# **Numerical analysis** in the age of **data science** through the **Solvability Complexity Index Hierarchy**

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# When can algorithms be trusted?

- **Ex1: Data-driven dynamical systems** **Error control and verification?**
- **Ex2: Trustworthiness in AI** **Stability and accuracy guarantees?**

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- **Ex2: Trustworthiness in AI** — **Stability and accuracy guarantees?**

**Why is this question essential?**

- Bedrock of numerical analysis.
- Reliable computations to back-up and test theories.
- Computed “solutions” meaningless without understanding error.

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**Toolkit** for classifying the difficulty of computational problems and proving the optimality of algorithms.

# Talk outline

- **Example 1:** Rigorous and verifiable data-driven dynamical systems
  - **Upper bounds (on difficulty):** Positive results on what’s possible.
- **A toolkit:** Solvability Complexity Index Hierarchy
  - Classification for infinite-dimensional spectral problems and beyond.
- **Example 2:** Smale's 18th problem, “What are the limits of AI?”
  - **Lower bounds (on difficulty):** Use SCI techniques to prove impossibility results.

**Toolkit** for classifying the difficulty of computational problems and proving the optimality of algorithms.

# Example 1: Rigorous and verifiable data-driven dynamical systems

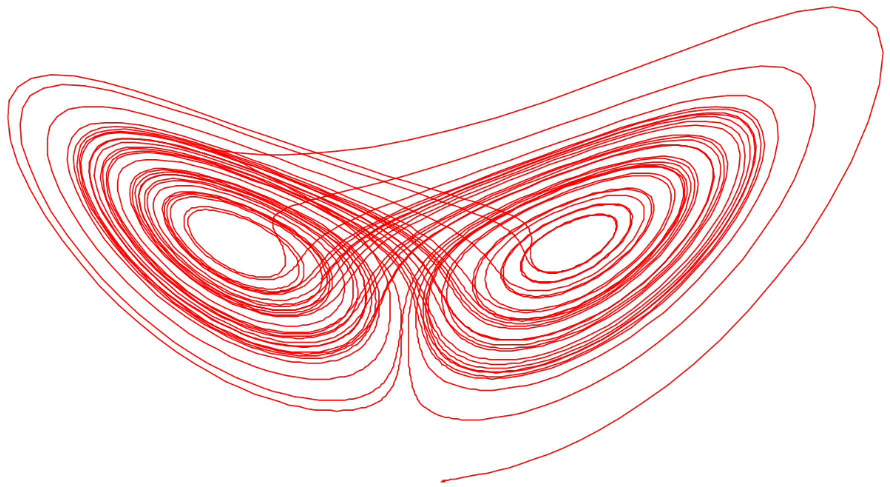
**Upper bounds:** Positive results on what's possible.

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



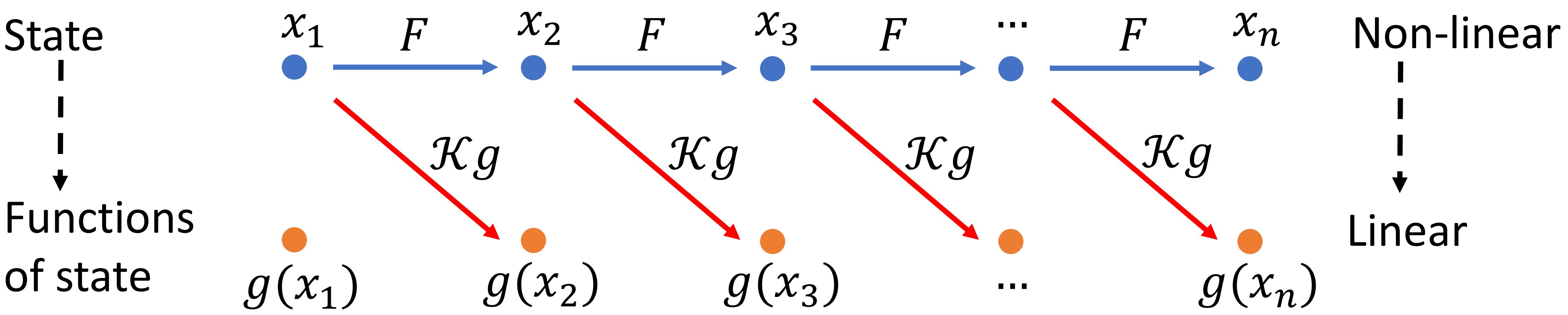
**Can we develop verified methods?**

# 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 $\omega$, with inner product $\langle \cdot, \cdot \rangle$.


- Koopman, "*Hamiltonian systems and transformation in Hilbert space*," **PNAS**, 1931.
- Koopman, v. Neumann, "*Dynamical systems of continuous spectra*," **PNAS**, 1932.

# Koopman mode decomposition

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

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

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.

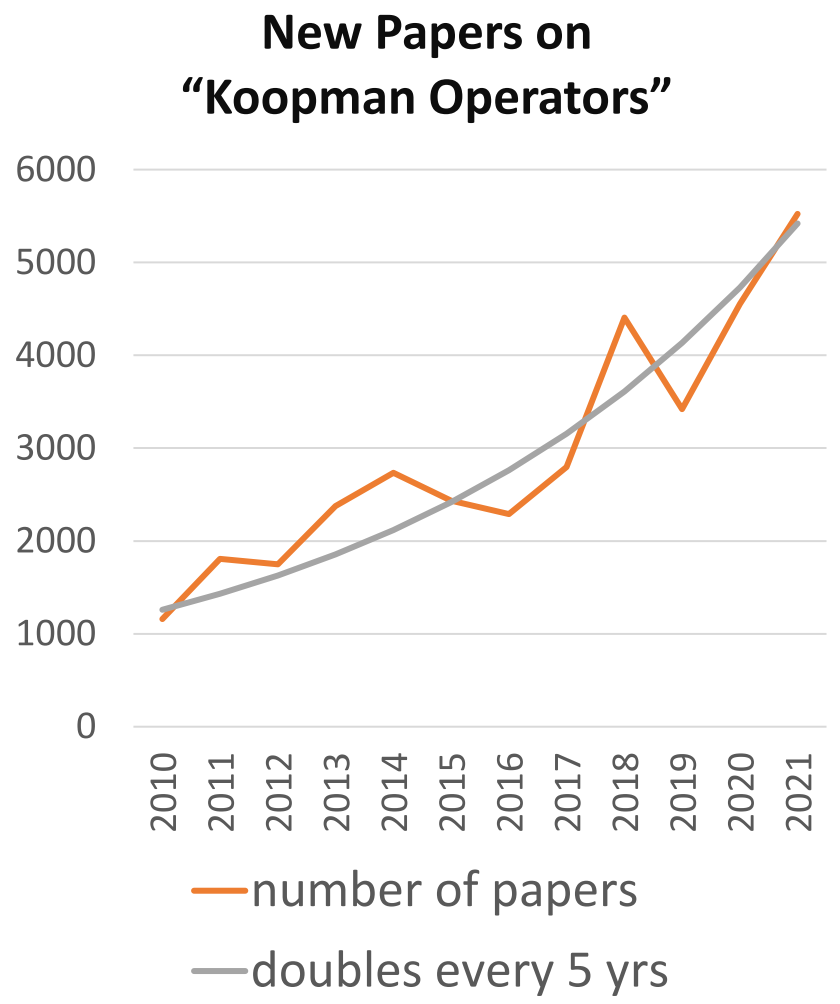
# Koopmania*: a revolution in the big data era

≈35,000 papers over last decade!

***Very* little on convergence guarantees or verification.**

**Why is this lacking?**

- K. operators have been distinct from NA community.
- Dealing with infinite dim. is notoriously hard …




**Wikipedia*: *"its wild surge in popularity is sometimes jokingly called 'Koopmania'"*

# Can we compute spectral properties in inf. dim.?

$$\mathrm{Spec}(\mathcal{K}) = \{\lambda \in \mathbb{C} : \mathcal{K} - \lambda I \text{ is not invertible}\}$$

*"Operators that arise in practice are not **diagonalized**, and it is often very hard to locate the spectrum. Thus, one has to settle for numerical approximations. Unfortunately, there are **no proven general techniques**."* W. Arveson, Berkeley (1994)

**Naïve:** $\mathcal{K} \longrightarrow \mathbb{K} \in \mathbb{C}^{N\times N}$ + compute e-values, **problems:**

1) **"Too much":** Approximate spurious modes $\lambda \notin \mathrm{Spec}(\mathcal{K})$ - "spectral pollution"
2) **"Too little":** Miss parts of $\mathrm{Spec}(\mathcal{K})$
3) **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.

# Dynamic Mode Decomposition (DMD)

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

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

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

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

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


- Schmid, “*Dynamic mode decomposition of numerical and experimental data,*” **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.

# Residual DMD (ResDMD): Approx. $\mathcal{K}$ and $\mathcal{K}^*\mathcal{K}$

$$\langle \psi_k, \psi_j \rangle \approx \sum_{m=1}^{M} w_m \overline{\psi_j(x^{(m)})}\, \psi_k(x^{(m)}) = [\underbrace{\Psi_X{}^* W \Psi_X}_{G}]_{jk}$$

$$\langle \mathcal{K}\psi_k, \psi_j \rangle \approx \sum_{m=1}^{M} w_m \overline{\psi_j(x^{(m)})}\, \underbrace{\psi_k(y^{(m)})}_{[\mathcal{K}\psi_k](x^{(m)})} = [\underbrace{\Psi_X{}^* W \Psi_Y}_{K_1}]_{jk}$$

Error control

$$\langle \mathcal{K}\psi_k, \mathcal{K}\psi_j \rangle \approx \sum_{m=1}^{M} w_m \overline{\psi_j(y^{(m)})}\, \psi_k(y^{(m)}) = [\underbrace{\Psi_Y{}^* W \Psi_Y}_{K_2}]_{jk}$$

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


- 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.

# Example of an upper bound

$$\mathrm{res}(\lambda, \mathbf{g}) = \sqrt{\frac{\mathbf{g}^*\left[K_2 - \lambda {K_1}^* - \bar{\lambda} K_1 + |\lambda|^2 G\right]\mathbf{g}}{\mathbf{g}^* G \mathbf{g}}}, \qquad \mathrm{Spec}_\varepsilon(\mathcal{K}) = \cup_{\|\mathcal{B}\| \le \varepsilon} \mathrm{Spec}(\mathcal{K} + \mathcal{B})$$

1. Compute $G, K_1, K_2 \in \mathbb{C}^{N\times N}$.
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 $\mathrm{Spec}_\varepsilon(\mathcal{K})$), $\{g_k : \tau_k < \varepsilon\}$ ($\varepsilon$-pseudo-eigenfunctions).

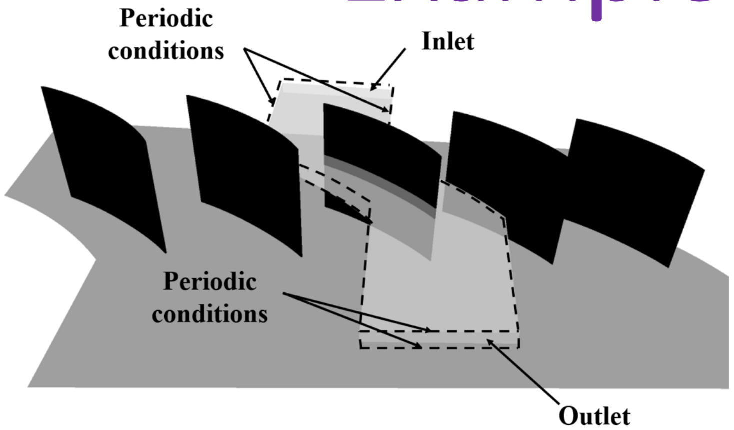
**First convergent method for general $\mathcal{K}$**

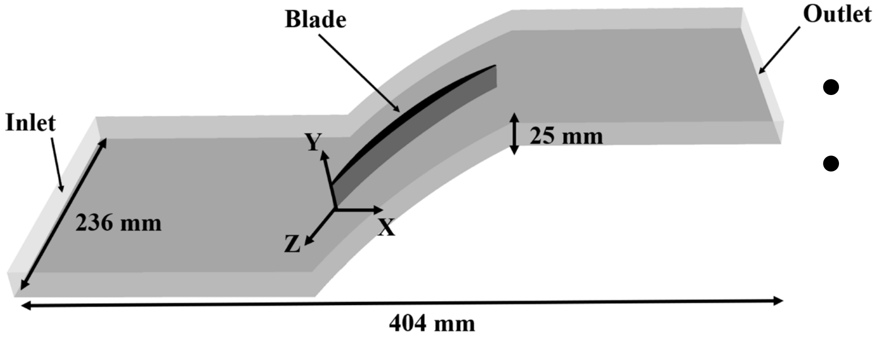
**Theorem**: Suppose the quadrature rule converges.
- **Error control:** $\{z_k : \tau_k < \varepsilon\} \subseteq \mathrm{Spec}_\varepsilon(\mathcal{K})$ (as $M \to \infty$)
- **Convergence:** Converges locally uniformly to $\mathrm{Spec}_\varepsilon(\mathcal{K})$ (as $N \to \infty$)

Similarly, overcome: **1) "too much", 2) "too little", 3) cts spectra, 4) verification.**

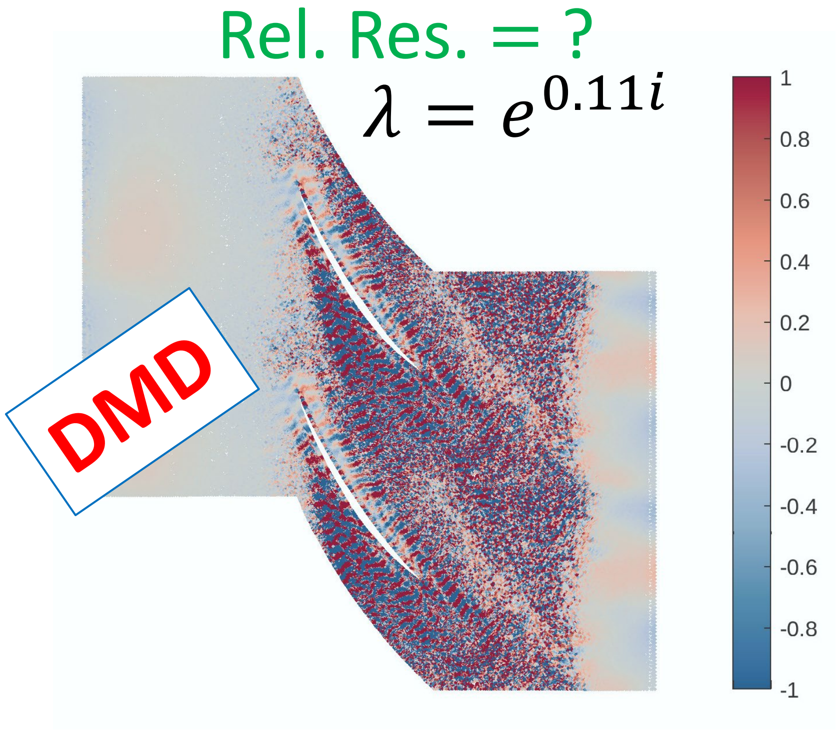
**Paves the way for rigorous data-driven Koopmania!**

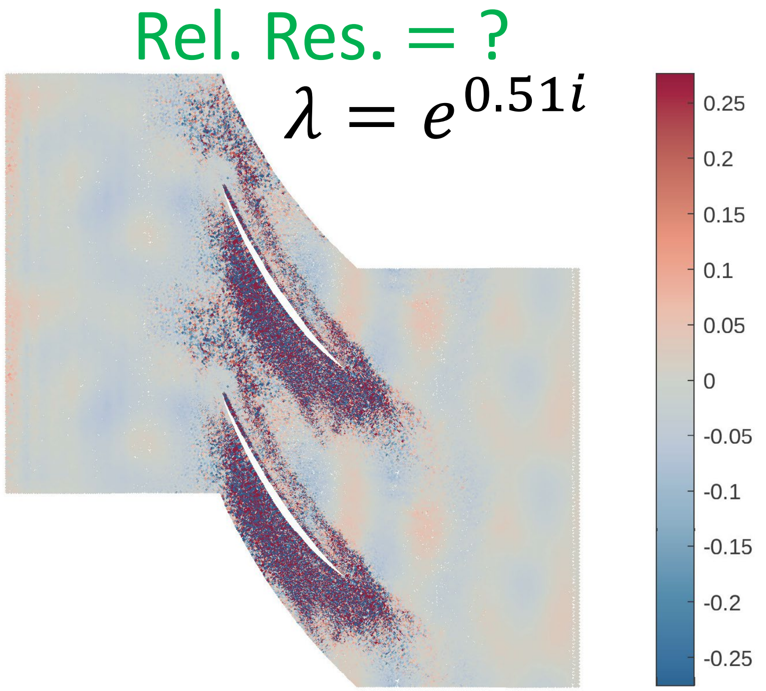
# Example: pressure field of turbulent flow

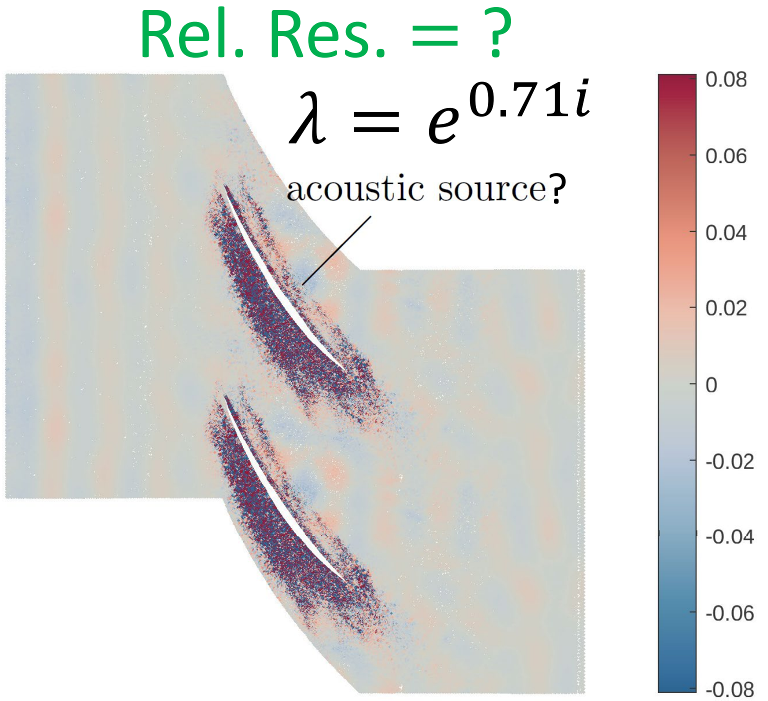


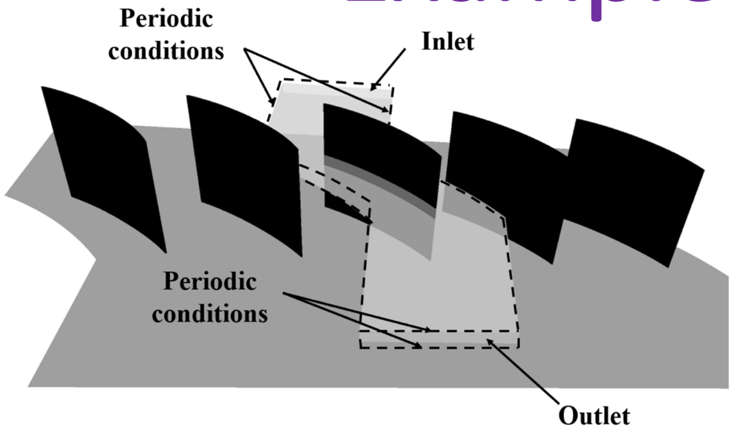

- Reynolds number $\approx 3.9 \times 10^5$
- Ambient dimension $\approx 300{,}000$ (number of measurement points)

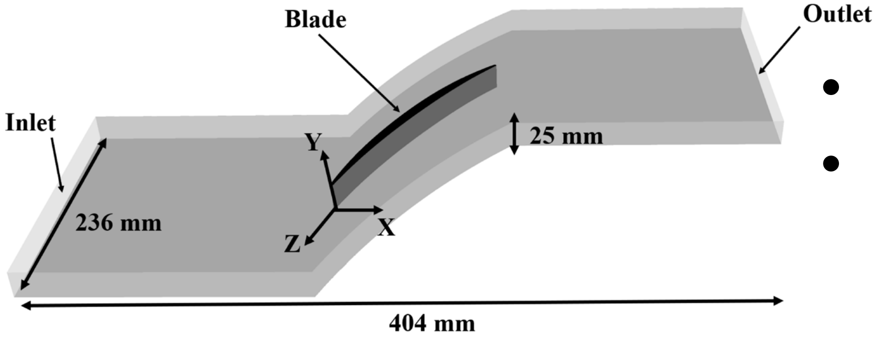


# Example: pressure field of turbulent flow

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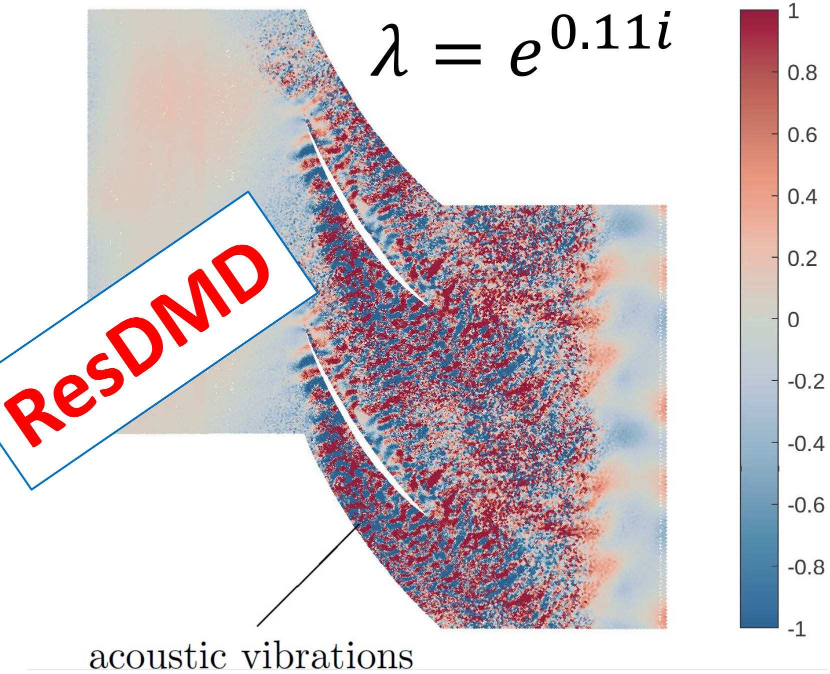
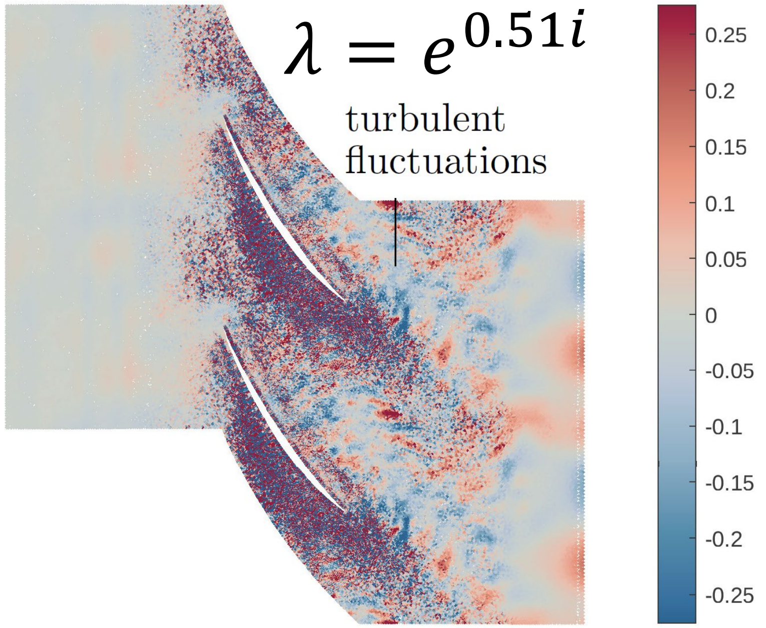
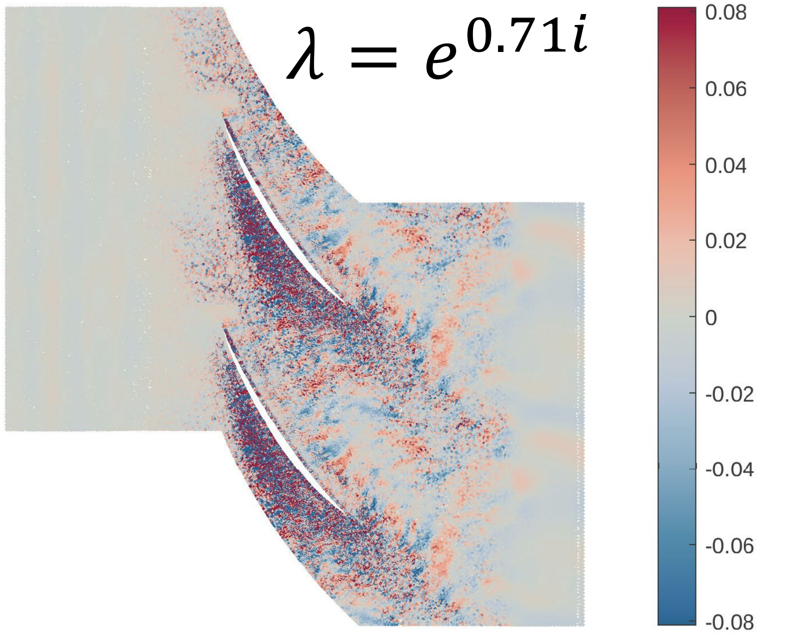
Rel. Res. $\leq 0.0054$




Rel. Res. $\leq 0.0128$




Rel. Res. $\leq 0.0196$



Previous algorithm $\Gamma_M$ (with adaptive $N = N(M)$):

$$\lim_{\varepsilon\downarrow 0}\lim_{M\to\infty}\Gamma_M\left(\left\{x^{(m)}, y^{(m)} = F\left(x^{(m)}\right)\right\}_{m=1}^{M}, \varepsilon\right) = \mathrm{Spec}(\mathcal{K})$$

Phenomena of "successive limits" widespread…

# A toolkit: Solvability Complexity Index Hierarchy

# Solvability Complexity Index Hierarchy

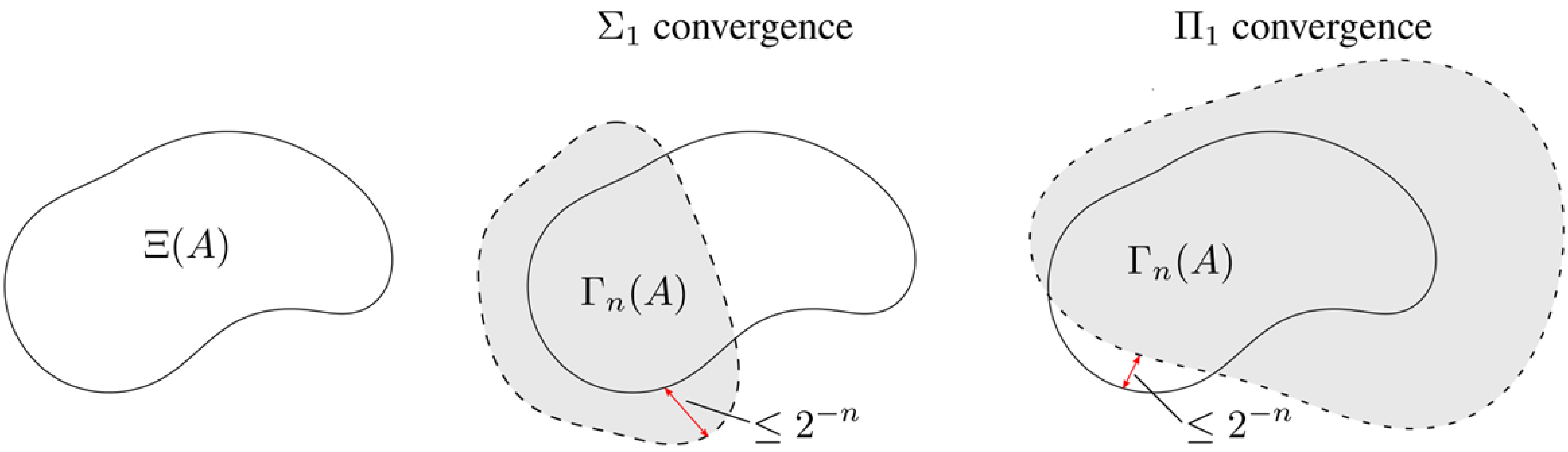
For $A \in \Omega$, want to compute $\Xi\colon \Omega \to (\mathcal{M}, d)$ metric space

- $\Delta_0$: Problems solved in finite time (v. rare).
- $\Delta_1$: Problems solved in "one limit" with full error control:
$$d(\Gamma_n(A), \Xi(A)) \leq 2^{-n}$$
- $\Delta_2$: Problems solved in "one limit" (SCI=1):
$$\lim_{n\to\infty} \Gamma_n(A) = \Xi(A)$$
- $\Delta_3$: Problems solved in "two successive limits" (SCI=2):
$$\lim_{n\to\infty} \lim_{m\to\infty} \Gamma_{n,m}(A) = \Xi(A)$$

and so on…


- C., *"The Foundations of Infinite-Dimensional Spectral Computations,"* **Cambridge**, PhD thesis.
- Ben-Artzi, C., Hansen, Nevanlinna, Seidel, *"On the solvability complexity index hierarchy and towers of algorithms."*
- Hansen, *"On the solvability complexity index, the $n$-pseudospectrum and approximations of spectra of operators,"* **JAMS**, 2011.
- McMullen, *"Families of rational maps and iterative root-finding algorithms,"* **Annals of Mathematics**, 1987.
- Smale, *"The fundamental theorem of algebra and complexity theory,"* **Bulletin of the AMS**, 1981.

# Error control for spectral problems




- $\Sigma_1 \subsetneq \Delta_2$: $\lim_{n\to\infty} \Gamma_n(A) = \Xi(A)$, $\max_{z\in\Gamma_n(A)} \mathrm{dist}\big(z, \Xi(A)\big) \leq 2^{-n}$
- $\Pi_1 \subsetneq \Delta_2$: $\lim_{n\to\infty} \Gamma_n(A) = \Xi(A)$, $\max_{z\in\Xi(A)} \mathrm{dist}(z, \Gamma_n(A)) \leq 2^{-n}$

**NB: Typically, eigensolvers for PDEs prove $\Delta_2$, not optimal $\Sigma_1$…**

# $\Sigma_1$ example: e-values with guaranteed error bounds

$$A = -\nabla^2 + x^2 + V(x) \text{ on } \mathbb{R}^1$$

| $V$ | $\cos(x)$ | $\tanh(x)$ | $\exp(-x^2)$ | $1/(1+x^2)$ |
|---|---|---|---|---|
| $E_0$ | 1.7561051579 | 0.8703478514 | 1.6882809272 | 1.7468178026 |
| $E_1$ | 3.3447026910 | 2.9666370800 | 3.3395578680 | 3.4757613534 |
| $E_2$ | 5.0606547136 | 4.9825969775 | 5.2703748823 | 5.4115076464 |
| $E_3$ | 6.8649969390 | 6.9898951678 | 7.2225903394 | 7.3503220313 |
| $E_4$ | 8.7353069954 | 8.9931317537 | 9.1953373991 | 9.3168983920 |

Can deal with mix of cts and discrete spectra, other domains, other PDEs etc.

# Small sample of classification theorems

Increasing difficulty →

**Error control**

$$
\begin{array}{ccccccccccccccc}
\Pi_0 & & & & \Pi_1 & & & & \Pi_2 & & & & \Pi_3 & & \\
\| & & & \rotatebox{45}{$\subsetneq$} & & \rotatebox{-45}{$\subsetneq$} & & \rotatebox{45}{$\subsetneq$} & & \rotatebox{-45}{$\subsetneq$} & & \rotatebox{45}{$\subsetneq$} & & \cdot^{\cdot^{\cdot}} & \\
\Delta_0 & \subsetneq & \Delta_1 & \subsetneq & \Sigma_1 \cup \Pi_1 & \subsetneq & \Delta_2 & \subsetneq & \Sigma_2 \cup \Pi_2 & \subsetneq & \Delta_3 & \subsetneq & \Sigma_3 \cup \Pi_3 & \ldots & \\
\| & & & \rotatebox{-45}{$\subsetneq$} & & \rotatebox{45}{$\subsetneq$} & & \rotatebox{-45}{$\subsetneq$} & & \rotatebox{45}{$\subsetneq$} & & \rotatebox{-45}{$\subsetneq$} & & \ddots & \\
\Sigma_0 & & & & \Sigma_1 & & & & \Sigma_2 & & & & \Sigma_3 & &
\end{array}
$$

# Small sample of classification theorems

Increasing difficulty

**Error control**

$$\begin{array}{ccccccccccccccc}
\Pi_0 & & & & & \Pi_1 & & & & \Pi_2 & & & & \Pi_3 & \\
\| & & & & \rotatebox{45}{$\subsetneq$} & & \rotatebox{-45}{$\subsetneq$} & & \rotatebox{45}{$\subsetneq$} & & \rotatebox{-45}{$\subsetneq$} & & \rotatebox{45}{$\subsetneq$} & & \ddots \\
\Delta_0 & \subsetneq & \Delta_1 & \subsetneq & \Sigma_1 \cup \Pi_1 & & \subsetneq & \Delta_2 & \subsetneq \Sigma_2 \cup \Pi_2 \subsetneq & & & \Delta_3 & \subsetneq \Sigma_3 \cup \Pi_3 & \ldots & \\
\| & & & & \rotatebox{-45}{$\subsetneq$} & & \rotatebox{45}{$\subsetneq$} & & \rotatebox{-45}{$\subsetneq$} & & \rotatebox{45}{$\subsetneq$} & & \rotatebox{-45}{$\subsetneq$} & & \iddots \\
\Sigma_0 & & & & & \Sigma_1 & & & & \Sigma_2 & & & & \Sigma_3 &
\end{array}$$

Spectra of $\mathcal{K}$

Continuous spectra of $\mathcal{K}$ (different regularity assumptions)

# Small sample of classification theorems

Increasing difficulty

**Error control**

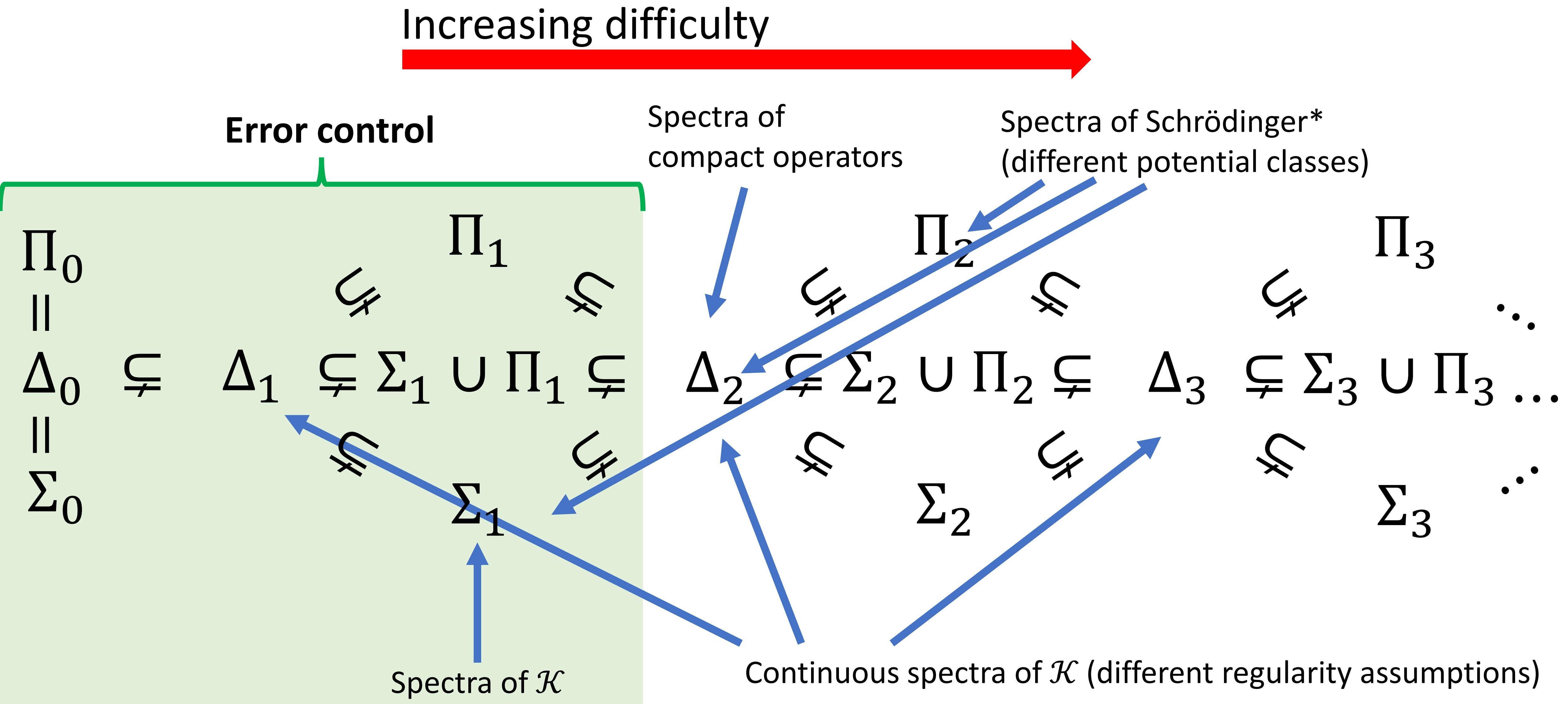
Spectra of compact operators

$$
\begin{tikzcd}
\Pi_0 \arrow[d, phantom, "\Vert"] & & \Pi_1 \arrow[dr, phantom, "\subsetneq"] & & \Pi_2 \arrow[dr, phantom, "\subsetneq"] & & \Pi_3 \arrow[dr, phantom, "\iddots"] & \\
\Delta_0 \arrow[r, phantom, "\subsetneq"] \arrow[d, phantom, "\Vert"] & \Delta_1 \arrow[ur, phantom, "\subsetneq"] \arrow[dr, phantom, "\subsetneq"] & \Sigma_1 \cup \Pi_1 \arrow[l, phantom, "\supsetneq"] \arrow[r, phantom, "\subsetneq"] & \Delta_2 \arrow[ur, phantom, "\subsetneq"] \arrow[dr, phantom, "\subsetneq"] & \Sigma_2 \cup \Pi_2 \arrow[l, phantom, "\supsetneq"] \arrow[r, phantom, "\subsetneq"] & \Delta_3 \arrow[ur, phantom, "\subsetneq"] \arrow[dr, phantom, "\subsetneq"] & \Sigma_3 \cup \Pi_3 \arrow[l, phantom, "\supsetneq"] & \dots \\
\Sigma_0 & & \Sigma_1 \arrow[ur, phantom, "\subsetneq"] & & \Sigma_2 \arrow[ur, phantom, "\subsetneq"] & & \Sigma_3 \arrow[ur, phantom, "\ddots"] &
\end{tikzcd}
$$

Spectra of $\mathcal{K}$

Continuous spectra of $\mathcal{K}$ (different regularity assumptions)

# Small sample of classification theorems




*Open problem of Schwinger*: “The special canonical group,” “Unitary operator bases,” PNAS, 1960.

# Small sample of classification theorems

Increasing difficulty

**Error control**

Spectra of compact operators

Spectra of Schrödinger* (different potential classes)

$$\Pi_0 = \Delta_0 = \Sigma_0$$

$$\Delta_0 \subsetneq \Delta_1 \subsetneq \Sigma_1 \cup \Pi_1 \subsetneq \Delta_2 \subsetneq \Sigma_2 \cup \Pi_2 \subsetneq \Delta_3 \subsetneq \Sigma_3 \cup \Pi_3 \ldots$$

$$\Delta_1 \subsetneq \Pi_1 \subsetneq \Delta_2, \quad \Delta_1 \subsetneq \Sigma_1 \subsetneq \Delta_2, \quad \Delta_2 \subsetneq \Pi_2 \subsetneq \Delta_3, \quad \Delta_2 \subsetneq \Sigma_2 \subsetneq \Delta_3, \quad \Delta_3 \subsetneq \Pi_3 \ldots, \quad \Delta_3 \subsetneq \Sigma_3 \ldots$$

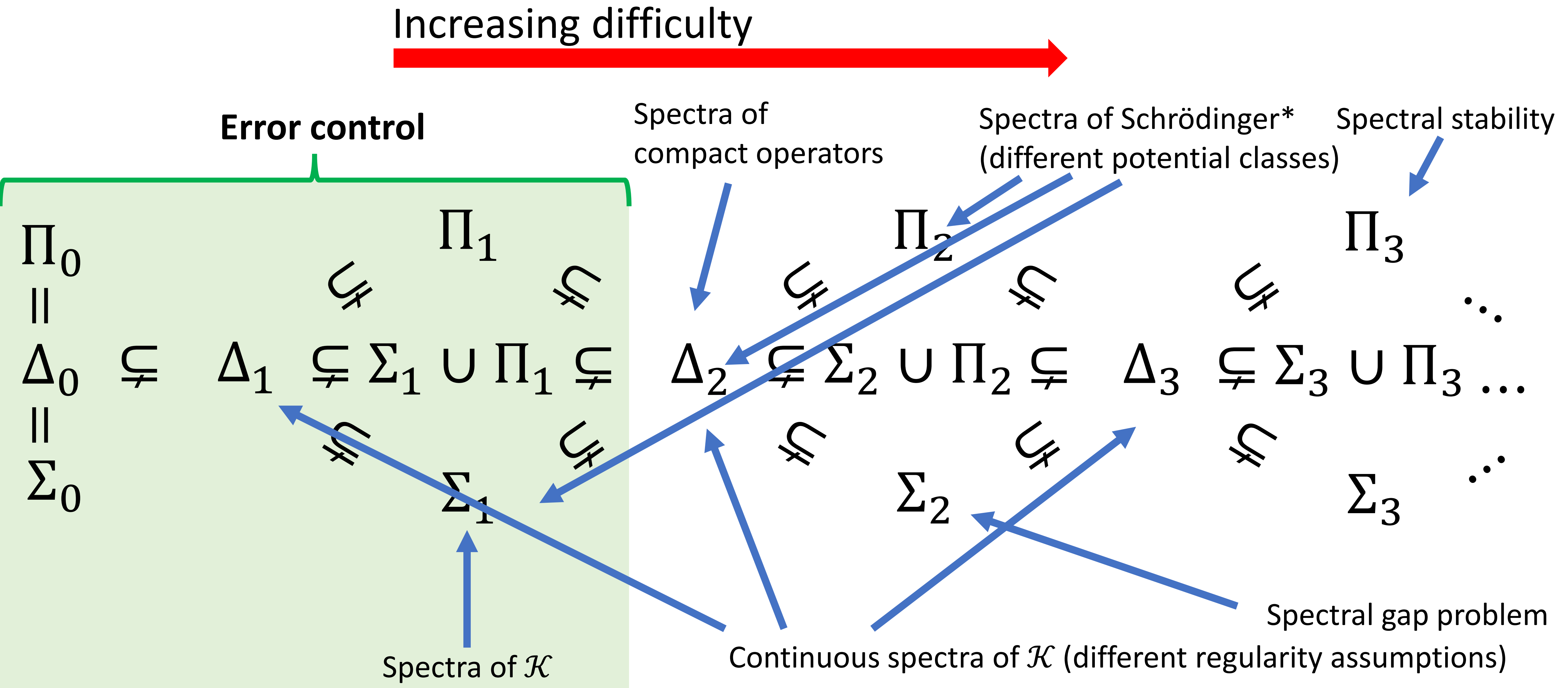
Spectra of $\mathcal{K}$

Spectral gap problem

Continuous spectra of $\mathcal{K}$ (different regularity assumptions)

*_Open problem of Schwinger_: "The special canonical group," "Unitary operator bases," PNAS, 1960.

# Small sample of classification theorems




**Open problem of Schwinger*: “The special canonical group,” “Unitary operator bases,” PNAS, 1960.

# Some success stories in inf. dim. spec. comp.

- Spectra with $\Sigma_1$ error control (v. large class of disc. ops and PDEs)
  - C., Roman, Hansen, *"How to compute spectra with error control,"* **PRL**, 2019.
  - C., Hansen, *"The foundations of spectral computations via the solvability complexity index hierarchy,"* **JEMS**, under revisions.
- Spectral measures and type (classification varies from $\Delta_1$ to $\Sigma_3$)
  - Webb, Olver, *"Spectra of Jacobi operators via connection coefficient matrices,"* **CIMP**, 2021.
  - C., *"Computing spectral measures and spectral types,"* **CIMP,** 2021.
  - C., Horning, Townsend, *"Computing spectral measures of self-adjoint operators,"* **SIAM Rev**, 2021.
- Resonances ($\Delta_2 \backslash \Sigma_1 \cup \Pi_1$)
  - Ben-Artzi, Marletta, Rösler, *"Computing scattering resonances,"* **JEMS**, 2022.
  - Ben-Artzi, Marletta, Rösler, *"Computing the sound of the sea in a seashell,"* **FOCM**, 2022.
- Zoo of problems (e.g., fractal dims, capacity, radii etc.) – up to $\Sigma_6$!!!!
  - C., *"On the computation of geometric features of spectra of linear operators on Hilbert spaces,"* **FOCM**, under revisions.

**General technique for lower bounds by embedding combinatorial problems.**


E.g., ground state of quasicrystal


E.g., continuous spectra of graphene

# Remarks

- Any model of computation.
  (lower bds universal, upper bds can be realized via interval arith.)
- Practical: “Spot” info or subclass needed to lower difficulty.
- Tells us what we can or cannot do.
- Existing hierarchies become special cases.
- **Extends beyond spectral problems:** 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, …

# Example 2: Smale's 18th problem “What are the limits of AI?”

*“Very often, the creation of a technological artifact precedes the science that goes with it. The steam engine was invented before thermodynamics. Thermodynamics was invented to explain the steam engine, essentially the* ***limitations*** *of it.* ***What we are after is the equivalent of thermodynamics for intelligence.****”* Yann LeCun

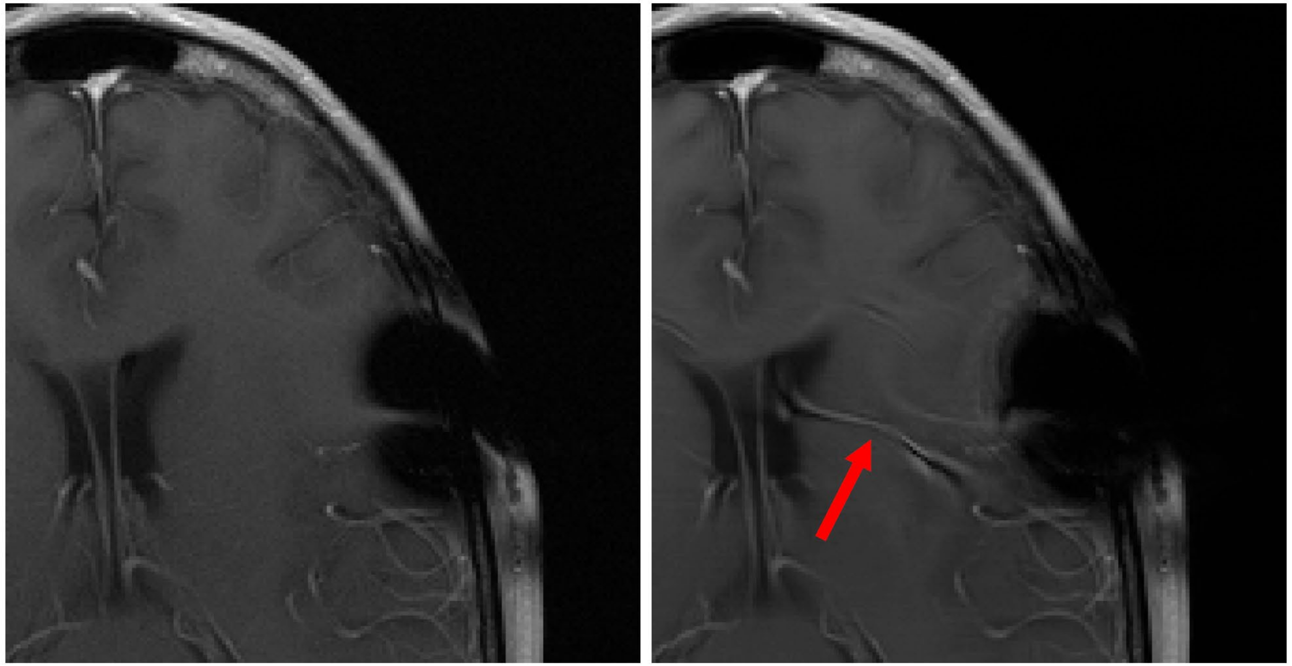
**Lower bounds:** Use SCI techniques to prove impossibility results.

(Different techniques needed for training problems.)

**S. Smale’s list of problems for the 21st century (requested by V. Arnold), inspired by Hilbert’s list*

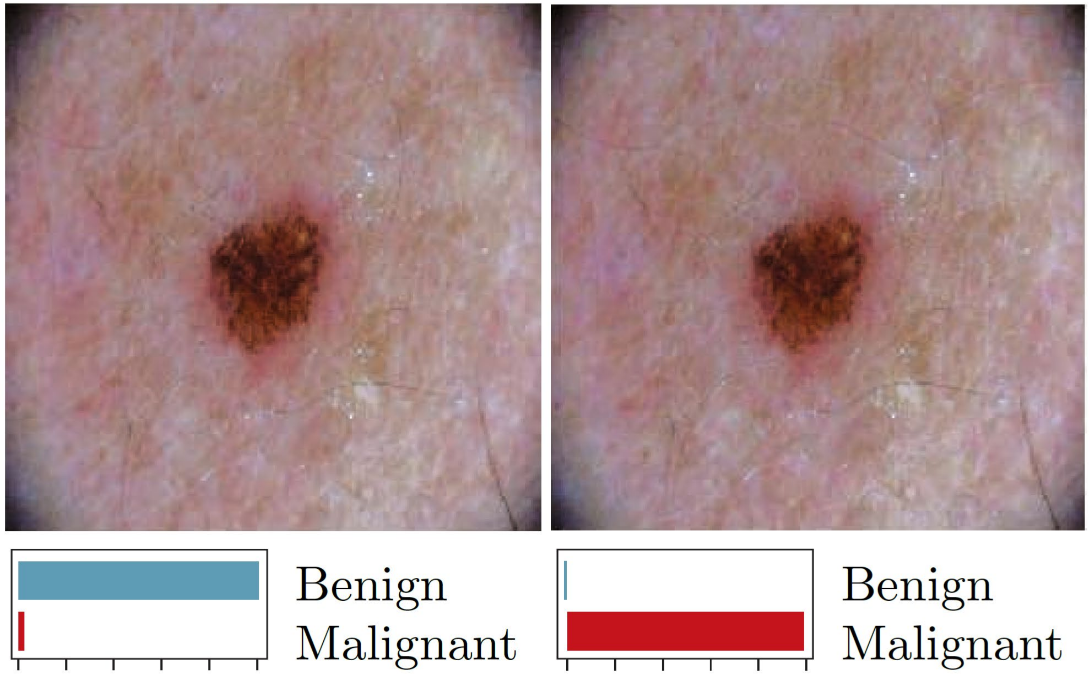
# Problem: hallucinations and instability

## Hallucinations in image reconstruction




“**AI generated hallucination**”, from Facebook and NYU’s ***FastMRI challenge*** 2020

## Instabilities in medical diagnosis




From Finlayson et al., “*Adversarial attacks on medical machine learning,*” **Science**, 2019.

**When can we make AI robust and trustworthy?**

# Example of the limits of deep learning

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

E.g., suppose we want to solve (holds for much more general problems)

$$\min_{x \in \mathbb{C}^N} \|x\|_{l^1} + \lambda \|Ax - y\|_{l_2}^2$$

$$A \in \mathbb{C}^{m \times N} \text{ (modality}, m < N), \qquad S = \{y_j\}_{j=1}^{R} \text{ (samples)}$$

Arises when given $y \approx Ax + e$.

Allow arbitrary precision of training data.

Enforce condition numbers bounded by 1.

# Example of the limits of deep learning

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

**Theorem**: Pick positive integers $n \geq 3$ and $M$. Class of problems such that:

- (**Not trainable**) No algorithm (even random) can train a neural network with $\boldsymbol{n}$ **digits** of accuracy over the dataset with probability greater than 1/2.
- (**Not practical**) $\boldsymbol{n-1}$ **digits** of accuracy possible over the dataset, but any training algorithm requires **arbitrarily large training data**.
- (**Trainable and practical**) $\boldsymbol{n-2}$ digits of accuracy possible over the dataset via training algorithm using $\boldsymbol{M}$ **training data**.

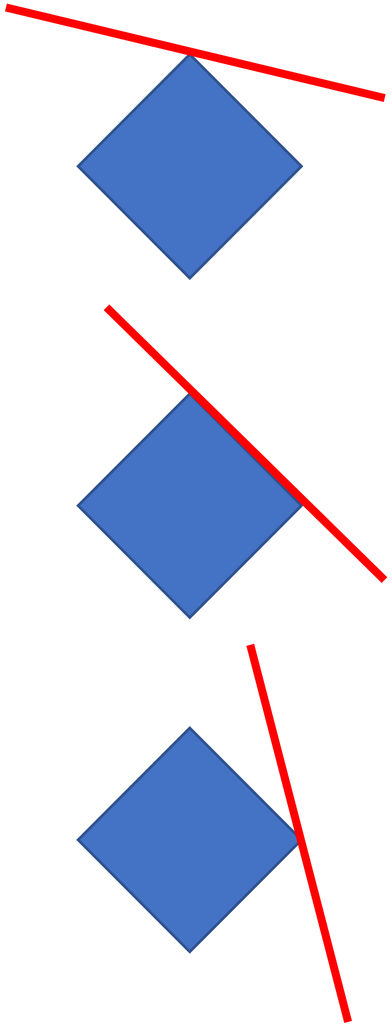
Holds for any architecture, any precision of training data.

$\Longrightarrow$ **Classification theory telling us what can and cannot be done**


- C., Antun, Hansen, "*The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem,*" **PNAS**, 2022.
- Antun, C., Hansen, *"Proving Existence Is Not Enough: : Mathematical Paradoxes Unravel the Limits of Neural Networks in Artificial Intelligence,"* **SIAM News**, May 2022.
- Choi, *"Some AI Systems May Be Impossible to Compute,"* **IEEE Spectrum**, March 2022.

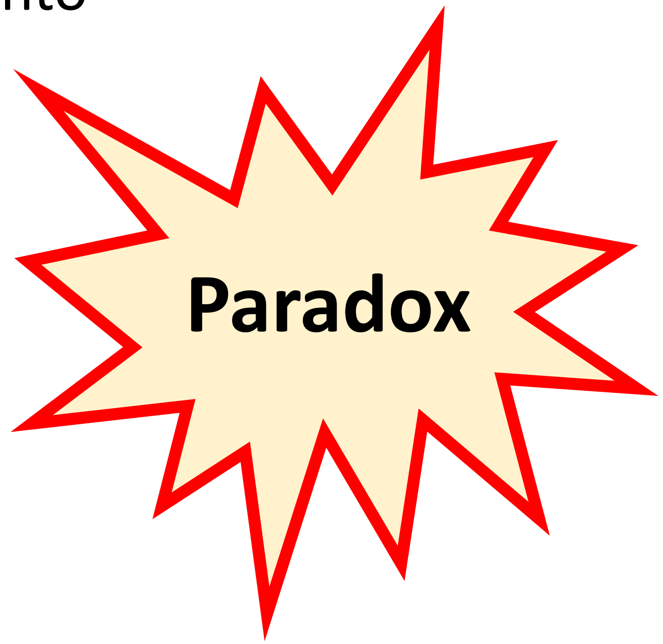
# Idea of mechanism

Phase transitions

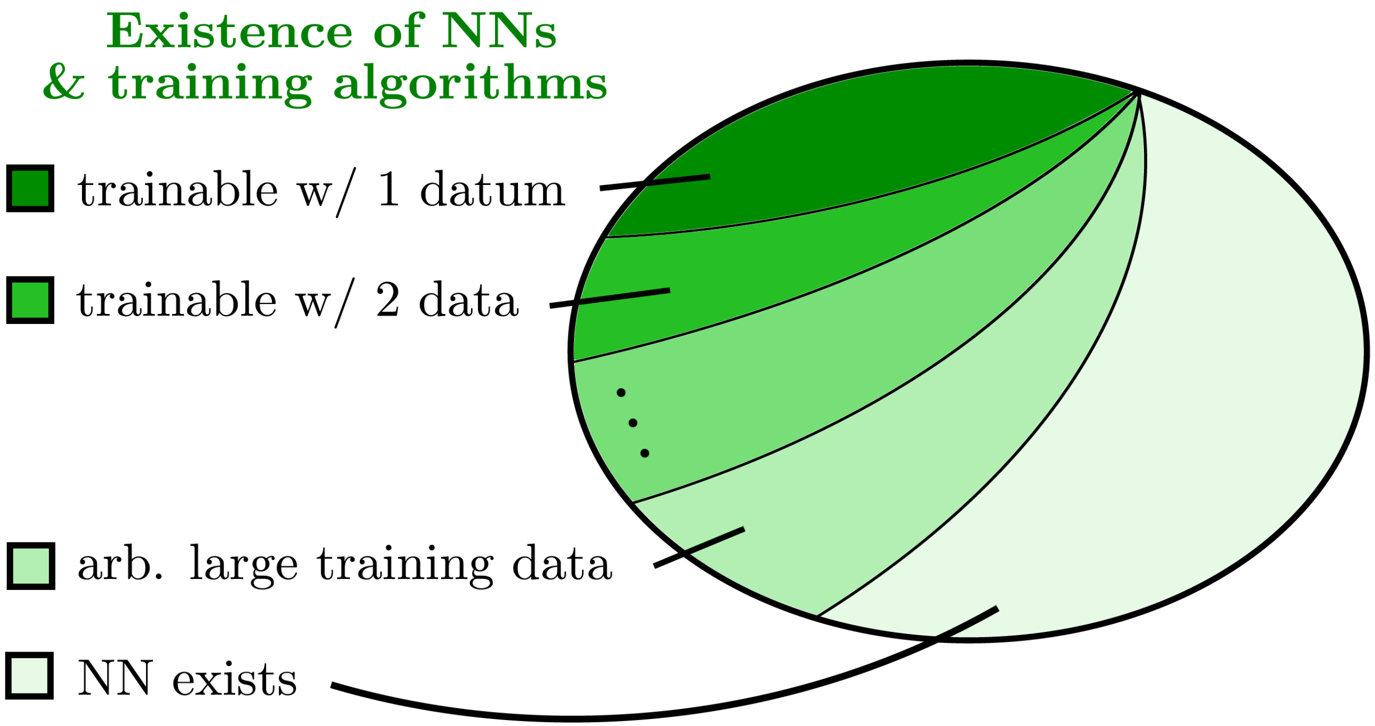


SCI machinery for embedding into
<u>well-conditioned</u> problems

General lemma
(works in other scenarios)

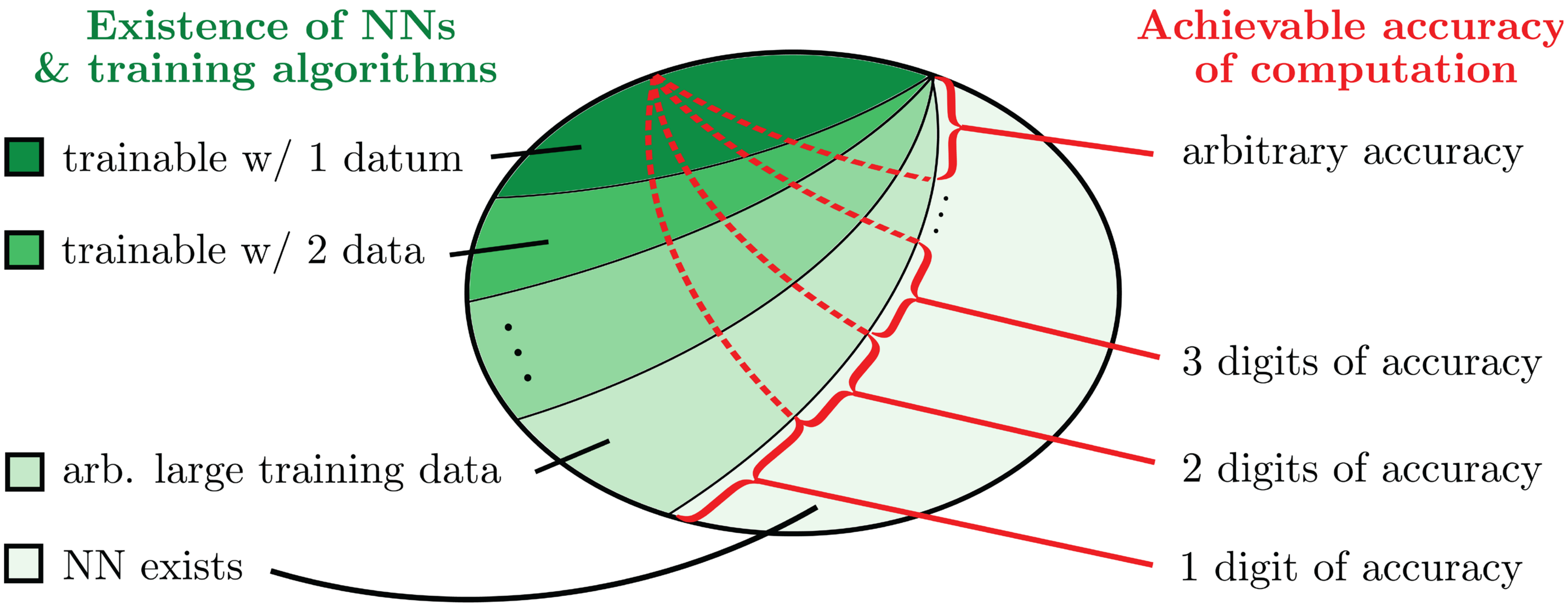


# The world of neural networks




**Given a problem and conditions, where does it sit in this diagram?**

# The world of neural networks




**Given a problem and conditions, where does it sit in this diagram?**

# Example counterpart theorem

**Certain conditions:** stable neural networks trained with exponential accuracy.
E.g., *approximate Łojasiewicz-type inequality*:

$$(1) \quad \min_{x \in \mathbb{C}^N} f(x) \quad \text{s.t.} \quad \|Ax - y\| \leq \varepsilon$$

$$\text{dist}(x, \text{solution}) \leq \alpha([f(x) - f^*] + [\|Ax - y\| - \varepsilon] + \delta)$$

**F**ast **I**terative **RE**started **NET**works (FIRENETs)
(unrolled primal-dual with novel restart scheme)

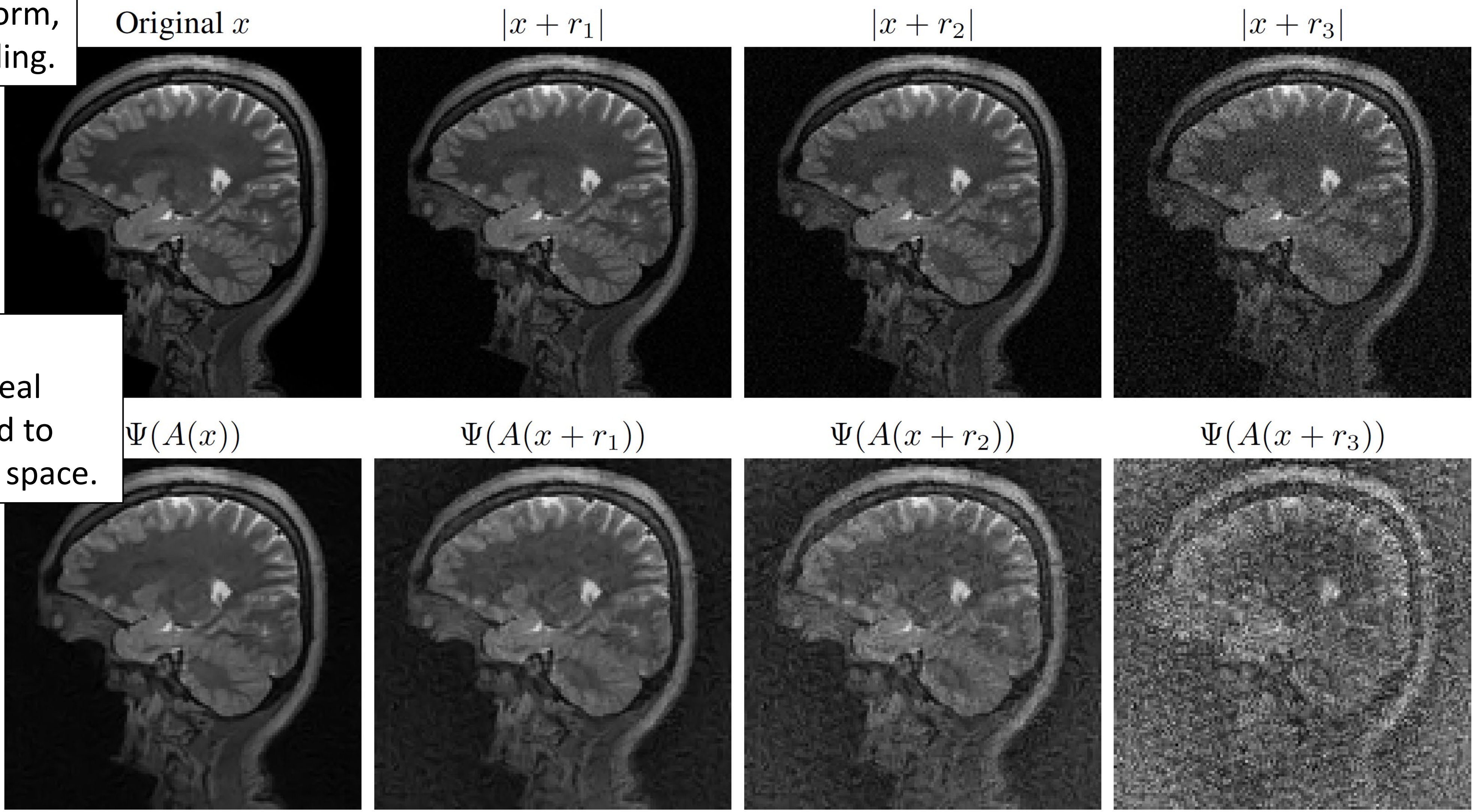
**Theorem**: Training algorithm that, under above assumption, produces *stable* neural networks $\varphi_n$ of width $O(N)$, depth $O(n)$, guaranteed worst bound

$$\text{dist}(\varphi_n(y), \text{solution}) \lesssim e^{-n} + \delta$$


- C., Antun, Hansen, "*The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem,*" **PNAS**, 2022.
- C., "*WARPd: A linearly convergent first-order method for inverse problems with approximate sharpness conditions,*" **SIIMS**, to appear.

# Example of severe instability

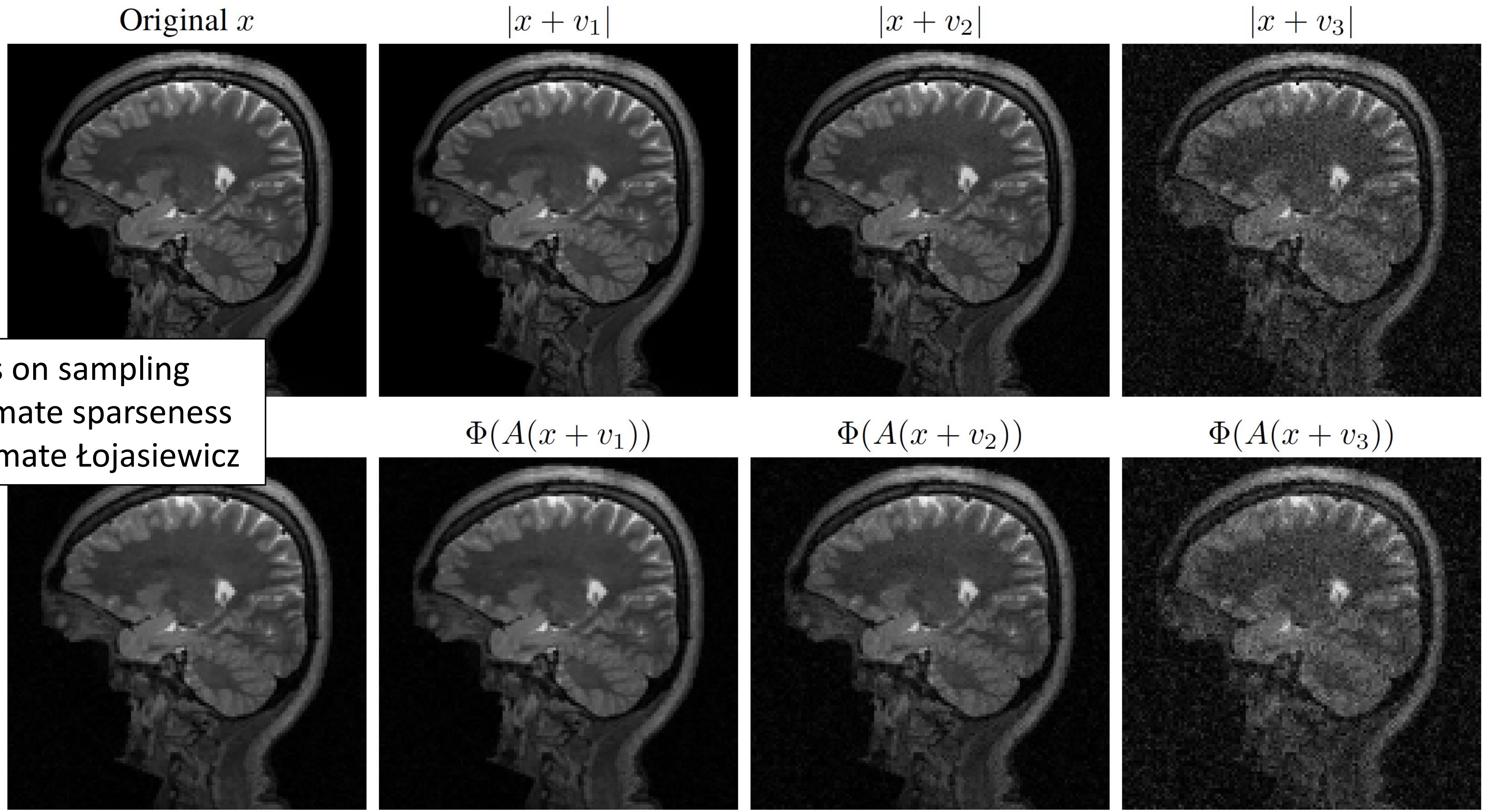
MRI: discrete 2D Fourier transform, 60% subsampling.




Perturbations computed in real space, mapped to measurement space.

- Zhu et al., *"Image reconstruction by domain-transform manifold learning,"* **Nature,** 2018.
- Antun et al., *"On instabilities of deep learning in image reconstruction and the potential costs of AI,"* **PNAS**, 2020.

# FIRENET: provably stable (even to adversarial examples) and accurate




Assumptions on sampling and approximate sparseness give approximate Łojasiewicz

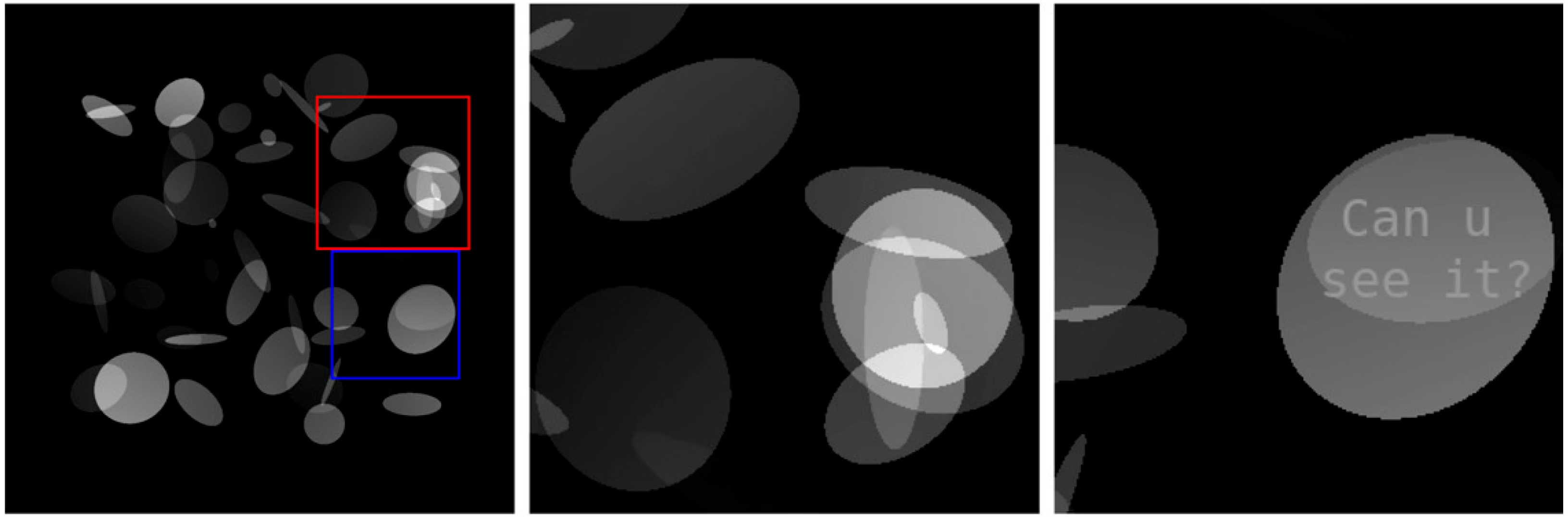
- C., Antun, Hansen, "*The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem*," **PNAS**, 2022.

# Key pillars: stability and accuracy

MRI: discrete 2D Fourier transform, 15% subsampling.

All networks trained on 5000 images of ellipses

Original $x$ (full size) | Original (cropped, red frame) | Original + detail $(x + h_1)$ (cropped, blue frame)

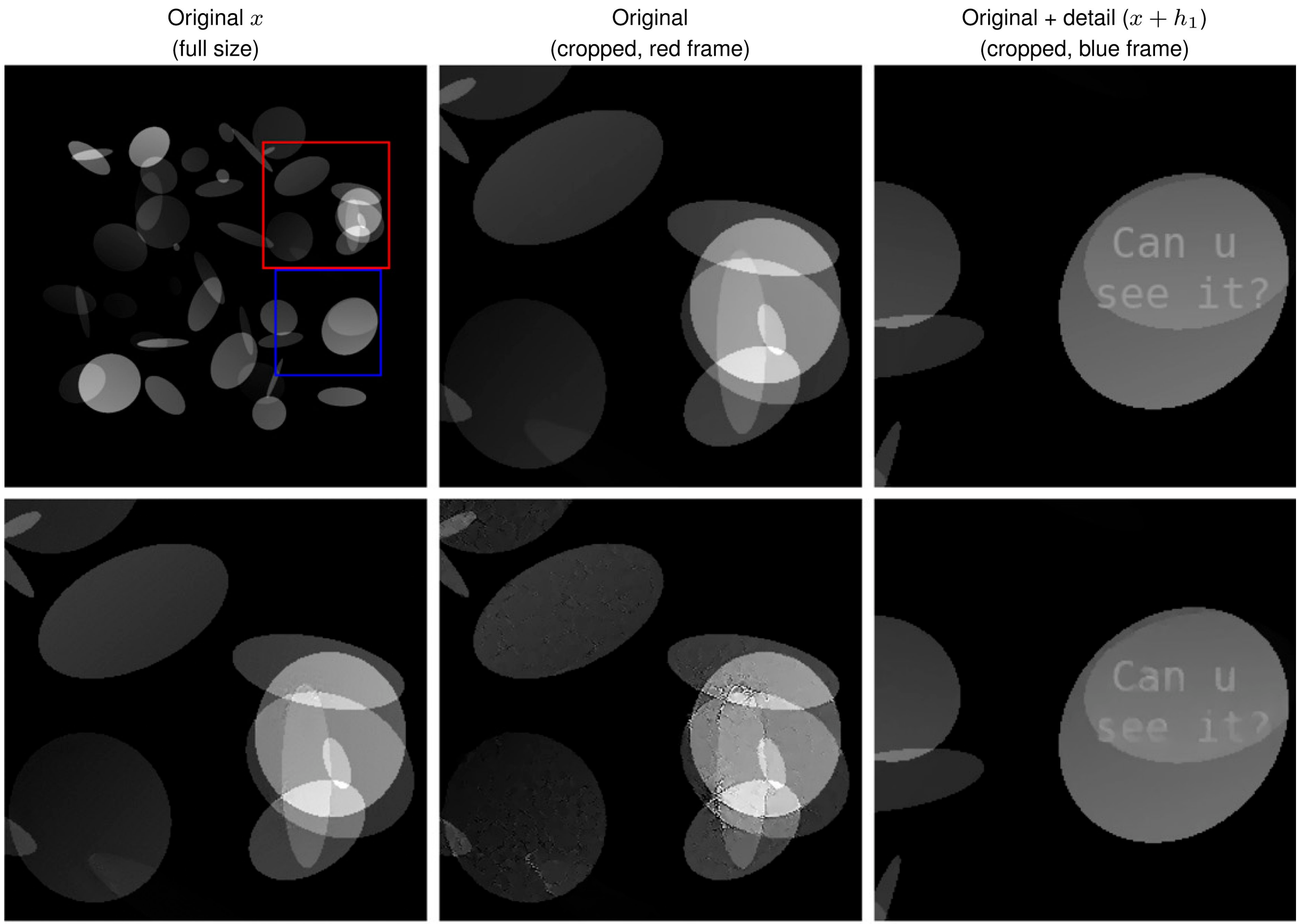



- C., Antun, Hansen, "*The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem,*" **PNAS**, 2022.

# U-Net with no noise: accurate but unstable



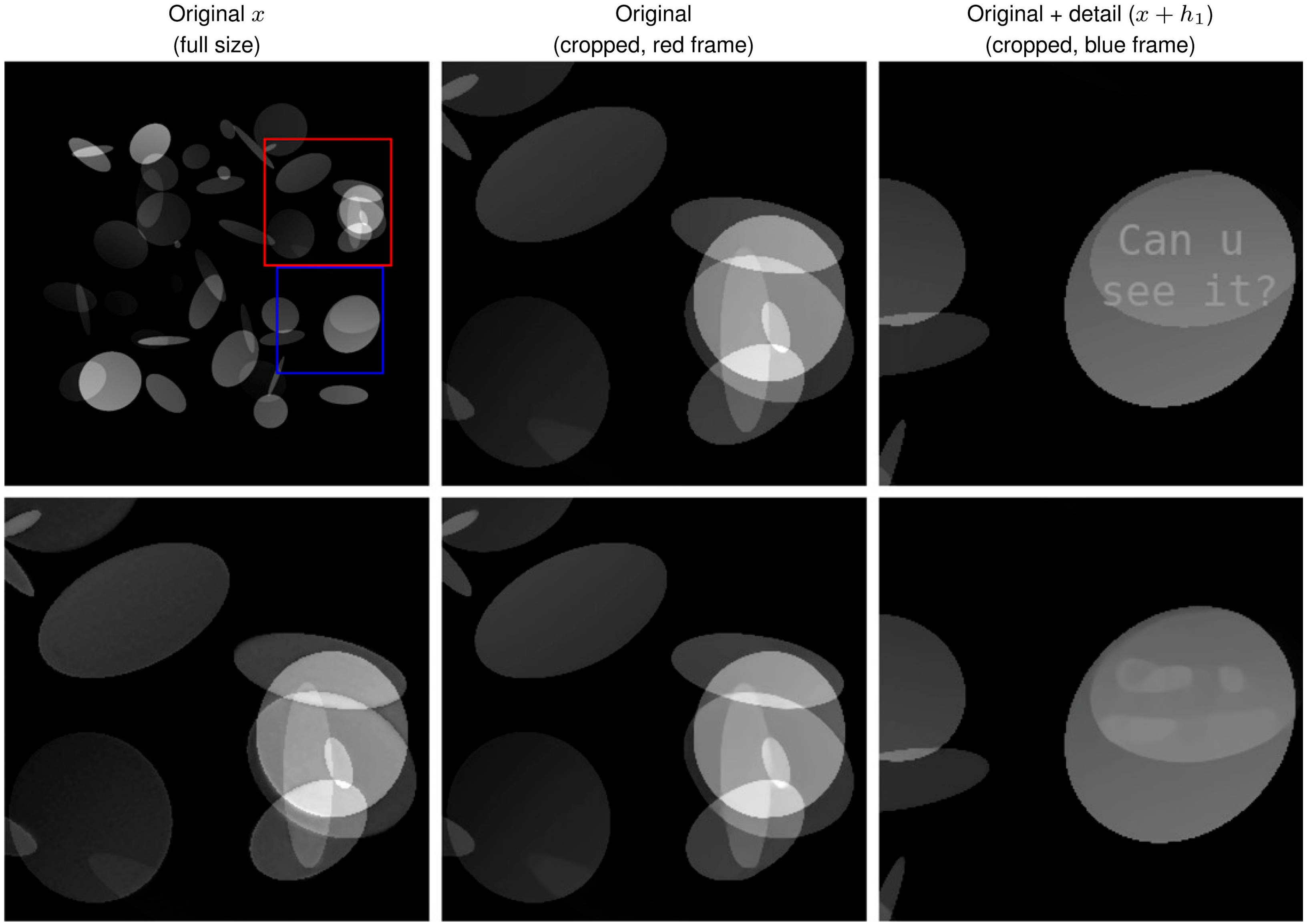
U-Net: standard neural network architecture for imaging. Approx 4 million parameters.




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

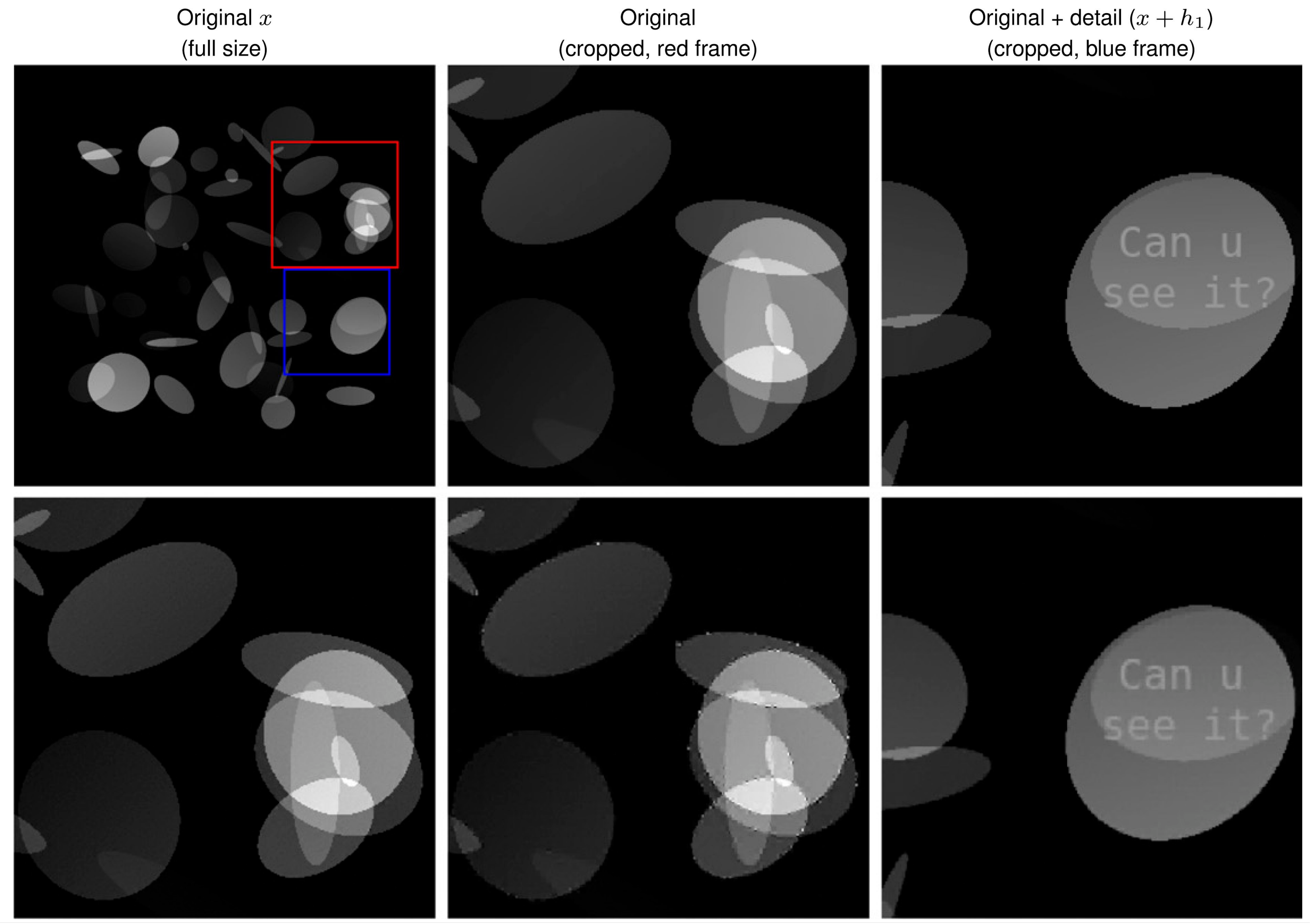
# U-Net with noise: stable but inaccurate






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

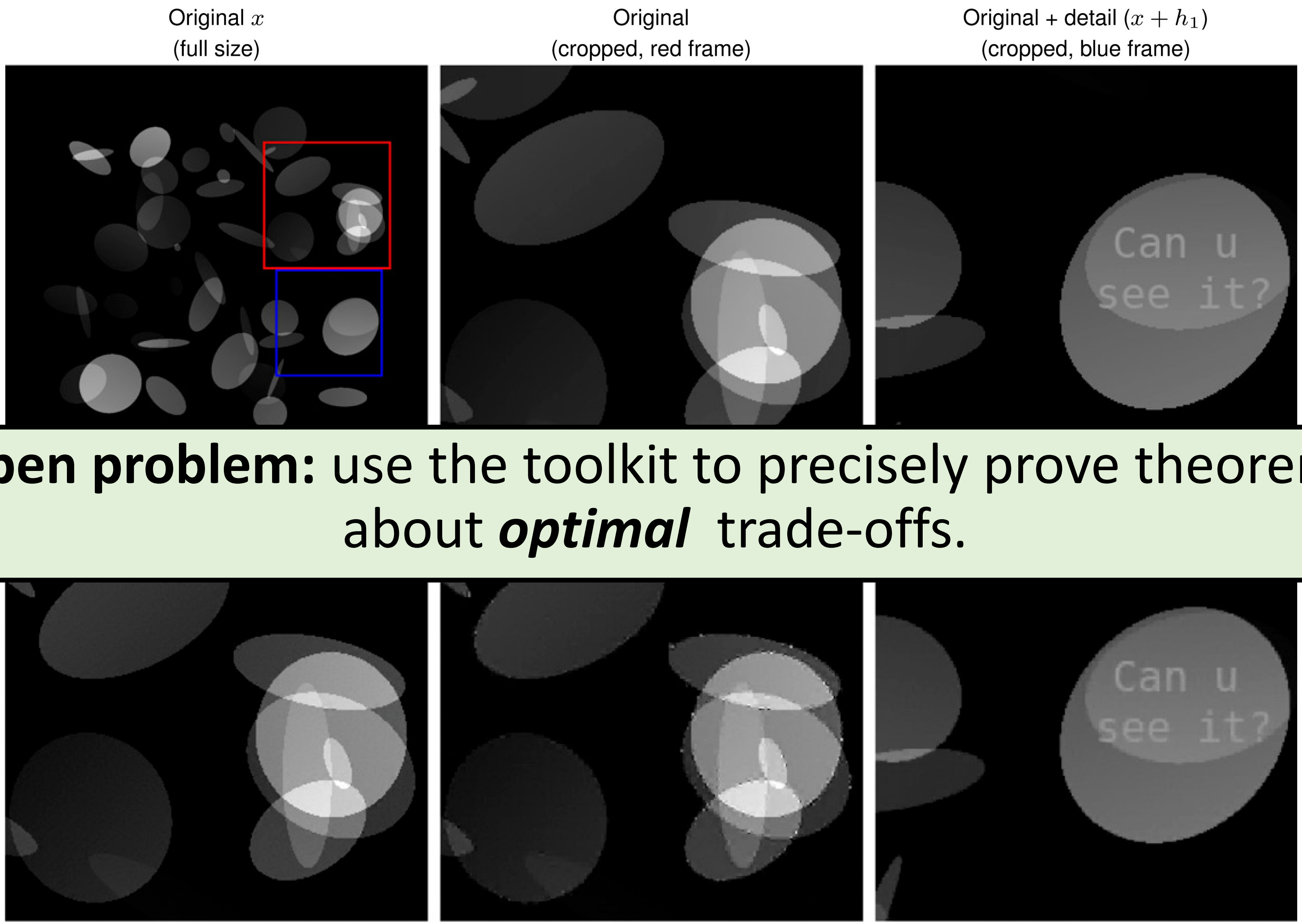
# FIRENET: balances stability and accuracy?




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

# FIRENET: balances stability and accuracy?






**Open problem:** use the toolkit to precisely prove theorems about ***optimal*** trade-offs.

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

# Summary: When can algorithms be trusted?

**Toolkit** + **programme**:

- Classifying the difficulty of computational problems
- Proving the optimality of algorithms.

Two **examples**:

- Rigorous and verifiable data-driven dynamical systems: <u>use the residual!</u>
- Computational boundaries in AI: <u>we need foundations!</u>

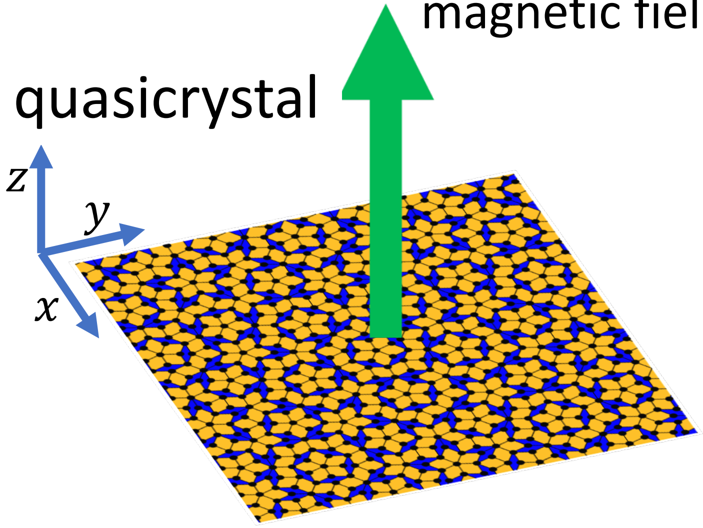
Building blocks for further problems in data analysis and beyond …

# Additional slides

# Example of “too much” (spectral pollution)

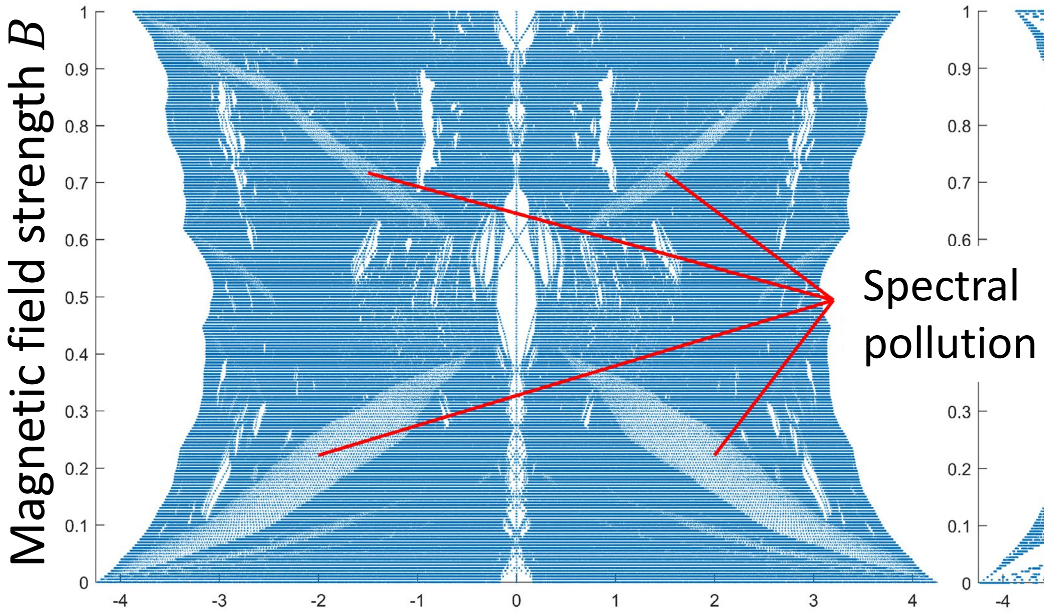
$B$: perpendicular magnetic field

quasicrystal




Infinite matrix: discrete Schrödinger operator

**Naïve method**

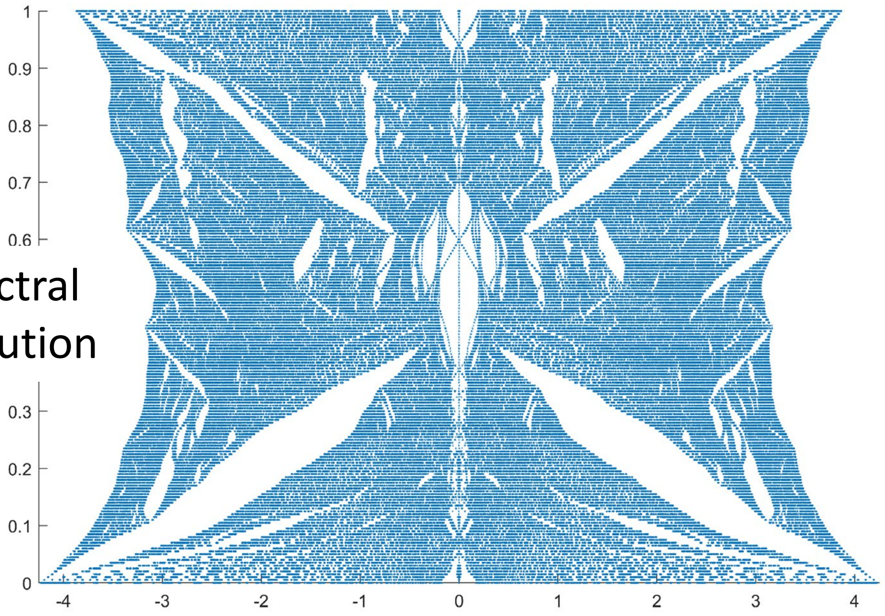



Approx. of spectrum (energy)

**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.

# Convergence of quadrature

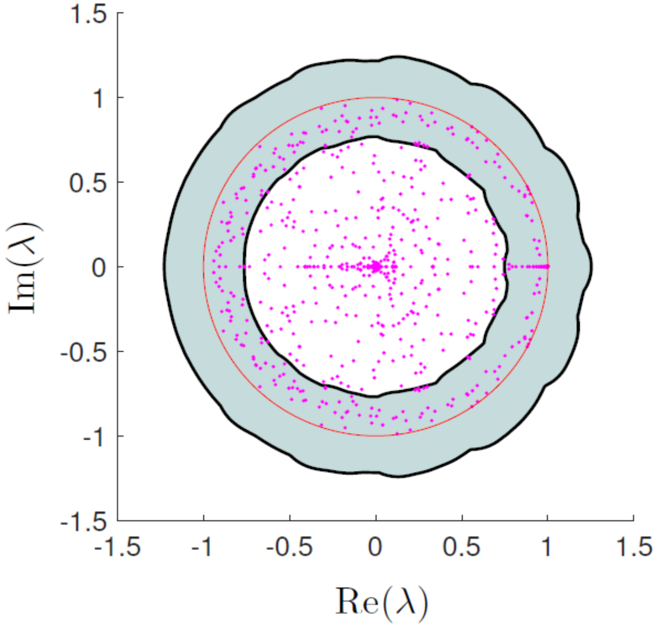
E.g., $\langle \mathcal{K}\psi_k, \psi_j \rangle = \lim_{M\to\infty} \sum_{m=1}^{M} w_m \overline{\psi_j(x^{(m)})}\, \underbrace{\psi_k(y^{(m)})}_{[\mathcal{K}\psi_k](x^{(m)})}$

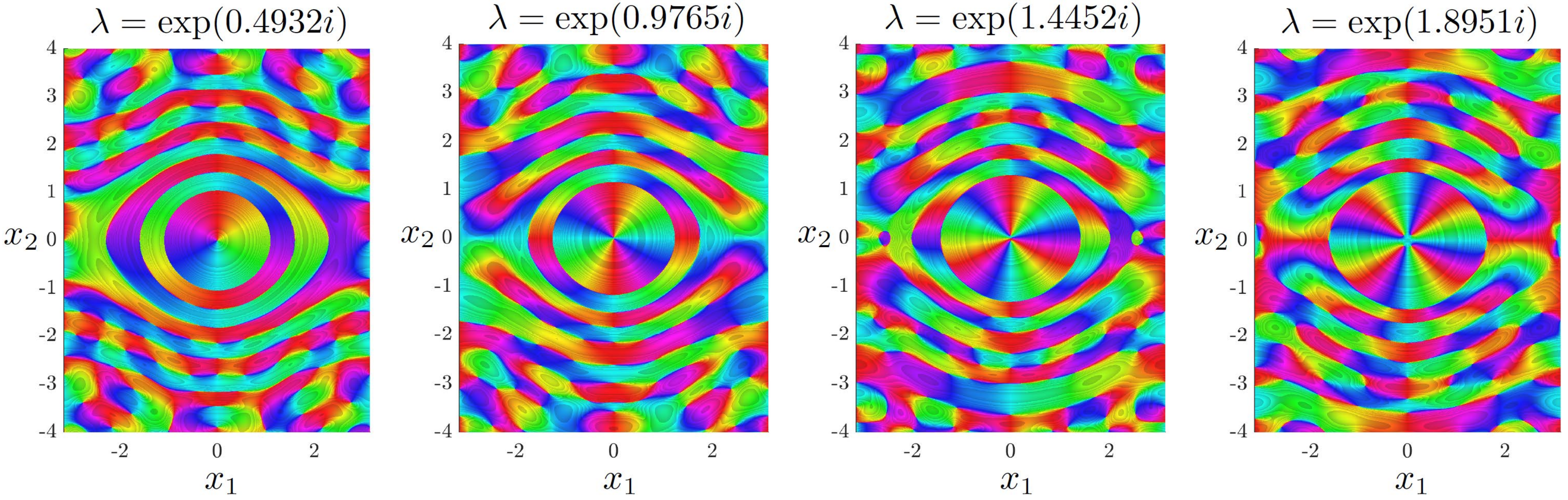
Three examples:

- **High-order quadrature:** $\{x^{(m)}, w_m\}_{m=1}^{M}$ $M$-point quadrature rule.
  Rapid convergence. Requires free choice of $\{x^{(m)}\}_{m=1}^{M}$ and small $d$.
- **Random sampling:** $\{x^{(m)}\}_{m=1}^{M}$ selected at random.
  Large $d$. Slow Monte Carlo $O(M^{-1/2})$ rate of convergence.
- **Ergodic sampling:** $x^{(m+1)} = F(x^{(m)})$.
  Single trajectory, large $d$. Requires ergodicity, convergence can be slow.

Most common

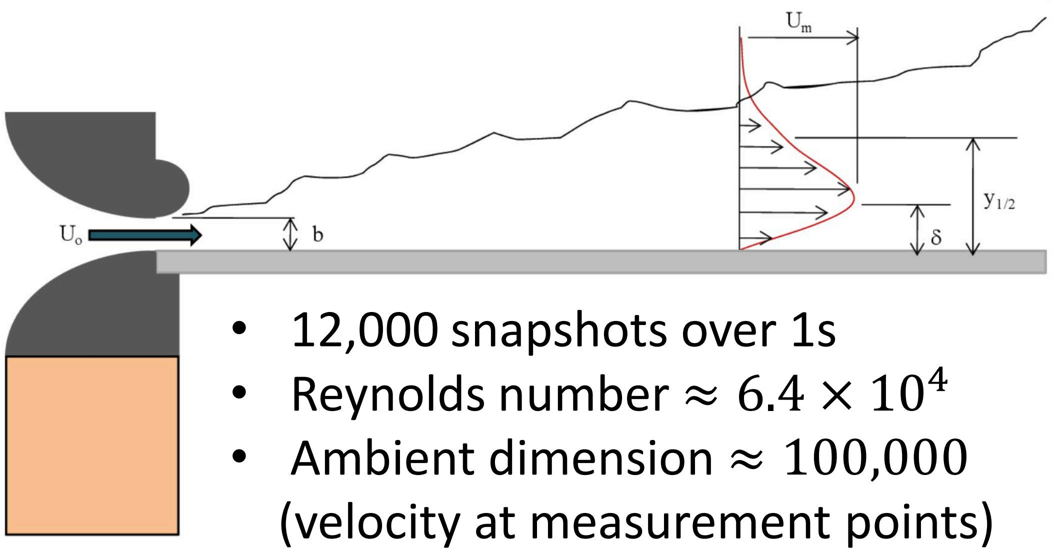
# Example: pendulum

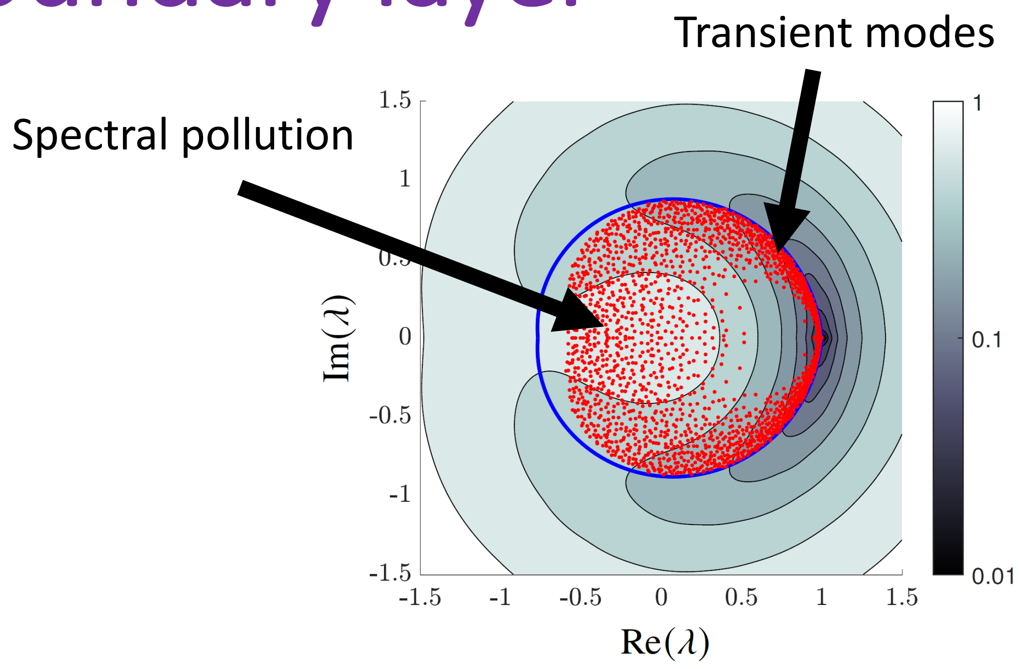



- C., Townsend, *"Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems,"* **Communications on Pure and Applied Mathematics**, under review.

# Example: wall-jet boundary layer

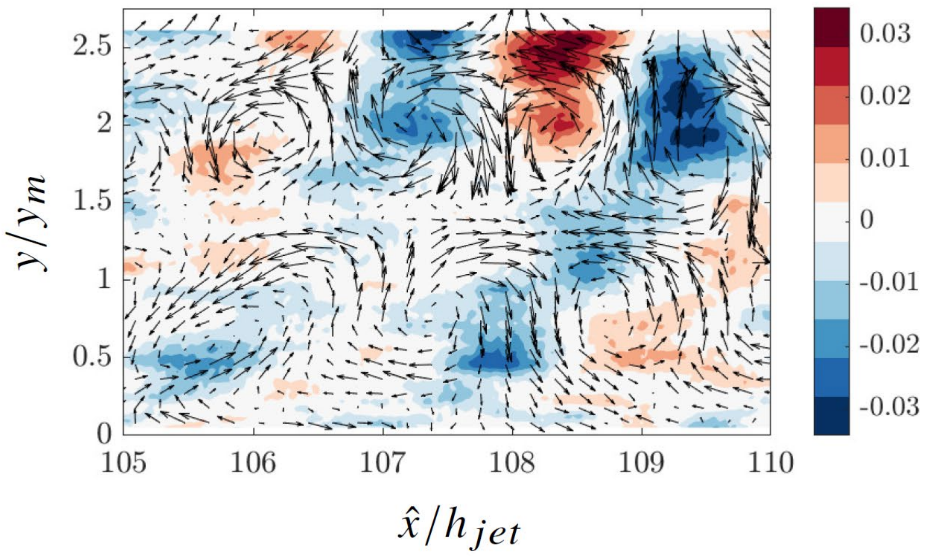


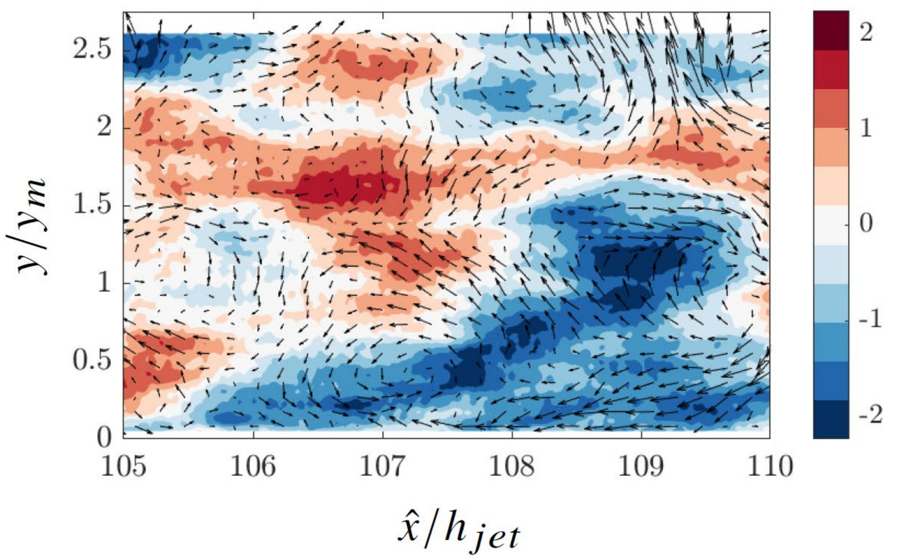

- 12,000 snapshots over 1s
- Reynolds number $\approx 6.4 \times 10^4$
- Ambient dimension $\approx 100{,}000$ (velocity at measurement points)

*Raw measurements provided by Máté Szőke (Virginia Tech)

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




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



# Koopman mode decomposition ($\mathbb{K}V = V\Lambda$)

Standard Koopman mode decomposition (order modes by $|\Lambda|$):

$$g(x) \approx \underbrace{[\psi_1(x) \quad \cdots \quad \psi_{N_K}(x)]V}_{\text{approx Koopman e-functions}} \underbrace{\left(V\sqrt{W}\Psi_X\right)^{\dagger}\sqrt{W}[g(x^{(1)}) \quad \cdots \quad g(x^{(M)})]^{\mathrm{T}}}_{\text{Koopman modes}}$$

$$\overset{?}{\Rightarrow} g(x_n) \approx \underbrace{[\psi_1(x) \quad \cdots \quad \psi_{N_K}(x)]V}_{\text{approx Koopman e-functions}} \Lambda^n \underbrace{\left(V\sqrt{W}\Psi_X\right)^{\dagger}\sqrt{W}[g(x^{(1)}) \quad \cdots \quad g(x^{(M)})]^{\mathrm{T}}}_{\text{Koopman modes}}$$

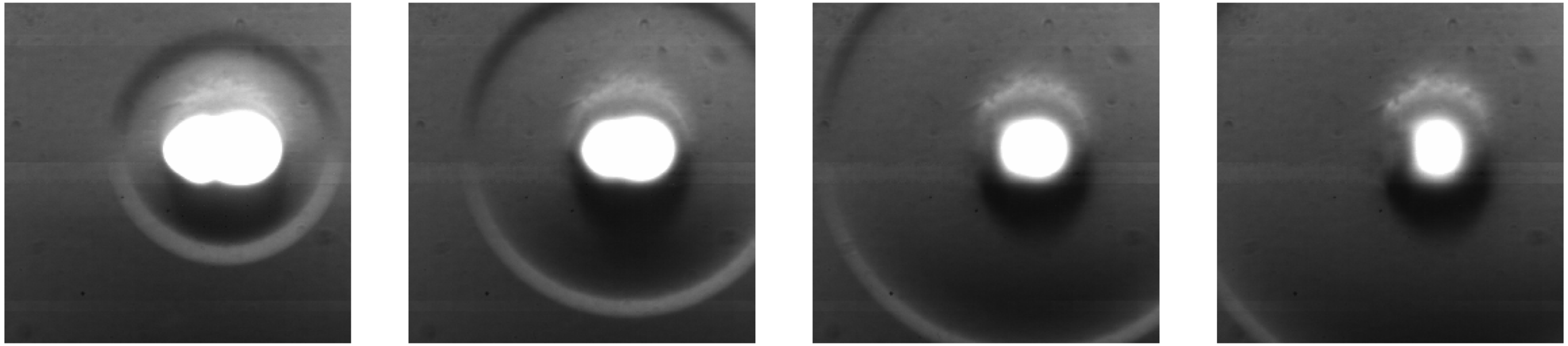
Residual Koopman mode decomposition (order modes by $\mathrm{res}(\lambda, \mathbf{v})$):

Controllable error

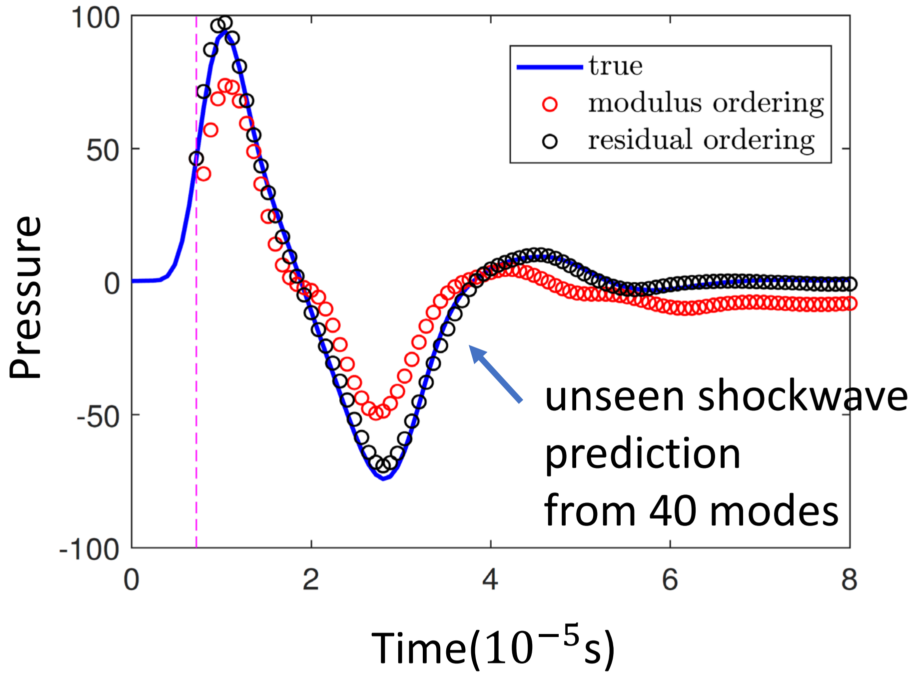
$$g(x) \approx \underbrace{[\psi_1(x) \quad \cdots \quad \psi_{N_K}(x)]V_{(\varepsilon)}}_{\text{approx Koopman e-functions}} \underbrace{\left(V_{(\varepsilon)}\sqrt{W}\Psi_X\right)^{\dagger}\sqrt{W}[g(x^{(1)}) \quad \cdots \quad g(x^{(M)})]^{\mathrm{T}}}_{\text{Koopman modes}}$$

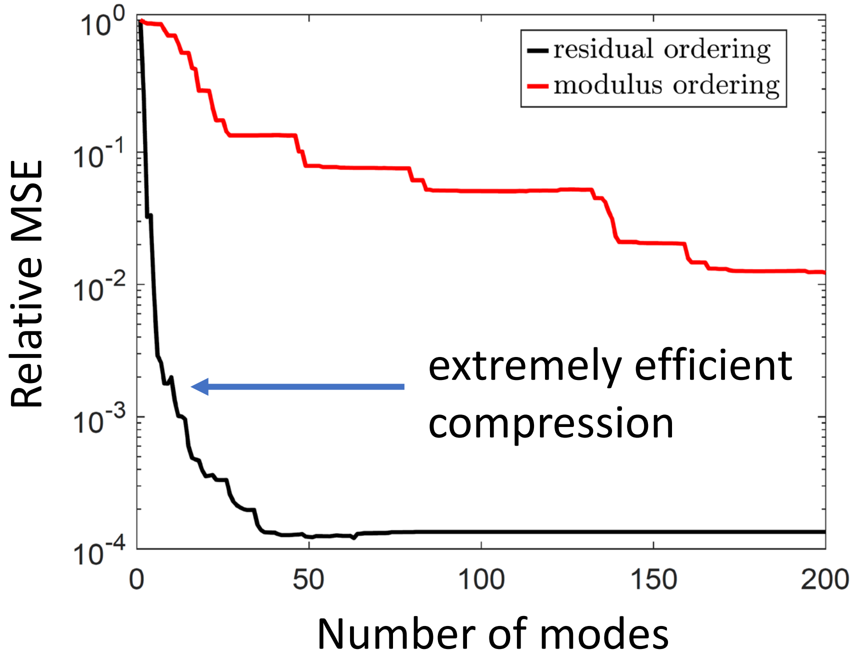
$$g(x_n) \approx \underbrace{[\psi_1(x_0) \quad \cdots \quad \psi_{N_K}(x_0)]V_{(\varepsilon)}}_{\text{approx Koopman e-functions}} \Lambda_{(\varepsilon)}^n \underbrace{\left(V_{(\varepsilon)}\sqrt{W}\Psi_X\right)^{\dagger}\sqrt{W}[g(x^{(1)}) \quad \cdots \quad g(x^{(M)})]^{\mathrm{T}}}_{\text{Koopman modes}}$$

# Example: laser-induced plasma



a) $t = 5\ \mu s$ b) $t = 10\ \mu s$ c) $t = 15\ \mu s$ d) $t = 20\ \mu s$



# Example: ionization probabilities in < 1 second

$$[Au](r) = -\frac{d^2u}{dr^2}(r) + \left(\frac{l(l+1)}{r^2} + \frac{e^{-r}-1}{r}\right)u(r), \qquad r > 0$$

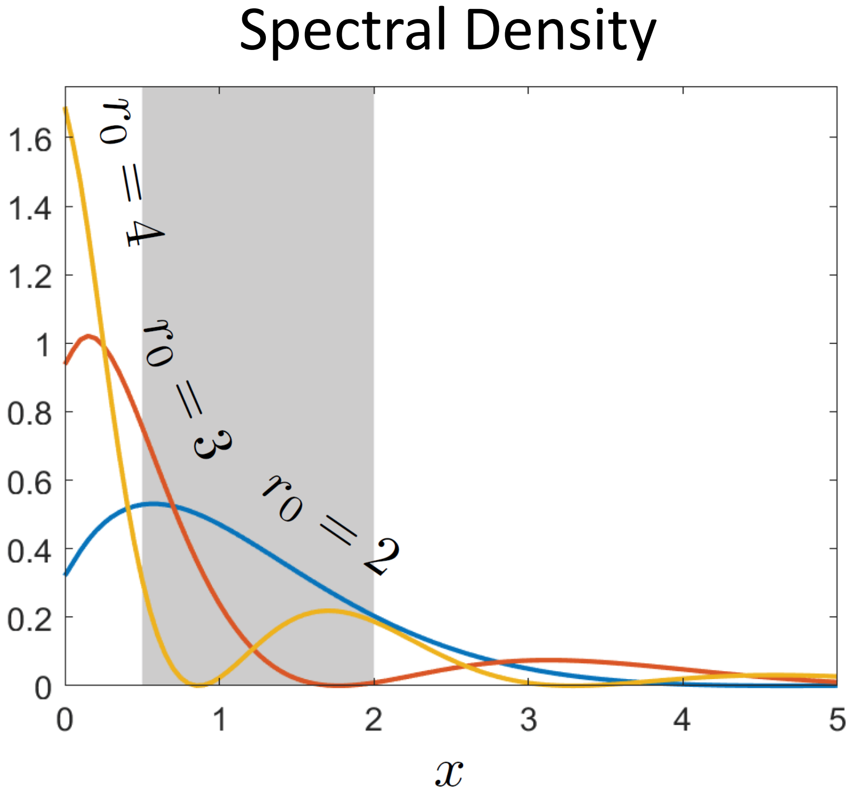
Hellman potential

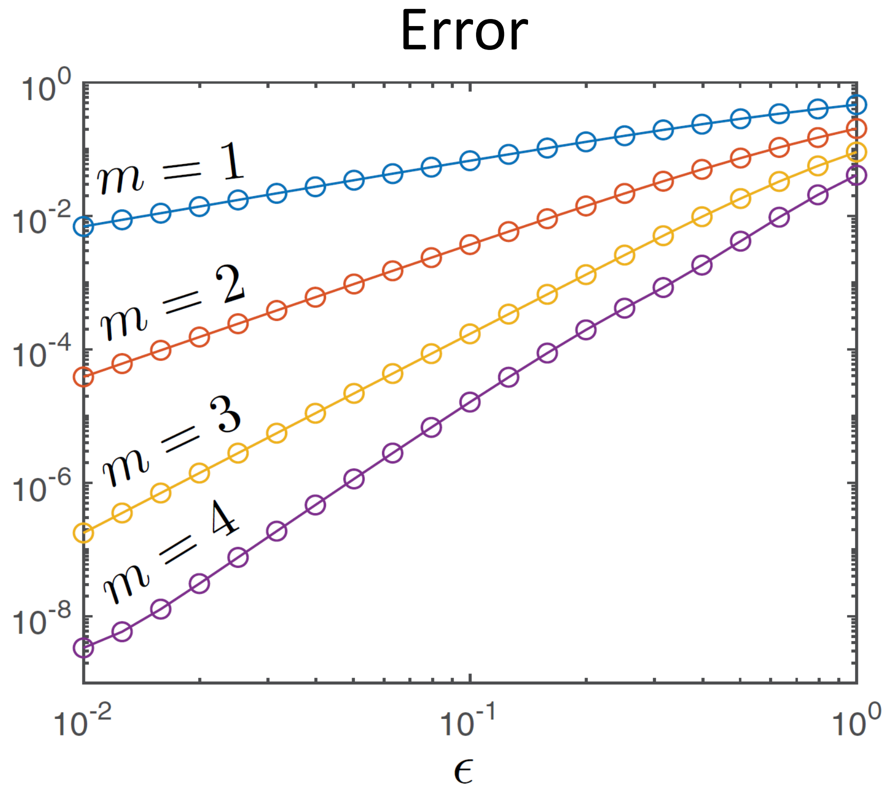
```
c = sqrt(pi/8)*(2-igamma(1/2,8)/gamma(1/2));      % Norm squared
g = @(r) exp(-(r-2).^2)/sqrt(c);                  % Measure wrt g(r)
V={@(r) 0, @(r) exp(-r)-1, 1};                    % Potential, l=1
[xi, wi] = chebpts(20,  [1/2 2]);                 % Quadrature rule
nu = rseMeas(V, g, xi, 0.1, 'Order', 4);          % epsilon=0.1, m=4
ion_prob = wi * nu;                               % Ionization prob
```

# Example: ionization probabilities in < 1 second

$$[Au](r) = -\frac{d^2u}{dr^2}(r) + \left(\frac{l(l+1)}{r^2} + \frac{e^{-r}-1}{r}\right)u(r), \qquad r > 0$$

Hellman potential



# Extensions to PDEs

- Operator A on $\mathbb{R}^d$ of form

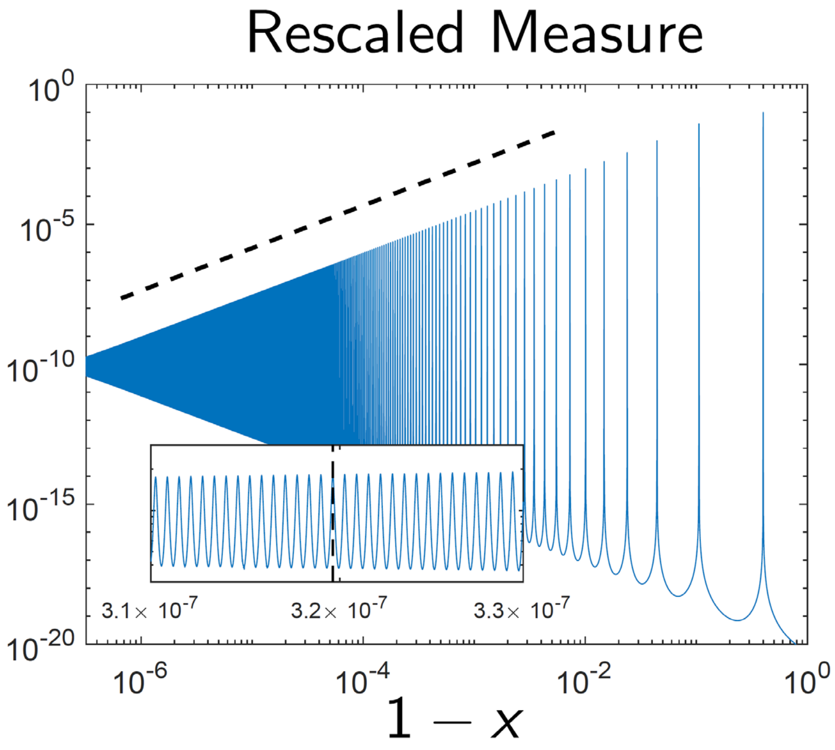
$$[Au] = \sum_{k \in \mathbb{Z}_{\geq 0}^d, |k| \leq N} c_k(x)[\partial^k u](x)$$

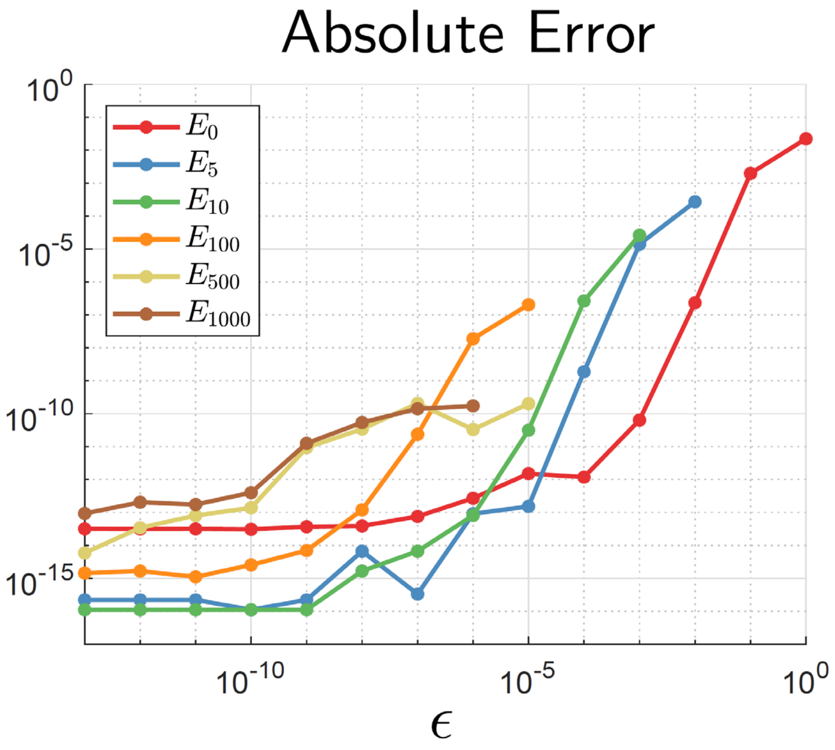
- Assume coefficients are
  - Polynomially bounded
  - Locally bounded total variation
- Build matrix representation using quasi-Monte Carlo integration.

$\rightarrow$ Sample coefficients to compute $\mathrm{Spec}(A)$ with error control!

**NB:** works for spectral methods, FEM, etc.

# Eigenvalues of Dirac operator



# Example of impossibility theorem for subsampled discrete cosine transform

| $\min_k \operatorname{dist}(\Psi_n(y_k), \Xi(A, y_k))$ | $\min_k \operatorname{dist}(\Phi_n(y_k), \Xi(A, y_k))$ | prec. of training data | $10^{-n}$ |
|---|---|---|---|
| 0.2999690 | 0.2597827 | $m = 10$ | $10^{-1}$ |
| 0.3000000 | 0.2598050 | $m = 20$ | $10^{-1}$ |
| 0.3000000 | 0.2598052 | $m = 30$ | $10^{-1}$ |
| 0.0030000 | 0.0025980 | $m = 10$ | $10^{-3}$ |
| 0.0030000 | 0.0025980 | $m = 20$ | $10^{-3}$ |
| 0.0030000 | 0.0025980 | $m = 30$ | $10^{-3}$ |
| 0.0000030 | 0.0000015 | $m = 10$ | $10^{-6}$ |
| 0.0000030 | 0.0000015 | $m = 20$ | $10^{-6}$ |
| 0.0000030 | 0.0000015 | $m = 30$ | $10^{-6}$ |

Impossibility of computing approximations of the neural network to arbitrary accuracy. We demonstrate the impossibility statement on fast iterative restarted networks $\Phi_n$ and learned iterative shrinkage thresholding algorithm networks $\Psi_n$. The table reveals the shortest $l_2$ distance between the networks' output and the problem's true solution for different values of $m$ (precision of training data is $2^{-m}$). Neither of the trained neural networks can compute the existing correct neural network to accuracy $10^{-n}$, but both compute approximations that are accurate to $10^{-n+1}$.

# Stabilising unstable neural networks

$\Psi(\tilde{y}),\ \tilde{y} = Ax + e_3$ | $\Phi\left(\tilde{y}, \Psi(\tilde{y})\right)$ | FIRENET rec. from $y = Ax + \tilde{e}_3$ | AUTOMAP+FIRENET rec. from $y = Ax + \hat{e}_3$