An ALE Finite Element Method for Vorticity-Streamfunction Formulation with Species Transport Equation

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Outline

1. Introduction
2. Mathematical Model
3. Computational Code
4. Validation
5. Results
6. Conclusion

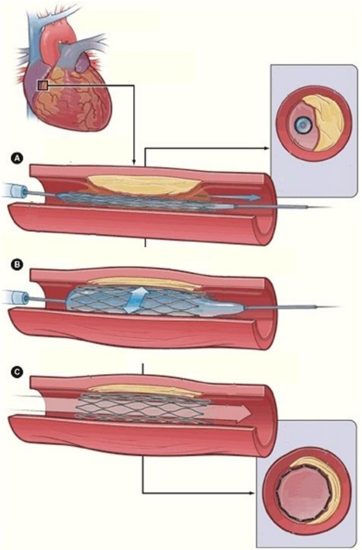
Introduction

Motivation:

- Ischaemic heart disease and stroke have remained the leading death causes globally in the last 15 years [1]

Goals:

- To develop a ALE-FE code for the Vorticity-Streamfunction Formulation
- To create new drug-eluting stent design patent



[1] World Health Organization, 2018, "The top 10 causes of death". *www.who.int/news-room/fact-sheets/detail/the-top-10-causes-of-death* [Online accessed 06-04-20 08:27pm]

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Arbitrary Lagrangian-Eulerian (ALE)

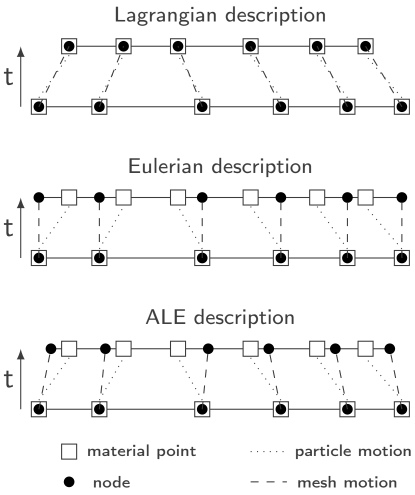
The Arbitrary Lagrangian-Eulerian combines the classical motion descriptions, while it provides [2]:

Advantages:

- Simulations in fluid-structure and moving boundary problems

Disadvantages:

- The computational mesh requires an extensive topological treatment



[2] Donea, J., Huerta, A., Ponthot, J.-P. and Rodríguez-Ferran, A. (2004). Arbitrary Lagrangian–Eulerian Methods. In Encyclopedia of Computational Mechanics *doi:10.1002/0470091355.ecm009*

Governing Equations

Assumptions [3]:

1. Continuum hypothesis
2. Homogeneous and Isotropic
3. Incompressible
4. Newtonian
5. Constant Mass Difusivity
6. Single-phase Flow
7. Two-dimensional flow

$$\frac{\partial \omega_z}{\partial t} + (\mathbf{v} - \hat{\mathbf{v}}) \cdot \nabla \omega_z = \frac{1}{Re} \nabla^2 \omega_z$$

$$\nabla^2 \psi = -\omega_z$$

$$\frac{\partial e}{\partial t} + (\mathbf{v} - \hat{\mathbf{v}}) \cdot \nabla e = \frac{1}{ReSc} \nabla^2 e$$

- If the mesh velocity field $\hat{\mathbf{v}} = \mathbf{v}$ (*Lagrangian*) or $\hat{\mathbf{v}} = 0$ (*Eulerian*)
- The material velocity field $\mathbf{v} = (v_x, v_y)$ is calculated by: $v_x = \partial\psi/\partial y$ and $v_y = -\partial\psi/\partial x$

[3] Panton, R. (2013). Incompressible Flow John Wiley & Sons, Ltd

Semi-Lagrangian Method

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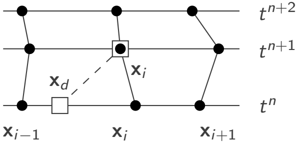
The convective term was replaced by material derivative in the direction of characteristic trajectory, that is: $\frac{D(\cdot)}{Dt} = \frac{\partial(\cdot)}{\partial t} + (\mathbf{v} - \hat{\mathbf{v}}) \cdot \nabla(\cdot)$

$$\frac{D\omega_z}{Dt} = \frac{1}{Re}\nabla^2\omega_z$$

$$\nabla^2\psi = -\omega_z$$

$$\frac{De}{Dt} = \frac{1}{ReSc}\nabla^2 e$$

The departure node is calculated by $x_d^n = x_i^{n+1} - (\mathbf{v} - \hat{\mathbf{v}})\,\Delta t$. Then, a searching procedure is required to find x_d^n using barycentric coordinates



Semi-Lagrangian Method

The implicit semi-Lagrangian time discretization provides [4]:

Advantages:

- Symmetric linear systems
- Unconditionnal stability

Disadvantages:

- Numerical Diffusion
- Searching procedure may lead to excessive computational cost if it is not well designed

$$\frac{\omega_i^{n+1} - \omega_d^n}{\Delta t} = \frac{1}{Re}\nabla^2 \omega^{n+1}$$

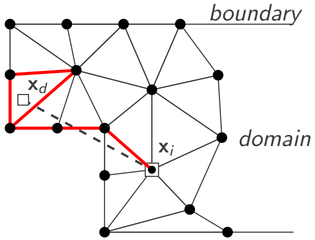
$$\nabla^2 \psi = -\omega$$

$$\frac{e_i^{n+1} - e_d^n}{\Delta t} = \frac{1}{ReSc}\nabla^2 e^{n+1}$$

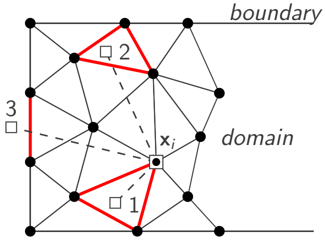
[4] Pironneau, O. On the transport-diffusion algorithm and its applications to the Navier-Stokes equations. Numer. Math. 38, 309–332 (1982). *https://doi.org/10.1007/BF01396435*

Searching Procedure

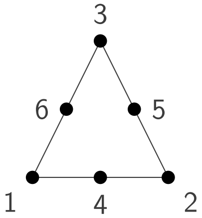
The start searching procedure was used. This procedure has presented an acceptable computational cost, in addition to the concave domains can be used



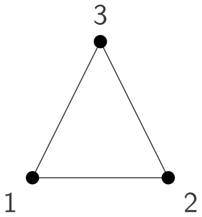
The searching procedure must be prepared for three situations that may occur. After the departure node is found, the interpolation is performed



Galerkin FE Method



Quad Element



Linear Element

$$\left[\frac{\mathbf{M}}{\Delta t} + \frac{\mathbf{K}}{Re}\right] \omega_i^{n+1} = \frac{\mathbf{M}}{\Delta t} \omega_d^n$$

$$\mathbf{K}\psi = \mathbf{M}\omega$$

$$\left[\frac{\mathbf{M}}{\Delta t} + \frac{\mathbf{K}}{ReSc}\right] e_i^{n+1} = \frac{\mathbf{M}}{\Delta t} e_d^n$$

- The material velocity field is calculated by:
  $\mathbf{M} v_x = \mathbf{G_y} \psi$
  $\mathbf{M} v_y = -\mathbf{G_x} \psi$

Mesh Velocity

The computational mesh velocity $\hat{\mathbf{v}}$ is defined as a linear combination of other velocities, such as:

$$\hat{\mathbf{v}} = \beta_1 \mathbf{v}_1 + \beta_2 \mathbf{v}_2$$

where, $\mathbf{v}_1$ is the Lagrangian velocity, $\mathbf{v}_2$ is the Laplacian Smoothing velocity, β_1 and β_2 are the parameters control the Lagrangian and Laplacian motion respectively.

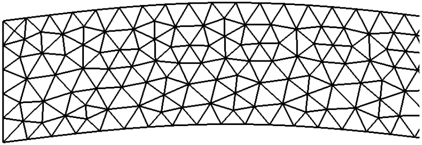
Laplacian Smoothing

To avoid the fast degradation of the computational elements due to ALE description, it was used the Laplacian Smoothing Method [5]

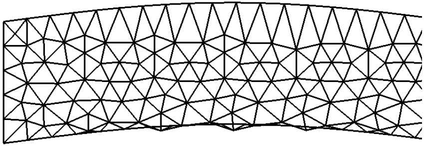
The new node position $\hat{\mathbf{x}}_\mathbf{i}$ can be approximated by:

$$\hat{\mathbf{x}}_\mathbf{i} = w_{ij} \sum_{j}^{N_1} (\mathbf{x}_j - \mathbf{x}_i)$$

where, N_1 is the 1-ring neighbors of the node, w_{ij} is the weight and was calculated by the inverse distance from neighbors vertices



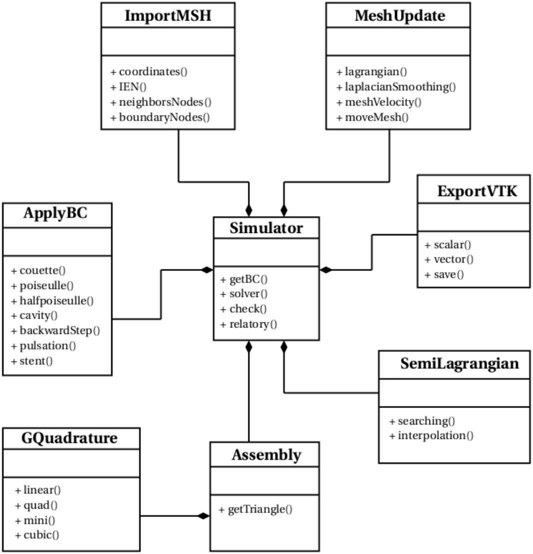
with Laplacian Smoothing



no Laplacian Smoothing

[5] Zheng, Y. Lewis, R. Gethin, D., Three-dimensional unstructured mesh generation: Part 2. surface meshes. Computer Methods in Applied Mechanics and Engineering, Amsterdam: North-Holland Pub. Co., c1972-, v. 134, n. 3, p. 269–284, 1996.

Code Framework



Simplified Class Diagram

Computational Cost

Process	AVG Computational Cost (%)
Mesh import	1.24
Assembly	73.87
BC Apply	6.70
Mesh update	10.05
Semi-Lagrangian	2.27
Vorticity Solver	5.51
VTK export	0.36

Average computational cost for the linear triangular element.

Solution Algorithm

1. Import mesh
2. Calculate Gaussian Quadradure and Assemble Matrix
3. Apply Boundary Conditions
4. Calculate Laplacian smoothing and ALE velocity
5. Move Nodes
6. Calculate semi-Lagrangian Method
7. Calculate Gaussian Quadrature and Assemble Matrix
8. Apply Boundary Conditions
9. Calculate vorticity field
10. Calculate streamfunction field
11. Calculate velocity field
12. Calculate concentration field

Repeat the procedure
for the next time step
until the steady state

Validation - Poiseuille Flow

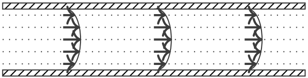
Inflow condition: $v_x = u_{analytical}, \ v_y = 0$

Top plate: $v_x = 0, \ v_y = 0, \ \psi = 1$

Bottom plate: $v_x = 0, \ v_y = 0, \ \psi = 0$

Vorticity condition: $\omega = \nabla \times \mathbf{v}$

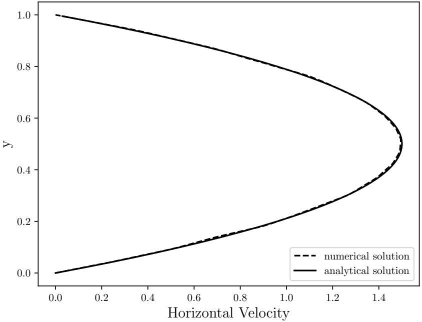
$\beta_1 = 0 \qquad \beta_2 = 1$

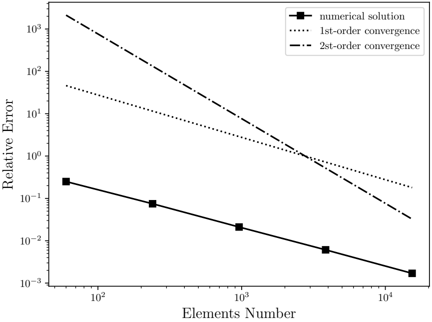


Nodes: 3835

Elements: 7299

Relative Error: 0.4%





Validation - Symmetric Poiseuille Flow

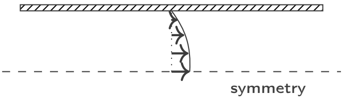
Inflow condition: $v_x = u_{analytical}$, $v_y = 0$

Top plate: $v_x = 0$, $v_y = 0$, $\psi = 1$

Symmetric axis: $v_y = 0$, $\psi = 0$

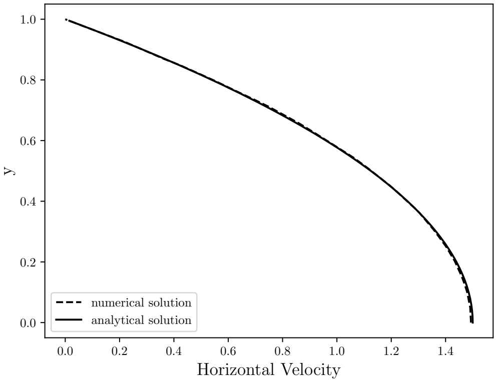
Vorticity condition: $\omega = \nabla \times \mathbf{v}$

$\beta_1 = 0$ $\qquad \beta_2 = 1$



Nodes: 3835

Elements: 7299



Validation - Lid Driven Cavity Flow

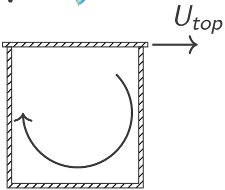
Bottom and side plates: $v_x = 0$, $v_y = 0$ e $\psi = 0$

Top plate: $v_x = 1$, $v_y = 0$ e $\psi = 0$

Vorticity condition: $\omega = \nabla \times \mathbf{v}$

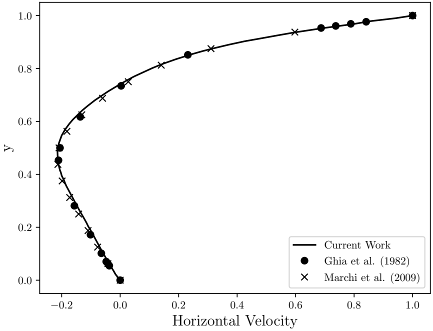
$\beta_1 = 0$ $\beta_2 = 1$

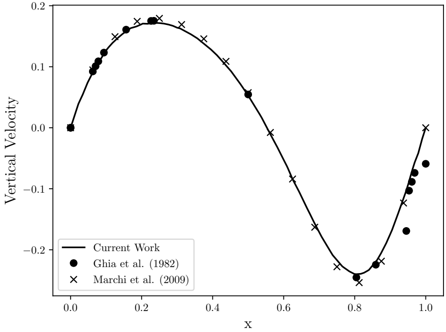
$Re = 100$



Nodes: 1563

Elements: 2988

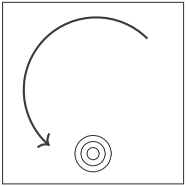




Validation - Pure Advection Flow

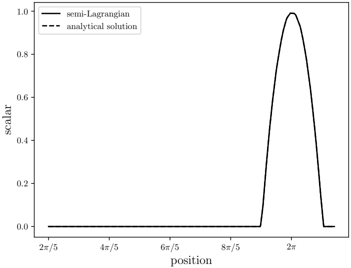
Assumptions

1. Continuum hypothesis
2. Homogeneous and Isotropic
3. Incompressible
4. Newtonian
5. Two-dimensional Flow
6. Single-phase Flow
7. High Reynolds number ($Re = \infty$)

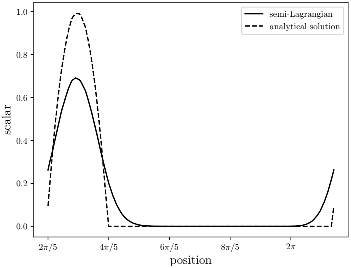


$$\frac{\partial \alpha}{\partial t} + \mathbf{v} \cdot \nabla \alpha = 0$$

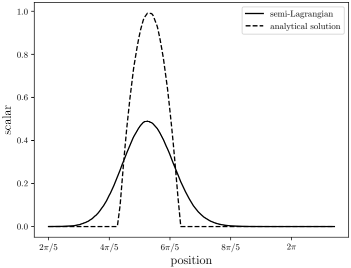
Linear Triangular Element



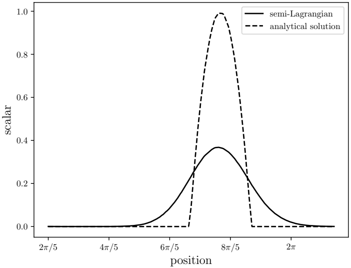
initial



1/4 rotation

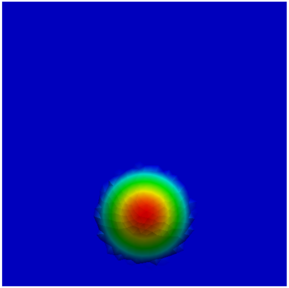


1/2 rotation

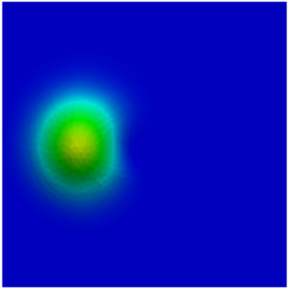


3/4 rotation

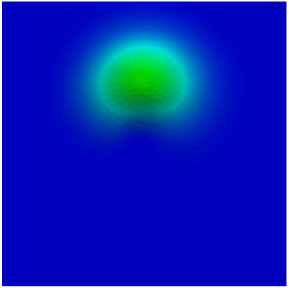
Linear Triangular Element



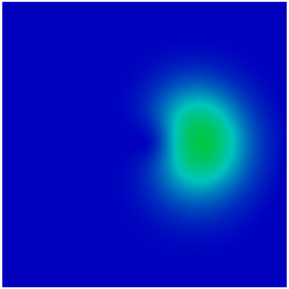
initial



1/4 rotation

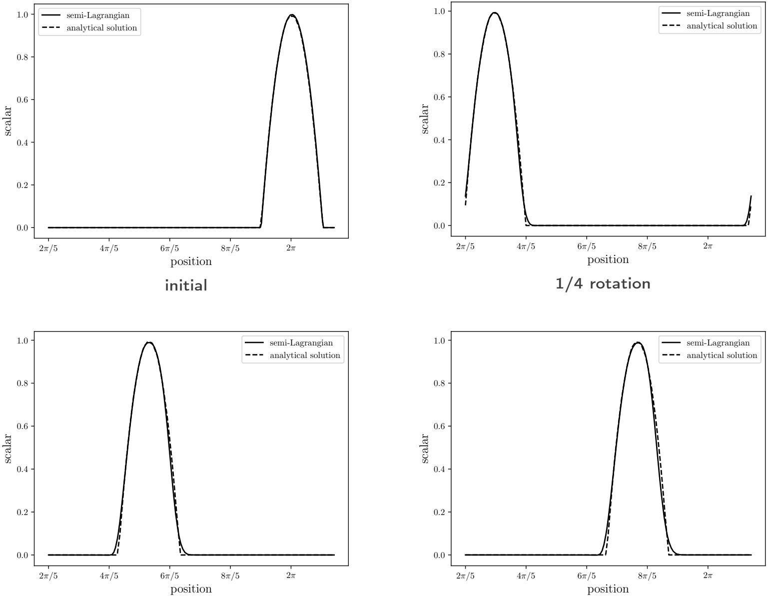


1/2 rotation



3/4 rotation

Quadratic Triangular Element



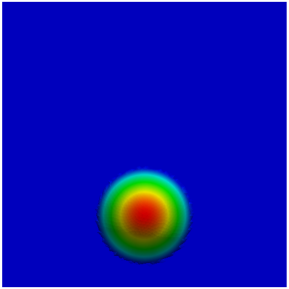
initial

1/4 rotation

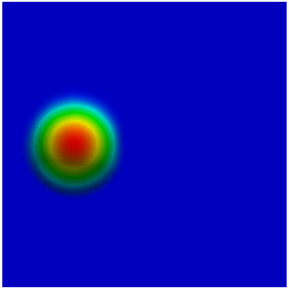
1/2 rotation

3/4 rotation

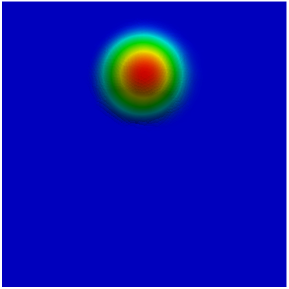
Quadratic Triangular Element



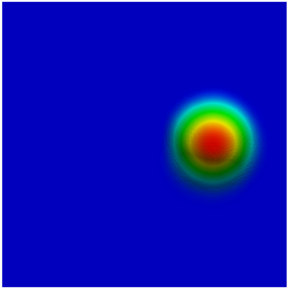
initial



1/4 rotation



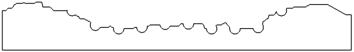
1/2 rotation



3/4 rotation

Results

(a)



(b)

Non-dimensional symmetric geometry for blood flow in coronary artery with drug-eluting stent placed by Wang et al. (2017): (a) Curved Channel with Stent (b) Real Channel with Stent.

Inflow condition: $v_x = u_{analytical}, \ v_y = 0;$

Top plate: $v_x = 0, \ v_y = 0, \ \psi = 1;$

Symmetry condition: $v_y = 0, \ \psi = 0;$

Drug-eluting stent: $v_x = 0, \ v_y = 0, \ \psi = 1, \ e = 1$

Vorticity condition: $\omega = \nabla \times \mathbf{v}$

$\beta_1 = 0 \qquad \beta_2 = 1$

$R = 0.0015m$

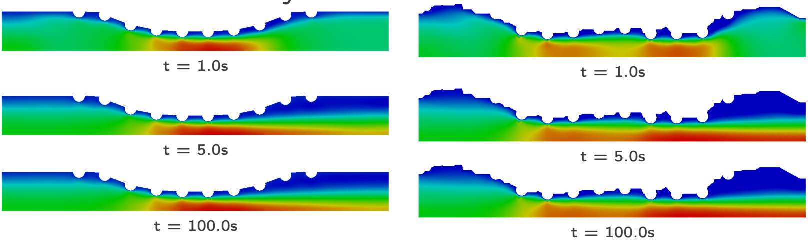
$\mu = 0.0035Pa.s$

$\rho = 1060kg/m^3$

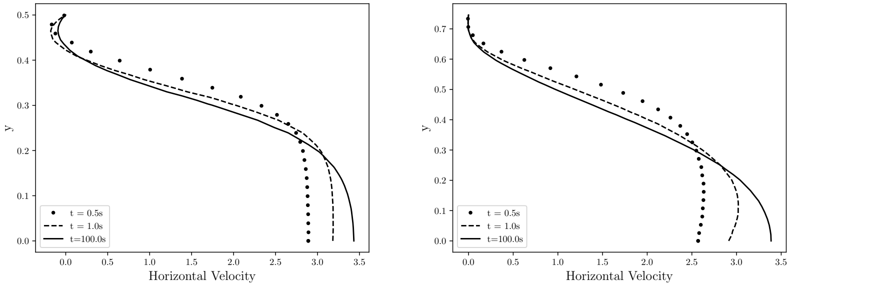
$u = 12cm/s$

$Re = 54.5$

Results - Velocity Field

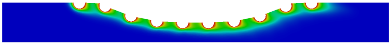


Evolution in time and space of velocity field:
Curved Channel (left column) and Real Channel (right column)

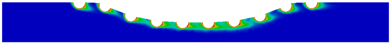


Evolution of velocity profile in centerline ($x = 0.5L$):
(a) Curved Channel and (b) Real Channel

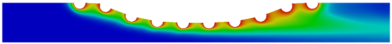
Results - Concentration Field



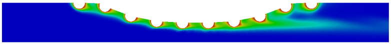
t = 1.0s



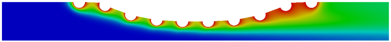
t = 1.0s



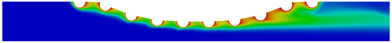
t = 5.0s



t = 5.0s

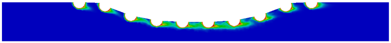


t = 100.0s

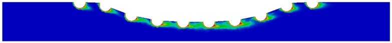


t = 100.0s

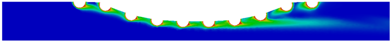
Evolution in time and space of concentration field in Curved Channel: $Sc = 1$ (left column) and $Sc = 10$ (right column)



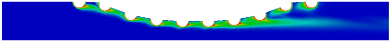
t = 1.0s



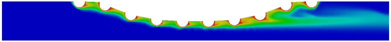
t = 1.0s



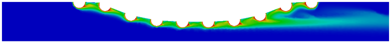
t = 5.0s



t = 5.0s



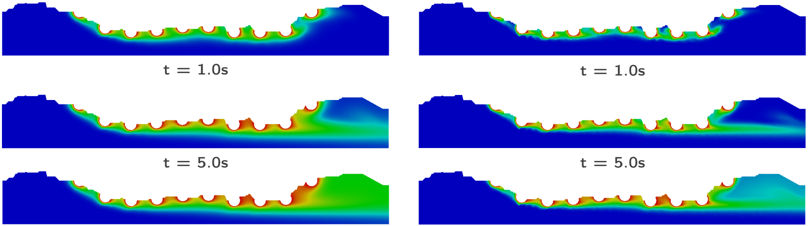
t = 100.0s



t = 100.0s

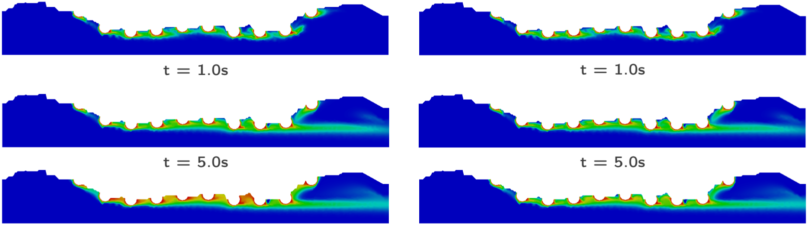
Evolution in time and space of concentration field in Curved Channel: $Sc = 100$ (left column) and $Sc = 1000$ (right column)

Results - Concentration Field



t = 1.0s | t = 1.0s
t = 5.0s | t = 5.0s
t = 100.0s | t = 100.0s

Evolution in time and space of concentration field in Real Channel:
$Sc = 1$ (left column) and $Sc = 10$ (right column)



t = 1.0s | t = 1.0s
t = 5.0s | t = 5.0s
t = 100.0s | t = 100.0s

Evolution in time and space of concentration field in Real Channel:
$Sc = 100$ (left column) and $Sc = 1000$ (right column)

Conclusion

1. The ALE description allows to perform simulations in the fluid-structure and moving boundary problems, in addition it is possible to assign several mesh velocity values in specific regions of the problem in order to improve the accuracy of the numerical results

2. The searching procedure of the semi-Lagrangian Method used in this work was well designed since it corresponds to only 2% of average computational cost of the numerical simulation. Therefore, the methos showed to be very useful due to the unconditionnal stability and symmetric linear system

3. As expected, the chemical species transport in blood flow is directly influenced by Schmidt number, where the diffusion is increased as the Schmidt number decreases. It is possible that the density and viscosity of the blood are affected by chemical species diffusion. However, this influence is not considered in this work

Further developments:

1. Increase assembly performance
2. The use of primitive variables in the 3D Navier-Stokes equation
3. Blood flow model as a multiphase problem
4. Blood flow model as a non-Newtonian fluid

Thank you!

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