LA-UR-24-26584

Approved for public release; distribution is unlimited.

Title: Mori-Zwanzig dimensionality reduction for turbulent flows

Author(s): Livescu, Daniel
Lin, Yen Ting
Tian, Yifeng
Woodward, Michael Joseph
Barnett, Joel Ryan

Intended for: Advancing fluid and soft-matter dynamics with machine learning and data science, 2024-06-04 (Madison, Wisconsin, United States)
Web

Issued: 2024-07-02

Mori-Zwanzig dimensionality reduction for turbulent flows

Daniel Livescu

Senior Scientist

CCS-2, Los Alamos National Laboratory

Acknowledgements: Yen Ting Lin (CCS-3),
Yifeng Tian (CCS-3)
Michael Woodward (CCS-2)
Joel Barnett (UCLA)

Los Alamos NATIONAL LABORATORY EST.1943

LDRD

NNSA National Nuclear Security Administration

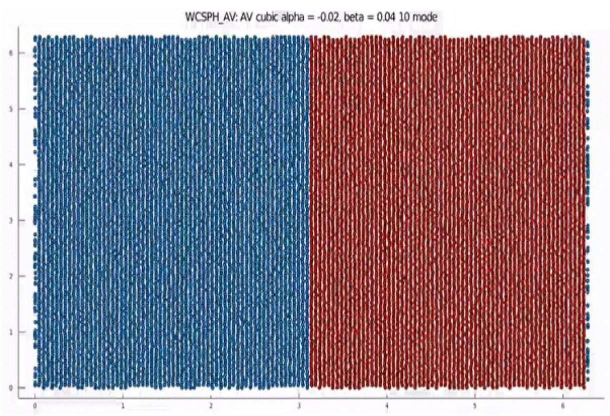
Turbulence strongly coupled across broad range of scale

- Need tractable models
- Data-Driven Discovery
  - Machine Learning inspired by nature: Eagles' nervous system learned a model for controlling turbulent flow.
- Encode physical symmetries and conservation laws

PIML models show significant better match and generalizability error compared to physics blind models.

Example: Learning Lagrangian dynamics using the framework of SPH (Woodward et al, PRF 2023; Tian et al, PNAS 2023).

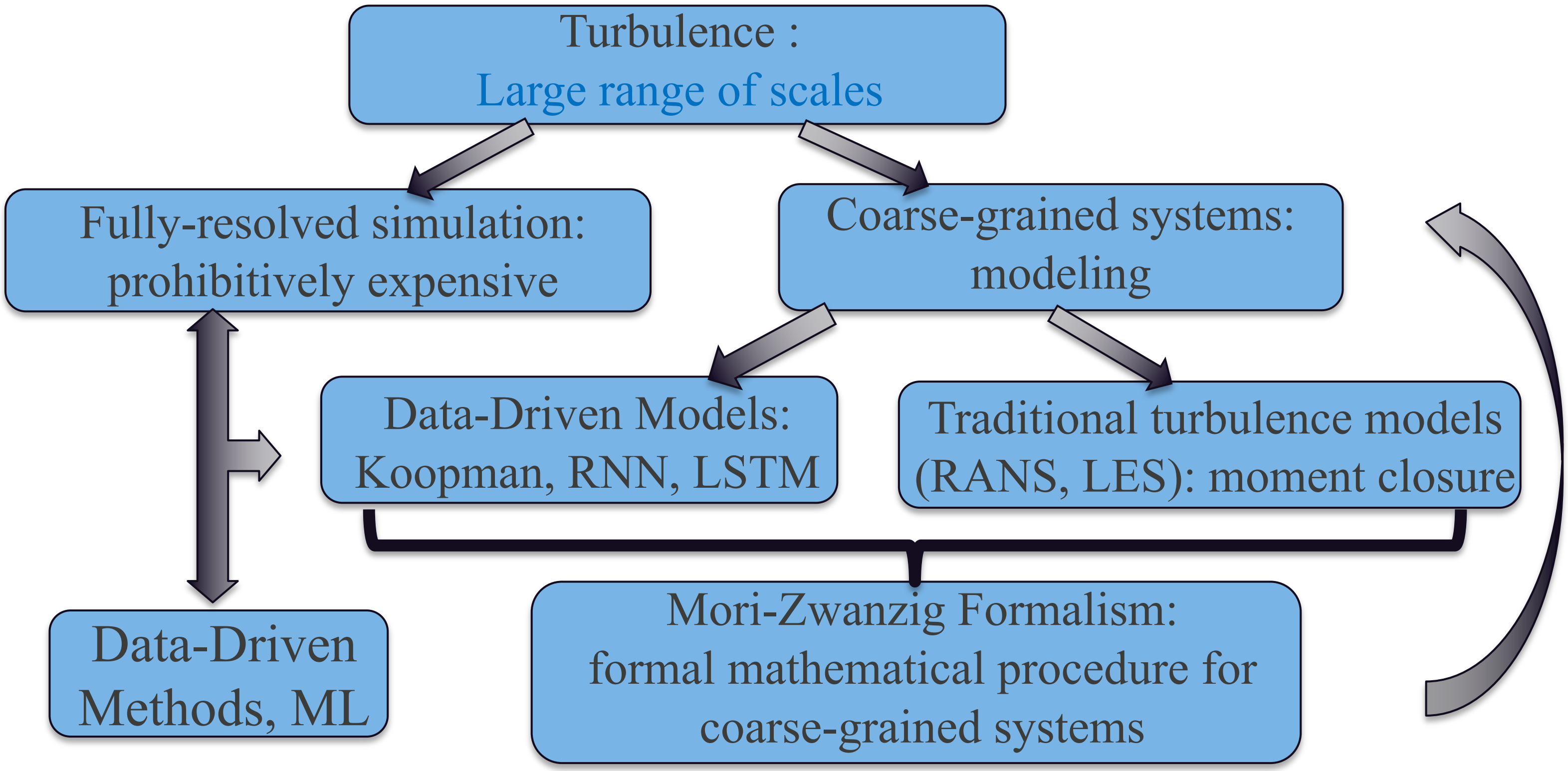
- **Goal:** Build effective Lagrangian models that capture turbulent dynamics on resolved scales using particle-based methods
- **Model:** Smooth Particle Hydrodynamics (SPH): Maps a continuous field onto a series of discrete particles carrying fluid quantities in the Lagrangian frame.
- **Approach:** Learn (estimate) parameters and functions from turbulence data.



Hierarchy of reduced order models, show increasingly better match with DNS data and generalizability error.

1. Physics-blind: NODE (Neural ODEs)
2. Replace terms on the right hand side with NNs
3. Add symmetries
4. Physics-informed: follow the full structure and symmetries of SPH model

The Mori-Zwanzig Formalism can be used as a general structure to formulate the turbulence closure problem.



Full order model is described by Direct Numerical Simulations of Navier-Stokes equations.

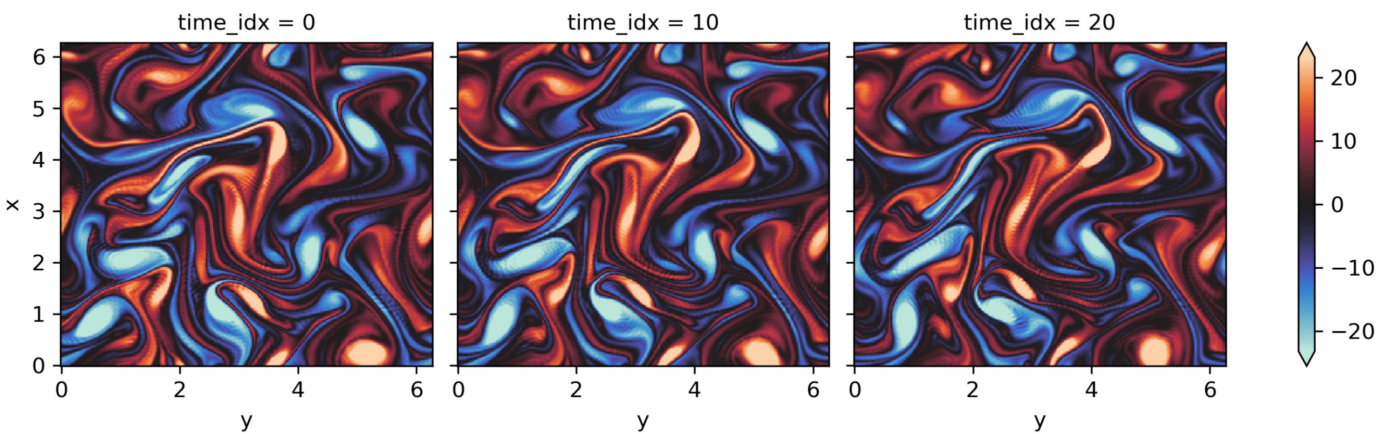
Full order model in semi-discrete form:

$$\frac{d\,\boldsymbol{u}(t)}{d\,t} = \boldsymbol{R}\big(\boldsymbol{u}(t)\big) \qquad \boldsymbol{u}(0) = \boldsymbol{u}_0$$

$$\boldsymbol{u} \in \mathbb{R}^N \qquad \boldsymbol{R}: \mathbb{R}^N \to \mathbb{R}^N$$

For Navier-Stokes equations represented on a discrete grid with grid point i:

$$\boldsymbol{u}_i = \left(\boldsymbol{v}, \rho, e, Y_{\boldsymbol{1}\ldots\boldsymbol{N_s}}\right)_i$$

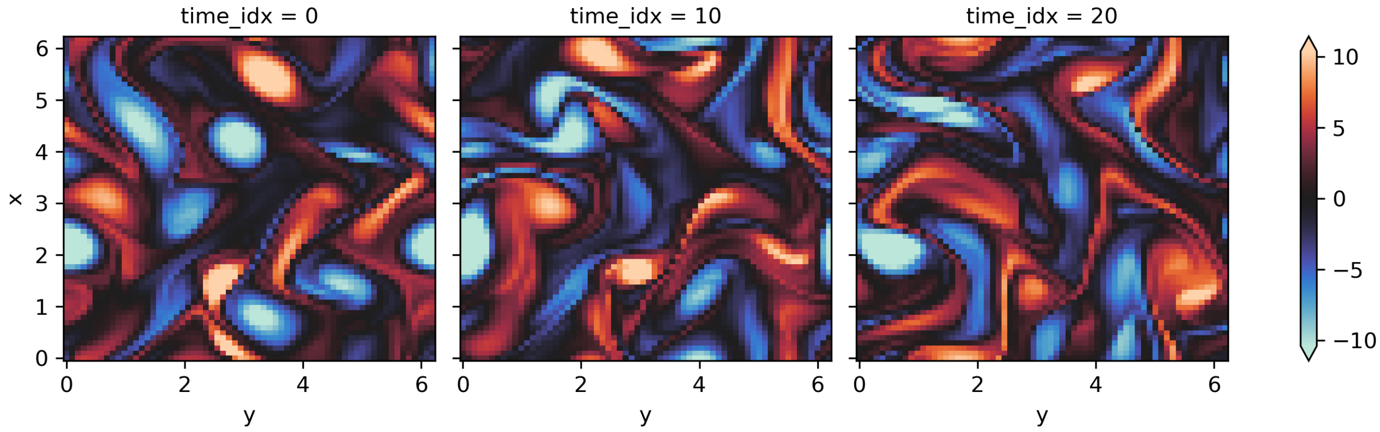


To reduce the dimensionality of the problem, define a reduced set of "observables."

Let $\boldsymbol{g}(\boldsymbol{u}(\boldsymbol{u}_0, t)), \boldsymbol{g}: \mathbb{R}^N \rightarrow \mathbb{R}^D$, D<M, be a set of observables at time t.

For example:

$$\frac{d}{dt}\boldsymbol{u} = \boldsymbol{R}(\boldsymbol{u}), \boldsymbol{u} \in \mathbb{R}^N \xrightarrow[\mathbb{R}^N \text{ to } \mathbb{R}^D,\, D \ll N]{\text{Coarse-graining}} \frac{d}{dt}\boldsymbol{g} \approx \underbrace{\widehat{\boldsymbol{R}}(\boldsymbol{g})}_{\text{Resolved}} + \underbrace{model(\boldsymbol{g})}_{\text{Under-resolved}}, \boldsymbol{g} \in \mathbb{R}^D$$



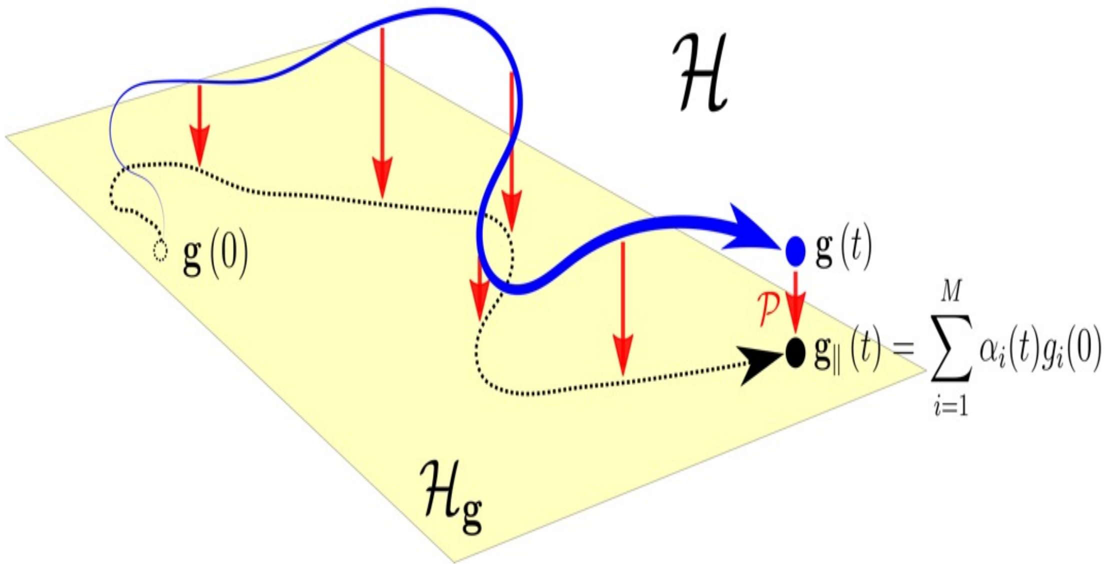
Mori-Zwanzig formalism, first introduced in statistical mechanics, can be expressed as an exact framework for reduced order models.

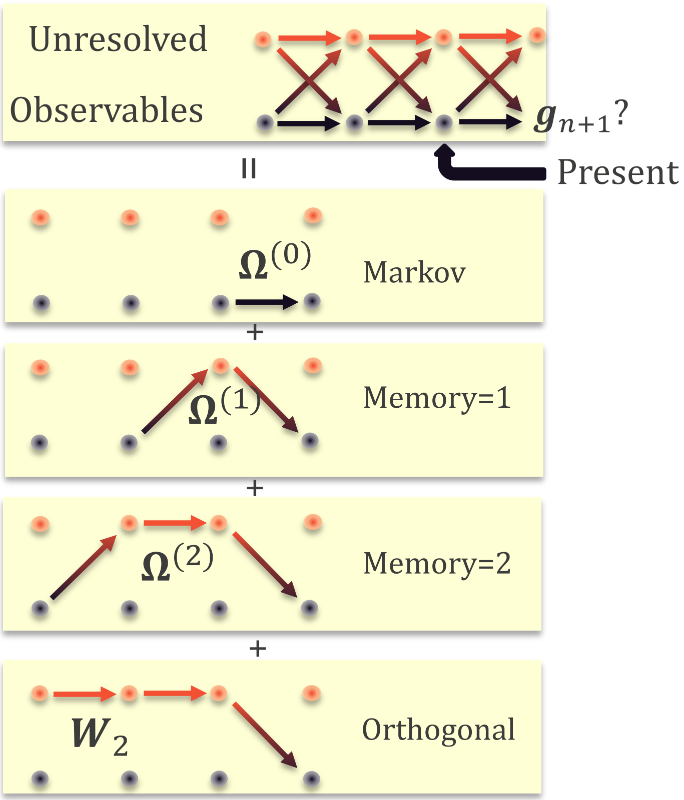
- **[Mori65] and [Zwanzig73] show that the evolution of coarse-grained/resolved observables satisfies the Generalized Langevin Equation (GLE):**

$$\frac{d}{dt}\boldsymbol{g}(\boldsymbol{u}_0,t) = \underbrace{\boldsymbol{M}(\boldsymbol{g}(\boldsymbol{u}_0,t))}_{\text{Markovian term}} - \int_0^t \underbrace{\boldsymbol{K}(\boldsymbol{g}(\boldsymbol{u}_0,t-s),s)ds}_{\text{Memory kernel}} + \underbrace{F(\boldsymbol{u}_0,t)}_{\text{Orthogonal dynamics}}$$

- To define the MZ operators, need to introduce a projection operator $\boldsymbol{P}$ that maps the full space N onto the reduced space D, i.e. it maps functions f: $\mathbb{R}^N \rightarrow \mathbb{R}^N$ onto the subspace $Span\{g_1(u_0) \ldots . g_D(u_0)\}$.
- Using $\boldsymbol{P}$, the operators $\boldsymbol{M}$, $\boldsymbol{K}$ and $\boldsymbol{F}$ can be expressed based on the initial system, e.g. $\boldsymbol{M} = [\boldsymbol{PR}](\boldsymbol{u}(\boldsymbol{u}_0,t))$.
- Orthogonal dynamics and memory kernel are related through Generalized Fluctuation-Dissipation (GFD) relation.
- Discrete version (Lin, Tian, Livescu, Anghel 2021): $\boldsymbol{g}_{n+1} = \sum_{l=0}^{n} \boldsymbol{\Omega}^{(l)}(\boldsymbol{g}_{n-l}) + \boldsymbol{W}_n$

Mori-Zwanzig formalism has an intuitive geometrical representation.





Mori-Zwanzig formalism is a generalization of the Dynamic Mode Decomposition (Lin, Tian, Livescu, Anghel SIADS 2021).

- If the inner product on full space is used to define the projection operator as

$$\boldsymbol{P} f\big(\boldsymbol{g}(\boldsymbol{u}_0)\big) \equiv \sum_{i,j=1}^{D} < f, g_i > [\boldsymbol{C}_0^{-1}]_{ij} g_j(u_0),$$

where $\boldsymbol{C}_0^{-1}$ is the inverse of the covariance matrix $< g_i, g_j >$ (Mori's finite rank projection), then the GLE becomes linear:

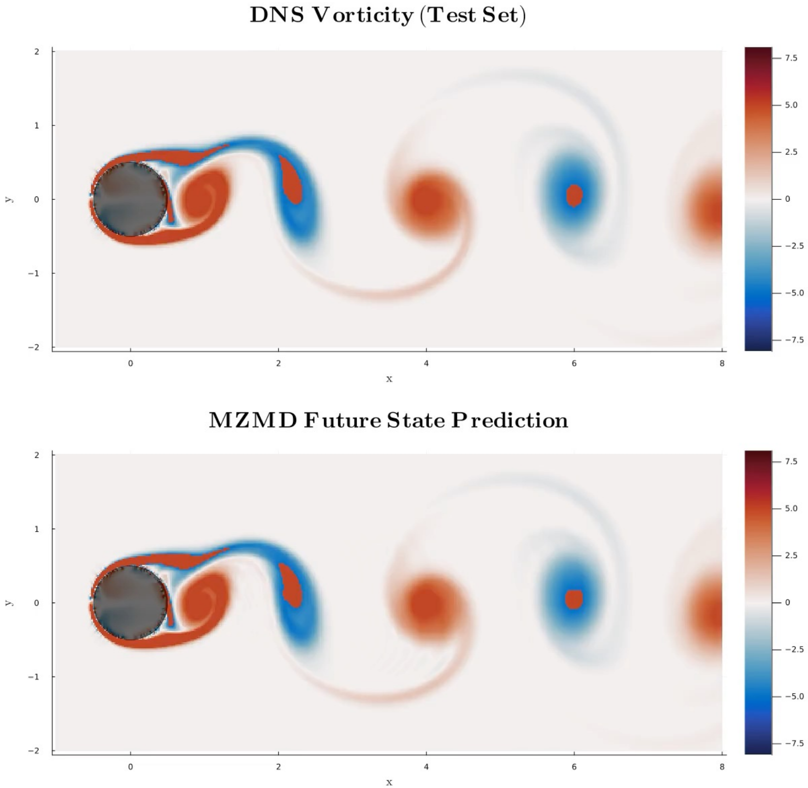
$$\frac{d}{dt} g_i(\boldsymbol{u}_0, t) = \sum_{j=1}^{D} [\boldsymbol{M}]_{ij} g_j(\boldsymbol{u}_0, t) - \int_0^t \sum_{j=1}^{D} [\boldsymbol{K}(t-s)]_{ij} g_j(\boldsymbol{u}_0, t)\, ds + F(\boldsymbol{u}_0, t)$$

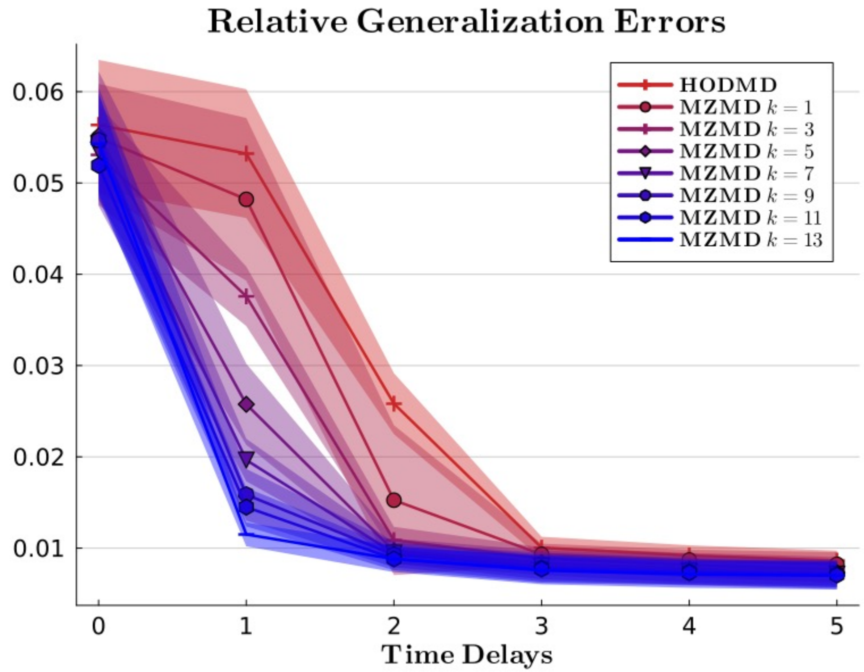
- **Generalized Fluctuation-Dissipation (GFD) relation:** $\boldsymbol{K}(s) = -< \boldsymbol{F}(s), \boldsymbol{F}(0)^T > \boldsymbol{C}_0^{-1}$

- Learning $\boldsymbol{M}$ and $\boldsymbol{K}$ becomes a convex problem in the Koopman formulation of dynamical systems and we have devised efficient algorithms for learning them based on **GFD** (Lin, Tian, Livescu, Anghel SIADS 2021).

- **Keeping only the Markov term recovers the DMD/EDMD formulation**.

Mori-Zwanzig formalism is also a generalization of Higher Order DMD (HODMD) and can be combined with time delay embedding.





Usual Mori-Zwanzig formalism approaches model the memory kernels, as it is computationally unfeasible to extract them exactly.

- Summary for the discrete representation:

$$\begin{cases} \boldsymbol{g}_{n+1} \triangleq \mathcal{K}_\Delta^n \boldsymbol{g} = \sum_{\ell=0}^{n} \boldsymbol{\Omega}^{(\ell)} \circ \boldsymbol{g}_{n-\ell} + \boldsymbol{W}_n \quad \text{(Generalized Langevin Equation)} \\ \boldsymbol{\Omega}^{(\ell)} \coloneqq \mathcal{P}\mathcal{K}_\Delta[(1-\mathcal{P})\mathcal{K}_\Delta]^l \quad (\ell = 0\text{: Markov, } \ell > 0\text{: memory kernel}) \\ \boldsymbol{W}_n \coloneqq [(1-\mathcal{P})\mathcal{K}_\Delta]^{n+1}(\boldsymbol{g}) \quad (\text{orthogonal dynamics, } \mathcal{P}\boldsymbol{W}_n = 0) \end{cases}$$

Here, $\mathcal{K}_\Delta$ is the Koopman transfer operator, i.e. $\frac{d}{dt}\phi = R(\phi) \Rightarrow \boldsymbol{g}_{n+1} = \mathcal{K}_\Delta \boldsymbol{g}_n$

We have derived computationally efficient recursive relations (using the GFD relation) to extract the *operators* $\boldsymbol{\Omega}^0, \boldsymbol{\Omega}^{(\boldsymbol{1})}, \ldots, \boldsymbol{\Omega}^{(\boldsymbol{n})}$:

- For Mori's linear projection in Lin, Tian, Livescu, Anghel SIADS 2021.
- Reformulating the projection as nonlinear regression (with various regression bases, including spline and CNNs) in Lin, Tian, Perez, Livescu SIADS 2023.

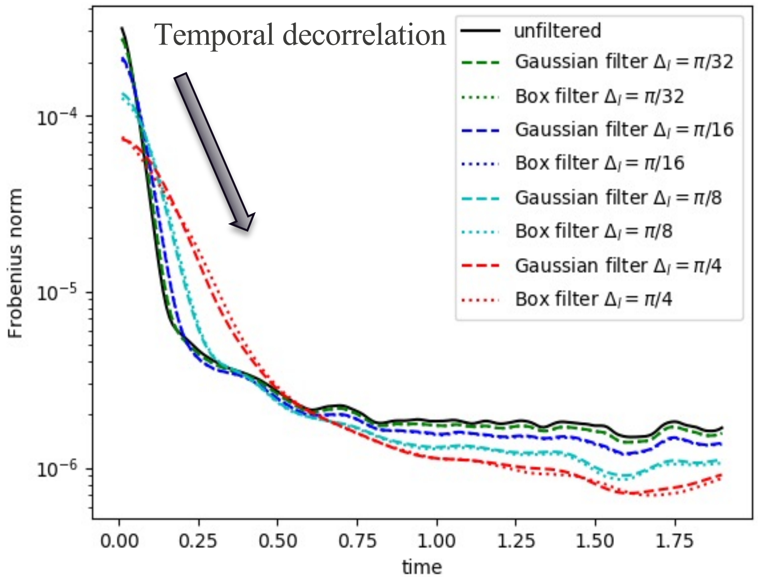
We first applied the Mori-Zwanzig decomposition to isotropic turbulence (Tian, Lin, Anghel, Livescu POF 2021).

- Direct Numerical Simulation of incompressible N-S equation on a 128x128x128 mesh, with Taylor Reynolds number ≈100.
- A long trajectory (1000 integral time scales) of 3D Snapshots (approx. 100,000) with small time interval $\mathrm{d}t$ ≈ 10*Kolmogorov timescale are used for learning
- Coarse-graining is performed by applying a filter (Gaussian/Box) to the chosen observable with various filter sizes Δ_l, and then coarsely sampled on a 4x4x4 grid.
- Rotational invariance and translation invariance are implemented to impose symmetries on the learned kernel, and thus reduce the samples size for statistical convergence.
- Different types of observables are selected based on physical intuition and governing equation.

First data-driven extraction of memory kernel of homogeneous isotropic turbulence shows that memory length is finite!

Effects of spatial filters on the memory kernel

- Two filter types: Gaussian, box
- Various filtering length scale Δ_l



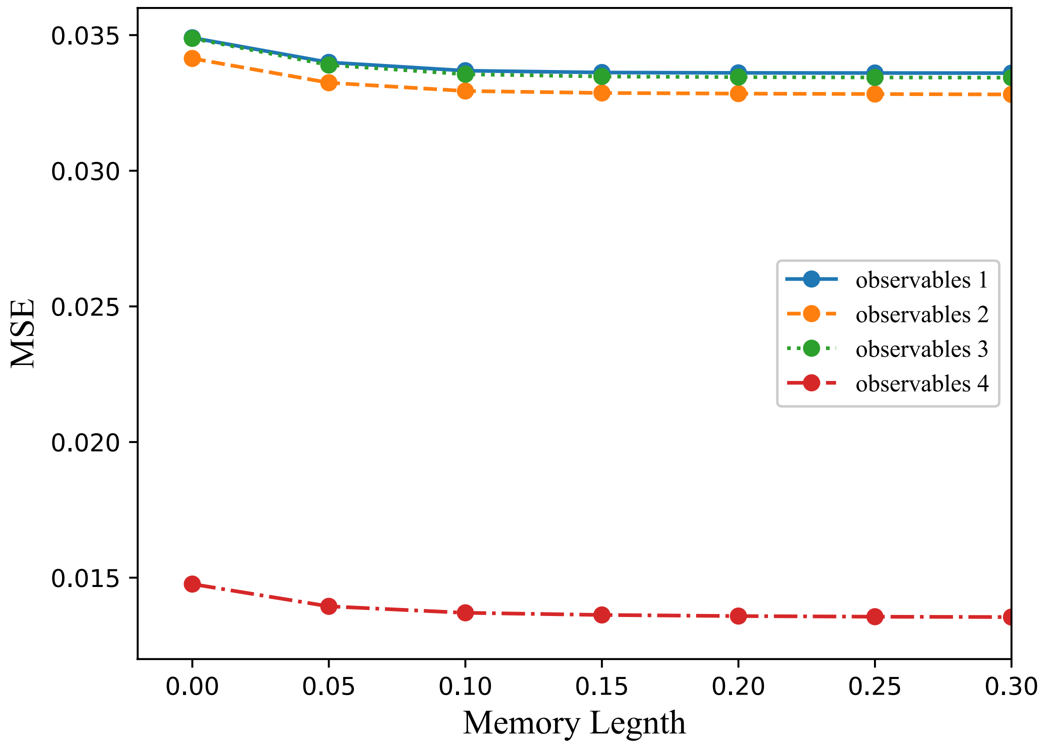
- Finite memory length: memory kernel norm drops to 1% within 10% of the integral time scale.
- The filter type does not affect the memory kernel significantly.
- As the filter size increases, the memory length also increases.

Finding the optimal observables that represent the dominant/slow dynamics of a nonlinear system is an important topic in MZ learning.

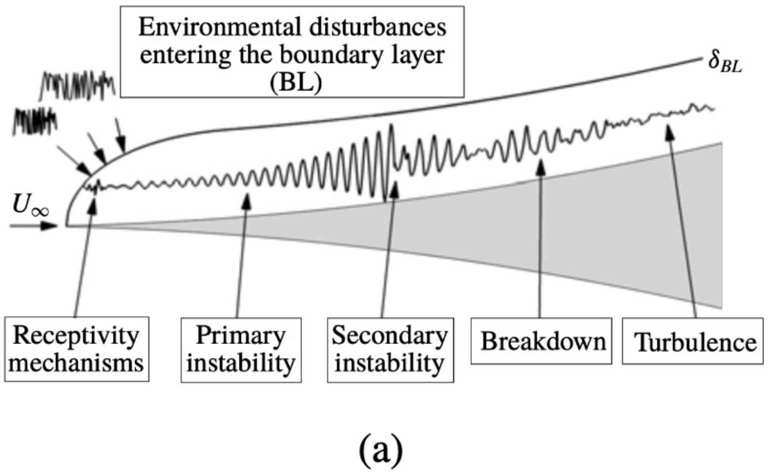
The types of observables considered:

- **Observables set 1:** $\tilde{u}$, $\tilde{v}$, $\tilde{w}$
- **Observables set 2 (moment closure): 1,** $\tilde{u}$, $\tilde{v}$, $\tilde{w}$, $\tilde{u}\tilde{u}$, $\tilde{v}\tilde{v}$, $\tilde{w}\tilde{w}$, $\tilde{u}\tilde{v}$, $\tilde{u}\tilde{w}$, $\tilde{v}\tilde{w}$, $\widetilde{uu}$-$\tilde{u}\tilde{u}$, $\widetilde{vv}$-$\tilde{v}\tilde{v}$, $\widetilde{ww}$-$\tilde{w}\tilde{w}$, $\widetilde{uv}$-$\tilde{u}\tilde{v}$, $\widetilde{uw}$-$\tilde{u}\tilde{w}$, $\widetilde{vw}$-$\tilde{v}\tilde{w}$)
- **Observables set 3 (physical intuition): 1,** $\tilde{u}$, $\tilde{v}$, $\tilde{w}$, $\frac{\partial \tilde{u}}{\partial x}, \frac{\partial \tilde{v}}{\partial y}, (\frac{\partial \tilde{w}}{\partial z}), \frac{\partial \tilde{u}}{\partial y}+\frac{\partial \tilde{v}}{\partial x}, \frac{\partial \tilde{u}}{\partial z}+\frac{\partial \tilde{w}}{\partial x}, \frac{\partial \tilde{v}}{\partial z}+\frac{\partial \tilde{w}}{\partial y}, \frac{\partial \tilde{u}}{\partial y}-\frac{\partial \tilde{v}}{\partial x}, \frac{\partial \tilde{u}}{\partial z}-\frac{\partial \tilde{w}}{\partial x}, \frac{\partial \tilde{v}}{\partial z}-\frac{\partial \tilde{w}}{\partial y}, \tilde{u}\tilde{u}+\tilde{v}\tilde{v}+\tilde{w}\tilde{w}, S_{ij}S_{ij}, W_{ij}W_{ij}$
- **Observables set 4 (direct equation): 1,** $\tilde{u}$, $\tilde{v}$, $\tilde{w}$, $\frac{\partial \widetilde{uu}}{\partial x}, \frac{\partial \widetilde{vv}}{\partial y}, \frac{\partial \widetilde{ww}}{\partial z}, \frac{\partial \widetilde{uv}}{\partial x}, \frac{\partial \widetilde{uv}}{\partial y}, \frac{\partial \widetilde{uw}}{\partial x}, \frac{\partial \widetilde{uw}}{\partial z}, \frac{\partial \widetilde{vw}}{\partial y}, \frac{\partial \widetilde{vw}}{\partial z}, \frac{\partial \tilde{P}}{\partial x}, \frac{\partial \tilde{P}}{\partial y}, \frac{\partial \tilde{P}}{\partial z}$

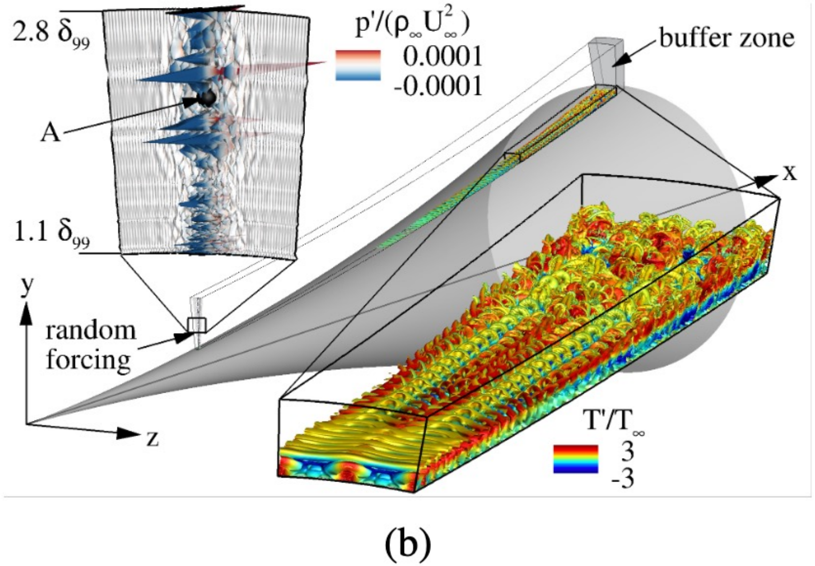
Including memory effects and using appropriate observables can significantly decrease prediction error!



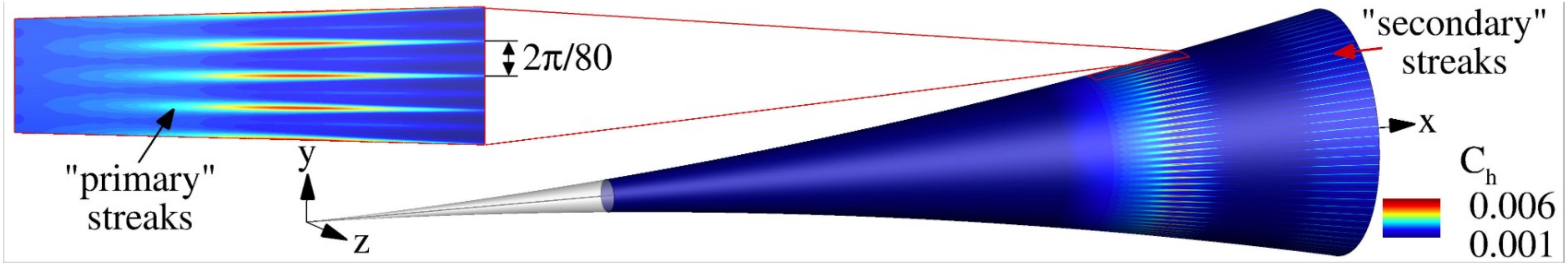
Currently applying the approach to better understand and control boundary layer transition for hypersonic flight (Woodward et al 2023).



(a)



(b)



[C. Hader, H. Fasel JFM 2019]

We introduce Mori-Zwanzig Mode Decomposition, as a generalization of Dynamic Mode Decomposition.

- Full state GLE: $\boldsymbol{x}_{n+1} = \boldsymbol{\Omega}_0^{(x)} \cdot \boldsymbol{x}_n + \ldots + \boldsymbol{\Omega}_k^{(x)} \cdot \boldsymbol{x}_{n-k},$

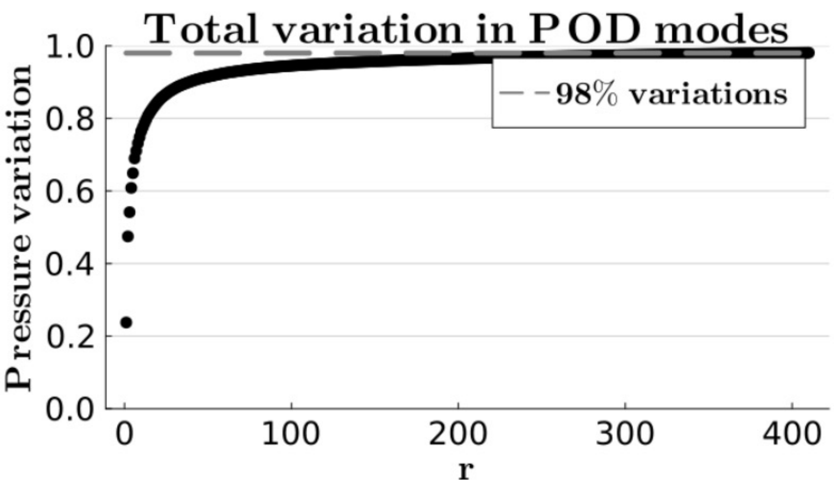
as a model for: $\boldsymbol{x}_{n+1} = \boldsymbol{F}(\boldsymbol{x}_n), \quad \boldsymbol{x}(0) = \boldsymbol{x}_0,$

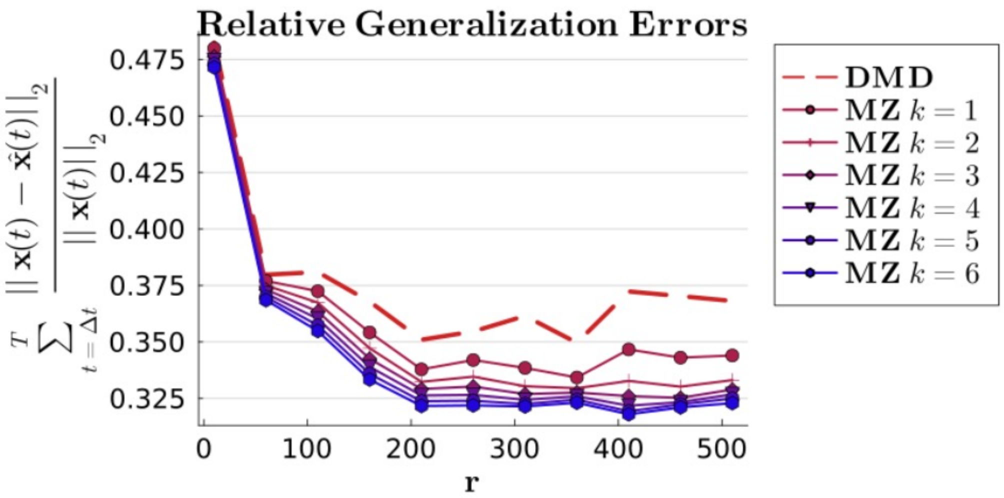
- Apply SVD to full snapshot time data: $\boldsymbol{X} = [\boldsymbol{x}_0, \ldots, \boldsymbol{x}_\tau] \approx \boldsymbol{U}_r \boldsymbol{\Sigma}_r \boldsymbol{V}_r^*$
- Define observables using a reduced set of POD modes as: $\boldsymbol{g} = \boldsymbol{U}_r^* \boldsymbol{X}$
- Reduced GLE: $\boldsymbol{g}_{n+1} = \boldsymbol{\Omega}_0^{(g)} \cdot \boldsymbol{g}_n + \ldots + \boldsymbol{\Omega}_k^{(g)} \cdot \boldsymbol{g}_{n-k},$

where projected memory kernels are: $\boldsymbol{\Omega}_i^{(g)} = \boldsymbol{U}_r^* \boldsymbol{\Omega}_i^{(x)} \boldsymbol{U}_r$

- The modes can be found from the companion matrix: $\boldsymbol{C}_g = \begin{bmatrix} \boldsymbol{\Omega}_0 & \boldsymbol{\Omega}_1 & \ldots & \boldsymbol{\Omega}_k \\ \boldsymbol{I} & \boldsymbol{0} & \ldots & \boldsymbol{0} \\ & \ddots & & \\ \boldsymbol{0} & \ldots & \boldsymbol{I} & \boldsymbol{0} \end{bmatrix}$

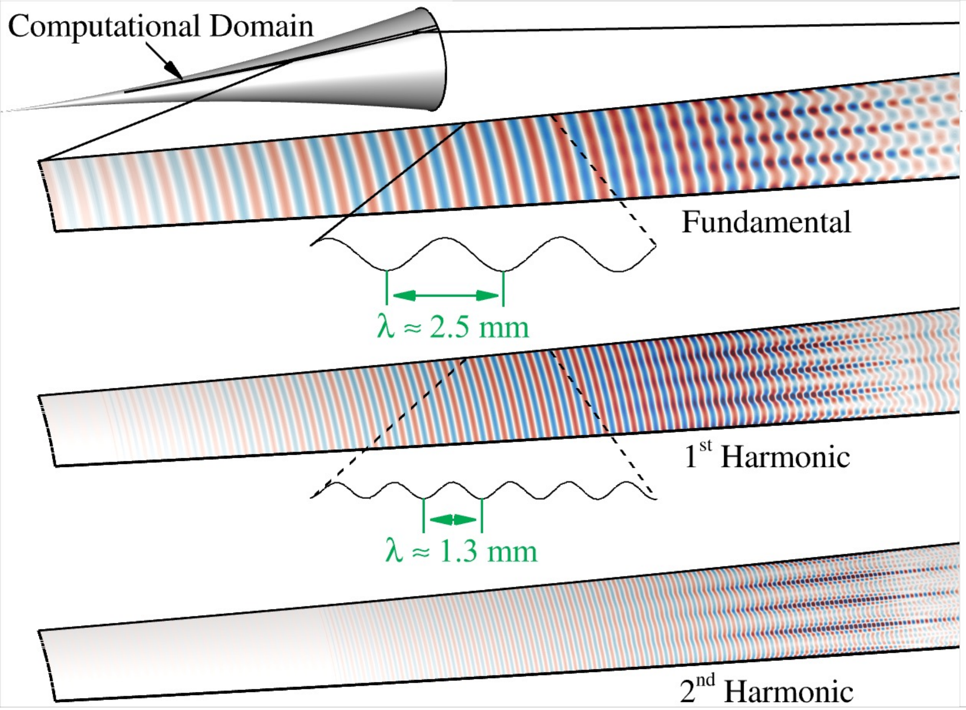
The memory terms in MZMD improve the generalization error over DMD.



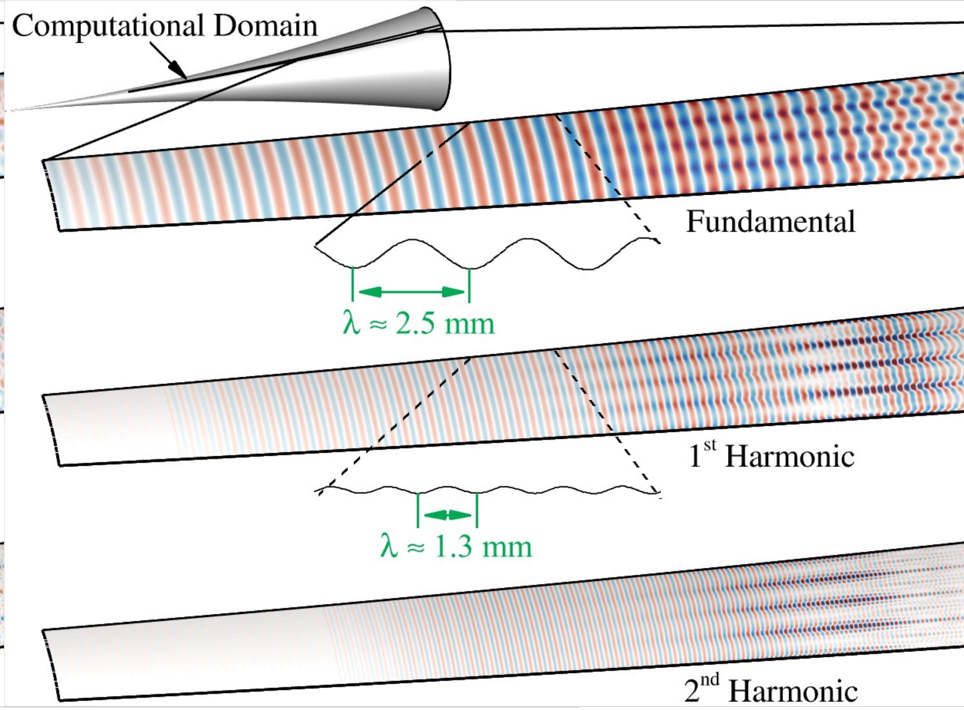


The memory terms in MZMD improve the representation of the primary and secondary modes.

MZMD modes

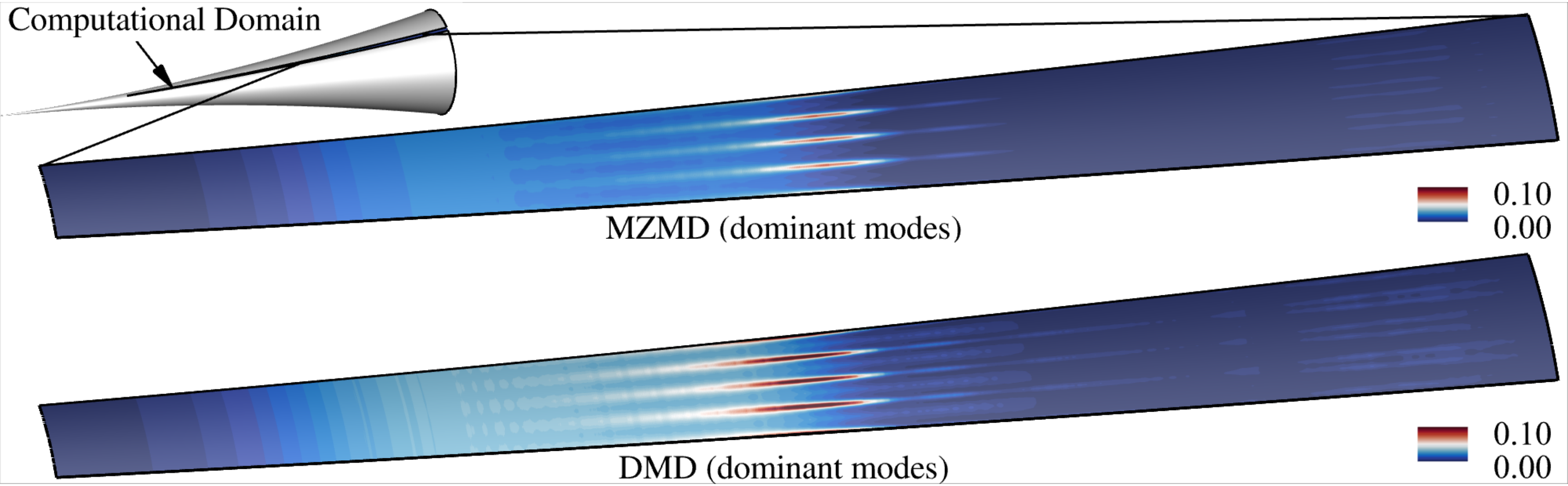


DMD modes



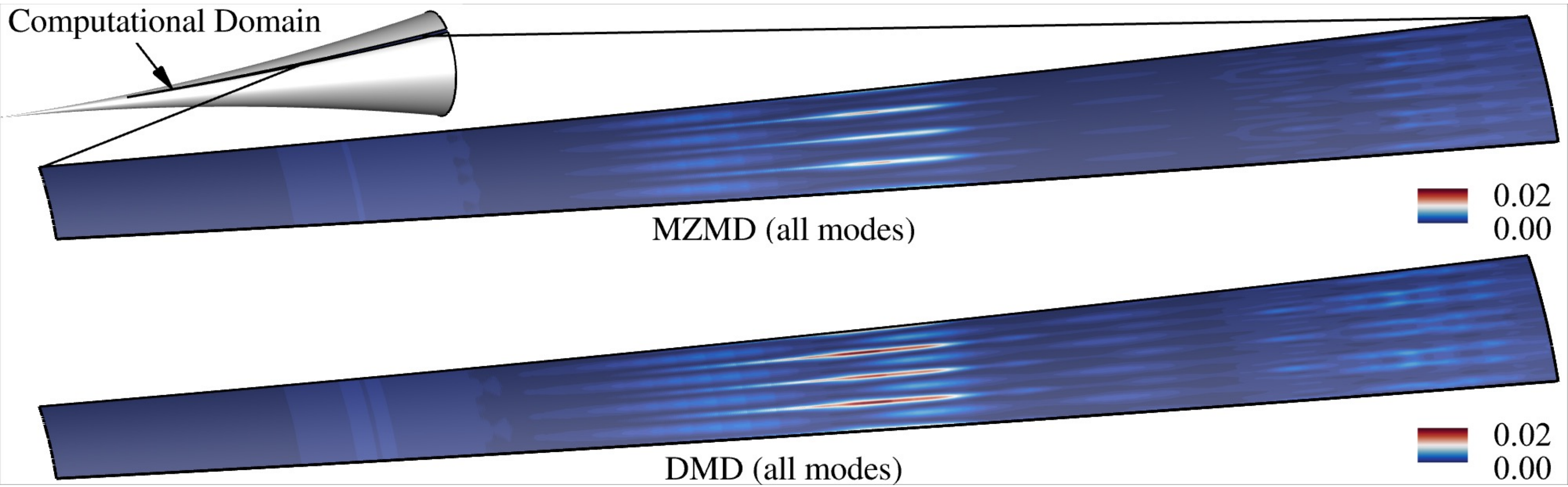
The memory terms in MZMD improve the representation of the primary and secondary modes.

Pointwise relative error over time

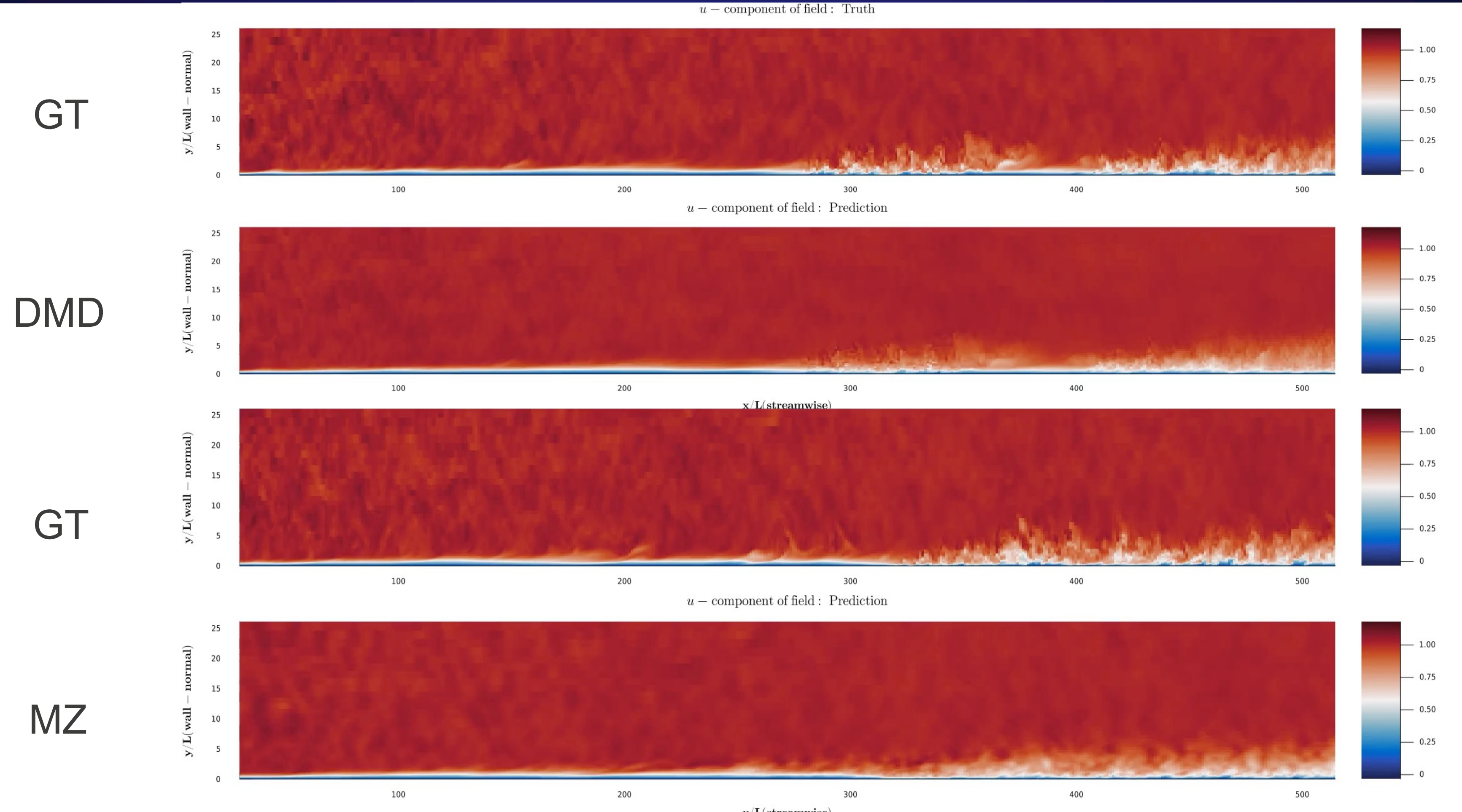


The memory terms in MZMD improve the representation of the primary and secondary modes.

Pointwise relative error over time



By including memory effects, MZ can predict the flow longer than current data driven models (Woodward et al, AIAA 2023)



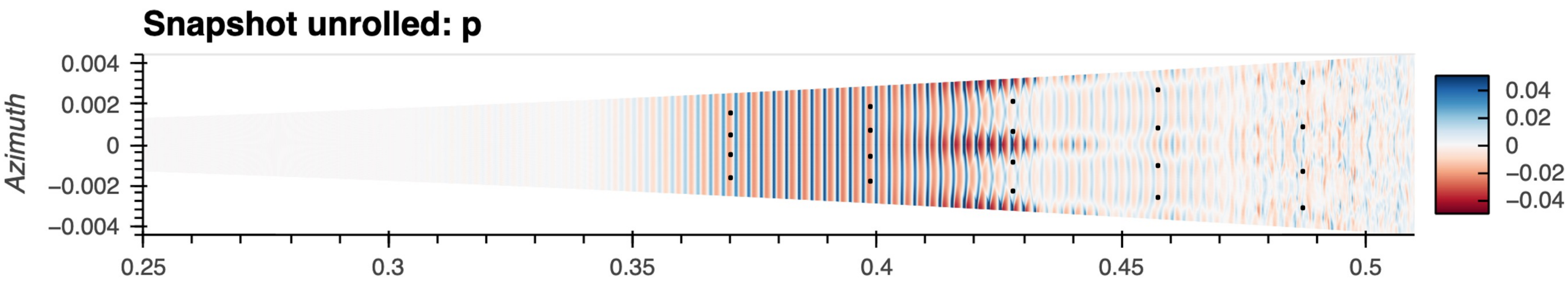
MZMD improves mode representation and prediction compared to DMD with similar compiutational costs.

Memory	$k = 0$	$k = 1$	$k = 2$	$k = 3$	$k = 4$	$k = 5$	$k = 6$
MZMD: Learning (ms)	83.5	112.4	127.1	157.7	198.1	241.0	289.5
MZMD: Future state prediction (s)	2.505	2.502	2.508	2.516	2.525	2.537	2.546

- **Learning**: MZMD only 0.1% more expensive than DMD
- **Prediction**: MZMD only 1% more expensive than DMD
- **Accuracy**: up to 32% relative improvement in accuracy
- **Memory**: easily portable to existing DMD code
- **GFD**: Enforces generalized fluctuation dissipation relation

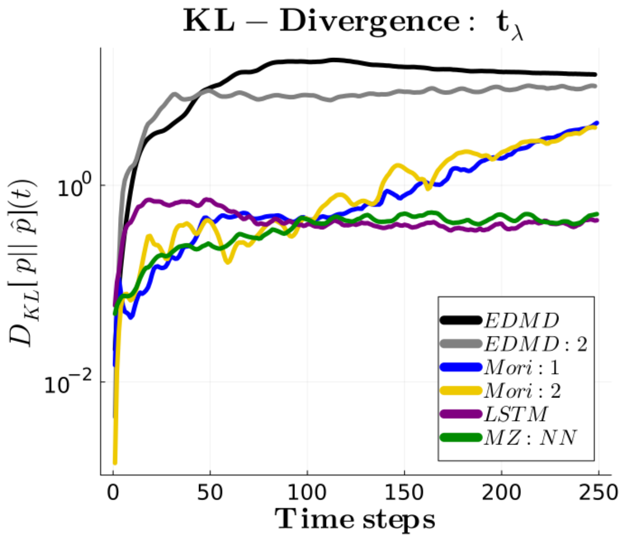
MZ formalism can also be used as ROM for the control problem.

Define the observables as the pressure values at an array of sensors:



- Using regression-based projection allows NNs to be used to learn MZ operators.

- MZ-NN performs best, LSTM similar results (however less formal and interpretable)



Mori-Zwanzig dimensionality reduction for turbulent flows