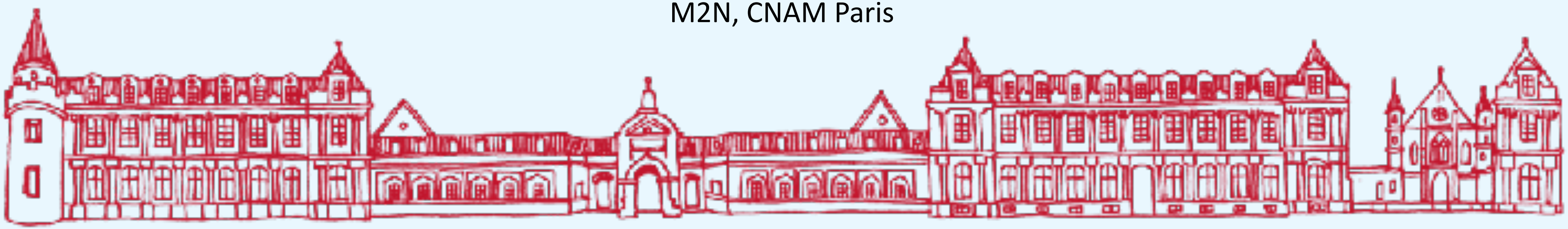
Ismael Zighed

Predictive data-driven models: A Shift in Perspective

Taraneh Sayadi

M2N, CNAM Paris



le cnam

Numerical models (Digital Twin)

Fidelity

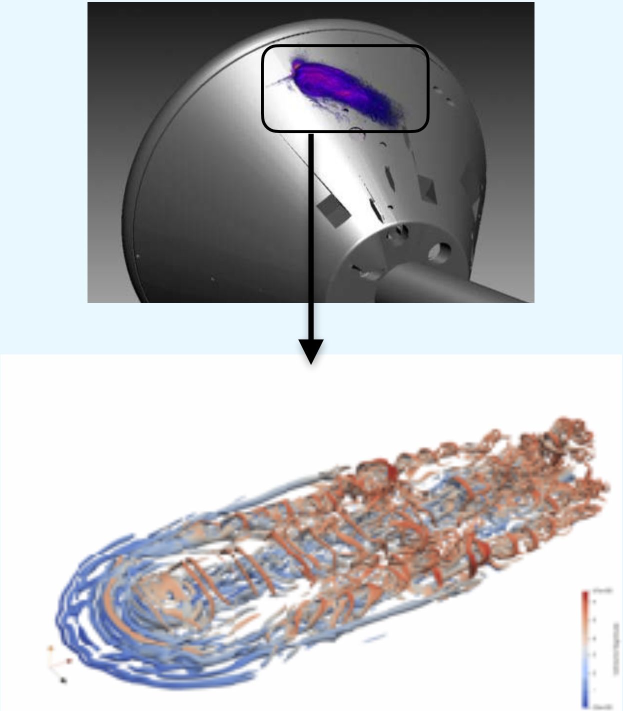
Governing equations (GE)

Approximated GE

Reduced-Order Models (ROM)

Efficiency

Ivey et al. 2011



ESA

Numerical models (Digital Twin)

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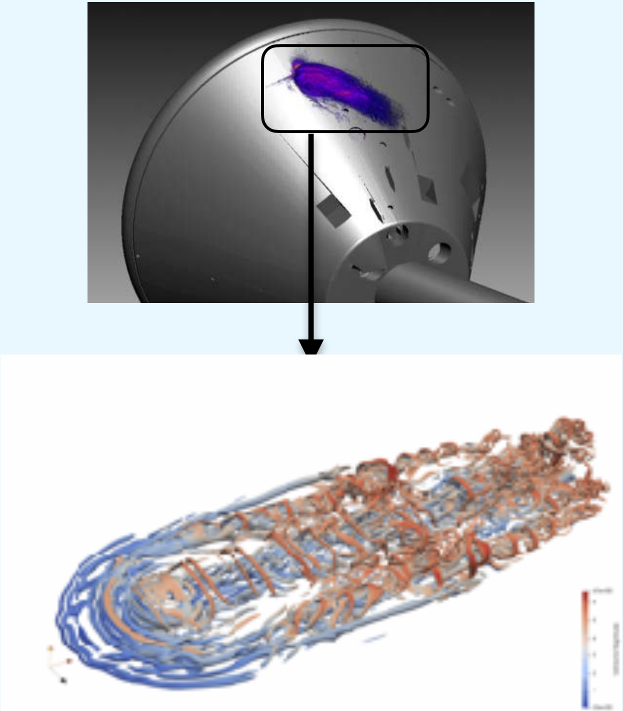
Efficiency

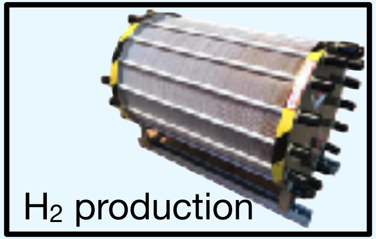
Ivey et al. 2011



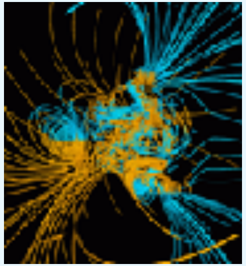
Design, Inverse Problems, …

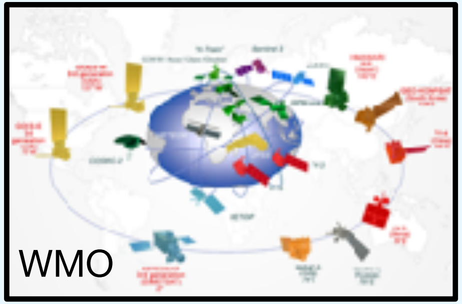
- Transport

- Energy



- Physical systems





Requirements

Multi-query applications

—> O(100) function evaluations (**operating conditions of the system**)

ROM

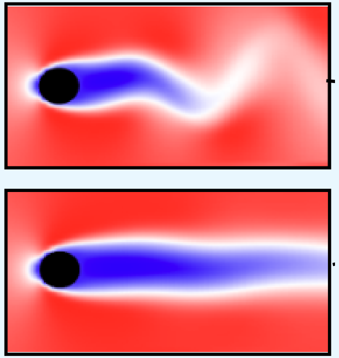
Requirements:

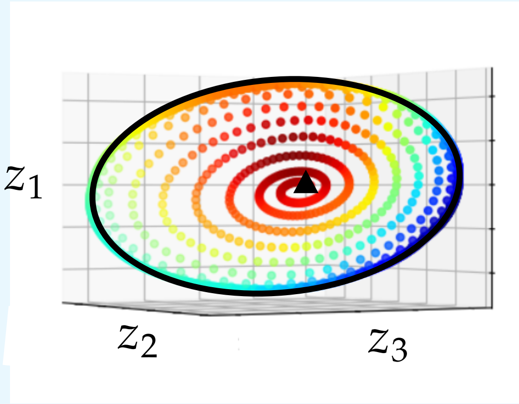
- Predictive
- Robust
- Parametrised
- Cheap

High-dimensional Problems

Assumption:

Although the system is high-dimensional, the dynamics evolve on a lower dimensional manifold



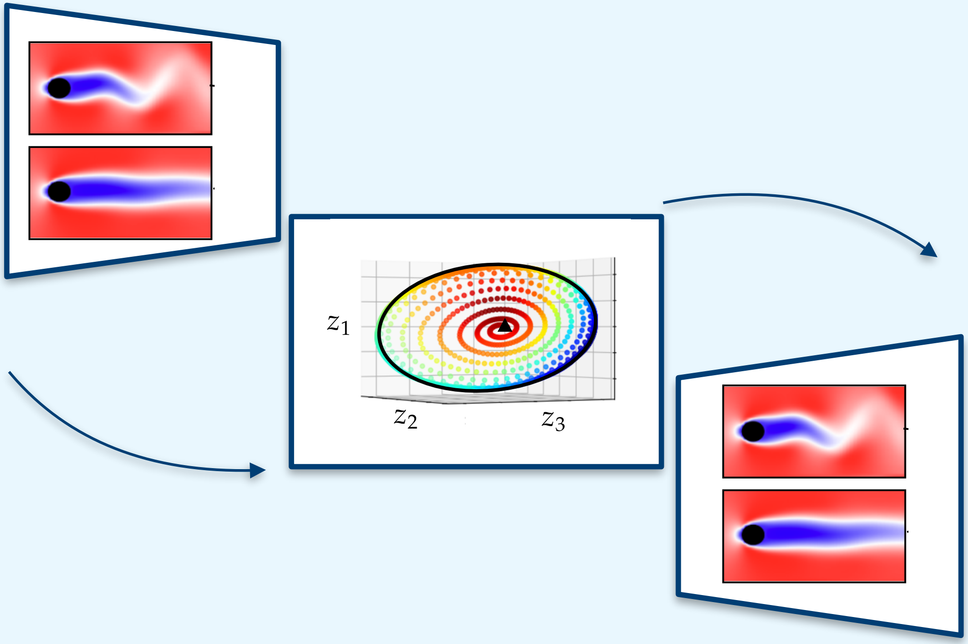


Approach

1. **Compression —>** dimensionality reduction

2. **Dynamics** in the lower-dimensional manifold

3. **Decompression**



Intrusive techniques

- **Projection techniques**
  - ➡ POD —> linear
  - ➡ POD-DEIM
  - ➡ Galerking projection
  - ➡ Petrov-Galerkin projection with hyper-reduction

- **Adaptive projection techniques**

The DGDD method for reduced-order modeling of conservation laws

Sébastien Riffaud[a,b,*], Michel Bergmann[a,b], Charbel Farhat[c,d,e], Sebastian Grimberg[c], Angelo Iollo[a,b]

[a] *IMB, UMR 5251, Univ. Bordeaux, 33400 Talence, France*
[b] *INRIA Bordeaux Sud-Ouest, Team MEMPHIS, 33400 Talence, France*
[c] *Department of Aeronautics and Astronautics, Stanford University, Stanford, CA 94305, USA*
[d] *Department of Mechanical Engineering, Stanford University, Stanford, CA 94305, USA*
[e] *Institute for Computational and Mathematical Engineering, Stanford University, Stanford, CA 94305, USA*

Predictive Reduced Order Modeling of Chaotic Multi-scale Problems Using Adaptively Sampled Projections

Cheng Huang
University of Kansas, Lawrence, KS

Karthik Duraisamy
University of Michigan, Ann Arbor, MI

Nonintrusive - data-driven techniques

Linear reduction

- DMD
- *Koopman ?*

Nonlinear reduction

- SSM
- MZ-formalism

Properties of Immersions for Systems with Multiple Limit Sets with Implications to Learning Koopman Embeddings ⋆

Zexiang Liu [a] Necmiye Ozay [a] Eduardo D. Sontag [b]

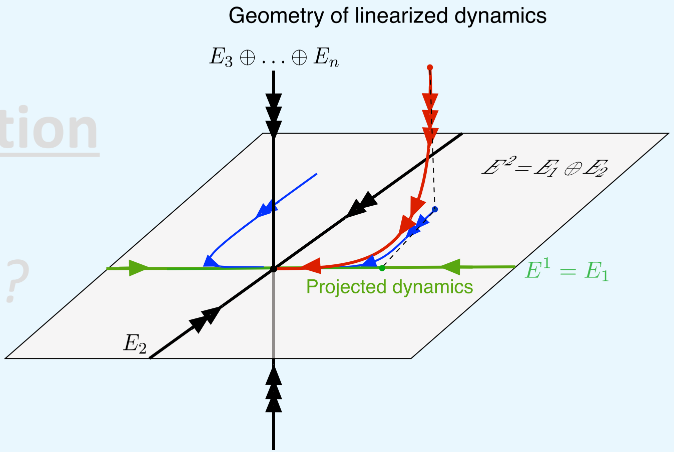
Nonlinear model reduction to temporally aperiodic spectral submanifolds

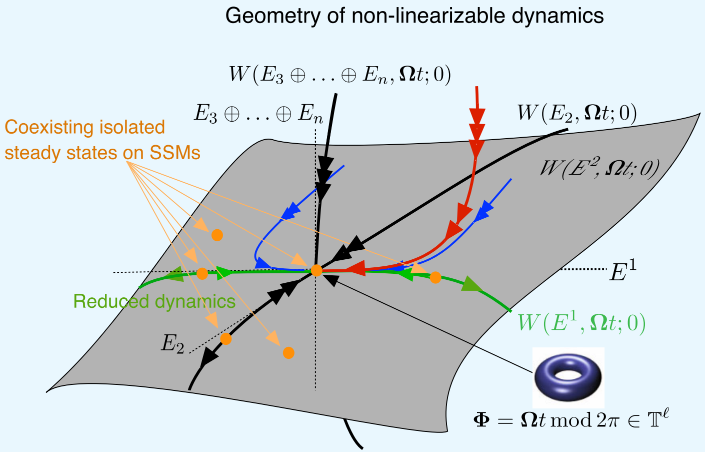
Cite as: Chaos 34, 043152 (2024); doi: 10.1063/5.0187080
Submitted: 10 November 2023 · Accepted: 1 April 2024 ·
Published Online: 26 April 2024

View Online

George Haller[a] and Roshan S. Kaundinya

Nonintrusive - data-driven techniques





Linear reduction

- DMD
- *Koopman ?*

Nonlinear reduction

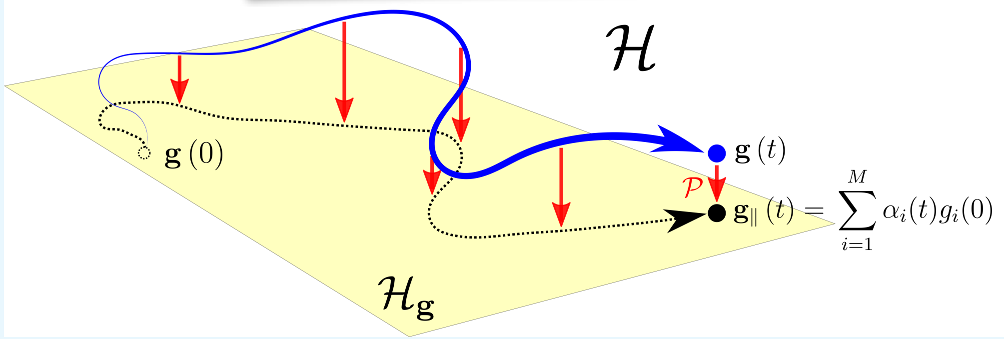
- SSM
- MZ-formalism

M. Cenedese, J. Axås, B. Bäuerlein, K. Avila and G. Haller. Data-driven modeling and prediction of non-linearizable dynamics via spectral submanifolds. *Nature Communications*, **13** (2022) 872.

MZ - formalism

Data-driven learning for the Mori–Zwanzig formalism: a generalization of the Koopman learning framework

Yen Ting Lin[1,*], Yifeng Tian[2], Marian Anghel[1], and Daniel Livescu[2]



$$\frac{d\boldsymbol{\Phi}(t)}{dt} = S(\boldsymbol{\Phi}(t)), \quad \boldsymbol{\Phi}(0) = \boldsymbol{\Phi}_0,$$

$$\frac{\partial g(x,t)}{\partial t} = \mathcal{L}\{g(x,t)\} \quad , \quad g(0,t) = g_0$$

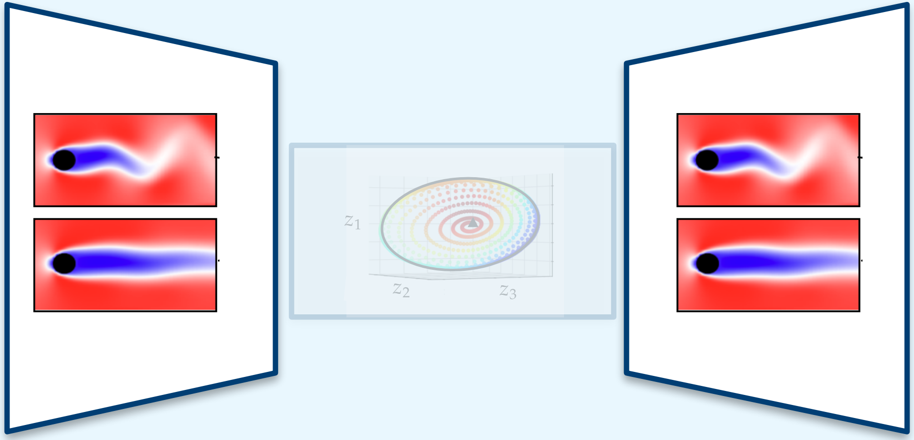
$$\frac{\partial}{\partial t}\hat{\mathbf{g}}(\boldsymbol{\Phi}_0, t) = \underbrace{\mathcal{P}\mathcal{L}\hat{\mathbf{g}}(\boldsymbol{\Phi}_0, t)}_{\text{Markov}} + \underbrace{\int_0^t \mathcal{P}\mathcal{L}e^{s\mathcal{Q}\mathcal{L}}\mathcal{Q}\mathcal{L}\hat{\mathbf{g}}(\boldsymbol{\Phi}_0, t-s)ds}_{\text{Memory}} + \underbrace{e^{t\mathcal{Q}\mathcal{L}}\mathcal{Q}\mathcal{L}\hat{\mathbf{g}}(\boldsymbol{\Phi}_0)}_{\text{Noise}}$$

How does this all translate into an ML architecture?

ML-based Compression

Compression/decompression

- PCA —> Linear
- AE / VAE —> nonlinear



Identification of the observables !

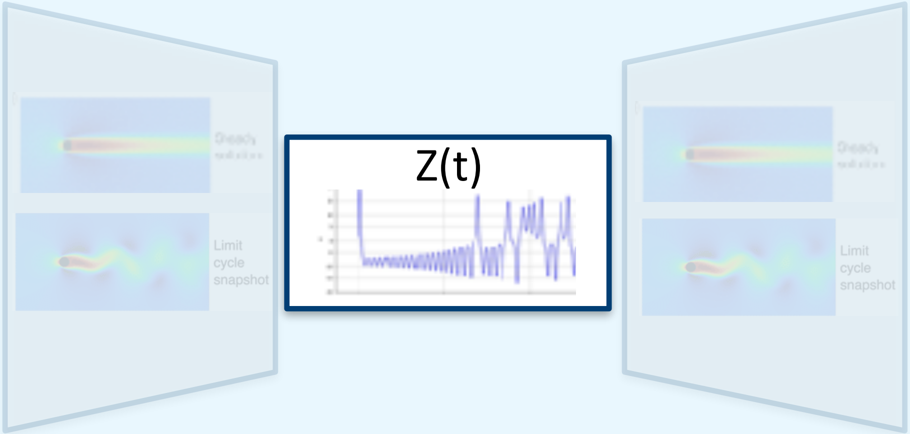
$$\frac{\partial}{\partial t}\underline{\hat{\mathbf{g}}(\boldsymbol{\Phi}_0,t)} = \underbrace{\mathcal{P}\mathcal{L}\hat{\mathbf{g}}(\boldsymbol{\Phi}_0,t)}_{\text{Markov}} + \underbrace{\int_0^t \mathcal{P}\mathcal{L}e^{s\mathcal{Q}\mathcal{L}}\mathcal{Q}\mathcal{L}\hat{\mathbf{g}}(\boldsymbol{\Phi}_0,t-s)ds}_{\text{Memory}} + \underbrace{e^{t\mathcal{Q}\mathcal{L}}\mathcal{Q}\mathcal{L}\hat{\mathbf{g}}(\boldsymbol{\Phi}_0)}_{\text{Noise}}$$

Dynamic Reconstruction

Dynamics in the latent space

- Neural ODEs [1]
- ESN [2]
- LSTM [3]
- **Transformers**

Haller et al. 2022



[1] E. Menier, M.A. Bucci, M. Yagoubi, L. Mathelin, M. Schoenauer, CD-ROM: Complemented Deep - Reduced order model, Computer Methods in Applied Mechanics and Engineering. 410 (2023).
[2] A. Racca, NAK Doan, L. Magri. Predicting turbulent dynamics with the convolutional autoencoder echo state network. Journal of Fluid Mechanics. 975:A2. doi:10.1017/jfm.2023.716 (2023).
[3] P. Gupta, P.J. Schmid, D. Sipp, T. Sayadi & G. Rigas. Mori–Zwanzig latent space Koopman closure for nonlinear autoencoder. Proc. R. Soc. A.481, http://doi.org/10.1098/rspa.2024.0259 (2025)

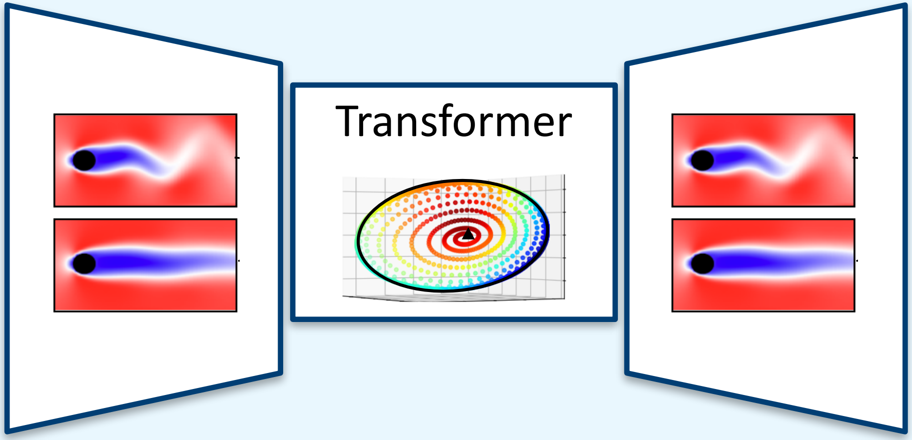
MZ formalism - ML architecture

Observable space : $\hat{\mathrm{g}}(\boldsymbol{\Phi}_0, t)$

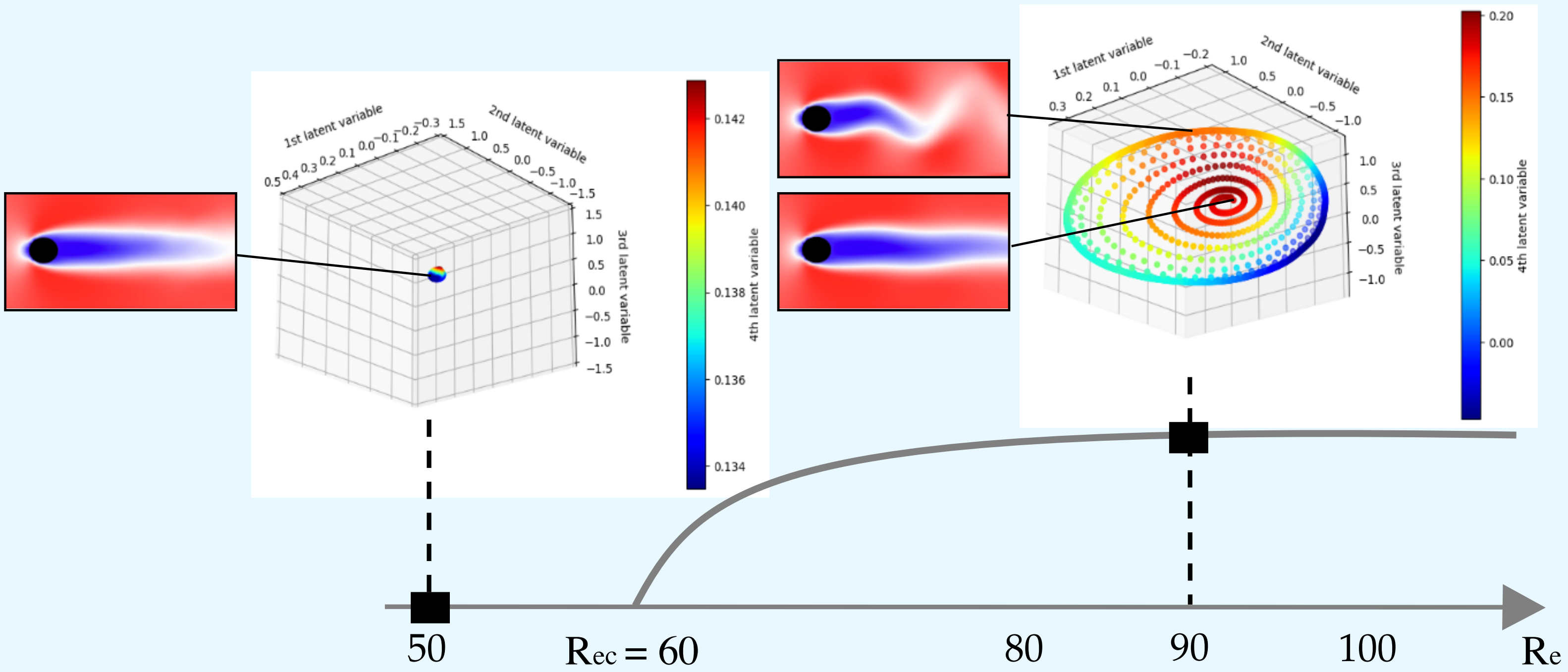
$$\frac{d\boldsymbol{\Phi}(t)}{dt} = S(\boldsymbol{\Phi}(t)), \quad \boldsymbol{\Phi}(0) = \boldsymbol{\Phi}_0,$$

$$\frac{\partial}{\partial t}\hat{\mathrm{g}}(\boldsymbol{\Phi}_0, t) = \underbrace{\mathcal{PL}\hat{\mathrm{g}}(\boldsymbol{\Phi}_0, t)}_{\text{Markov}} + \underbrace{\int_0^t \mathcal{PL}e^{s\mathcal{QL}}\mathcal{QL}\hat{\mathrm{g}}(\boldsymbol{\Phi}_0, t-s)ds}_{\text{Memory}} + \cancel{\underbrace{e^{t\mathcal{QL}}\mathcal{QL}\hat{\mathrm{g}}(\boldsymbol{\Phi}_0)}_{\text{Noise}}}$$

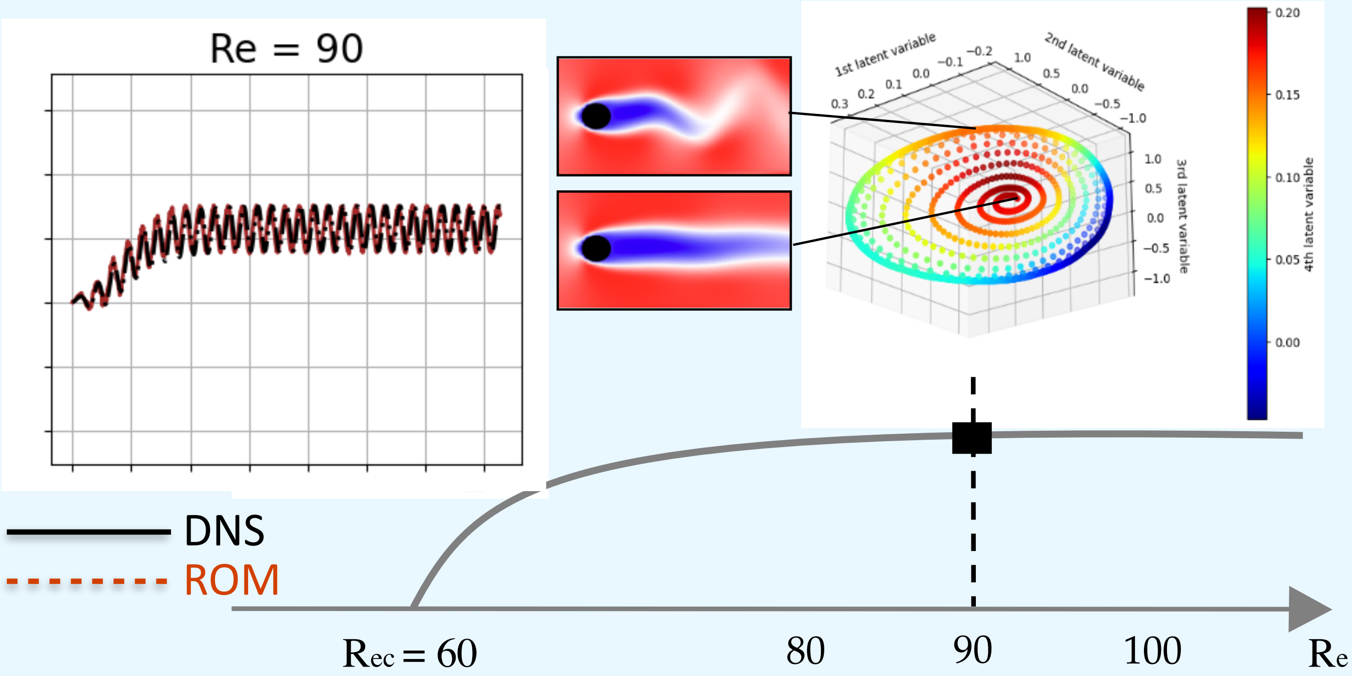
Parametrised!



Flow Around a Cylinder

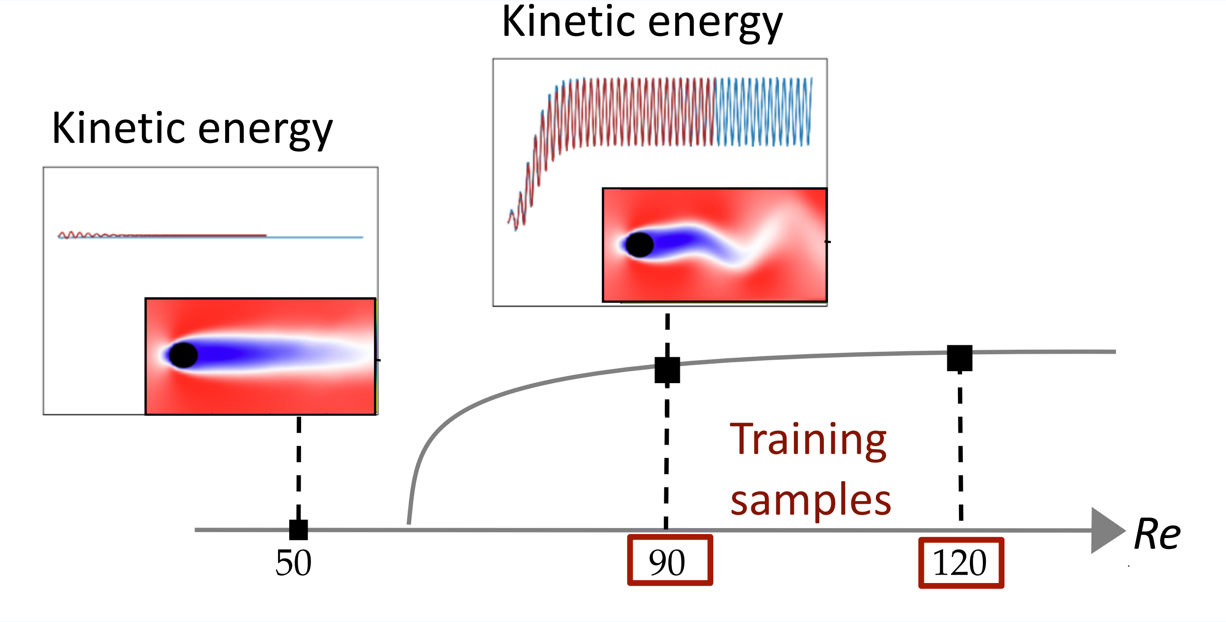


Predictive …



Re = 90
DNS
ROM
1st latent variable
2nd latent variable
3rd latent variable
4th latent variable
$Re_{ec} = 60$
80
90
100
Re

Predictive …


Kinetic energy
Kinetic energy
Training
samples
50
90
120
Re

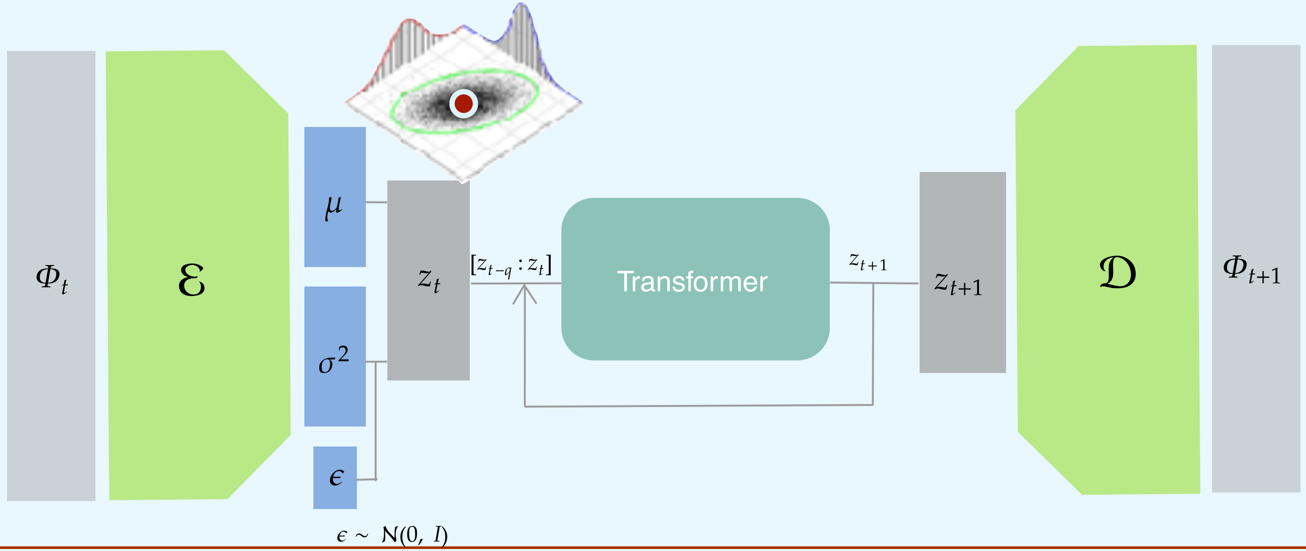
Move from deterministic representation in the latent space to a stochastic one!

Probabilistic Representation

Variational AutoEncoder (VAE)

- Encoder maps each point into a distribution within the latent space
- Distribution is computed using **Kullback-Leiber Divergence (KLD)** assuming **Gaussian distribution**

$$\mathcal{L} = \frac{\lambda}{m}\Big(\sum_{k=0}^{m} \|\phi_{n-q:n} - \mathcal{DE}(\phi_{n-q:n})\| + \beta.\mathrm{KLD}\Big) + \frac{1}{m}\sum_{k=0}^{m} \|z_{n+1:n+h} - \hat{z}_{n+1:n+h}\| + \frac{1}{m}\sum_{k=0}^{m} \|\phi_{n+1:n+h} - \mathcal{D}(\hat{z}_{n+1:n+h})\|.$$



How can the information be used?

- Data-assimilation —> reducing training data
- Uncertainty quantification

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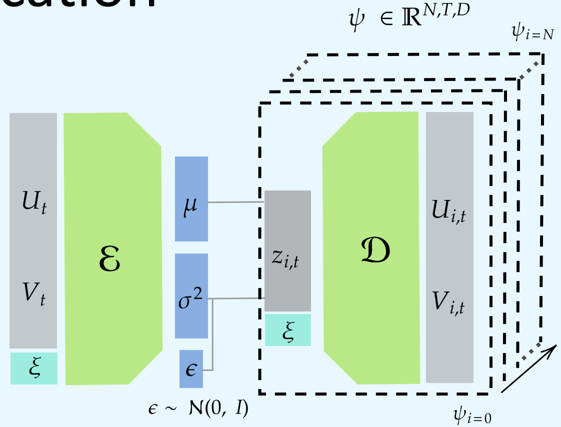
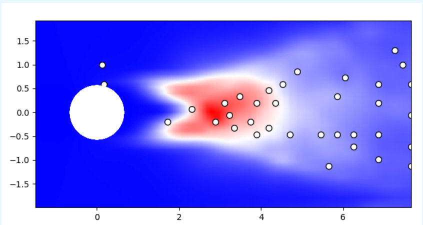
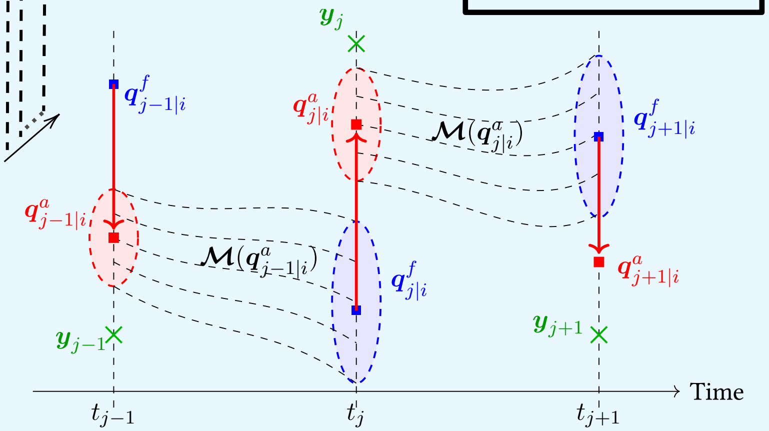
- **Data-assimilation —> reducing training data**
- Uncertainty quantification



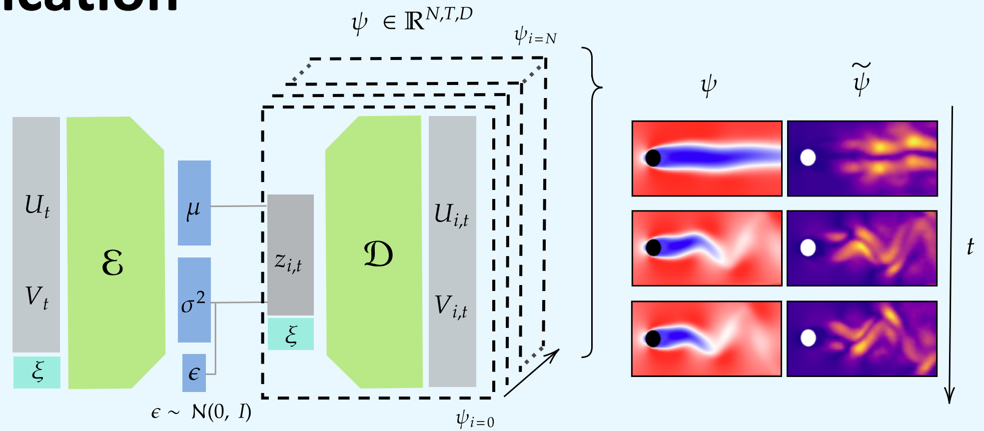


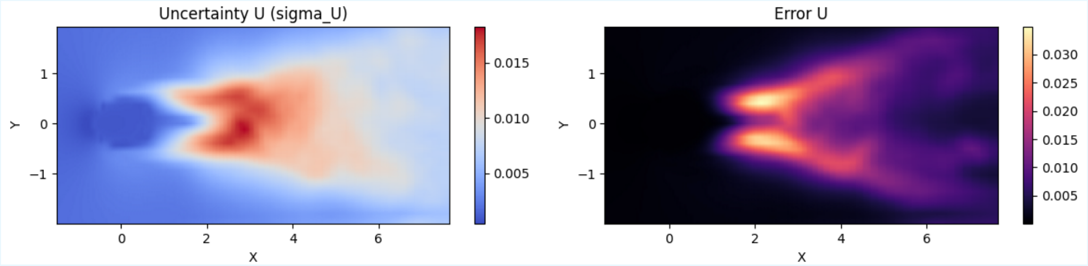
Villiers *et al*. 2025



How can the information be used?

- Data-assimilation —> reducing training data
- **Uncertainty quantification**





What about chaotic systems?

What is the current SoA

Data-driven modeling and forecasting of chaotic dynamics on inertial manifolds constructed as spectral submanifolds

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Submitted: 4 October 2023 · Accepted: 6 March 2024 ·
Published Online: 26 March 2024

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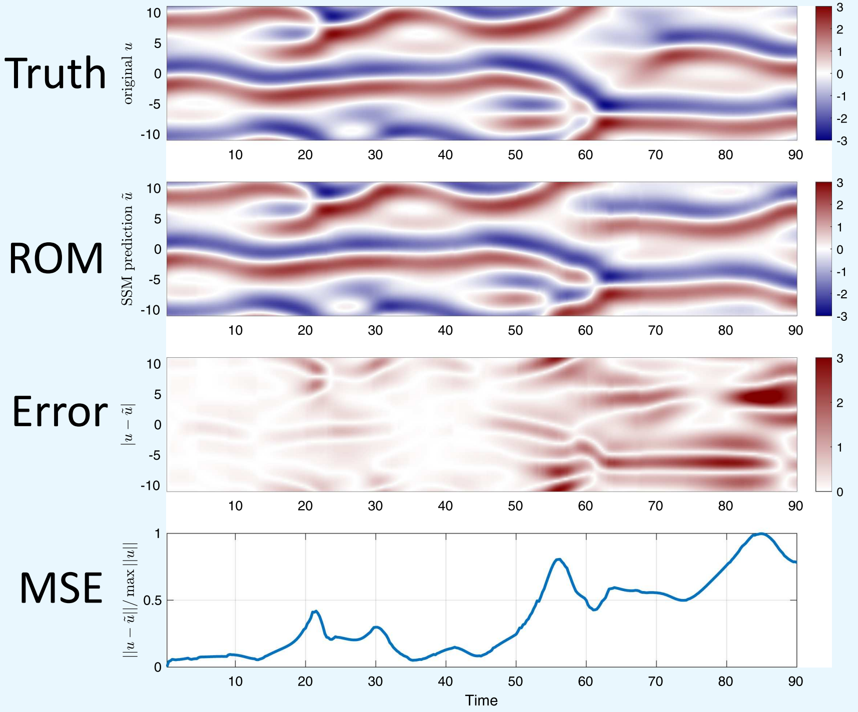
Aihui Liu, Joar Axås, and George Haller[a)]



What is the ultimate goal of these models ?

- Image reconstruction ?
- Acceptable dynamical/statistical behaviour

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- Image reconstruction ?
- Acceptable dynamical/statistical behaviour

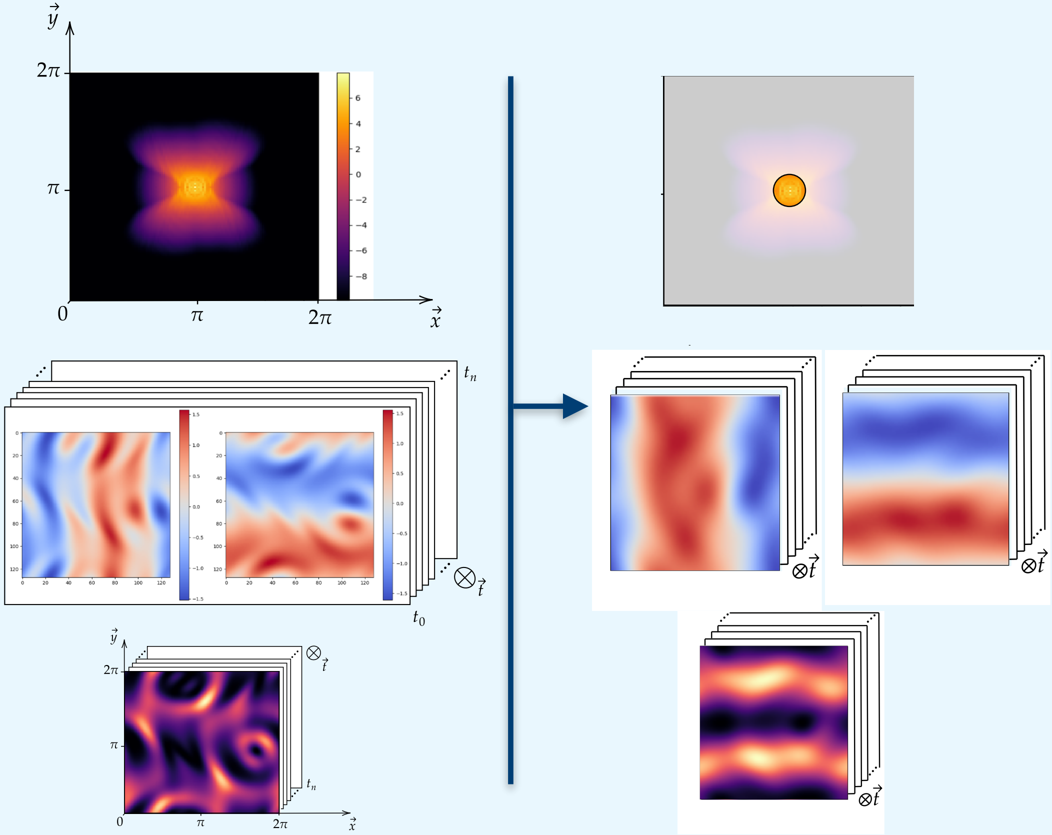
Decompose the process into two steps : (scale separation)

I. **Large scales** —> predicted by ROM (FORECAST)

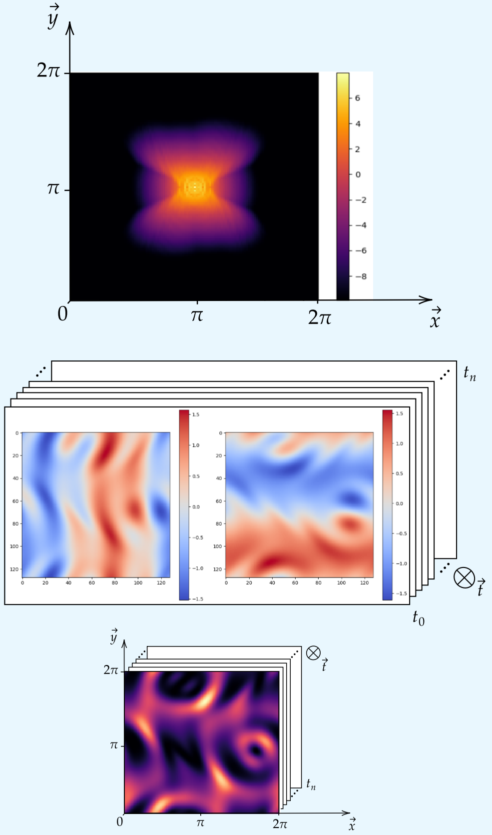
+

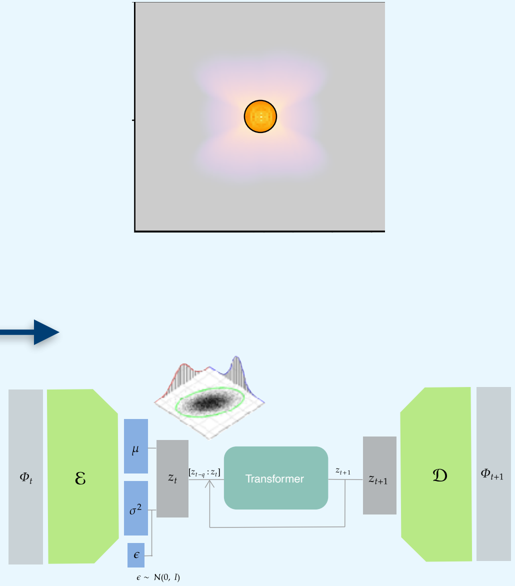
II. **Small scales** —> Stochastic closure (Closure)

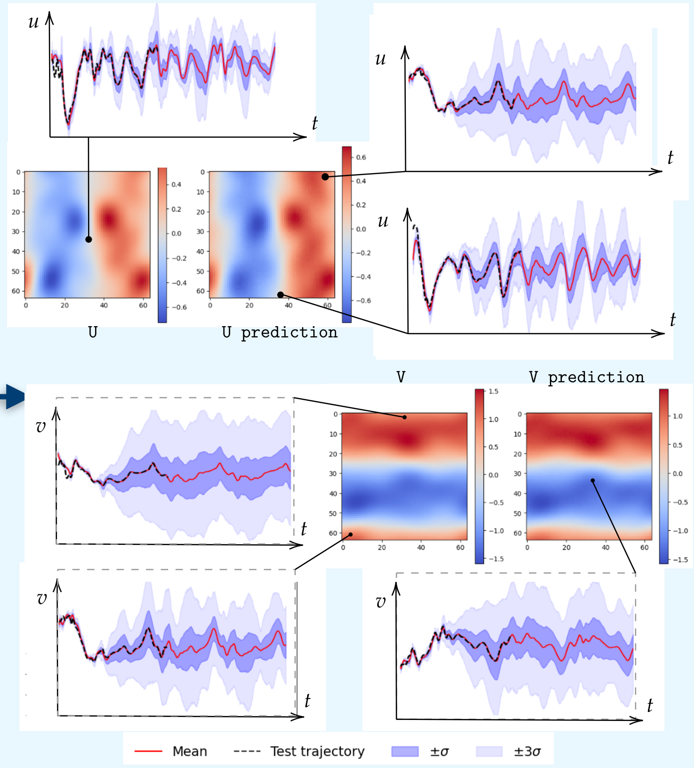
I. Large Scales



I. Large Scales







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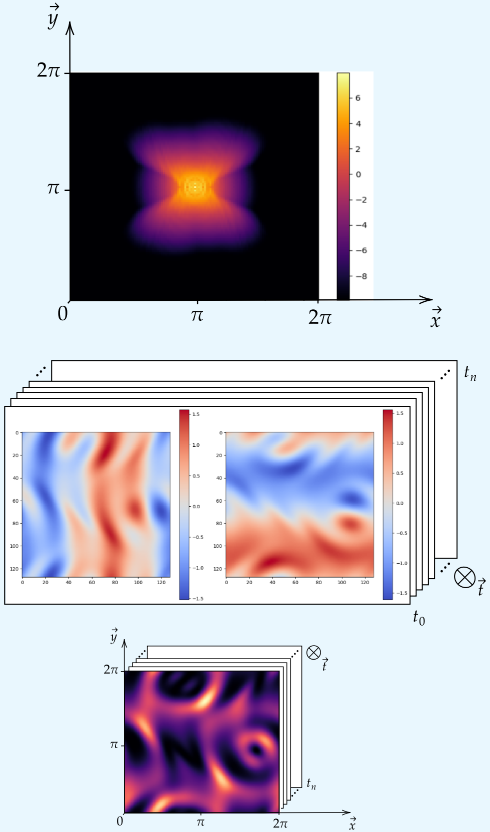
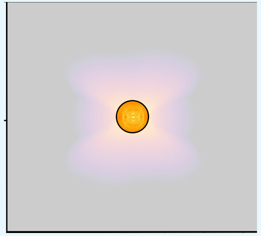
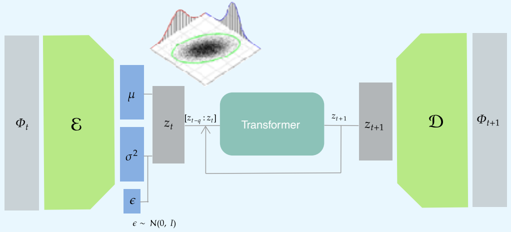
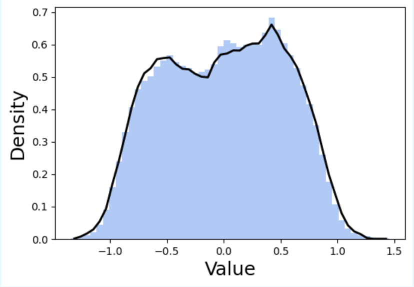
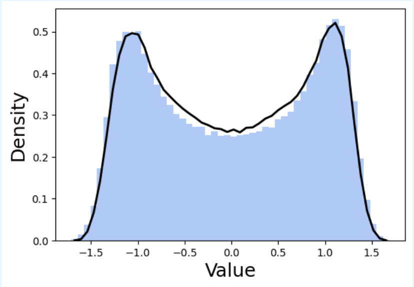








(a) Comparison of the density of U and its prediction



(b) Comparison of the density of V and its prediction

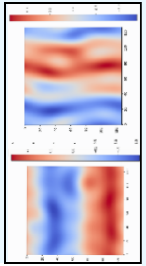
Prediction - Histogram — True - PDF

II. Closure

Make use of the existing coherence —> **dimensionality reduction**

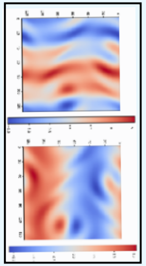
Filtered

$\widehat{\varphi}$



DNS

φ



Assumptions:

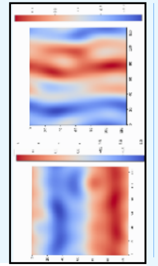
- Closure is independent of the dynamics.
- Can be performed on a reduced space.

II. Closure

Make use of the existing coherence —> **dimensionality reduction**

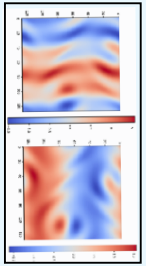
Filtered

$\widehat{\varphi}$



DNS

φ



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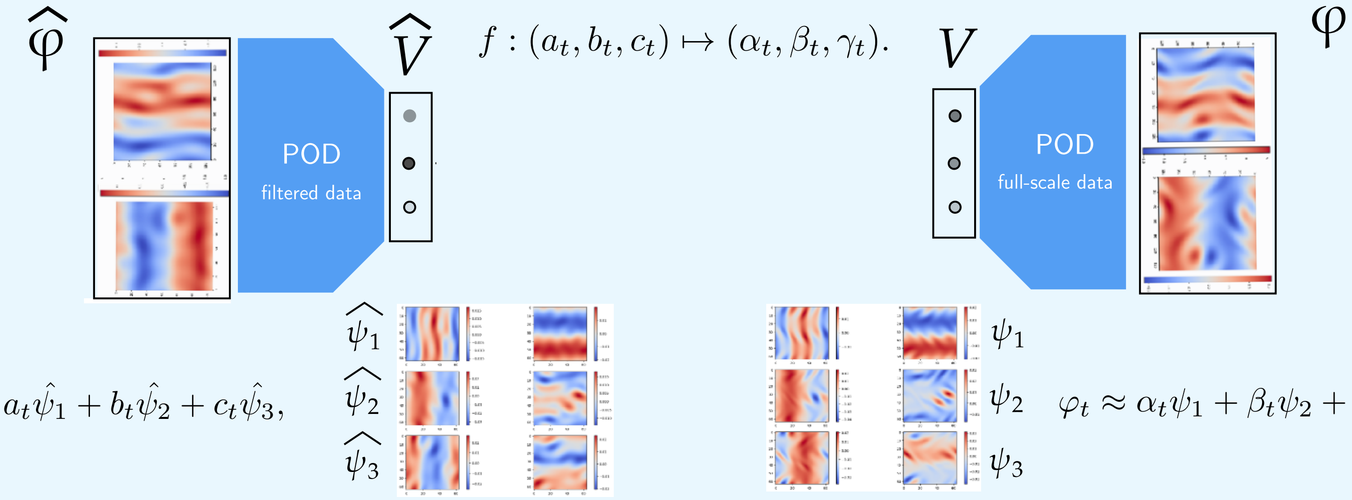
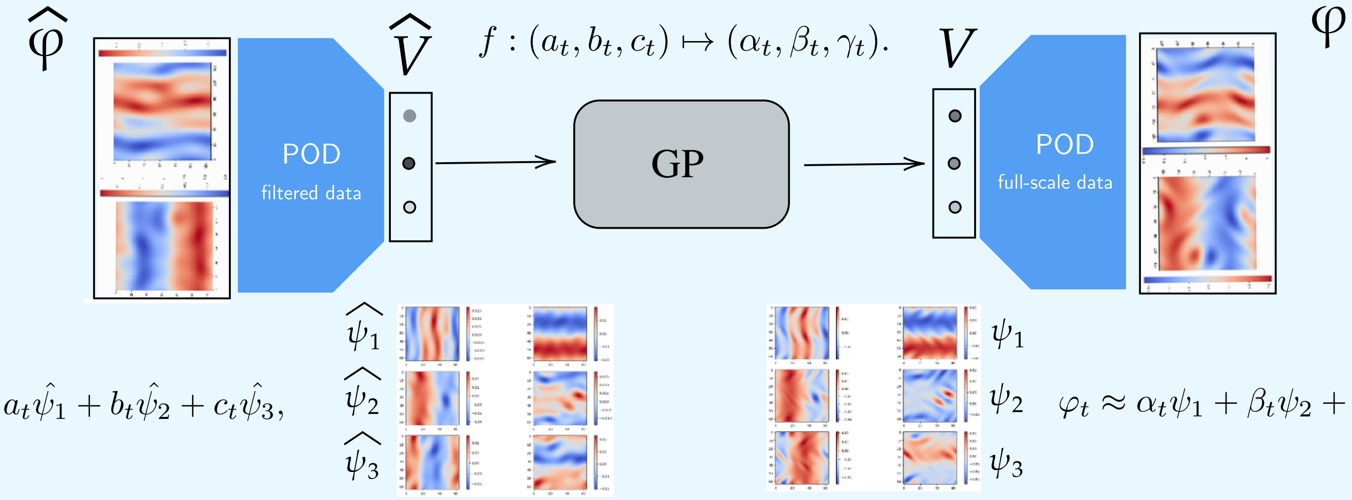


$$\hat{\varphi}_t \approx a_t\hat{\psi}_1 + b_t\hat{\psi}_2 + c_t\hat{\psi}_3,$$

$$\varphi_t \approx \alpha_t\psi_1 + \beta_t\psi_2 + \gamma_t\psi_3,$$

II. Closure

Make use of the existing coherence —> **dimensionality reduction**

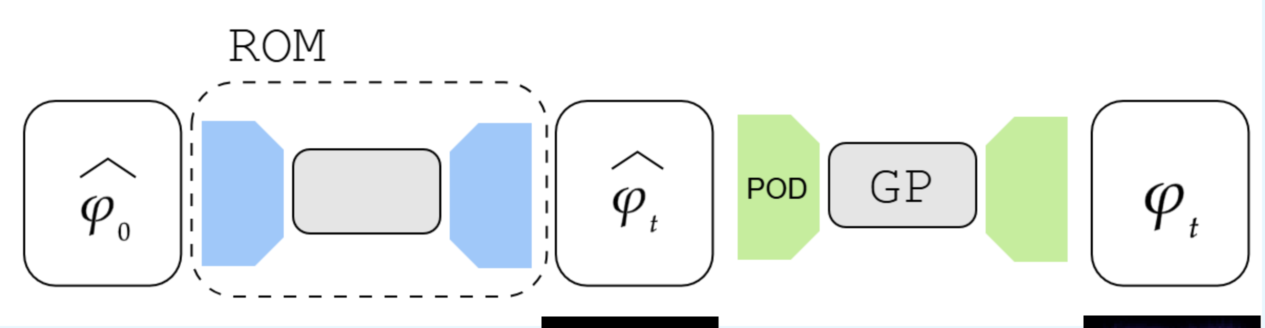


$$\hat{\varphi}_t \approx a_t \hat{\psi}_1 + b_t \hat{\psi}_2 + c_t \hat{\psi}_3,$$

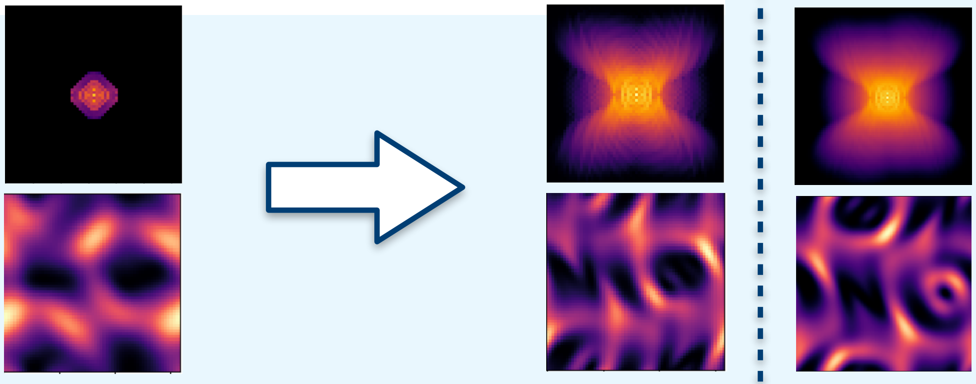
$$\varphi_t \approx \alpha_t \psi_1 + \beta_t \psi_2 + \gamma_t \psi_3,$$

Full model —> I + II

Make use of the existing coherence —> **dimensionality reduction**

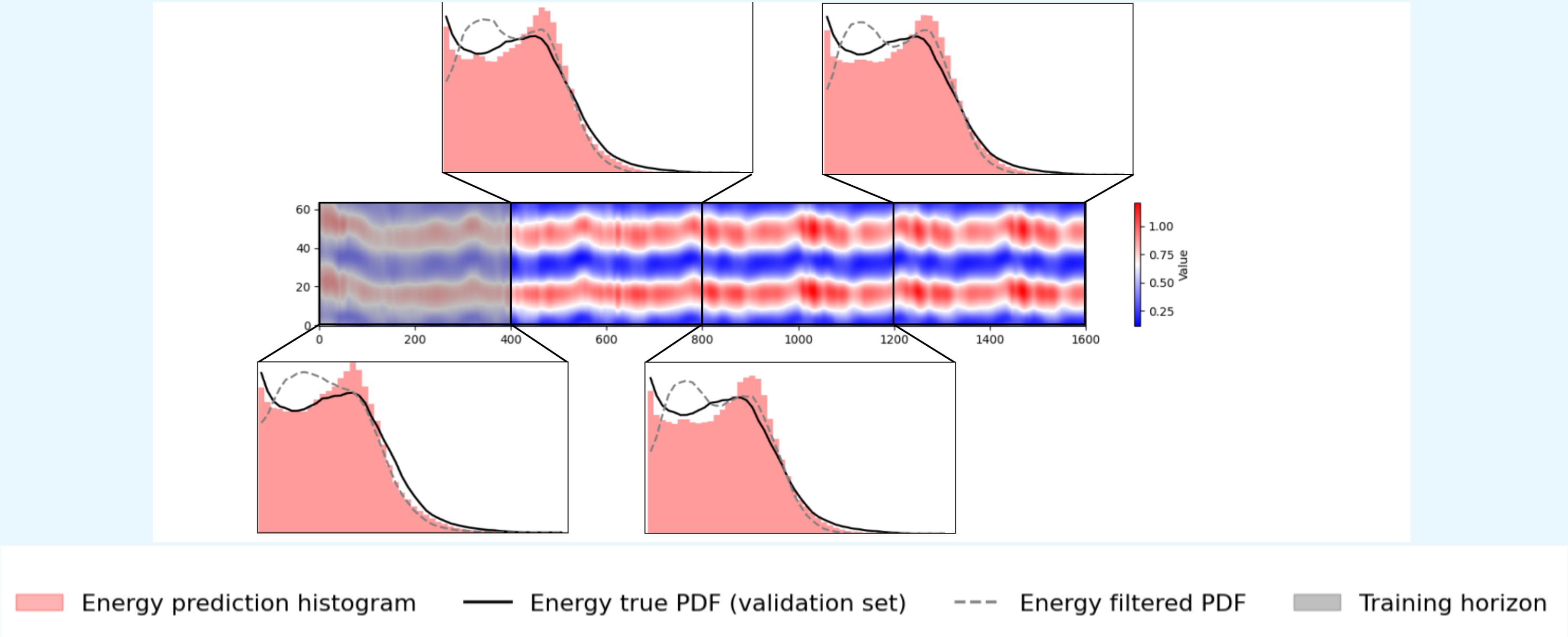


Truth



Moments should match not images!

Long-time Forecasting



Last Words …

- Advances has been made regarding AI-driven ROMs
  - Specially in domains with access to big data

Article

Probabilistic weather forecasting with machine learning

https://doi.org/10.1038/s41586-024-08252-9

Received: 30 April 2024

Accepted: 18 October 2024

Ilan Price[1,2]✉, Alvaro Sanchez-Gonzalez[1,2], Ferran Alet[1,2], Tom R. Andersson[1,2], Andrew El-Kadi[1], Dominic Masters[1], Timo Ewalds[1], Jacklynn Stott[1], Shakir Mohamed[1], Peter Battaglia[1]✉, Remi Lam[1]✉ & Matthew Willson[1]✉

Article

End-to-end data-driven weather prediction

https://doi.org/10.1038/s41586-025-08897-0

Received: 10 July 2024

Accepted: 12 March 2025

Anna Allen[1,11]✉, Stratis Markou[2,11]✉, Will Tebbutt[2,9], James Requeima[3], Wessel P. Bruinsma[4], Tom R. Andersson[5,10], Michael Herzog[6], Nicholas D. Lane[1], Matthew Chantry[7], J. Scott Hosking[5,8] & Richard E. Turner[2,8]✉

Some more last words …

- When applied to engineering applications
  - Data is scarce comparatively —> data-assimilation
  - Stochastic approach for complex systems
  - Taking advantage of prior physical knowledge

A change in perspective is necessary !