Numerical investigation of blood flows with slip boundary conditions

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AND PHYSICS
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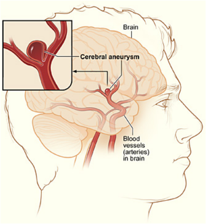
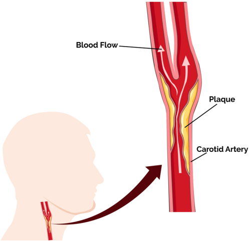
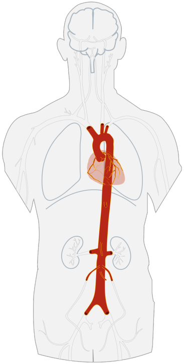
Motivation - blood flows

Examples

- Flows in aneurysms - predicting problematic cases
- Flows in carotids - plaque deposition and stenosis
- Flows in aorta - artificial replacemnts, pathological wall changes

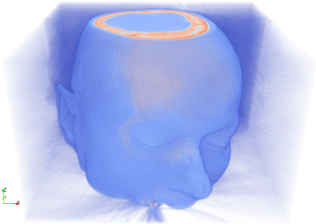






Motivation - typical work pipeline

using your favorite tools: Vascular Modelling Toolkit `www.vmtk.org`, Itk-SNAP `www.itksnap.org`...



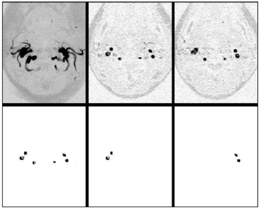
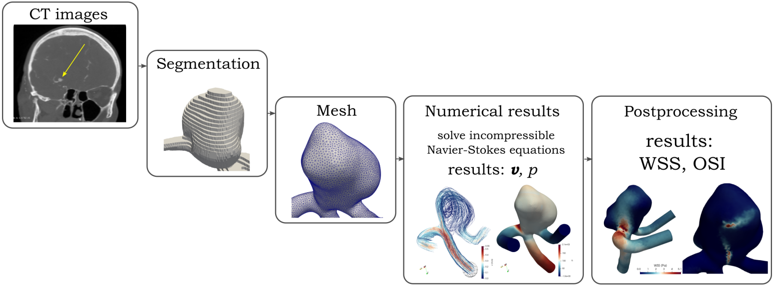


Figure 9: CT image processing.



Model Problem - Descending Aorta

$$\rho(\nabla \mathbf{v})\mathbf{v} - \operatorname{div} \mathbb{T}(\mathbf{v}, p) = \mathbf{0} \quad \text{in } \Omega$$

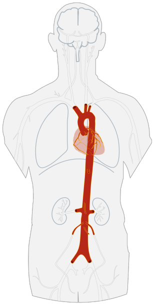
$$\mathbb{T}(\mathbf{v}, p) = -p\mathbb{I} + 2\mu\mathbb{D}(\mathbf{v}) \quad \text{in } \Omega$$

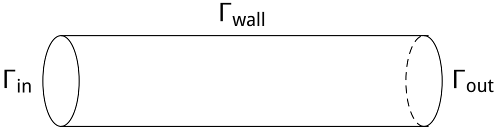
$$\operatorname{div} \mathbf{v} = 0 \quad \text{in } \Omega$$

$$\mathbf{v} = \mathbf{v}_{\text{in}} \quad \text{on } \Gamma_{\text{in}}$$

$$(\mathbb{T}(\mathbf{v}, p)\,\mathbf{n}) \cdot \mathbf{n} = \frac{1}{2}\rho\,(\mathbf{v} \cdot \mathbf{n})_-^2 \quad \text{and} \quad \mathbf{v}_{\text{t}} = \mathbf{0} \quad \text{on } \Gamma_{\text{out}}$$

$$\theta\,\mathbf{v}_{\text{t}} + \gamma_*(1-\theta)(\mathbb{T}(\mathbf{v}, p)\,\mathbf{n})_{\text{t}} = \mathbf{0} \quad \text{and} \quad \mathbf{v} \cdot \mathbf{n} = 0 \quad \text{on } \Gamma_{\text{wall}}$$





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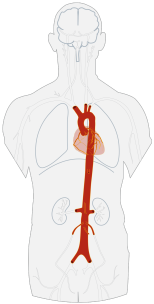

Why to use Navier slip boundary condition:

- for blood suggested by some experiment [Nubar (1973), Hershey (1965)]
- possible bc for models based on mixture/suspension
- compensation of geometry uncertainity [Nolte (2019)]

Model Problem - Descending Aorta

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{\color{blue}\rho}(\nabla \mathbf{v})\mathbf{v} - \operatorname{div} \mathbb{T}(\mathbf{v}, p) &= \mathbf{0} && \text{in } \Omega \\
\mathbb{T}(\mathbf{v}, p) &= -p\,\mathbb{I} + 2{\color{blue}\mu}\mathbb{D}(\mathbf{v}) && \text{in } \Omega \\
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\end{aligned}
$$

$$
\begin{aligned}
\mathbf{v} &= {\color{red}\mathbf{v}_{\text{in}}} && \text{on } \Gamma_{\text{in}} \\
(\mathbb{T}(\mathbf{v}, p)\,\mathbf{n}) \cdot \mathbf{n} = \frac{1}{2}\,{\color{blue}\rho}\,(\mathbf{v} \cdot \mathbf{n})_-^2 \quad \text{and} \quad \mathbf{v}_{\text{t}} &= \mathbf{0} && \text{on } \Gamma_{\text{out}} \\
{\color{red}\theta}\,\mathbf{v}_{\text{t}} + \gamma_*(1 - {\color{red}\theta})(\mathbb{T}(\mathbf{v}, p)\,\mathbf{n})_{\text{t}} = \mathbf{0} \quad \text{and} \quad \mathbf{v} \cdot \mathbf{n} &= 0 && \text{on } \Gamma_{\text{wall}}
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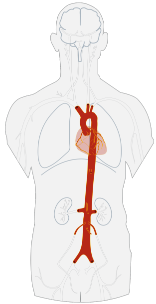
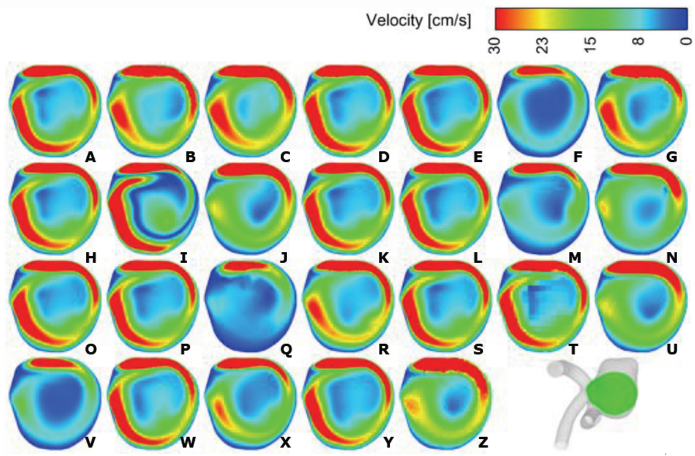


- μ, ρ: use tabular data or patient specific measurements
- θ, $\mathbf{v}_{\text{in}}$: difficult or impossible to measure directly

Discretization

- time discretization: BDF-k, Crank-Nicholson scheme (TS object in PETSc)
- space discretization: FEM P_1^+/P_1 (MINI), P_2/P_1 (Taylor-Hood) or stabilized P_1/P_1 on tetrahedrons
- nonlinear solver - Newton method, NGMRES with nonlinear preconditioning by quasi-Newton with laged Jacobian (SNES/NPC objects from PETSc)
- Core problem: Solve large, sparse, non-symmetric, indefinite linear system of equations. (direct sparse multifrontal method - MUMPS)

Aneurysm challenge



Results from 26 groups on the prescribed plane for the second case
16 groups used plug flow, 12 groups used Ansys software

G. Janiga et al. (2015): *The Computational Fluid Dynamics Rupture Challenge 2013*

Hemodynamic risk indicators

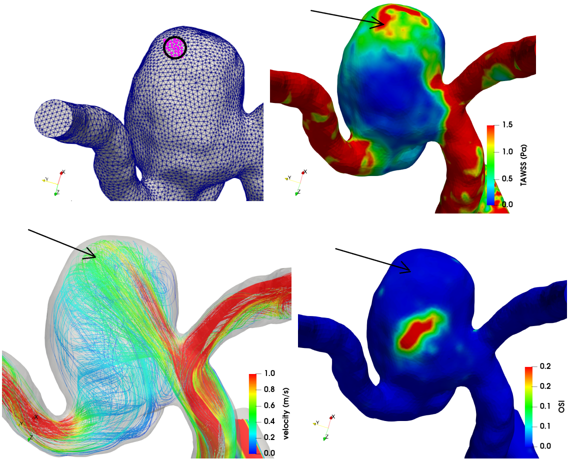
- Wall shear stress (WSS): the tangential part of the traction force

$$\mathbf{WSS} = (\mathbb{T}\boldsymbol{n})_\tau = \mathbb{T}\boldsymbol{n} - (\mathbb{T}\boldsymbol{n} \cdot \boldsymbol{n})\boldsymbol{n},$$

- Oscillatory shear index (OSI): measures WSS oscillations
- Oscillatory velocity index (OVI): measures oscillations of velocity

$$\mathrm{OI}_{\mathbf{a}} = \frac{1}{2}\left(1 - \frac{\left|\int_0^T \mathbf{a}\,\mathrm{dt}\right|}{\int_0^T |\mathbf{a}|\,\mathrm{dt}}\right)$$

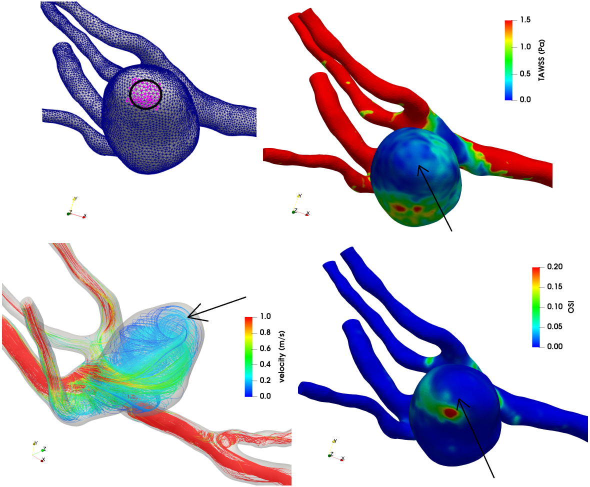
Ruptured aneurysms



Correlation of hemodynamic parameters to the site of the rupture.

A. Hejčl et al. (2019): Hemodynamics in ruptured intracranial aneurysms

Ruptured aneurysms



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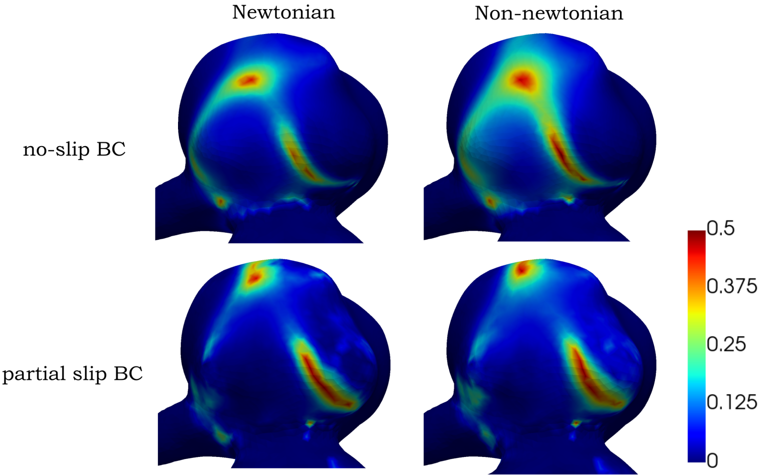
Comparison - non-Newtonian vs Navier slip



OSI/OVI for two different models (Newtonian and Carreau–Yasuda) and slip parameters (no-slip and partial slip with $\theta = 0.95$).

Flow in descending aorta

- Geometry segmented from MRI image
- Available velocity image from MRI

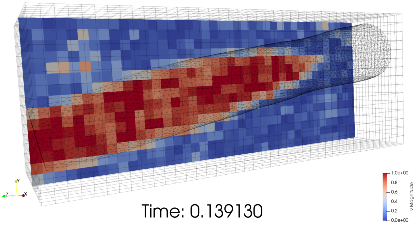


Figure: 4D-PC MRI data

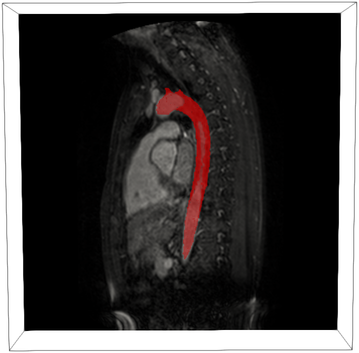


Figure: Geometry segmentation

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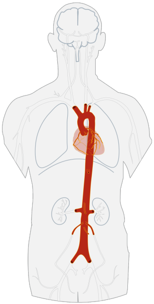

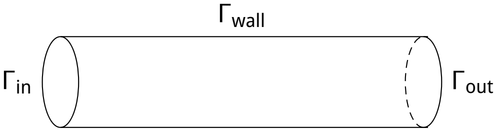

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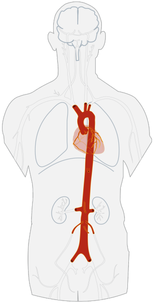
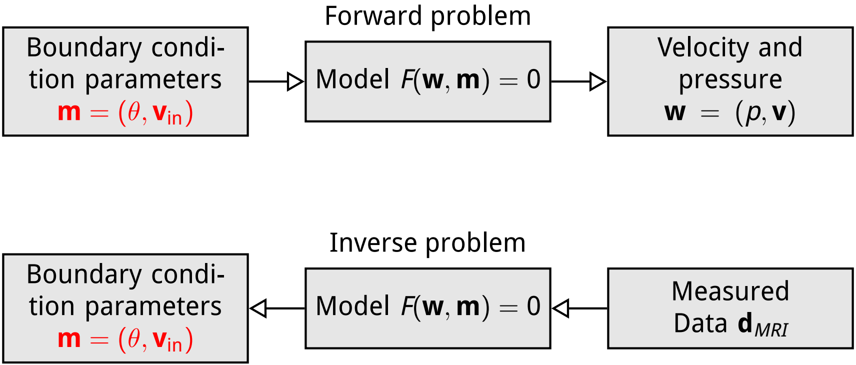
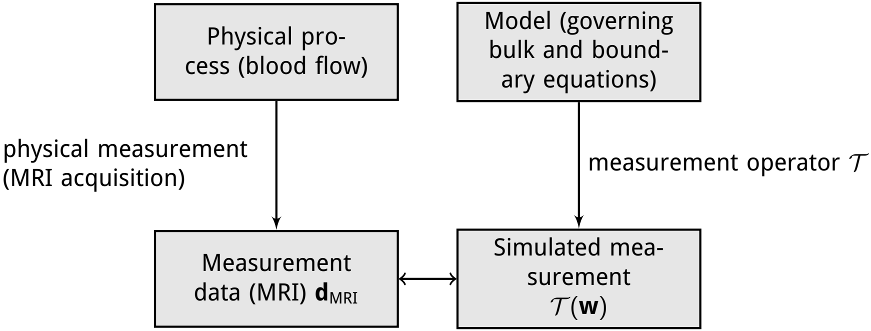


- μ, ρ: use tabular data or patient specific measurements
- $\theta, \mathbf{v}_{\text{in}}$: difficult or impossible to measure directly
- Simplified notation:
  - unknown parameters: $\mathbf{m} = (\theta, \mathbf{v}_{\text{in}})$
  - PDE solution: $\mathbf{w} = (p, \mathbf{v})$
  - model: $F(\mathbf{w}, \mathbf{m}) = 0$

Inverse Problem



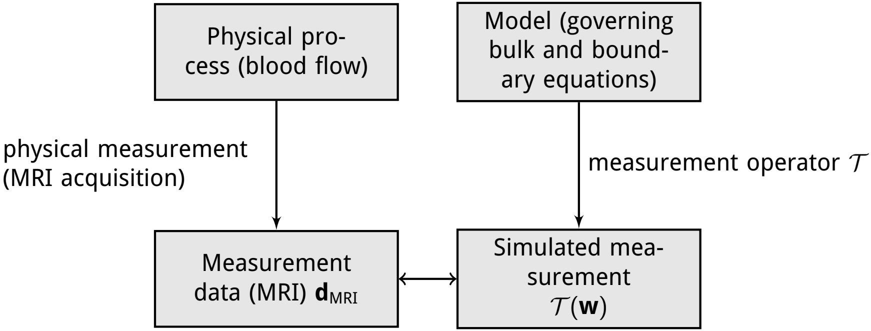
Variational Data Assimilation



- minimize an error functional $\mathcal{J}$ subject to PDE $F(\mathbf{w}, \mathbf{m}) = 0$

$$\mathcal{J}(\mathbf{w}, \mathbf{m}) = \frac{1}{2} ||\mathcal{T}(\mathbf{w}) - \mathbf{d}_{\mathrm{MRI}}||^2$$

Variational Data Assimilation



- minimize an error functional $\mathcal{J}_R$ subject to PDE $F(\mathbf{w}, \mathbf{m}) = 0$

$$\mathcal{J}_R(\mathbf{w}, \mathbf{m}) = \frac{1}{2}||\mathcal{T}(\mathbf{w}) - \mathbf{d}_{\text{MRI}}||^2 + \frac{\alpha}{2}||\mathbf{m}||^2$$

- α: Tikhonov regularization weight

Adjoint Based Approach

Data: $\mathbf{m}^0$
for $i = 0, 1, 2 \ldots$ **do**
  if *stopping criterion is fulfilled* **then**
    stop the optimization
  else
    find $\mathbf{w}(\mathbf{m}^i)$ by solving the PDE equations $F(\mathbf{w}, \mathbf{m}) = 0$ with $\mathbf{m}^i$;
    find λ^i by solving the adjoint equations $\left(\frac{\partial F}{\partial \mathbf{w}}\right)^* (\lambda^i) = \frac{\partial \mathcal{J}_R}{\partial \mathbf{w}}$ for $\mathbf{m}^i$ and $\mathbf{w}(\mathbf{m}^i)$;
    evaluate $\hat{\mathcal{J}}_R(\mathbf{m}^i) = \mathcal{J}_R(\mathbf{w}(\mathbf{m}^i), \mathbf{m}^i)$;
    compute $\frac{\partial \hat{\mathcal{J}}_R}{\partial \mathbf{m}}(\mathbf{m}^i) = -\left\langle \lambda^i, \frac{\partial F}{\partial \mathbf{m}} \right\rangle + \frac{\partial \mathcal{J}_R}{\partial \mathbf{m}}$;
    determine $\mathbf{m}^{i+1}$ using the chosen optimization algorithm;

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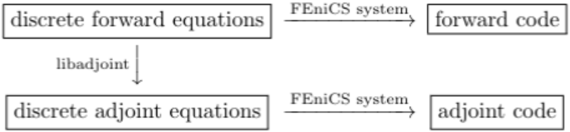
FEniCS PROJECT
dolfin-adjoint
Firedrake

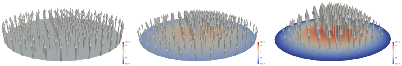


Application to descending aorta flow problem

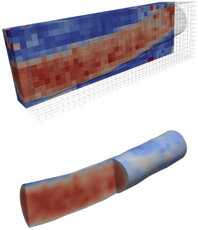
- Controls: $\mathbf{m} = (\theta, \mathbf{v}_{\text{in}})$, PDE solution: $\mathbf{w} = (\mathbf{v}, p)$

$$\mathcal{J}_R\left((\mathbf{v}, p), (\theta, \mathbf{v}_{\text{in}})\right) = \frac{1}{2\,\ell^3} ||\mathbf{v} - \mathbf{d}_{\text{MRI}}||^2_{L^2(\Omega)} + \frac{\alpha}{2} ||\nabla \mathbf{v}_{\text{in}}||^2_{L^2(\Gamma_{\text{in}})} + \frac{\beta}{2\,\ell^2} ||\mathbf{v}_{\text{in}} - \mathbf{v}_{\text{analytic}}(V, \theta)||^2_{L^2(\Gamma_{\text{in}})}$$

- $\mathbf{v}_{\text{analytic}}(V, \theta)$: analytic solution for Poiselle flow for given V and



$\mathbf{d}_{\text{MRI}}$:



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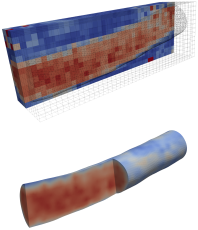

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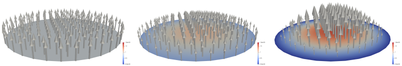

- finite elements: P1P1 + IP stabilization, MINI or Hood-Taylor
- Picard/Newton iterations

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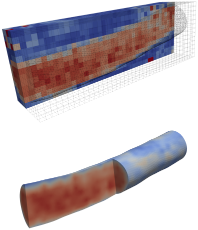

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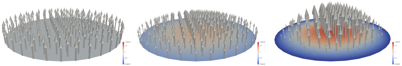
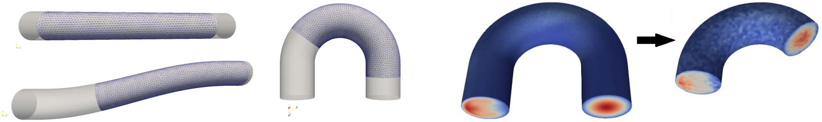


- finite elements: P1P1 + IP stabilization, MINI or Hood-Taylor
- Picard/Newton iterations
- optimization algorithm: L-BGFS-B (from scipy library) or IPOPT (box constraint for $\theta \in [0, 1]$)

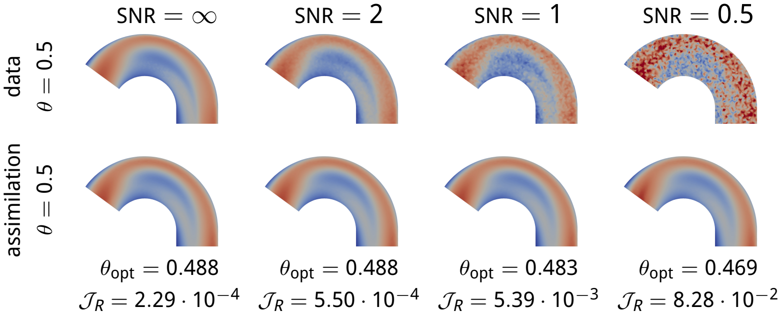
Experiments on Artificial Data in 3D: Setup

- *A. Jarolímová, JH* (2024), *Determination of Navier's slip parameter using variational data assimilation*, *arXiv::2402.04766*



- reference velocity computed for $\theta \in [0.2, 0.5, 0.8, 1.0]$, $V = 0.1$
- inf-sup stable element, $\mathbf{v}_{\text{in}} = \mathbf{v}_{\text{analytic}}(V, \theta)$
- interpolation to shorter and coarser mesh
- addition of Gaussian noise

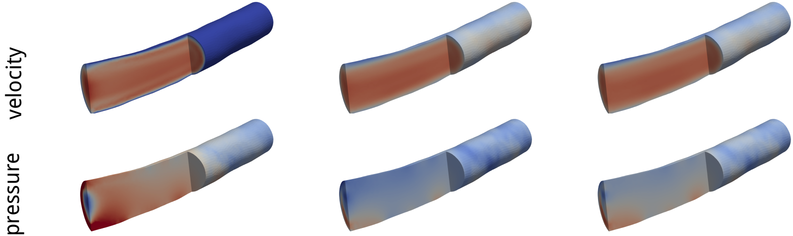
Experiments on Artificial Data in 3D



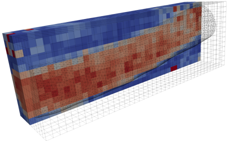
- low sensitivity to the amount of Gaussian noise
- results independent of initial guess
- P1P1 with IP stabilization - sensitive to the stabilization weight α_v

Experiments on Real Data

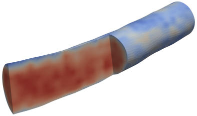
no-slip	Navier's slip	non-const. Navier's slip



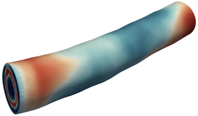
no-slip	Navier's slip	non-const. Navier's slip
$\theta = 1.0$	$\theta_{\text{opt}} = 0.216$	$\text{avg}(\theta_{\text{opt}}) = 0.415$
$\mathcal{J}_R = 0.44218$	$\mathcal{J}_R = 0.16389$	$\mathcal{J}_R = 0.15996$
iterations: 50	iterations: 125	iterations: 681



MRI data



interpolated data



θ_{opt}

Summary

- Blood flow simulations almost exclusively done with no-slip boundary condition. However there are substantial reasons to consider *slip* boundary condition.
- The slip parameter almost imposlible to measure - can be deduced from velocity mesurements (4D-PC MRI - can give velocity field).
- Slip parameter determination robust with respect to data noise.
- The local amount of slip on boundary can possibly indicate either physical state of the wall (inflamation, calcification) or just error in boundary segmentation
- Firedrake/dolfin-adjoint - tool for easy implmentation of the whole pde-constraint minimization problem. 👍