Boundary conditions involving pressure for the Stokes problem and applications in computational hemodynamics

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VIVABRAIN: Virtual angiography simulation from 3D and 3D+t brain vascular models

Real MRA images → 3D vascular models → 3D+t simulation of blood flow → Computational meshes

Goal: Closing the Loop!

N. Passat et al. From Real MRA to Virtual MRA: Towards an Open-Source Framework, MICCAI 2016.
Cerebral venous network: mathematical model

**Blood:** homogeneous, incompressible fluid, with “standard” Newtonian behavior, quasi-steady Navier-Stokes equations:

\[
\rho \frac{\partial \mathbf{u}}{\partial t} - 2 \nabla \cdot (\mu \mathbf{D}(\mathbf{u})) + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla p = 0, \quad \text{in } \Omega \times I
\]

\[
\nabla \cdot \mathbf{u} = 0, \quad \text{in } \Omega \times I
\]

+ Initial and boundary conditions,

where:
- \( \mathbf{u} \) and \( p \) velocity and pressure of the fluid;
- \( \mathbf{D}(\mathbf{u}) = \frac{1}{2} (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \) strain rate tensor;
- \( \sigma(\mathbf{u}, p) = -p \mathbf{I} + 2\mu \mathbf{D}(\mathbf{u}) \) Cauchy stress tensor;
- \( \rho \) and \( \mu \) density and dynamic viscosity of the fluid.

Cerebral venous network: boundary conditions

- **Wall:**
  - \( u = 0 \) (if rigid walls); or
  - \( u = \) velocity of the structure (if elastic walls, fluid-structure coupling).

- **Inflow / Outflow:**
  - Dirichlet BC: if velocity measures available (rarely the case);
  - Neumann / Robin / Non Standard BC: if pressure, flow rate or other data given.

1, internal jugular veins. 2, vein of Galen. 3, straight sinus. 4, confluence of sinuses. 5, lateral sinus (transverse portion). 6, lateral sinus (sigmoid portion). 7, superior sagittal sinus. 8, internal cerebral vein. 9, basilar vein. 10, superior cerebral veins. 11, superior anastomotic veins.
For $\varepsilon = 0$ (Stokes) and $\varepsilon = 1$ (Navier-Stokes), consider the problem:

$$
-\mu \Delta u + \varepsilon (u \cdot \nabla)u + \nabla p = f, \quad \text{in } \Omega,
$$

$$
\nabla \cdot u = 0, \quad \text{in } \Omega,
$$

$$
u = u_1, \quad \text{on } \Gamma_1,
$$

$$
u \times n = u_2 \times n, \quad \text{on } \Gamma_2,
$$

$$
p + \frac{\varepsilon}{2} |u|^2 = p_2, \quad \text{on } \Gamma_2,
$$

where $\partial \Omega = \overline{\Gamma}_1 \cap \overline{\Gamma}_2$ and $\Gamma_1 \cup \Gamma_2 = \emptyset$ represents a partition without overlap of the boundary of a connected bounded domain $\Omega$.  

First works on this topic:


A lot of subsequent literature on boundary conditions on the pressure.

Recent developments:

Variational formulation

Define:

\[
 a(u, v) = \mu \int_{\Omega} (\nabla \times u) \cdot (\nabla \times v) \, dx, \quad N(u, v, w) = \int_{\Omega} [((\nabla \times u) \times v) \cdot w] \, dx
\]

\[
 b(v, q) = -\int_{\Omega} q \nabla \cdot v \, dx, \quad L(v) = \int_{\Omega} f \cdot v - \int_{\Gamma_2} p_2 v \cdot n \, ds.
\]

Main results:

- the problem of finding \((u, p)\) in an appropriate space, such that
  \[
  a(u, v) + \varepsilon N(u, u, v) + b(v, p) = L(v)
  \]
  for all test function \(v\) and \(b(u, q) = 0\) for all test function \(q\) is well posed.
- discretization by FEM + a priori and a posteriori analysis.
- numerical simulations: penalty method.

Key ingredient: rotational formulation for the equation, based on:

\[
 -\Delta u = \nabla \times (\nabla \times u) - \nabla (\nabla \cdot u).
\]
Steady Stokes problem:

\[-2\mu \nabla \cdot (D(u)) + \nabla p = f, \quad \text{in} \ \Omega,\]
\[\nabla \cdot u = 0, \quad \text{in} \ \Omega,\]
\[u = 0, \quad \text{on} \ \Gamma_1,\]
\[u \times n = 0 \quad \text{and}\]
\[p = p_0, \quad \text{on} \ \Gamma_2,\]

where

\[\partial \Omega = \bar{\Gamma}_1 \cap \bar{\Gamma}_2, \quad \text{with} \ \Gamma_1 \cup \Gamma_2 = \emptyset \quad \text{and with} \ \Gamma_2 \ \text{planar}.\]

Remarks:

- Continuous level: the two formulations are equivalent, since
  \[\nabla \cdot u = 0 \Rightarrow \nabla \cdot (\nabla u + \nabla u^T) = \Delta u.\]
- Modeling standpoint (e.g. fluid-structure problems): it might be useful to work with the symmetric tensor, since it gives directly the natural boundary condition for the structure problem.
Variational formulation

\[ 2\mu \int_{\Omega} D(u) : D(v) \, dx - \int_{\Gamma_2} \sigma(u, p) n \cdot v \, ds - \int_{\Omega} p \nabla \cdot v \, dx = \int_{\Omega} f \cdot v \, dx, \quad \forall v \in V, \]

where \( V = \{ v \in [H^1(\Omega)]^d : v = 0 \text{ on } \Gamma_1 \} \).

**Theorem**

For any velocity normal surface \( \Gamma \subset \partial \Omega \), the normal component of the normal traction is given by

\[ (\sigma(u, p)n) \cdot n = -(p + 2\mu |u|_\kappa), \]

where \( \kappa \) is the mean curvature of \( \Gamma \). Furthermore, in the case where \( \Gamma \) is a planar surface, this reduces to the pressure condition

\[ (\sigma(u, p)n) \cdot n = -p. \]


Consequently, on \( \Gamma_2 \) (planar):

\[ \sigma(u, p)n = -pn + \tau(u, p). \]
Variational formulation

Introduce a Lagrange multiplier $\lambda = \tau(u, p)$, then:

$$2\mu \int_{\Omega} D(u) : D(v) \, dx - \int_{\Omega} p \nabla \cdot v \, dx + \int_{\Gamma_2} p_0 n \cdot v \, ds - \int_{\Gamma_2} \lambda \cdot v \, ds = \int_{\Omega} f \cdot v \, dx.$$ 

Remark

$$u \times n = 0 \iff u \cdot t = 0,$$

for all unitary vector $t$ with $t \cdot n = 0$

$$\Leftrightarrow c(u, \lambda) = 0,$$

for all $\lambda \in \Lambda$,

where

$$c(u, \lambda) = \int_{\Gamma_2} u \cdot \lambda \, ds,$$

and

$$\Lambda = \{ \eta \in [H^{-1/2}(\Gamma_2)]^d : \eta \cdot n = 0 \}.$$
Variational formulation: main result

Problem:

Find \( u \in V, \ p \in L^2(\Omega), \ \lambda \in \Lambda \) such that for all \( v \in V, \ q \in L^2(\Omega), \ \eta \in \Lambda \):

\[
2\mu \int_{\Omega} D(u) : D(v) \, dx - \int_{\Omega} p \nabla \cdot v \, dx - c(v, \lambda) = \int_{\Omega} f \cdot v \, dx - \int_{\Gamma_2} p_0 n \cdot v \, ds
\]

\[
\int_{\Omega} q \nabla \cdot u \, dx = 0
\]

\[
c(u, \eta) = 0.
\]

Theorem

The previous problem admits a unique solution \( (u, p, \lambda) \) which verifies

\[
\|u\|_{1,\Omega} + \|p\|_{0,\Omega} + \|\lambda\|_{-1/2,\Gamma_2} \lesssim \|f\|_{V'} + \inf_{v \in V} \frac{\int_{\Gamma_2} p_0 n \cdot v \, ds}{\|v\|_{1,\Omega}} \lesssim \|f\|_{0,\Omega} + \|p_0\|_{0,\Gamma_2}.
\]

Moreover, if \( u \in [C^2(\Omega)]^d, \ p \in C^1(\Omega) \), then \( (u, p) \) is the solution to the Stokes problem and \( \lambda \) verifies

\[
\lambda = \tau(u, p).
\]
Variational formulation: construction of $c$

The two dimensional case:

$\Lambda$ is isomorphic to $H^{-1/2}(\Gamma_2)$ and

$$c(v, \lambda) = \int_{\Gamma_2} \lambda t \cdot v \, ds.$$ 

The three dimensional case:

$\Lambda$ is isomorphic to $[H^{-1/2}(\Gamma_2)]^2$ and

$$c(v, \lambda) = \int_{\Gamma_2} (v \times n) \cdot C\lambda \, ds,$$

with

$$C = \alpha \begin{pmatrix} 0 & n_2 \\ 0 & -n_1 \\ 1 & 0 \end{pmatrix}, \quad \text{and} \quad \alpha = (1 - n_3^2)^{-1/2}. $$
**Discretization strategy**

**Notations (three-dimensional case):**

- $\mathcal{T}_h$: shape regular, quasi uniform, and such that for all $K \in \mathcal{T}_h$ with $K \cap \Gamma \neq \emptyset$ either $K \cap \Gamma \subset \bar{\Gamma}_1$ or $K \cap \Gamma \subset \bar{\Gamma}_2$.

- $V_h \subseteq V$, $Q_h \subset L^2(\Omega)$ such that:

\[
\inf_{p_h \in Q_0^h} \sup_{u \in V_h \cap [H^1_0(\Omega)]^3} \frac{\int_{\Omega} p_h \nabla \cdot u_h \, dx}{\|u\|_{1,\Omega} \|p\|_{0,\Omega}} \gtrsim 1,
\]

where $Q_0^h = \{q_h \in Q_h : \int_{\Omega} q_h = 0\}$.

- $V_h|_{\Gamma_2} = [W_h]^3$ and $\Lambda_h$ the image of $[W_h]^2$ by the previous isomorphism.
Discrete problem: main result

**Problem:** Find $u_h \in V_h$, $p \in Q_h$, $\lambda \in \Lambda_h$ such that $\forall \, v_h \in V_h$, $q_h \in Q_h$, $\eta_h \in \Lambda_h$

$$2\mu \int_{\Omega} D(u_h) : D(v_h) \, dx - \int_{\Omega} p_h \nabla \cdot v_h \, dx - c(v_h, \lambda_h) = \int_{\Omega} f \cdot v_h \, dx - \int_{\Gamma_2} p_0 n \cdot v_h \, ds$$

$$\int_{\Omega} q_h \nabla \cdot u_h \, dx = 0$$

$$c(u_h, \eta_h) = 0.$$

**Theorem**

There exists $h_0$ such that, if $h \leq h_0$, the previous problem admits a unique solution $(u_h, p_h, \lambda_h)$ which verifies

$$\|u_h\|_{1, \Omega} + \|p\|_{0, \Omega} + \|\lambda_h\|_{-1/2, \Gamma_2} \lesssim \|f\|_{0, \Omega} + \|p_0\|_{0, \Omega}.$$

Moreover the following error estimate holds:

$$\|u - u_h\|_{1, \Omega} + \|p - p_h\|_{0, \Omega} \lesssim \inf_{v_h \in V_h^0} \|u - v_h\|_{1, \Omega} + \inf_{q_h \in Q_h} \|q - q_h\|_{0, \Omega},$$

where $V_h^0 = \ker C_h = \{u_h \in V_h : \int_{\Gamma_2} (u_h \times n) \cdot C \lambda \, ds = 0, \forall \lambda \in \Lambda_h\}.$
Error estimate

Classical case of Taylor-Hood inf-sup stable finite element spaces:

\[ V_h = \{ u \in [C^0(\Omega)]^3 : \forall K \in T_h u|_K \in [P^k(K)]^3 \}, \]
\[ Q_h = \{ p \in C^0(\Omega) : \forall K \in T_h p|_K \in P^{k-1}(K) \}. \]

Corollary

For \( u \in [H^{k+1}(\Omega)]^3 \) and \( p \in H^k(\Omega) \) we have

\[ \| u - u_h \|_{1,\Omega} + \| p - p_h \|_{0,\Omega} \lesssim h^k (\| u \|_{k+1,\Omega} + \| p \|_{k,\Omega}). \]

⇒ optimal convergence rates.
A word of caution: case of curved $\Gamma_2$

- **Continuous framework**: similar results when changing the pressure boundary condition into

  $$p + 2\mu |\mathbf{u}|_\kappa = p_0, \quad \text{on } \Gamma_2.$$ 

- **Discrete level**: need to use

  $$B^T(W_h)^3 \subseteq (W_h)^3, \quad B(W_h)^3 \subseteq (W_h)^3,$$

  where

  $$B = \begin{pmatrix} \alpha n_2 & -\alpha n_1 & 0 \\ \alpha n_3 n_1 & \alpha n_2 n_3 & \alpha(n_3^2 - 1) \end{pmatrix}. $$

  but this doesn’t automatically hold for curved boundaries!

**Key assumption**: on all the connected components of $\Gamma_2$ the normal $\mathbf{n}$ is constant.
Feel++ Finite Element Embedded Library and Language in C++

A Domain Specific Language for PDEs embedded in C++ providing a syntax very close to the mathematical language.

Features

- Supports generalized arbitrary order Galerkin methods (cG, dG) in 1D, 2D and 3D.
- Supports simplex, hypercube and high order meshes.
- Supports seamless parallel computing.
- Supports large scale parallel linear and non-linear solvers (PETSc/SLEPc).
- Enables a wide range of modeling and numerical choices.

Problem 1: Stokes flow in a curved tube

Torus sector with square cross-section for \( \theta = \frac{\pi}{6} \).

**Analytic solution:**

\[
\begin{align*}
    p_{\text{ex}}(r, \theta, z) &= \frac{p_{\text{in}}(\theta - \alpha_1) + p_{\text{out}}(\alpha_2 - \theta)}{\alpha_2 - \alpha_1}, \\
    u_{\text{ex}}(r, \theta, z) &= [0, \frac{p_{\text{in}} - p_{\text{out}}}{\alpha_2 - \alpha_1} \left( \frac{1}{2} r \ln(r) + C \frac{1}{r} + D r \right), 0]^T,
\end{align*}
\]

where

\[
C = \frac{1}{2} \frac{r_1^2 r_2^2 \ln(r_1) - \ln(r_2)}{r_1^2 - r_2^2}, \quad D = -\frac{1}{2} \frac{r_1^2 \ln(r_1) - r_2^2 \ln(r_2)}{r_1^2 - r_2^2}.
\]
Problem 1: results

Torus geometry for $\theta = \frac{\pi}{6}$: velocity and pressure profiles.

Logarithmic plots of the errors for the velocity and pressure, as functions of the mesh size.
Problem 2: physiological flow in a realistic geometry

<table>
<thead>
<tr>
<th></th>
<th>$h_{\text{min}}$</th>
<th>$h_{\text{max}}$</th>
<th>$h_{\text{average}}$</th>
<th>$N_{\text{elt}}$</th>
<th>$N_{\text{dof}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>M0</td>
<td>0.104</td>
<td>3.702</td>
<td>0.840</td>
<td>775 242</td>
<td>3 777 309</td>
</tr>
<tr>
<td>M1</td>
<td>0.083</td>
<td>3.060</td>
<td>0.697</td>
<td>1 234 148</td>
<td>5 886 029</td>
</tr>
<tr>
<td>M2</td>
<td>0.071</td>
<td>2.784</td>
<td>0.607</td>
<td>1 840 209</td>
<td>8 596 453</td>
</tr>
<tr>
<td>M3</td>
<td>0.050</td>
<td>2.190</td>
<td>0.478</td>
<td>3 528 238</td>
<td>16 086 516</td>
</tr>
<tr>
<td>M4</td>
<td>0.047</td>
<td>1.940</td>
<td>0.408</td>
<td>5 441 080</td>
<td>24 456 367</td>
</tr>
</tbody>
</table>

Table: Meshes of the cerebral venous network.

Boundary conditions:

- Inlet sections connected to the superior sagittal sinus: $p = 6.75 \text{mmHg}$
- Inlet sections connected to the straight sinus: $p = 6.58 \text{mmHg}$
- Right outlet section: $p = 5.85 \text{mmHg}$, left outlet section: $p = 6.14 \text{mmHg}$.
- Lateral walls: $u = 0$. 
Problem 2: results

Cerebral venous hemodynamics obtained by imposing a pressure drop between the inlet and outlet.
Problem 2: results and numerical strategy

<table>
<thead>
<tr>
<th>FlowRate0 [$m^3/s$]</th>
<th>FlowRate1 [$m^3/s$]</th>
<th>MeanPressure [$mmHg$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>M0 4.24732 · 10^{-6}</td>
<td>3.18926 · 10^{-6}</td>
<td>6.51364</td>
</tr>
<tr>
<td>M1 4.27849 · 10^{-6}</td>
<td>3.20839 · 10^{-6}</td>
<td>6.51337</td>
</tr>
<tr>
<td>M2 4.29280 · 10^{-6}</td>
<td>3.21806 · 10^{-6}</td>
<td>6.51328</td>
</tr>
<tr>
<td>M3 4.31223 · 10^{-6}</td>
<td>3.23130 · 10^{-6}</td>
<td>6.51314</td>
</tr>
<tr>
<td>M4 4.31968 · 10^{-6}</td>
<td>3.23678 · 10^{-6}</td>
<td>6.51309</td>
</tr>
</tbody>
</table>

Mesh refinement effect.

<table>
<thead>
<tr>
<th>Strategy $P^{GASM}$</th>
<th>Strategy $P^{LOCK}_1$</th>
<th>Strategy $P^{LOCK}_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>M0 163[420]</td>
<td>20[174]</td>
<td>67[86]</td>
</tr>
<tr>
<td>M1 366[393]</td>
<td>45[267]</td>
<td>161[123]</td>
</tr>
<tr>
<td>M2 1080[429]</td>
<td>84[369]</td>
<td>271[143]</td>
</tr>
<tr>
<td>M4 x</td>
<td>898[791]</td>
<td>1960[175]</td>
</tr>
</tbody>
</table>

Time comparison for three preconditioning strategies (in seconds). In brackets, the number of iteration used by solver.
Conclusion.

- Stokes problem with non standard boundary conditions involving the pressure: “classical problem”, novel method based on a Lagrange multiplier formulation.
- Continuous and discrete analysis.
- New applications in view.

Perspectives.

- Improve linear solvers robustness and flexibility, by means of well-suited block-preconditioning strategies.
- Extend the analysis to curved boundaries, Navier-Stokes problem and some non-Newtonian models.
- Explore connections between the Lagrange multipliers technique and Nitsche-based methods.
- Refine analysis, include more data and validate results for the cerebral venous network.
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- Feel++ Community www.feelpp.org
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Thank you for your attention!