BOUNDARY CONTROL PROBLEMS IN HEMODYNAMICS

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Motivation

- The progress of medical imaging techniques, blood flow modelling, and computational capacity allow us to consider the possibility of obtaining patient specific simulations.
- Numerical simulations must be reliable
- Important flow indicators as the Wall Shear Stress are highly sensitive to the geometry and the parameters in the model. But those are hard to "guess"!
    - Missing link: use the available data to make simulations reliable...

Motivation

- The progress of medical imaging techniques, blood flow modelling, and computational capacity allow us to consider the possibility of obtaining patient specific simulations.
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  - Missing link: use the available data to make simulations reliable...

The Cardiovascular System - too large to model in detail

Fig: *medicalnoises.com*

- Aorta with characteristic diameter 2.5 cm
- 50 arteries with diameter $1 - 10$ mm
- 10^3 arteries with diameter $0.5 - 1$ mm
- 10^4 arterioles with diameter $0.01 - 0.5$ mm
- 10^6 capillaries with diameter $0.006 - 0.01$ mm

[Thiriet, Parker, *Physiology and pathology of the cardiovascular system*, Cardiovascular Mathematics, 2009]

Blood Composition

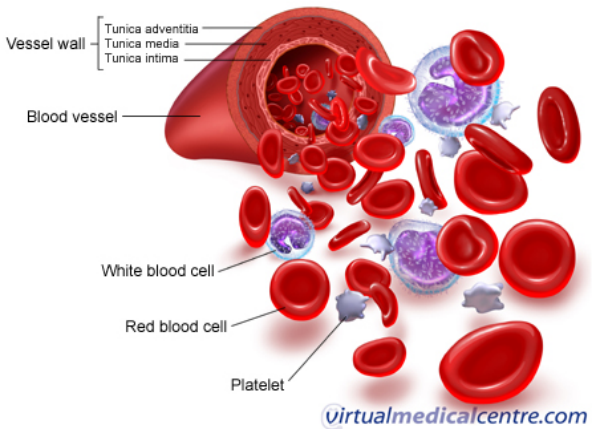

Fig: *myvmc.com*

Blood is a suspension of particles in the plasma (92% of water)

- Red Blood Cells (RBC) - $6-8\ \mu m/\ 4-6\times 10^6$ per mm^3 (45% of blood volume)
- White Blood Cells - $8-18\ \mu m\ /\ 4-10\times 10^3$ per mm^3
- Platelets

[Robertson, Sequeira, Kameneva, *Hemorheology*, in: Hemodynamic Flows, Birkhäuser, 2008]

Viscosity laws for shear-thinning behavior

- $\mu(\dot{\gamma}) = \mu_\infty + \frac{\mu_0 - \mu_\infty}{(1+(\lambda\dot{\gamma})^2)^{\frac{1-n}{2}}}$ $\rightarrow$ Carreau model
  - $\mu_0 = 4.56 \cdot 10^{-2}\, Pa.s, \quad \mu_\infty = 3.2 \cdot 10^{-3}\, Pa.s$
  - $n = 0.344, \quad \lambda = 10.3\, s$
- $\mu(\dot{\gamma}) = \mu_\infty + \frac{\mu_0 - \mu_\infty}{(1+(\lambda\dot{\gamma})^b)^{\frac{1-n}{b}}}$ $\rightarrow$ Carreau-Yasuda model
  - $\mu_0 = 6.57 \cdot 10^{-2}\, Pa.s, \quad \mu_\infty = 4.47 \cdot 10^{-3}\, Pa.s$
  - $n = 0.34, \quad b = 1.76, \quad \lambda = 10.4\, s$
- $\mu(\dot{\gamma}) = \mu_\infty + \frac{\mu_0 - \mu_\infty}{(1+(\lambda\dot{\gamma})^b)^a}$ $\rightarrow$ Generalized Cross model
  - $\mu_0 = 1.6 \cdot 10^{-1}\, Pa.s, \quad \mu_\infty = 3.6 \cdot 10^{-3}\, Pa.s$
  - $a = 1.23, \quad b = 0.64, \quad \lambda = 8.2\, s$

- *Robertson et al.*, Hem. Fl. Mod. An. Sim., 2008.
- *Gambaruto et al.*, Math. BioSc. Eng., 2011.
- *Bodnar, Sequeira, Prosi*, App. Math. Comp., 2011.

Optimal Control in Cardiovascular Mathematics

Optimal Control techniques can be useful to model the cardiovascular system:

- Shape optimization: Rozza, Quarteroni,...
- Inverse problems (parameter estimation): Marsden, Gerbeau, Moireau, Figueroa, Vignon-Clementel, Veneziani, Vergara, ...
- Boundary data reconstruction: D'Elia, Perego, Veneziani

Optimal Control in Cardiovascular Mathematics

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- Boundary data reconstruction: D'Elia, Perego, Veneziani, Guerra, Tiago, Sequeira
- Boundary location: Gambaruto, Tiago, Sequeira

Model for medium size arteries with rigid walls - The Generalized Navier-Stokes Equations

$$\begin{cases} \rho(\dfrac{d\mathbf{u}}{dt} + \mathbf{u}\cdot\nabla\mathbf{u}) = div\ (\tau(D\mathbf{u})) - \nabla p + \mathbf{f} & \text{in } \Omega \\ div\,\mathbf{u} = 0 & \text{in } \Omega, \\ \mathbf{u} = 0 & \text{on } \Gamma_{wall} \\ \mathbf{u} = \mathbf{g} & \text{on } \Gamma_{in} \\ (-p\mathbf{I} + 2\nu(\dot{\gamma})D\mathbf{u})\cdot\mathbf{n} = P_{out} & \text{on } \Gamma_{out}. \end{cases}$$

where $\tau(D\mathbf{u}) = 2\nu(\sqrt{D\mathbf{u} : D\mathbf{u}})D\mathbf{u} = 2\nu(\dot{\gamma})D\mathbf{u}$

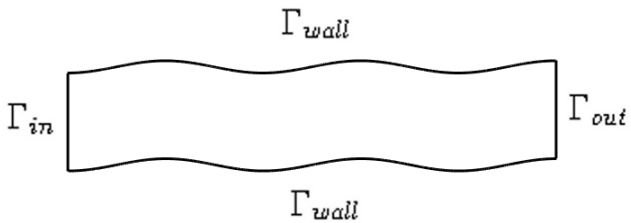
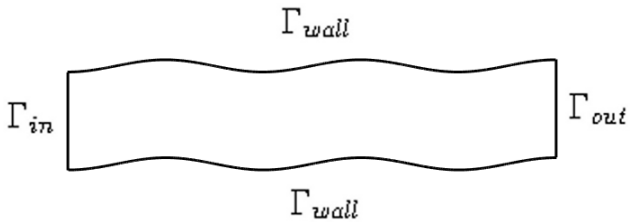


Fig: Domain representation

The optimal control problem: velocity tracking (steady flow)

$$\begin{cases} -div\ (\tau(D\mathbf{u})) + \rho\mathbf{u}\cdot\nabla\mathbf{u} + \nabla p = \mathbf{f} & \text{in } \Omega \\ div\,\mathbf{u} = 0 & \text{in } \Omega \\ \mathbf{u} = 0 & \text{on } \Gamma_{wall} \\ \mathbf{u} = \mathbf{g} & \text{on } \Gamma_{in} \\ (-p\mathbf{I} + 2\nu(\dot{\gamma})D\mathbf{u})\cdot\mathbf{n} = 0 & \text{on } \Gamma_{out}. \end{cases}$$



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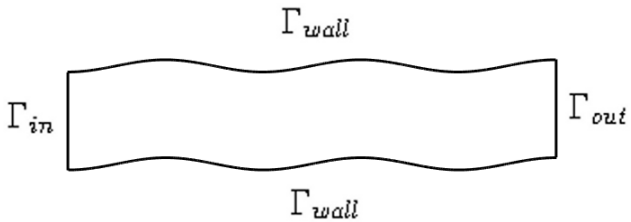

Fig: Domain representation

The optimal control problem: velocity tracking

$$\mathbf{J}(\mathbf{u}, \mathbf{g}) = \beta_1 \int_{\Omega_{part}} |\mathbf{u} - \mathbf{u}_d|^2 dx + \beta_2 \int_{\Gamma_{in}} |\mathbf{g}|^2 ds + \beta_3 \int_{\Gamma_{in}} |\nabla_s \mathbf{g}|^2 ds$$

The optimal control problem: velocity tracking

Minimize

$$\mathbf{J}(\mathbf{u}, \mathbf{g}) = \beta_1 \int_{\Omega_{part}} |\mathbf{u} - \mathbf{u}_d|^2 dx + \beta_2 \int_{\Gamma_{in}} |\mathbf{g}|^2 ds + \beta_3 \int_{\Gamma_{in}} |\nabla_s \mathbf{g}|^2 ds$$

subject to

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Remark:

In: *"D'Elia, A. Veneziani, Methods for assimilating blood velocity measures in hemodynamics simulations: preliminary results, Procedia Comput. Sci., 2010."* *the control was taken as the pressure - Neumann control.*

Theoretical frame: Non-Newtonian case

Existence results and optimality conditions for distributed and boundary control, Neumann type.

$$\mathbf{J}(\mathbf{u}, \mathbf{g}) = \frac{1}{2}\int_{\Omega} |\mathbf{u} - \mathbf{u}_d|^2 dx + \frac{w_2}{2}\int_{\Omega} |g|^2 ds$$

for generalized Newtonian models

Eduardo Casas, Fernandez, Nadir Arada, Telma Guerra.

Theoretical frame: Newtonian case

Existence results and optimality conditions for full Dirichlet boundary control

$$\mathbf{J}(\mathbf{u}, \mathbf{g}) = \frac{1}{2}\int_{\Omega} |\mathbf{u} - \mathbf{u}_d|^2 dx + \frac{w_2}{2}\int_{\partial\Omega} |g|^2 ds$$

Gunzburger, Casas, Manservisi, Fursikov, De los Reyes, Kunish,....

- Gunzburger, Hou, Svobodny, RAIRO- Mod. Math. An. Num., 1991
- De los Reyes, Kunisch, Num. An., 2005
- Manservisi, I.J. Num. An. Mod., 2007
- De los Reys, Yousept, J. Math. An. App., 2009

Except in

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Existence results and optimality conditions for full Dirichlet boundary control

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Theoretical Frame: Direct Problem

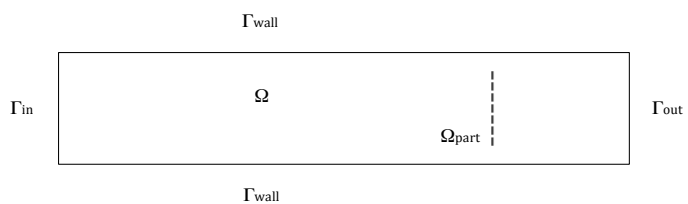
$$\begin{cases} -\nu \triangle \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p = \mathbf{f} & \text{in } \Omega, \\ div\, \mathbf{u} = 0 & \text{in } \Omega, \\ \mathbf{u} = 0 & \text{on } \Gamma_{wall} \\ \mathbf{u} = \mathbf{g} & \text{on } \Gamma_{in} \\ \nu \dfrac{d\mathbf{u}}{d\mathbf{n}} - \mathbf{n}p = 0 & \text{on } \Gamma_{out}. \end{cases}$$

Definition

Let $\mathbf{g} \in \mathbf{H}_0^1(\Gamma_{in})$, $\mathbf{f} \in \mathbf{L}^{\frac{3}{2}}(\Omega)$. We say that $\mathbf{u} \in \mathbf{V}_{\Gamma_{wall}}$ is a weak solution of (NS) if $\gamma_{\Gamma_{in}} \mathbf{u} = \mathbf{g}$ and

$$-\nu \int_\Omega \nabla \mathbf{u} : \nabla \mathbf{v}\, dx + \int_\Omega (\mathbf{u} \cdot \nabla)\mathbf{u}\mathbf{v}\, dx = \int_\Omega \mathbf{f}\mathbf{v}\, dx,$$

for all $\mathbf{v} \in \mathbf{V}_D$.



$$H_0^1(\Gamma_{in}) = \left\{ v \in L^2(\Gamma_{in}) \mid \nabla_s v \in L^2(\Gamma_{in}),\ \gamma_{\partial\Gamma_{in}} v = 0 \right\}$$

$$\mathbf{V}_{\Gamma_{wall}} = \left\{ \mathbf{v} \in H^1(\Omega) :\ \gamma_{\Gamma_{wall}} \mathbf{v} = 0,\ div\, \mathbf{v} = 0 \right\}$$

$$\mathbf{V}_{\Gamma_D} = \left\{ \mathbf{v} \in H^1(\Omega) :\ \gamma_{\Gamma_D} \mathbf{v} = 0,\ div\, \mathbf{v} = 0 \right\}$$

Theoretical Frame: Direct Problem

Theorem

Let $g \in \mathbf{H}_0^1(\Gamma_{in})$ such that $\|g\|_{\mathbf{H}_0^1(\Gamma_{in})} \leq \rho$, for $\rho > 0$ sufficiently small, and $f \in \mathbf{L}^{\frac{3}{2}}(\Omega)$. Then, there exists a unique weak solution $u \in \mathbf{V}_{\Gamma_{wall}}$ of the Navier-Stokes eq which verifies

$$\|u\|^2_{\mathbf{H}^1(\Omega)} \leq \alpha\left(\|g\|^2_{\mathbf{H}_0^1(\Gamma_{in})}\right) + \|f\|^2_{\mathbf{L}^{\frac{3}{2}}(\Omega)}, \tag{1}$$

where $\alpha(s) = c(s^2 + s)$.

$$\mathbf{V}_{\Gamma_{wall}} = \left\{\mathbf{v} \in H^1(\Omega) : \gamma_{\Gamma_{wall}}\mathbf{v} = 0,\ div\,\mathbf{v} = 0\right\}$$

$$H_0^1(\Gamma_{in}) = \left\{v \in L^2(\Gamma_{in}) \mid \nabla_s v \in L^2(\Gamma_{in}),\ \gamma_{\partial\Gamma_{in}} v = 0\right\}$$

[Guerra, Sequeira, Tiago, *Existence of optimal boundary control for the Navier-Stokes equations with mixed boundary conditions*, Port. Math, 2015].

Theoretical Frame: Direct Problem - Some tools

- $H_{00}^{\frac{1}{2}}(\Gamma) = \left\{ g \in L^2(\Gamma) \mid \exists v \in H^1(\Omega),\ v_{|\partial\Omega} \in H^{\frac{1}{2}}(\partial\Omega),\ \gamma_\Gamma v = g,\ \gamma_{\partial\Omega\setminus\Gamma} v = 0 \right\}$

  closed subspace of $H^{\frac{1}{2}}(\Gamma)$.

- The continuous embeddings $H_0^1(\Gamma) \subset H_{00}^{\frac{1}{2}}(\Gamma)$ and $H_{00}^{\frac{1}{2}}(\Gamma) \subset L^2(\Gamma)$

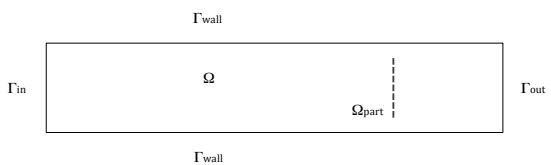
  [R. Dautray, J. L. Lions, *Mathematical Analysis and Numerical Methods for Science and Technology*, 2000]

- Extension operator from $\hat{H}^{\frac{1}{2}}(\Gamma_{in} \cup \Gamma_{out})$ to $\mathbf{V}_{\Gamma_{wall}}$

  $\hat{H}^{\frac{1}{2}}(\Gamma_1 \cup \Gamma_2) = \left\{ (g_1, g_2) \in H_{00}^{\frac{1}{2}}(\Gamma_1) \times H_{00}^{\frac{1}{2}}(\Gamma_2) \mid \int_{\Gamma_1} g_1 \cdot n\, ds + \int_{\Gamma_2} g_2 \cdot n\, ds = 0 \right\}$

Lemma

Let $(g_1, g_2) \in \hat{H}^{\frac{1}{2}}(\Gamma_{in} \cup \Gamma_{out})$. Then there is a bounded extension operator $E : \hat{H}^{\frac{1}{2}}(\Gamma_{in} \cup \Gamma_{out}) \to \mathbf{V}_{wall}$, $\forall v \in \mathbf{V}_{wall}$, such that for $v = E(g_1, g_2)$ we have $g_1 = \gamma_{\Gamma_{in}} v$, $g_2 = \gamma_{\Gamma_{out}} v$.



- Theorem proof: Fixed point argument + Estimates for Stokes solution

Theoretical Frame: Control Problem - Existence Result

Minimize

$$\mathbf{J}(\mathbf{u}, \mathbf{g}) = \beta_1 \int_{\Omega_{part}} |\mathbf{u} - \mathbf{u}_d|^2 dx + \beta_2 \int_{\Gamma_{in}} |\mathbf{g}|^2 ds + \beta_3 \int_{\Gamma_{in}} |\nabla_s \mathbf{g}|^2 ds$$

[$\Omega_{part} = \cup_{i=1}^{m} s_i$ where S_i are cross sections of the "vessel" domain] subject to

$$\begin{cases} -\nu \triangle \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p = \mathbf{f} & \text{in } \Omega, \\ div\, \mathbf{u} = 0 & \text{in } \Omega, \\ \mathbf{u} = 0 & \text{on } \Gamma_{wall} \\ \mathbf{u} = \mathbf{g} & \text{on } \Gamma_{in} \\ \nu \dfrac{d\mathbf{u}}{d\mathbf{n}} - \mathbf{n}p = 0 & \text{on } \Gamma_{out}. \end{cases}$$

$$\mathbf{g} \in \mathcal{U}, \quad \mathbf{u} \in \mathbf{V}_{\Gamma_{wall}} = \left\{ \mathbf{v} \in H^1(\Omega) : \gamma_{\Gamma_{wall}} \mathbf{v} = 0,\ div\, \mathbf{v} = 0 \right\}$$

$$\mathcal{U} = \left\{ g \in H_0^1(\Gamma_{in}) \mid \|g\|_{H_0^1(\Gamma)} \leq \rho \right\} \subset \mathcal{U}_0$$

$$\mathcal{U}_0 = \left\{ g \in H_0^1(\Gamma_{in}) : \text{s.t. NSEq have a unique weak solution} \right\}.$$

[Guerra, Sequeira, Tiago, *Existence of optimal boundary control for the Navier-Stokes equations with mixed boundary conditions*, Port. Math, 2015].

Theoretical Frame: Control Problem - Tools

Direct Method of the Calculus of Variations

- Non-emptiness of admissible set
- Compactness of minimizing sequences
- J is weakly l.s.c (we need to check continuity and convexity properties)

Numerical Approach - Discretization

- Discretize then Optimize approach -
  - Discretize using Finite Element Methods + GLS stabilization:

Minimize

$$\mathbf{J}(\mathbf{u},\mathbf{g}) = \beta_1 \int_{\Omega_{part}} |\mathbf{u} - \mathbf{u}_d|^2 dx + \beta_2 \int_{\Gamma_{in}} |\nabla_s \mathbf{g}|^2 ds$$

subject to

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Numerical Approach - Discretization

- Discretize then Optimize approach -
  - Discretize using Finite Element Methods + GLS stabilization:

Minimize

$$J(U, G) = \beta_1 \langle U - U_d, M(U - U_d) \rangle_{N_u} + \beta_2 \langle G, NG \rangle_{N_g}$$

subject to

$$\begin{cases} \mathbf{Q}(U) + \mathbf{N}(U)U + B^T P = F(U) \\ BU = 0\,. \end{cases}$$

$$U = U(G)$$

Numerical Approach - Discretization

- Discretize then Optimize approach -
  - Discretize using Finite Element Methods + GLS stabilization:

the diffusion term:

$$\int_{\Omega} \nu \nabla \mathbf{u}_h : \nabla \mathbf{v}_h + \sum_{K \in \tau_h} \int_{K} -\nu \Delta \mathbf{u}_h \cdot \varphi(\mathbf{u}_h, \mathbf{v}_h).$$

the convective term:

$$\int_{\Omega} ((\mathbf{u}_h \cdot \nabla)\mathbf{u}_h) \cdot \mathbf{v}_h + \sum_{K \in \tau_h} \int_{K} ((\mathbf{u}_h \cdot \nabla)\mathbf{u}_h) \cdot \varphi(\mathbf{u}_h, \mathbf{v}_h).$$

$$\varphi(\mathbf{u}_h, \mathbf{v}_h) = \delta((\mathbf{u}_h \cdot \nabla)\mathbf{v}_h + \nu \triangle \mathbf{v}_h).$$

[Bazilevs, Hughes, et al, *Int. J. Numer. Meth. Fluids*, 2007]

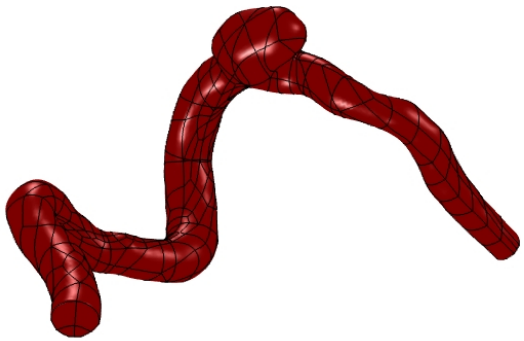
Numerical Approach- Optimization

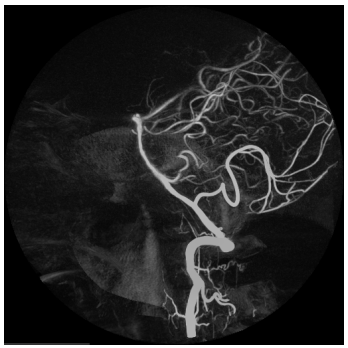
- Solve the Nonlinear Mathematical Programming (NMP) problem
  - Use Sequential Quadratic Programming (in SNOPT - Sparse Nonlinear Optimization + SQOPT)

$$\begin{cases} \min\limits_{g} Q(u(g), g) \\ L(u(g), g) = 0 \\ l_1 \leq G(u(g), g) \leq l_2 \end{cases}$$

[Gill, Murray, Saunders, *Siam Review*, 2005]

3D simulations: the case of a brain aneurysm





- Computational domain Segmented from Medical Images
- Mesh Tetrahedral and Hexahedral (boundary layers) elements
- Stabilized P1-P1 FEM. 213k dofs
- Finite Element Meth. solved with Comsol Multiphysics

Direct Solution - Data to be used

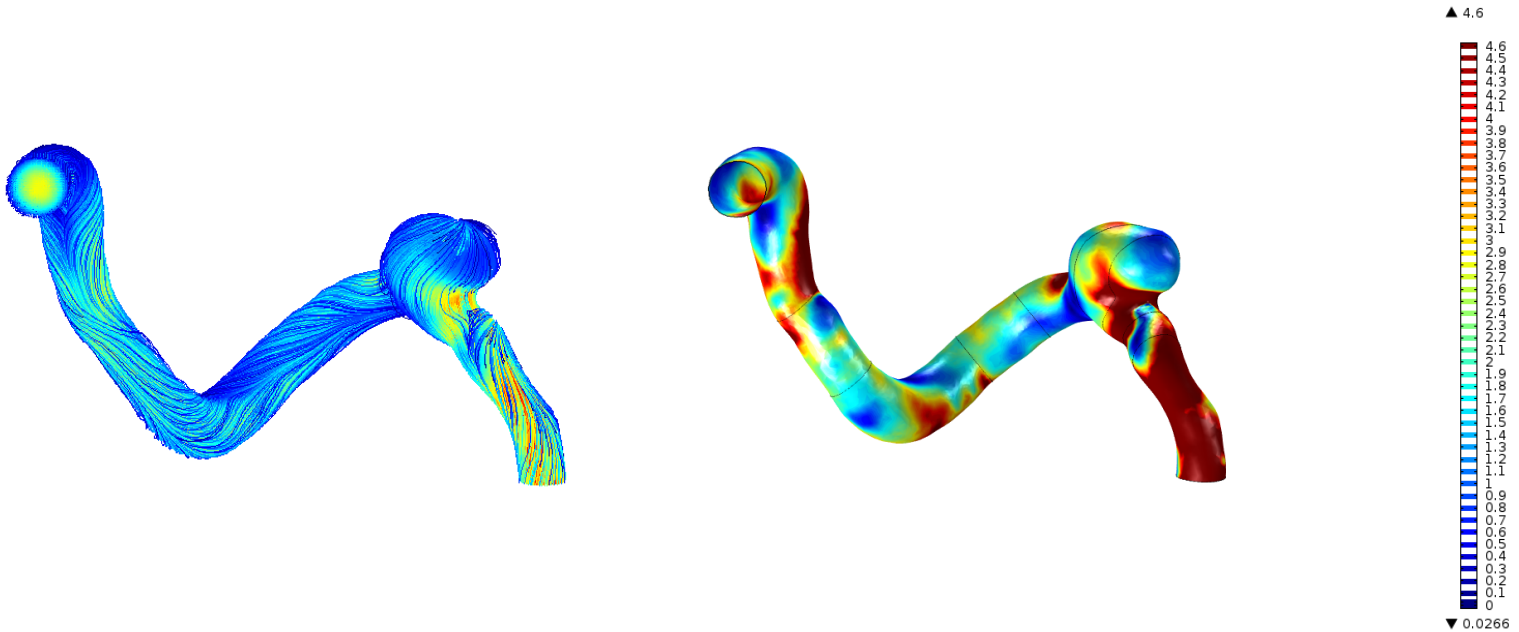
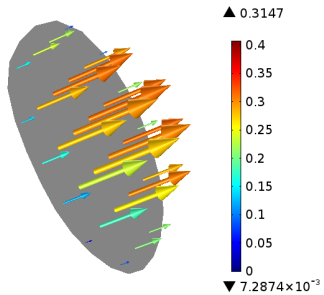


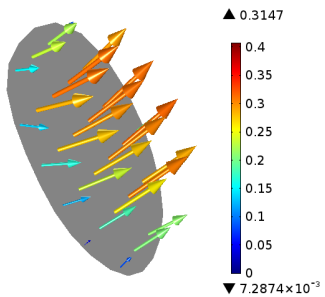
Fig: Left: Streamlines. Right: WSS (N/m^2) .

Naïve Solution: laminar inflow boundary, same flow rate Q



(a) Laminar Inlet for the naïve solution (u_Q).

(b) Domain of interest



(c) True velocity (u_d) at the inlet .

Control Problem

$$\min \mathbf{J}(\mathbf{u}, \mathbf{g}) = 1.e^{4} \int_{\Omega_{part}} |\mathbf{u} - \mathbf{u}_d|^2 dx + 1.e^{-3} \int_{\Gamma_{in}} |\nabla_s \mathbf{g}|^2 dx$$

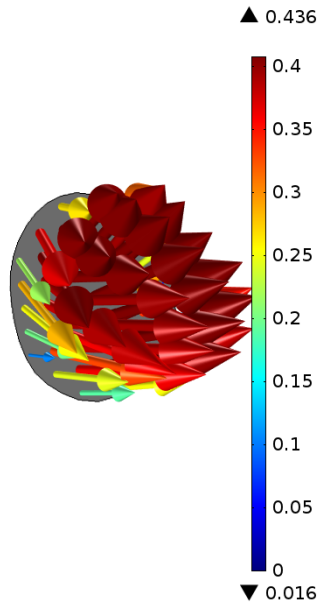
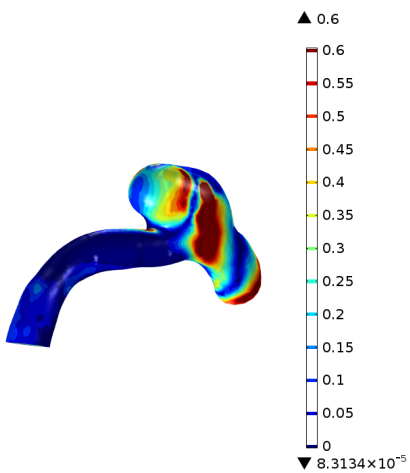


Fig: Left: Observations $\mathbf{u}_d$ in Ω_{part}. Right: Velocity vectors at Ω_{part}

Numerical Results: global view

Weights	Rel. Error Ω_{part}	Rel. error Ω
$\mathbf{u}$ vs $\mathbf{u}_d$, $\beta_1 = 1e^4$	0.06778	0.11732
$\mathbf{u}$ vs $\mathbf{u}_d$, $\beta_1 = 1e^5$	0.01381	0.0883
$\mathbf{u}_Q$ vs $\mathbf{u}_d$	0.10584	0.15199

Table: Errors relative to $\mathbf{u}_d$ for $\mathbf{u}_Q$ and the controlled solutions $\mathbf{u}$



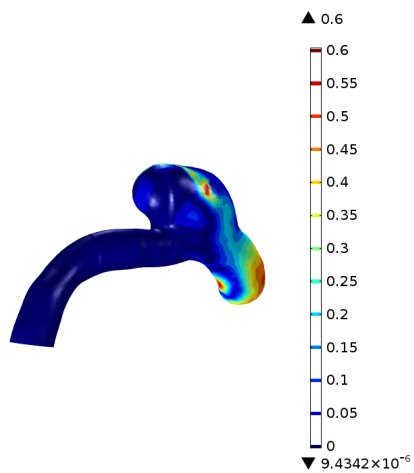
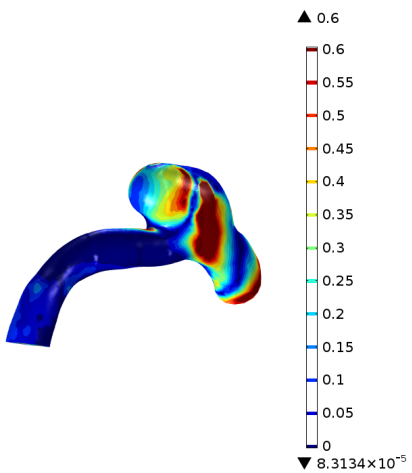


Fig: Left: Wall Shear Stress Relative Error of u_Q with respect to u_d. Right: Wall Shear Stress Relative Error of u with respect to u_d.

Numerical Results: 3D control - enriched data

Weights	Rel. Error Ω_{part}	Rel. error Ω
$\mathbf{u}$ vs $\mathbf{u}_d$, $\beta_1 = 1e^4$	0.0279	0.07548
$\mathbf{u}$ vs $\mathbf{u}_d$, $\beta_1 = 1e^5$	0.00524	0.03478
$\mathbf{u}_Q$ vs $\mathbf{u}_d$	0.10584	0.15199

Table: Errors relative to $\mathbf{u}_d$ for $\mathbf{u}_Q$ and the controlled solutions $\mathbf{u}$



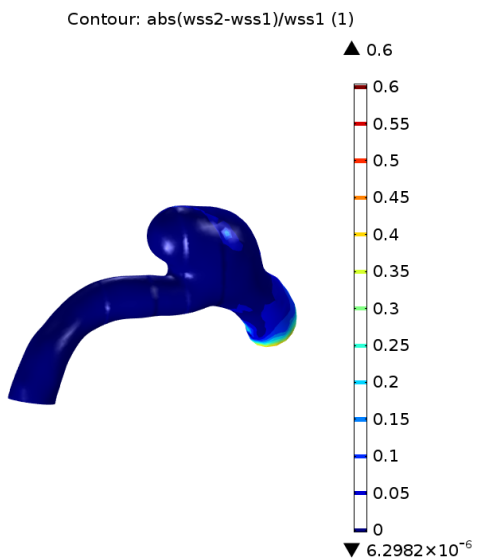


Fig: Left: Wall Shear Stress Relative Error of u_Q with respect to u_d. Right: Wall Shear Stress Relative Error of u with respect to u_d.

Future Work

- Theoretical frame:
  - Regularity;
  - Time dependent problems (ongoing).
- For the velocity reconstruction, use real data and time dependent model;
  - Deal with the presence of errors (from data or/and from the model) - Kalman filter.
  - Order reduction.
- 3D wall reconstruction (ongoing)

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References

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- Guerra, Sequeira, Tiago, *Existence of optimal boundary control for the Navier-Stokes equations with mixed boundary conditions*, Portugal. Math., 2015.

- Tiago, Gambaratuto, Sequeira, *Patient-specific blood flow simulations: setting Dirichlet boundary conditions for minimal error with respect to measured data*, Math. Model. Nat. Phenom., 2014.

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Thank you for your attention!

Wall Reconstruction

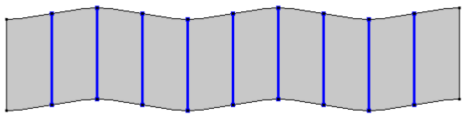
We can now choose the uncertain velocity profiles as the solution of the optimal control problem

$$\min_{\mathbf{g}\in\mathcal{A}} \mathbf{J}(\mathbf{g}) = \beta_1 \int_{\Omega_{Obs}} |\mathbf{u} - \mathbf{u}_d|^2 \, dx + \beta_2 \int_{\Gamma_c} |\nabla \mathbf{g}|^2 \, dx \tag{2}$$

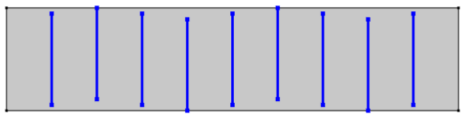
subject to

$$\begin{cases} -div\,\tau + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p = 0 & \text{in } \Omega \\ div\,\mathbf{u} = 0 & \text{in } \Omega, \\ \mathbf{u} = 0 & \text{on } \Gamma_{wall} \setminus \Gamma_c \\ \mathbf{u} = \mathbf{g} & \text{on } \Gamma_c \\ (-p\mathbf{I} + 2\nu D\mathbf{u})\cdot\mathbf{n} = 0 & \text{on } \Gamma_{out}. \end{cases} \tag{3}$$

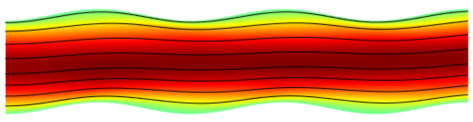
Example: Wavy Channel



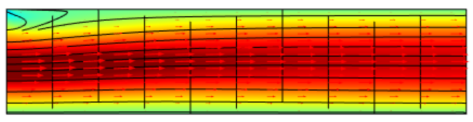
True geometry and observation sections



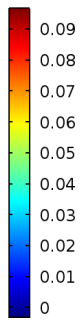
Approximated geometry

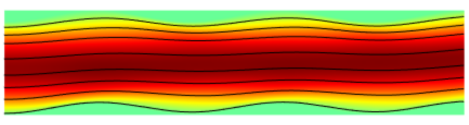


True solution

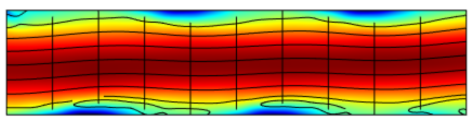


Initial guess

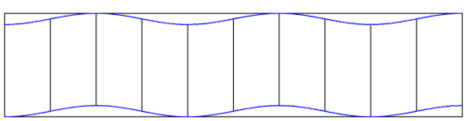




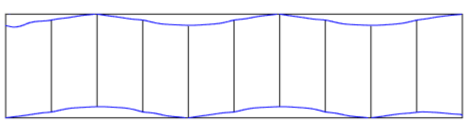
True solution extrapolated



Controlled solution

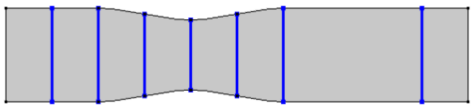


Zero contour for true solution extrapolated

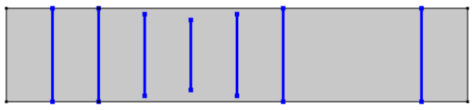


Zero contour of controlled solution

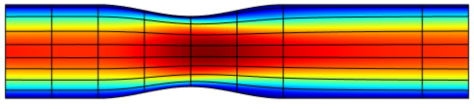
Example: Stenosis



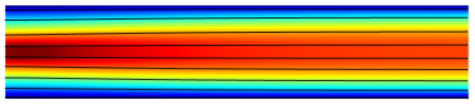
True geometry and observation sections



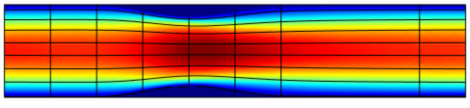
Approximated geometry



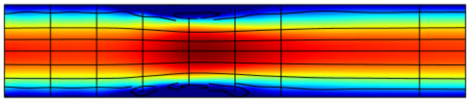
True solution



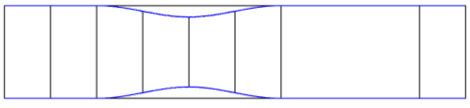
Initial guess



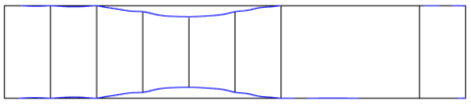
True solution extrapolated



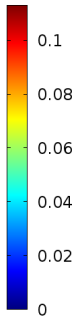
Controlled solution



Zero contour for true solution, extrapolated



Zero contour of controlled solution



Example: Saccular Aneurysm

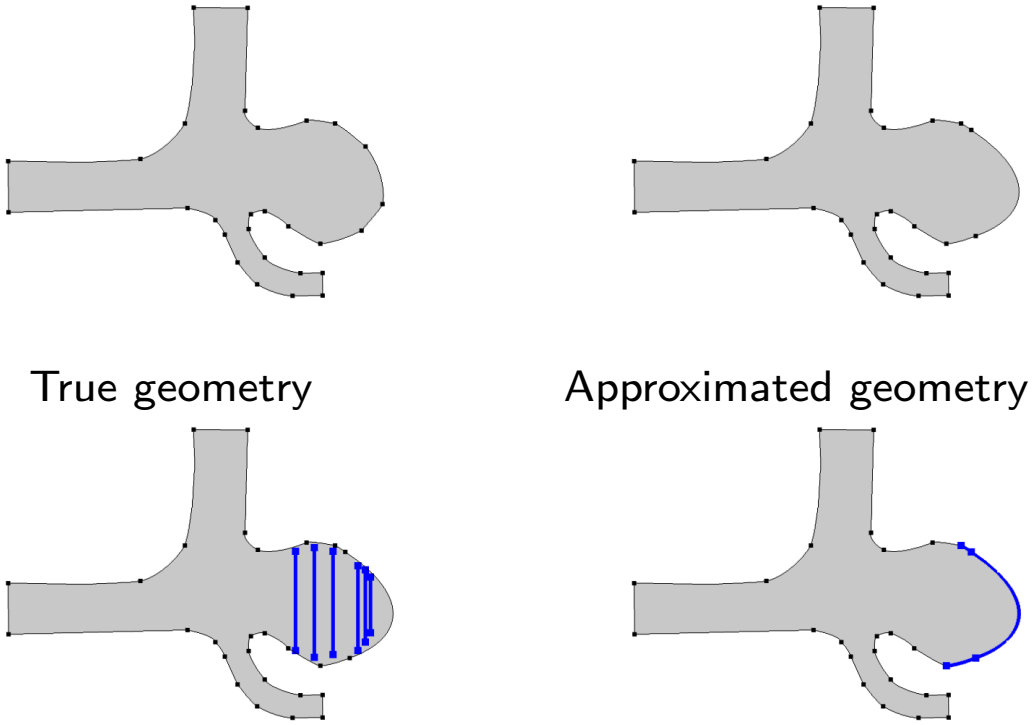


Fig: Top row left: original geometry. Top row right: approximated geometry. Bottom row left: observation sections Ω_{obs}. Bottom row right: the boundary to be controlled.

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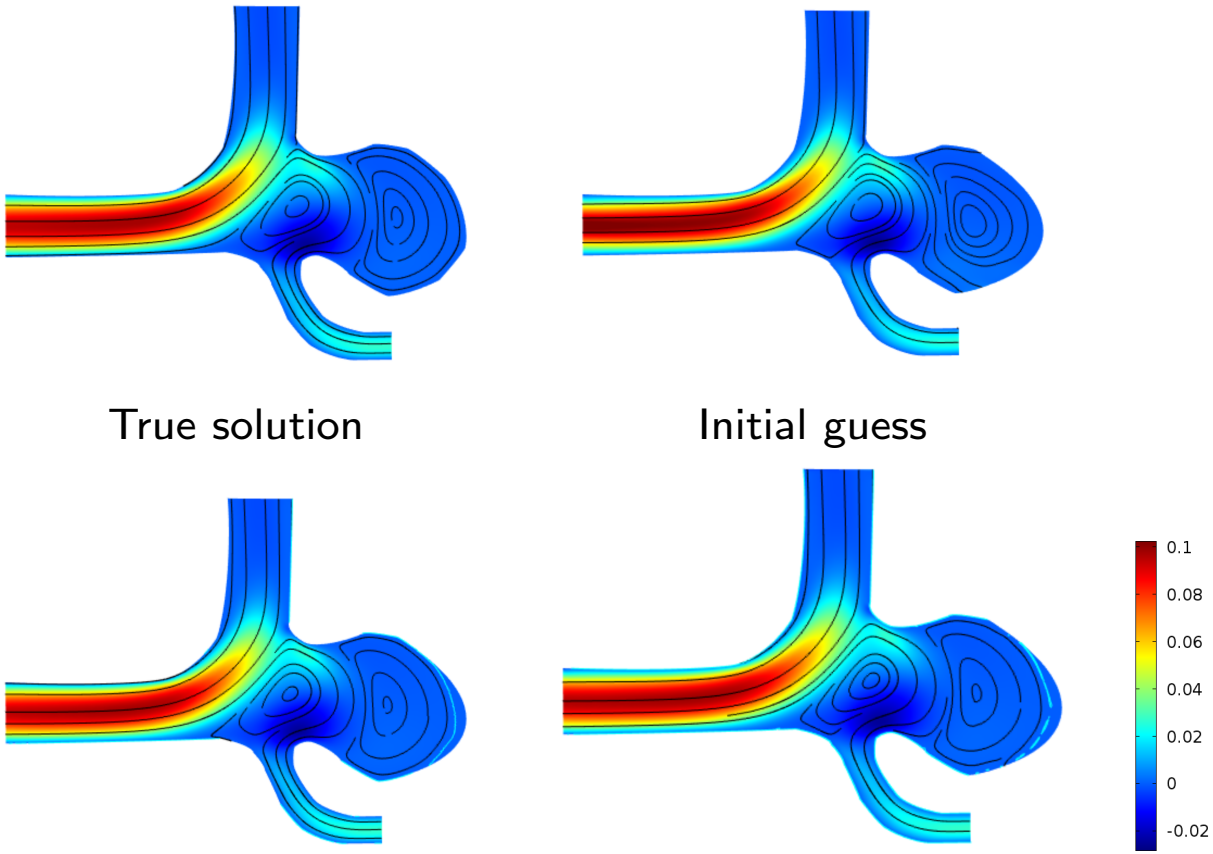

Fig: Top row left: solution for original geometry. Top row right: approximated solution using constant average velocity. Second row left: solution extrapolated for approximated geometry.