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

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8th FreeFem++'s days

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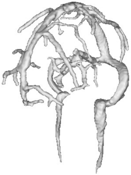
VIVABRAIN: *Virtual angiography simulation from 3D and 3D+t brain vascular models*

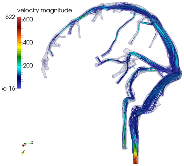
Real MRA images

3D vascular models



Virtual MRA

Goal: Closing the Loop!



3D+t simulation of blood flow

Computational meshes

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:

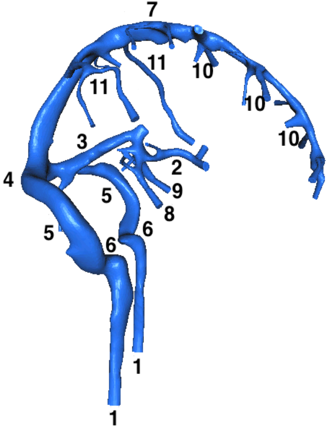
$$\begin{aligned} \rho\frac{\partial \mathbf{u}}{\partial t} - 2\nabla\cdot(\mu\mathbf{D}(\mathbf{u})) + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p &= \mathbf{0}, \quad \text{in } \Omega\times I \\ \nabla\cdot\mathbf{u} &= 0, \quad \text{in } \Omega\times I \end{aligned}$$

$+$ 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;
- $\boldsymbol{\sigma}(\mathbf{u}, p) = -p\mathbf{I} + 2\mu\mathbf{D}(\mathbf{u})$ Cauchy stress tensor;
- ρ and μ density and dynamic viscosity of the fluid.

O. Miraucourt, S. Salmon, M. Szopos, M. Thiriet. *Blood flow in the cerebral venous system: modeling and simulation*, CMBBE 2016, in press.

Cerebral venous network: boundary conditions



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.

- **Wall:**
  - $\mathbf{u} = \mathbf{0}$ (if rigid walls); or
  - $\mathbf{u} =$ 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.

Boundary conditions involving the pressure

For $\varepsilon = 0$ (Stokes) and $\varepsilon = 1$ (Navier-Stokes), consider the problem:

$$\begin{aligned}
-\mu\Delta\mathbf{u} + \varepsilon(\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p &= \mathbf{f}, \quad \text{in } \Omega,\\
\nabla\cdot\mathbf{u} &= 0, \quad \text{in } \Omega,\\
\mathbf{u} &= \mathbf{u_1}, \quad \text{on } \Gamma_1,\\
\mathbf{u}\times\mathbf{n} &= \mathbf{u_2}\times\mathbf{n}, \quad \text{on } \Gamma_2,\\
p + \frac{\varepsilon}{2}|\mathbf{u}|^2 &= p_2, \quad \text{on } \Gamma_2,
\end{aligned}$$

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

Related literature

- First works on this topic:
  - O. Pironneau. *Conditions aux limites sur la pression pour les équations de Stokes et de Navier-Stokes*, CRAS 1986.
  - C. Begue, C. Conca, F. Murat, O. Pironneau. *A nouveau sur les équations de Stokes et de Navier-Stokes avec des conditions aux limites sur la pression*, CRAS 1987.
  - C. Conca, F. Murat, O. Pironneau. *The Stokes and Navier-Stokes equations with boundary conditions involving the pressure*, Japan. J. Math. 1994.

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

- Recent developments:
  - C. Bernardi, T. Chacón-Rebollo, D. Yakoubi. *Finite element discretization of the Stokes and Navier-Stokes equations with boundary conditions on the pressure*, SINUM 2015.
  - T. Chacón-Rebollo, V. Girault, F. Murat, O. Pironneau. *Analysis of a Simplified Coupled Fluid-Structure Model for Computational Hemodynamics*, SINUM 2016.

Variational formulation

Define:

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

$$b(\mathbf{v},q) = -\int_\Omega q \nabla \cdot \mathbf{v}\, dx, \qquad L(\mathbf{v}) = \int_\Omega \mathbf{f} \cdot \mathbf{v} - \int_{\Gamma_2} p_2 \mathbf{v} \cdot \mathbf{n}\, ds.$$

Main results:

- the problem of finding $(\mathbf{u}, p)$ in an appropriate space, such that $a(\mathbf{u},\mathbf{v}) + \varepsilon N(\mathbf{u},\mathbf{u},\mathbf{v}) + b(\mathbf{v},p) = L(\mathbf{v})$ for all test function $\mathbf{v}$ and $b(\mathbf{u},q) = 0$ 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:

$$-\Delta \mathbf{u} = \nabla \times (\nabla \times \mathbf{u}) - \nabla(\nabla \cdot \mathbf{u}).$$

Today's talk

Steady Stokes problem:

$$\begin{aligned} -2\mu\nabla\cdot(\mathbf{D}(\mathbf{u}))+\nabla p &= \mathbf{f}, \quad \text{in } \Omega, \\ \nabla\cdot\mathbf{u} &= 0, \quad \text{in } \Omega, \\ \mathbf{u} &= \mathbf{0}, \quad \text{on } \Gamma_1, \\ \mathbf{u}\times\mathbf{n} &= \mathbf{0} \quad \text{and} \\ p &= p_0, \quad \text{on } \Gamma_2, \end{aligned}$$

where

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

Remarks:

- Continuous level: the two formulations are equivalent, since $\nabla\cdot\mathbf{u} = 0 \Rightarrow \nabla\cdot(\nabla\mathbf{u}+\nabla\mathbf{u}^T) = \Delta\mathbf{u}$.
- 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

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

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

Theorem

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

$$(\sigma(\mathbf{u}, p)\mathbf{n}) \cdot \mathbf{n} = -(p + 2\mu|\mathbf{u}|\kappa),$$

where κ is the mean curvature of Γ. Furthermore, in the case where Γ is a planar surface, this reduces to the pressure condition

$$(\sigma(\mathbf{u}, p)\mathbf{n}) \cdot \mathbf{n} = -p.$$

W.L. Barth, G.F Carey. *On a boundary condition for pressure-driven laminar flow of incompressible fluids*, IJNMF 2007.

Consequently, on Γ_2 (planar):

$$\sigma(\mathbf{u}, p)\mathbf{n} = -p\mathbf{n} + \boldsymbol{\tau}(\mathbf{u}, p).$$

Variational formulation

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

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

Remark

$$\begin{aligned} \mathbf{u} \times \mathbf{n} = \mathbf{0} \quad &\Leftrightarrow \quad \mathbf{u} \cdot \mathbf{t} = 0, \ \text{for all unitary vector } \mathbf{t} \text{ with } \mathbf{t} \cdot \mathbf{n} = 0 \\ &\Leftrightarrow \quad c(\mathbf{u}, \boldsymbol{\lambda}) = 0, \ \text{for all } \boldsymbol{\lambda} \in \boldsymbol{\Lambda}, \end{aligned}$$

where

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

and

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

Variational formulation: main result

Problem:

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

$$\begin{aligned} 2\mu \int_\Omega \mathbf{D}(\mathbf{u}) : \mathbf{D}(\mathbf{v})\, dx - \int_\Omega p \nabla \cdot \mathbf{v}\, dx - c(\mathbf{v}, \boldsymbol{\lambda}) &= \int_\Omega \mathbf{f} \cdot \mathbf{v}\, dx - \int_{\Gamma_2} p_0 \mathbf{n} \cdot \mathbf{v}\, ds \\ \int_\Omega q \nabla \cdot \mathbf{u}\, dx &= 0 \\ c(\mathbf{u}, \boldsymbol{\eta}) &= 0. \end{aligned}$$

Theorem

The previous problem admits a unique solution $(\mathbf{u}, p, \boldsymbol{\lambda})$ *which verifies*

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

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

$$\boldsymbol{\lambda} = \boldsymbol{\tau}(\mathbf{u}, p).$$

Variational formulation: construction of c

The two dimensional case:

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

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

The three dimensional case:

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

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

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 $K \cap \Gamma \subset \bar{\Gamma}_2$.

- $\boldsymbol{V}_h \subseteq \boldsymbol{V}$, $Q_h \subset L^2(\Omega)$ such that:

$$\inf_{p_h \in Q_h^0} \sup_{\mathbf{u} \in \boldsymbol{V}_h \cap [H_0^1(\Omega)]^3} \frac{\int_\Omega p_h \nabla \cdot \mathbf{u}_h \, dx}{\|\mathbf{u}\|_{1,\Omega} \|p\|_{0,\Omega}} \gtrsim 1,$$

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

- $\boldsymbol{V}_h|_{\Gamma_2} = [W_h]^3$ and $\boldsymbol{\Lambda}_h$ the image of $[W_h]^2$ by the previous isomorphism.

Discrete problem: main result

Problem: Find $\mathbf{u}_h \in \boldsymbol{V}_h$, $p \in Q_h$, $\boldsymbol{\lambda} \in \boldsymbol{\Lambda}_h$ such that $\forall$ $\mathbf{v}_h \in \boldsymbol{V}_h$, $q_h \in Q_h$, $\boldsymbol{\eta}_h \in \boldsymbol{\Lambda}_h$

$$\begin{aligned}
2\mu \int_\Omega \mathbf{D}(\mathbf{u}_h) : \mathbf{D}(\mathbf{v}_h) dx - \int_\Omega p_h \nabla \cdot \mathbf{v}_h dx - c(\mathbf{v}_h, \boldsymbol{\lambda}_h) &= \int_\Omega \mathbf{f} \cdot \mathbf{v}_h dx - \int_{\Gamma_2} p_0 \mathbf{n} \cdot \mathbf{v}_h ds \\
\int_\Omega q_h \nabla \cdot \mathbf{u}_h \, dx &= 0 \\
c(\mathbf{u}_h, \boldsymbol{\eta}_h) &= 0.
\end{aligned}$$

Theorem

There exists h_0 such that, if $h \le h_0$, the previous problem admits a unique solution $(\mathbf{u}_h, p_h, \boldsymbol{\lambda}_h)$ which verifies

$$\|\mathbf{u}_h\|_{1,\Omega} + \|p\|_{0,\Omega} + \|\boldsymbol{\lambda}_h\|_{-1/2,\Gamma_2} \lesssim \|\mathbf{f}\|_{0,\Omega} + \|p_0\|_{0,\Omega}.$$

Moreover the following error estimate holds:

$$\|\mathbf{u} - \mathbf{u}_h\|_{1,\Omega} + \|p - p_h\|_{0,\Omega} \lesssim \inf_{\mathbf{v}_h \in \boldsymbol{V}_h^0} \|\mathbf{u} - \mathbf{v}_h\|_{1,\Omega} + \inf_{q_h \in Q_h} \|q - q_h\|_{0,\Omega},$$

where $\boldsymbol{V}_h^0 = \ker C_h = \{\mathbf{u}_h \in \boldsymbol{V}_h : \int_{\Gamma_2} (\mathbf{u}_h \times \mathbf{n}) \cdot C\boldsymbol{\lambda}_h \, ds = 0, \ \forall \boldsymbol{\lambda}_h \in \boldsymbol{\Lambda}_h\}$.

Error estimate

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

$$
\begin{aligned}
\boldsymbol{V}_h &= \{\mathbf{u} \in [C^0(\Omega)]^3 : \ \forall K \in \mathcal{T}_h \ \mathbf{u}|_K \in [\mathbb{P}^k(K)]^3\}, \\
Q_h &= \{p \in C^0(\Omega) : \ \forall K \in \mathcal{T}_h \ p|_K \in \mathbb{P}^{k-1}(K)\}.
\end{aligned}
$$

Corollary

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

$$
\|\mathbf{u} - \mathbf{u}_h\|_{1,\Omega} + \|p - p_h\|_{0,\Omega} \lesssim h^k(\|\mathbf{u}\|_{k+1,\Omega} + \|p\|_{k,\Omega}).
$$

$\Rightarrow$ optimal convergence rates.

A word of caution: case of curved Γ_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

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

where

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

but this doesn't automatically hold for curved boundaries!

Key assumption: on all the connected components of Γ_2 the normal $\mathbf{n}$ is constant.

Numerical framework `http://www.feelpp.org` `www.cemosis.fr.`

Feel++ Finite Element Embedded Library and Language in C++

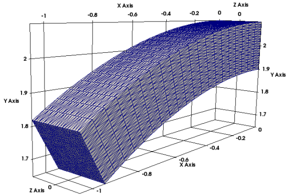
A Domain Specific Language for PDEs embedded in C++ providing a syntax very close to the mathematical language.

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.

C. Prud'Homme, V. Chabannes, V. Doyeux, M. Ismail, A. Samake, G. Pena. *Feel++: A Computational Framework for Galerkin Methods and Advanced Numerical Methods*, ESAIM: Procs 2012.

Problem 1: Stokes flow in a curved tube



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

Analytic solution:

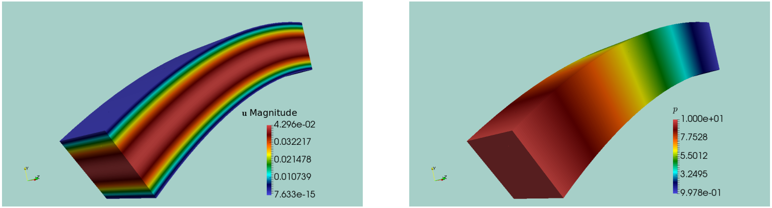
$$p_{ex}(r, \theta, z) = \frac{p_{in}(\theta - \alpha_1) + p_{out}(\alpha_2 - \theta)}{\alpha_2 - \alpha_1},$$

$$\mathbf{u}_{ex}(r, \theta, z) = [0, \frac{p_{in} - p_{out}}{\alpha_2 - \alpha_1}(\frac{1}{2} r \ln(r) + C\frac{1}{r} + Dr), 0]^T,$$

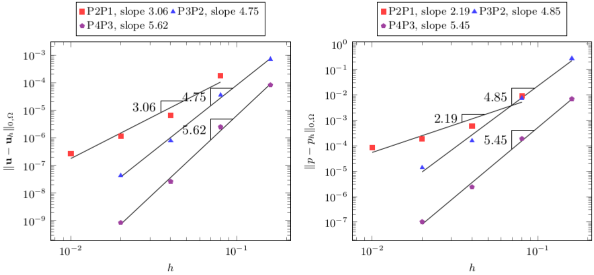
where

$$C = \frac{1}{2} r_1^2 r_2^2 \frac{\ln(r_1) - \ln(r_2)}{r_1^2 - r_2^2}, \qquad D = -\frac{1}{2} \frac{r_1^2 \ln(r_1) - r_2^2 \ln(r_2)}{r_1^2 - r_2^2}.$$

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

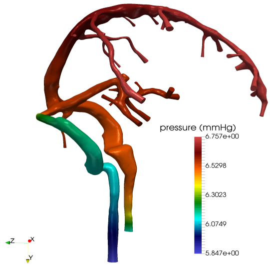
	h_{min}	h_{max}	$h_{average}$	N_{elt}	N_{dof}
M0	0.104	3.702	0.840	775 242	3 777 309
M1	0.083	3.060	0.697	1 234 148	5 886 029
M2	0.071	2.784	0.607	1 840 209	8 596 453
M3	0.050	2.190	0.478	3 528 238	16 086 516
M4	0.047	1.940	0.408	5 441 080	24 456 367

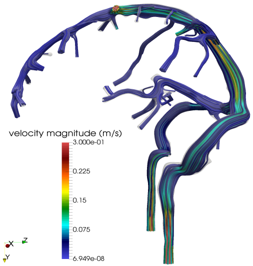
Table: Meshes of the cerebral venous network.

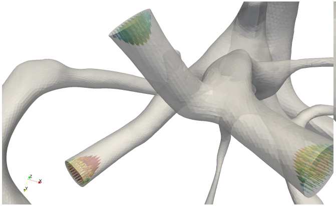
Boundary conditions:

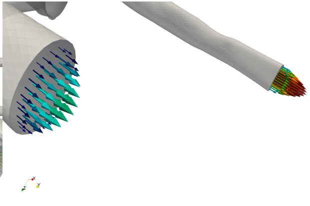
- Inlet sections connected to the superior sagittal sinus: $p = 6.75 mmHg$
- Inlet sections connected to the straight sinus: $p = 6.58 mmHg$
- Right outlet section: $p = 5.85 mmHg$, left outlet section: $p = 6.14 mmHg$.
- Lateral walls: $\mathbf{u} = \mathbf{0}$.

Problem 2: results









Inlet sections

Outlet Sections

Cerebral venous hemodynamics obtained by imposing a pressure drop between the inlet and outlet

Problem 2: results and numerical strategy

	FlowRate0 $[m^3/s]$	FlowRate1 $[m^3/s]$	MeanPressure $[mmHg]$
M0	$4.24732 \cdot 10^{-6}$	$3.18926 \cdot 10^{-6}$	6.51364
M1	$4.27849 \cdot 10^{-6}$	$3.20839 \cdot 10^{-6}$	6.51337
M2	$4.29280 \cdot 10^{-6}$	$3.21806 \cdot 10^{-6}$	6.51328
M3	$4.31223 \cdot 10^{-6}$	$3.23130 \cdot 10^{-6}$	6.51314
M4	$4.31968 \cdot 10^{-6}$	$3.23678 \cdot 10^{-6}$	6.51309

Mesh refinement effect.

	Strategy P^{GASM}	Strategy P_1^{BLOCK}	Strategy P_2^{BLOCK}
M0	163[420]	20[174]	67[86]
M1	366[393]	45[267]	161[123]
M2	1080[429]	84[369]	271[143]
M3	4616[522]	293[660]	707[196]
M4	x	898[791]	1960[175]

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

Conclusion and future directions

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.

Acknowledgment

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- Cemosis `www.cemosis.fr`.
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Thank you for your attention!