Reduced basis method for the reliable model reduction of Navier-Stokes equations in cardiovascular modelling

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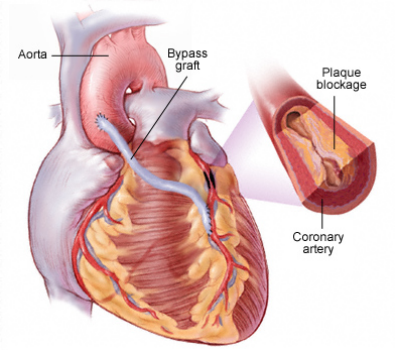
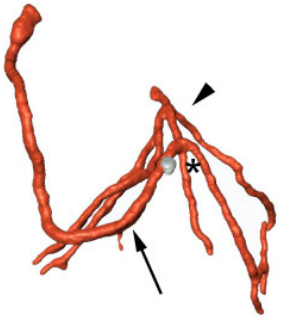
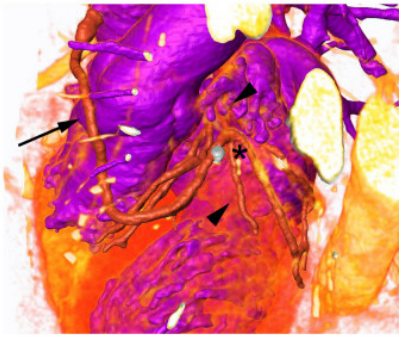
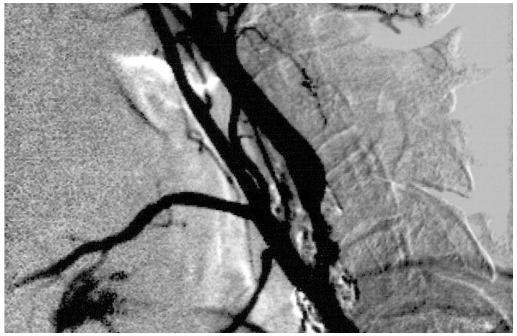
Challenges in modelling the human cardiovascular system

- Human cardiovascular system is a complex flow network of different spatial and temporal scales.
- When investigating fluid flow processes the flow geometries are changing over time. The geometric variation causes a strong nonlinearity in the equations.
- Medical professionals are interested in accurate simulation of spatial quantities, such as wall shear stresses at the location of a possible pathology.
- Computational costs can become unacceptably high, especially if the objective is to model the entire network, and strategies to reduce numerical efforts and model order are being developed.









Parametric incompressible Navier-Stokes equations (steady case)

We consider the following model problem:

For a given parameter vector $\mu \in \mathscr{D} \subset \mathbb{R}^P$, find $U(\mu) \in X$ s.t.

$$a(U(\mu), V; \mu) = f(V; \mu) \quad \forall V \in X, \forall \mu \in \mathscr{D}$$

where $U := (\mathbf{u}, p)$ and $V := (\mathbf{v}, q)$ consist of the velocity field and the pressure, the product space $X = \mathscr{V} \times \mathscr{Q} \subset [H^1(\Omega)]^2 \times L^2(\Omega)$, and the problem consists of a linear part a_0 and a nonlinear (quadratic in U) part a_1:

$$a(U, V; \mu) := a_0(U, V; \mu) + a_1(U, U, V; \mu) \quad \forall U, V \in X, \forall \mu \in \mathscr{D}$$

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For example, if the parameter is simply $\mu = \nu$ (fluid viscosity), we have

$$a_0(U, V; \mu) = \int_\Omega [\mu \nabla \mathbf{u} : \nabla \mathbf{v} - p \operatorname{div}(\mathbf{v}) - q \operatorname{div}(\mathbf{u})] \, d\Omega$$

$$a_1(U, W, V) = \int_\Omega \mathbf{v} \cdot (\mathbf{u} \cdot \nabla) \mathbf{w} \, d\Omega$$

$+$ appropriate boundary conditions.

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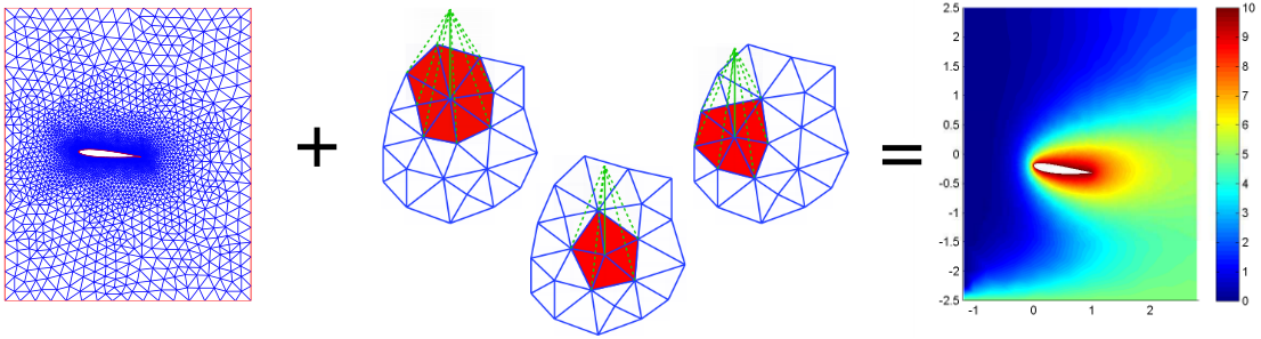
Typically we are interested in linear functionals of the field solutions (outputs) $s(\mu) := \ell(U(\mu))$, i.e. need to find a reduced model $\widetilde{s}(\mu)$ that has is within **certified** tolerance of the actual outputs: $|s(\mu) - \widetilde{s}(\mu)| <$ TOL for all $\mu \in \mathscr{D}$.

Finite element approximation to the Navier-Stokes solution



- Starting from initial guess U^0, solve at each step k of a FP iteration for U^k s.t.

$$a_0(U^k, V; \mu) + a_1(U^{k-1}, U^k, V) = f(V) \quad \forall V \in \mathscr{V} \times \mathscr{Q}$$

until convergence.

- Stable discretization with $\mathbb{P}_2/\mathbb{P}_1$ FE spaces for velocity and pressure

$$\mathscr{V}_h := \{\mathbf{v} \in C(\Omega, \mathbb{R}^d) : \mathbf{v}|_K \in [P_2(K)]^2, \quad \forall K \in \mathscr{T}_h\} \subset \mathscr{V}$$
$$\mathscr{Q}_h := \{q \in C(\Omega, \mathbb{R}) : q|_K \in P_1(K), \quad \forall K \in \mathscr{T}_h\} \subset \mathscr{Q}.$$

- Galerkin projection in FE space: solve at each step k for U_h^k s.t.

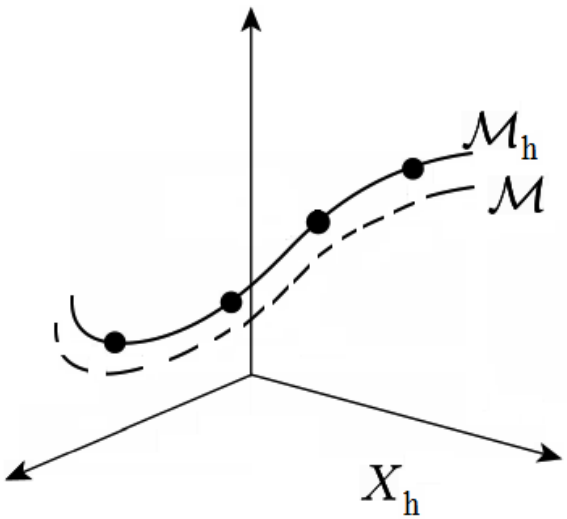
$$a_0(U_h^k, V_h; \mu) + a_1(U_h^{k-1}, U_h^k, V_h) = f(V_h) \quad \forall V_h \in \mathscr{V}_h \times \mathscr{Q}_h$$

until convergence.

Similar approach for the Newton's method...

Reduced basis approximation of the finite element solution

1. Assumption: parametric manifold of FE solutions $\mathscr{M}_h \subset X_h$ is 1) low dimensional and 2) depends smoothly on μ (valid for small Reynolds number)
2. Choose a representative set of parameter values $\mu^1, \ldots, \mu^N$
3. Snapshot solutions $\mathbf{u}_h(\mu^1), \ldots, \mathbf{u}_h(\mu^N)$ span a subspace $\mathscr{V}_h^N$ for the velocity and $p_h(\mu^1), \ldots, p_h(\mu^N)$ span a subspace $\mathscr{Q}_h^N$ for the pressure
4. Galerkin reduced basis: given $\mu \in \mathscr{D}$, find $U_h^N(\mu) \in X_h^N$ s.t.
$$a_0(U_h^{k,N}, V_h^N; \mu) + a_1(U_h^{k-1,N}, U_h^k, V_h^N) = f(V_h^N) \quad \forall V_h^N \in X_h^N$$
5. Adaptive sampling procedure (greedy algorithm) for the choice of $\mu^1, \ldots, \mu^N$



$$\mathscr{M} = \{U(\mu) \in X;\ \mu \in \mathscr{D}\}$$
$$\mathscr{M}_h = \{U_h(\mu) \in X_h;\ \mu \in \mathscr{D}\}$$

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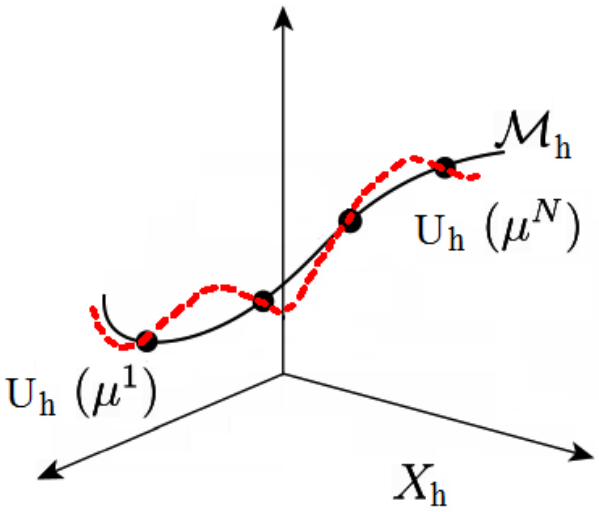

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$$\mathscr{M}_h = \{U_h(\mu) \in X_h;\ \mu \in \mathscr{D}\}$$

$$X_h^N = \text{span}\{U_h(\mu^i),\quad i = 1, \ldots, N\}$$

Reliability / accuracy ?

1. is based on the quality of the sampling
2. relies on computable and rigorous a posteriori error estimator $\Delta_N(\mu)$:

$$\|U_h(\mu) - U_h^N(\mu)\|_X \leq \Delta_N(\mu), \qquad |s(\mu) - s^N(\mu)| \leq \Delta_N^s(\mu) = \|\ell\|_{X_h'} \Delta_N(\mu)$$

A posteriori error estimation of the reduced basis approximation

(Veroy-Patera 2005) If $\tau_N(\mu) < 1$ and $\beta_h(\mu) > 0$ there exists a unique solution $U_h(\mu)$ s.t.

$$||U_h(\mu) - U_h^N(\mu)||_X \leq \Delta_N(\mu) =: \frac{\beta_h(\mu)}{\rho(\mu)} \left[1 - \sqrt{1 - \tau_N(\mu)}\right]$$

Here:

- $\beta_h(\mu)$ is the Babuska inf-sup constant that needs to be estimated

$$\inf_{W \in X_h} \sup_{V \in X_h} \frac{da(U_h(\mu);\mu)(W,V)}{||W||||V||} = \beta_h(\mu) > \beta_0 > 0$$

  for the Fréchet derivative of $a(U, W, V)$ w.r.t first argument at U_h
- $\rho(\mu)$ is a Sobolev embedding constant that needs to be estimated
- $\tau_N(\mu) := \frac{2\rho(\mu)\varepsilon_N(\mu)}{\beta_h(\mu)^2}$, where $\varepsilon_N(\mu) := ||f(\cdot;\mu) - a(U_h^N, \cdot;\mu)||_{X_h'}$ is the RB residual

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Note: for large viscosity we obtain the Stokes equations and the estimator simplifies to

$$||U_h(\mu) - U_h^N(\mu)|| \leq \Delta_N(\mu) = \frac{\varepsilon_N(\mu)}{\beta_h(\mu)} \Bigg\} \text{ key ingredients}$$

Generalization of reduced basis method to parametric geometries

Parametrized formulation on fixed reference domain (Rozza 2009)

Evaluate output of interest $s(\mu) = \ell(U_h(\mu))$

$$\text{s.t.} \quad U_h = (\mathbf{u}_h(\mu), p(\mu)) \in \mathscr{V}_h(\widehat{\Omega}) \times \mathscr{Q}_h(\widehat{\Omega}) \quad \text{solves}$$

$$a(U_h(\mu), V_h; \mu) = f(V_h; \mu) \qquad \forall\ V_h \in X(\widehat{\Omega})$$

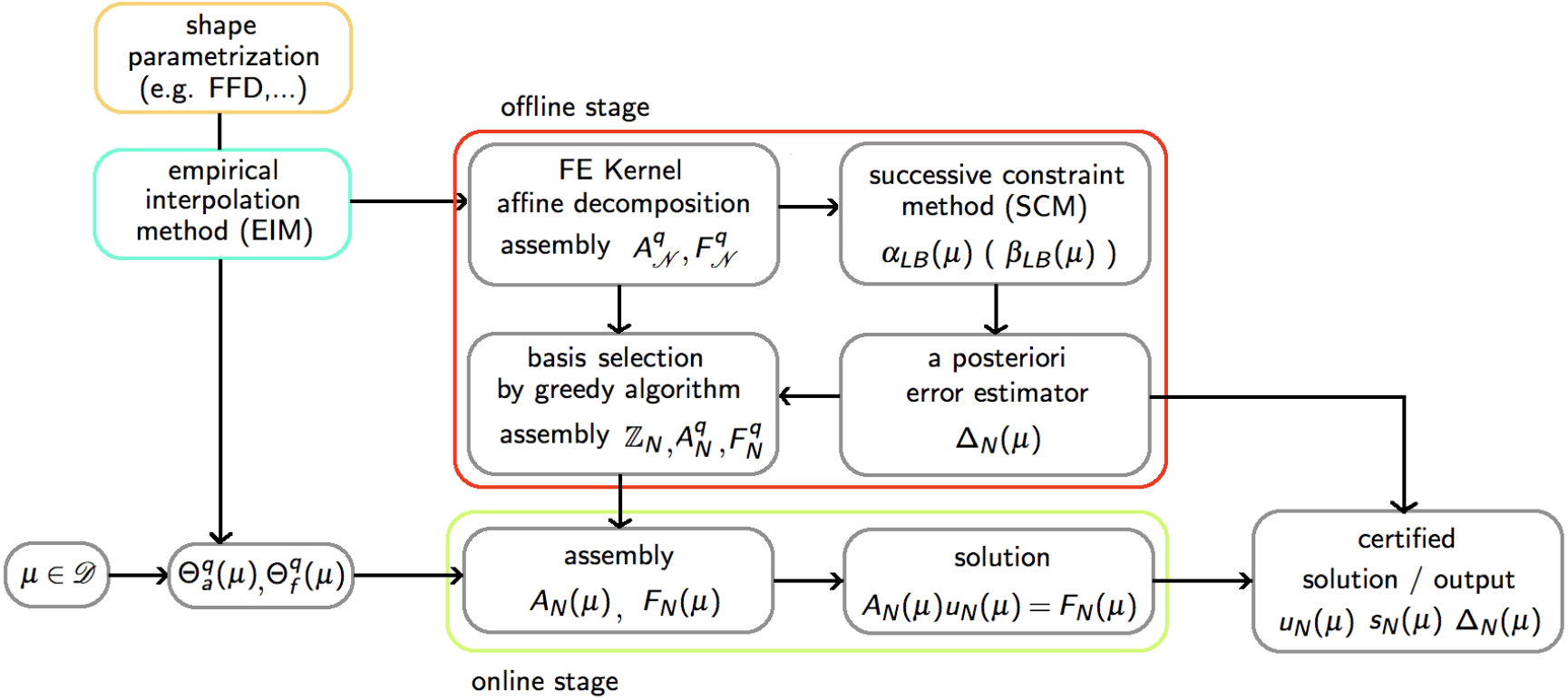
$$a((\mathbf{v}, p), (\mathbf{w}, q); \mu) = \int_{\widehat{\Omega}} \frac{\partial \mathbf{v}}{\partial x_i} \nu_{ij}(x, \mu) \frac{\partial \mathbf{w}}{\partial x_j} d\Omega - \int_{\widehat{\Omega}} p \chi_{ij}(x, \mu) \frac{\partial w_j}{\partial x_i} d\Omega - \int_{\widehat{\Omega}} q \chi_{ij}(x, \mu) \frac{\partial v_j}{\partial x_i} d\Omega,$$

- The parametrized (original) domain $\Omega(\mu)$ is the image of a reference domain $\widehat{\Omega}$ through a parametric mapping $T(\cdot; \mu) : \widehat{\Omega} \to \Omega(\mu)$
- One possible parametrization using free-form deformations (L.-Rozza 2009)
- Transformation tensors ($\mathbf{J}_T = \mathbf{J}_T(x, \mu) =$ Jacobian of $T(x, \mu)$)

$$\nu(x, \mu) = \mathbf{J}_T^{-1} \nu^o \mathbf{J}_T^{-T} |\mathbf{J}_T| \quad \text{and} \quad \chi(x, \mu) = \mathbf{J}_T^{-1} \chi^o |\mathbf{J}_T|$$

- Problem reduced to a parametric PDEs system on $\widehat{\Omega}$ (reference domain)

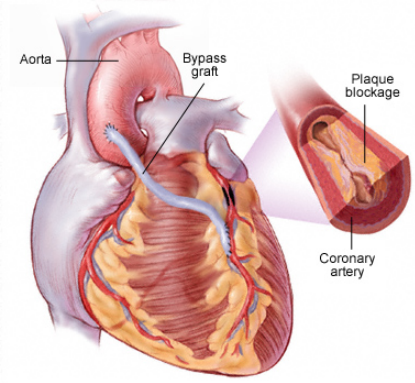
Reduced basis offline/online computational framework



- Offline stage involves precomputation of structures required for the certified error estimate and choice of the reduced basis functions.
- Online stage has complexity only depending on N and allows evaluation of output $s(\mu)$ for any $\mu \in \mathscr{D}$ with a certified error bounds.

Shape Optimization of Aorto-Coronaric Bypass Grafts

- Shape optimization of cardiovascular geometries helps to avoid post-surgical complications
- Local fluid patterns (vorticity) and wall shear stress are strictly related to the development of cardiovascular diseases



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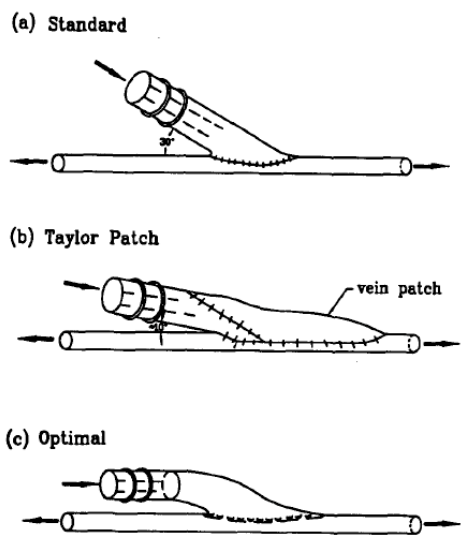
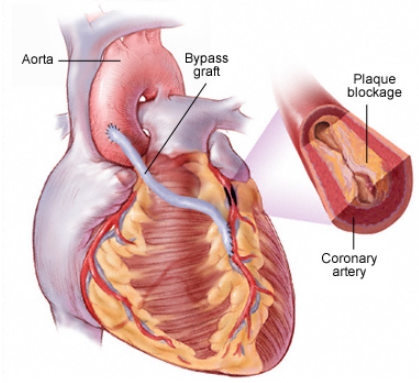


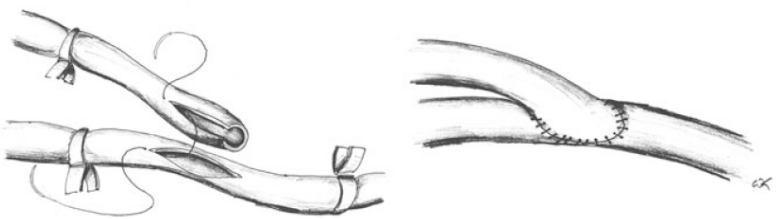
Shape optimization problem [Agoshkov-Quarteroni-Rozza 2006]

$$\min J(\Omega;\mathbf{v}) \quad \text{s.t.}$$

$$\begin{cases} -\nu\Delta\mathbf{v}+\nabla p=\mathbf{f} & \text{in } \Omega \\ \nabla\cdot\mathbf{v}=0 & \text{in } \Omega \\ \mathbf{v}=\mathbf{v}_g & \text{on } \Gamma_D := \partial\Omega\setminus\Gamma_{out}, \\ -p\cdot\mathbf{n}+\nu\dfrac{\partial\mathbf{v}}{\partial\mathbf{n}}=\mathbf{0} & \text{on } \Gamma_{out} \end{cases}$$

$$J_o(\Omega;\mathbf{v})=\int_{\Omega^{df}}|\nabla\times\mathbf{v}|^2 d\Omega, \qquad J_o(\Omega;\mathbf{v})=-\int_{\partial\Omega}\nu\frac{\partial\mathbf{v}}{\partial\mathbf{n}}\cdot\mathbf{t}\,d\Gamma_o$$



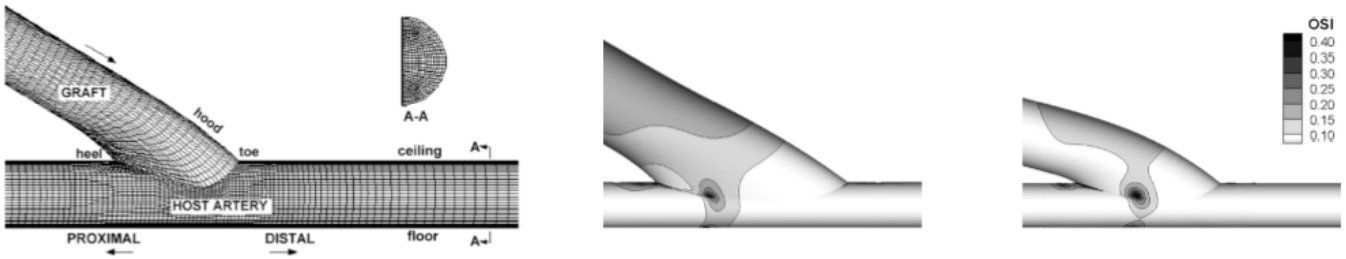


Pictures taken from: Lei et al., J Vasc. Surg. 25(1997),637-646; Loth et al., Annu. Rev. Fluid Mech. 40(2008),367-393.

Shape optimization of aorto-coronaric bypass grafts

A possible free-form deformation approach [Manzoni-Quarteroni-Rozza 2010]

- Several analyses show a deep impact of the graft-artery diameter ratio Φ and anastomotic angle α on shear stress and vorticity distributions



Oscillatory shear stress with different graft-artery diameter ratios Φ and anastomotic angles α.
Picture taken from F.L. Xiong, C.K. Chong, Med. Eng. & Phys. 30(2008),311-320.

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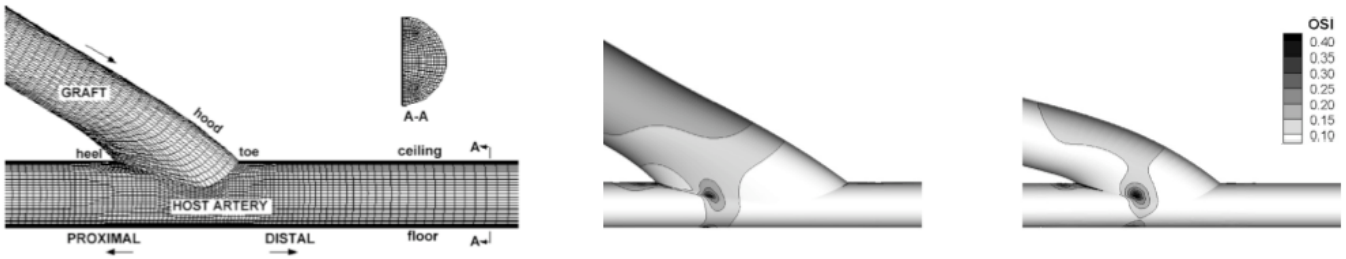

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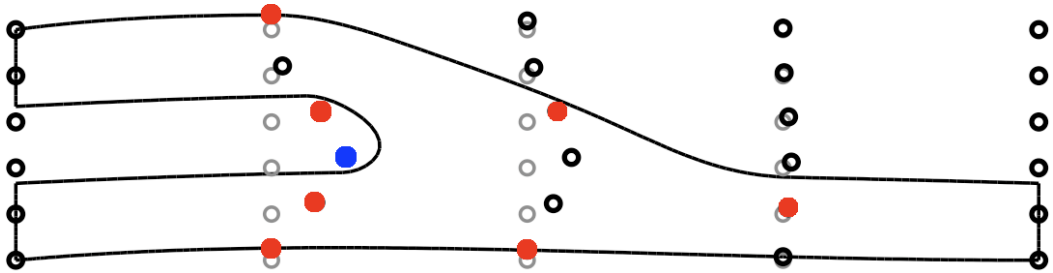
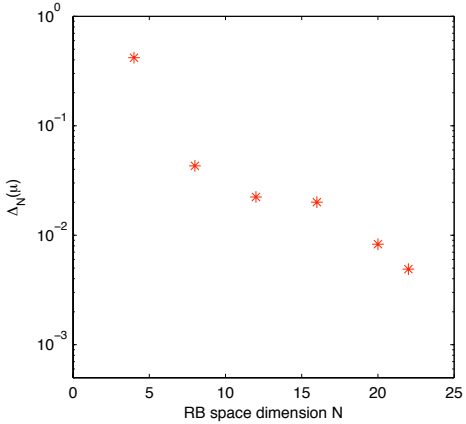
- In order to get a low-dimensional FFD parametrization we need to maximize the influence of the control points by placing them close to the sensitive regions



- 8 parameters (7 vertical • and 1 horizontal • displacements) to control the anastomotic angle, the graft-artery diameter ratio, the upper side, the lower wall

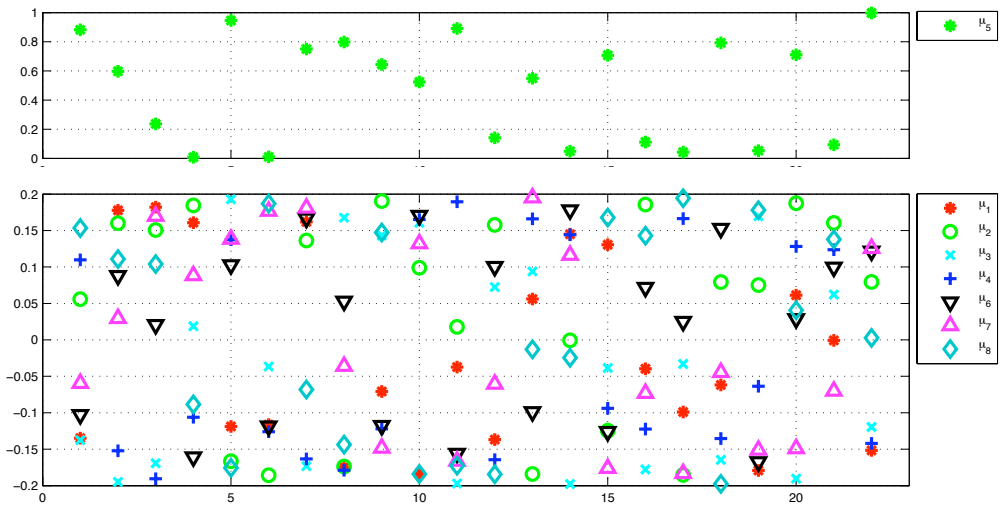
Shape optimization of aorto-coronaric bypass grafts

RB approximation space construction



Number of FE dof $\mathcal{N}_{\mathbf{v}} + \mathcal{N}_p$	35997
Lattice FFD control points $\mathbf{P}_{i,j}$	5×6
Number of design variables P	8
Number of RB functions N	22
Error tolerance RB greedy ε_{tol}^{RB}	5×10^{-3}
Affine operator components Q	222

Error estimation (energy norm) for RB space construction (greedy procedure) and selected snapshots

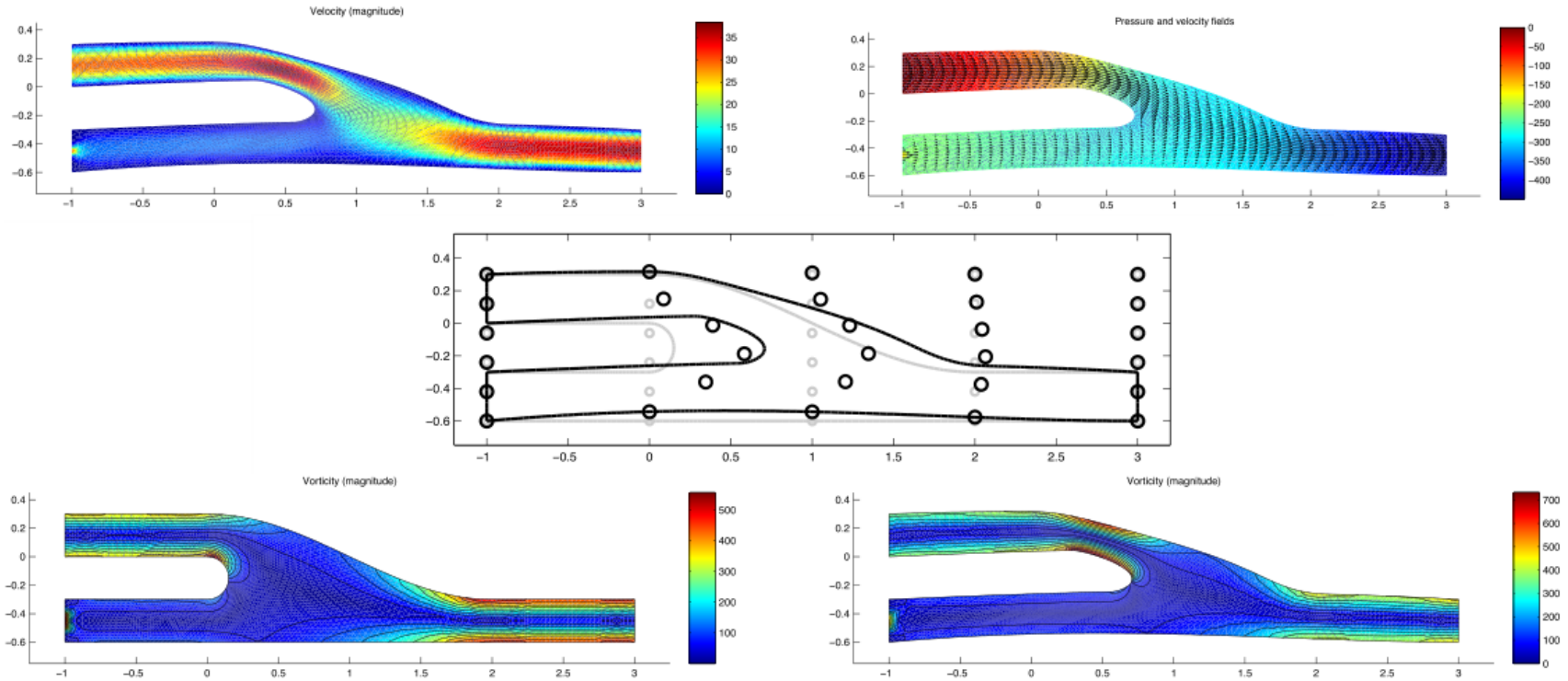


Reduction in linear system dimension	500:1
Computational speedup (single flow simulation)	107
Reduction in parametric complexity w.r.t. explicit nodal deformation	102:1

Shape optimization of aorto-coronaric bypass grafts

Vorticity Minimization (downfield region)

- Automatic iterative minimization procedure (sequential quadratic programming)
- Vorticity evaluation by using the reduced basis velocity at each step [Manzoni-Quarteroni-Rozza 2010]



Optimized bypass anastomosis and Stokes flow (velocity magnitude and pressure)
Optimal (black) and unperturbed (grey) configurations of FFD parametrization
Vorticity magnitude for the unperturbed (left) and optimal (right) configuration

Reduction of time-dependent Navier-Stokes (ongoing work)

One-dimensional prototype problem (viscous Burgers' equation): find $u(\mu) \in L^2(0,T;V) \cap C^0([0,T];L^2(\Omega))$ s.t.

$$\frac{d}{dt}(u(\mu),v) + \mu \int_\Omega u_x(\mu) v_x \, dx - \frac{1}{2} \int_\Omega u^2(\mu) v_x \, dx = f(v) \quad \forall v \in V$$

where $\Omega = (0,1)$ and $V \subset H^1(\Omega)$.

- Time discretization with implicit Euler $\Longrightarrow$ time-discrete equations
- Spatial discretization with FEM + reduced basis reduction as before
- Stability constant $\rho_N := \inf_{v \in V} \frac{da(u_h^{N,k})(v,v)}{||v||_X}$ not necessarily positive!
- A posteriori estimator (Nguyen-Rozza-Patera 2009) for $k = 1, \ldots, \frac{T}{\Delta t}$

$$||u_h^k(\mu) - u_h^{N,k}(\mu)|| \leq \triangle_N^k(\mu) := \sqrt{\frac{\frac{\Delta t}{\mu} \sum_{m=1}^k \left(\varepsilon_N^2(t^m;\mu) \prod_{j=1}^{m-1} (1 + \Delta t \rho_N(t^j;\mu)) \right)}{\prod_{m=1}^k (1 + \Delta t \rho_N(t^m;\mu))}}$$

BUT the error bound grows exponentially in time

Conclusions

- Reduced basis methods a reliable MOR method for parametric PDEs
- Parameters can also describe the (variable) flow geometry
- Certified error bounds for spatial outputs of reduced field variables
- Extensions to noncoercive (Stokes) and nonlinear (Navier-Stokes) cases
- Future work
  - Time-dependent Navier-Stokes, improved error estimates
  - Reduction of coupled multiphysics problems
  - Parameter identification and inverse problems

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