Data, dynamics, and manifolds

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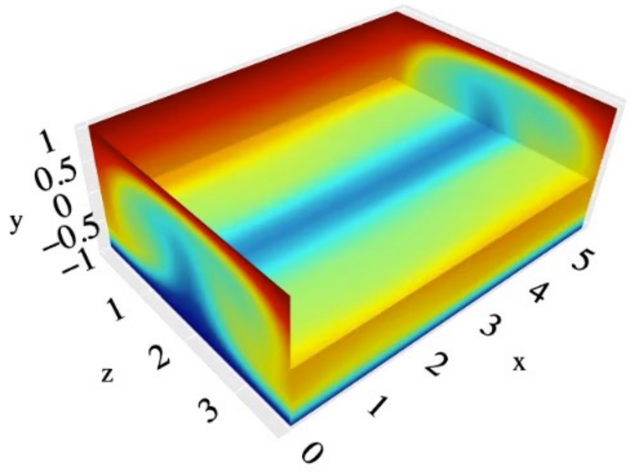
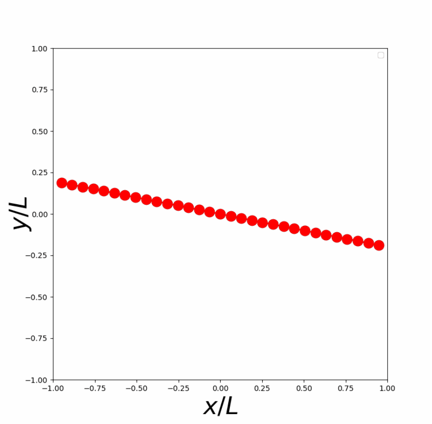
Complex dynamics with many degrees of freedom

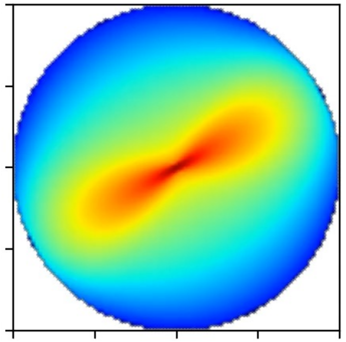
- In many applications we have large amounts of high-dimensional data from experiments or high-resolution simulations
- Dynamics may be very complex in space and time
- Modeling is computationally expensive and limits simulation-based design and control applications

Turbulent Fluid Flow



Microstructure in a complex fluid





Aim: Data-based modeling of complex systems, especially in fluid mechanics –keeping only *essential* degrees of freedom.

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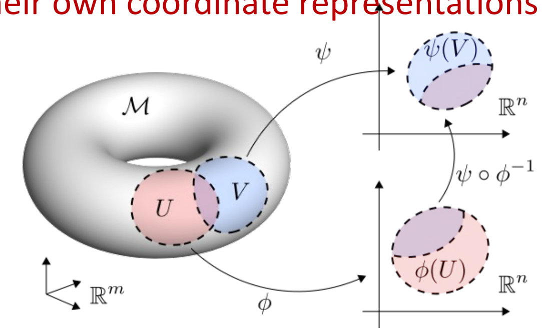
Data, dynamics, and manifolds

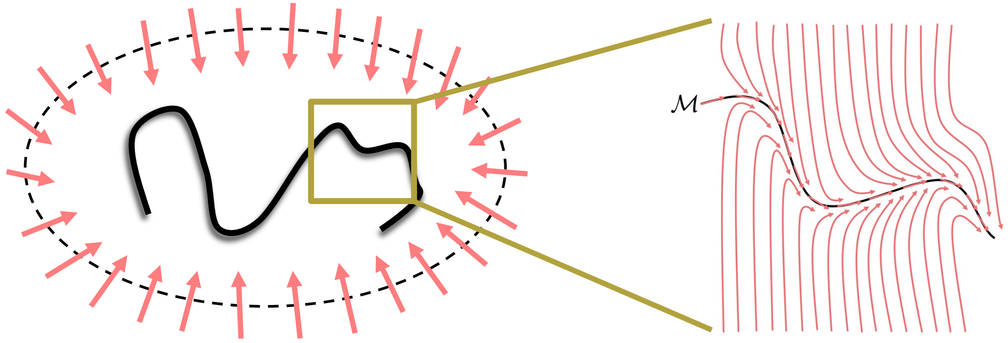
Manifold: generalization of curve or surface – can *locally* represent with Cartesian coords.

- **Dynamics:** invariant manifolds are surfaces in state space that trajectories stay on forever, and a stable manifold is approached by nearby trajectories
  - Invariant manifolds organize dynamics and contain long-time behavior
  - Diffusion/viscosity → strong damping of short wavelengths → long-time dynamics of dissipative PDEs lie on a finite-dimensional invariant manifold
- **Machine learning:** "Manifold hypothesis": idea that real-world data in *d* dimensions lies on a manifold with far fewer dimensions – partial explanation for the success of neural networks to represent and classify data.
- Unless the data is very simple, we don't know in advance the dimension on the manifold it lies on.

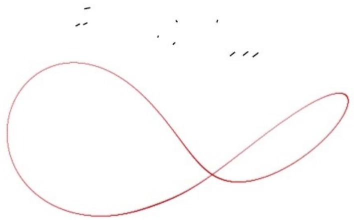
Manifold and local regions ("charts") with their own coordinate representations



State space of a dynamical system with a stable manifold – arrows are trajectories

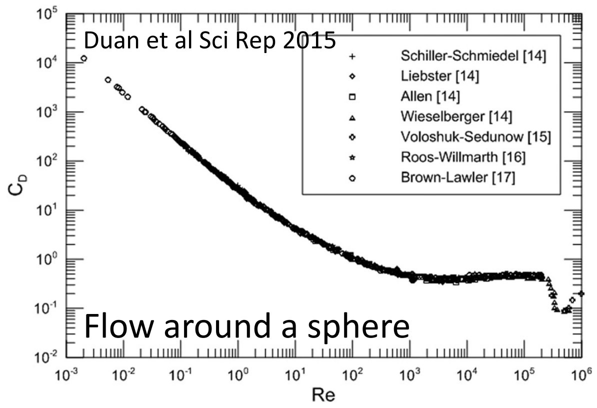


Initial conditions approaching a stable oscillatory solution (1D manifold)



Data, dynamics, and symmetry

Exploiting symmetry enables more effective use of data

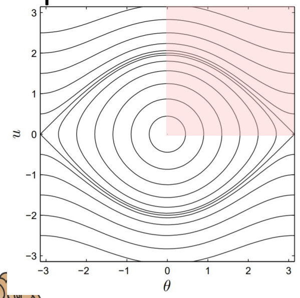


Independence of physical laws from units of measurements = a form of dilation symmetry → dimensional analysis

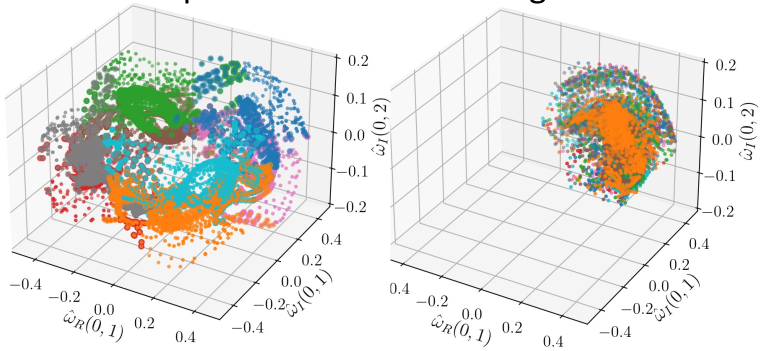
Drag force, velocity, viscosity, density, diameter → drag coefficient, Reynolds number

Periodic domain & translation equivariance
→ data can be separated into pattern and phase -- i.e. we don't have to learn separate representations of the same pattern at different rotation angles

State space for pendulum



State space for chaotic Kolmogorov flow



Symmetries in physical space lead to symmetries between different parts of state space
→ we only have to capture dynamics in part of state space and symmetry gives us the rest

Linot & G, PRE 2020, Zeng & G. PRE 2021, Perez de Jesus & G. 2023

Overview: toward minimal data-driven models of complex dynamics

"Data-driven manifold dynamics (DManD)"

Overall Aim: **From data**, efficiently/*minimally* approximate $\mathcal{M}$ and the dynamics on it for complex/chaotic processes

- Short-time predictions (always limited quantitatively for chaotic systems)
- Long-time statistics – overall "shape" of the dynamics in state space

- **Coordinate transformations** between full state space *H* and lower-dimensional manifold $\mathcal{M}$
  - Reduced description contains the essential structures of the flow -- autoencoders
  - Combine clustering with local representations to obtain global minimal-dimensional representations
- **ODE models** for the dynamics on the manifold (again in neural network form)
  - Respect Markovian nature of the original dynamical system
  - Allow effective use of widely spaced data – no time derivatives should need to be estimated from data
- Exploit continuous and discrete symmetries
- Allow for actuation and exploit low-dimensional representation for control
- Apply to complex flow problems – a particular target is drag reduction in wall turbulence

Other manifold-based approaches: Kevrekidis, Koumoutsakos, Haller,…

Basic Framework

Mapping to Manifold Coordinates (Autoencoder)

$$u \xrightarrow{\chi} h \xrightarrow{\check{\chi}} \tilde{u}$$

$$u \in \mathbb{R}^d$$
$$h \in \mathbb{R}^{d_h}, \; d_h \ll d$$

Data

Input $[u(t_1), u(t_2), \ldots, u(t_M)]$

Output $[u(t_1), u(t_2), \ldots, u(t_M)]$

Loss $\min_{\theta_1,\theta_2} \sum_i^M ||u_i - \check{\chi}(\chi(u_i;\theta_1);\theta_2)||^2$

NN parameters

Prediction $\tilde{u}_i$

- It can be advantageous to work in the PCA basis -- efficiency, interpretability
- Symmetry reduction (split out spatial phase from pattern) improves representation

Linot and G., PRE (2020), Chaos (2022). Perez De Jesus and G. PRF (2023)

Evolution in Manifold Coordinates (Neural ODE)

$$\dot{h} = g(h)$$

Data (already processed through autoencoder)

Input $[h(t_1), h(t_2), \ldots, h(t_M)]$

Output $[h(t_1+\tau), h(t_2+\tau), \ldots, h(t_M+\tau)]$

Loss $\min_{\phi} \sum_i ||\Delta h(t_i+\tau) - \int_{t_i}^{t_i+\tau} \tilde{g}(h(t);\phi)\, dt||^2$

NN parameters

Time-integration of ODE

- To determine gradient of loss
  - Treat ODE as constraint, use adjoint method
  - Or just do automatic differentiation through an ODE solver
  - Adding an explicit dissipative term can stabilize (Linot et al 2023)

Chen et al., NeurIPS (2018)

Data-driven manifold dynamics of turbulent Couette flow

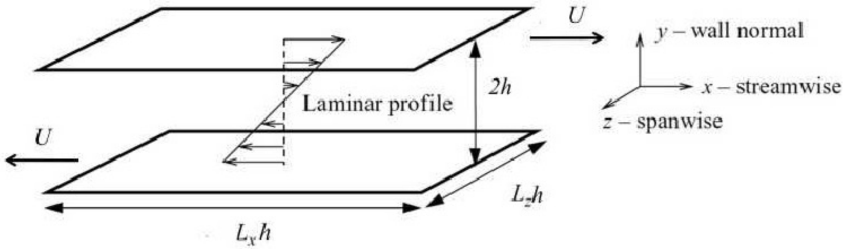
Minimal turbulent Couette flow: the essence of near-wall turbulence

Turbulence near walls has a universal basic structure:

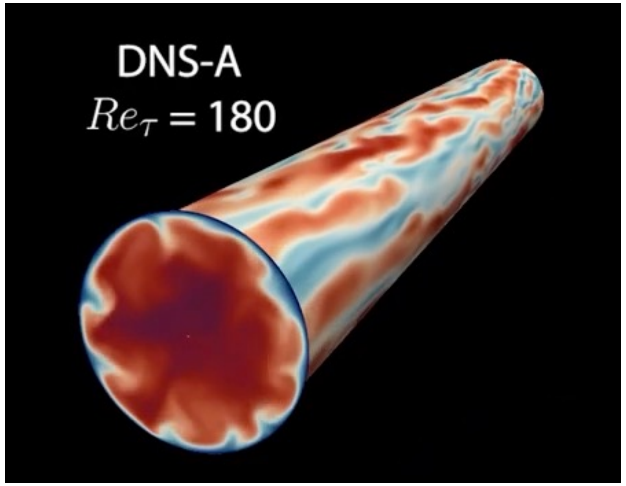
- Quasistreamwise vortices
- Low- and high-speed streaks as slow- and fast-moving fluid is carried around by the vortices
- "Streak breakdown" events with strong three-dimensionality
- Characteristic spacing in units based on wall shear stress

Plane Couette flow at low Reynolds number in small domains is the minimal physical system that displays this structure:

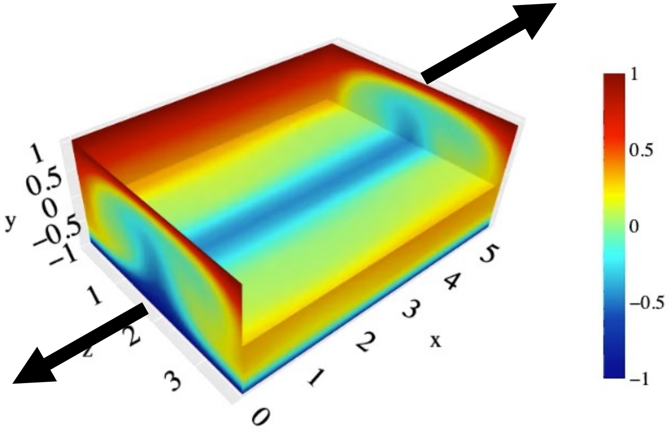
- "Minimal flow unit" (MFU) (Hamilton, Kim, Waleffe 1995)
- Fully resolved simulation (32x35x32x3)=10^5 dimensions at Re=400



Streamwise velocity evolution



Pipe flow
(Ceci et al 2021)



Couette flow

What's the actual minimal number of dimensions required to capture this flow?

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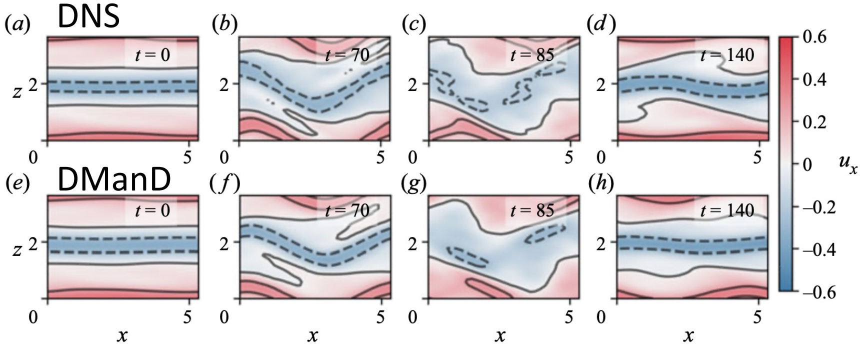
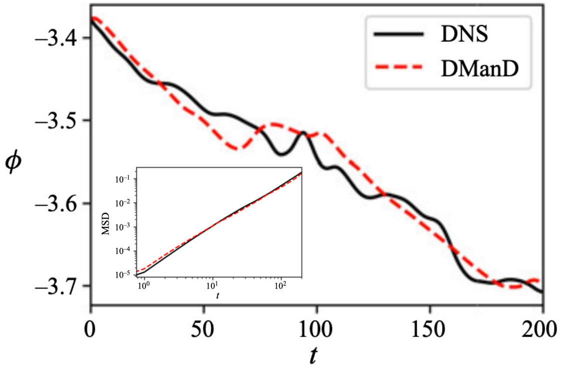
Manifold dynamics: plane Couette flow (10^5 → 18 dimensions)

Short-time predictions

Reliably tracks dynamics through "streak breakdown" process that characterizes intermittent behavior in near-wall turbulence



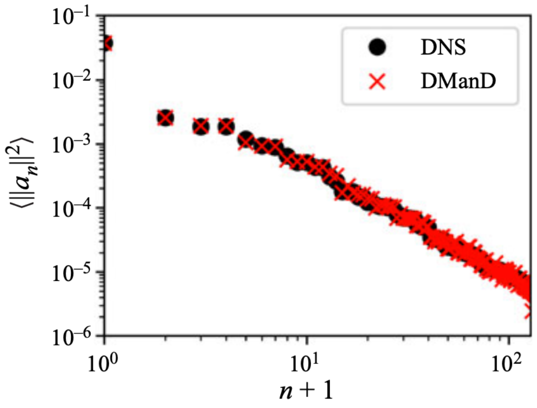
Phase dynamics – including "diffusion" of streak pattern – is captured



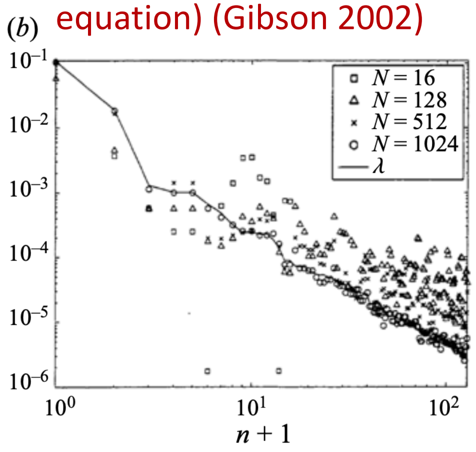
Long-time statistics

Much better performance than POD Galerkin

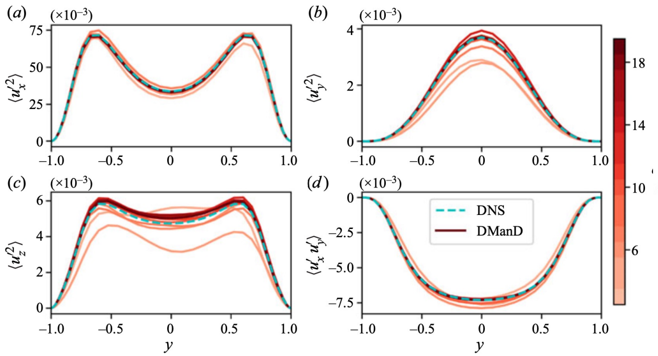
RMS POD mode amplitudes (d_h=18)



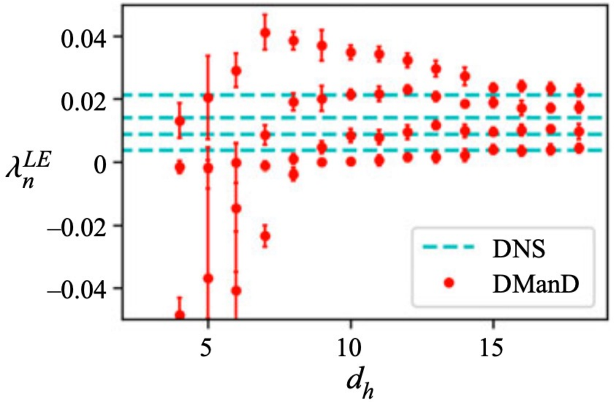
POD-Galerkin (i.e data + governing equation) (Gibson 2002)



Reynolds stresses



Leading Lyapunov exponents



Linot & G. JFM (2023)

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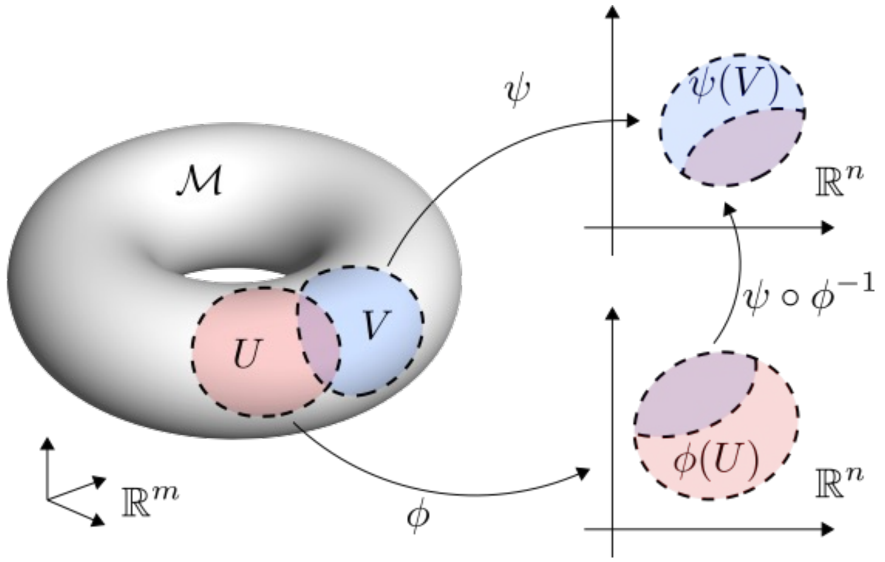
DManD with local representations and models

Global intrinsic-dimensional representation of a manifold

Example: global Cartesian representation of a torus is not possible in two dimensions – need to embed in 3D.



Working representation of a manifold: an **atlas of charts**

Chart: 2 ingredients

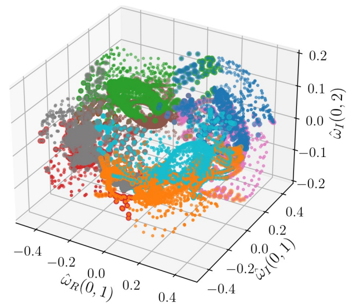
1. An open subset of $\mathcal{M}$ (the coordinate domain U)
2. A continuous, *one-to-one* map ϕ taking us from $U \subseteq \mathcal{M} \subseteq \mathbb{R}^m$ to $\phi(U) \subseteq \mathbb{R}^n$

Atlas: a collection of charts whose (Cartesian) coordinate domains cover $\mathcal{M}$

1. Patch the manifold into overlapping coordinate domains (k-means clustering)
2. For each patch, train an autoencoder
3. For each patch, train a neural network to learn dynamics in reduced space

Why complicate our lives with this more complex representation?

- Necessary for *minimal-dimension* representation of an arbitrary manifold (e.g. torus) – *any standard global manifold representation is a "one-chart" method and cannot be minimal-dimensional in general*
- Advantageous for systems with complex dynamics such as intermittency – different structure to dynamics in different parts of state space
- Natural formalism for systems with discrete symmetries – charts related by symmetry operations



"Charts and Atlases for Nonlinear Data-Driven Dynamics on Manifolds = CANDyMan"

Floryan & G. Nature Mach Int 2022, Fox et al, PRE (2023), Perez De Jesus et al ArXiv (2023)

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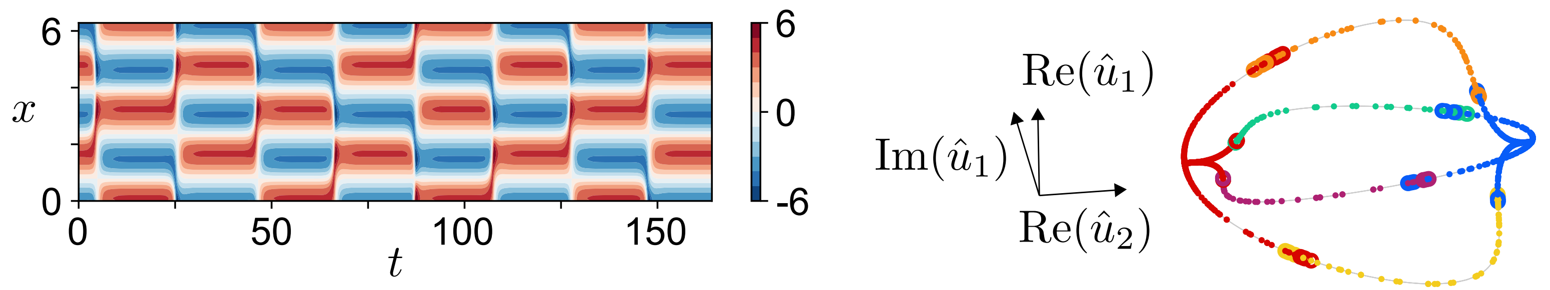
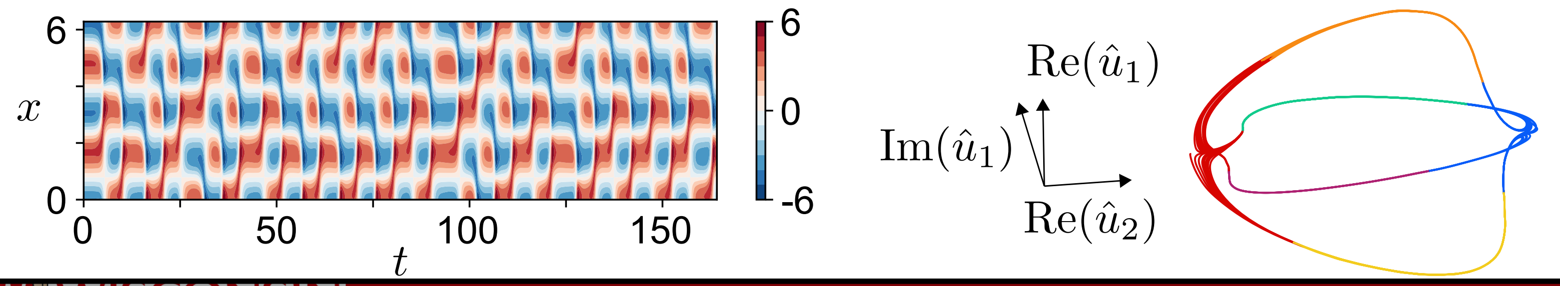
A challenging problem: bursting dynamics of a PDE

Data from Kuramoto-Sivashinsky equation



Atlas with 6 charts

3-dimensional dynamical model



Key challenges:

- Disparate time scales: fast bursts between quiescent cells
- Very thin state space structure
- Sensitive, non-periodic dynamics

CANDyMan:

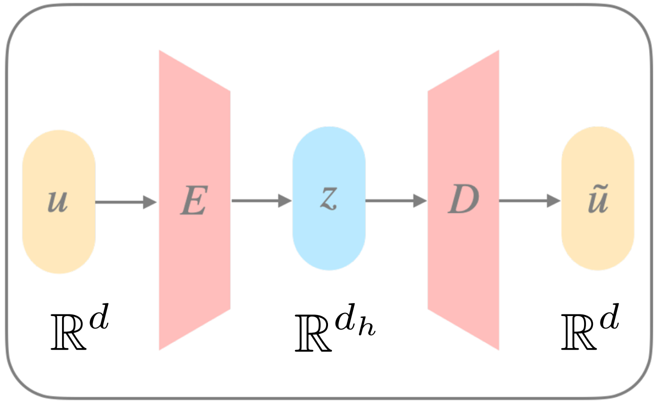
- Captures structure of attractor in 3D model
- The only quantitative discrepancy is the length of the quiescent portions
- Sensitivity of quiescent periods to model error arises from logarithmic divergence of time spent near saddle points

“One-chart” method fails badly even at 6 dimensions – cannot capture shape of attractor

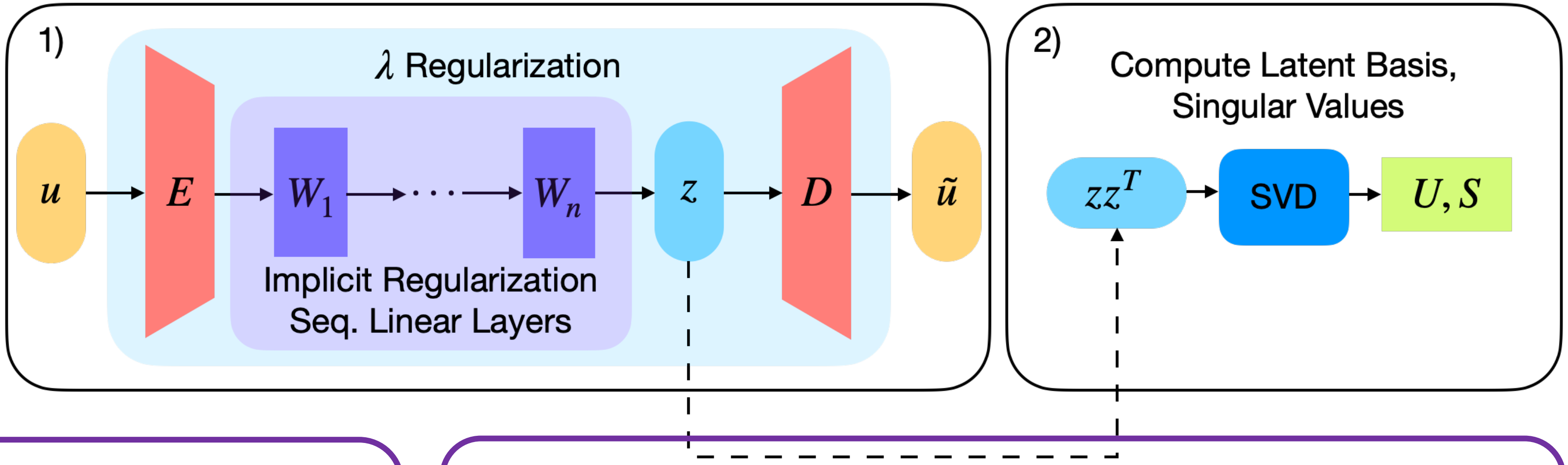
How many dimensions?

Formulation: IRMAE-WD

Classical autoencoder (AE)



Implicit rank-minimizing autoencoder with weight-decay (IRMAE-WD)



Framework automatically learns a latent space to span only the ~minimal necessary directions needed to parameterize the data:

$$\mathcal{L}(u; \theta_E, \theta_D) = \langle ||u - \mathcal{D}(\mathcal{E}(u; \theta_E); \theta_D)||^2 \rangle + \frac{\lambda}{2} ||w||_p^2$$

Only need to train one model to estimate $d_{\mathcal{M}}$, whereas other AE methods require training an array of models

Framework utilizes several low-rank driving forces:

- *Implicit regularization*[1,2,3]: internal linear layers drive/accelerate convergence to low rank latent space
- *Weight decay λ* [4]: breaks degeneracies in SGD dynamics introduced by linear layers —prevents "drift" of trailing singular values

Performing PCA on the learned latent space yields:

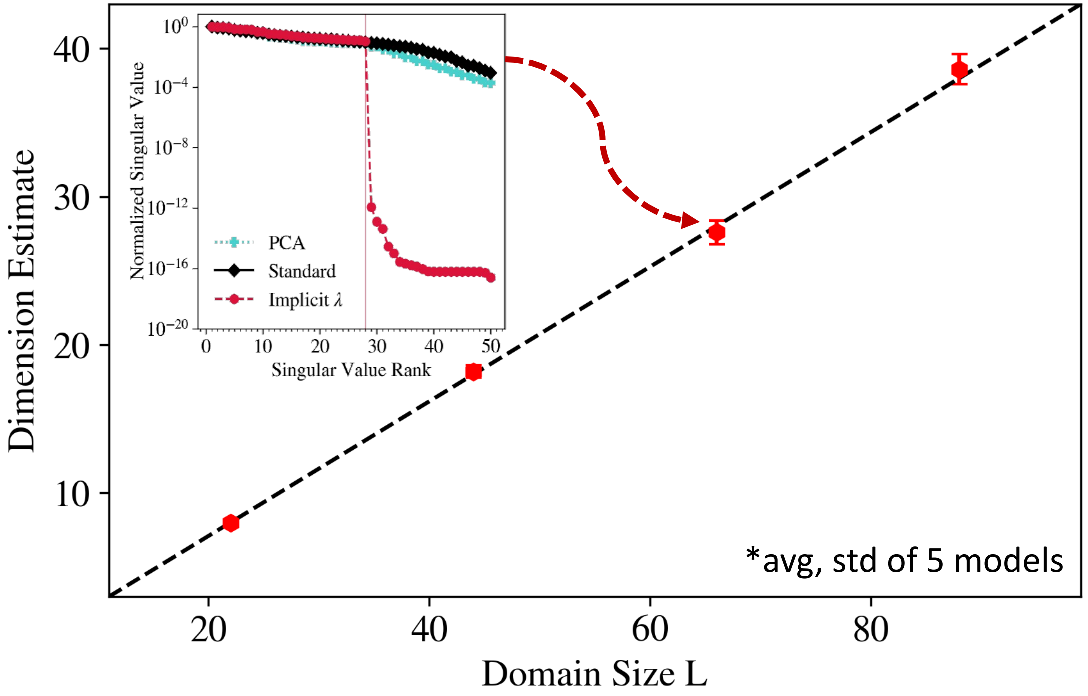
- *Manifold dimension:* singular value spectra of covariance
- *Manifold coordinates:* singular vectors

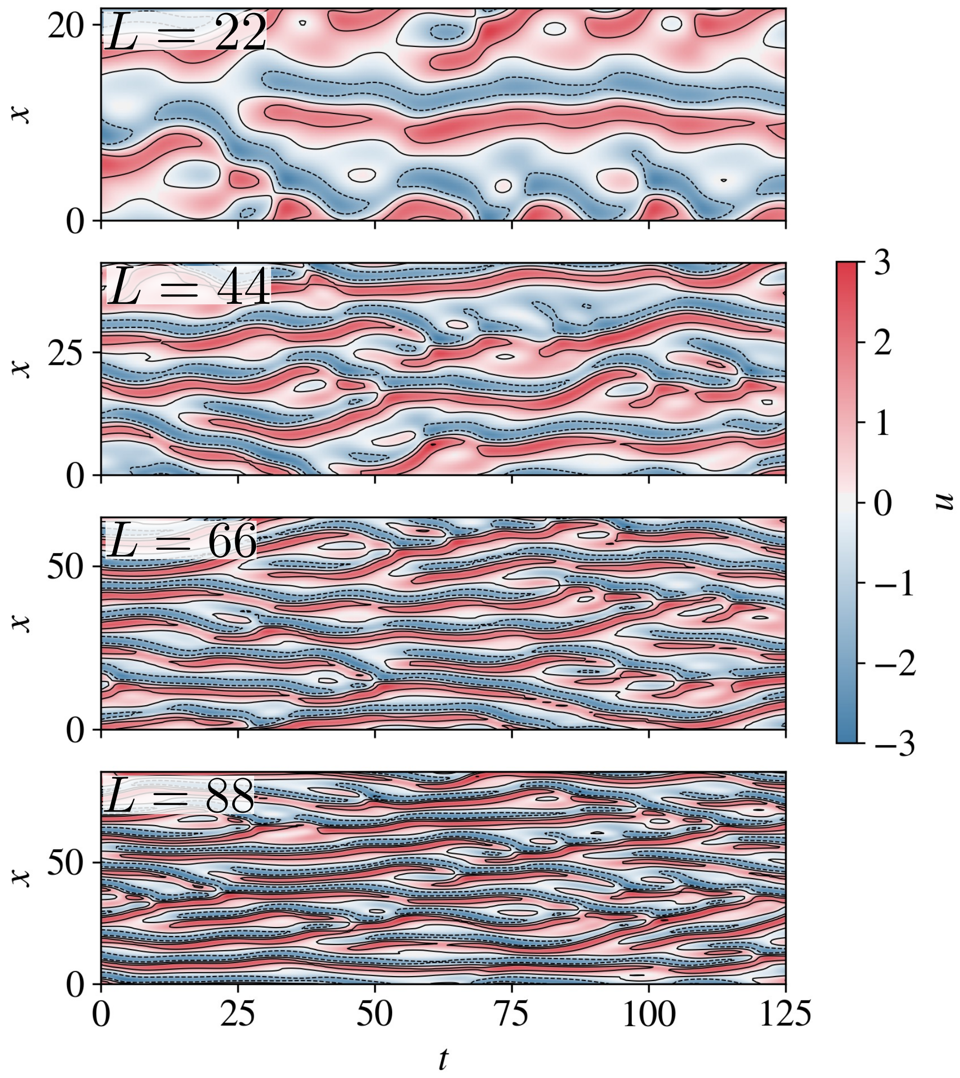
[1]: Arora et al., Neurips 2019
[2]: Gunasekar et al., Neurips 2019
[3]: Jing et al., Neurips 2020
[4]: Mousavi-Hosseini et al., ArXiv 2022

Dimension vs domain size: Kuramoto-Sivashinsky

- We apply our method to the Kuramoto-Sivashinsky Eq. for increasingly large domain sizes of L=22, 44, 66, 88
- **We achieve accurate & precise estimates for larger domain sizes *L* and demonstrate linear scaling in manifold dimension [1]**
- **Can use for dynamic model as above**

[1]: Yang, PRL 2009

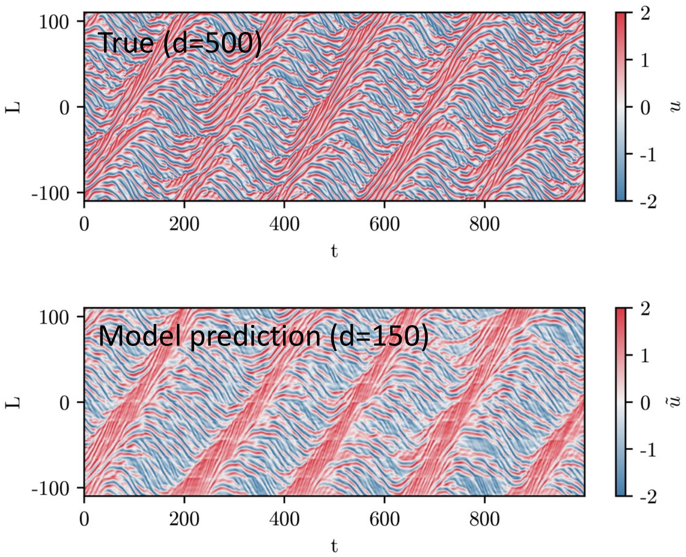




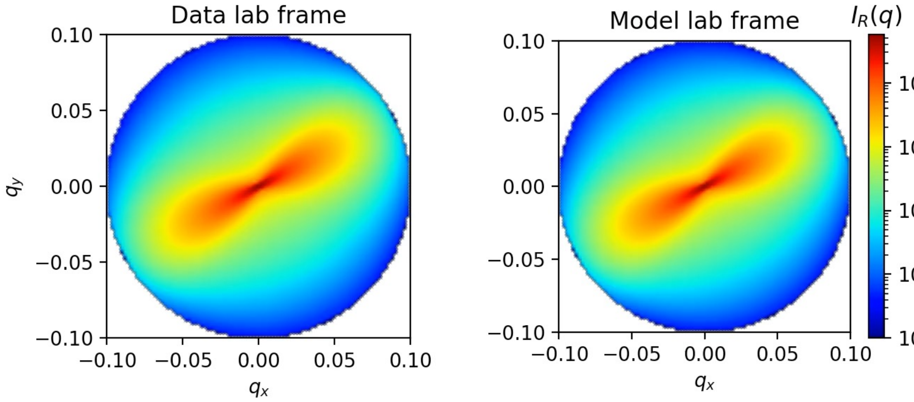
What's next?

- More complex systems
- Improved methods to estimate manifold dimension and representation (TDA tools, improvements over simple clustering)
- Distributed/hierarchical models for systems with multiscale dynamics
- Approximate methods for dynamics with very high dimension – keep the "thick" directions, model the "thin" ones
- Building more physics into data-driven reduced-order models
- Improved robustness for IRMAE-WD in high-dimensional ambient spaces
- Data-driven modeling of microstructure and stress in flowing complex fluids: dynamic symmetry – material frame indifference

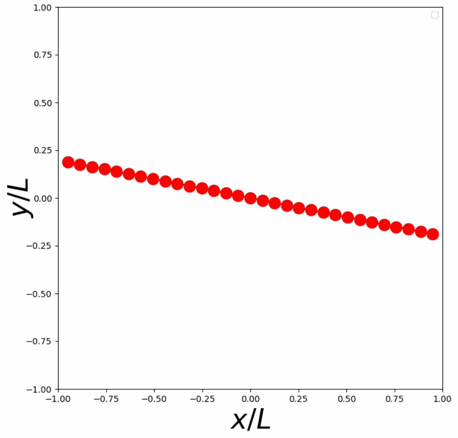
KSE dynamics with large scale forcing: hierarchical AE/NODE



DManD predictions of x-ray scattering pattern along a streamline
Young et al Rheol Acta 2023



DmanD model of sedimenting flexible fiber
(black – true, red – 4D DManD model)



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Thanks!