PDEs-Constrained Optimal Control Problems with Reduction Strategies for Biomedical Applications: Time-Dependent Analysis

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Objective

In this poster, we present a computational approach tailored for biomedical applications, leveraging parametrized optimal control problems ($\text{OCP}_{\boldsymbol{\mu}}$) and reduction techniques. Our method involves solving unsteady Navier-Stokes (N-S) equations using a Galerkin finite element approach, with specified initial and/or boundary conditions, while minimizing a cost functional. Choosing appropriate boundary conditions is crucial, particularly in biomedical simulations of the cardiovascular system. These conditions heavily influence computed pressure and flow rates, both clinically significant parameters. To address this, we employ control as an outflow boundary, coupled with proper orthogonal decomposition reduction methods, to compute flow fields in three-dimensional bifurcation vascular networks efficiently.

Problem Definition

Considering a spatial-temporal domain $\Omega\times(0,T)\subset\mathbf{R}^{n_{\text{sd}}}\times(0,T)$, where $n_{\text{sd}}=3$ represents the spatial dimension and T is the final time of the physiological event. The boundary $\Gamma=\Gamma_{\text{w}}\cup\Gamma_{\text{in}}\cup\Gamma_{\text{out}}$, where Γ_{w}, Γ_{in}, and Γ_{out}, respectively, represent the wall, inlet, and outflow boundaries of the computational geometry. We aim at solving $\text{OCP}_{\boldsymbol{\mu}}$ with parametric dependence, for which the optimal solution depends on the parameter vector $\boldsymbol{\mu}\in\mathcal{D}$, where $\mathcal{D}\in\mathbb{R}^P$ is the parameter space with $P\geq 1$.
The parametrized optimal control problem ($\text{OCP}_{\boldsymbol{\mu}}$) reads:

$$\text{find}\quad u(t,\boldsymbol{\mu})\in\mathcal{U},\qquad u(t,\boldsymbol{\mu})=\operatorname{argmin}\left(J\left(\mathbf{v}(t,\boldsymbol{\mu}),u(t,\boldsymbol{\mu});\boldsymbol{\mu}\right)\right), \tag{1}$$

for any given $\boldsymbol{\mu}\in\mathcal{D}$, where $u(t,\boldsymbol{\mu})\in\mathcal{U}$ is the control variable, $J(\cdot,\cdot;\boldsymbol{\mu})$ is the cost functional, and $\mathbf{v}(t,\boldsymbol{\mu})\,(=(\boldsymbol{v}(t,\boldsymbol{\mu}),p(t,\boldsymbol{\mu})))\in\mathbb{V}\times\mathbb{P}$ is the solution of the following state equation represented by the unsteady, incompressible N-S equations with the given initial and boundary conditions. Consider the functional spaces: $\mathbb{V}=L^2\left(0,T;[H^1_\Gamma(\Omega)]^{n_{\text{sd}}}\right)\cap H^1\left(0,T;[H^1_\Gamma(\Omega)^*]^{n_{\text{sd}}}\right)$, and $\mathbb{P}=L^2\left(0,T;L^2(\Omega)\right)$ are known as *state spaces* of velocity and pressure, respectively. The symbol $*$ represents the *dual space* of the funcational space, also consider the *control space* $\mathcal{U}$ as $L^2\left(0,T;[L^2(\Omega)]^{n_{\text{sd}}}\right)$.
The cost functional $\mathcal{J}$ is expressed as:

$$\mathcal{J}(\mathbf{v},u;\boldsymbol{\mu})=\frac{1}{2}\int_0^T\int_\Omega m(\mathbf{v}(\boldsymbol{\mu})-v_d(\boldsymbol{\mu}),\mathbf{v}(\boldsymbol{\mu})-v_d(\boldsymbol{\mu});\boldsymbol{\mu})+\frac{\alpha}{2}\int_0^T\int_\Omega n(u(\boldsymbol{\mu}),u(\boldsymbol{\mu});\boldsymbol{\mu}), \tag{2}$$

where $m(\mathbf{v}(\boldsymbol{\mu})-v_d(\boldsymbol{\mu}),\mathbf{v}-v_d(\boldsymbol{\mu}))=\|\mathbf{v}(\boldsymbol{\mu})-v_d(\boldsymbol{\mu})\|^2_{\mathbb{V}}$ a symmetric, continuous and non-negative form associated with the velocity state space over Ω while $n(u(\boldsymbol{\mu}),u(\boldsymbol{\mu});\boldsymbol{\mu})=\|u(\boldsymbol{\mu})\|^2_{\mathcal{U}}$ is symmetric, coercive and bounded bilinear form associated with the control space.
The cost functional is *subjected to the Galerkin variational formulation of the* parametrized unsteady N-S equations, *state equations*, reads:

$$\begin{aligned}
\frac{\partial\mathbf{v}(\boldsymbol{\mu})}{\partial t}+\left(\mathbf{v}(\boldsymbol{\mu})\cdot\nabla\right)\mathbf{v}(\boldsymbol{\mu})+\nabla p(\boldsymbol{\mu})&=\nu\,\Delta\mathbf{v}(\boldsymbol{\mu}), && \text{in } \Omega\times(0,T),\\
\nabla\cdot\mathbf{v}(\boldsymbol{\mu})&=0, && \text{in } \Omega\times(0,T),\\
\mathbf{v}(\boldsymbol{\mu})&=-\frac{\nu}{R_{in}}\left(1-\frac{r^2}{R_{in}^2}\right)\mathbf{n}_{in}, && \text{on } \Gamma_{in}\times(0,T),\\
\mathbf{v}(\boldsymbol{\mu})&=0, && \text{on } \Gamma_{w}\times(0,T),\\
(\nu\,\nabla\mathbf{v}(\boldsymbol{\mu})-p(\boldsymbol{\mu}))\cdot\mathbf{n}&=u(\boldsymbol{\mu}), && \text{on } \Gamma_{out}\times(0,T),\\
\mathbf{v}(\boldsymbol{\mu})\,(\mathbf{x},0)&=\mathbf{v}_0(\boldsymbol{\mu}), && \text{on } \Omega\times\{0\},
\end{aligned} \tag{3}$$

wherein p represents the pressure, $\mathbf{v}$ denotes the velocity vector, and $\mathbf{n}$ signifies the unit outward normal vector on the boundary Γ. The kinematic viscosity is denoted by ν. Additionally, wherein r represents the radius of cross-sections computed using centerlines, R_{in} denotes the radius of inlet cross-sections, and $u(\mu)$ is the control set as an outflow boundary. Here, $\alpha>0$ is a predetermined constant, and $v_d(\boldsymbol{\mu})\in\mathcal{Z}$ represents a desired velocity within the observation space $\mathcal{Z}\supset\mathbb{V}$. The strategies for solving $\text{OCP}_{\boldsymbol{\mu}}$ are elaborated in the reports [1, 3, 4], addressing diverse types of parametrized PDEs that define the dynamical systems. Our methodology follows the *optimize-discretize-reduce* approach. In the optimization step, we formulate a coupled optimality system satisfying the first-order **Karush-Kuhn-Tucker** optimality conditions for the Lagrangian operator ($\mathcal{L}$) with the adjoint variable z, which is

$$\nabla\mathcal{L}(\mathbf{v},u,z;\boldsymbol{\mu})[\mathbf{s},q,\kappa]=0. \tag{4}$$

Software

RBniCS
https://www.rbnicsproject.org/

MULTIPHENICS
https://mathlab.sissa.it/multiphenics

References

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Reduced Order Methodology

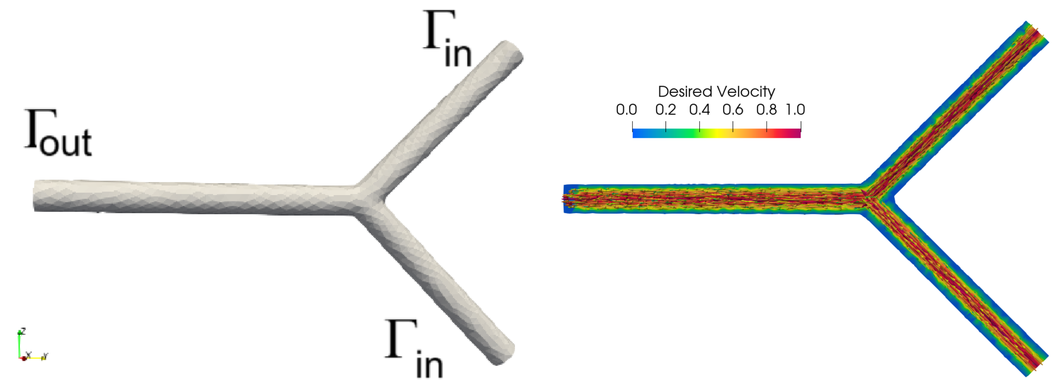
We apply the Galerkin finite element (FE) method to discretize the system described in 3, which is computationally demanding with the dimension of $\mathcal{N}$. To address this challenge, we employ proper orthogonal decomposition (POD)-Galerkin [2], a technique that effectively reduces computational costs while preserving the essential physical features of the model. For any parameter $\boldsymbol{\mu}\in\mathcal{D}$, we aim to find the reduced basis pair $(\mathbf{x}_N(\boldsymbol{\mu}),p_N(\boldsymbol{\mu}))\in\mathbb{V}\times\mathbb{P}\times\mathcal{U}$, where $N\ll\mathcal{N}$, is given as:

$$\begin{cases}
A(x_N,\omega;\boldsymbol{\mu})+B(\omega,p_N;\boldsymbol{\mu})+\mathcal{E}(v_N,s_N,\omega;\boldsymbol{\mu})\\
\quad+\mathcal{E}(s_N,v_N,\omega;\boldsymbol{\mu})=\int_0^T\langle\mathcal{F}(\boldsymbol{\mu}),w_N\rangle\mathrm{d}t, \qquad \forall\omega\in\mathbb{V},\\
B(x_N,\kappa;\boldsymbol{\mu})+\mathcal{E}(v_N,v_N,\kappa;\boldsymbol{\mu})=\int_0^T\langle\mathcal{G}(\boldsymbol{\mu}),\kappa\rangle\mathrm{d}t, \qquad \forall\kappa\in\mathbb{Q}.
\end{cases} \tag{5}$$

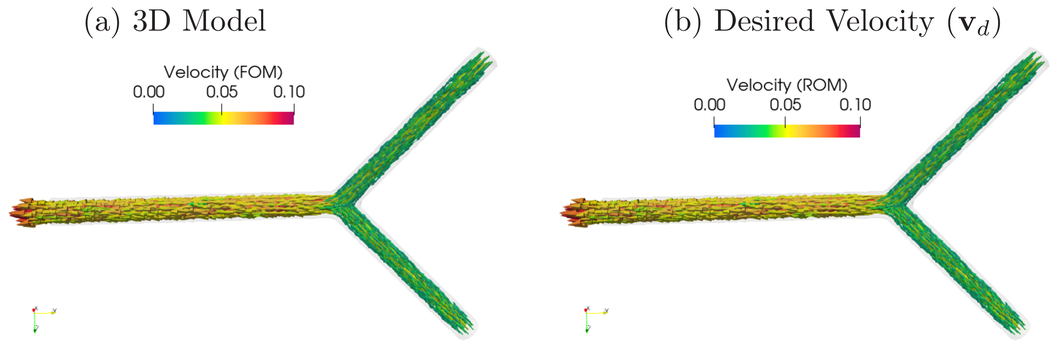
These terms represent the variational operators of the system of equations (2-4) in low-dimensional form. We used the *offline-online strategy* for solving the FE assembled system.

Numerical Results

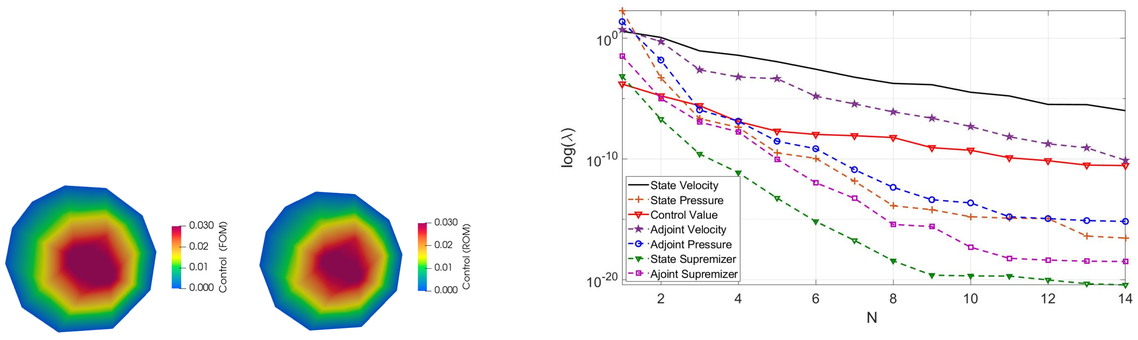
In the cardiovascular system, achieving accurate initial conditions is crucial, often requiring optimization through periodicity computations over the heartbeat; therefore, we consider $\mathbf{v}_0(\mu)=0$ in this computation. We consider the dependent parameter $\boldsymbol{\mu}$ as $\nu\in(0.0,50.0]$, and time $T=1.0s$ with time-step $\Delta t=0.05s$.



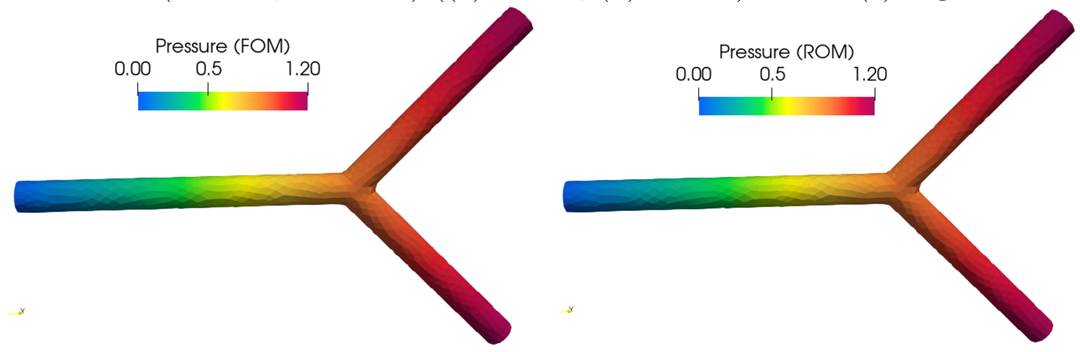
(a) 3D Model (b) Desired Velocity ($\mathbf{v}_d$)



Velocity Distribution ($\nu=1.5$, $T=0.5s$) (Left: FOM , Right: ROM)



Control ($\nu=1.5$, $T=0.5s$) ((a): FOM, (b): ROM) (c) Eigenvalues



Pressure Distribution ($\nu=1.5$, $T=0.5s$)(Left: FOM, Right: ROM)

The flow fields and control exhibit comparable behavior in both *offline* and *online* phases.
Future perspective: We will extend our analysis to patient-specific models, exploring various configurations of boundary conditions and controls.

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