Reduced order methods for parametrized optimal flow control problems: applications in biomedical and environmental marine sciences

Maria Strazzullo[1], Zakia Zainib[1], Francesco Ballarin[1], and Gianluigi Rozza[1]

[1]mathLab, Mathematics area, SISSA - International School for Advance Studies, Trieste, Italy

1. Introduction & motivation

Reduced order methods for **parametrized optimal flow control problems** (OFCP($\boldsymbol{\mu}$)) are a **reliable and rapid approach** to manage wide classes of problems, in different fields [2, 3]. We focus on applications in life sciences, specifically in **biomedical and environmental sciences**.
Among biomedical problems, we focus on the application of reduced order optimal flow control framework in **patient-specific hemodynamics modeling** along with **patient-specific geometrical data assimilation** for coronary artery bypass grafts (CABGs)[1, 5]. Applications arising in **environmental marine sciences** and engineering are also presented: reduced optimal control framework is a useful approach to **monitor, manage** and **predict** (possibly dangerous) marine phenomena [4].

2. Reduced order parametrized optimal control model

Problem description: Let $\mathcal{D} \subset \mathbb{R}^p, p \in \mathbb{N}$ be a set of parameters characterizing geometrical and/or physical properties, $\mathcal{F}$ be residual of non-linear partial differential equations modeling fluid flow state and $\mathcal{J}$ be a desired objective functional. Parametrized optimal flow control problem is defined as:

Given $\boldsymbol{\mu} \in \mathcal{D}$, find optimal pair $(\boldsymbol{s}(\boldsymbol{\mu}), \boldsymbol{u}(\boldsymbol{\mu}))$ of fluid state and control variables such that

$$\min_{(\boldsymbol{s}(\boldsymbol{\mu}),\boldsymbol{u}(\boldsymbol{\mu}))} \mathcal{J}(\boldsymbol{s}, \boldsymbol{u}; \boldsymbol{\mu}) \text{ subject to } \mathcal{F}(\boldsymbol{s}, \boldsymbol{u}; \boldsymbol{\mu}) = 0.$$

For solution methodology we adopt *optimize-discretize-reduce* approach. The optimization step comprises of derivation of coupled optimality system in monolithic structure, by satisfying first order **Karush-Kuhn-Tucker** optimality conditons for Lagrangian $\mathcal{L}$ with adjoint $\boldsymbol{z}$, that is,

$$\nabla\mathcal{L}(\boldsymbol{s}, \boldsymbol{u}, \boldsymbol{z}; \boldsymbol{\mu})[\boldsymbol{\xi}, \boldsymbol{\pi}, \boldsymbol{\kappa}] = \nabla(\mathcal{J}(\boldsymbol{s}, \boldsymbol{u}; \boldsymbol{\mu}) + \langle \mathcal{F}(\boldsymbol{s}, \boldsymbol{u}; \boldsymbol{\mu}), \boldsymbol{z} \rangle)[\boldsymbol{\xi}, \boldsymbol{\pi}, \boldsymbol{\kappa}] = 0 \tag{1}$$

We implement Galerkin finite element methods to discretize and numerically approximate the solution to system (1), however the computations need to be performed in repetitive environment for different parametrized scenarios and hence, require days. To overcome this high computational expense, we utilize **proper orthogonal decomposition (POD)–Galerkin** which constructs a reduced order manifold from Galerkin finite element solutions preserving sufficient energy such that full order solution manifold is approximated by the reduced order manifold. We, then, explore solution in the reduced order spaces with **computational expense of a few seconds** thanks to low dimensions of solution spaces and **offline-online phase decomposition** of POD–Galerkin.

3(a). Aims in marine sciences

Loss of pollutant in the Gulf of Trieste, Italy:
we bring the concentration of the pollutant y under a safeguard y_d.
Nonlinear solution tracking North Atlantic Ocean:
match the solution (y) to a current profile based on experimental data (Gulf Stream dynamics) y_d
In both cases we minimise the functional

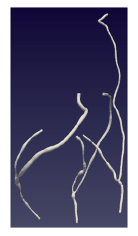
$$\frac{1}{2}\|y(\boldsymbol{\mu}) - y_d(\boldsymbol{\mu})\|^2_{L^2(\Omega_{OBS})} + \frac{\alpha}{2}\|u(\boldsymbol{\mu})\|^2_{L^2(\Omega_u)}$$

with respect

$(y, u) \in H^1(\Omega) \times L^2(\Omega_u)$ trough a distributed control.

4(a). Biomedical applications

Patient-specific coronary artery bypass grafts (CABGs) constructed from clinical images as computational domain Ω.

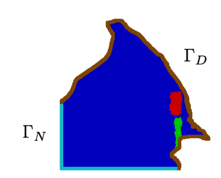


Objectives:

(i). Tracking patient-specific clinically acquired physiological data ($\boldsymbol{v_d}$) through minimization of $\mathcal{J} = \int_\Omega |\boldsymbol{v} - \boldsymbol{v_d}|^2 d\Omega$.
(ii). Quantifying outflow boundary conditions through boundary control $\boldsymbol{u}(\partial\Omega)$ to achieve (i).
(iii). Simulating different $\boldsymbol{\mu}$-dependent hemodynamics scenarios to achieve (i), in real-time.

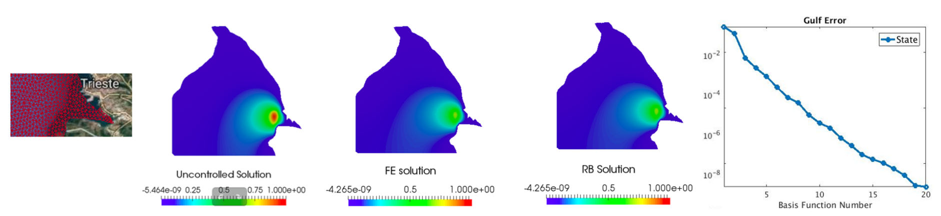
3(b). Applications in environmental marine sciences (with R. Mosetti[2])

Loss of pollutant in the Gulf of Trieste, Italy
The parameter $\boldsymbol{\mu} \in [0.5, 1] \times [-1, 1] \times [-1, 1]$ describes regional winds action and how they affect the diffusion of the pollutant.



Boundaries:
Γ_D = coasts, Γ_N = Adriatic Sea.
Subdomains:
Ω_{OBS} = Area of Miramare;
Ω_u = Source of pollutant (in front of the city of Trieste).

State Equation: Advection Diffusion $\mu_1 \Delta y + [\mu_2, \mu_3] \cdot \nabla y = \chi_{\Omega_u} u$

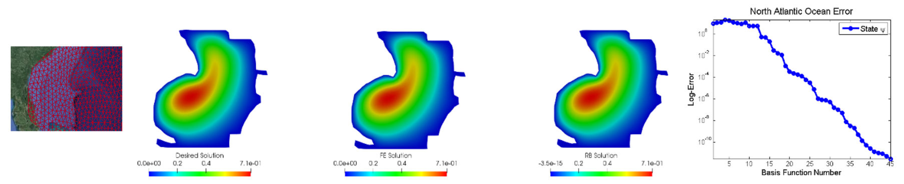


Comments:
We reproduced the **actual physical domain** thanks to **satellite images**. We solved an uncontrolled pollutant loss in order to understand how to manage this kind of dangerous situation. **Reduced** and **Finite Element** solutions **match**. The norm error between Finite Element and reduced solution is shown with respects the basis number N ($\sim 10^{-7}$). **Time of a run**: $t_\mathcal{N} = 2.79s$, $t_N = 2.41 \cdot 10^{-2}s$. **Dimensions**: $\mathcal{N} = 5639$ and $N = 20$.

Nonlinear solution tracking North Atlantic Ocean:
The parameter $\boldsymbol{\mu} \in [0.07^3, 1] \times [10^{-4}, 1] \times [10^{-4}, 0.045^2]$ describes the actual diffusivity and advection effects of the Ocean dynamic.

State Equation: Quasi-Geostrophic Equations $\mu_3 \dfrac{\partial y}{\partial x_1}\dfrac{\partial q}{\partial x_2} - \dfrac{\partial y}{\partial x_1}\dfrac{\partial q}{\partial x_2} = u - \mu_1 q + \mu_2 \Delta q,$
where $q = \Delta y$ and *no slip* boundary conditions are applied.

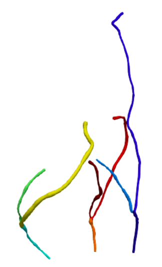
Streamline Formulation: y = streamfunction, q = −vorticity. The velocity field $\boldsymbol{u}$ of Oceanic current could be recovered by $(u_1, u_2) = (y_{x_2}, -y_{x_1})$
Domains: $\Omega_{OBS} = \Omega_u = \Omega$.



Comments:
We reproduced the Florida peninsula working on **satellite images**. Experimental data helped us to build the target function y_d. **Desired state**, **reduced** and **Finite Element** solutions **match**. The norm error between Finite Element and reduced solution is shown with respects the basis number N ($\sim 10^{-8}$). **Time of a run**: $t_\mathcal{N} = 5.59s$, $t_N = 2.38 \cdot 10^{-1}s$. **Dimensions**: $\mathcal{N} = 6490$ and $N = 25$.

4(b). Applications in cardiovascular problems (with P. Triverio[3] and L. Jiménez-Juan[4])

We assume blood to be **Newtonian** fluid and **vessel walls** to be **rigid** and **non-permeable**. Furthermore, we consider steady **Navier-Stokes equations** to model blood flow, that is,



- Γ_{in} := inlets
- Γ_w := walls
- Γ_o := outlets

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

$$\mathcal{J}(\boldsymbol{v}(\boldsymbol{\mu}), p(\boldsymbol{\mu}), \boldsymbol{u}(\boldsymbol{\mu})) = \frac{1}{2}\int_\Omega |\boldsymbol{v}(\boldsymbol{\mu}) - \boldsymbol{v_d}|^2 + \frac{\alpha}{2}\int_{\Gamma_o} |\boldsymbol{u}(\boldsymbol{\mu})|^2$$

Parametrized Poiseuille inflow velocity:

$$\boldsymbol{v_{in}}(\boldsymbol{\mu}) = -\frac{\eta\mu}{R_{in}}\left(1 - \frac{r^2}{R_{in}^2}\right)\boldsymbol{n_{in}},$$

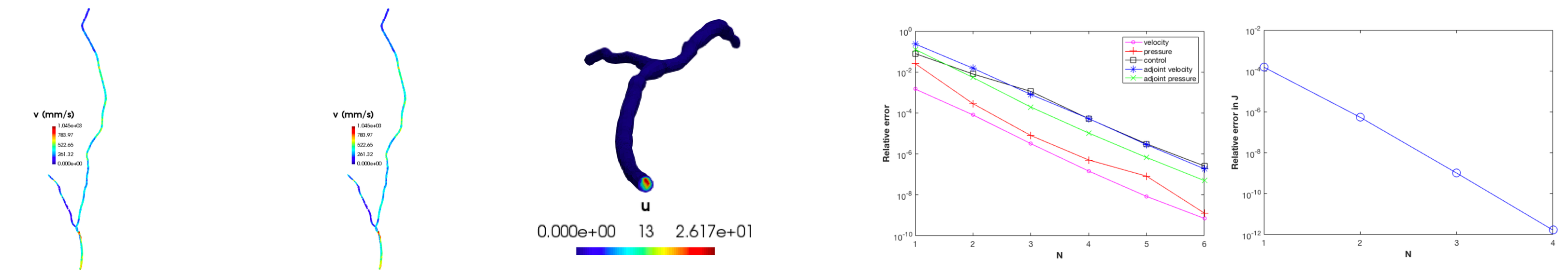
where $\boldsymbol{n_{in}}$ is outward normal to inlet

Parabolic desired velocity:

$$\boldsymbol{v_d} = v_o\left(1 - \frac{r^2}{R^2}\right)\boldsymbol{t_c}, \text{ where}$$

$\boldsymbol{t_c}$ is tangent along axial direction of centerlines

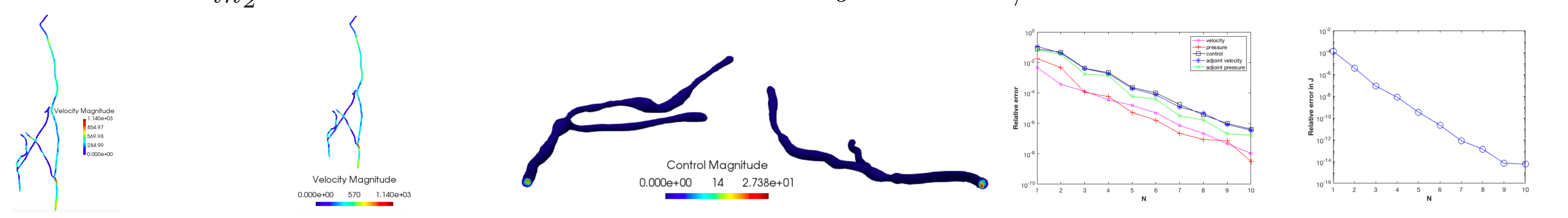
Case I: **Single graft connection: between right internal mammary artery and left anterior descending artery**. $\boldsymbol{\mu} = Re \in [70, 80]$.



FE approx. of velocity | POD approx. of velocity | Boundary control magnitude | Relative error for variables | Relative error for reduction in $\mathcal{J}$

Results showed that a total of 55 reduced bases sufficiently approximate Galerkin finite element spaces comprising of 433288 degrees of freedom, along with $\sim O(10^7)$ reduction in relative error for each variable and similar behavior for $\mathcal{J}$. Moreover computational time is reduced from 1214.3 seconds to 109.3 seconds (online phase).

Case II: **Double graft connections: between right internal mammary artery (RIMA) and left anterior descending artery (LAD), and saphenuous vein (SV) and first obtuse marginal artery (OM1).** $\boldsymbol{\mu} = \left(Re|_{\Gamma_{in_1}}, Re|_{\Gamma_{in_2}}\right) \in [45, 50] \times [70, 80]$, where Γ_{in_1} denotes inlets of SV and OM1 and Γ_{in_2} denotes inlets of RIMA and LAD. $v_o = 350$mm/s.



FE approx. of velocity | POD approx. of velocity | Boundary control magnitude | Relative error for variables | Relative error for reduction in $\mathcal{J}$

Results showed that a total of 93 reduced bases sufficiently approximate Galerkin finite element spaces comprising of 715462 degrees of freedom, along with $\sim O(10^6)$ reduction in relative error for each variable and similar behavior for $\mathcal{J}$. Moreover computational time is reduced from 1848.13 seconds to 202.27 seconds (online phase).

5. Softwares

mathlab.sissa.it/rbnics
mathlab.sissa.it/multiphenics

6. Future perspectives

In environmental sciences a needed development involves **time dependent optimal control** problems. This formulation could be applied in **climatological applications**, in order to forecast and predict possible scenarios in a reliable way. The time dependent model will make simulations more realistic and suited to actual ecological and environmental challenges, as well as more computationally demanding. Therefore, reduced order modeling is a suitable and versatile approach to be exploited.
Furthermore, for cardiovascular applications we propose integration of this framework with shape parametrization and implementation of reduced order methods to gain **reduction in parametric spaces**, in addition to reduced solution spaces. This shall better predict hemodynamics behavior based on computations in different **stenosis shape-dependent scenarios** and thus, the model shall be more feasible for clinical studies.

References

[1] F. Ballarin, E. Faggiano, A. Manzoni, A. Quarteroni, G. Rozza, S. Ippolito, C. Antona, and R. Scrofani. Numerical modeling of hemodynamics scenarios of patient-specific coronary artery bypass grafts. *Biomechanics and Modeling in Mechanobiology*, 16(4):1373–1399, 2017.
[2] F. Ballarin, A. Manzoni, A. Quarteroni, and G. Rozza. Supremizer stabilization of POD–Galerkin approximation of parametrized steady incompressible Navier–Stokes equations. *International Journal for Numerical Methods in Engineering*, 102(5):1136–1161, 2015.
[3] J. S. Hesthaven, G. Rozza, and B. Stamm. *Certified Reduced Basis methods for parametrized partial differential equations.* SpringerBriefs in Mathematics. Springer International Publishing, 2015.
[4] M. Strazzullo, F. Ballarin, R. Mosetti, and G. Rozza. Model reduction for parametrized optimal control problems in environmental marine sciences and engineering. *SIAM Journal on Scientific Computing*, 40(4):B1055–B1079, 2018.
[5] 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. *In preparation*, 2019.

[2]OGS, Trieste, Italy; [3]University of Toronto, Canada; [4]Sunnybrook Health Sciences Centre, Toronto, Canada.

Acknowledgements

We acknowledge the support by European Union Funding for Research and Innovation – Horizon 2020 Program – in the framework of European Research Council Executive Agency: Consolidator Grant H2020 ERC CoG 2015 AROMA-CFD project 681447 “Advanced Reduced Order Methods with Applications in Computational Fluid Dynamics”.