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Modeling and Complexity Reduction in PDES for Multiphysics

Reduced basis methods for parametrized PDEs, optimal control and shape optimization

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Outline

1. Reduced basis methods

2. Shape parametrization techniques

3. Reduced framework for optimal control/shape optimization

4. Applications in haemodynamics

(Joint with G.Rozza and A.Manzoni)

Reduced Basis Method: Motivations

- ✓ **Parametrized PDEs** problems (parameters μ can be physical - as material properties, boundary data, source terms - or geometrical)
- ✓ **Prediction of engineering outputs** associated with PDEs
- ✓ **Many query** (e.g. control, optimization) and **Real-time** (e.g. parameter estimation, rapid simulation) contexts
- ✓ **Improve** computational performance by using problems of lower dimensions
- ✓ **Offline/Online** decomposition stratagem. Heavy computations (μ-independent) carried out offline provide a database of solutions used for each new online evaluation (μ-dependent)

Formulation

$\mathrm{Pb}(\mu; u(\mu))$

PDE$_\mu$ (weak formulation)

$$u(\mu) \in X : \quad a(u(\mu), v; \mu) = F(v) \qquad \forall v \in X$$
$$s(\mu) = l(u(\mu))$$

$\mathrm{Pb}_{\mathcal{N}}(\mu; u^{\mathcal{N}}(\mu))$

Truth Approximation (FEM)

$$u^{\mathcal{N}}(\mu) \in X^{\mathcal{N}} : \quad a(u^{\mathcal{N}}(\mu), v; \mu) = F(v) \qquad \forall v \in X^{\mathcal{N}}$$
$$s^{\mathcal{N}}(\mu) = l(u^{\mathcal{N}}(\mu))$$

Sampling
Space Construction

OFFLINE

$$S_N = \{\mu^i, \quad i = 1, \dots, N\}$$
$$X_N = \mathrm{span}\{u^{\mathcal{N}}(\mu^i), \quad i = 1, \dots, N\}$$
$$\dim(X_N) = N \ll \mathcal{N} = \dim(X^{\mathcal{N}})$$

$\mathrm{Pb}_N(\mu; u_N(\mu))$

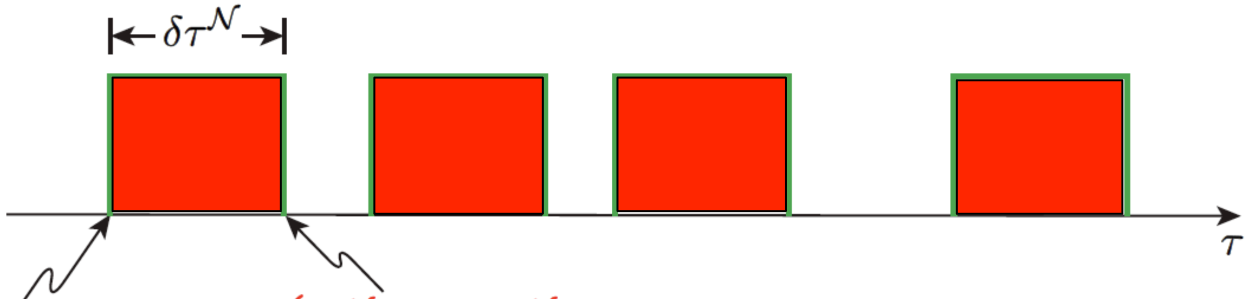
Reduced Basis approximation

Galerkin Projection

ONLINE

$$u_N(\mu) \in X_N : \quad a(u_N(\mu), v; \mu) = F(v) \qquad \forall v \in X_N$$
$$s_N(\mu) = l(u_N(\mu))$$

Classical Approach (e.g. Finite Element Method)

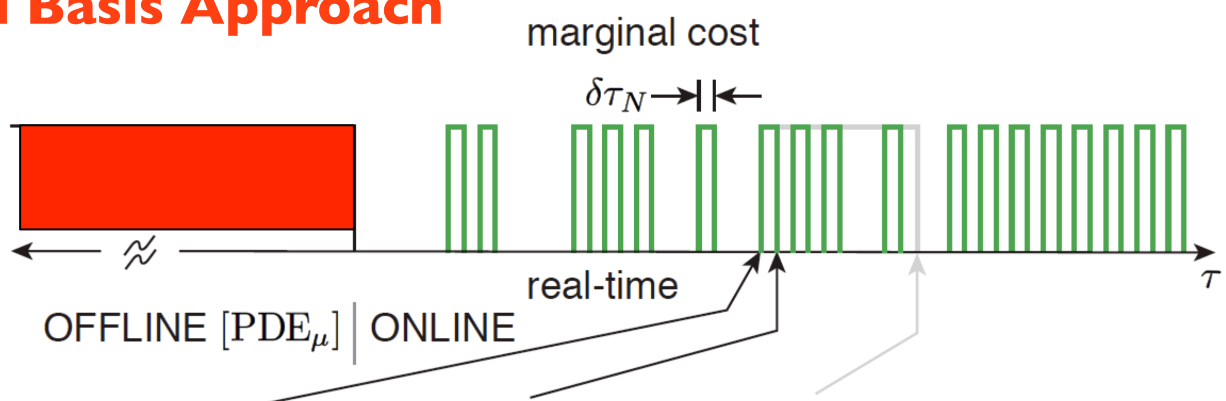


input μ $\xrightarrow{\text{PDE}_\mu}$

$$\begin{cases} u^{\mathcal{N}}(\mu) \in X^{\mathcal{N}} \approx u(\mu) \in X & \text{field} \\ s^{\mathcal{N}}(\mu) = \ell(u^{\mathcal{N}}(\mu)) \approx s(\mu) = \ell(u(\mu)) & \text{scalar output} \end{cases}$$

$\mathcal{N}$ = degrees of freedom in finite element approximation space

Reduced Basis Approach

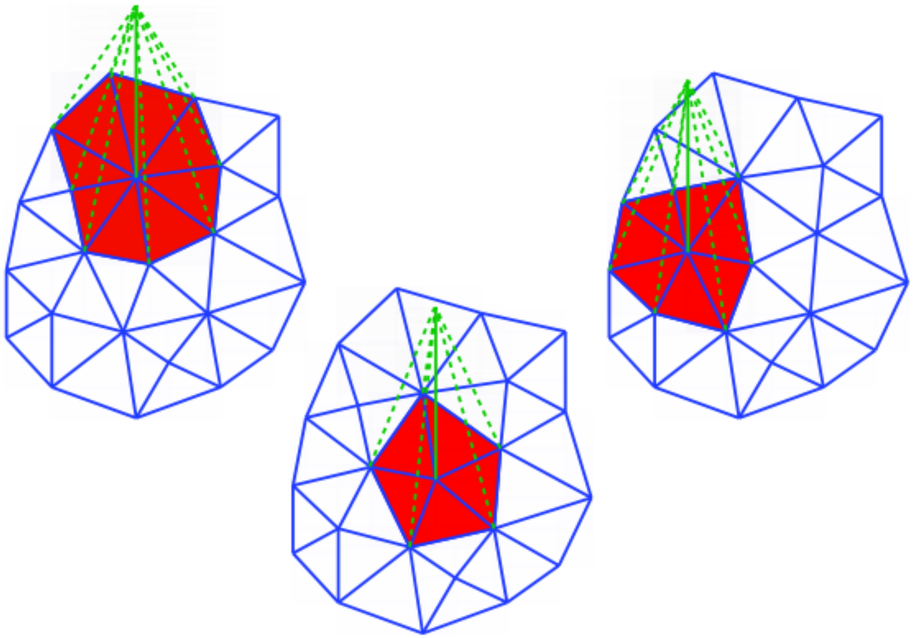


input μ $\xrightarrow{\text{PDE}_\mu}$

$$\begin{cases} u_N(\mu) \in X_N \approx u^{\mathcal{N}}(\mu) \in X^{\mathcal{N}} & \text{field} \\ s_N(\mu) = \ell(u_N(\mu)) \approx s^{\mathcal{N}}(\mu) = \ell(u^{\mathcal{N}}(\mu)) & \text{scalar output} \end{cases}$$

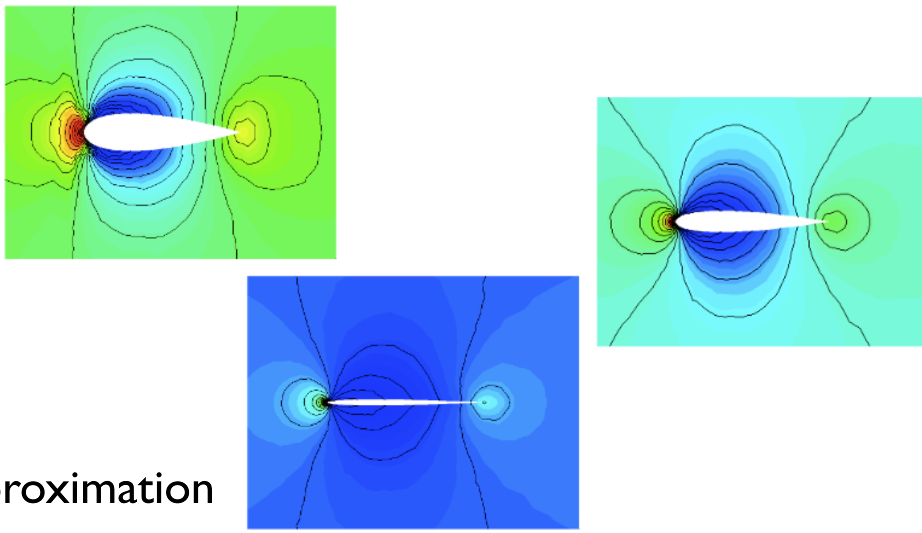
N = degrees of freedom in reduced basis approximation space

Finite Element “vs” Reduced Basis Methods



FE basis functions

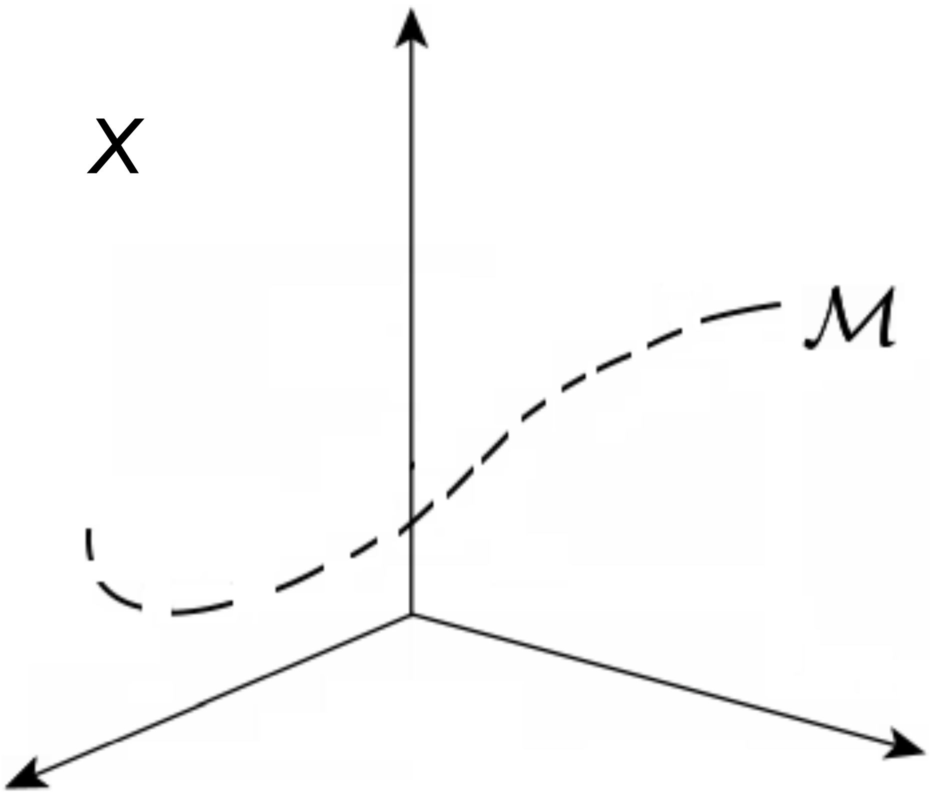
Locally supported basis functions
Generic, for different problems
Big linear systems / sparse matrices
A priori estimates readily available



RB basis functions

Globally supported basis functions
Constructed for specific problem
Small linear systems / full matrices
A posteriori estimates provide reliability of approximation

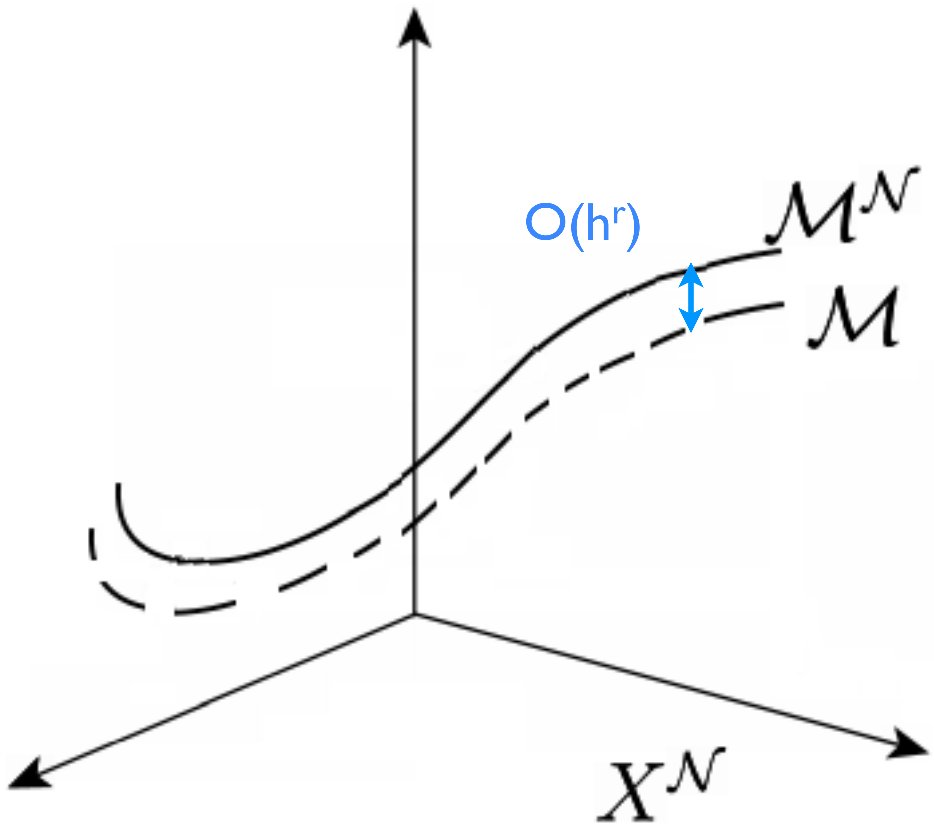
Spaces



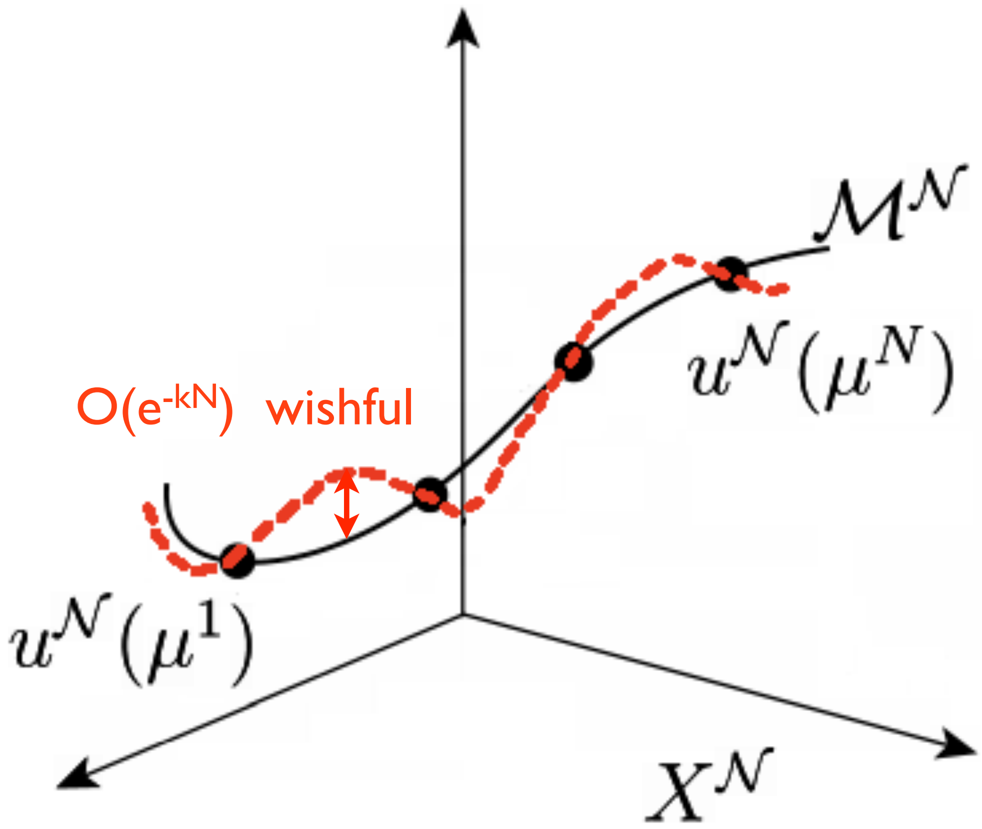
$$\mathcal{M} = \{u(\mu);\ \mu \in \mathscr{D}\}$$

$$u(\mu) \in X$$

Spaces



$$\mathcal{M}^{\mathcal{N}} = \{u^{\mathcal{N}}(\mu);\ \mu \in \mathscr{D}\}$$
$$u^{\mathcal{N}}(\mu) \in X^{\mathcal{N}}$$

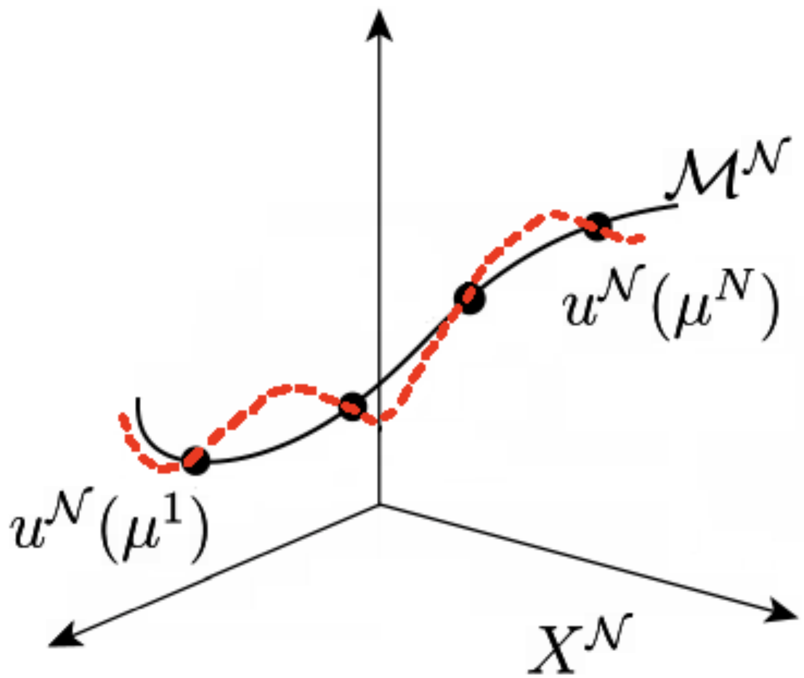


$$X_N = \text{span}\{u^{\mathcal{N}}(\mu^i), \quad i = 1, \dots, N\}$$

$$\dim(X_N) = N \ll \mathcal{N} = \dim(X^{\mathcal{N}})$$

Ingredients

1. Guess: low dimensional manifold $\mathcal{M}^{\mathcal{N}}$ - smooth dependence on μ
2. (Adaptive) sampling procedure for parameter exploration (greedy algorithm)
3. Evaluation procedure: (optimal) Galerkin projection
4. Offline/Online computational stratagem



Potential accuracy (based on a-priori analysis)

For an elliptic coercive problem, with P = 1 parameter, we have the following a priori result:

$$\frac{\|u^{\mathcal{N}}(\mu) - u_N(\mu)\|_\mu}{\|u^{\mathcal{N}}(\mu)\|_\mu} \leq \exp\left\{-\frac{N-1}{N_{crit}-1}\right\}, \quad \forall \mu \in \mathscr{D}$$

for $N \geq N_{crit} = 1 + \left[2e \ \ln\left(\frac{\mu_{max}}{\mu_{min}}\right)\right]_+$ with the following (equi-ln) parameter distribution:

$$\mu^n = \mu^{min} \exp\left\{\frac{n-1}{N-1} \ln\left(\frac{\mu_{max}}{\mu_{min}}\right)\right\}, \quad n = 1, \ldots, N$$

$$X_N = \text{span}\{u^{\mathcal{N}}(\mu^n), 1 \leq n \leq N\}$$

Note: no dependence on spatial regularity,
no dependence on $\mathcal{N}$; weak dependence on μ_{min}/μ_{max} (Maday, Patera,...)

$\|w\|_\mu = (w,w)_\mu^{1/2}$ is the energy norm given by: $(w,v)_\mu = a(w,v;\mu), \ \forall w,v \in X$

Reliability (based on a-posteriori error estimates)

1. depends on quality/meaningfulness of X_N
2. is based on the quality of the sampling
3. relies on rigorous a posteriori error analysis:

$$\|u^{\mathcal{N}}(\mu) - u_N(\mu)\|_X \leq \Delta_N(\mu) \qquad |s^{\mathcal{N}}(\mu) - s_N(\mu)| \leq \Delta_N^s(\mu)$$

$$\Delta_N(\mu) = \|r(\cdot;\mu)\|_{(X^{\mathcal{N}})'} / \alpha_{lb}^{\mathcal{N}}(\mu) \qquad \Delta_N^s(\mu) = \|l\|_{(X^{\mathcal{N}})'} \Delta_N(\mu)$$

- ✓ dual norm of the residual $r(v;\mu) = F(v;\mu) - a(u_N(\mu), v;\mu), \quad \forall v \in X^{\mathcal{N}}$
- ✓ lower bound $\alpha_{lb}^{\mathcal{N}}$ of the coercivity constant (in the elliptic, coercive case):

$$\alpha^{\mathcal{N}}(\mu) = \inf_{w \in X^{\mathcal{N}}} \frac{a(w,w;\mu)}{\|w\|_X^2}$$

- ✓ In the more general case, if $a(\cdot,\cdot;\mu) : X_1 \times X_2 \to \mathbb{R}$, $\alpha_{lb}^{\mathcal{N}}$ is replaced by the lower bound of the Babuska inf-sup constant

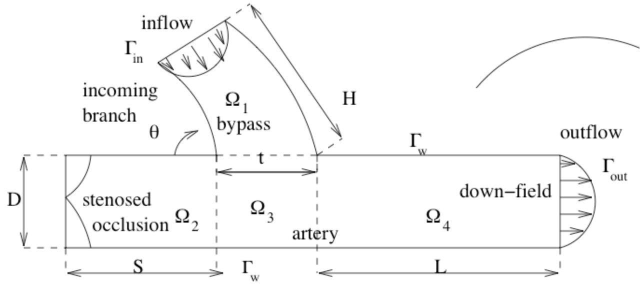
$$\beta^{\mathcal{N}}(\mu) = \inf_{w \in X_1^{\mathcal{N}}} \sup_{w \in X_2^{\mathcal{N}}} \frac{a(v,w;\mu)}{\|v\|_{X_1} \|w\|_{X_2}}$$

Elliptic coercive PDEs (affinely parametrized)

Weak formulation (Diffusion-advection-reaction problem)

For $\mu \in \mathscr{D} \subset \mathbb{R}^P$, evaluate

$$s^o(\mu) = l^o(u^o(\mu))$$



where $u^o(\mu) \in X(\Omega_o(\mu))$ satisfies:

$$a_o(u^o(\mu), v; \mu) = F_o(v; \mu), \qquad \forall v \in X(\Omega_o(\mu))$$

with

$$a_o(w, v; \mu) = \sum_{k=1}^{K_{dom}} \int_{\Omega_o^k(\mu)} \begin{bmatrix} \frac{\partial w}{\partial x_{o1}} & \frac{\partial w}{\partial x_{o2}} & w \end{bmatrix} \mathscr{K}_{o,ij}^k(\mu) \begin{bmatrix} \frac{\partial v}{\partial x_{o1}} \\ \frac{\partial v}{\partial x_{o2}} \\ v \end{bmatrix} d\Omega_o$$

Our problem is originally posed on the "original" domain $\Omega_o(\mu)$

Elliptic coercive PDEs (affinely parametrized)

Parametrized formulation

Problem reduced to a parametric PDEs system on Ω (reference domain)

For $\mu \in \mathscr{D} \subset \mathbb{R}^P$, evaluate $s(\mu) = l(u(\mu); \mu)$

where $u(\mu) \in X(\Omega)$ satisfies:

$$a(u(\mu), v; \mu) = F(v; \mu), \qquad \forall v \in X$$

with

$$a(w, v; \mu) = \sum_{k=1}^{K_{dom}} \int_{\Omega^k} \begin{bmatrix} \frac{\partial w}{\partial x_1} & \frac{\partial w}{\partial x_2} & w \end{bmatrix} \mathscr{K}_{ij}^k(\mu) \begin{bmatrix} \frac{\partial v}{\partial x_1} \\ \frac{\partial v}{\partial x_2} \\ v \end{bmatrix} d\Omega$$

and (transformation tensor)

$$\mathscr{K}^k(x; \mu) = \det(J_T^k(x; \mu)) J_T^{-1}(x; \mu) \mathscr{K}_o^k(\mu) J_T^{-T}(x; \mu)$$

All the parametric "dirtyness" is now embedded into $\mathscr{K}^k(x; \mu)$

Formulation

Elliptic coercive PDEs (affinely parametrized)

Parametrized formulation: definitions

μ : input parameter

$\mathscr{D}$: parameter domain in $\mathbb{R}^P$

X : function space, $H_0^1(\Omega) \subset X \subset H^1(\Omega)$

$s(\mu)$: output

$l(\cdot;\mu)$: output functional (linear, affine in μ, $L^2(\Omega)$ - bounded, $\forall\ \mu \in \mathscr{D}$)

u : field variable

$a(\cdot,\cdot;\mu)$: bilinear form (linear, affine in μ, X-continue, X-coercive, $\forall\ \mu \in \mathscr{D}$)

$F(\cdot;\mu)$: linear form (linear, affine in μ, X-bounded, X-coercive, $\forall\ \mu \in \mathscr{D}$)

Assumption: affine parametric dependence

$$a(v,w;\mu) = \sum_{q=1}^{Q_a} \Theta_a^q(\mu) a^q(v,w) \qquad F(w;\mu) = \sum_{q=1}^{Q_f} \Theta_f^q(\mu) F^q(w)$$

where $\Theta(\mu)$ represent coefficients and geometry

We transform, piecewise affinely, $\Omega_o^k(\mu) \rightarrow (\mu - \text{independent})\ \Omega^k$

Finite element ("truth") solution (never computed!!)

Elliptic coercive PDEs (affinely parametrized)

FEM (truth) approximation

For $\mu \in \mathscr{D} \subset \mathbb{R}^P$, evaluate

$$s^{\mathcal{N}}(\mu) = l(u^{\mathcal{N}}(\mu);\mu)$$

where $u^{\mathcal{N}}(\mu) \in X^{\mathcal{N}}$ satisfies:

$$a(u^{\mathcal{N}}(\mu), v; \mu) = F(v;\mu), \qquad \forall v \in X^{\mathcal{N}}$$

being $X^{\mathcal{N}} \subset X$ a sequence of (conforming) finite elements FE approximation spaces indexed by $\dim(X^{\mathcal{N}}) = \mathcal{N}$

The reduced basis (RB) approximation will be built in lieu of the FE solution, error will be measured (and certified) wrt the FE solution

Other discretization techniques instead of finite elements may also be used.

Elliptic coercive PDEs (affinely parametrized)

Reduced Basis Approximation

For $\mu \in \mathscr{D} \subset \mathbb{R}^P$, evaluate

$$s_N(\mu) = l(u_N(\mu); \mu)$$

where $u_N(\mu) \in X_N$ satisfies:

$$a(u_N(\mu), v; \mu) = F(v; \mu), \qquad \forall v \in X_N$$

Reduced linear system

Since $X_N = \text{span}\{\zeta_i^{\mathcal{N}},\ 1 \le i \le N\},\quad N = 1, \dots, N_{max}$ and

$$u_N(\mu) = \sum_{n=1}^{N} u_{Nn}(\mu) \zeta_n^{\mathcal{N}}$$

we look for $\mathbf{u}_N(\mu) \in \mathbb{R}^N$ s.t.

$$\sum_{j=1}^{N} \underbrace{a(\zeta_j^{\mathcal{N}}, \zeta_i^{\mathcal{N}}; \mu)}_{A_N(\mu)\, \in\, \mathbb{R}^{N \times N}} \mathbf{u}_{Nj}(\mu) = \underbrace{F(\zeta_i^{\mathcal{N}}; \mu)}_{F_N(\mu) \in\, \mathbb{R}^N}, \qquad 1 \le i \le N$$

Formulation

Elliptic coercive PDEs (affinely parametrized)

Offline/Online computational stratagem

$$\sum_{j=1}^{N}\left[\; \underbrace{\sum_{j=1}^{N} a(\zeta_j^{\mathcal{N}},\zeta_i^{\mathcal{N}};\mu)}_{A_N(\mu)\,\in\,\mathbb{R}^{N\times N}} \mathbf{u}_{Nj}(\mu) = \underbrace{F(\zeta_i^{\mathcal{N}};\mu)}_{F_N(\mu)\in\,\mathbb{R}^{N}}, \qquad 1 \le i \le N \quad i \le N \;\right]$$

$A_N(\mu) \in \mathbb{R}^{N\times N}$

$F_N(\mu) \in \mathbb{R}^{N}$

$$s_N(\mu) = l\left(\sum_{j=1}^{N} u_{Nj}(\mu)\zeta_n^{\mathcal{N}}\right) = \sum_{j=1}^{N} u_{Nn}(\mu)\, \underbrace{l(\zeta_j^{\mathcal{N}})}_{L_N\,\in\,\mathbb{R}^{N}}$$

OFFLINE	Heavy computations (solutions database / structures), performed once	$C(\mathcal{N})$
ONLINE	Fast solution/output evaluation (for each new parameter value)	$C(N, Q_a, Q_f)$

Elliptic coercive PDEs (affinely parametrized)

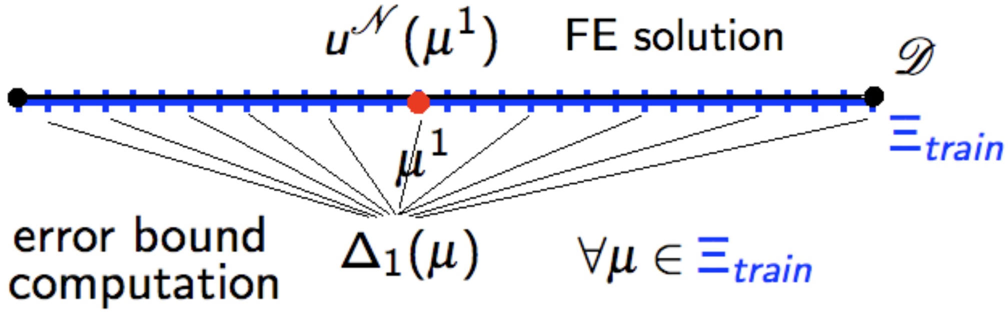
RB space construction: greedy sampling

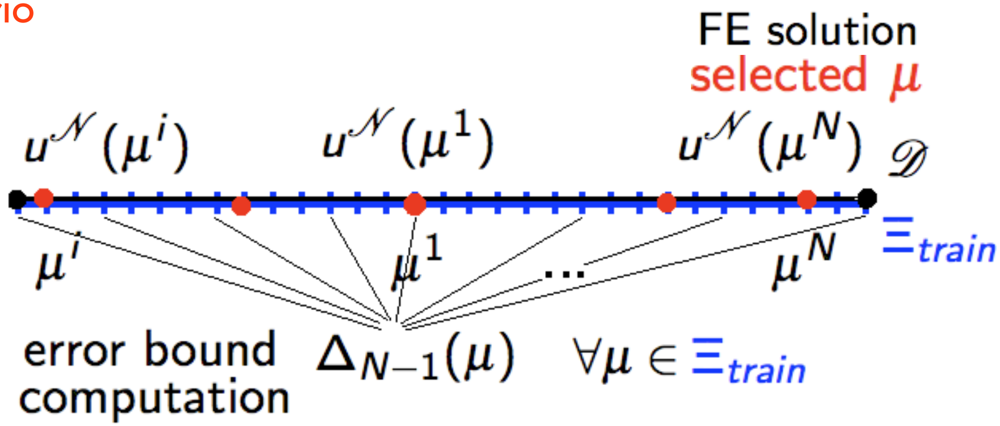
Given a train sample $\Xi_{train} \subset \mathscr{D}$, $\mu^1 \in \Xi_{train}$ and a tolerance ε_{tol}^{RB}

```
S_1 = {μ^1};
compute u^N(μ^1);
X_1 = span{u^N(μ^1)};
for N = 2 : N_max
    μ^N = arg max_{μ∈Ξ_train} Δ_{N-1}(μ);
    ε_{N-1} = Δ_{N-1}(μ^N);
    if ε_{N-1} ≤ ε_tol^RB
        N_max = N - 1;
    end;
    compute u^N(μ^N);
    S_N = S_{N-1} ∪ {μ^N};
    X_N = X^N_{N-1} ∪ span{u^N(μ^N)};
end.
```

Worst case scenario selection

Space enrichment



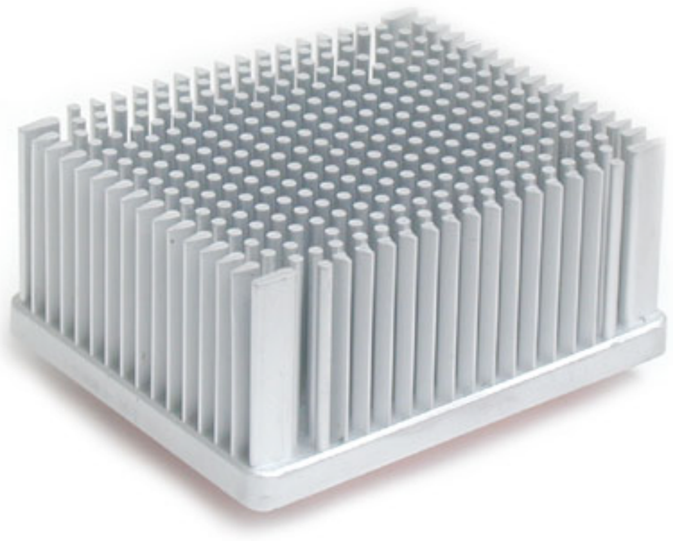


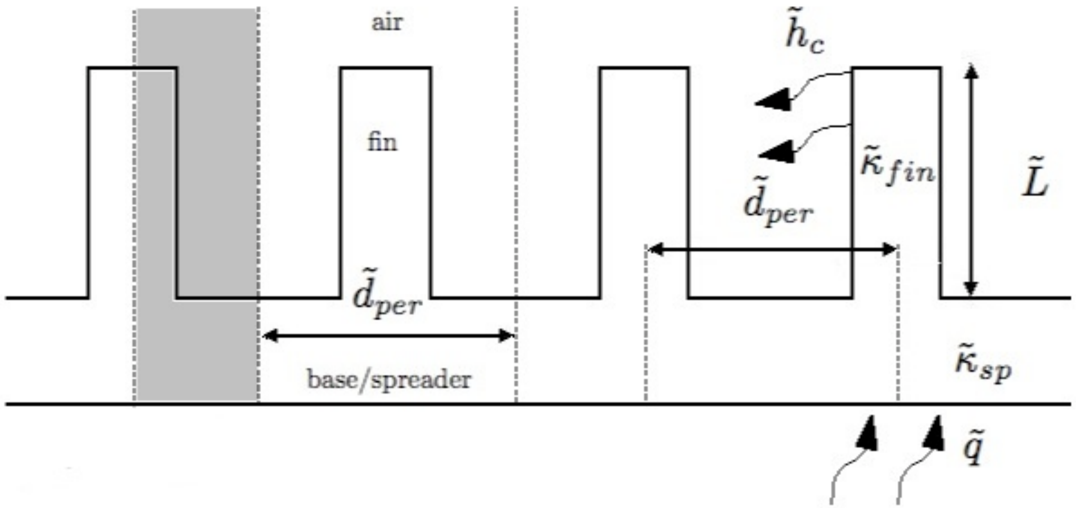
Strategy for train sample: uniform sampling, log-uniform san

In the Proper Orthogonal Decomposition (POD) FE solutions $X_N^{\mathcal{N}\,\mathrm{POD}} = \arg \inf_{X_N^{\mathcal{N}} \subset \mathrm{span}\{u^{\mathcal{N}}(\mu)\,|\,\mu \in \Xi_{train}\}} \| u^{\mathcal{N}} - \Pi_{X_N^{\mathcal{N}}} u^{\mathcal{N}} \|_{L^2(\Xi_{train};X)}$ would be computed $\forall \mu \in \Xi_{train}$

Model Problem: a thermal fin

- ✓ Heat sink designed for thermal management of high-density electronic components
- ✓ Shaded computational domain due to assumed periodicity/symmetry (multi-fin sink)
- ✓ Output of interest : temperature at the base of the spreader

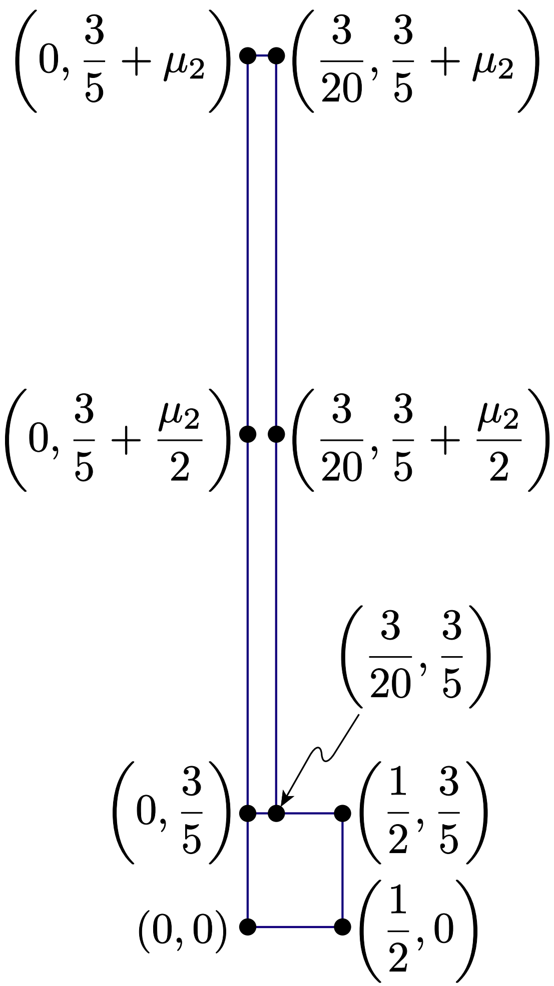




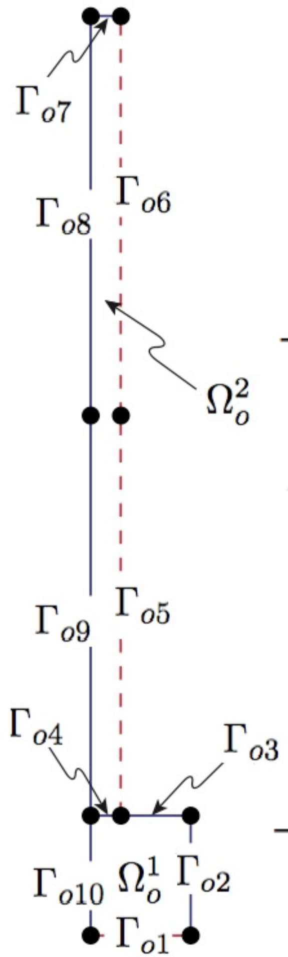
Physical and geometrical parametrization

$\mu_1 = \mathrm{Bi} = \tilde{h}_c \tilde{d}_{\mathrm{per}} / \tilde{\kappa}_{\mathrm{fin}}$	Biot number	$\mu_1 \in [0.01, 0.5]$
$\mu_2 = L = \tilde{L} / \tilde{d}_{\mathrm{per}}$	nondimensional fin height	$\mu_2 \in [2, 8]$
$\mu_3 = \kappa = \tilde{\kappa}_{\mathrm{sp}} / \tilde{\kappa}_{\mathrm{fin}}$	spreader-to-fin conductivity ratio	$\mu_3 \in [1, 10]$

Geometry



Temperature field



$$\frac{\partial u^o}{\partial \mathbf{n}} = 0$$

$$-\nabla \cdot (1 \nabla u^o) = 0$$

$$\frac{\partial u^o}{\partial \mathbf{n}} + \mu_1 u^o = 0$$

$$-\nabla \cdot (\mu_3 \nabla u^o) = 0$$

$$\mu_3 \frac{\partial u^o}{\partial \mathbf{n}} = 1$$

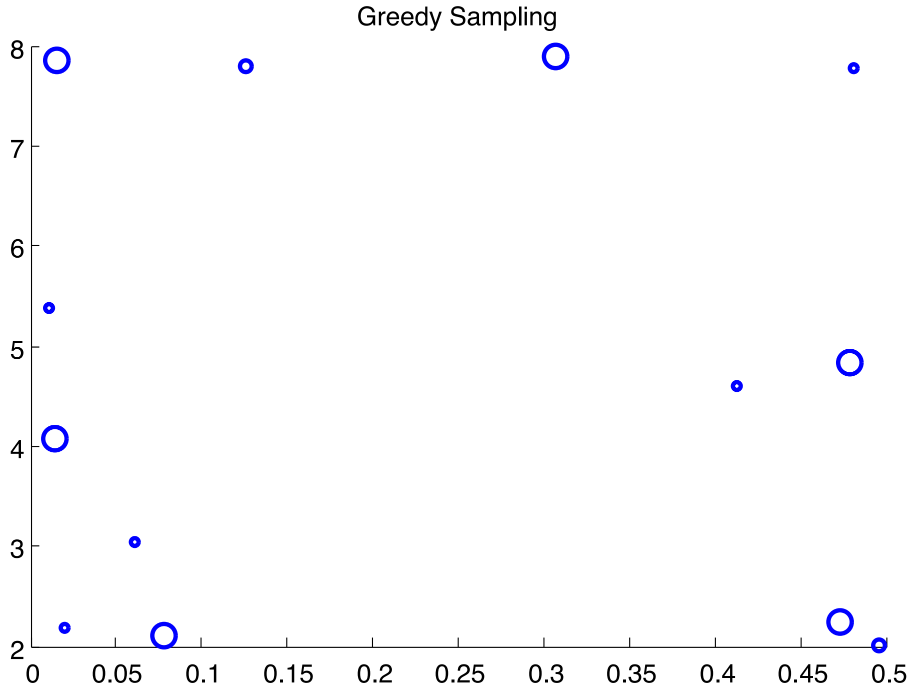
Output of interest

$$s(\mu) = 2 \int_{\Gamma_{o1}} u^o(\mu)$$

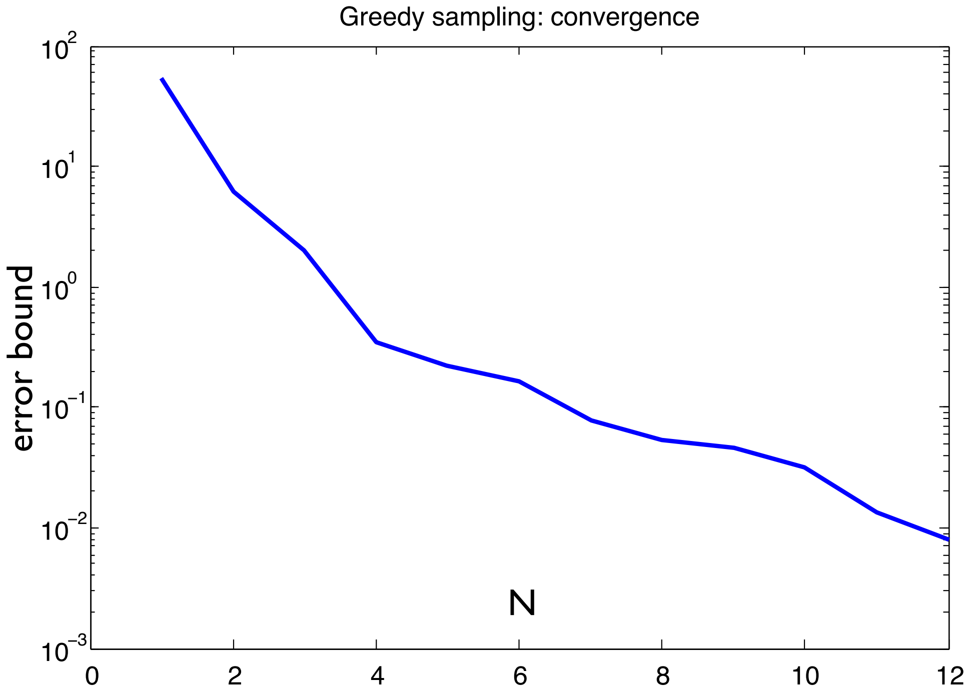
Model Problem: a thermal fin

Greedy sampling procedure

Number of FE dof	1116
Number of RB functions N (tol = 0.01)	12
Reduction in linear system dimension	100:1



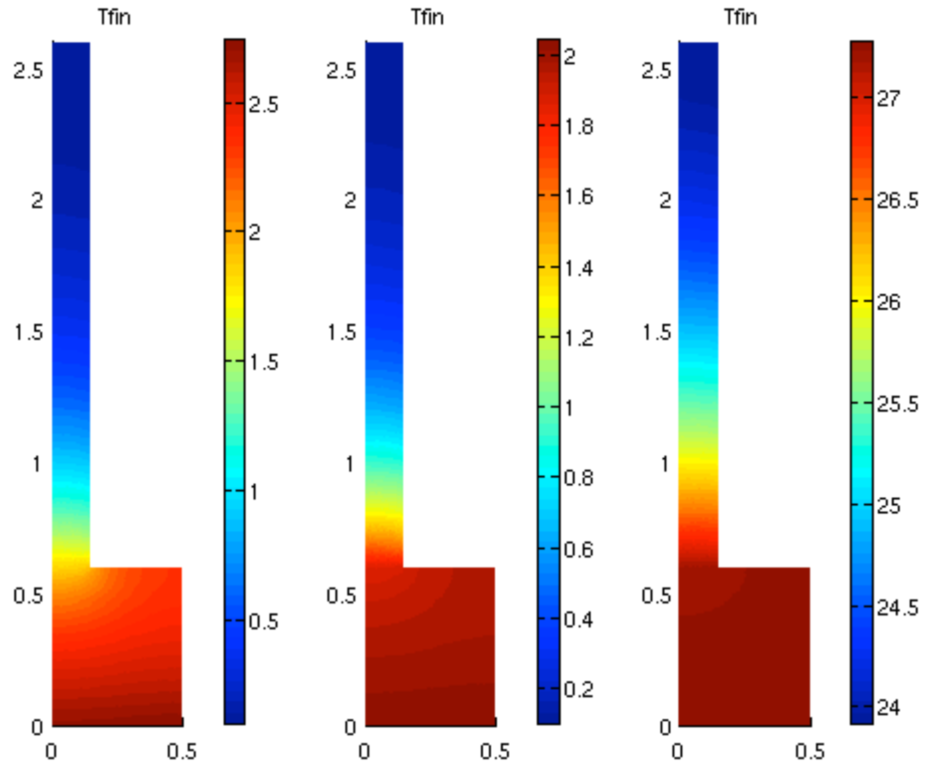
Selected parameter points
(plot referred to the (μ_1, μ_2) - axis, being the radius of the points proportional to μ_3)



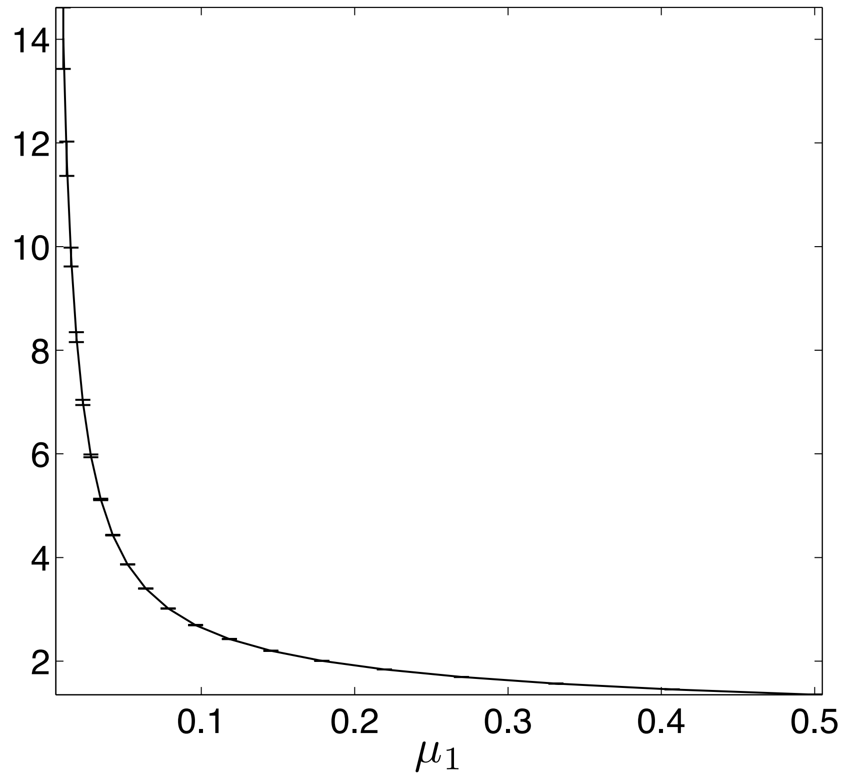
Error bound on solution as measure of the convergence of the sampling procedure
(stop tolerance = 0.01)

Model Problem: a thermal fin

Computed output and solution visualization



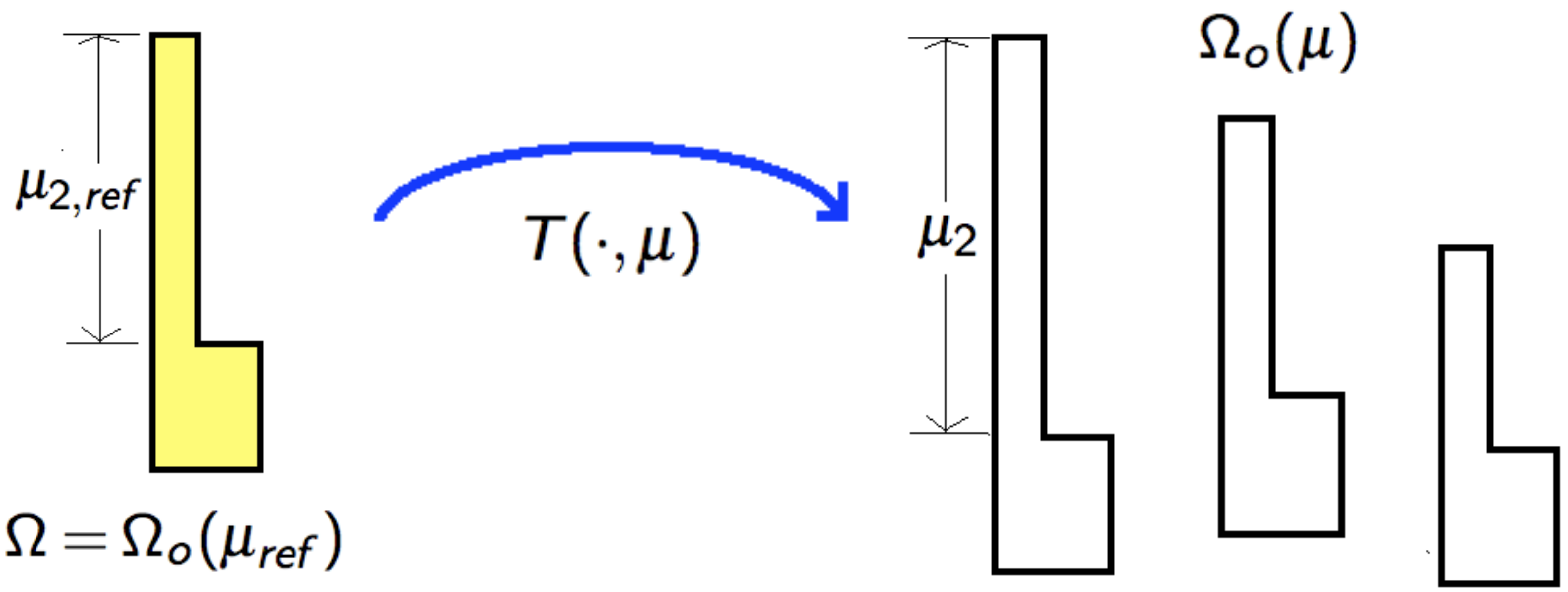
RB temperature field for different choices of parameters (fixed geometry μ_2): $\mu = (0.5, 2, 1)$, $\mu = (0.5, 2, 5)$, $\mu = (0.01, 2, 10)$



RB output and RB error bars $[s_N(\mu) - \Delta_N^s(\mu), s_N(\mu) + \Delta_N^s(\mu)]$ as a function of μ_1 for $\mu_2 = 2$, $\mu_3 = 1$

Formulation

- ✓ Our problem is originally posed on the "original" domain
- ✓ If a subset of parameters μ is made of geometrical parameters, we need a reference domain to compare (and combine) FE solutions that would be otherwise computed on different domains and grids



- ✓ The parametrized original domain $\Omega_o(\mu)$ is the image of a reference domain Ω through an affine parametric mapping $T(\cdot,\mu) : \Omega \rightarrow \Omega_o(\mu)$

Elliptic coercive PDEs (affinely parametrized)

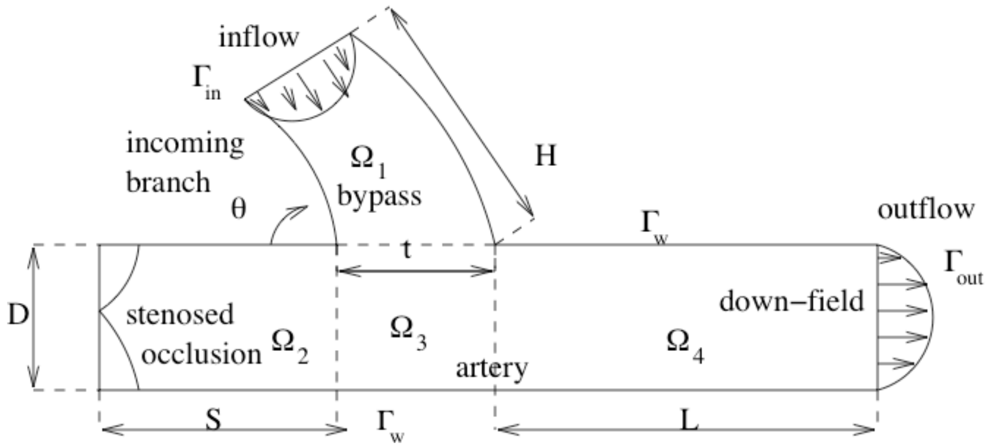
Parametrized formulation

- ✓ Our global transformation $T(\cdot,\mu):\Omega\rightarrow\Omega_o(\mu)$ can be seen as the union of **local affine mapping** on subdomains (triangles, elliptical/curvy triangles)

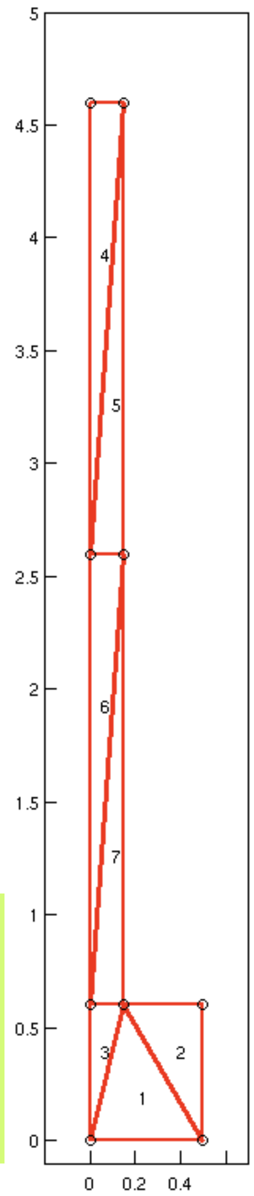
$$\Omega_o(\mu)=\bigcup_{k=1}^{K_{\mathrm{dom}}}\Omega_o^k(\mu)\qquad \Omega_o^k(\mu)=T^k(\Omega^k;\mu),\quad 1\leq k\leq K_{\mathrm{dom}}$$

$$T^k(\cdot,\mu):\Omega^k\rightarrow\Omega_o^k(\mu),\,1\leq k\leq K_{\mathrm{dom}}$$

- ✓ A fixed reference domain $\Omega\equiv\Omega_o(\mu_{\mathrm{ref}})$ is used for all FE computations, with $\Omega^k=\Omega_o^k(\mu_{\mathrm{ref}}),\,1\leq k\leq K_{\mathrm{dom}}$



Problem reduced to a parametric PDEs system on Ω (reference domain)



Outline

1. Reduced basis methods

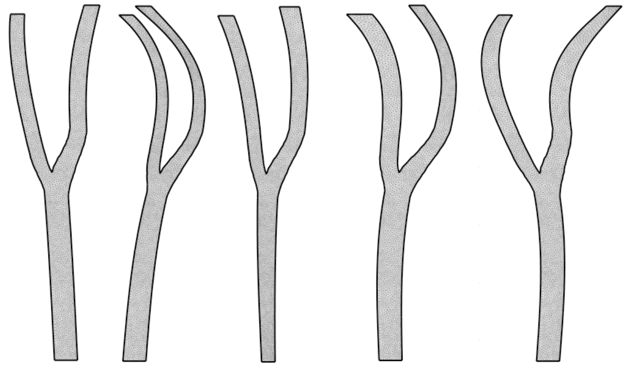
2. Shape parametrization techniques

3. Reduced framework for optimal control/shape optimization

4. Applications in haemodynamics

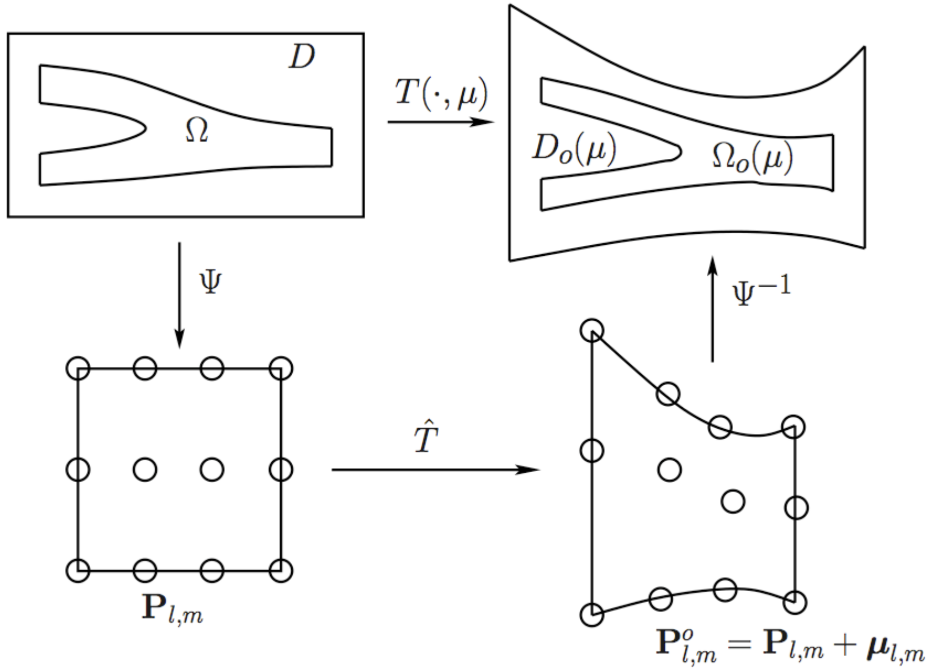
Shape Parametrization Techniques

- ✓ RB framework requires a geometrical map $T(\cdot\,;\mu): \Omega \rightarrow \Omega_o(\mu)$ in order to combine discretized solutions for the space construction
- ✓ This procedure enables to avoid shape deformation and remeshing (that, e.g. normally occur at each step of an iterative optimization procedure)
- ✓ Reduction in the complexity of parametrization: versatility, low-dimensionality, automatic generation of maps, capability to represent realistic configurations, ...



Left: Different carotid bifurcation specimens obtained by autopsy (adults aged 30-75); picture taken from Z. Ding et al., Journal of Biomechanics 34 (2001), 1555-1562.
Right: Different carotid bifurcation obtained through radial basis functions techniques.

Free-Form Deformation techniques



FFD mapping

$$D_o(\mu) = \Psi^{-1} \circ \hat{T} \circ \Psi(D,\mu)$$

$$\Omega_o(\mu) = \Psi^{-1} \circ \hat{T} \circ \Psi(\Omega,\mu)$$

$$\hat{T}(\hat{\mathbf{x}},\mu) = \sum_{l=0}^{L} \sum_{m=0}^{M} b_{l,m}^{L,M}(\hat{\mathbf{x}})(\mathbf{P}_{l,m} + \mu_{l,m})$$

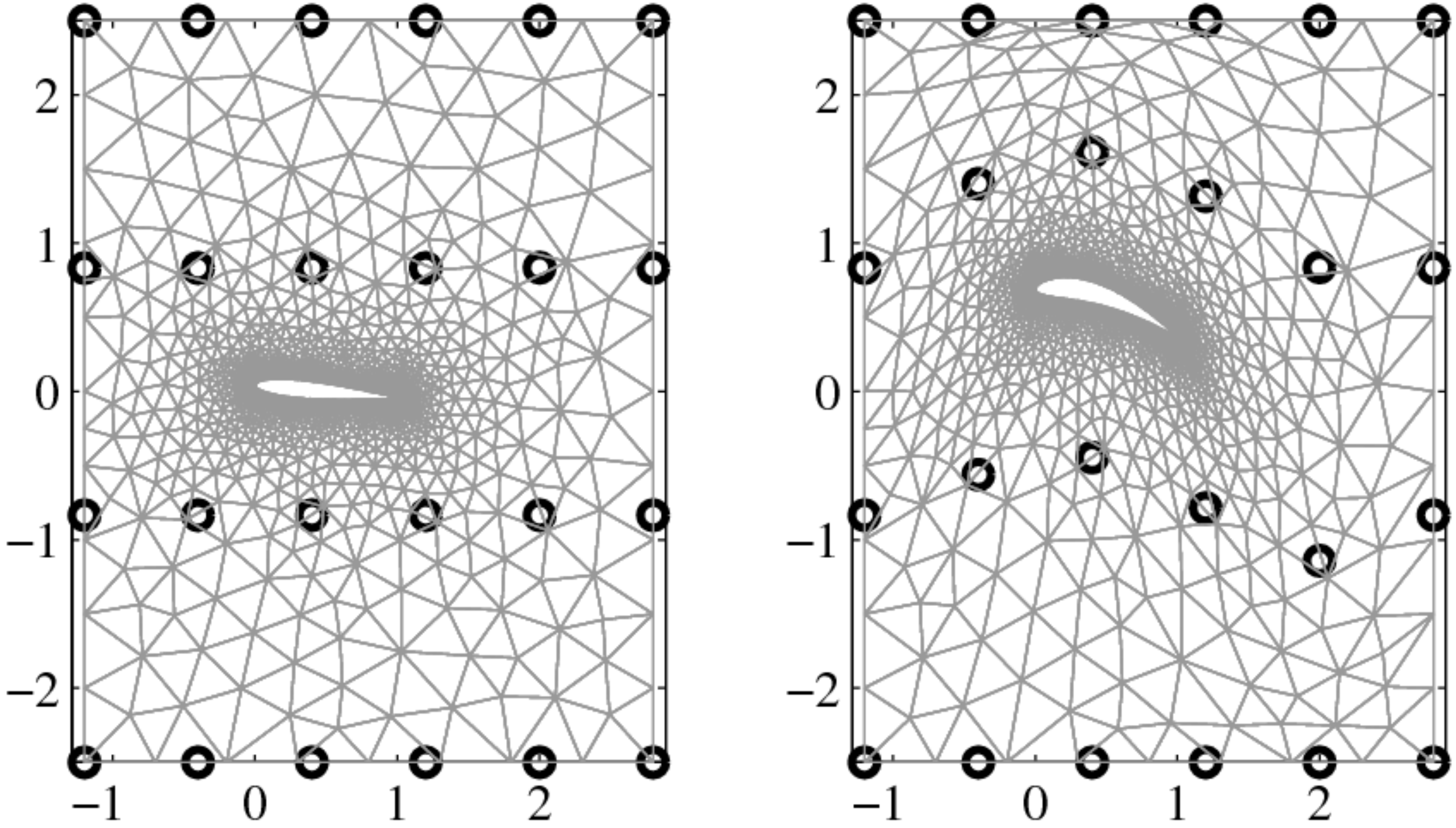
where

$$b_{l,m}^{L,M}(s,t) = b_l^L(s) b_m^M(t) = \binom{L}{l}\binom{M}{m}(1-s)^{L-l}s^l(1-t)^{M-m}t^m$$

(Bernstein polynomials)

Parameters $\mu_1, \ldots, \mu_P$ are chosen according to a given prolem-dependent criterium.
They induce the displacements of some (selected) control points.
Only a subset of them can be used as active unknowns - they univocally identify the map.

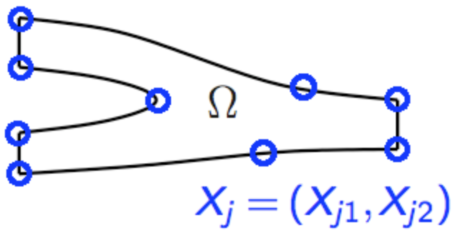
Shape Parametrization by FFD

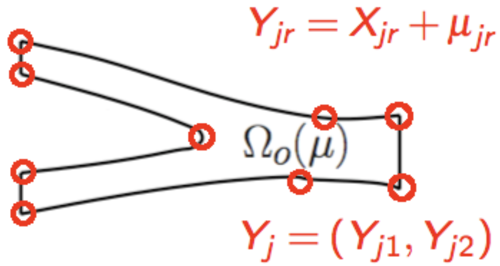


Free-Form Deformation (reference configuration and deformed configuration) for an airfoil problem.
Parameters are given by the vertical displacements of the eight central control points
(only eight active parameters are used).

Option II: shape parametrization by RBF

Radial Basis Functions technique





RBF mapping

$$T(x) = Q_r(x) + \sum_{i=1}^{k} w_i \ \sigma(\|x - X_i\|)$$

Ingredients

- $\mathbf{X_j}_{j=1}^{k}, \mathbf{Y_j}_{j=1}^{k} \in \mathbb{R}^{k\times 2}$ initial/deformed position of control points
- $Q_r(\cdot)$ is a low-degree polynomial function (in our case $r = 1$, $Q_1(x) = c + Ax$)
- $\{w_j\}_{j=1}^{k}$, $w_i \in \mathbb{R}^2$ set of weights corresponding to the k control points
- $\sigma(\cdot)$ is the basis function; e.g. $\sigma(h) = h^3$, $\exp(-Ch^2)$, $h^2 \log(h), \ldots$

Construction

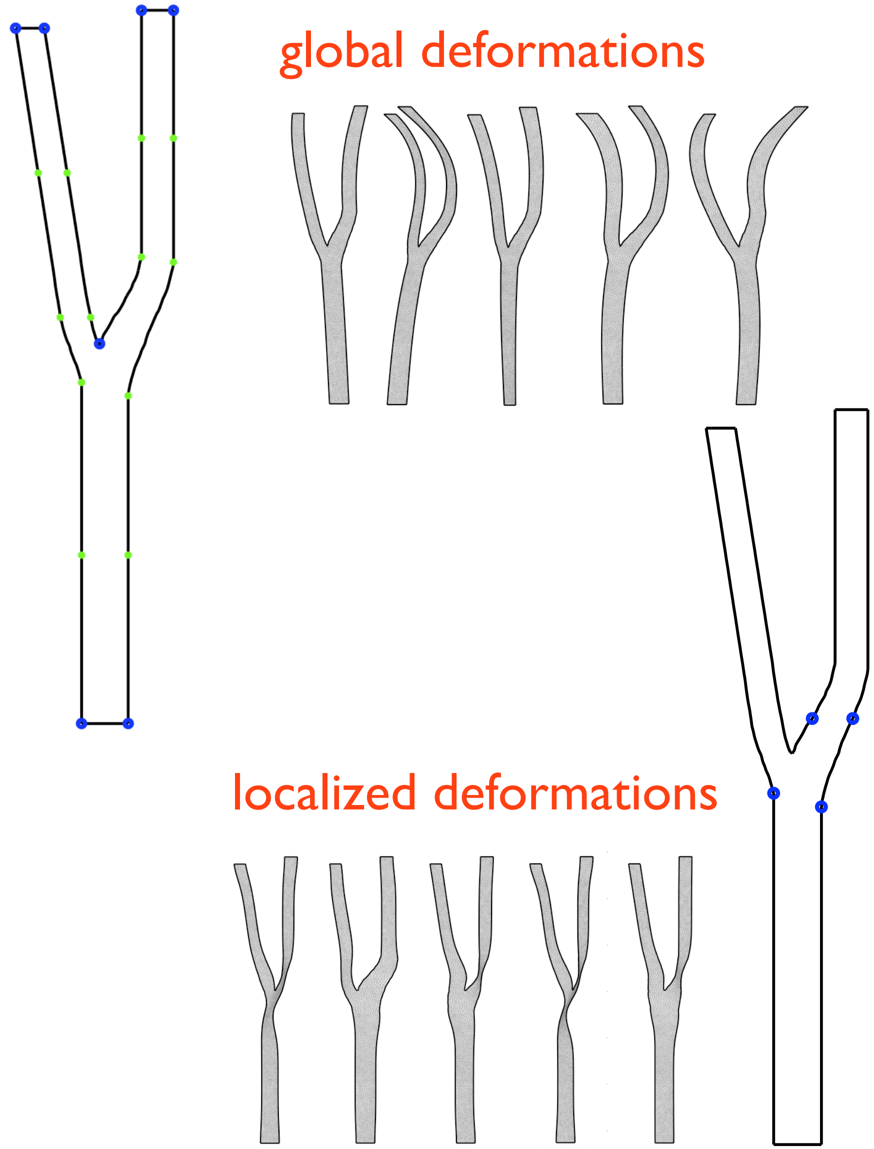
- RBF is function of $2k + 6$ coefficients: $c \in \mathbb{R}^2$, $A \in \mathbb{R}^{2\times 2}$, $W \in \mathbb{R}^{k\times 2}$ given by

$$\begin{bmatrix} S & \mathbb{I}_k & \mathbf{X} \\ \mathbb{I}_k^T & \mathbf{0} & \mathbf{0} \\ \mathbf{X}^T & \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} W(\mu) \\ (c(\mu))^T \\ (A(\mu))^T \end{bmatrix} = \begin{bmatrix} \mathbf{Y}(\mu) \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}$$

- Constraints: $2k$ interpolation $(Y_j) = T(X_j)$ + 6 “side” $\mathbb{I}_k^T W = X^T W = 0$
- Parameters $\mu_1, \ldots, \mu_P$ = displacements of some (selected) control points

Radial Basis Functions techniques

- ✓ Control positions can be freely chosen (they can be scattered in the domain and do not have to reside on a regular lattice)
- ✓ RBF techniques are interpolatory: each control point of the initial shape is mapped onto the corresponding control point of the deformed one
- ✓ Depending on the choice of control points, either global or localized deformations can be described



Outline

1. Reduced basis methods
2. Shape parametrization techniques
3. Reduced framework for optimal control/shape optimization
4. Applications in haemodynamics

How to make profit of RB in the framework of optimal control?

Framework: optimal control/shape optimization or more general inverse problems related with geometry/shape variation

Goal: optimize some output of interest

$$\text{find} \quad \hat{U} = \arg \min_{U \in \mathscr{U}_{ad}} J_o(Y(U))$$

- control variable $\quad U = (u, \Omega_o) \in \mathscr{U}_{ad} = U_{ad} \times \mathscr{O}_{ad}$
- original domain $\Omega_o \in \mathscr{O}_{ad}$, control function $u \in U_{ad}$
- state variable $Y = Y(U) \in \mathscr{Y}(\Omega_o)$ solution of

$$Y \in \mathscr{Y}(\Omega_o): \quad A_o(Y, W; U) = F_o(W; U), \quad \forall W \in \mathscr{Y}(\Omega_o).$$

High computational costs because:

- optimal control/shape optimization problems require multiple evaluations of outputs depending on state variables (or even domain geometry) during iterative procedures
- classical discretization techniques are expensive when geometry keeps changing

How to make profit of RB in the framework of optimal control?

Improving computational efficiency by (e.g.):

- introducing a low-dimensional **parametrization** to describe the control space (and reduce the geometrical complexity in the case of shape optimization)
  - **optimal control**: $u = u(\mu)$ (straightforward...)
  - **shape optimization**: $\Omega_o = \Omega_o(\mu)$ (shape parametrization)

  being $\mu = (\mu_1, \dots \mu_p) \in \mathscr{D} \subset \mathbb{R}^p$

- solving parametric PDEs using **reduced basis** methods for computational reduction

Assumption: we focus on shape optimization problems, with $U = \Omega_o$

Parametric optimization problem

$$\text{find} \quad \hat{\mu} = \arg \min_{\mu \in \mathscr{D}_{ad}} J_o(Y(\mu))$$

where $\mathscr{D}_{ad} \subseteq \mathscr{D}$ and $Y(\mu)$ solves

$$Y(\mu) \in \mathscr{Y}(\Omega_o(\mu)) : \quad A_o(Y(\mu), W; \mu) = F_o(W; \mu), \quad \forall W \in \mathscr{Y}(\Omega_o(\mu)).$$

How to make profit of RB in the framework of optimal control?

Recipe

Step 1: parametrized formulation on a reference (parameter independent) domain:

μ-parametrized optimization problem

$$\text{find} \quad \hat{\mu} = \arg\min_{\mu \in \mathscr{D}_{ad}} s(\mu) = J(Y(\mu)) \quad \text{s.t.}$$

$$Y(\mu) \in \mathscr{Y} : \; A(Y(\mu), W; \mu) = F(W; \mu), \quad \forall W \in \mathscr{Y}.$$

since the reduced basis method relies on the combination of pre-computed solutions, that would be otherwise computed on different domains.

Step 2: solve the reduced basis (RB) problem

RB μ-parametrized optimization problem

$$\text{find } \hat{\mu} = \arg\min_{\mu \in \mathscr{D}_{ad}} s_N(\mu) = J(Y_N(\mu)) \;\; \text{s.t.}$$

$$Y_N(\mu) \in \mathscr{Y}_N : \; A(Y_N(\mu), W; \mu) = F(W; \mu), \quad \forall W \in \mathscr{Y}_N.$$

Outline

1. Reduced basis methods
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The Context

1. From clinical imaging to computational grid

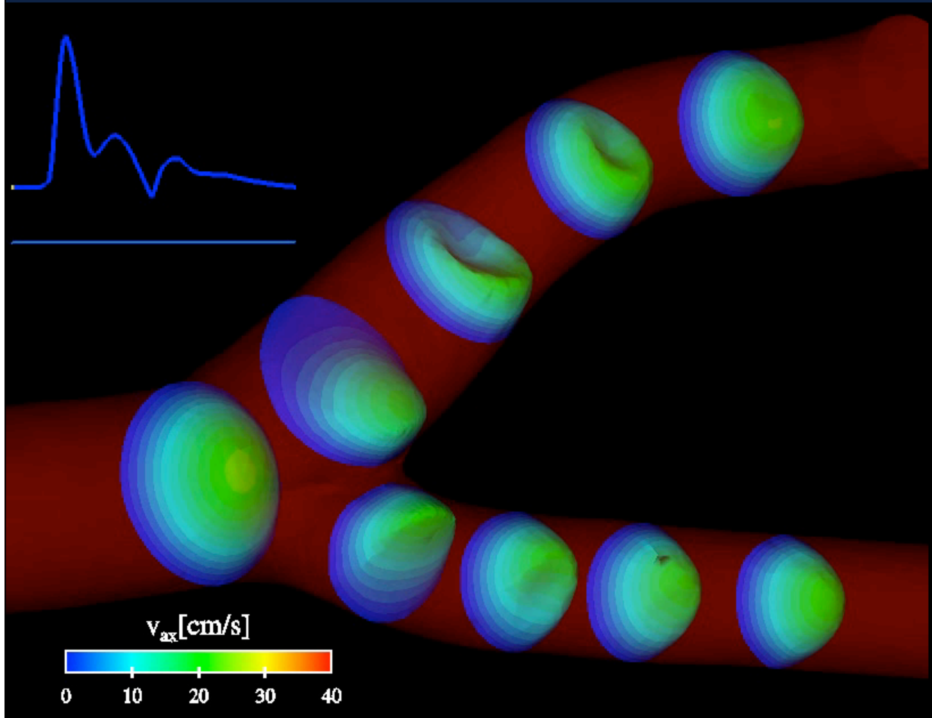
2. Mathematical Modeling

3. Computing

4. Verification Validation

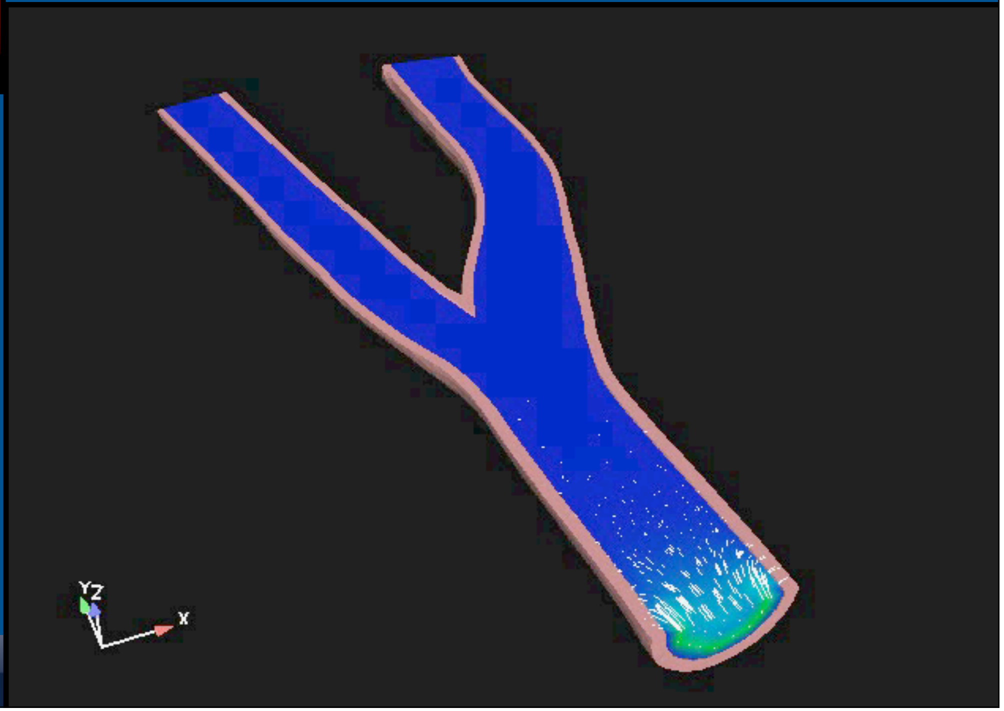
5. Clinical Applications

Handling Complexity



NS equations, rigid walls,
one heartbeat

FSI in carotid artery,
one heartbeat



Blood flow FSI - The equations

A coupled fluid-structure problem

Equations for the geometry:

$$\hat{\eta}_f = \text{Ext}(\hat{\eta}_{s|\hat{\Gamma}}),\ \hat{\mathbf{w}} = \frac{\partial \hat{\eta}_f}{\partial t}, \Omega_f(t) = (I + \hat{\eta}_f)(\hat{\Omega}_f)$$

Equations for the fluid:

$$\frac{\rho_f}{J_{\hat{\mathcal{A}}}} \frac{\partial J_{\hat{\mathcal{A}}} \mathbf{u}_f}{\partial t}_{|\hat{\mathbf{x}}} + \text{div}(\rho_f \mathbf{u}_f \otimes (\mathbf{u}_f - \mathbf{w}) - \sigma_f(\mathbf{u}_f, P)) = 0, \quad \text{in} \quad \Omega_f(t)$$

$$\text{div}\mathbf{u}_f = 0, \quad \text{in} \quad \Omega_f(t)$$

$$\mathbf{u}_f = \mathbf{u}_D, \quad \text{on} \quad \Gamma_{f,D}$$

$$\sigma_f(\mathbf{u}_f, P)\mathbf{n}_f = \mathbf{g}_{f,N}, \quad \text{on} \quad \Gamma_{f,N}$$

$$\mathbf{u}_f = \mathbf{w}, \quad \text{on} \quad \Gamma(t)$$

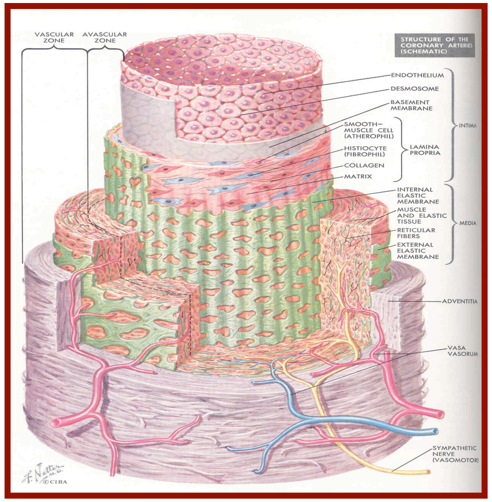
Equations for the structure:

$$\hat{\rho}_{s,0} \frac{\partial^2 \hat{\eta}_s}{\partial t^2} - \text{div}_{\hat{\mathbf{x}}}(\hat{\mathbf{F}}_s \hat{\Sigma}) = 0, \quad \text{in} \quad \hat{\Omega}_s$$

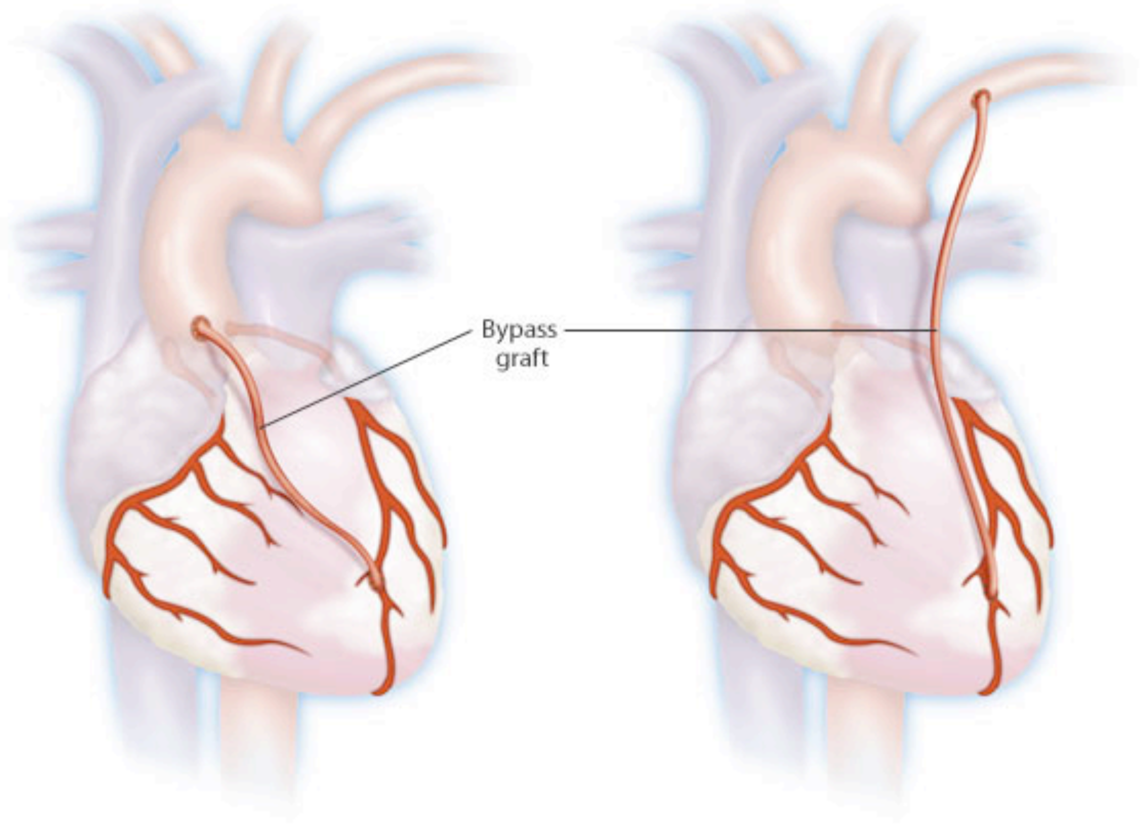
$$\hat{\eta}_s = 0 \quad \text{on} \quad \hat{\Gamma}_{s,D}$$

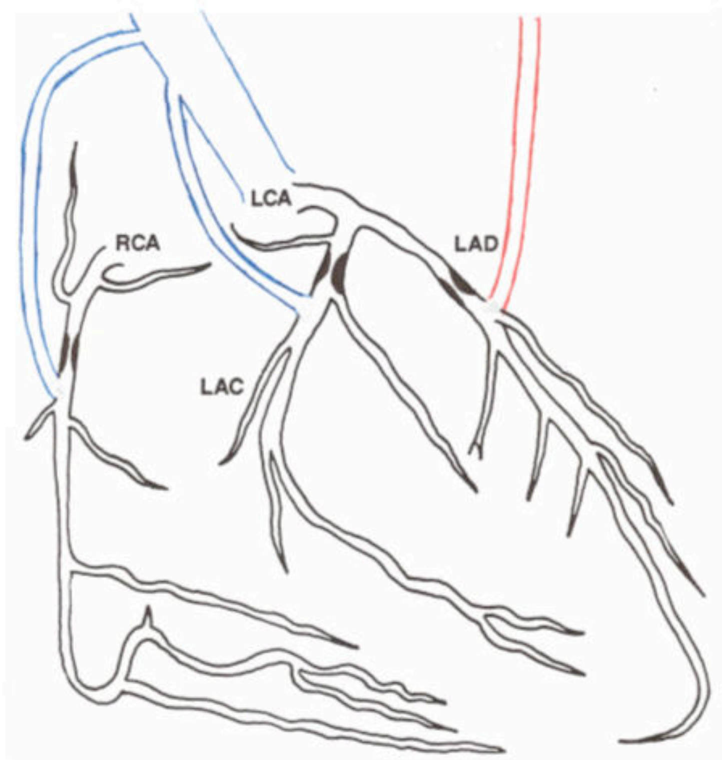
$$\hat{\mathbf{F}}_s \hat{\Sigma} \hat{\mathbf{n}}_s = \hat{J}_s |\hat{\mathbf{F}}_s^{-T} \hat{\mathbf{n}}_s| \hat{\mathbf{g}}_{s,N}, \quad \text{on} \quad \hat{\Gamma}_{s,N}$$

$$\hat{\mathbf{F}}_s \hat{\Sigma} \hat{\mathbf{n}}_s = \hat{J}_s \hat{\sigma}_f(\mathbf{u}_f, P) \hat{\mathbf{F}}_s^{-T} \hat{\mathbf{n}}_s, \quad \text{on} \quad \hat{\Gamma}$$

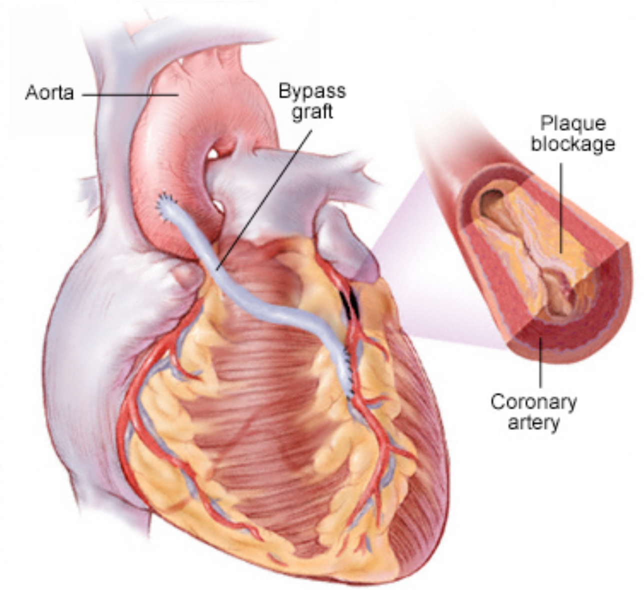


Shape Optimization of a bypass graft





Shape Optimization of a bypass graft



- Shape optimization of cardiovascular geometries may help to prevent post-surgical complications
- Local fluid patterns (vorticity) and wall shear stress are strictly related to the thickening caused by atherosclerotic obstructions, which is the principal disease process in venous bypass grafting
- Blood flow in coronary arteries can be modeled by means of Stokes equations (low velocity in vessels of small diameter)

Shape optimization by flow control

(minimization of blood vorticity in the down-field region of the bypass)

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

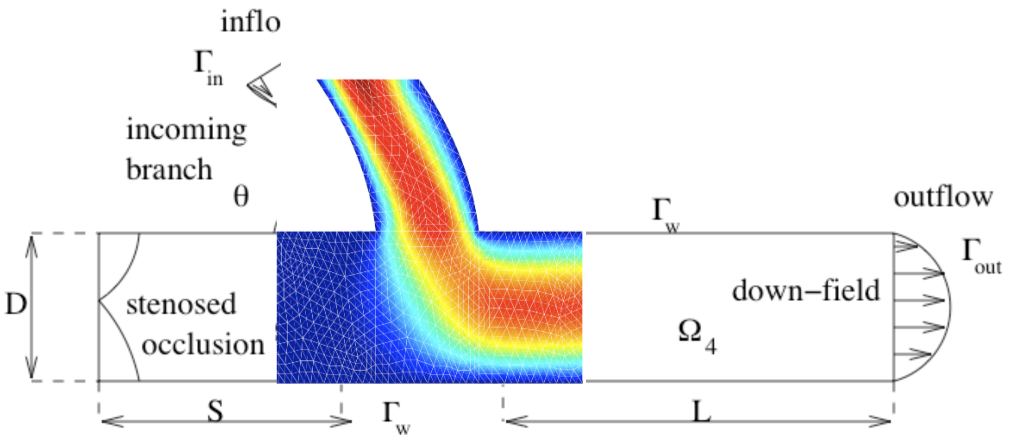
$$\begin{cases} -\nu\Delta\mathbf{v} + \nabla p = \mathbf{f} & \text{in } \Omega_o \\ \nabla\cdot\mathbf{v} = 0 & \text{in } \Omega_o \\ \mathbf{v} = \mathbf{v}_g & \text{on } \Gamma_D := \partial\Omega_o \setminus \Gamma_{out}, \\ -p\cdot\mathbf{n} + \nu\dfrac{\partial\mathbf{v}}{\partial\mathbf{n}}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

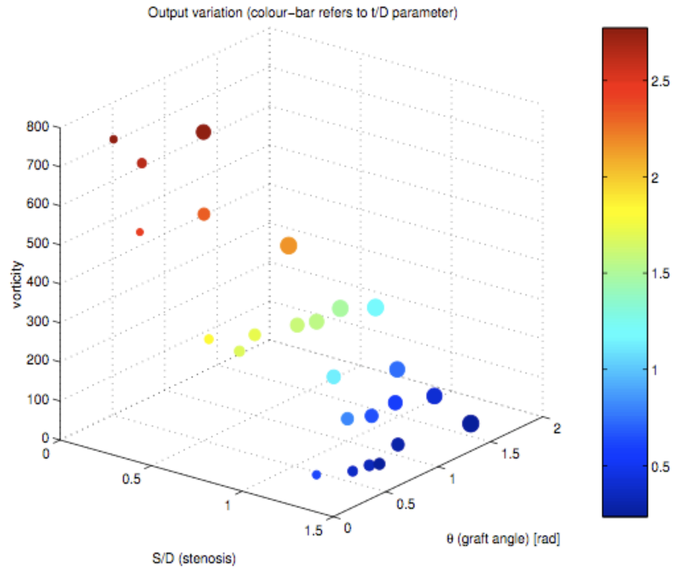
$$J_o(\Omega_o; \mathbf{v}) = \int_{\Omega_o^{df}} |\nabla\times\mathbf{v}|^2 d\Omega_o,$$

$$J_o(\Omega_o; \mathbf{v}) = -\int_{\partial\Omega_o} \nu\frac{\partial\mathbf{v}}{\partial\mathbf{n}}\cdot\mathbf{t}\, d\Gamma_o$$

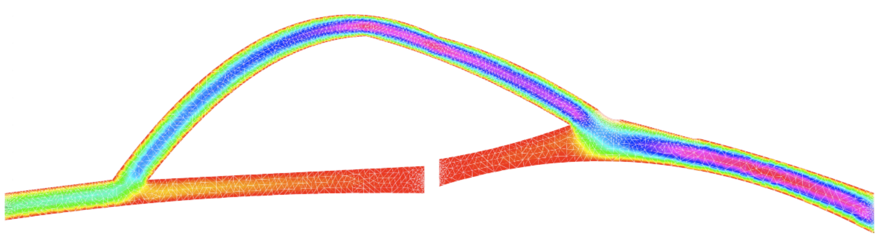
Parametric Shape Optimization

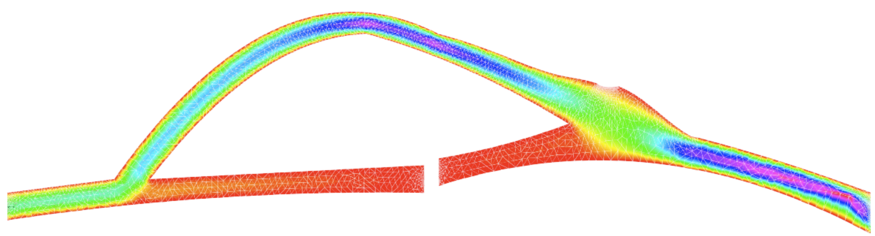
✓ Input parameters as geometrical properties





✓ Input parameters as variables describing the boundary shape

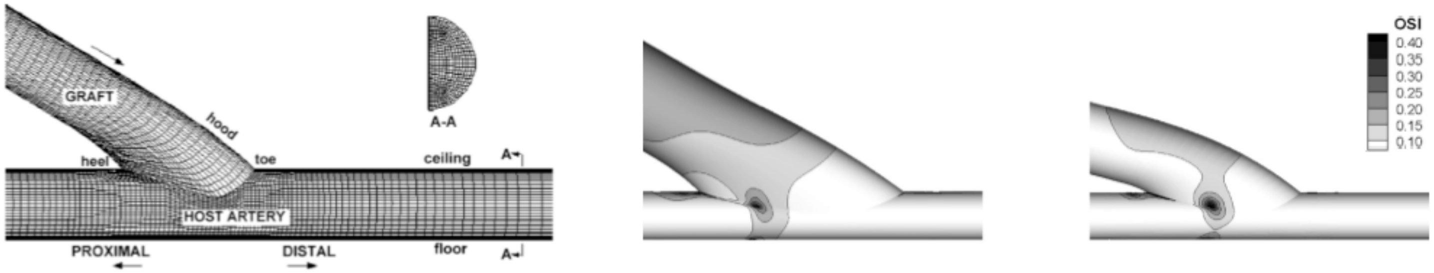




A RB + FFD approach

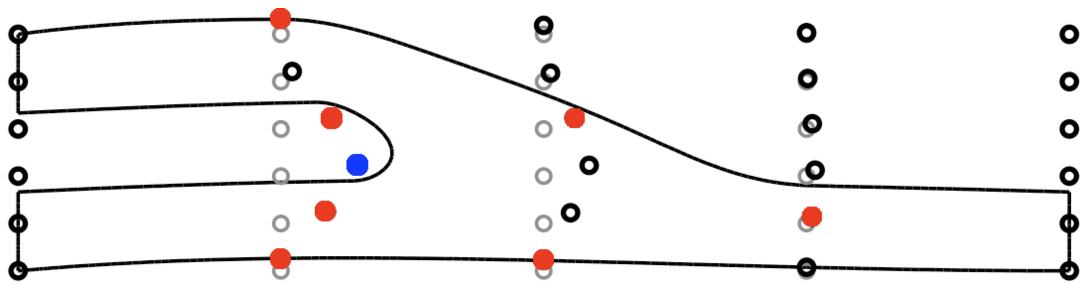
✓ **Many-query problem**: shape optimization by iterative procedure

✓ 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.

✓ 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

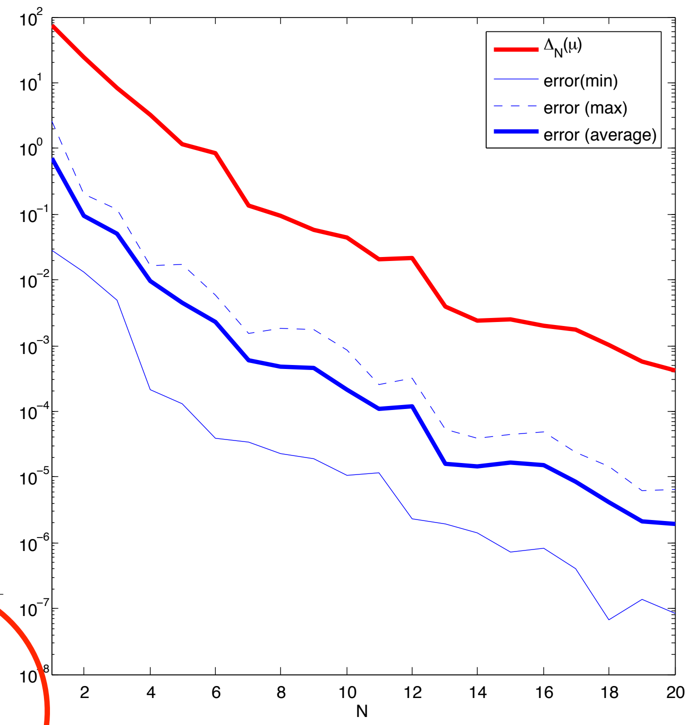


✓ We choose 8 parameters (7 vertical • and 1 horizontal • displacements) to control the anastomotic angle, the graft-artery diameter ratio, the upper side, the lower wall.

Shape Optimization of a bypass graft

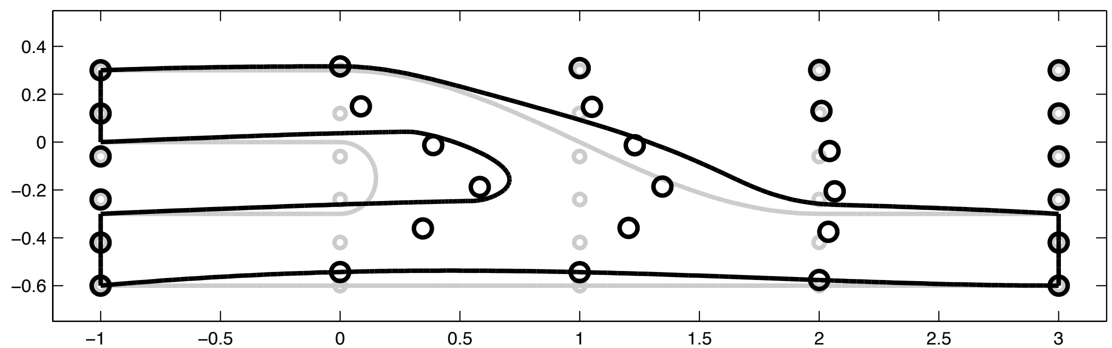
Construction of the RB space

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	20
Error tolerance RB greedy ε_{tol}^{RB}	5×10^{-3}
Affine operator components Q	222



Computational Reduction

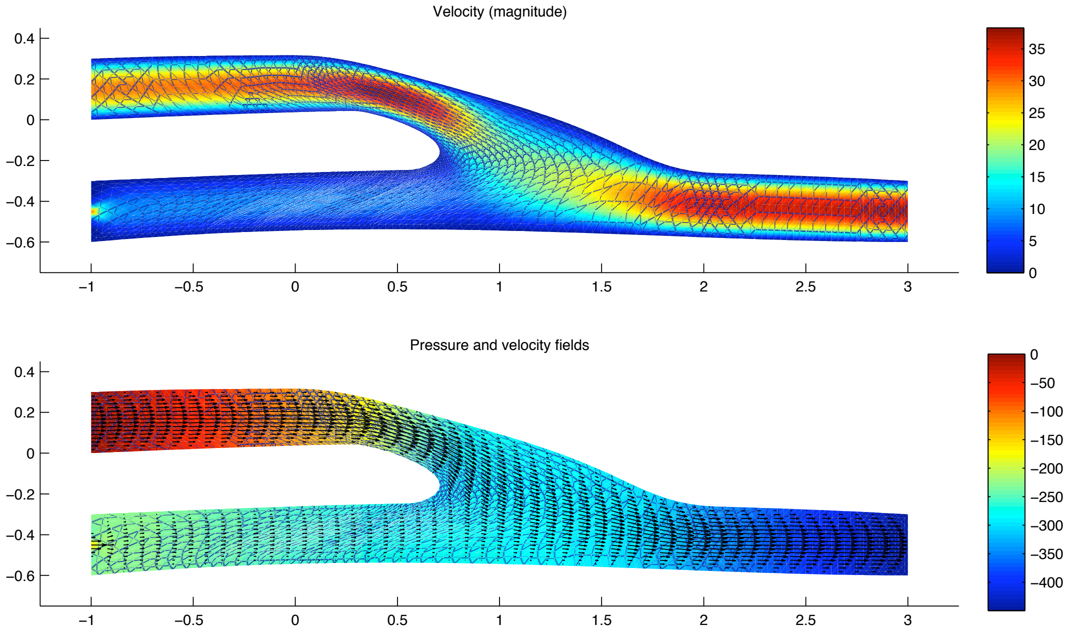
Reduction in linear system dimension	500:1
Computational speedup (single flow simulation	107
Reduct. in param. complexity (w.r.t. mesh motion)	102:1



Initial and optimal bypass configuration

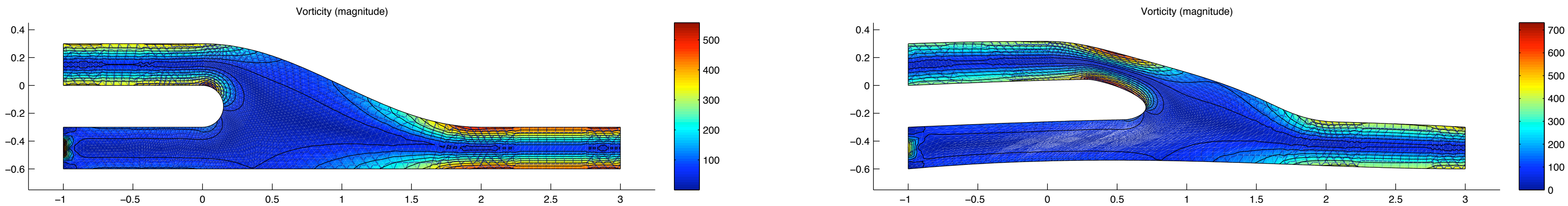
Shape Optimization of a bypass graft

- ✓ Automatic iterative minimization procedure (SQP, sequential quadratic programming)
- ✓ Vorticity evaluation by using the reduced basis velocity at each step



Velocity and pressure field (RB approximation) for the optimal bypass configuration

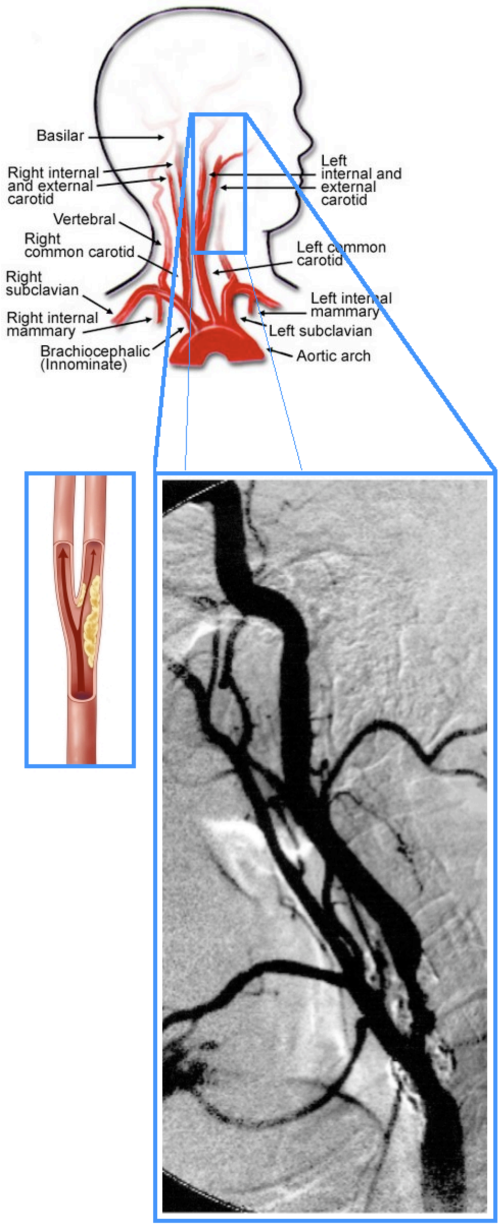
Vorticity reduction (downfield) = 45%



Vorticity field (magnitude) for the initial and the optimal bypass configuration

A. Manzoni, G. Rozza, A.Q., Shape optimization for viscous flows by reduced basis methods and free-form deformation, submitted

Fast blood flow simulation



Vessels geometry strongly influences haemodynamics behaviour

- Study the influence of the vessel shape on blood flow
- Real-time evaluation of flow indexes related with geometry variation that assess/measure arteries occlusion risk (e.g. vorticity, viscous energy dissipation)

Output evaluation problem:

$$\text{evaluate} \quad J_o(\Omega_o;\mathbf{u}) = \int_{\Omega_o} |\nabla \mathbf{u}|^2 d\Omega_o \quad \text{s.t.}$$

$$\begin{cases} -\nu \Delta \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p = \mathbf{f} & \text{in } \Omega_o \\ \nabla\cdot\mathbf{u} = 0 & \text{in } \Omega_o \\ \mathbf{u} = \mathbf{u}_g & \text{on } \Gamma_w^o := \partial\Omega_o \setminus \Gamma_{out}^o \\ -p\cdot\mathbf{n} + \nu \dfrac{\partial \mathbf{u}}{\partial \mathbf{n}} = \mathbf{0} & \text{on } \Gamma_{out}^o \end{cases}$$

Interesting case: stenosed carotid artery bifurcation

- Shape analysis can be useful also for carotid stenting
- The curved (proximal) portions of the internal carotid arteries exhibit a great shape variety

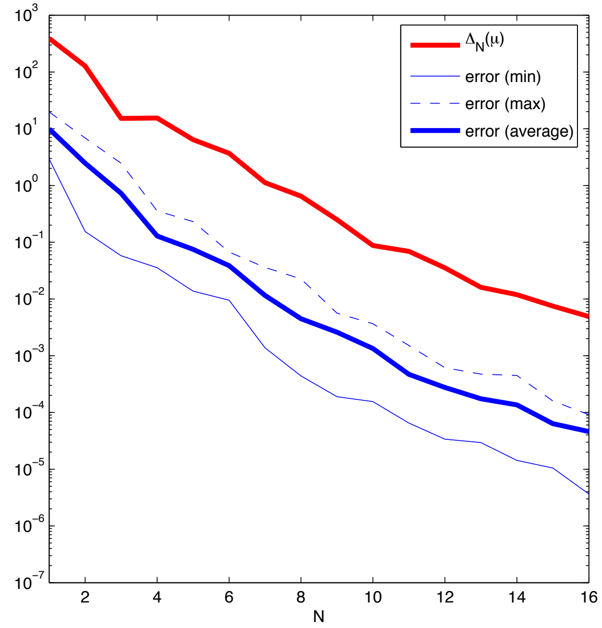
Fast blood flow simulation

Construction of the RB space

Number of FE dof $\mathcal{N}_v + \mathcal{N}_p$	24046
Number of RB functions N	16
Number of design variables P	7

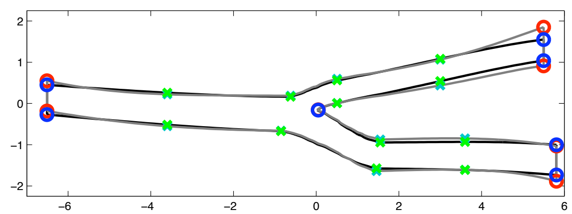
Linear system dimension reduction	500:1
FE evaluation t_{FE} (s)	217.76
RB evaluation t_{RB}^{online} (s)	2.31

- Error estimation and • true error RB vs. FE approximation



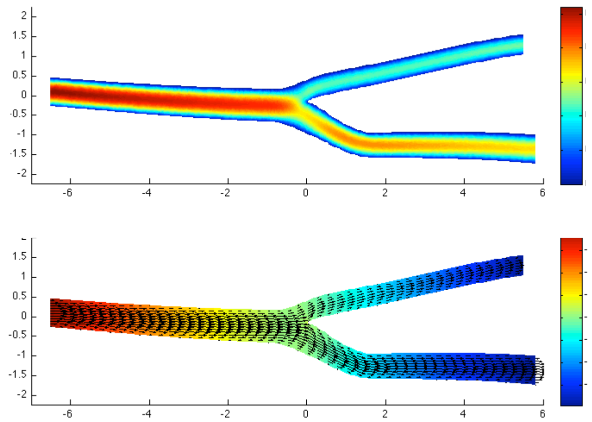
CPU-Shape reconstruction

t = 5.35s



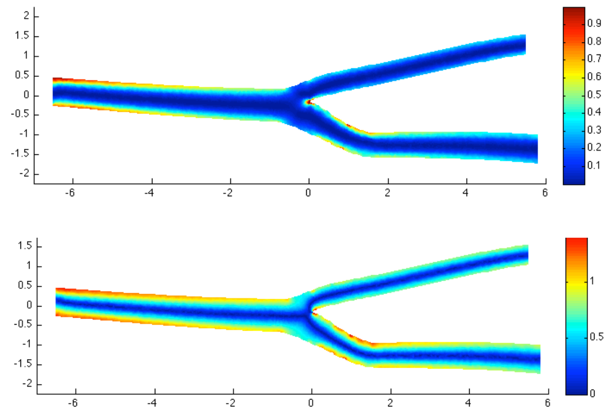
CPU-RB flow simulation

t = 2.31s



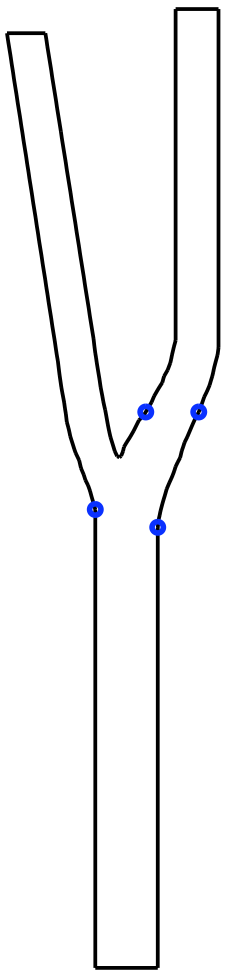
CPU-Output evaluation

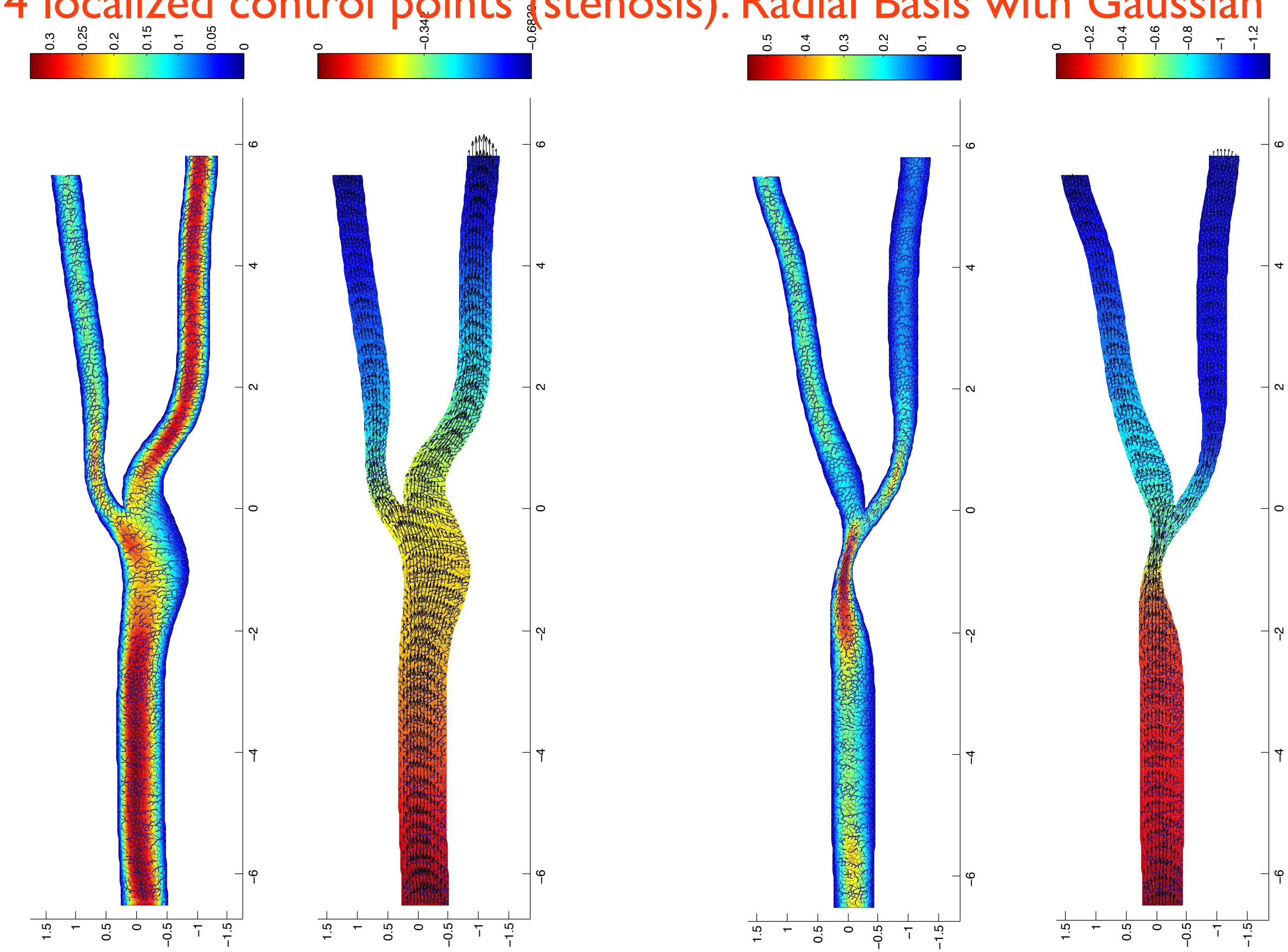
t = 1.54s



Fast blood flow simulation

Local deformations - 4 localized control points (stenosis). Radial Basis with Gaussian kernel

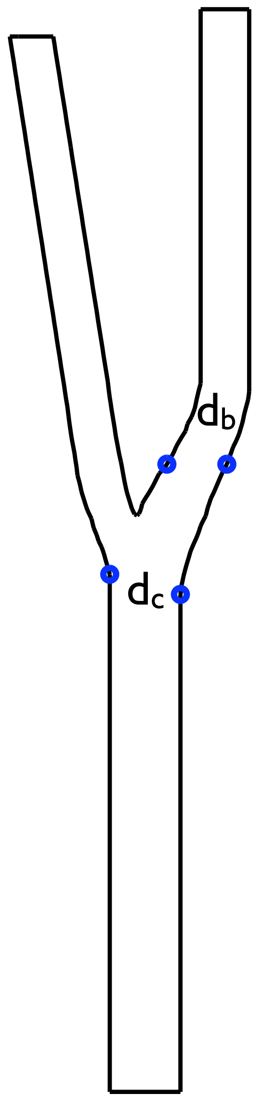


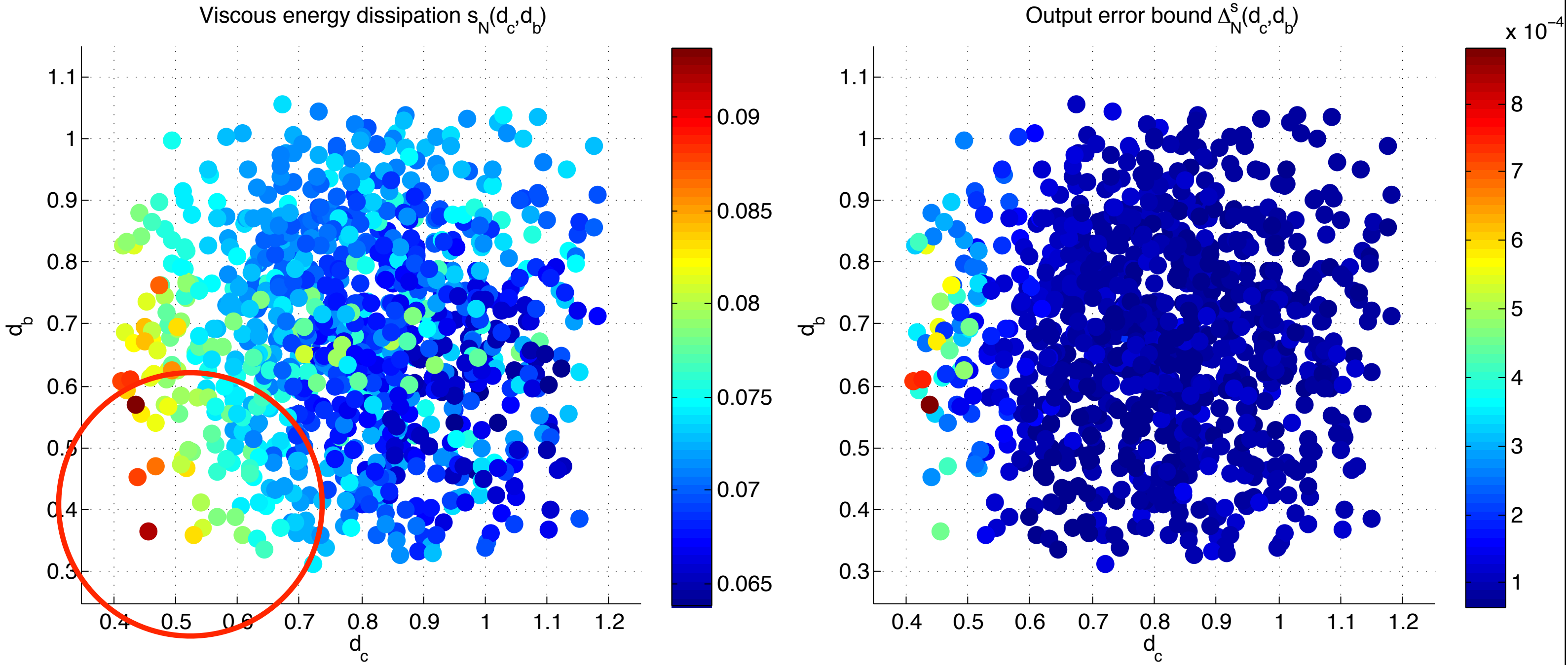


- ✓ Blood flows in different stenosed parametrized geometries, described by P = 4 parameters (horizontal displacements of the ● control points)
- ✓ Each RB online evaluation takes about 2.5 seconds

Fast blood flow simulation

Shape Sensitivity





Viscous energy dissipation and estimated error between RB and FE approximations for 1000 parametrized configurations

- ✓ Viscous energy dissipation for 1000 different parametrized configurations
- ✓ Flow disturbances caused by stenoses lead to higher values of the dissipated energy, the maximum occurring for the smallest diameters on both sections.