A machine learning-based reduced order model for the investigation of the haemodynamics in coronary artery bypass grafts

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Introduction

A machine learning **Reduced Order Model** (ROM) is developed in order to ensure rapid computations in a patient-specific **Coronary Artery Bypass Graft** (CABG). Both physical and geometrical parameters of clinical interest are introduced. An expensive offline phase performs a large number of high-fidelity solutions and generates the Reduced Basis (RB) with the **Proper Orthogonal Decomposition** (POD). Then, **feedforward Neural Networks** (NNs) are trained to interpolate the reduced coefficients. During the online stage, the behaviour of the system in the parameter space is available for real-time evaluation.
We consider two applications:

1. the ROM is implemented for the reconstruction of pressure, velocity and Wall Shear Stress (WSS) computed by the **Navier-Stokes** (N-S) equations. The inlet flow rate and the severity of the stenosis are considered as parameters in the reduced framework [2].
2. The ROM approach is used within an **Optimal Control Problem** (OCP) in order to match measured clinical data with numerical outcomes, varying the Reynolds (Re) number [4]. This approach is introduced to overcome the issues arising from unrealistic outlet boundary conditions, which can lead to doubtful predictions.

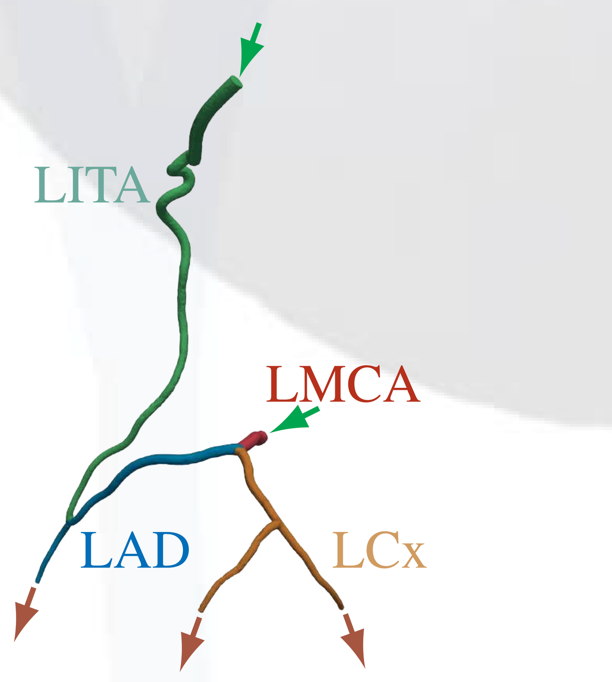
Full order model - 1

This work starts from [1], but it recasts the problem in a **Finite Volume** (FV) environment. Therefore, the geometrical parametrization of the domain changes accordingly.

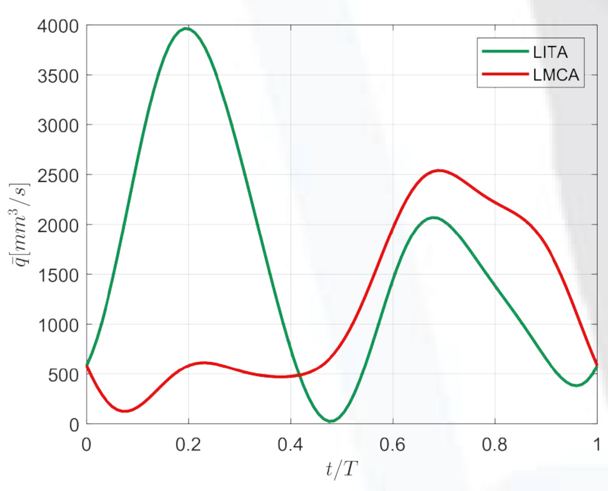
The dynamics of the blood flow is described by parametrized incompressible N-S equations:

$$\begin{cases} \partial_t \boldsymbol{v}(\boldsymbol{\mu}) + \nabla\cdot(\boldsymbol{v}(\boldsymbol{\mu})\otimes\boldsymbol{v}(\boldsymbol{\mu})) + \nabla p(\boldsymbol{\mu}) - \nu\Delta\boldsymbol{v}(\boldsymbol{\mu}) = 0, \\ \nabla\cdot\boldsymbol{v}(\boldsymbol{\mu}) = 0. \end{cases}$$

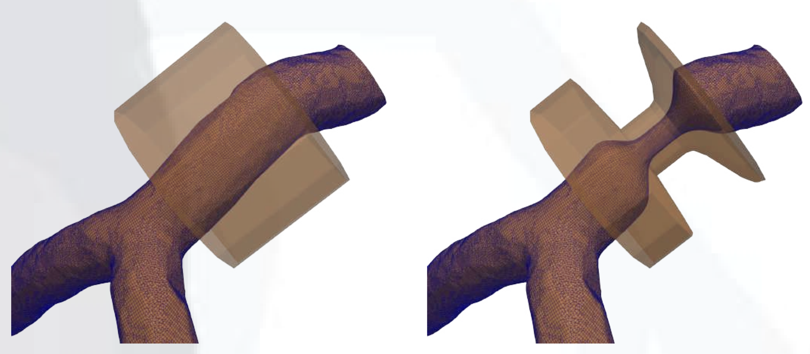
The parameters $\boldsymbol{\mu}$ are the **degree of the stenosis** in the Left Main Coronary Artery (LMCA) and the **inflow boundary conditions**.



The boundary conditions are:



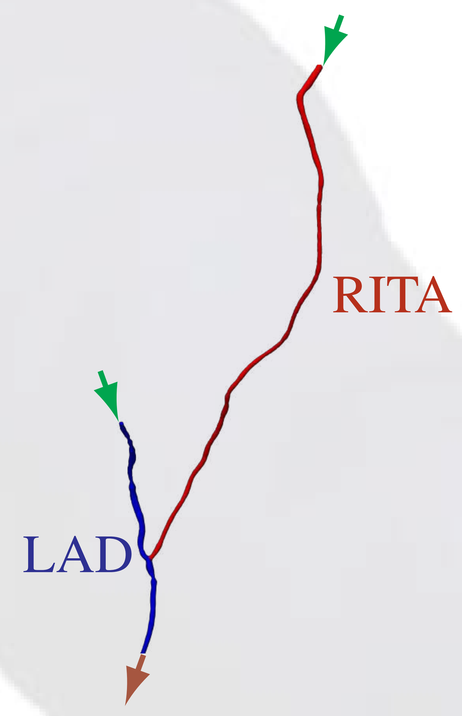
The **free form deformation** is used to introduce the stenosis in the LMCA:



OpenFOAM is used to find the FV high fidelity solutions, varying the parameters.

Optimal control approach - 2

Our OCP starts from [3] and finds the **Finite Element** (FE) solutions varying the inlet **Re** number.



The main ingredients are:

(a) steady-state incompressible N-S equations

$$\begin{cases} -\nu\Delta\boldsymbol{v}(\boldsymbol{\mu}) + (\boldsymbol{v}(\boldsymbol{\mu})\cdot\nabla)\boldsymbol{v}(\boldsymbol{\mu}) + \nabla p(\boldsymbol{\mu}) = 0, \\ \nabla\cdot\boldsymbol{v}(\boldsymbol{\mu}) = 0, \end{cases}$$

(b) with boundary conditions

$$\begin{cases} \boldsymbol{v}(\boldsymbol{\mu}) = \boldsymbol{v}_{\text{in}}(\boldsymbol{\mu}), & \text{on} \quad \Gamma_{\text{inlet}}, \\ -\nu(\nabla\boldsymbol{v}(\boldsymbol{\mu}))\boldsymbol{n} + p(\boldsymbol{\mu})\boldsymbol{n} = \boldsymbol{u}(\boldsymbol{\mu}), & \text{on} \quad \Gamma_{\text{outlet}}, \\ \boldsymbol{v}(\boldsymbol{\mu}) = \boldsymbol{0}, & \text{on} \quad \Gamma_{\text{wall}}, \end{cases}$$

(c) the **objective functional** to optimize is

$$\mathscr{I} = \frac{1}{2}\int_\Omega |\boldsymbol{v}(\boldsymbol{\mu}) - \boldsymbol{v}_{\text{m}}|^2 d\Omega + \frac{\alpha}{2}\int_{\Gamma_{\text{outlet}}} |\boldsymbol{u}(\boldsymbol{\mu})|^2 d\Gamma.$$

> Given $\boldsymbol{\mu}$, find $(\boldsymbol{v}(\boldsymbol{\mu}), p(\boldsymbol{\mu}), \boldsymbol{u}(\boldsymbol{\mu}))$ such that the objective functional $\mathscr{I}$ in (c) is minimized under the constrain (a)-(b).

In our work, the desired blood flow velocity and the boundary conditions are:

$$\boldsymbol{v}_{\text{in}} = \frac{\eta Re}{R_{\text{in}}}\Big(1 - \frac{r^2}{R_{\text{in}}^2}\Big)\boldsymbol{n}_{\text{in}}, \quad \boldsymbol{v}_{\text{m}} = v_{\text{const}}\Big(1 - \frac{r^2}{R^2}\Big)\boldsymbol{t}_{\text{c}}.$$

Python libraries **FEniCS** and **multiphenics** are used.

Reduced order model

The **POD-NN** is the **data-driven** method employed in these works to speed up high fidelity (FV and FE) simulations.

- Let $\bar{\Phi}$ be the variable of interest. The **POD** algorithm performs a SVD for the snapshots matrix:

$$S_\Phi = \begin{Bmatrix} \bar{\Phi}_1(\boldsymbol{\mu}_1) & \cdots & \bar{\Phi}_1(\boldsymbol{\mu}_L) \\ \vdots & \vdots & \vdots \\ \bar{\Phi}_{N_\delta}(\boldsymbol{\mu}_1) & \cdots & \bar{\Phi}_{N_\delta}(\boldsymbol{\mu}_L) \end{Bmatrix}.$$

The firsts $R \ll L$ left eigenvectors compose the RB:

$$V_\delta = [\boldsymbol{w}_1|\dots|\boldsymbol{w}_R] \in \mathbb{R}^{N_\delta\times R}.$$

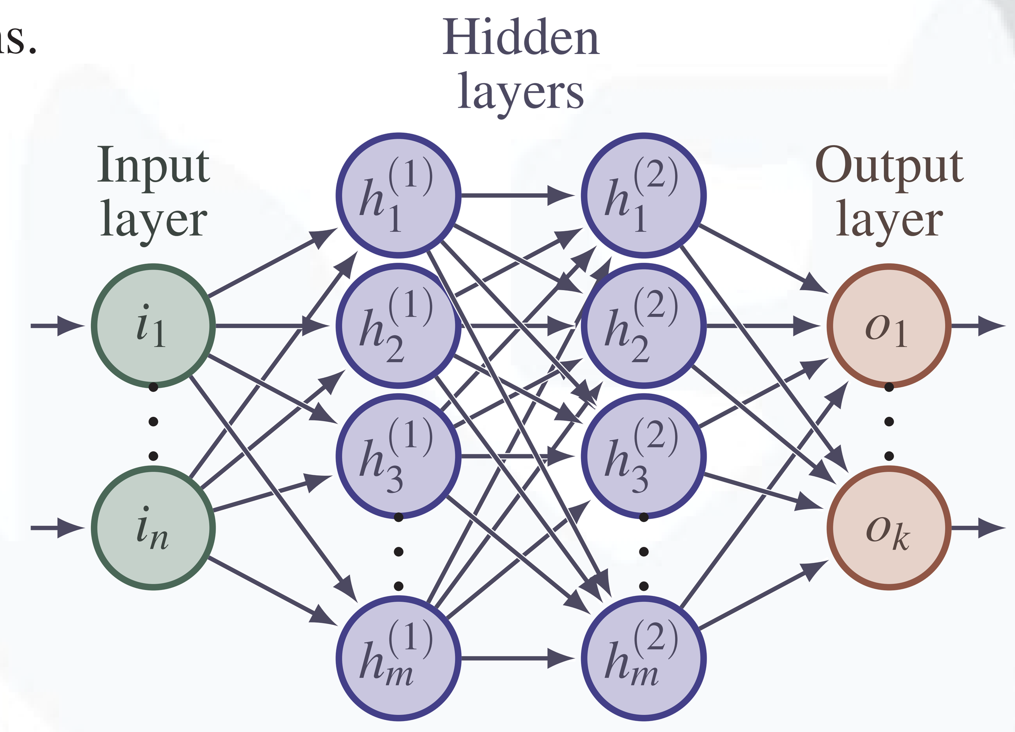
- Since the reduced solution is:

$$\Phi_{\text{r}}(\boldsymbol{\mu}_l) = \sum_{r=1}^{R}({V_\delta}^T\bar{\Phi}(\boldsymbol{\mu}_l))_r\boldsymbol{w}_r, \quad l = 0,\dots,L,$$

an **interpolation** of the reduced coefficients

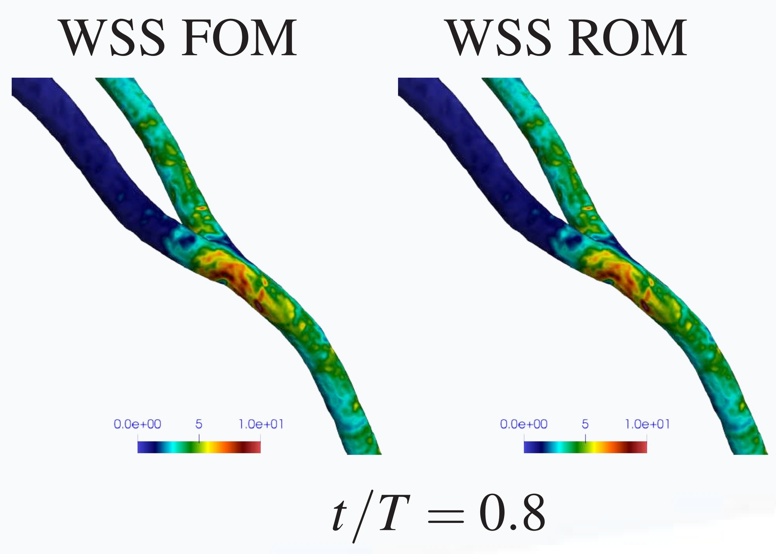
$$\pi : \boldsymbol{\mu}_l \mapsto [({V_\delta}^T\bar{\Phi}(\boldsymbol{\mu}_l))_r]_{r=1}^R, \quad l = 1,\dots,L,$$

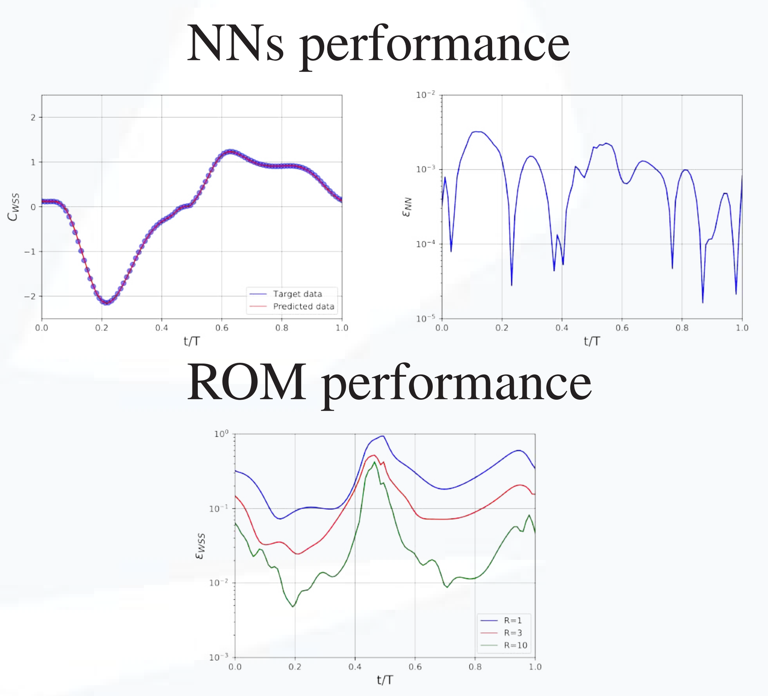
is carried out through **feedforward NNs**.



Results - 1

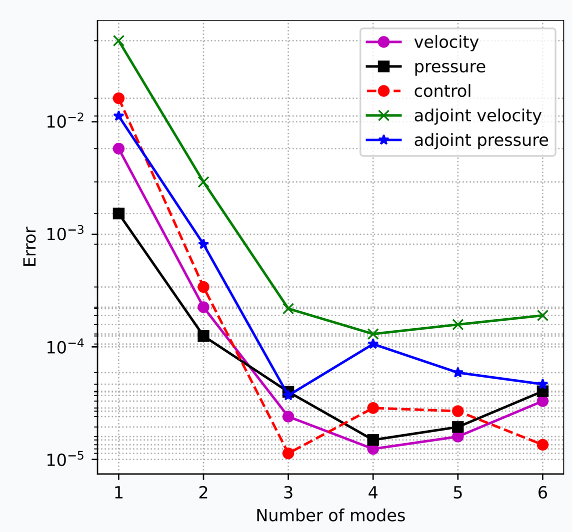
The speed-up is about $\mathscr{O}(10^5)$.

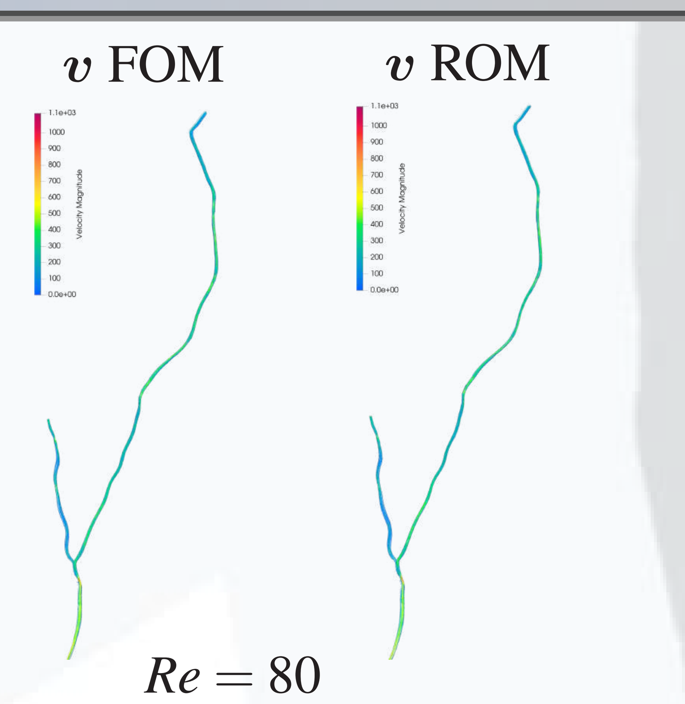




Results - 2

The speed-up is $\mathscr{O}(10^6)$, 4 times larger than POD-Galerkin of [3].





[1] F. Ballarin et al., *Fast simulations of patient-specific haemodynamics of coronary artery bypass grafts based on a POD–Galerkin method and a vascular shape parametrization*, Journal of Computational Physics, 315, 609-628, 2016
[2] P. Siena at al., *Data-driven reduced order modelling for patient-specific hemodynamics of coronary artery bypass grafts with physical and geometrical parameters*, arXiv preprint arXiv:2203.13682, 2022
[3] Z. Zainib at al., *Reduced order methods for parametric optimal flow control in coronary bypass grafts, toward patient-specific data assimilation*, International Journal for Numerical Methods in Biomedical Engineering, 37, e3367, 2021
[4] C. Balzotti at al., *A data-driven reduced order method for parametric optimal blood flow control: application to coronary bypass graft*, arXiv preprint arXiv:2206.15384, 2022
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