Reduced order methods for parametric optimal flow control in patient-specific coronary bypass grafts: geometrical reconstruction, data assimilation

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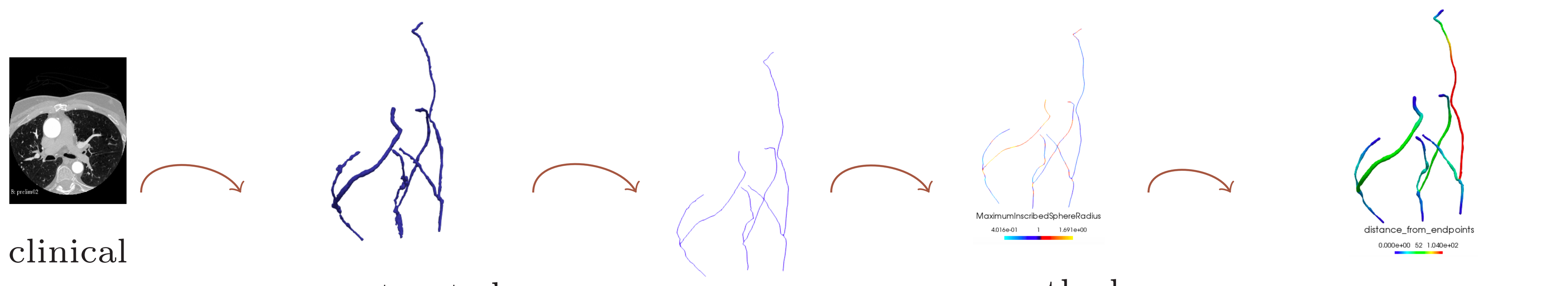
1. Introduction & motivation

Projection based **reduced order methods** [2] aim for exploring solutions in a **low dimensional manifold**, a projection of high dimensional solution manifold. Such techniques can be applied to a wide range of problems including **optimal flow control problems** (OFCPs) governed by partial differential equations (PDEs) [3], with the goal to solve the problem in a many-query **parameter dependent** context.
Here, we focus on applications in biomedical sciences, specifically on the application of reduced OFCPs to **patient-specific coronary artery bypass grafts (CABGs)** [1] with the aim to **minimize the misfit** between clinical measurements and numerical simulations [4].

2. Geometrical reconstruction



clinical image → reconstructed structure → centerlines → smoothed centerlines → smooth reconstructed geometry

From clinical image to smooth patient-specific geometry

3. Parametrized optimal control model

Let $\Omega \in \mathbb{R}^3$ be the patient-specific CABG geometry with boundary $\partial\Omega = \Gamma_{in} \cup \Gamma_w \cup \Gamma_o$, where $\Gamma_{in}, \Gamma_w, \Gamma_o$ denote the inlets, walls and outlet of the CABG. Let $\mathcal{D} \subset \mathbb{R}^\gamma, \gamma \in \mathbb{N}$ be a set of physical parameters, $\boldsymbol{v} \in V(\Omega)$ and $p \in P(\Omega)$ be state velocity and pressure and $\boldsymbol{u} \in U(\Gamma_o)$ be the unknown control variables. Parametrized optimal flow control problem, constrained by steady incompressible Navier-Stokes equations, reads:

Given $\boldsymbol{\mu} \in \mathcal{D}$, find optimal pair $(\boldsymbol{v}(\boldsymbol{\mu}), p(\boldsymbol{\mu}), \boldsymbol{u}(\boldsymbol{\mu})) \in V \times P \times U$ such that,

$$\min_{(\boldsymbol{v},p,\boldsymbol{u})} \mathcal{J}(\boldsymbol{v},p,\boldsymbol{u},\boldsymbol{\mu}) = \frac{1}{2}\underbrace{\|\boldsymbol{v}(\boldsymbol{\mu}) - \boldsymbol{v}_d\|_V^2}_{m(\boldsymbol{v}(\boldsymbol{\mu})-\boldsymbol{v}_d, \boldsymbol{v}(\boldsymbol{\mu})-\boldsymbol{v}_d)} + \frac{\alpha}{2}\underbrace{\|\boldsymbol{u}(\boldsymbol{\mu})\|_U^2}_{n(\boldsymbol{u}(\boldsymbol{\mu}),\boldsymbol{u}(\boldsymbol{\mu}))}, \text{ subject to,} \quad (1)$$

$$\begin{cases} -\eta\Delta\boldsymbol{v}(\boldsymbol{\mu}) + (\boldsymbol{v}(\boldsymbol{\mu})\cdot\nabla)\boldsymbol{v}(\boldsymbol{\mu}) + \nabla p(\boldsymbol{\mu}) = \boldsymbol{0}, & \text{in } \Omega \\ \nabla\cdot\boldsymbol{v}(\boldsymbol{\mu}) = 0, & \text{in } \Omega \\ \boldsymbol{v}(\boldsymbol{\mu}) = \boldsymbol{v}_{in}(\boldsymbol{\mu}), & \text{on } \Gamma_{in} \\ \boldsymbol{v}(\boldsymbol{\mu}) = \boldsymbol{0}, & \text{on } \Gamma_w \\ \eta\nabla\boldsymbol{v}(\boldsymbol{\mu})\cdot\boldsymbol{n} - p(\boldsymbol{\mu})\boldsymbol{n} = \boldsymbol{u}(\boldsymbol{\mu}) & \text{on } \Gamma_o, \end{cases} \quad (2)$$

where $\boldsymbol{n}$ is unit outward normal and $\boldsymbol{v}_{in}(\boldsymbol{\mu}) = -\frac{\eta\mu}{R_{in}}\left(1 - \frac{r^2}{R_{in}^2}\right)\boldsymbol{n}_{in}$ is parametrized inflow velocity with $\boldsymbol{n}_{in}$ denoting outward normal to Γ_{in}. Moreover, $\boldsymbol{v}_d$ is desired velocity, distributed through $v_{const}\left(1 - \frac{r^2}{R^2}\right)\boldsymbol{t}_c$, across Ω.

4. Reduced order parametrized optimal control model

Let $X_N = V_N \times P_N \times U_N$ be the reduced order state and control spaces and $Z_N = Z_{\boldsymbol{v}_N} \times Z_{p_N}$ be the reduced order adjoint spaces. The reduced order coupled optimality system, derived from first order **Karush-Kuhn-Tucker** optimality conditions, is defined as:

$$\begin{cases} \mathcal{A}(\mathbf{x}_N, \mathbf{y}_N; \boldsymbol{\mu}) + \mathcal{B}(\mathbf{y}_N, \boldsymbol{z}_N; \boldsymbol{\mu}) + \mathcal{E}(\boldsymbol{v}_N, \boldsymbol{w}_N, \mathbf{y}_{\boldsymbol{v}_N}; \boldsymbol{\mu}) + \mathcal{E}(\boldsymbol{w}_N, \boldsymbol{v}_N, \mathbf{y}_{\boldsymbol{v}_N}; \boldsymbol{\mu}) = \langle \mathcal{H}(\boldsymbol{\mu}), \mathbf{y}_N \rangle, \\ \mathcal{B}(\mathbf{x}_N, \boldsymbol{\kappa}_N; \boldsymbol{\mu}) + \mathcal{E}(\boldsymbol{v}_N, \boldsymbol{v}_N, \boldsymbol{\kappa}_{\boldsymbol{w}_N}; \boldsymbol{\mu}) = \boldsymbol{0}, \end{cases} \quad (3)$$

where, $\mathcal{B} : X_N \times Z_N \to \mathbb{R}$ is operator associated to linear part of weak formulation of state constraints (2), $\mathcal{E}$ is associated to non-linear terms, $\mathcal{A} = m(\boldsymbol{v}_N(\boldsymbol{\mu}), \mathbf{y}_{\boldsymbol{v}_N}) + \alpha n(\boldsymbol{u}_N(\boldsymbol{\mu}), \mathbf{y}_{\boldsymbol{u}_N})$ and $\mathcal{H}(\boldsymbol{\mu}) = m(\boldsymbol{v}_d, \mathbf{y}_{\boldsymbol{v}_N})$.
Thanks to the saddle-point structure of system (3), the parametrized optimal flow control problem can be written in the following algebraic form: *Given $\boldsymbol{\mu} \in \mathcal{D}$, find $(\mathbf{x}_N, \boldsymbol{z}_N) \in X_N \times Z_N$ such that,*

$$\begin{bmatrix} M(\boldsymbol{\mu}) + \tilde{E}(\mathbf{w}(\boldsymbol{\mu}); \boldsymbol{\mu}) & 0 & 0 & A(\boldsymbol{\mu}) + E(\mathbf{v}_N(\boldsymbol{\mu}); \boldsymbol{\mu}) & B(\boldsymbol{\mu}) \\ 0 & 0 & 0 & B^T(\boldsymbol{\mu}) & 0 \\ 0 & 0 & \mathrm{N}(\boldsymbol{\mu}) & C(\boldsymbol{\mu}) & 0 \\ A(\boldsymbol{\mu}) + E(\mathbf{v}(\boldsymbol{\mu}); \boldsymbol{\mu}) & B^T(\boldsymbol{\mu}) & C(\boldsymbol{\mu}) & 0 & 0 \\ B(\boldsymbol{\mu}) & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{v}(\boldsymbol{\mu}) \\ \mathbf{p}(\boldsymbol{\mu}) \\ \mathbf{u}(\boldsymbol{\mu}) \\ \mathbf{w}(\boldsymbol{\mu}) \\ \mathbf{q}(\boldsymbol{\mu}) \end{bmatrix} = \begin{bmatrix} \mathbf{h}(\boldsymbol{\mu}) \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{f}(\boldsymbol{\mu}) \\ \mathbf{g}(\boldsymbol{\mu}) \end{bmatrix}. \quad (4)$$

Here $A(\boldsymbol{\mu}) \in \mathbb{R}^{N_{\boldsymbol{v}}} \times \mathbb{R}^{N_{\boldsymbol{w}}}$, $B(\boldsymbol{\mu}) \in \mathbb{R}^{N_q} \times \mathbb{R}^{N_{\boldsymbol{v}}}$, $B^T(\boldsymbol{\mu}) \in \mathbb{R}^{N_p} \times \mathbb{R}^{N_{\boldsymbol{w}}}$, $C(\boldsymbol{\mu}) \in \mathbb{R}^{N_{\boldsymbol{u}}} \times \mathbb{R}^{N_{\boldsymbol{w}}}$, $M(\boldsymbol{\mu}) \in \mathbb{R}^{N_{\boldsymbol{v}}} \times \mathbb{R}^{N_{\boldsymbol{v}}}$, $N(\boldsymbol{\mu}) \in \mathbb{R}^{N_{\boldsymbol{u}}} \times \mathbb{R}^{N_{\boldsymbol{u}}}$, $E(\boldsymbol{\mu}) \in \mathbb{R}^{N_{\boldsymbol{v}}} \times \mathbb{R}^{N_{\boldsymbol{w}}}$ and $\tilde{E}(\boldsymbol{\mu}) \in \mathbb{R}^{N_{\boldsymbol{v}}} \times \mathbb{R}^{N_{\boldsymbol{v}}}$ are the stiffness matrices associated to the operators in (3).

5. Numerical results

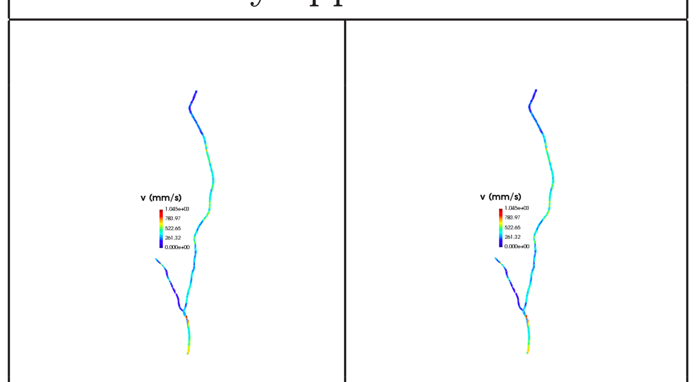
Case I : One graft connection

Graft connection: between right internal mammary artery (**RIMA**) (green) & left anterior descending artery (**LAD**)(red).

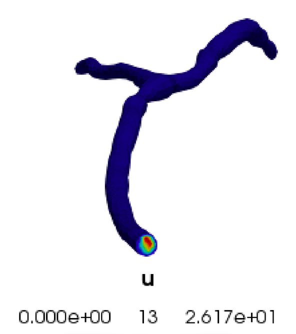
Parameters = Reynolds number, i.e., $\mu = Re|_{\Gamma_{in}} \in \mathcal{D} = [70, 80]$

Ω_1

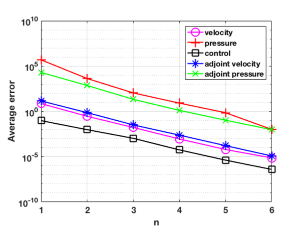
Velocity approximations



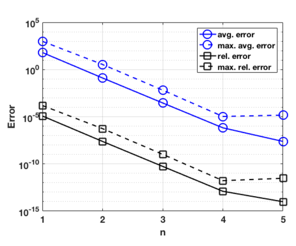
Galerkin FEM | POD–Galerkin



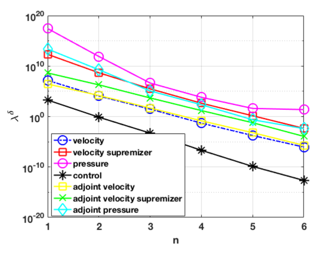
Boundary control magnitude



Average error for variables



Avg. and rel. errors for $\mathcal{J}$



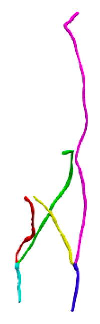
Eigenvalues reduction

In this case, 99.9% energy of full order solution spaces is captured within **6 POD modes** reducing the dimensions of the problem from **433288 dofs** to **79 reduced bases**. Furthemore, the errors in velocity and pressure approximations are reduced to $\mathbf{10^{-5}}$ and $\mathbf{10^{-3}}$, respectively. A similar behavior is depicted for $\mathcal{J}$ and the computational time is reduced from **1214.3** seconds to **109.3** seconds (online phase).

Case II : Two grafts connections

Graft connections: between right internal mammary artery (**RIMA**) (magenta) & left anterior descending artery (**LAD**) (yellow), and between saphenous vein (**SV**) (green) and first obtuse marginal artery (**OM1**) (red).

Parameters = Reynolds number, i.e., $(\mu_1, \mu_2) = \left(Re|_{\Gamma_{in_1}}, Re|_{\Gamma_{in_2}}\right) \in \mathcal{D} = [70, 80] \times [45, 50]$

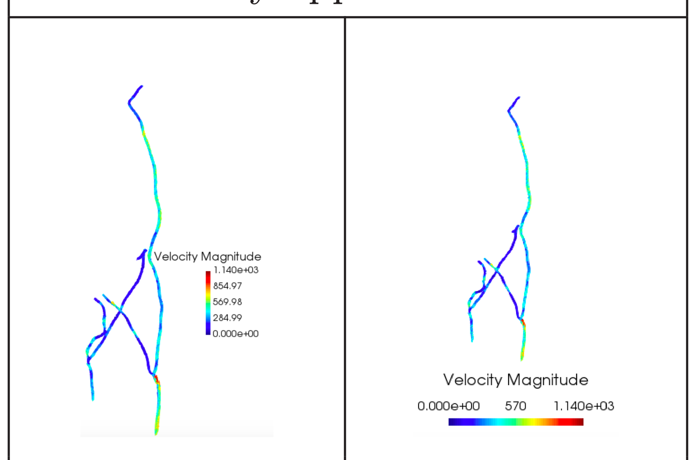


Ω_2

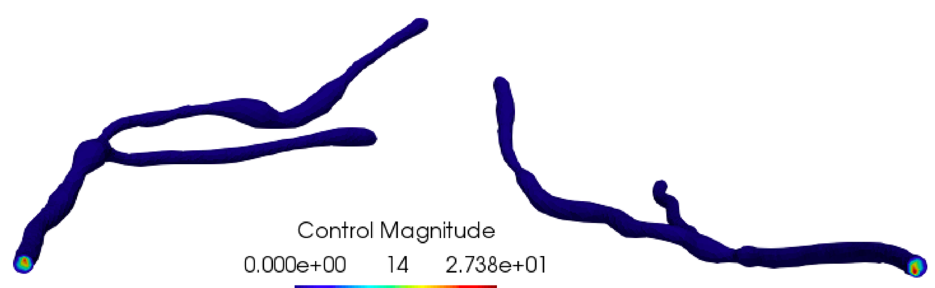
Γ_{in_1} := inlets of RIMA and LAD

Γ_{in_2} := inlets of SV and OM1

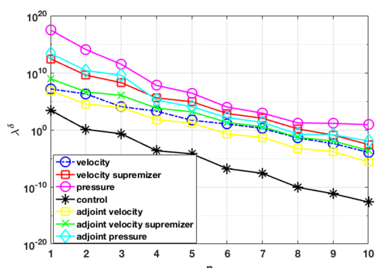
Velocity approximations



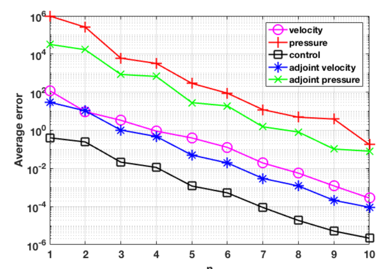
Galerkin FEM | POD–Galerkin



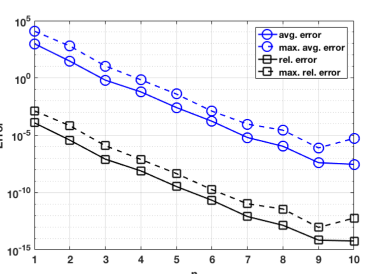
Boundary control magnitude



Eigenvalues reduction



Average error for variables



Avg. and rel. errors for $\mathcal{J}$

In this case, **Galerkin finite element spaces** have **715462 dofs**. In reduced order problem, **10 POD modes** capture 99.9% energy of Galerkin finite element spaces. Thus, reduced order spaces spanned by **132 reduced bases** sufficiently approximate full order solutions, reducing the error in velocity and pressure approximations to $\mathbf{10^{-5}}$ and $\mathbf{10^{-3}}$, respectively. A similar behavior is depicted for $\mathcal{J}$ and the computational time is reduced from **1848.13** seconds to **202.27** seconds (online phase).

6. Software

mathlab.sissa.it/rbnics

mathlab.sissa.it/multiphenics

7. Future perspectives

We further propose implementation of reduced order methods in shape parametrization context to gain **reduction in parametric spaces**, in addition to reduced solution spaces. This shall better predict hemodynamics behavior, dependent upon extent of stenosis and thus, the model shall be more feasible for clinical studies.

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[4] Z. Zainib, F. Ballarin, G. Rozza, P. Triverio, L. Jiménez-Juan, and S. Fremes. Reduced order methods for parametric optimal flow control in coronary bypass grafts: patient-specific data assimilation and geometrical reconstruction. *International Journal for Numerical Methods in Biomedical Engineering, Submitted*, 2019.

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