Real-time reduced basis techniques in arterial bypass geometries

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Abstract

The reduced basis method on parametrized domains is applied to approximate blood flow through an arterial bypass. The aim is to provide (a) a sensitivity analysis for relevant geometrical quantities in bypass configurations and (b) rapid and reliable prediction of integral functional outputs (such as fluid mechanics indexes). The goal of this investigation is (i) to achieve design indications for arterial surgery in the perspective of future development for prosthetic bypasses, (ii) to develop numerical methods for optimization and design in biomechanics, and (iii) to provide an input–output relationship led by models with lower complexity and computational costs than the complete solution of fluid dynamics equations by a classical finite element method.

Keywords: Design of improved biomechanical devices; Parametrized PDEs; Generalized Stokes problem; Reduced basis methods; Arterial bypass optimization, Haemodynamics

1. Design and optimization in arterial bypass configurations

When a coronary artery is affected by a stenosis, the heart muscle cannot be properly oxygenated through blood. Aorto-coronaric anastomosis restores the oxygen amount through a bypass surgery overcoming an occlusion. At present, different kinds and shapes of aorto-coronaric bypasses are available and, consequently, different surgery procedures can be devised to set up a bypass. Numerical simulation of physiological flows allows better understanding of phenomena involved in coronary diseases (see [1]) and a potential reduction of surgical and post-surgical failures. It may also suggest new means in bypass surgical procedures as well as with less invasive methods to devise improved bypass configuration (see [2] and [3]). Efficient schemes for reduced basis techniques [4] applied to parametrized partial differential equations (P^2DEs) have been developed to provide useful and real-time indications (outputs) in a repetitive design environment as optimization requires and a sensitivity analysis on important geometrical quantities, such as bypass diameter t, arterial diameter D, stenosis length S, graft angle θ, bypass bridge height H, as shown in Fig. 1. See [5] for a more general framework.

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2. Reduced basis technique for Stokes equations in parametrized domains

The essential properties of a reduced basis method, i.e. (i) the rapid convergence of global reduced basis approximations (Galerkin projection onto a space W_N spanned by solutions of the governing partial differential equations at N selected points in parameter space); (ii) the off-line/on-line computational procedures which decouple the generation and projection stages of the approximation process (for the parameter-affine problems) and (iii) the operation count for the on-line stage – given a new parameter value, we calculate the output of interest – which depends only on N (typically very small) and the parametric complexity of the problem, have allowed computational economies of several orders of magnitude. In the perspective of using low-order methods for real-time pre-process optimization and then higher fidelity method in feedback, at this stage we have adopted the steady Stokes fluid model which provides good approximation in mid-size arteries with low Reynolds number and low mean velocity. A two-dimensional parametrized bypass configuration (Fig. 1) has been built, assembling four simple subdomains. We build a system of P^2DEs depending on a set of geometrical parameters (μ) as coefficients. The Stokes problem on a reference domain Ω in its weak formulation reads:

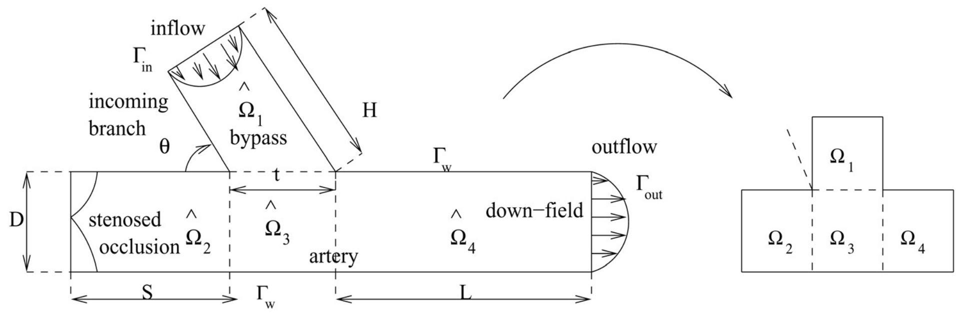

Fig. 1. Schematic bypass configuration and reference domain.

find $\mathbf{u} \in Y = H^1_{\Gamma_D}(\Omega) \times H^1_{\Gamma_D}(\Omega),\ p \in Q = L^2(\Omega),$
$\Omega \subset \mathbb{R}^2$:

$$\begin{cases} \mathcal{A}(\mu;\ \mathbf{u}(\mu),\ \mathbf{w}) + \mathcal{B}(\mu;\ p(\mu),\ \mathbf{w}) = \langle F_s, \mathbf{w} \rangle + \langle F^0, \mathbf{w} \rangle, \\ \quad \forall \mathbf{w} \in Y \\ \mathcal{B}(\mu;\ q, \mathbf{u}(\mu)) = \langle G^0, q \rangle\ \forall q \in Q. \end{cases} \tag{1}$$

F^0, G^0 are terms due to non-homogeneous Dirichlet boundary condition on Γ_{in} (homogeneous Dirichlet on Γ_w and Neumann free-stress condition on $\Gamma_N = \Gamma_{out}$); $\Gamma_D = \Gamma_{in} \cup \Gamma_w$ (Fig. 1). F_s is a distributed force term. In our case: $\Omega = \bigcup_{r=1}^{R} \Omega_r$, $R = 4$. The true domain $\hat{\Omega}$ of Fig. 1 has been traced back to a *reference domain* by an *affine mapping* of the subdomains $\hat{\Omega}_r$ into Ω_r. For any $\hat{x} \in \hat{\Omega}_r$, $r = 1, \ldots, R$, its image $x \in \Omega_r$ is given by $x = \mathcal{G}^r(\mu; \hat{x}) = G^r(\mu)\hat{x} + g^r, 1 \le r \le R$, we thus write $\frac{\partial}{\partial \hat{x}_i} = \frac{\partial x_j}{\partial \hat{x}_i} \frac{\partial}{\partial x_j} = G^r_{ji}(\mu) \frac{\partial}{\partial x_j}$, $1 \le i, j \le d = 2$, and in the reference domain Ω we have:

$$\mathcal{A}(\mu,\ \mathbf{u},\ \mathbf{w}) = \sum_{r=1}^{R} \int_{\Omega_r} \frac{\partial \mathbf{u}}{\partial x_i} \Big(G^r_{ii'}(\mu) \hat{\nu}_{i'j'} G^r_{jj'}(\mu) det(G^r(\mu))^{-1} \Big) \frac{\partial \mathbf{w}}{\partial x_j} d\Omega \ \ \forall \mathbf{w} \in Y \tag{2}$$

$$\mathcal{B}(\mu, p,\ \mathbf{w}) = -\sum_{r=1}^{R} \int_{\Omega_r} p \Big(G^r_{ij}(\mu) det(G^r(\mu))^{-1} \Big) \frac{\partial w_j}{\partial x_i} d\Omega \ \ \forall \mathbf{w} \in Y \tag{3}$$

$$\langle F_s, \mathbf{w} \rangle = \sum_{r=1}^{R} \int_{\Omega_r} \Big(\hat{f}^r det(G^r(\mu))^{-1} \Big) \mathbf{w} d\Omega;\ \langle F^0, \mathbf{w} \rangle = -\langle \mathcal{A} g_{in}, \mathbf{w} \rangle;\ \langle G^0, q \rangle = \langle \mathcal{B} q, g_{in} \rangle \tag{4}$$

where $\hat{\nu}_{i,j} = \nu \delta_{i,j}$, g_{in} is the term due to boundary inflow condition and $\hat{f}_r$ the force field. We introduce the parameter vector $\mu = \{t, D, L, S, H, \theta\} \in \mathcal{D}^\mu \subset \mathbb{R}^P$, $\mathcal{D}^\mu$ is given by:

$$[t_{min}, t_{max}] \times [D_{min}, D_{max}] \times [L_{min}, L_{max}] \times [S_{min}, S_{max}] \times [H_{min}, H_{max}] \times [\theta_{min}, \theta_{max}]$$

The *transformation tensors* for bilinear forms are defined as follows:

$$\nu^r_{ij}(\mu) = G^r_{ii'}(\mu) \hat{\nu}_{i'j'} G^r_{jj'}(\mu) det(G^r(\mu))^{-1}, 1 \le i,j \le 2, \quad r = 1, \ldots, R$$

Then in our case:

$$\nu^1 = \nu \begin{bmatrix} \frac{t}{H} & -\tan\theta \\ -\tan\theta & \frac{1+\tan^2\theta}{t} H \end{bmatrix};\ \ \nu^2 = \nu \begin{bmatrix} \frac{S}{D} & 0 \\ 0 & \frac{D}{S} \end{bmatrix}; \quad \nu^3 = \nu \begin{bmatrix} \frac{t}{D} & 0 \\ 0 & \frac{D}{t} \end{bmatrix};\ \ \nu^4 = \nu \begin{bmatrix} \frac{L}{D} & 0 \\ 0 & \frac{D}{L} \end{bmatrix} \tag{5}$$

The tensors for *pressure and divergence forms* are:

$$\mathcal{X}^r_{ij}(\mu) = G^r_{ij} det(G^r(\mu))^{-1}, 1 \le i,j \le 2, r = 1, \ldots, R$$

and are given by:

$$\mathcal{X}^1 = \begin{bmatrix} t-H & \tan\theta \\ 0 & H \end{bmatrix};\ \ \mathcal{X}^2 = \begin{bmatrix} S & 0 \\ 0 & D \end{bmatrix}; \quad \mathcal{X}^3 = \begin{bmatrix} t & 0 \\ 0 & D \end{bmatrix};\ \ \mathcal{X}^4 = \begin{bmatrix} L & 0 \\ 0 & D \end{bmatrix} \tag{6}$$

Furthermore, we may define

$$\Theta^{q(i,j,r)}(\mu) = \nu^r_{ij}(\mu),\ \ \Big\langle \mathcal{A}^{q(i,j,r)} \mathbf{u}, \mathbf{w} \Big\rangle = \int_{\Omega_r} \frac{\partial \mathbf{u}}{\partial x_i} \frac{\partial \mathbf{w}}{\partial x_j} d\Omega \tag{7}$$

$$\Phi^{s(i,j,r)}(\mu) = \mathcal{X}^r_{ij}(\mu),\ \ \Big\langle \mathcal{B}^{s(i,j,r)} p, \mathbf{w} \Big\rangle = -\int_{\Omega_r} p \frac{\partial w_i}{\partial x_j} d\Omega \tag{8}$$

for $1 \le r \le R$, $1 \le i, j \le d = 2$. So:

$$\mathcal{A}(\mu, \mathbf{u}, \mathbf{w}) = \sum_{q=1}^{Q^a} \Theta^q(\mu)\mathcal{A}(\mathbf{u}, \mathbf{w})^q;$$

$$\mathcal{B}(\mu, p, \mathbf{w}) = \sum_{s=1}^{Q^b} \Phi^s(\mu)\mathcal{B}(p, \mathbf{w})^s$$

in our case $Q^a = 20$ and $Q^b = 9$, in reality max $(Q^a) = d \times d \times d \times R = 32$ and max $(Q^b) = d \times d \times R = 16$.

In the reduced basis approximation we take some suitable samples $S_N^\mu = \{\mu^1, \ldots, \mu^N\}$, where $\mu^n \in \mathcal{D}^\mu$, $n = 1, \ldots, N$.

The *reduced basis pressure space* is Q_N = span $\{\xi_n, n = 1, \ldots, N\}$, where $\xi_n = p(\mu^n)$.

The *reduced basis velocity space* is Y_N^μ = span $\{\sigma_n, n = 1, \ldots, 2N\}$ = span $\{\zeta_n, T^\mu \zeta_n, n = 1, \ldots, N\}$, where $\zeta_n = \mathbf{u}(\mu^n)$ and T^μ: $Q \to Y$ is the supremizer operator $(T^\mu q, \mathbf{w})_Y = \mathcal{B}(\mu; q, \mathbf{w};)$, $\forall$ $\mathbf{w} \in Y$. Using the *affine dependence* of $\mathcal{B}(q, \mathbf{w}, \mu)$ on the parameter and the *linearity of* T^μ we can write $T^\mu \xi = \sum_{q=1}^{Q^b} \Phi^q(\mu) T^q \xi$ for any ξ and μ. The problem in reduced basis approximation reads: find $(\mathbf{u}_N(\mu), p_N(\mu)) \in Y_N^\mu \times Q_N$

$$\begin{cases} \mathcal{A}(\mu; \mathbf{u}_N(\mu), \mathbf{w}) + \mathcal{B}(\mu; p_N(\mu), \mathbf{w}) = \langle F, \mathbf{w} \rangle, & \forall w \in Y_N^\mu \\ \mathcal{B}(\mu; q, \mathbf{u}_N(\mu)) = \langle G, q \rangle, \quad \forall q \in Q_N \end{cases} \tag{9}$$

The supremizers solutions guarantee the fulfillment of an equivalent *inf-sup* (LBB) condition: $\beta_N(\mu) \geq \beta(\mu) \geq \beta_0 > 0$, $\forall$ $\mu \in \mathcal{D}^\mu$ where
$\beta_N(\mu) = \inf_{q \in Q_N} \sup_{\mathbf{w} \in Y_N^\mu} \frac{\mathcal{B}(\mu; q, \mathbf{w})}{\|\mathbf{w}\| Y \|q\| Q}$ and
$\beta(\mu) = \inf_{q \in Q} \sup_{\mathbf{w} \in Y} \frac{\mathcal{B}(\mu; q, \mathbf{w})}{\|\mathbf{w}\| Y \|q\| Q}$ (see [6]).

For a new sample μ we look for a solution

$$\mathbf{u}_N(\mu) = \sum_{j=1}^{2N} \mathbf{u}_{Nj}(\mu)\sigma_j, \quad p_N(\mu) = \sum_{l=1}^{N} p_{Nl}(\mu)\xi_l$$

where the unknown coefficients are found as the solution of the following reduced basis linear system:

$$\begin{cases} \sum_{j=1}^{2N} A_{ij}^\mu \mathbf{u}_{Nj}(\mu) + \sum_{l=1}^{N} B_{il}^\mu p_{Nl}(\mu) = F_i^\mu & 1 \leq i \leq 2N \\ \sum_{j=1}^{2N} B_{jl}^\mu \mathbf{u}_{Nj}(\mu) = G_l^\mu \quad 1 \leq l \leq N \end{cases} \tag{10}$$

where:

$$A_{ij}^\mu = \sum_{k=1}^{Q^a} \Theta^k(\mu)\mathcal{A}(\sigma_i, \sigma_j)^k, \; B_{il}^\mu = \sum_{k=1}^{Q^b} \Phi^k(\mu)\mathcal{B}(\sigma_i, \xi_l)^k$$

$$F_i^\mu = \langle F, \sigma_i \rangle, \; G_l^\mu = \langle G, \xi_l \rangle, \; 1 \leq i,j \leq 2N, 1 \leq l \leq N$$

For further details on Stokes reduced basis approximation and other supremizers options see [7]. As a measure of blood flow perturbation we consider for example the mean blood velocity:

$$s(\mu) = \sum_{r=1}^{R} \frac{\int_{\Omega_r} |\mathbf{u}| d\Omega}{\int_{\Omega_r} d\Omega} \tag{11}$$

3. Some numerical results

With great computational cost savings we can provide in real time useful clinical indication dealing with a great number (i.e. hundreds) of bypass configurations and understand the role of each geometrical parameter and their reciprocal influence. Numerical results indicate a very good convergence behaviour and a tight control on the maximum N, i.e. on the dimension of reduced basis matrices, whose assembling computational costs are $O(Q^a\ (Q^b + 1)^2 4N^2)$ for the sub-matrix A, $O((Q^b + 1)^2 2N^2)$ for B, $O((Q^b + 1)\ N)$ for F and $O(9N^3)$ for the inversion of the global matrix. Numerical tests on the bypass configuration (Fig. 1) have been carried out imposing a mean Reynolds number of 10^3, a blood kinematic viscosity ν of $4 \cdot 10^{-6}$ m^2 s^{-1} and a force field: f = (0,9.8). Solutions used as basis functions are obtained by the Galerkin-finite element method with Taylor–Hood elements (P^2 and P^1 for velocity and pressure, respectively). Figure 2 shows good convergence of the errors (H^1 for velocity and L^2 for pressure) testing a great number of configurations. We have carried out three different medical application-oriented tests by our *input–output* methodology. Figure 3 shows the first case study where we have investigated the bypass graft angle perturbation (other parameters are frozen) measuring the increase of our output of interest, Eq.(11): varying θ from ~ 0 to $\frac{\pi}{3}$ the increase of the mean blood velocity is very high in the range $[0, \pi/6]$ and smoothed in the range $[\pi/6, \pi/3]$. Results are shown for different N to underline the fidelity of approximation

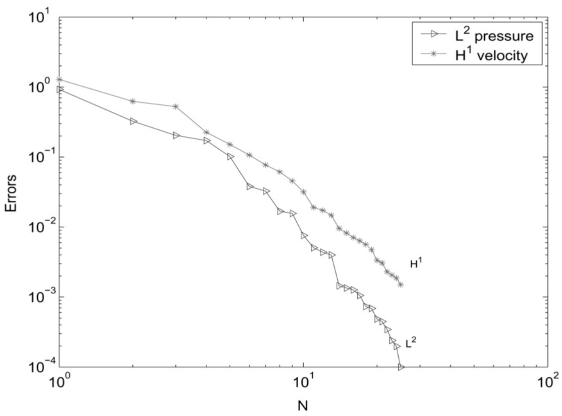

Fig. 2. Reduced basis convergence results: mean error on velocity and pressure.

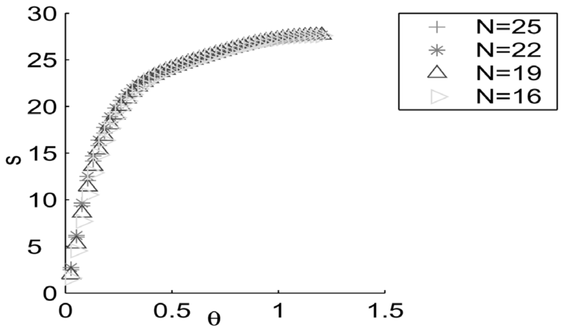

Fig. 3. Output s [$ms^{-1} \cdot 10^{-2}$] versus the parameter θ.

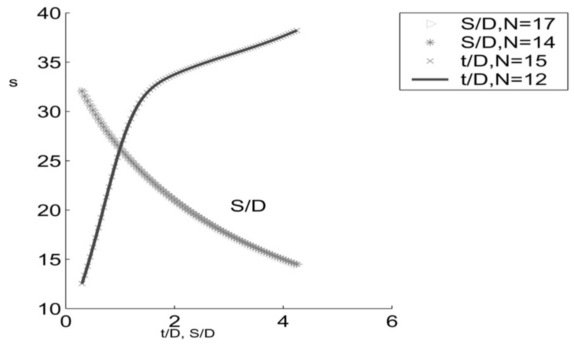

Fig. 4. Output s [$ms^{-1} \cdot 10^{-2}$] versus the ratios t/D and S/D.

with a few basis functions. Figure 4 shows the flow perturbations with respect to the quantity S/D: the ratio between the stenosis length and the arterial diameter (best performances when $S/D \geq 1$) and the quantity t/D (improving performances when the ratio is less than unity, i.e. bypass diameter smaller than arterial diameter).

4. Conclusion

Development guidelines are devoted to the application of reduced basis (i) to Navier–Stokes equations [8] in parametrized domains, (ii) in problems involving non-affine mapping dependence (introduction of curved walls) [9] and (iii) in using a great number of geometrical parameters.

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