Deep learning-based reduced order models for real-time approximation of nonlinear time-dependent parametrized PDEs

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Abstract

Conventional linear reduced order modeling techniques, such as, e.g., the reduced basis method, may incur in severe limitations when dealing with nonlinear time-dependent parametrized PDEs, featuring coherent structures that propagate over time such as transport, wave, or convection-dominated phenomena. In this work, we propose a new, nonlinear approach relying on deep learning (DL) algorithms to obtain accurate and efficient reduced order models (ROMs), whose dimensionality matches the number of system parameters.

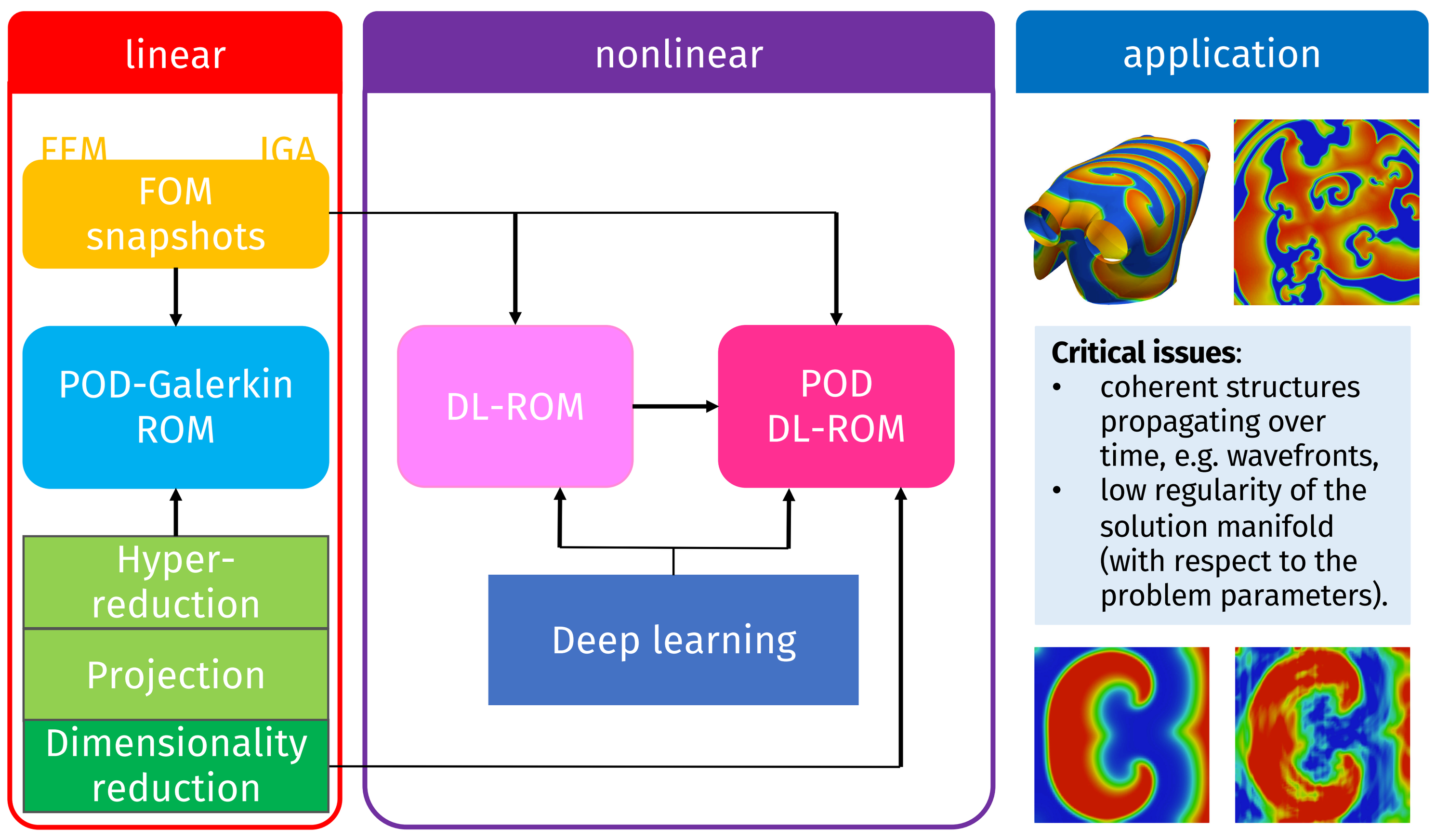
Introduction

Given $\mu \in \mathcal{P}$, we aim at solving the initial value problem

$$\begin{cases} \dot{\mathbf{u}}_h(t;\mu) = \mathbf{f}(t, \mathbf{u}_h(t;\mu); \mu) & t \in (0,T), \\ \mathbf{u}_h(0;\mu) = \mathbf{u}_0(\mu), \end{cases} \quad (1)$$

where $\mathcal{P} \subset \mathbb{R}^{n_\mu}$ is a bounded and closed set.

Reduced order modeling aims at replacing the FOM (1) by a model showing a much lower complexity but still able to express the physical features of the problem at hand.



Deep learning-based reduced order models

The POD-DL-ROM approximation $\tilde{\mathbf{u}}_h(t;\mu,\theta_{DF},\theta_D)$ of the FOM solution $\mathbf{u}_h(t;\mu)$ is given by

$$\tilde{\mathbf{u}}_h(t;\mu,\theta_{DF},\theta_D) = \mathbf{V}\tilde{\mathbf{u}}_N(t;\mu,\theta_{DF},\theta_D),$$

where $\tilde{\mathbf{u}}_N(t;\mu,\theta_{DF},\theta_D) = \mathbf{f}_N^D(\phi_n^{DF}(t;\mu,\theta_{DF});\theta_D)$.

- To describe the reduced dynamics on the nonlinear trial manifold $\tilde{\mathcal{S}}_N^n$, the intrinsic coordinates of the approximation $\tilde{\mathbf{u}}_N$ are defined as

$$\mathbf{u}_n(t;\mu) = \phi_n^{DF}(t;\mu,\theta_{DF}),$$

where $\phi_n(\cdot;\cdot,\theta_{DF}) : [0,T) \times \mathbb{R}^{n_\mu+1} \to \mathbb{R}^n$ is *a deep feedforward neural network*;

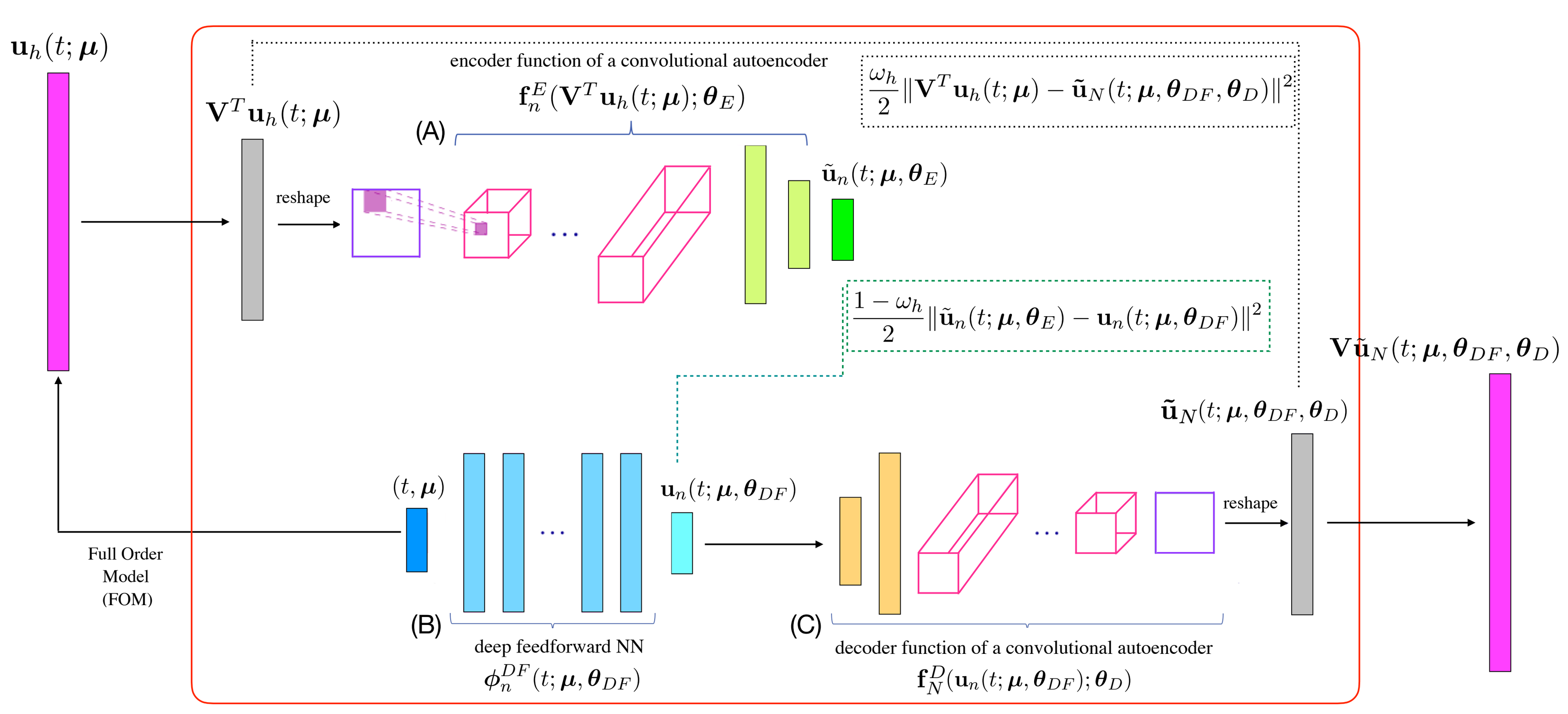
- to model the reduced nonlinear trial manifold $\tilde{\mathcal{S}}_N^n$, we employ the decoder function of a *convolutional autoencoder*, that is,

$$\tilde{\mathcal{S}}_N^n = \{\mathbf{f}_N^D(\phi_n^{DF}(t;\mu,\theta_{DF});\theta_D) \mid \mathbf{u}_n(t;\theta_{DF}) \in \mathbb{R}^n,\ t \in [0,T),\ \mu \in \mathcal{P} \subset \mathbb{R}^{n_\mu}\},$$

where $\mathbf{f}_N^D(\cdot;\theta_D) : \mathbb{R}^n \to \mathbb{R}^N$.

Computing the ROM approximation consists in solving an optimization problem (in the variable θ) where the **per-example loss function** is given by

$$\mathcal{L}(t^k,\mu_i;\theta) = \frac{\omega_h}{2}\|\mathbf{V}^T\mathbf{u}_h(t^k;\mu_i) - \tilde{\mathbf{u}}_N(t^k;\mu_i,\theta_{DF},\theta_D)\|^2 + \frac{1-\omega_h}{2}\|\tilde{\mathbf{u}}_n(t^k;\mu_i,\theta_E) - \mathbf{u}_n(t^k;\mu_i,\theta_{DF})\|^2$$



Proper Orthogonal Decomposition-enhanced Deep Learning-based Reduced Order Model (POD DL-ROM)

Main features:

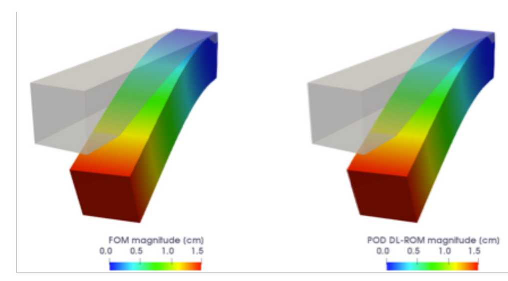
- POD-DL-ROMs learn, simultaneously, the **nonlinear trial manifold** and the nonlinear **reduced dynamics**;
- the POD-DL-ROM dimension is as close as possible to the **number of parameters** which the PDE solution depends upon;
- a prior dimensionality reduction, performed by means of **randomized POD,** and **pretraining** allow to drastically reduce training computational times.

Numerical results

Test 1: pretraining on 3D elastodynamics equations

P² FE method
Generalized-α method
N_h = 5674 (x3)
N = 64 (x3)
n = 2 (x3)

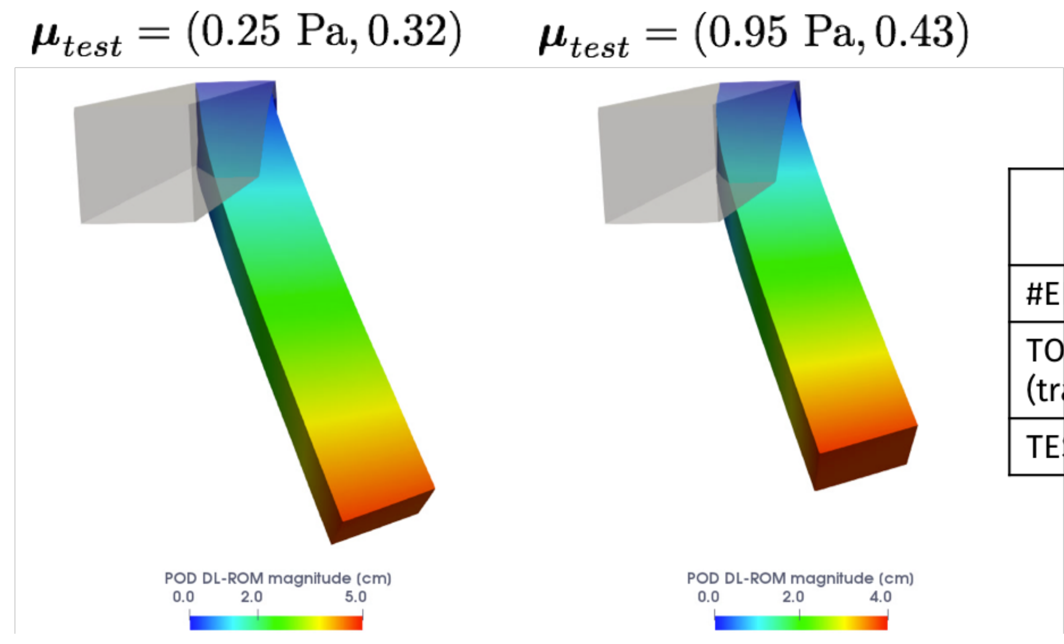
- $\mathcal{P} = [1,3]\mathrm{Pa} \times [0.25, 0.42]$
- St. Venant-Kirchhoff model
- **f** = 10^{-3} (-1, 0, -2)^T
- T = 15 s
- Δt = 0.2 s



$\mathcal{P} = [0.1, 1]\mathrm{Pa} \times [0.3, 0.45]$

- Neo-Hookean model
- **f** = 10^{-3} (-1t, 0, -2t)^T
- T = 22.5 s
- Δt = 0.25 s

$\mu_{test} = (0.25\ \mathrm{Pa}, 0.32)$ $\quad \mu_{test} = (0.95\ \mathrm{Pa}, 0.43)$

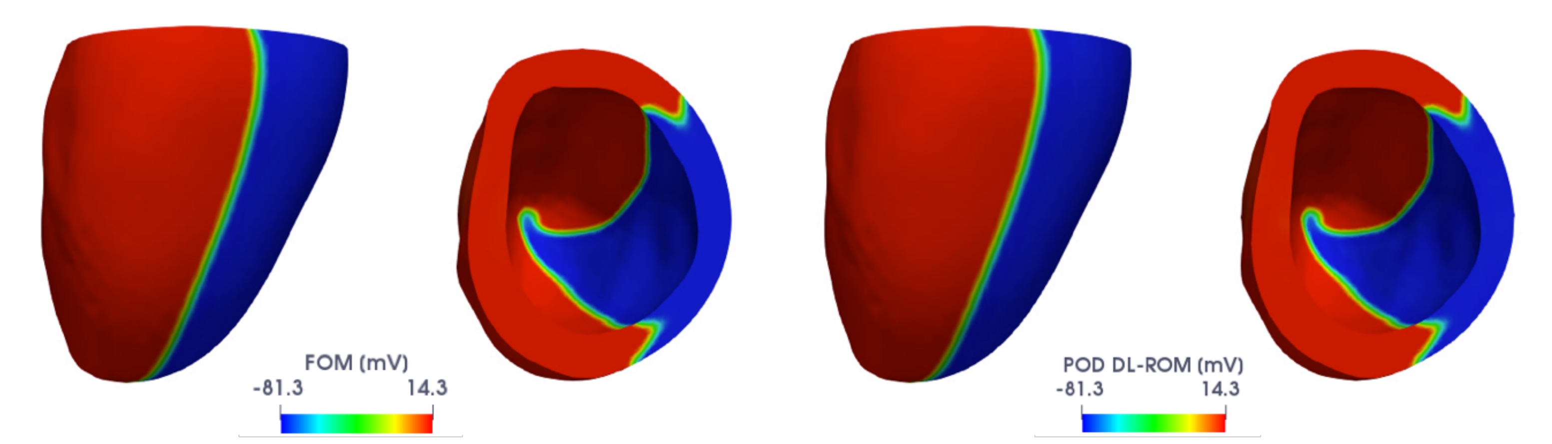


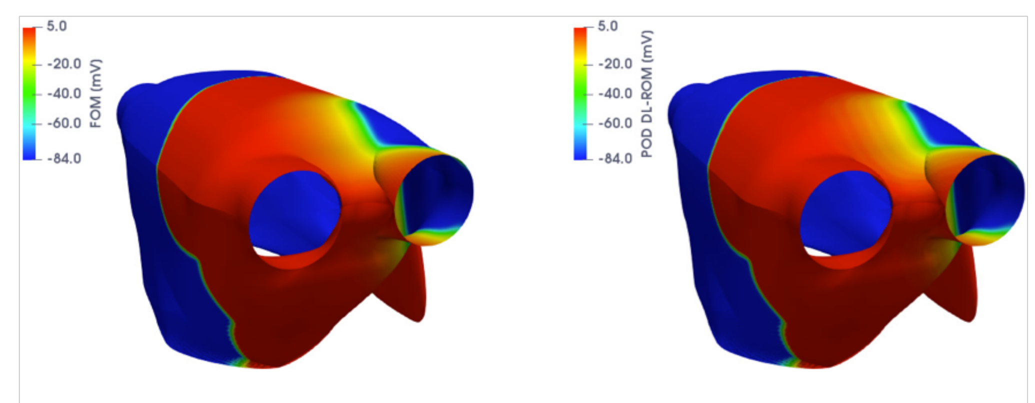
	POD DL-ROM	POD DL-ROM PRETRAINED
#EPOCHS	6490	1519
TOTAL TIME (train. + val.)	63 m	15 m
TEST	0.006 s	0.006 s

Test 2: cardiac electrophysiology on left ventricle and atrium

FOM (CPU)	POD-Galerkin ROM N_c = 4: train (CPU)	POD-Galerkin ROM N_c = 4: test (CPU)	POD DL-ROM: train (GPU)	POD DL-ROM: test (GPU)
3.5 h	28 h	120 s	49 m	0.25 s

- N_h = 65503
- N = 256
- n = 2
- N_{train} = 25
- N_t = 1000
- T = 0.3 s





FOM (CPU)	POD DL-ROM: train (GPU)	POD DL-ROM: test (GPU)
2 h	3.5 h	0.16 s

- N_h = 61732
- N = 256
- n = 2
- N_{train} = 21
- N_t = 500
- T = 0.2 s

References

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- S. Fresca et al. *Deep learning-based reduced order models in cardiac electrophysiology*. PLOS ONE, 15(10):1–32, 2020.
- S. Fresca et al. *POD-DL-ROM: enhancing deep learning-based reduced order models for nonlinear parametrized PDEs by proper orthogonal decomposition*. In preparation.
- https://github.com/stefaniafresca/DL-ROM

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