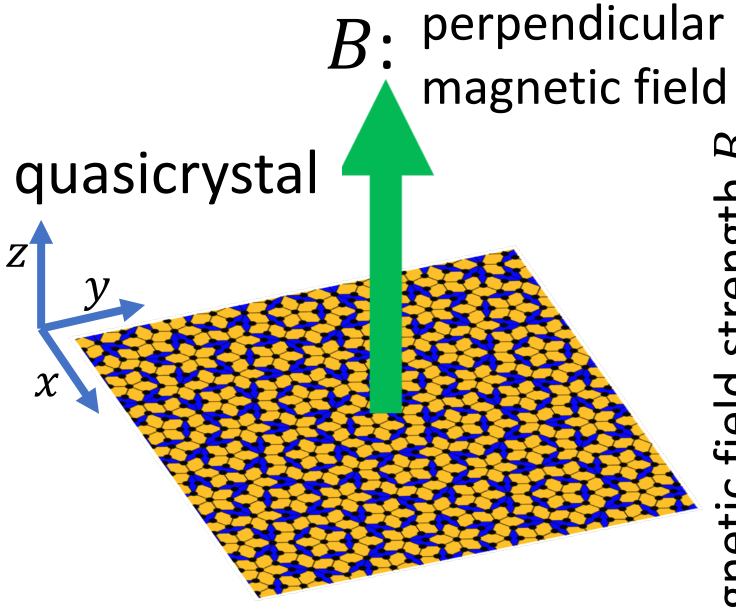
Four key challenges

$$\mathcal{K} \text{ "="} \begin{pmatrix} k_{11} & k_{12} & \cdots \\ k_{21} & k_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$, **naïve:** truncate to $\mathbb{K} \in \mathbb{C}^{N_K \times N_K}$ + compute e-values

1) **Too little:** Miss parts of $\mathrm{Spec}(\mathcal{K})$
2) **Too much:** Approximate spurious modes $\lambda \notin \mathrm{Spec}(\mathcal{K})$ - "spectral pollution"
3) **Lose continuous spectra.**
4) **Verification:** Which part of an approximation can we trust?

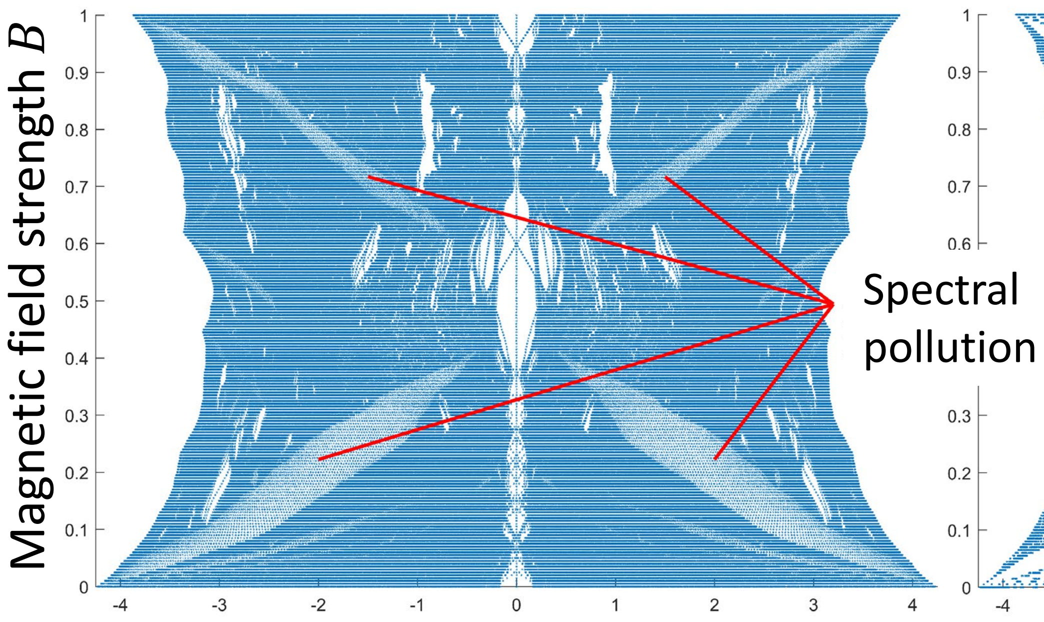
- Arveson, "*The role of C^*-algebras in infinite dimensional numerical linear algebra,*" **Contemp. Math.**, 1994.
- Davies, "*Linear operators and their spectra,*" **CUP**, 2007.
- Brunton, Kutz, "*Data-driven Science and Engineering: Machine learning, Dynamical systems, and Control,*" **CUP**, 2019.

Example of "too much" (spectral pollution)



Infinite matrix: discrete Schrödinger operator

Naïve method

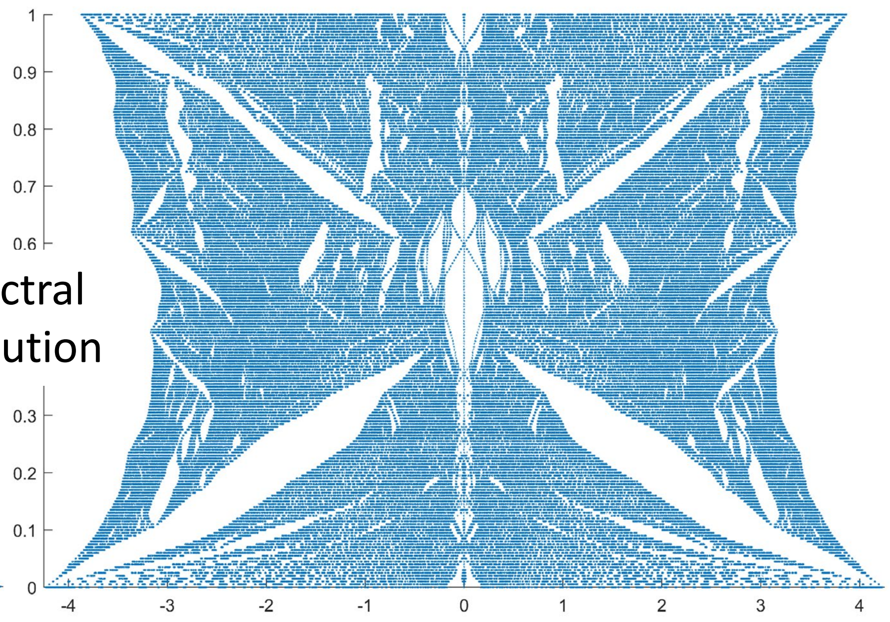


Approx. of spectrum (energy)

Spectral pollution

No error control

"Infinite-dimensional" method



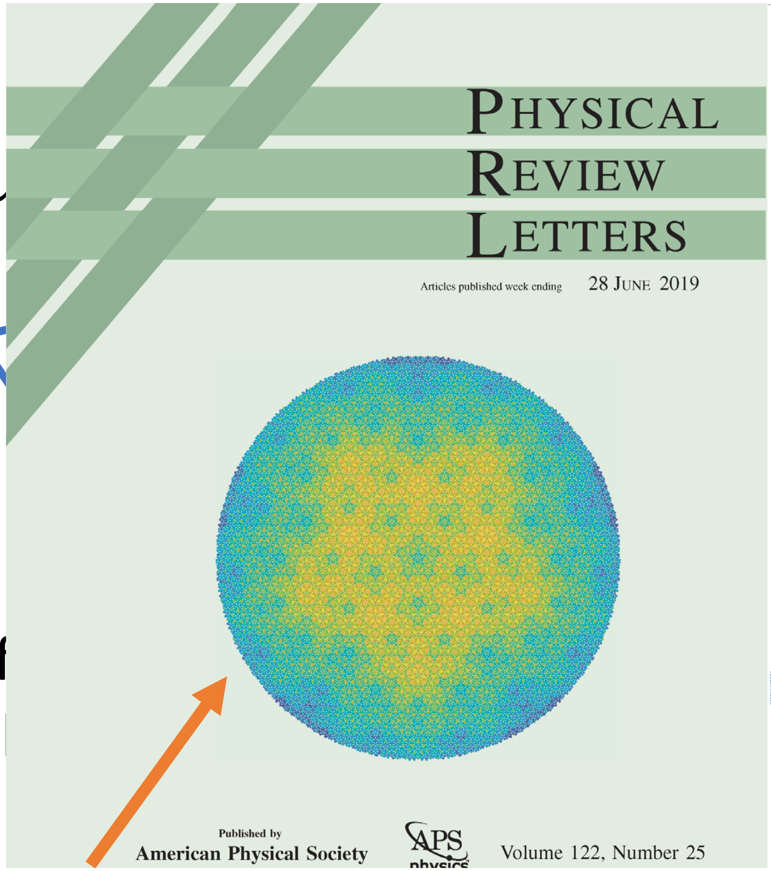
Approx. of spectrum (energy)

Convergent computation

Error control

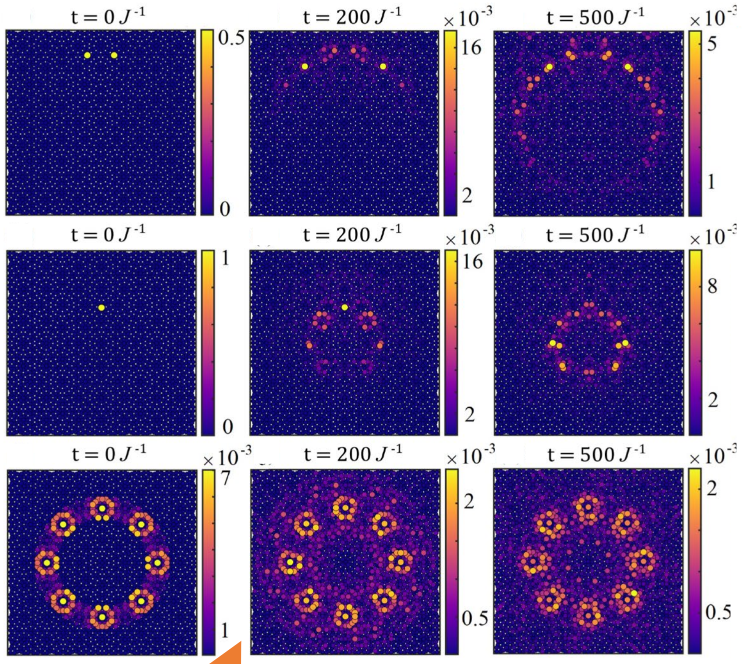
- C., Roman, Hansen, *"How to compute spectra with error control,"* **Physical Review Letters**, 2019.
- C., Horning, Townsend, *"Computing spectral measures of self-adjoint operators,"* **SIAM Review**, 2021.
- Johnstone, C., Nielsen, Öhberg, Duncan, *"Bulk Localised Transport States in Infinite and Finite Quasicrystals via Magnetic Aperiodicity."*

Example of "too much" (spectral pollution)



E.g., ground state of quasicrystal

E.g., continuous spectra of graphene



E.g., new states and phenomena: bulk localised transport states

- C., Roman, Hansen, "*How to compute spectra with error control,*" **Physical Review Letters**, 2019.
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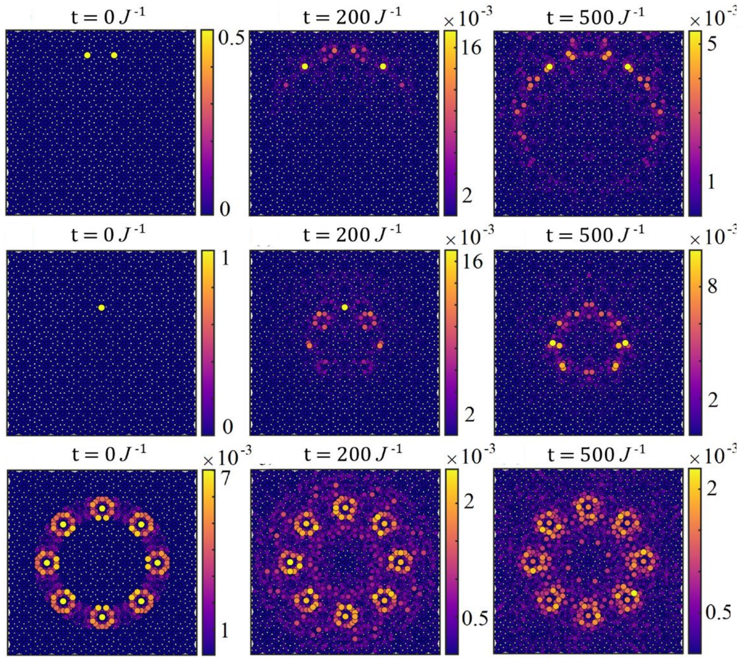

Now back to data-driven dynamical systems …

- C., Roman, Hansen, "*How to compute spectra with error control,*" **Physical Review Letters**, 2019.
- C., Horning, Townsend, "*Computing spectral measures of self-adjoint operators,*" **SIAM Review**, 2021.
- Johnstone, C., Nielsen, Öhberg, Duncan, "*Bulk Localised Transport States in Infinite and Finite Quasicrystals via Magnetic Aperiodicity.*"

Build the matrix: Dynamic Mode Decomposition (DMD)

Given dictionary $\{\psi_1, \dots, \psi_{N_K}\}$ of functions $\psi_j : \Omega \to \mathbb{C}$ $\boxed{\left\{x^{(m)}, y^{(m)} = F(x^{(m)})\right\}_{m=1}^{M}}$

$$\underbrace{\left[\begin{pmatrix} \psi_1(x^{(1)}) & \cdots & \psi_{N_K}(x^{(1)}) \\ \vdots & \ddots & \vdots \\ \psi_1(x^{(M)}) & \cdots & \psi_{N_K}(x^{(M)}) \end{pmatrix}^* \begin{pmatrix} w_1 & & \\ & \ddots & \\ & & w_M \end{pmatrix} \begin{pmatrix} \psi_1(x^{(1)}) & \cdots & \psi_{N_K}(x^{(1)}) \\ \vdots & \ddots & \vdots \\ \psi_1(x^{(M)}) & \cdots & \psi_{N_K}(x^{(M)}) \end{pmatrix}\right]_{jk}}_{G} \approx \langle \psi_k, \psi_j \rangle$$

$$\underbrace{\left[\begin{pmatrix} \psi_1(x^{(1)}) & \cdots & \psi_{N_K}(x^{(1)}) \\ \vdots & \ddots & \vdots \\ \psi_1(x^{(M)}) & \cdots & \psi_{N_K}(x^{(M)}) \end{pmatrix}^* \begin{pmatrix} w_1 & & \\ & \ddots & \\ & & w_M \end{pmatrix} \begin{pmatrix} \psi_1(y^{(1)}) & \cdots & \psi_{N_K}(y^{(1)}) \\ \vdots & \ddots & \vdots \\ \psi_1(y^{(M)}) & \cdots & \psi_{N_K}(y^{(M)}) \end{pmatrix}\right]_{jk}}_{K_1} \approx \langle \mathcal{K}\psi_k, \psi_j \rangle$$

Approximate $\mathcal{K}$ by $\mathbb{K} = G^{-1}K_1 \in \mathbb{C}^{N_K \times N_K}$

Open problems: 1) too little, 2) too much, 3) lose continuous spectra, 4) verification.

- Schmid, "*Dynamic mode decomposition of numerical and experimental data,*" **Journal of fluid mechanics**, 2010.
- 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,*" **Journal of Nonlinear Science**, 2015.

Key idea: Residual DMD (ResDMD)

$$\left.\begin{aligned}
&\underbrace{\left[\begin{pmatrix}\psi_1(x^{(1)}) & \cdots & \psi_{N_K}(x^{(1)})\\ \vdots & \ddots & \vdots\\ \psi_1(x^{(M)}) & \cdots & \psi_{N_K}(x^{(M)})\end{pmatrix}^* \begin{pmatrix}w_1 & & \\ & \ddots & \\ & & w_M\end{pmatrix} \begin{pmatrix}\psi_1(x^{(1)}) & \cdots & \psi_{N_K}(x^{(1)})\\ \vdots & \ddots & \vdots\\ \psi_1(x^{(M)}) & \cdots & \psi_{N_K}(x^{(M)})\end{pmatrix}\right]_{jk}}_{G} \approx \langle \psi_k, \psi_j \rangle\\
&\underbrace{\left[\begin{pmatrix}\psi_1(x^{(1)}) & \cdots & \psi_{N_K}(x^{(1)})\\ \vdots & \ddots & \vdots\\ \psi_1(x^{(M)}) & \cdots & \psi_{N_K}(x^{(M)})\end{pmatrix}^* \begin{pmatrix}w_1 & & \\ & \ddots & \\ & & w_M\end{pmatrix} \begin{pmatrix}\psi_1(y^{(1)}) & \cdots & \psi_{N_K}(y^{(1)})\\ \vdots & \ddots & \vdots\\ \psi_1(y^{(M)}) & \cdots & \psi_{N_K}(y^{(M)})\end{pmatrix}\right]_{jk}}_{K_1} \approx \langle \mathcal{K}\psi_k, \psi_j \rangle\\
&\underbrace{\left[\begin{pmatrix}\psi_1(y^{(1)}) & \cdots & \psi_{N_K}(y^{(1)})\\ \vdots & \ddots & \vdots\\ \psi_1(y^{(M)}) & \cdots & \psi_{N_K}(y^{(M)})\end{pmatrix}^* \begin{pmatrix}w_1 & & \\ & \ddots & \\ & & w_M\end{pmatrix} \begin{pmatrix}\psi_1(y^{(1)}) & \cdots & \psi_{N_K}(y^{(1)})\\ \vdots & \ddots & \vdots\\ \psi_1(y^{(M)}) & \cdots & \psi_{N_K}(y^{(M)})\end{pmatrix}\right]_{jk}}_{K_2} \approx \langle \mathcal{K}\psi_k, \mathcal{K}\psi_j \rangle
\end{aligned}\right\} \text{Approximate } \mathcal{K} \text{ and } \mathcal{K}^*\mathcal{K}$$

Residuals: $g = \sum_{j=1}^{N_K} \mathbf{g}_j \psi_j$, $\|\mathcal{K}g - \lambda g\|^2 \approx \mathbf{g}^*[K_2 - \lambda K_1{}^* - \bar{\lambda} K_1 + |\lambda|^2 G]\mathbf{g}$

- C., Townsend, "*Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems*," **Communications on Pure and Applied Mathematics**, under review.
- C., Ayton, Szőke, "*Residual Dynamic Mode Decomposition*," **Journal of Fluid Mechanics**, under review.
- Code: https://github.com/MColbrook/Residual-Dynamic-Mode-Decomposition (MATLAB and Python)
- C., "*Rigorous and data-driven Koopmanism*," **Proceedings of the XXI Householder Symposium** (invited plenary).

ResDMD: avoiding spectral pollution

$$\mathrm{res}(\lambda, g)^2 = \frac{\mathbf{g}^*\left[K_2 - \lambda {K_1}^* - \bar{\lambda} K_1 + |\lambda|^2 G\right]\mathbf{g}}{\mathbf{g}^* G \mathbf{g}}$$

Algorithm:

1. Compute $\mathbb{K} = G^{-1}K_1 \in \mathbb{C}^{N_K \times N_K}$, its eigenvalues and eigenvectors.
2. For each eigenpair (λ, g), compute $\mathrm{res}(\lambda, g)$.
3. Discard pairs with $\mathrm{res}(\lambda, g) > \varepsilon$ (input tolerance ε).

Theorem (no spectral pollution): Suppose the quadrature rule converges. Let Λ_M denote the eigenvalue output of above algorithm. Then

$$\limsup_{M \to \infty} \max_{\lambda \in \Lambda_M} \|(\mathcal{K} - \lambda)^{-1}\|^{-1} \leq \varepsilon$$

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BUT: Typically, does not capture all of spectrum!

ResDMD: computing pseudospectra and spectra

$$\mathrm{Spec}_\varepsilon(\mathcal{K}) = \bigcup_{\|\mathcal{B}\|\leq\varepsilon} \mathrm{Spec}(\mathcal{K}+\mathcal{B}), \qquad \lim_{\varepsilon\downarrow 0} \mathrm{Spec}_\varepsilon(\mathcal{K}) = \mathrm{Spec}(\mathcal{K})$$

Algorithm:

First convergent method for general $\mathcal{K}$

1. Compute $G, K_1, K_2 \in \mathbb{C}^{N_K \times N_K}$.
2. For z_k in comp. grid, compute $\tau_k = \min_{g=\sum_{j=1}^{N} \mathbf{g}_j \psi_j} \mathrm{res}(z_k, g)$, corresponding g_k (gen. SVD).
3. Output $\{z_k : \tau_k < \varepsilon\}$ (approx. of $\mathrm{Spec}_\varepsilon(\mathcal{K})$), $\{g_k : \tau_k < \varepsilon\}$ (ε-pseudo-eigenfunctions).

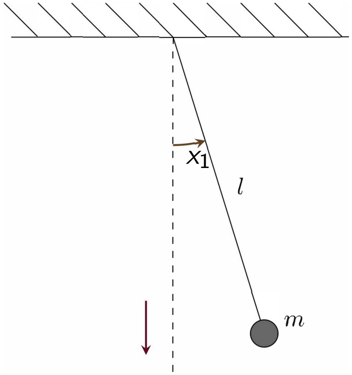
Theorem (full convergence): Suppose the quadrature rule converges.

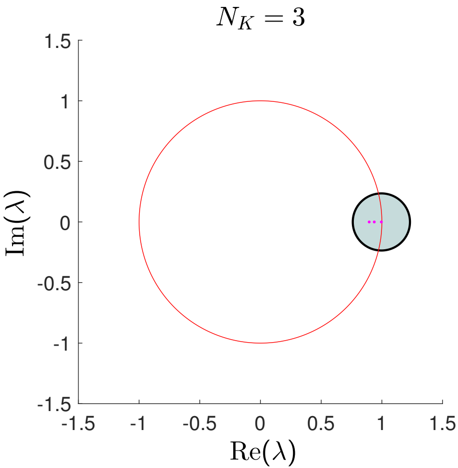
- **Error control:** $\{z_k : \tau_k < \varepsilon\} \subseteq \mathrm{Spec}_\varepsilon(\mathcal{K})$ (as $M \to \infty$)
- **Convergence:** Converges locally uniformly to $\mathrm{Spec}_\varepsilon(\mathcal{K})$ (as $N_K \to \infty$)

NB: Local optimisation strategy shrinks ε to compute $\mathrm{Spec}(\mathcal{K})$

Example: non-linear pendulum

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





Computed pseudospectra ($\varepsilon = 0.25$). Eigenvalues of $\mathbb{K}$ shown as dots (spectral pollution).

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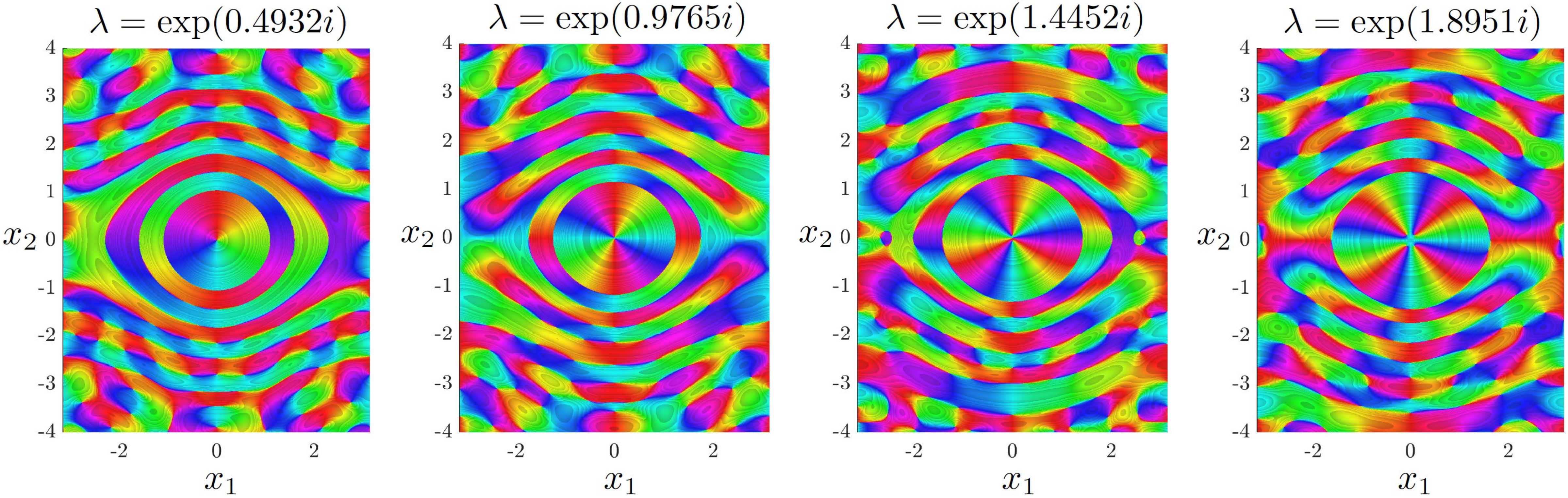


Colour represents complex argument, constant modulus shown as shadowed steps.
All residuals smaller than $\varepsilon = 0.05$ (made smaller by increasing N_K).

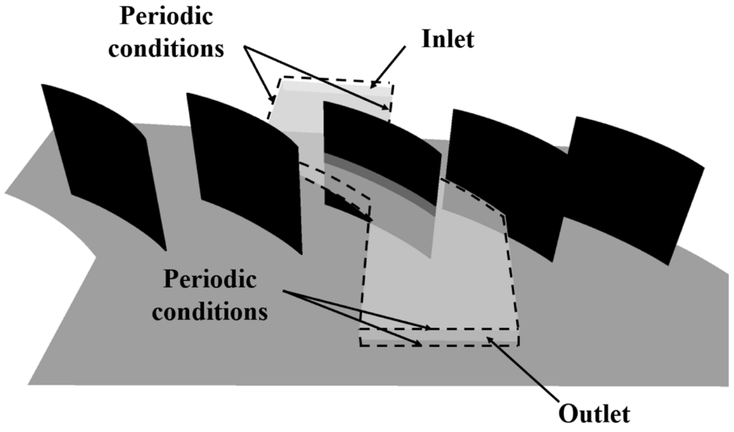
Large d (recall $\Omega \subseteq \mathbb{R}^d$)

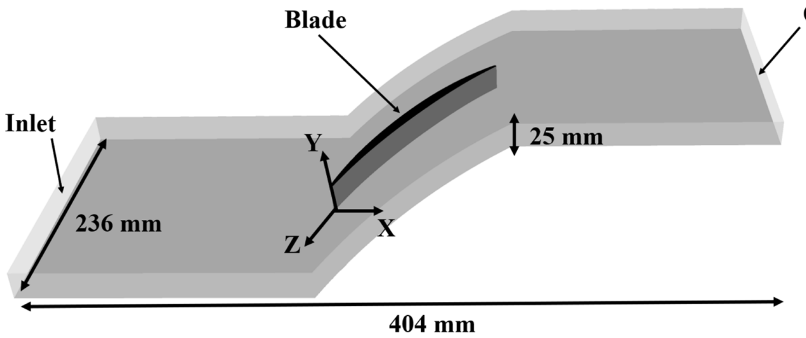
Error control → Rigorously ***verify*** learnt dictionary $\{\psi_1, \ldots, \psi_{N_K}\}$

E.g., kernel methods, neural networks, etc.

Deal with high-dimensional state-space Ω, ***robust*** and ***scalable***…

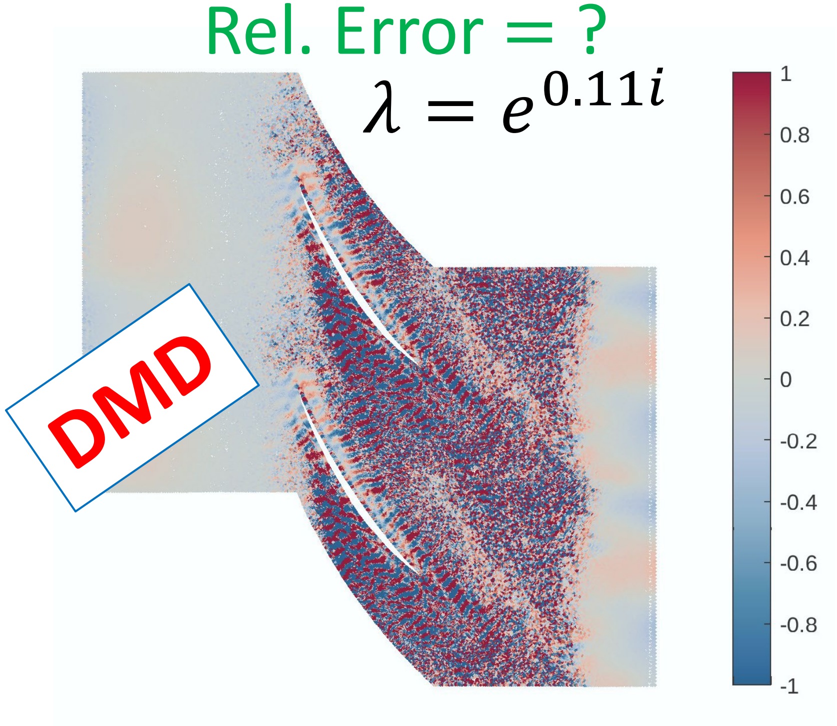
Example: pressure field of turbulent flow

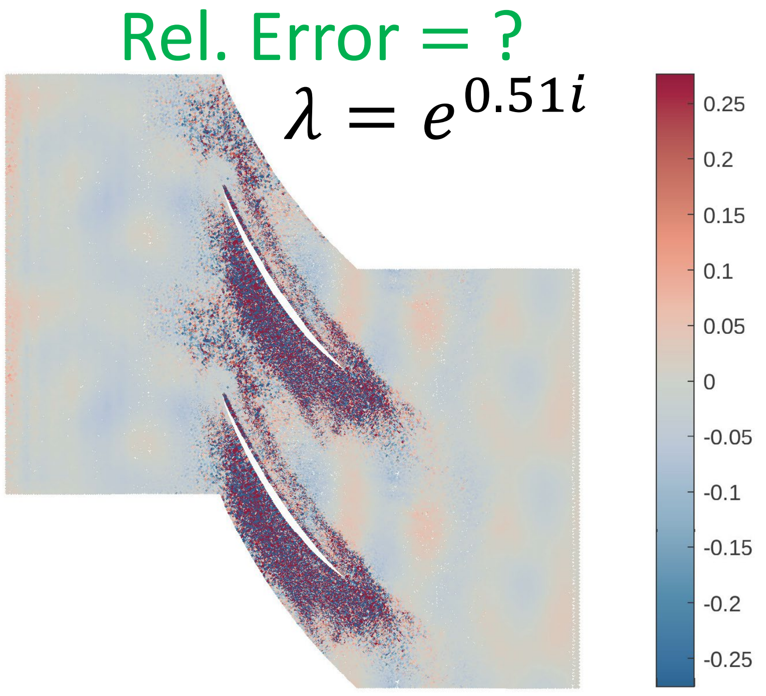


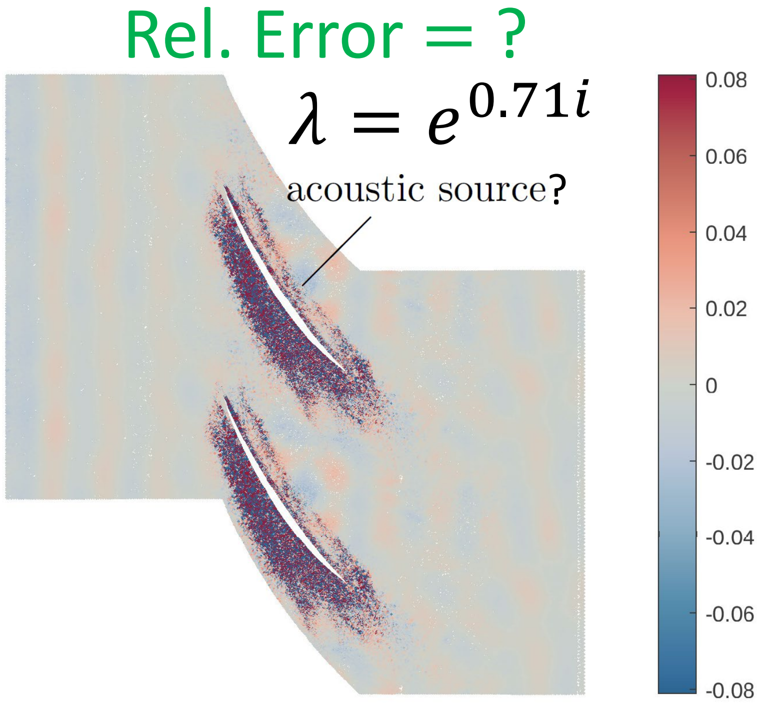


- Reynolds number $\approx 3.9 \times 10^5$
- Ambient dimension $\approx$ 300,000 (number of measurement points*)

*Raw measurements provided by Stephane Moreau (Sherbrooke)







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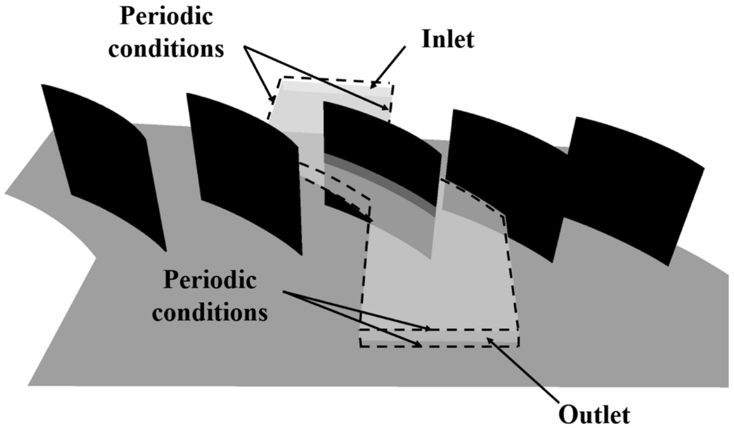

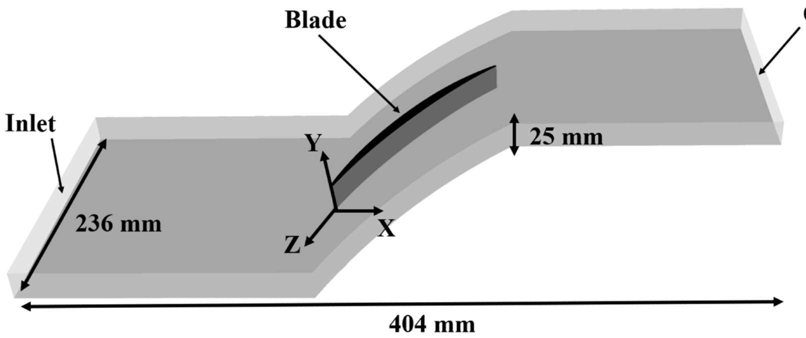

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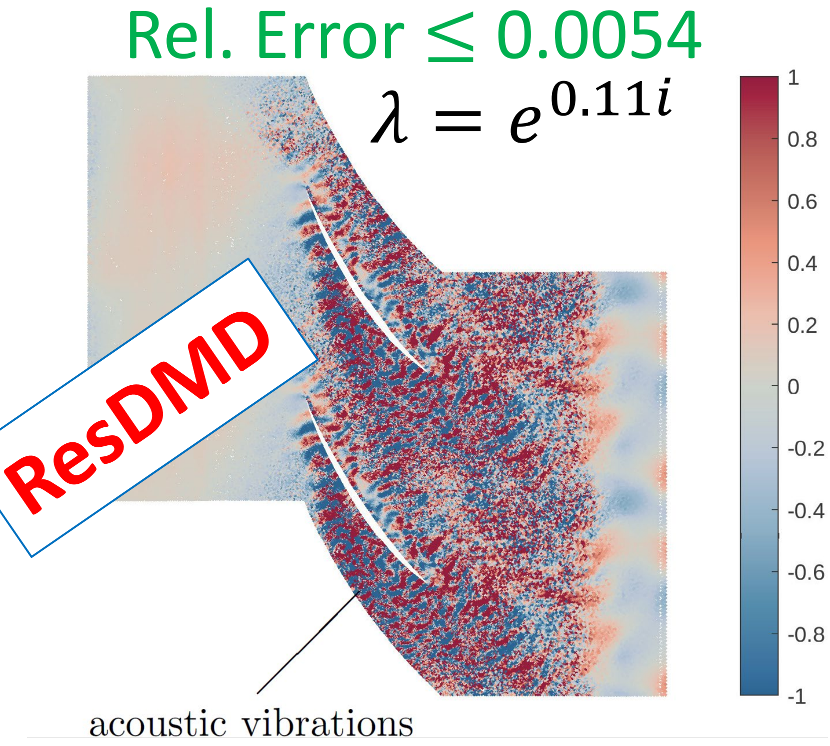
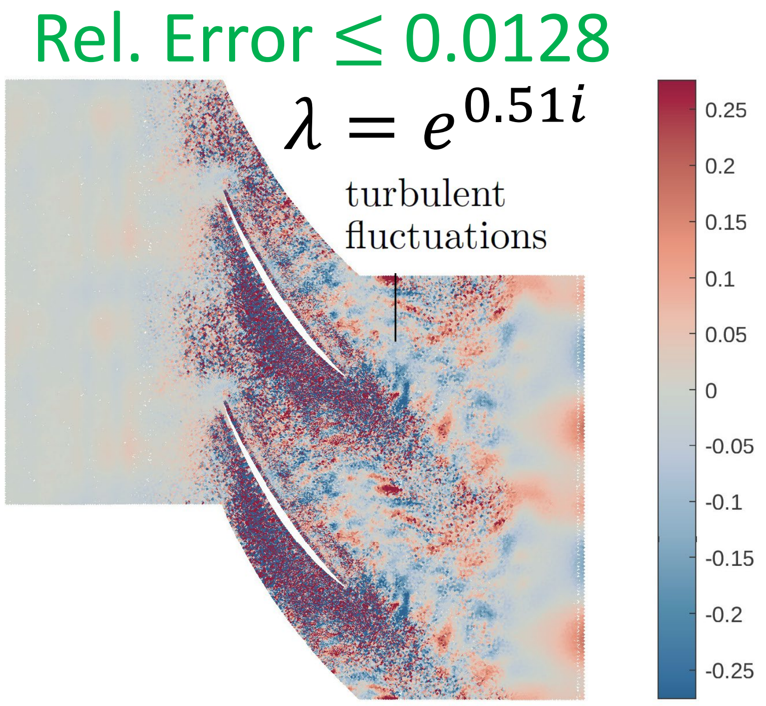
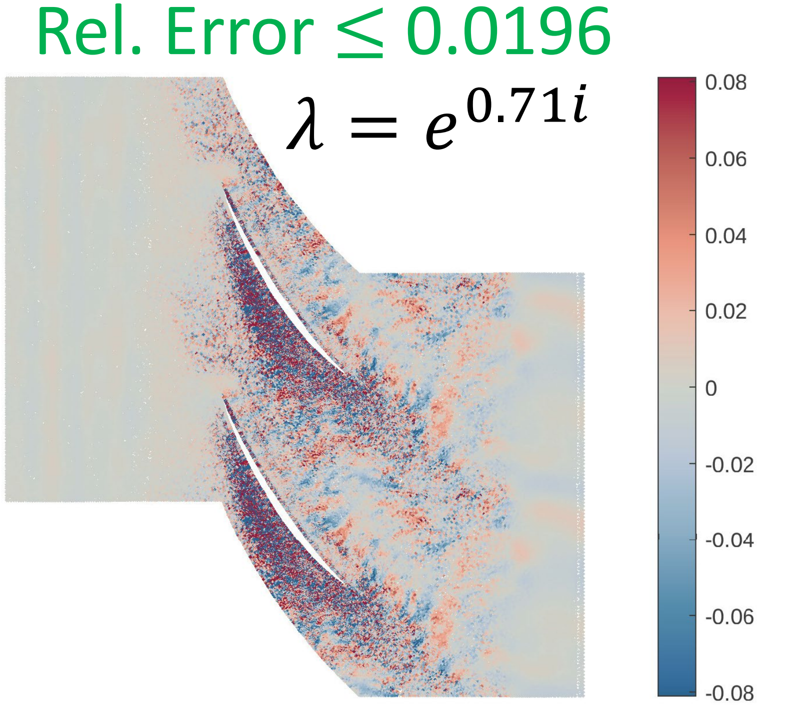
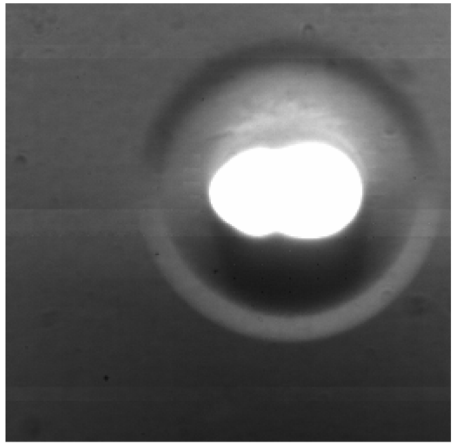


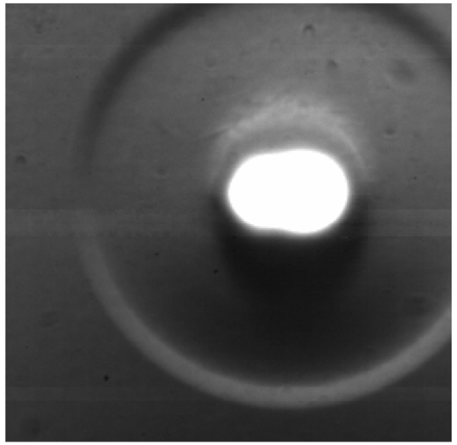




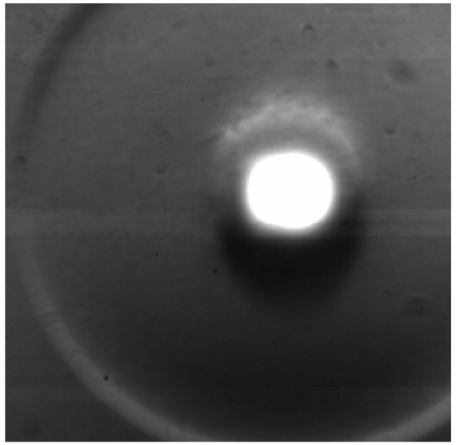
Example: laser-induced plasma



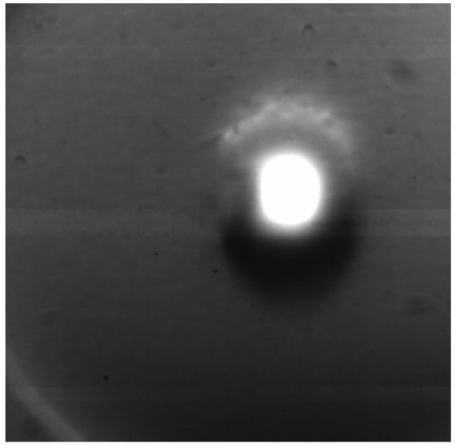
a) $t = 5\ \mu$s



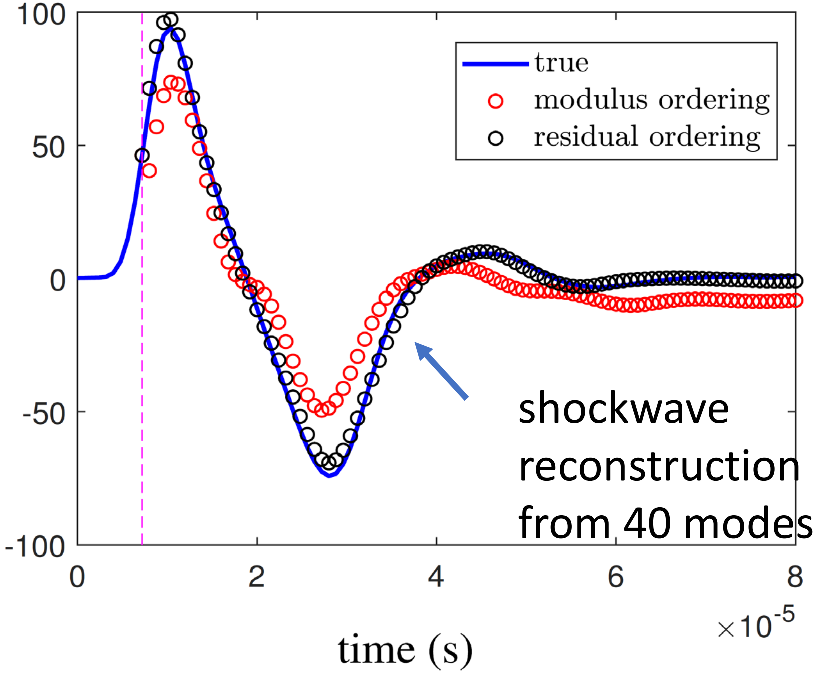
b) $t = 10\ \mu$s



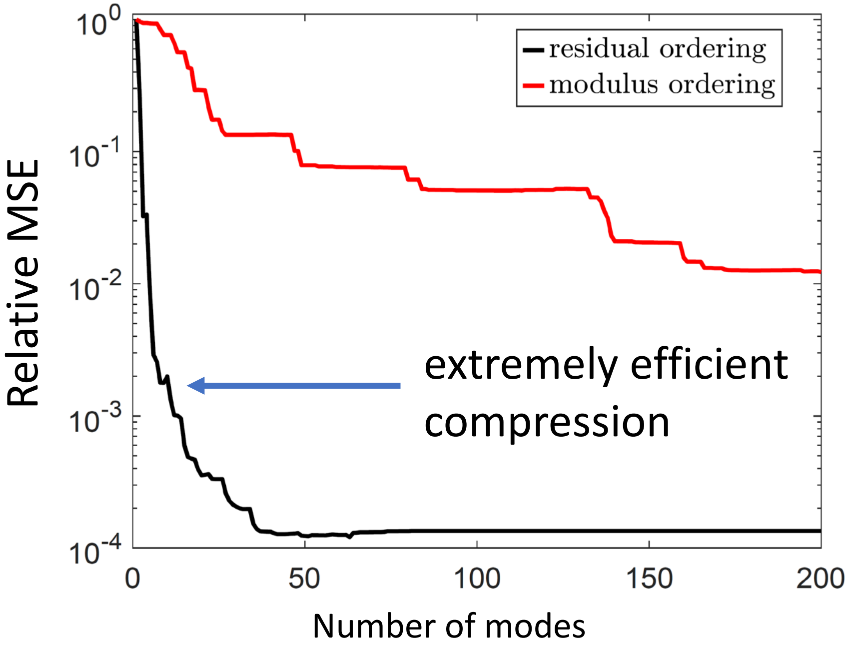
c) $t = 15\ \mu$s



d) $t = 20\ \mu$s



shockwave reconstruction from 40 modes



extremely efficient compression

Setup for continuous spectra

Now assume system is measure preserving

(e.g., Hamiltonian system, ergodic system, . . .)

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

Spectrum lives inside unit disk.

(For those interested: we consider canonical unitary extensions.)

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.:** Typically, no basis of e-vectors!
  Spectral theorem: (projection-valued) spectral measure E

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

- **Example:** $\nu_g(U) = \langle E(U)g, g\rangle$ prob. measures on $[-\pi, \pi]_{\mathrm{per}}$

Plemelj-type formula

$$\mathcal{C}_g(z) = \int_{-\pi}^{\pi} \frac{e^{i\theta}\,\mathrm{d}\nu_g(\theta)}{e^{i\theta} - z} = \begin{cases} \langle(\mathcal{K} - zI)^{-1}g, \mathcal{K}^* g\rangle, & \text{if } |z| > 1 \\ -z^{-1}\langle g, (\mathcal{K} - \bar{z}^{-1}I)^{-1}g\ \rangle, & \text{if } 0 < |z| < 1 \end{cases}$$

ResDMD computes
with error control

$$P_\varepsilon(\theta_0) = \frac{1}{2\pi} \frac{(1+\varepsilon)^2 - 1}{1 + (1+\varepsilon)^2 - 2(1+\varepsilon)\cos(\theta_0)}$$

Poisson kernel for
unit disk

$\boxed{\varepsilon = \text{“smoothing parameter”}}$

$$[P_\varepsilon * \nu_g](\theta_0) = \int_{-\pi}^{\pi} P_\varepsilon(\theta_0 - \theta)\,\mathrm{d}\nu_g(\theta) = \mathcal{C}_g\left(e^{i\theta_0}(1+\varepsilon)^{-1}\right) - \mathcal{C}_g\left(e^{i\theta_0}(1+\varepsilon)\right)$$

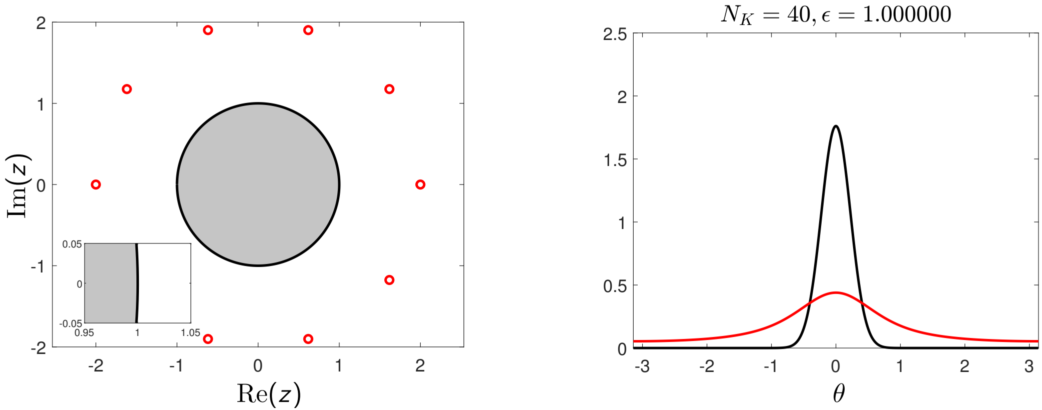
Example

$$\mathcal{K} = \begin{pmatrix} \overline{\alpha_0} & \overline{\alpha_1}\rho_0 & \rho_0\rho_1 & & & \\ \rho_0 & -\overline{\alpha_1}\alpha_0 & -\alpha_0\rho_1 & & & \\ & \overline{\alpha_2}\rho_1 & -\overline{\alpha_2}\alpha_1 & \overline{\alpha_3}\rho_2 & \rho_3\rho_2 & \\ & \rho_2\rho_1 & -\alpha_1\rho_2 & -\overline{\alpha_3}\alpha_2 & -\rho_3\alpha_2 & \ddots \\ & & & \overline{\alpha_4}\rho_3 & -\overline{\alpha_4}\alpha_3 & \ddots \\ & & & \ddots & \ddots & \ddots \end{pmatrix}$$

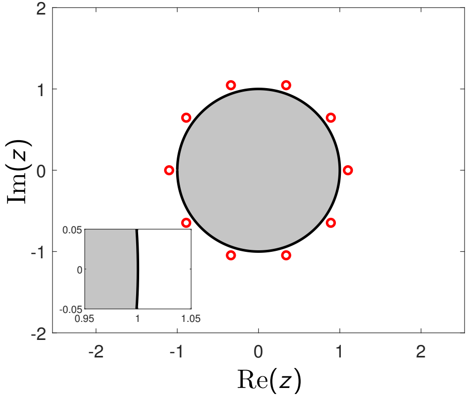
$$\alpha_j = (-1)^j 0.95^{(j+1)/2}, \qquad \rho_j = \sqrt{1 - |\alpha_j|^2}$$

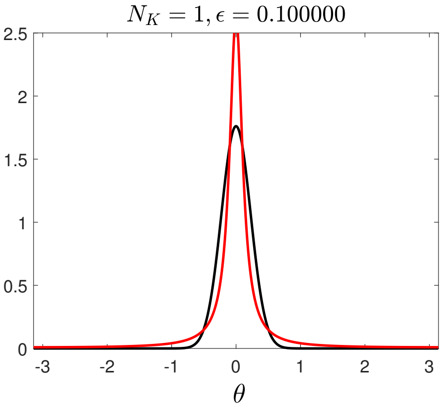
Generalised shift, typical building block of many dynamical systems.

Fix N_K, vary ε: unstable!

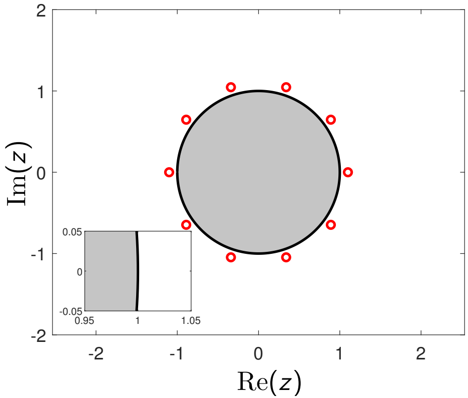


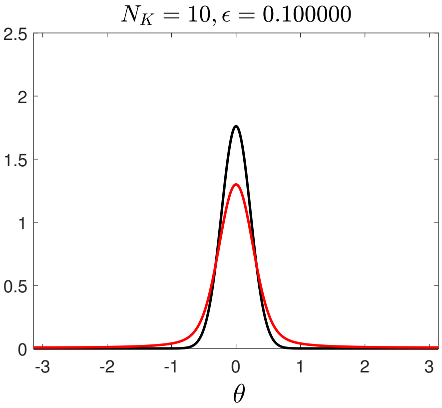
Fix ε, vary N_K: too smooth!





Adaptive: new matrix to compute residuals crucial

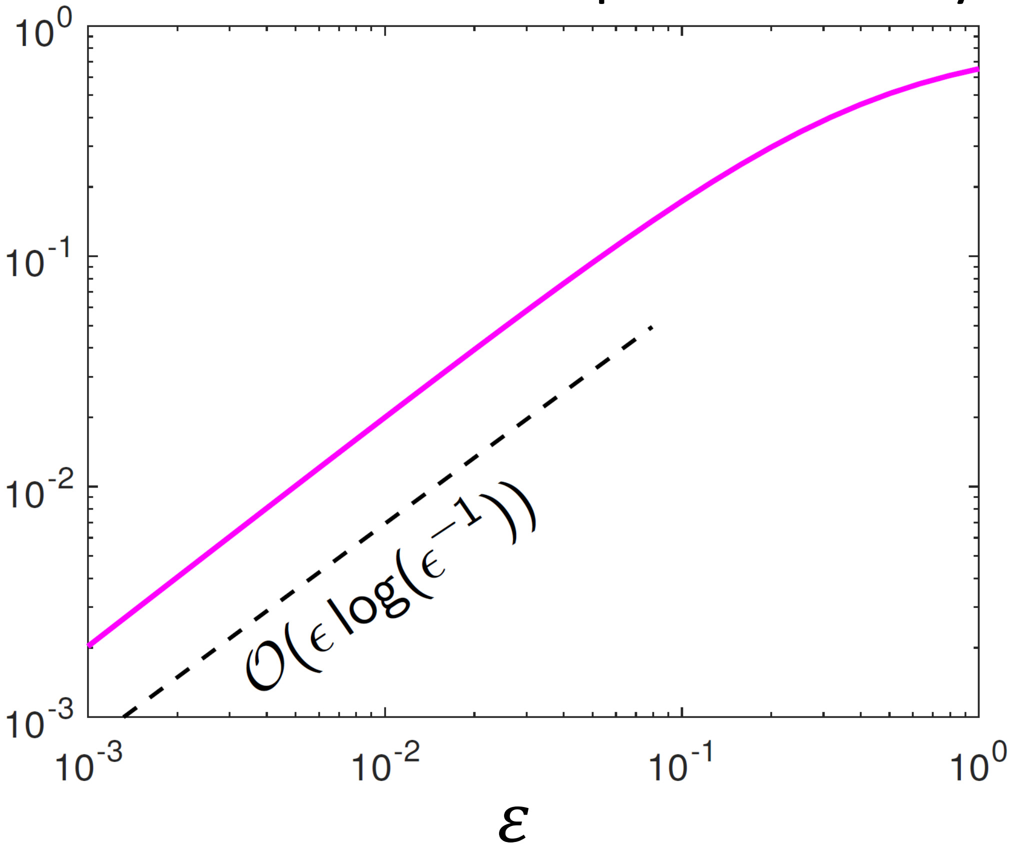




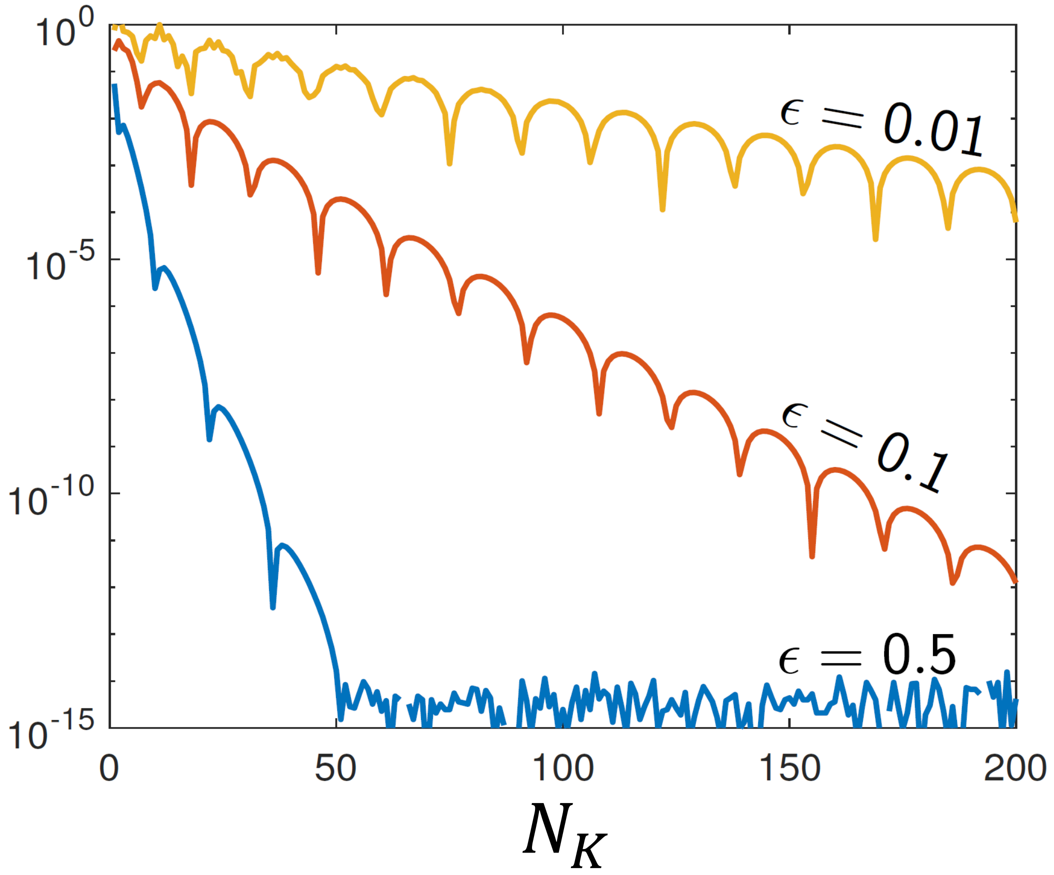
But … slow convergence

Problem: As $\varepsilon \downarrow 0$, error is $O(\varepsilon \cdot \log(1/\varepsilon))$ and $N_K(\varepsilon) \to \infty$.

Pointwise error for spectral density



Error due to discretisation



Small N_K critical in <u>data-driven</u> computations. Can we improve convergence rate?

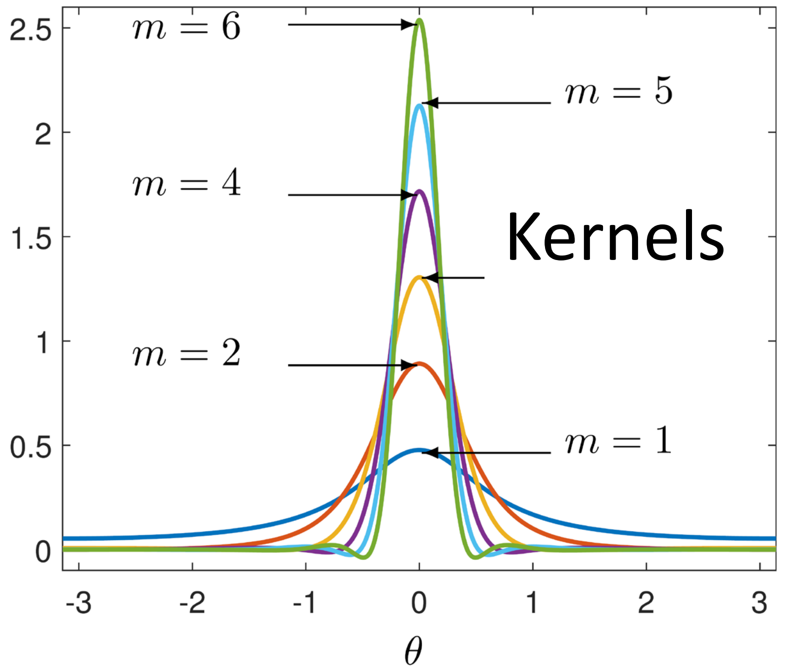
High-order rational kernels

mth order rational kernels:

$$K_\varepsilon(\theta) = \frac{e^{-i\theta}}{2\pi}\sum_{j=1}^{m}\left[\frac{c_j}{e^{-i\theta} - (1+\varepsilon\overline{z_j})^{-1}} - \frac{d_j}{e^{-i\theta} - (1+\varepsilon z_j)}\right]$$

$$[K_\varepsilon * \nu_g](\theta_0) = \sum_{j=1}^{m}\left[c_j\mathcal{C}_g\left(e^{i\theta_0}(1+\varepsilon\overline{z_j})^{-1}\right) - d_j\mathcal{C}_g\left(e^{i\theta_0}(1+\varepsilon z_j)\right)\right]$$

- Theory providing $\{c_j, d_j, z_j\}$
- Convolution computed with error control.
- $O(PN_K)$ cost for evaluation at P values of θ.



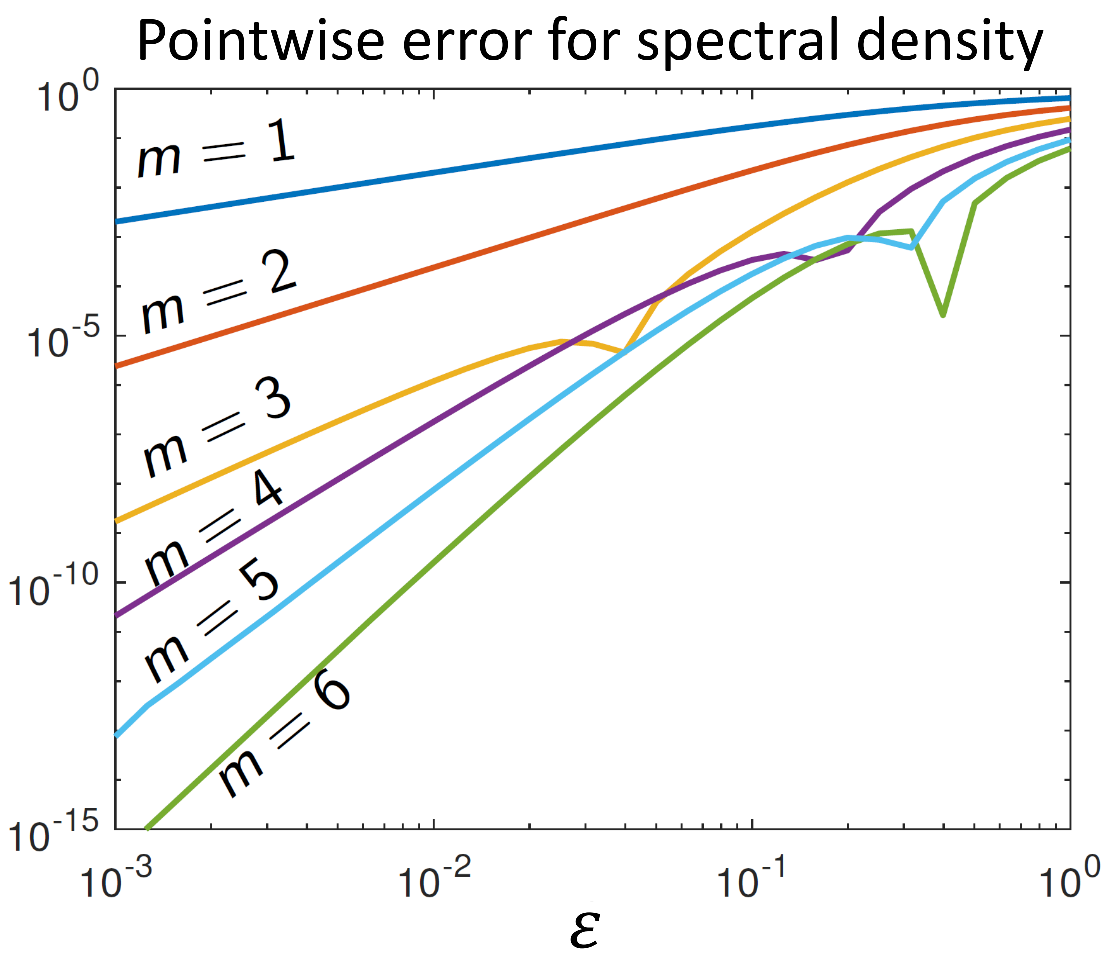
Convergence

Theorem: *Automatic* selection of $N_K(\varepsilon)$ with $O(\varepsilon^m \log(1/\varepsilon))$ convergence:

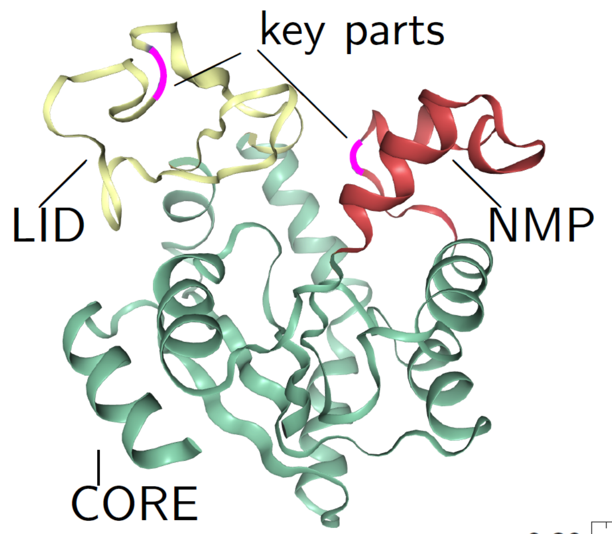
- Density of continuous spectrum.
  (pointwise and L^p)
- Integration against test functions.
  (weak convergence)

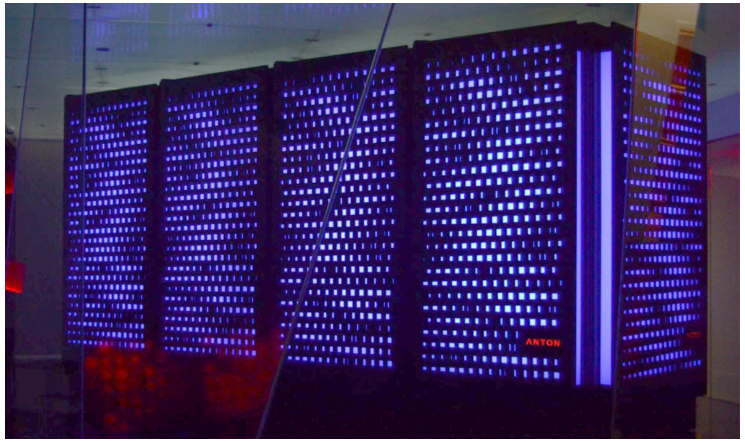
$$\int_{-\pi}^{\pi} h(\theta)\left[K_\varepsilon * \nu_g\right](\theta)\,\mathrm{d}\theta$$
$$= \int_{-\pi}^{\pi} h(\theta)\ \mathrm{d}\nu_g(\theta) + O(\varepsilon^m \log(1/\varepsilon))$$

Also recover discrete spectrum.

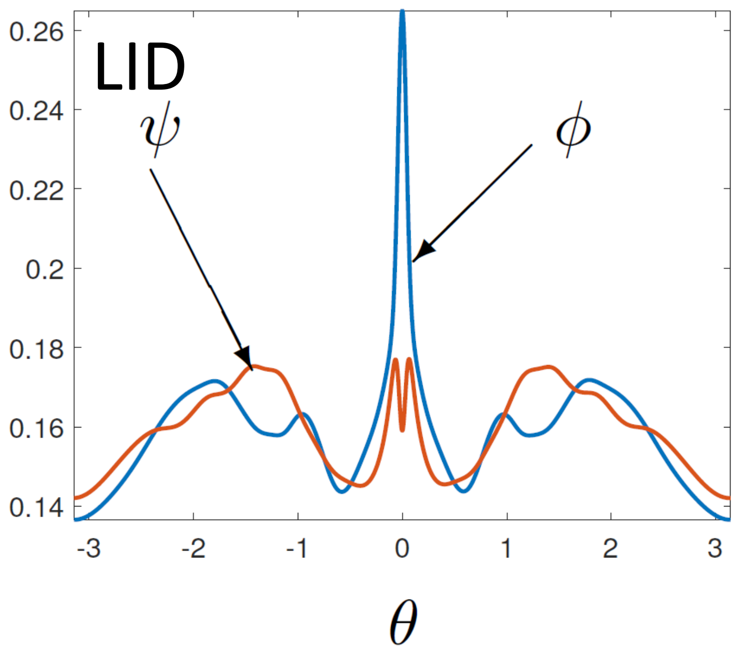


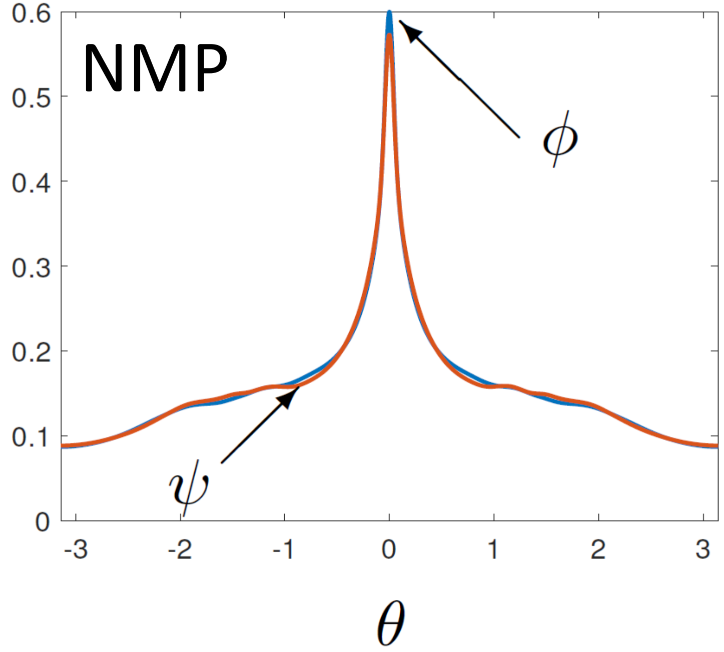
Example: molecular dynamics (Adenylate Kinase)





- All-atom equilibrium simulation for 1.004×10^{-6}s
- Ambient dimension $\approx 20{,}000$ (positions and momenta of atoms)
- 6th order kernel (spec res 10^{-6})



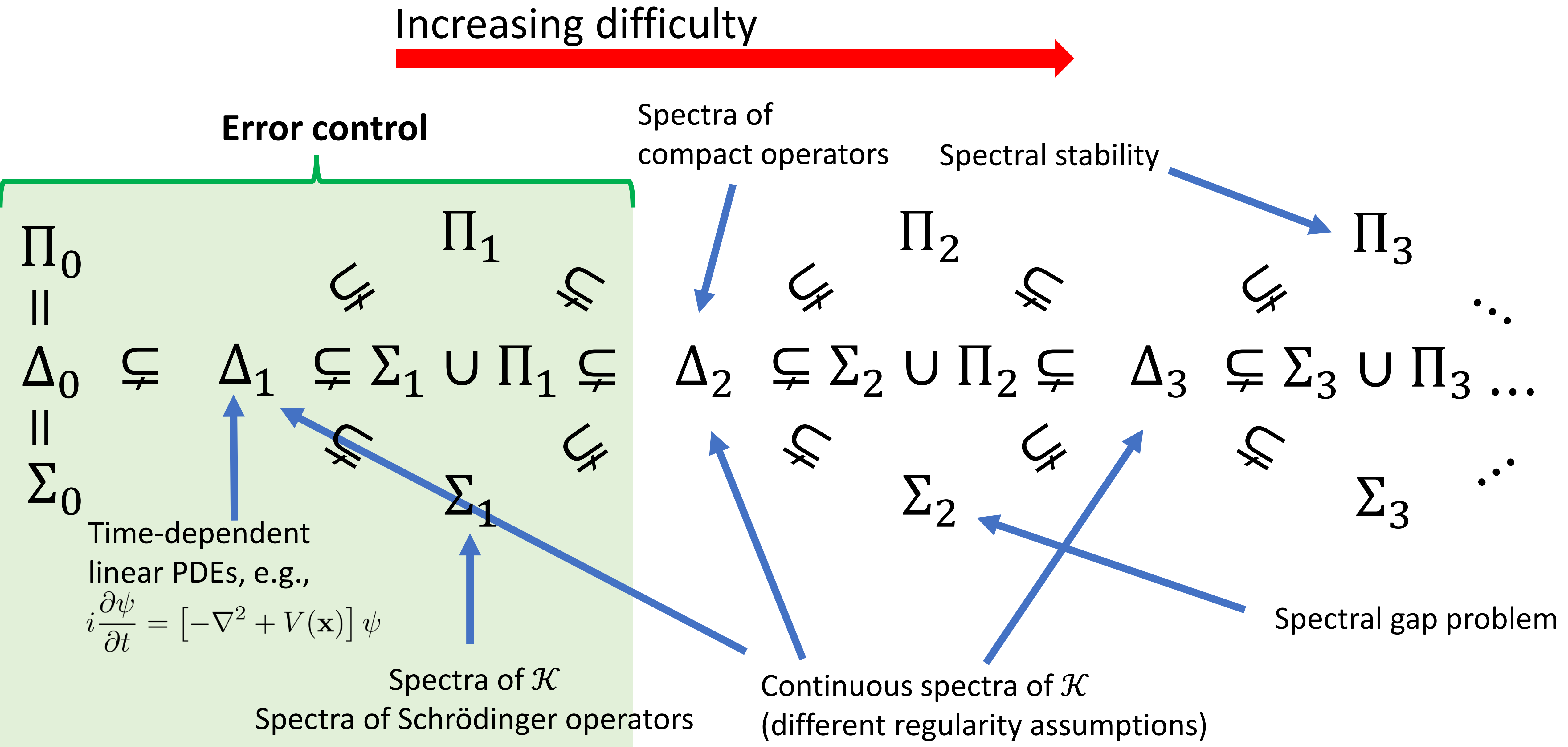


Wider programme: a toolkit

- Infinite-dimensional numerical analysis $\Longrightarrow$ **Compute spectral properties for the first time.**
- Solvability Complexity Index hierarchy $\Longrightarrow$ **Algorithms realise the boundaries of what's possible.**
- Builds on and extends work of **Turing**, **Smale**, and **McMullen.**
- **Extends to:** Foundations of AI, PDEs (e.g., time-dep. Schrödinger eq. on $L^2(\mathbb{R}^d)$ with error control), optimisation (e.g., guarantees), computer-assisted proofs, …

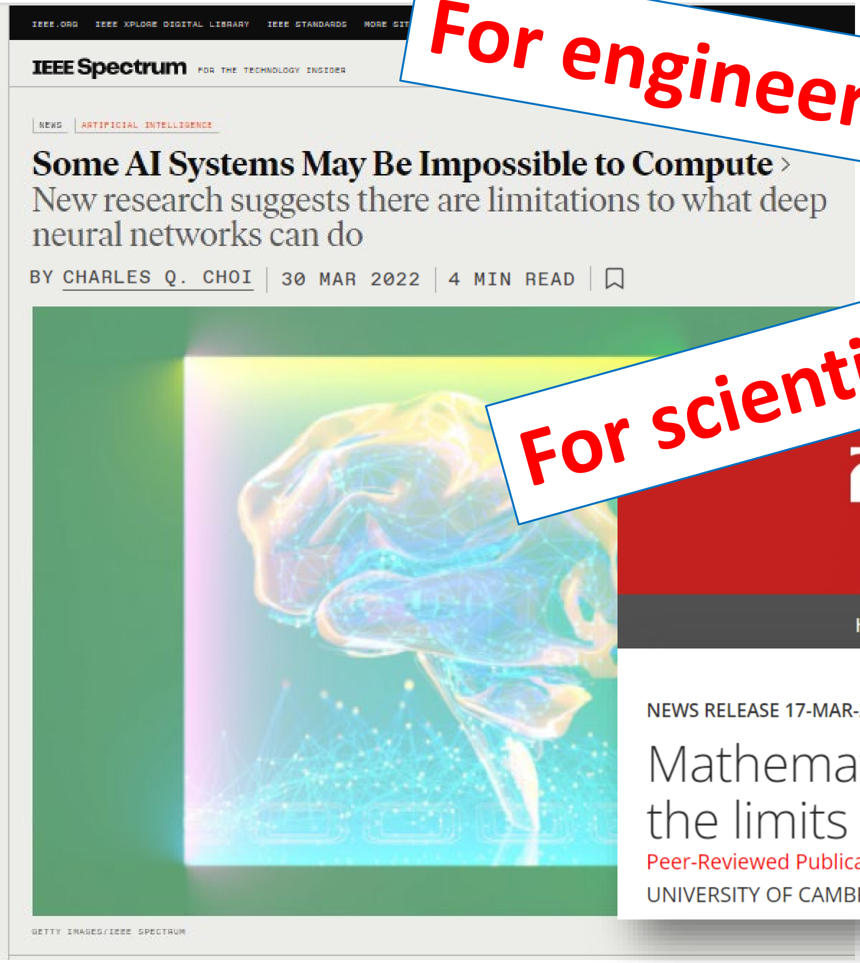
- C., *"On the computation of geometric features of spectra of linear operators on Hilbert spaces,"* **FOCM**, under revisions.
- C., *"Computing spectral measures and spectral types,"* **Communications in Mathematical Physics**, 2021.
- C., Horning, Townsend *"Computing spectral measures of self-adjoint operators,"* **SIAM Review**, 2021.
- C., Roman, Hansen, *"How to compute spectra with error control,"* **Physical Review Letters**, 2019.
- C., Hansen, *"The foundations of spectral computations via the solvability complexity index hierarchy,"* **JEMS**, under revisions.
- C., *"Computing semigroups with error control,"* **SIAM Journal on Numerical Analysis**, 2022.
- Software package (MATLAB): https://github.com/SpecSolve for PDEs, integral operators, infinite matrices.
- Smale, *"The fundamental theorem of algebra and complexity theory,"* **Bulletin of the AMS**, 1981.
- McMullen, *"Families of rational maps and iterative root-finding algorithms,"* **Annals of Mathematics**, 1987.

Sample of classification theorems



Paradox: "Nice" linear inverse problems where a stable and accurate neural network for image reconstruction exists, but it can never be trained!

For engineers



For scientists

For numerical analysts

- C., Antun, Hansen, "*The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem*," **Proceedings of the National Academy of Sciences**, 2022.

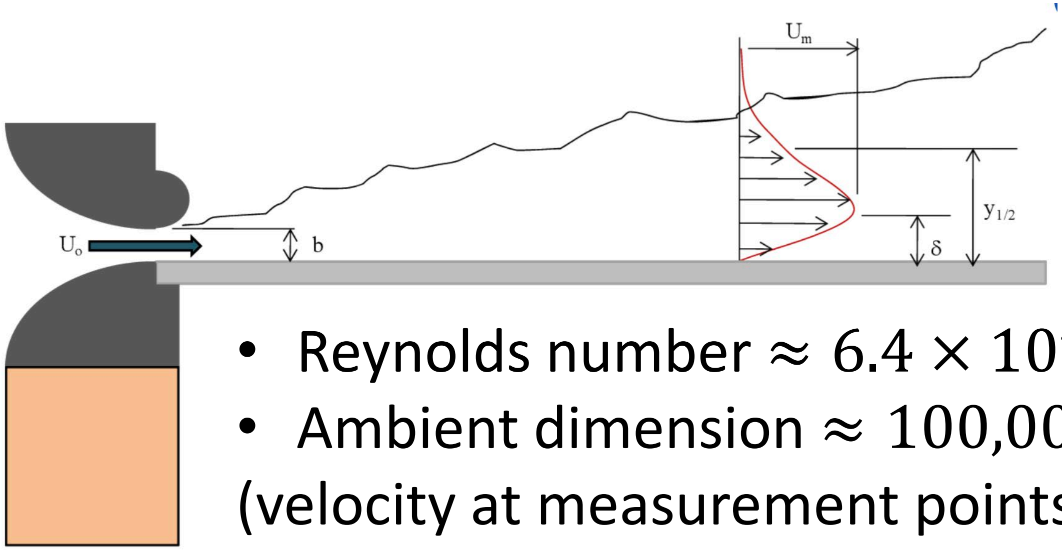
Summary

Rigorous + practical data-driven algorithms for spectral properties of Koopman operators.

- Spectra, pseudospectra and residuals of general Koopman operators (error control).
  - **Idea:** New matrix for residual ⇒ ResDMD.
- Spectral measures of measure-preserving systems with high-order convergence. Continuous spectra, discrete spectra and weak convergence.
  - **Idea:** Convolution with rational kernels via resolvent and ResDMD.
- Dealt with high-dimensional dynamical systems.
  - **Idea:** ResDMD to verify learned dictionaries.

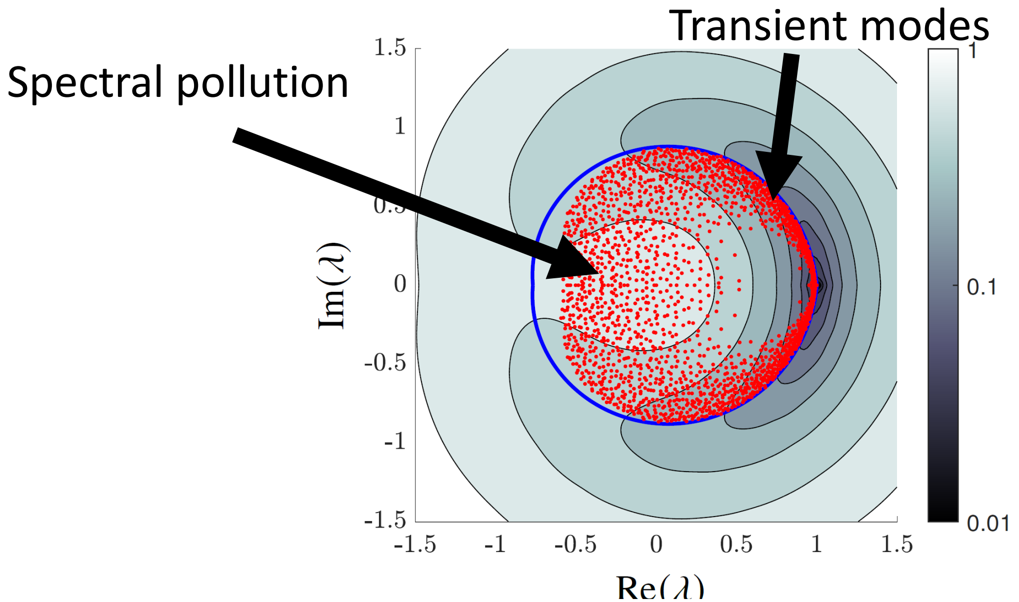
Part of a wider programme on foundations of computation and numerical analysis.

Example: wall-jet boundary layer

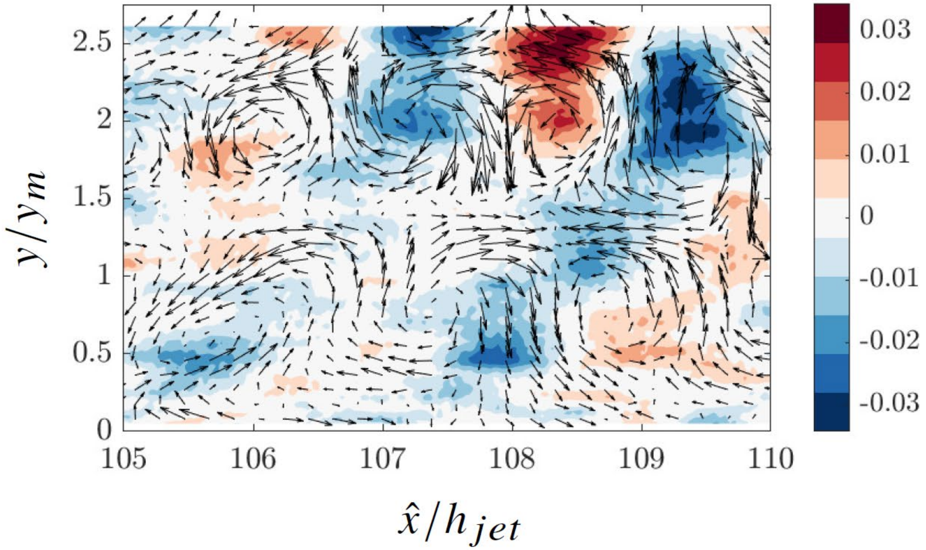


- Reynolds number $\approx 6.4 \times 10^4$
- Ambient dimension $\approx 100{,}000$

(velocity at measurement points)



$\lambda = 0.9439 + 0.2458i$, error ≤ 0.0765



$\lambda = 0.8948 + 0.1065i$, error ≤ 0.1105