CD-ROM – Complementary Deep - Reduced Order Model

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CD-ROM

Complementary Deep - Reduced Order Model

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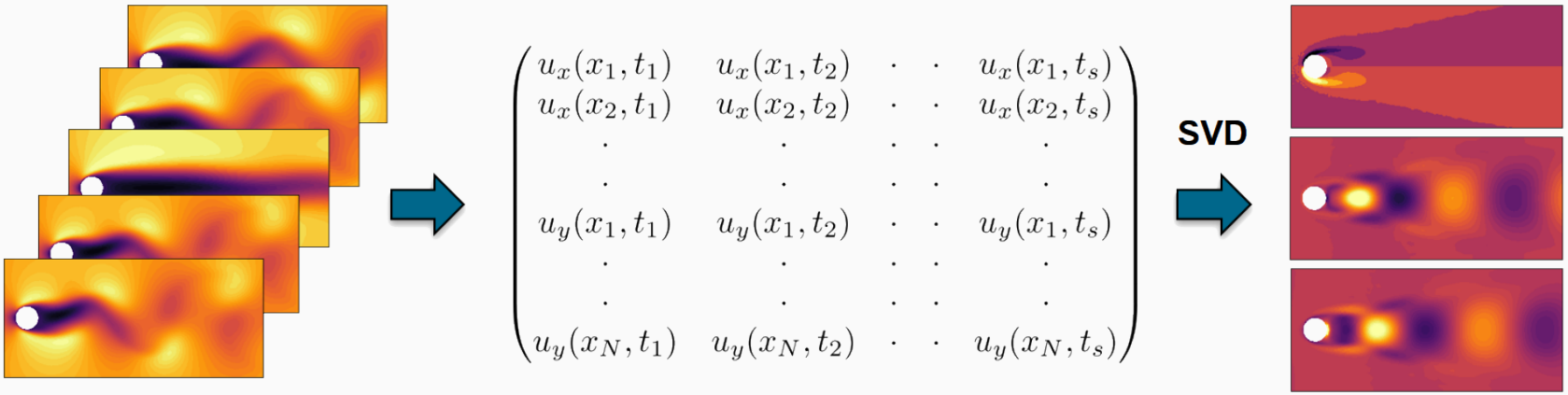
POD

- Proper Orthogonal Decomposition can be used to extract the principal modes (V) from a physical simulation :



- The flow approximates as a linear combination of a reduced number (r) of modes :

$$u(x,t) \approx \bar{u} = V(x)\alpha(t)$$

$$V \in \mathbb{R}^{n_x \times r}, \alpha \in \mathbb{R}^r$$

Galerkin Projection

- An equation for the coefficients of this simplified form is obtained through Galerkin Projection of the original system :

$$\frac{\partial u(x,t)}{\partial t} = g(u(x,t)),\ V^T u = \alpha$$

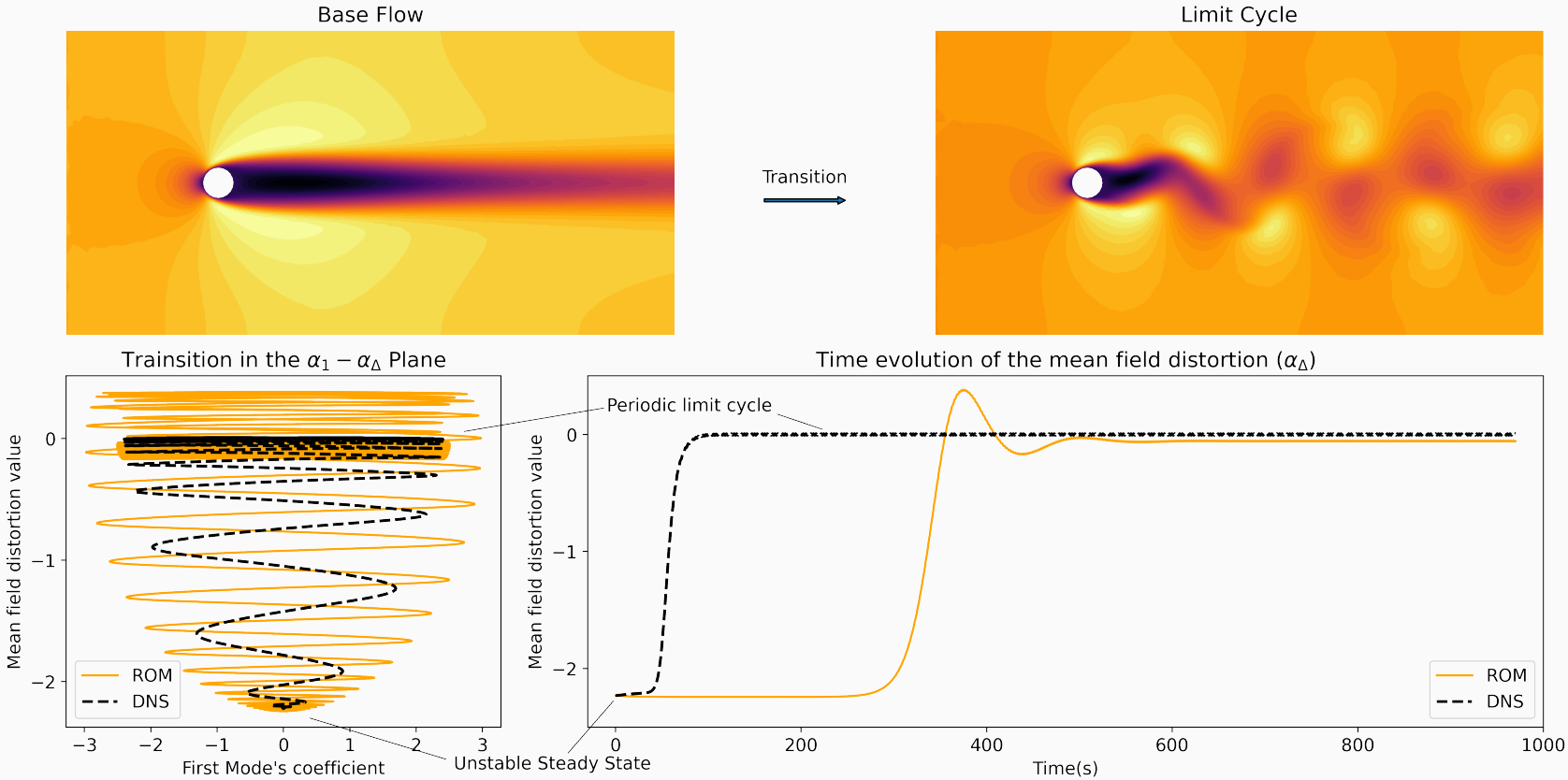
$$\implies \frac{d\alpha}{dt} = V^T g(u(x,t))$$

- The dynamics $g()$ of the reduced model are computed from the approximate solution, which introduces error :

$$\frac{d\alpha}{dt} \approx V^T g(\bar{u}) \neq V^T g(u(x,t))$$

ROM Errors

- In the case of a laminar 2-D cylinder flow, a 3 equation model can be used to capture the transient dynamics[1] :



[1] B. R. Noack et al., "A hierarchy of low-dimensional models for the transient and post-transient cylinder wake", Journal of Fluid Mechanics **497**, 335–363 (2003).

ROM Correction

- To address classical POD-Galerkin model's shortcomings, we propose to add a correction term to their dynamics :

$$\frac{d\alpha}{dt} = V^T g(u) = V^T g(\bar{u}) + f$$

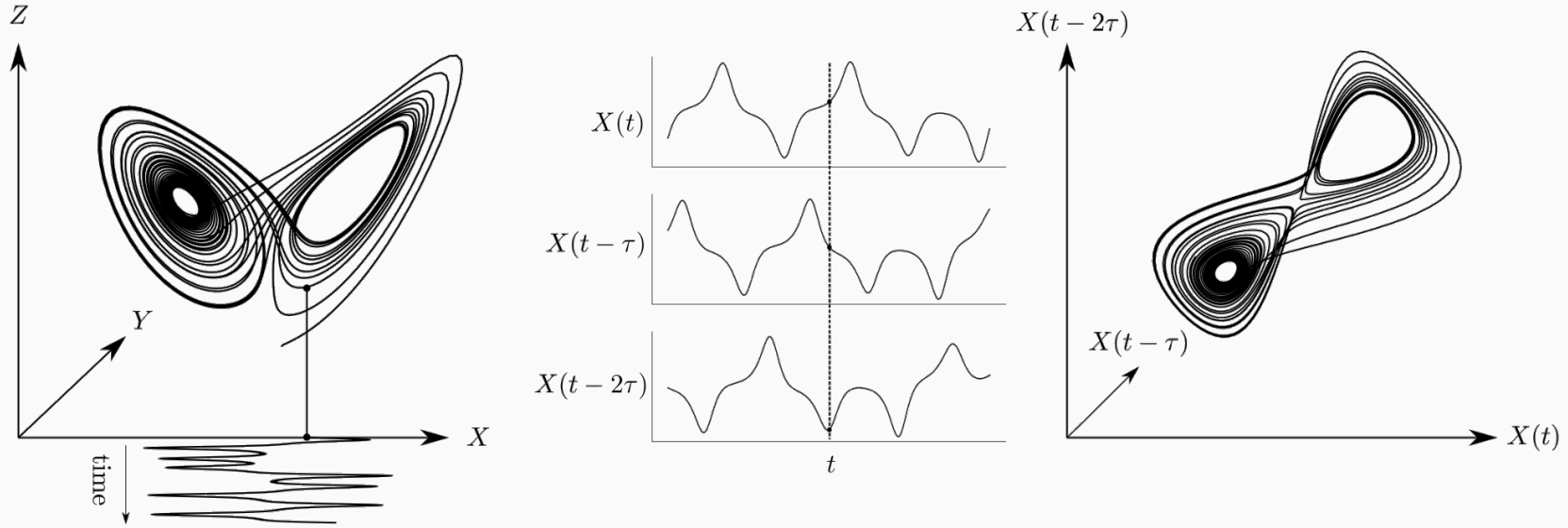
- This correction term depends on information outside of the POD basis:

Corrected ROM:

$$g(u) = g(VV^T u + (I - VV^T)u) \approx g(V\alpha) + g'_{V\alpha}(I - VV^T)u$$

Takens Theorem

- Following Takens's theorem, we can retrieve the information lost during the projection on the POD basis by considering the past states of the system :



DDE

- Delay Differential Equations can be used to aggregate information from the past in a time continuous manner :

$$\frac{dx}{dt} = f(t, x, y), \qquad y(t) = \int_{-\infty}^{t} x(\tau) e^{\lambda(\tau - t)} d\tau, \qquad \lambda \in \mathbb{R}_+$$

- These equations are solved as an augmented ODE system :

$$\begin{matrix} \frac{dx}{dt} \\ \frac{dy}{dt} \end{matrix} = \begin{matrix} f(t, x, y) \\ x - \lambda y \end{matrix}$$

Neural Correction Term

- We use Neural Networks to learn the ROM's correction from the memory y :

$$\begin{matrix} \frac{d\alpha}{dt} \\ \frac{dy}{dt} \end{matrix} = \begin{matrix} V^T g(V\alpha) & + & \mathcal{NN}(y) \\ \alpha & - & \lambda y \end{matrix}$$

- The information available in memory y is limited by its dimension :

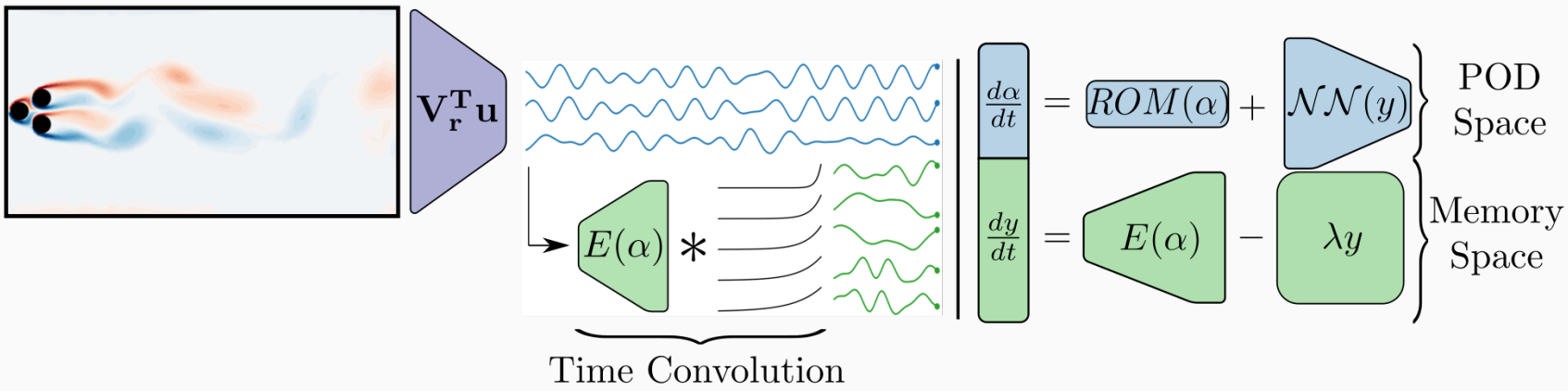
$$y(t) = \int_{-\infty}^{t} \alpha(\tau) e^{\lambda(\tau - t)} d\tau \implies dim(y) = dim(\alpha)$$

Encoders

- To address the bottleneck in the memory, we propose to add an encoder network to expand the dimension of the memory :

$$\begin{matrix} \frac{d\alpha}{dt} \\ \frac{dy}{dt} \end{matrix} = \begin{matrix} V^T g(V\alpha) & + & \mathcal{NN}(y) \\ E(\alpha) & - & \lambda y \end{matrix}$$

- Leading to the final CD-ROM formulation :



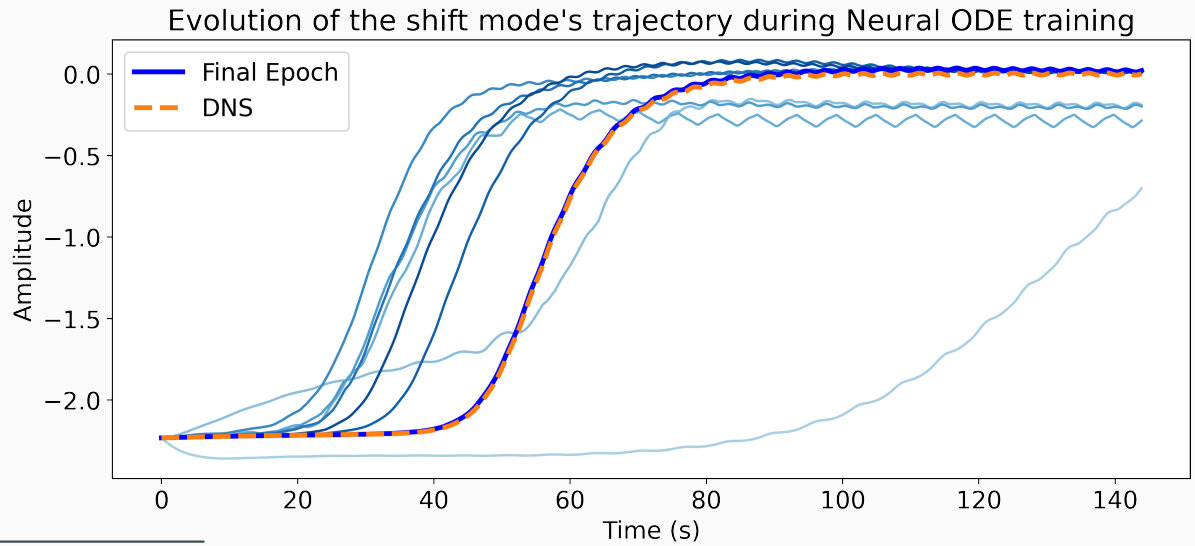
Training Data and Neural ODE

- Training data for the true ROM trajectories can be obtained from the snapshot data :

$$\hat{\alpha}_{t_i} = V^T u_{DNS,t_i}$$

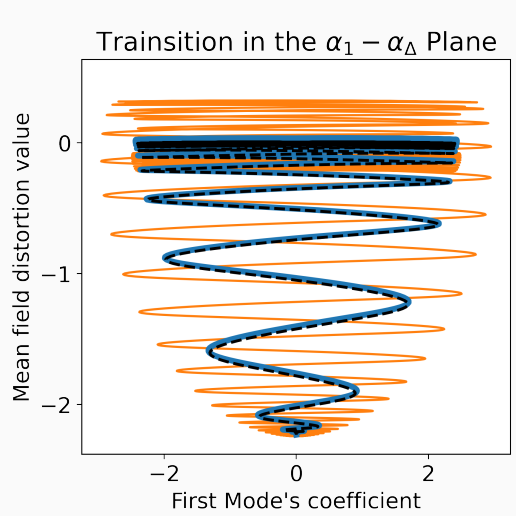
- The model can then be trained through adjoint backpropagation[2] :

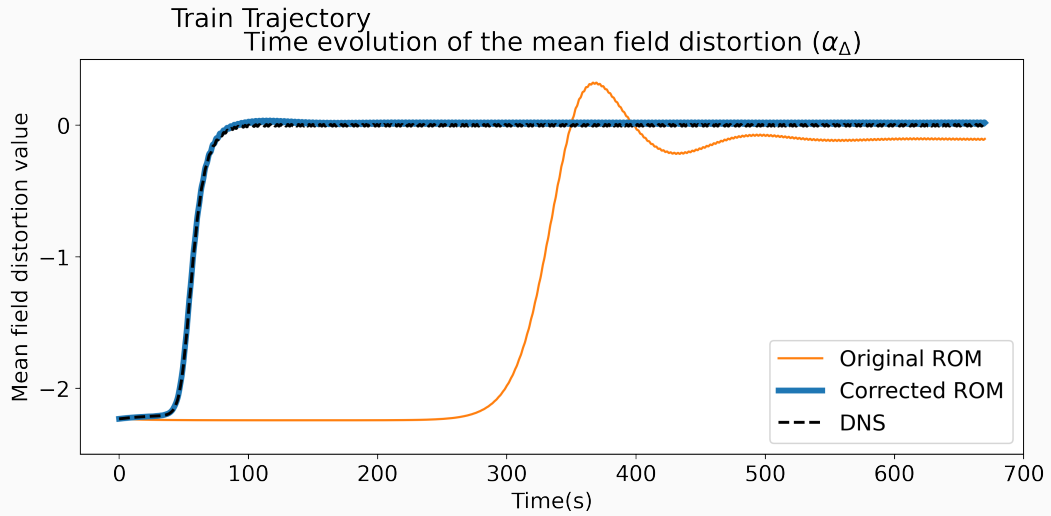
$$\mathcal{L}(\alpha) = \sum_{t_0}^{t_n} \|\alpha_{t_i} - \hat{\alpha}_{t_i}\|_2$$

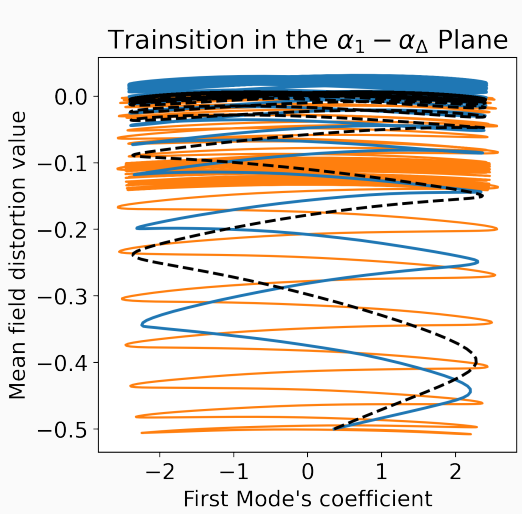


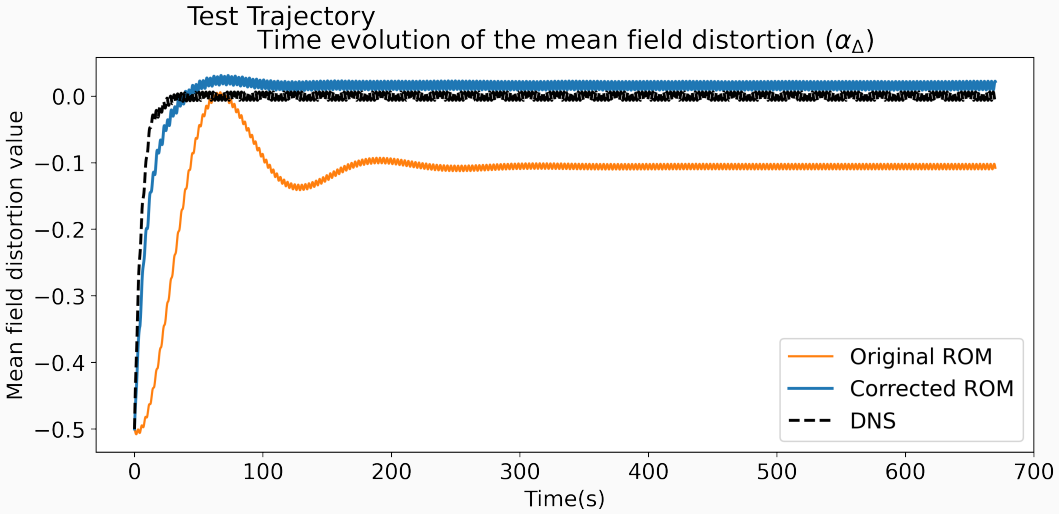
[2] R. T. Q. Chen et al., "Neural ordinary differential equations", (2019).

Cylinder Results



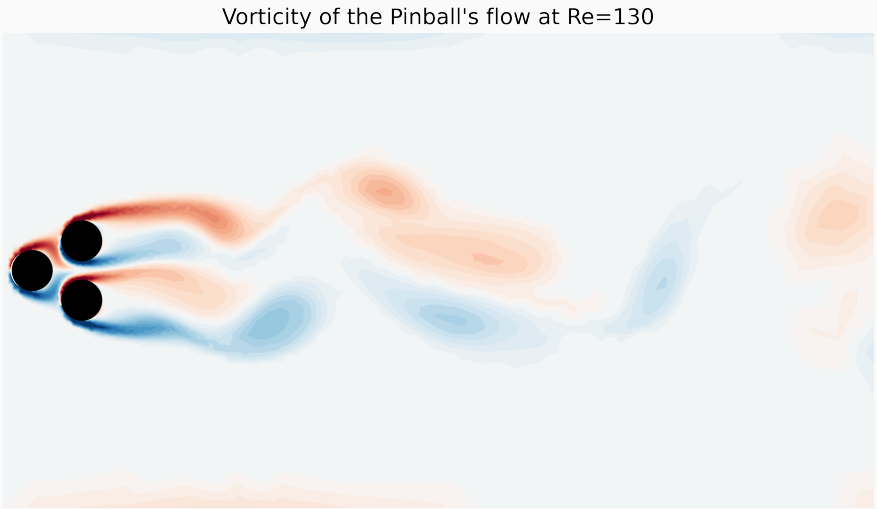


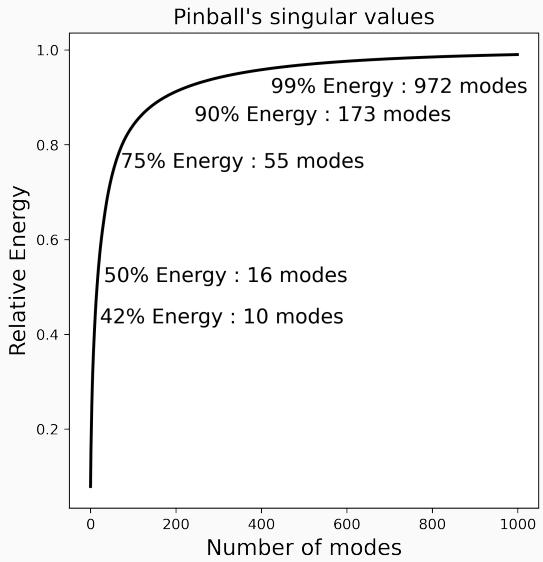




Chaotic Pinball

- We tested the approach on a more challenging case, the chaotic pinball[3]:





- Reminder : 8 modes are enough to capture 99 % of the cylinder flow's energy.

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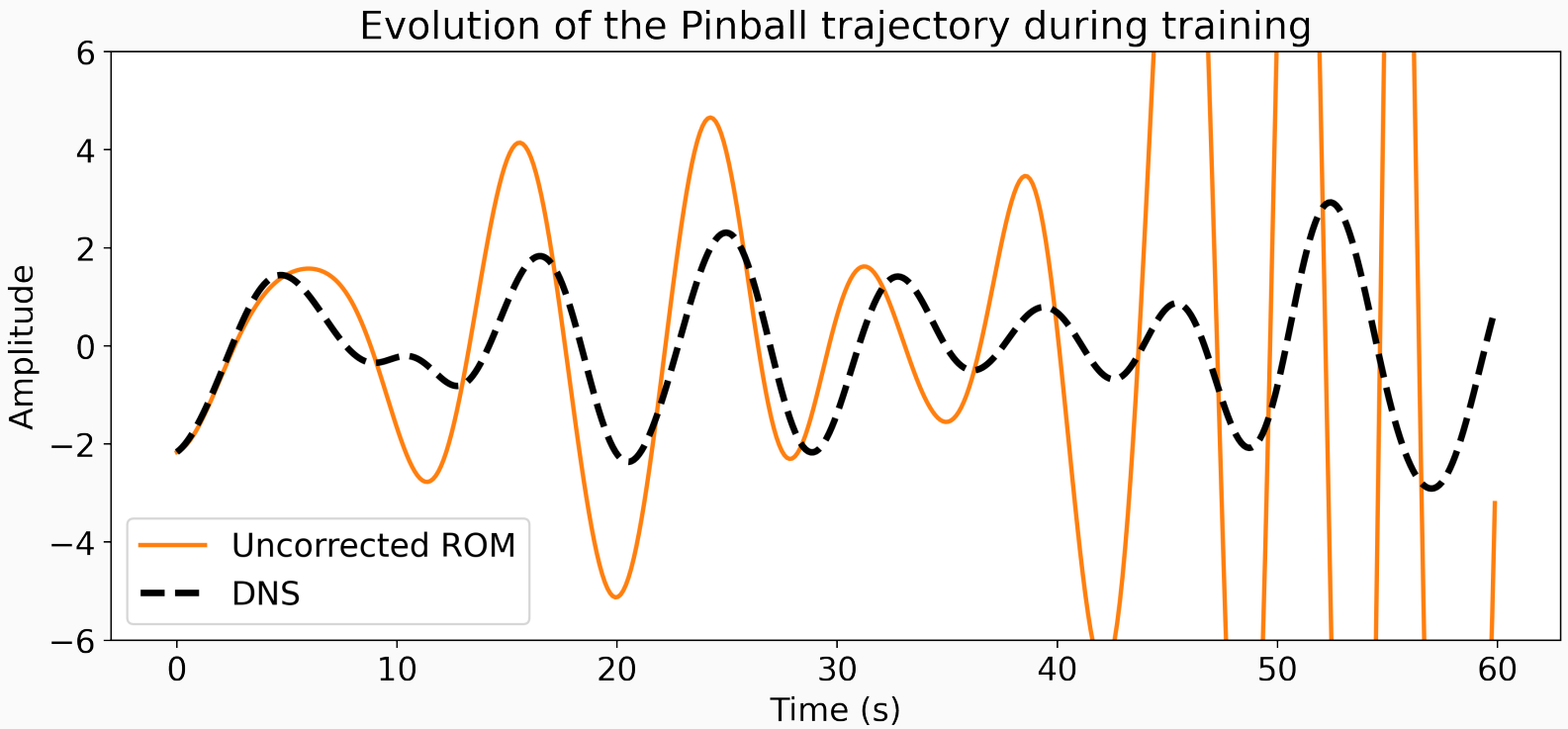
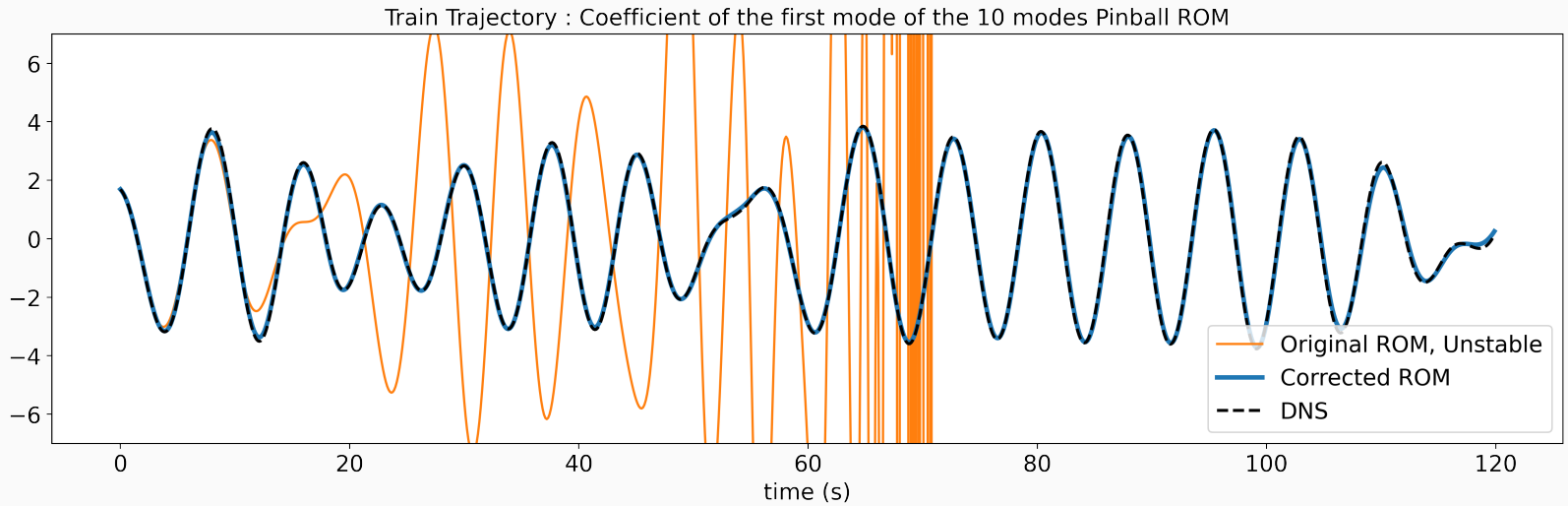
[3] N. Deng et al., "Low-order model for successive bifurcations of the fluidic pinball", Journal of Fluid Mechanics **884**, 10.1017/jfm.2019.959 (2019).

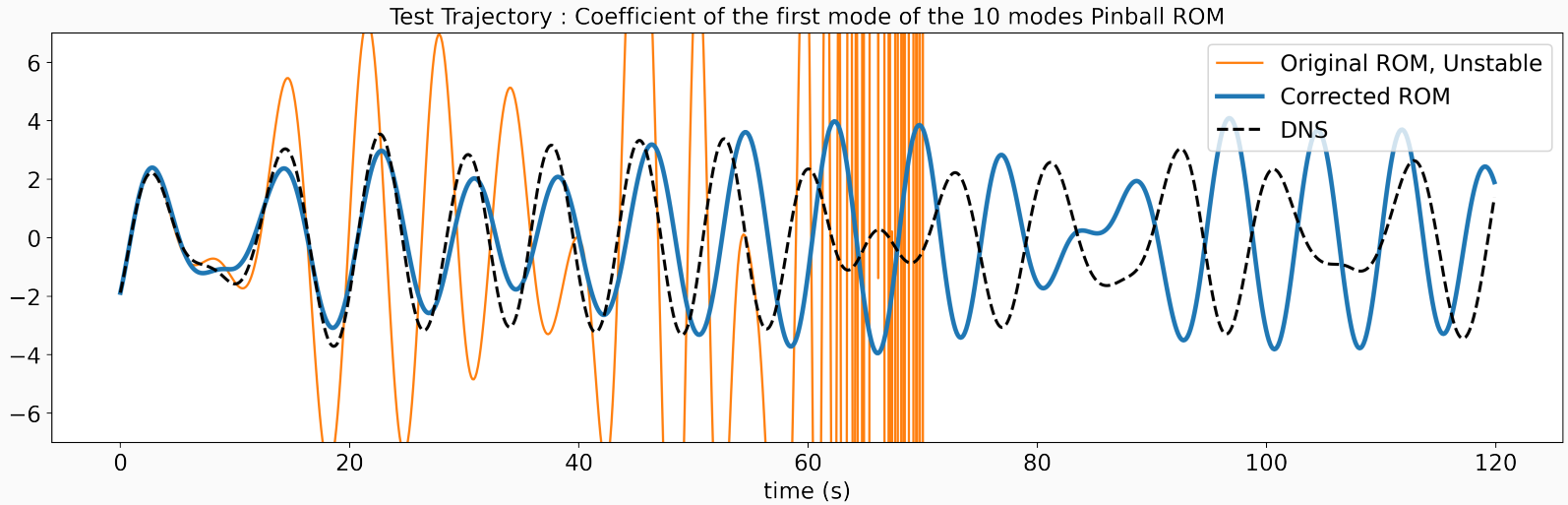
Unstable ROM

- Taking a very reduced number ($r = 10$) of modes for the pinball flow yields a very unstable model.



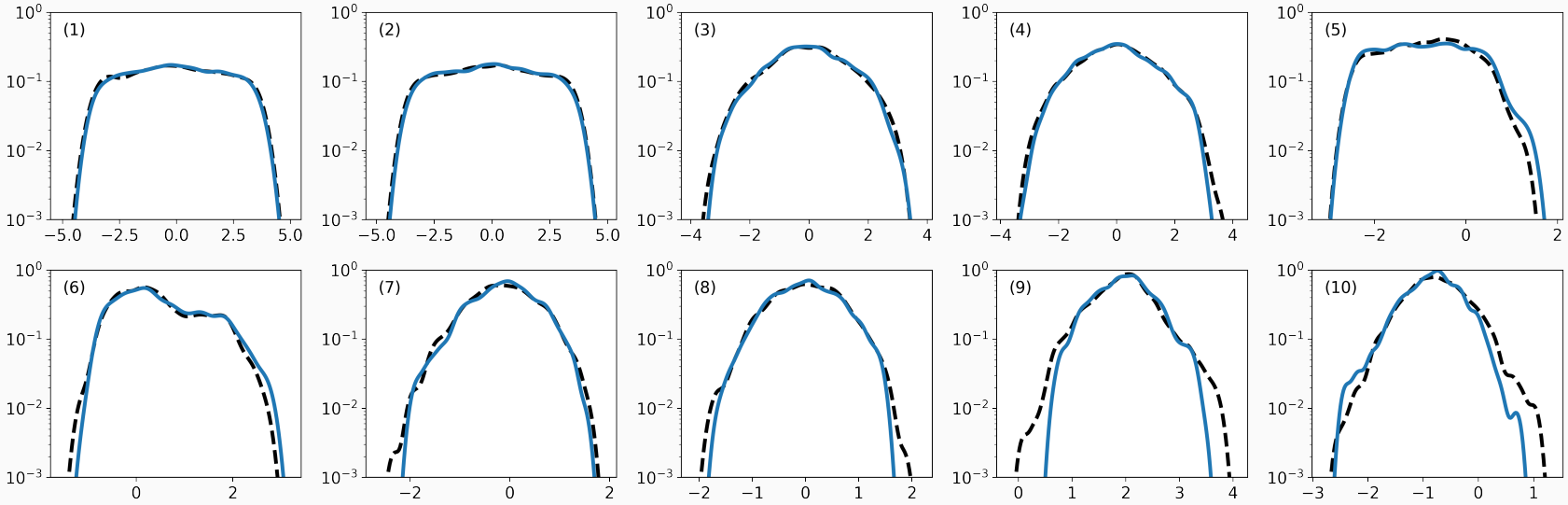
Pinball Results





Attractor Statistics

- The test trajectory presents statistics similar to the original attractor :



Probability density function of the amplitude of each mode over a trajectory of ≈ 1000 seconds. The CD-ROM results are presented in blue while the DNS is in black.

Attractor Statistics

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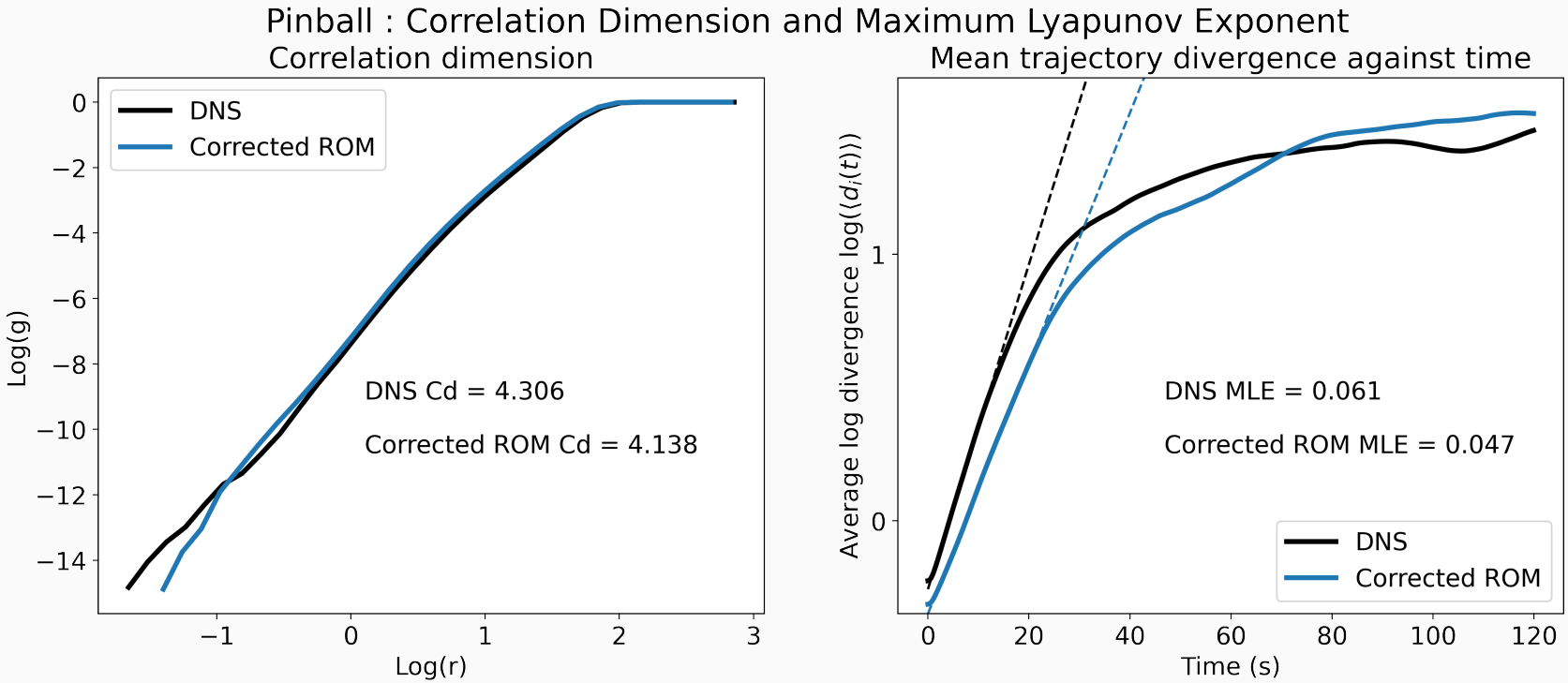


Time Horizons

- We can learn a different λ for each dimension of the memory :

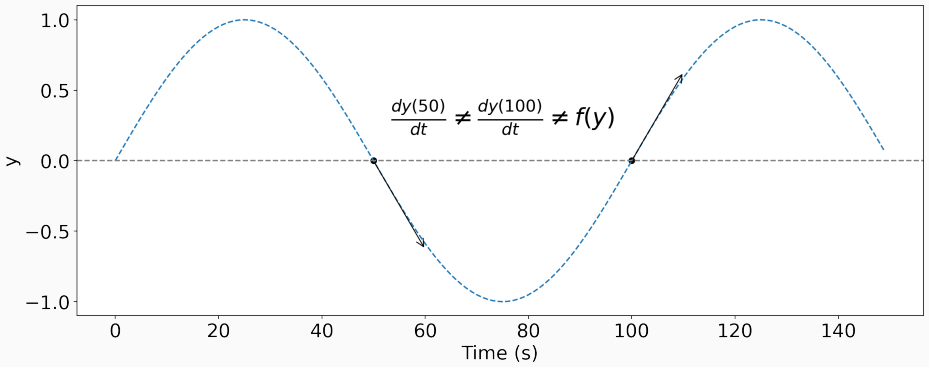
$$y(t) = \int_{-\infty}^{t} E(x(s))e^{\Lambda(s-t)}ds,\ \Lambda = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_N \end{bmatrix},\ N = dim(y)$$

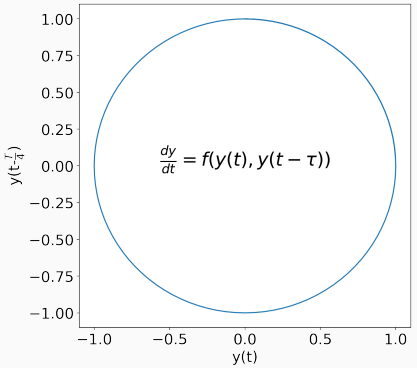
- Each λ_i defines the time horizon of each memory dimension, which can be computed as :

$$\tau_i = \frac{1}{\lambda_i}$$

Synthetic Experiment

- Sine waves are a good test-case to assess the ability of the CD-ROM to learn the time-horizons :

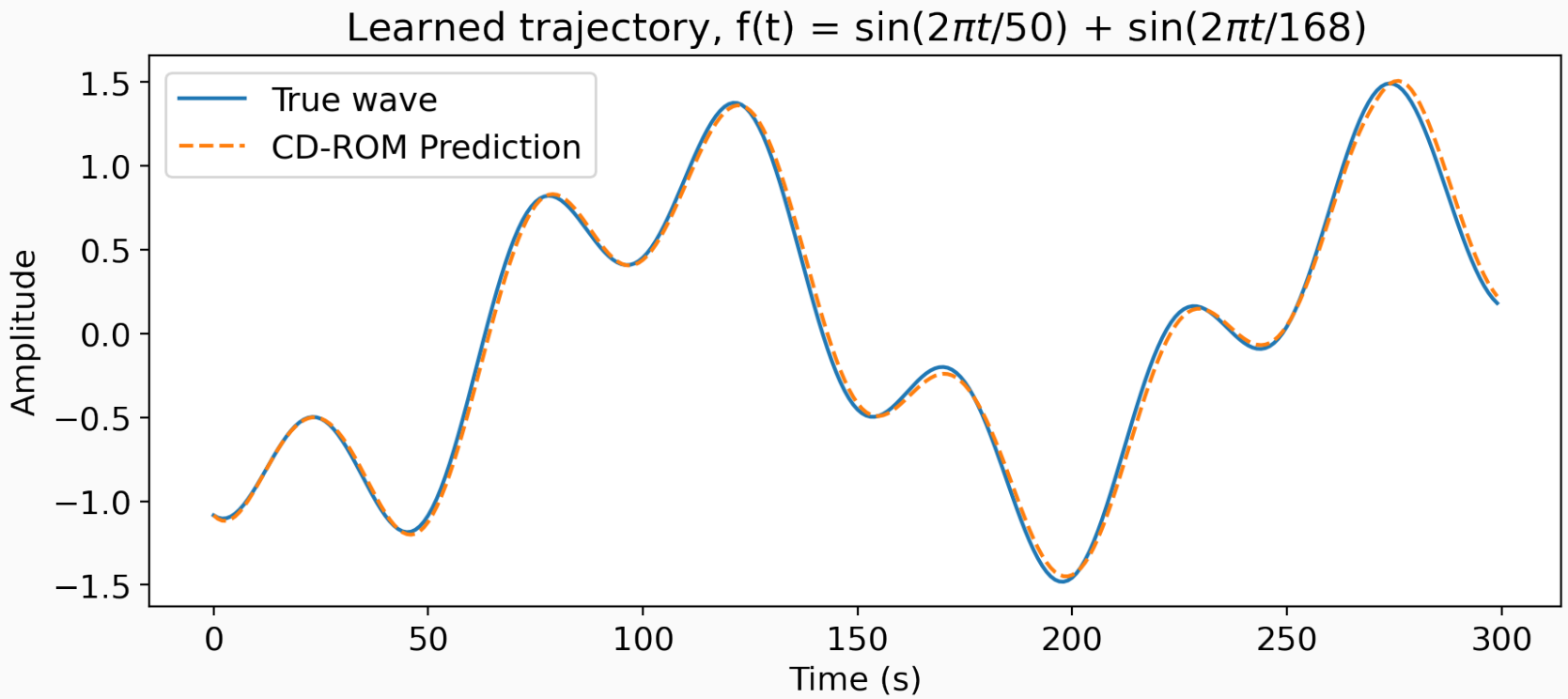




- With a wave of period T, using a delay of $\tau = \frac{T}{4}$ yields a perfect circle in phase space.

Trajectory Fit

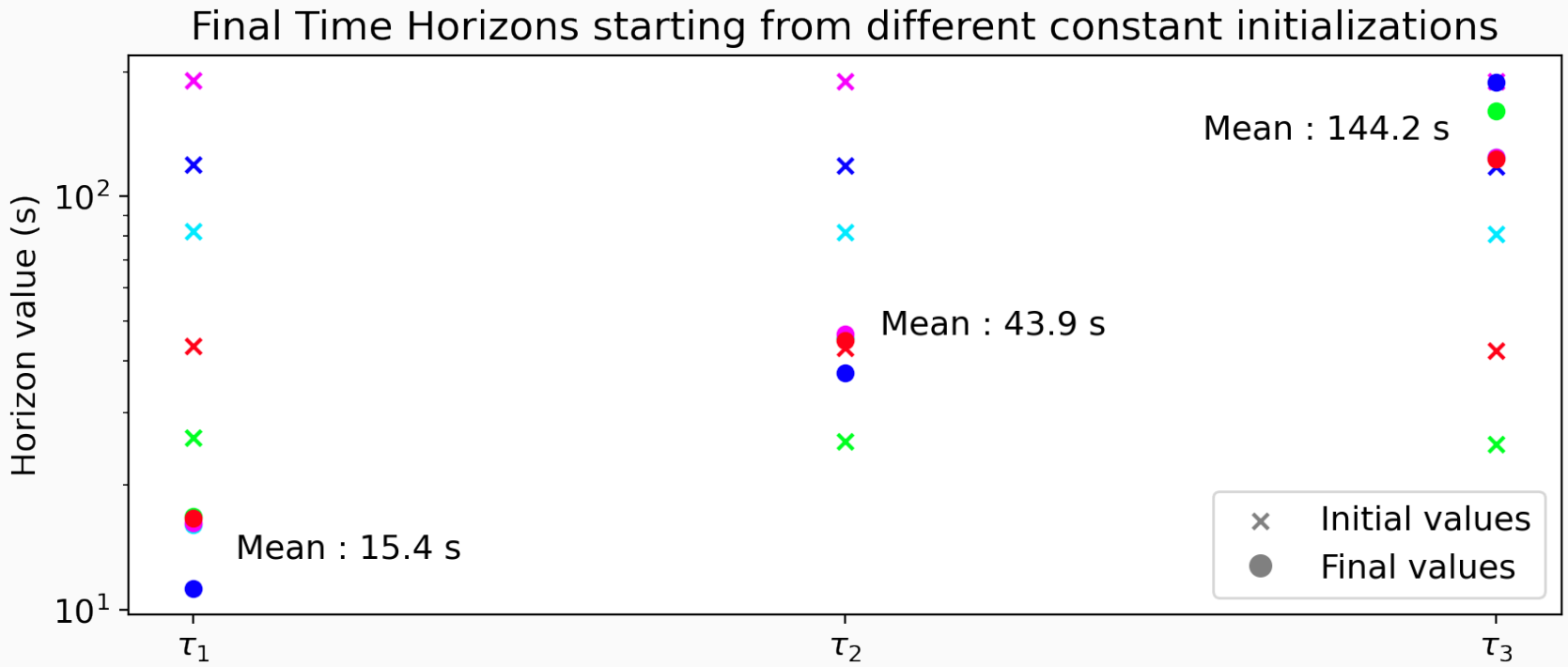
- We use a superposition of two waves of periods $T_1 = 50, T_2 = 168$:



- We need a memory of dimension 3 to represent the dynamics of the wave.

Learned Horizons

- Starting from varying initial conditions, the model learns similar horizons.



- $\tau_1 \approx 50/4, \qquad \tau_2 \approx 168/4, \qquad \tau_3 \approx 168$

Summary & Future Work

Summary :

- We propose a novel, time-continuous, neural architecture for modeling partially observable systems.
- It provides a computationally inexpensive and data-efficient correction to POD-Galerkin models, illustrated here in different flow configurations.
- Relevant and physically consistent time-constants are extracted from observations of the system.

- CD-ROM: Complementary Deep - Reduced Order model, Menier *et al.*, `https://arxiv.org/abs/2202.10746`

References

 B. R. Noack, K. Afanasiev, M. Morzyński, et al., "A hierarchy of low-dimensional models for the transient and post-transient cylinder wake", Journal of Fluid Mechanics **497**, 335–363 (2003).

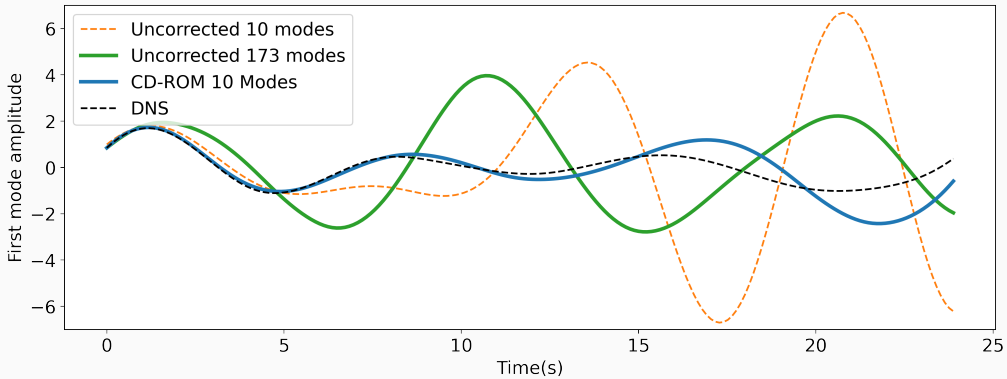
 R. T. Q. Chen, Y. Rubanova, J. Bettencourt, and D. Duvenaud, "Neural ordinary differential equations", (2019).

 N. Deng, B. R. Noack, M. Morzynski, et al., "Low-order model for successive bifurcations of the fluidic pinball", Journal of Fluid Mechanics **884**, 10.1017/jfm.2019.959 (2019).

Annex Slides

Computational Costs

- Although the CD-ROM increases the computational costs, it remains less expensive than bigger models :

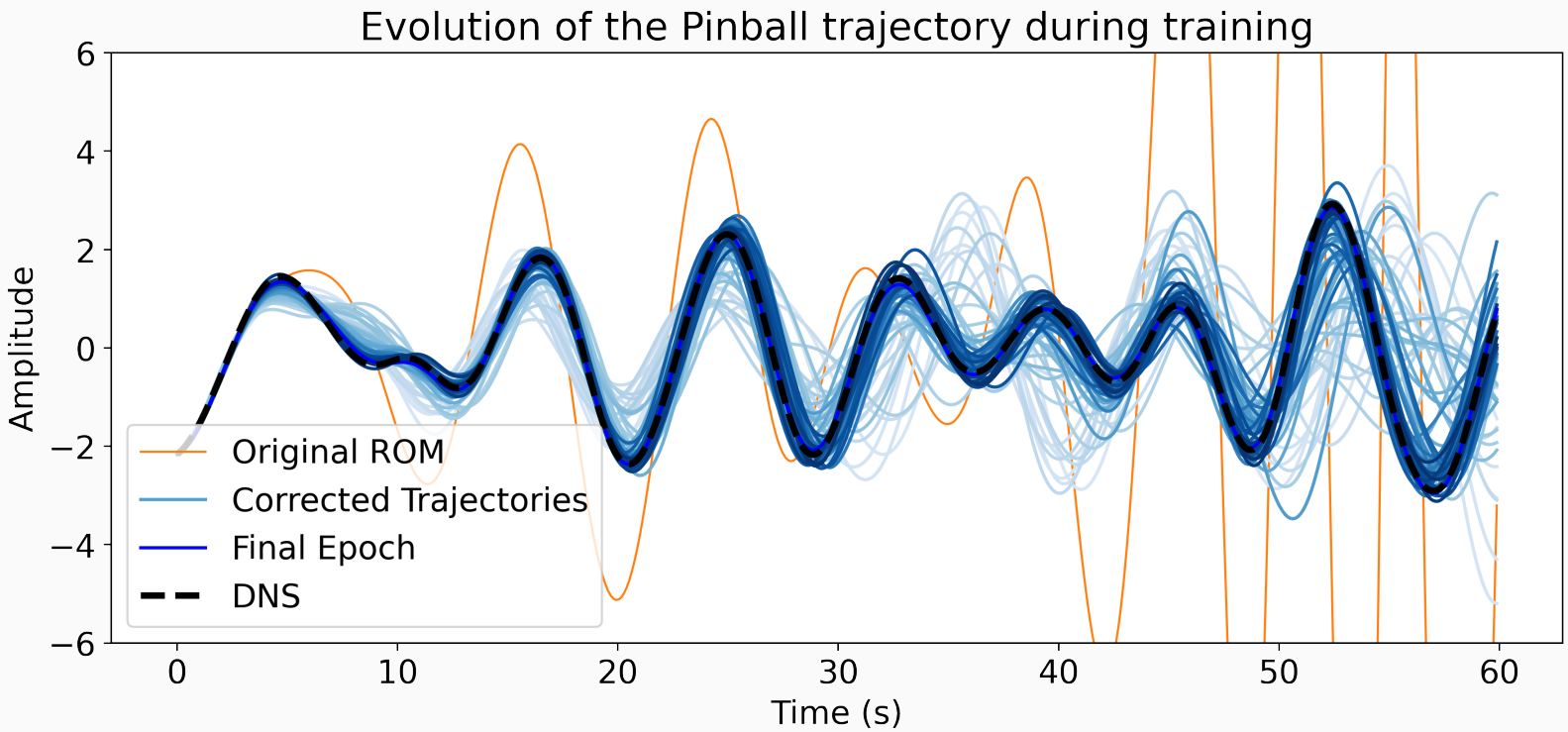


Integration times	
Uncorrected 10 modes	30 ms
Uncorrected 173 modes	550 ms
CD-ROM 10 modes	330 ms

Performance and computational cost of different models on a point outside the CD-ROM training basis.

Pinball Training

- This model can then be progressively corrected and stabilised through our approach :



Comparison with Reservoir Computing

- Echo State Networks are based on random matrices W_{in} and W :

$$Y_{t+1} = tanh(W_{in} \cdot x_t + W \cdot Y_t)$$
$$s.t.\ \rho(W) < 1$$

- Only the output operator is optimised to map the output sequence (O) to the memories :

$$x_t = W_{out} \cdot Y_t$$
$$W_{out} = Y^{\dagger} O$$

Comparison with RC

- Ignoring the non-linearity, the ESN becomes a linear dynamical system :

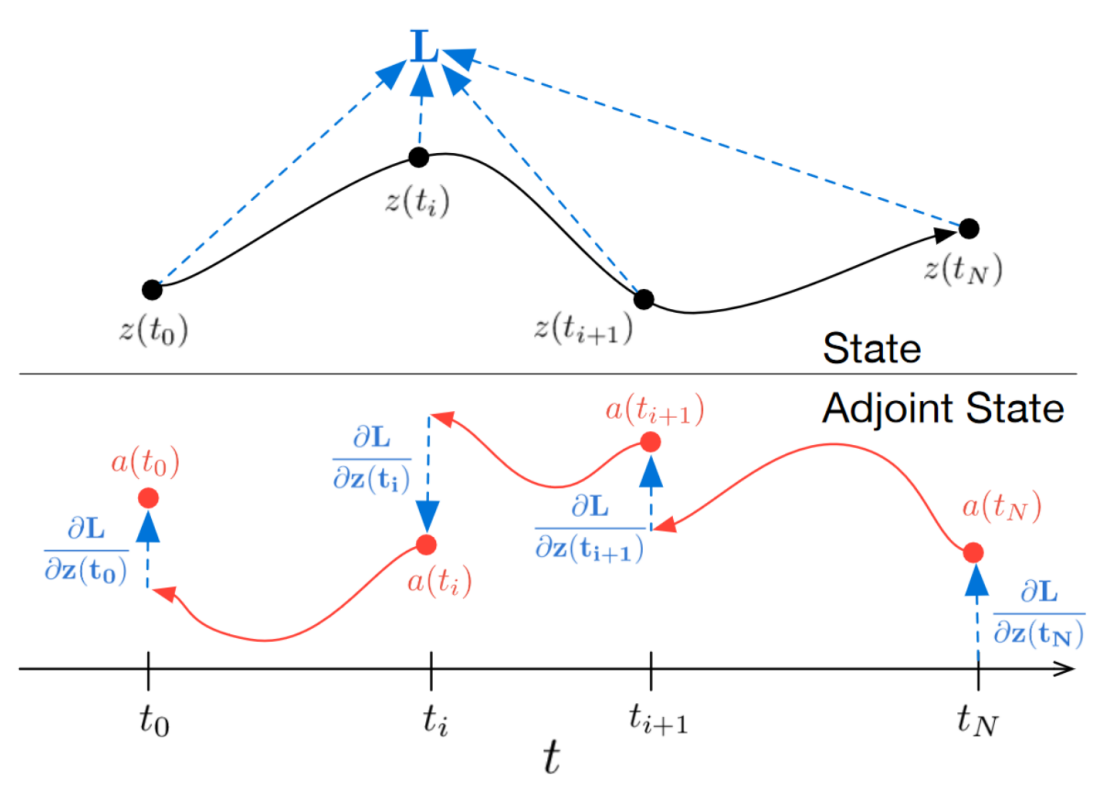
$$\begin{aligned} Y_{t+1} &= W_{in} \cdot x_t + W \cdot Y_t \\ &= Y_t + \Delta_t \frac{dY}{dt} \end{aligned} \quad \Longrightarrow \quad \frac{dY}{dt} = \frac{W_{in}}{\Delta_t} \cdot x(t) + \frac{W - I}{\Delta_t} Y(t)$$

- The operator $\bar{W} = \frac{W-I}{\Delta_t}$ eigenvalues have negative real part. It plays the same memory dissipation role as the Λ matrix in our architecture :

$$\begin{array}{lccccc} \textit{ESN :} & \frac{dY}{dt} & = & \frac{W_{in}}{\Delta_t} \cdot x & + & \frac{W-I}{\Delta_t} Y \\ \textit{Deep ROM :} & \frac{dY}{dt} & = & \textit{Enc}\,(x) & - & \Lambda Y \end{array}$$

Neural ODE

- With Neural ODEs[4] , we can back-propagate gradients through the simulation steps :



$$\frac{dz(t)}{dt} = f(z, t; \theta)$$

$$a(t) = \frac{dL}{dz}\Big|_t$$

$$\frac{da(t)}{dt} = -a(t)\frac{\partial f(z(t), t; \theta)}{\partial z}$$

$$\frac{dL}{d\theta} = -\int_{t_0}^{t_1} a(t)\frac{\partial f(z(t), t; \theta}{\partial \theta}$$

[4] R. T. Q. Chen et al., "Neural ordinary differential equations", (2019).

ROM NODE

- In our case, the Neural ODE corresponds to the complete ROM :

$$z = \begin{pmatrix} \alpha \\ y \end{pmatrix}$$

$$f(z, t; \theta) = \begin{matrix} \frac{1}{Re}\overline{K}\alpha - \alpha^T \overline{N}\alpha & + & \mathcal{NN}(y; \theta_1) \\ E(\alpha; \theta_2) & - & \Lambda y \end{matrix}$$

- Because the model is fully expressed with differentiable objects, the required jacobians can be easily evaluated through automatic differentiation.

Cylinder Hyperparameters

ReLU activation	
Encoder Network	
Layer 1	3 *neurons*
Layer 2	11 *neurons*
Layer 3	19 *neurons*
Layer 4	27 *neurons*
Correction Network	
Layer 1	30 *neurons*
Layer 2	30 *neurons*
Layer 3	30 *neurons*
Layer 4	3 *neurons*

Pinball Hyperparameters

Swish activation	
Encoder Network	
Layer 1	10 *neurons*
Layer 2	36 *neurons*
Layer 3	63 *neurons*
Layer 4	90 *neurons*
Correction Network	
Layer 1	100 *neurons*
Layer 2	500 *neurons*
Layer 3	500 *neurons*
Layer 4	10 *neurons*

Takens Theorem

- Discrete time delays are unsuitable for classical time integrators :