Numerical simulation of viscous biointerfaces coupling with fluid dynamics

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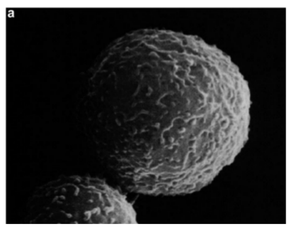
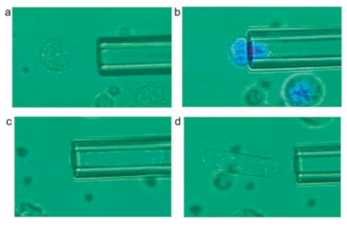
Biointerfaces coupling with fluid dynamics[5]

- The coupling of biology and fluid dynamics at the cell level is an active research field in understanding disease mechanisms and cell physiology.
  - Biological functions of cells are observed to be influenced by fluid dynamic forces. For example, fluid dynamic stress influences the adhesion of white blood cells to the interior surface of blood vessels (endothelium).
  - Blood cells also exert a strong influence on rheological properties of whole blood, e.g., non-Newtonian effects.
- We consider a white blood cell in a surrounding bulk fluid.





Models

- **Bulk fluid** : a simple Newtonian droplet model is considered.

$$\begin{cases} \rho_i\big(\mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u}\big) = \operatorname{div}(\sigma) + \rho_i\mathbf{g} \\ \qquad\qquad = -\nabla\mathbf{p} + \operatorname{div}\,(\mu_i\mathbf{D}(\mathbf{u})) + \rho_i\mathbf{g} & \text{in } \Omega_i \quad \text{for } i = 1,2 \\ \operatorname{div}\mathbf{u} = 0 & \text{in } \Omega_i \end{cases}$$

- **Interface condition** :
  - Continuity of velocity:

$$[\mathbf{u}] = 0 \qquad \text{on } \Gamma.$$

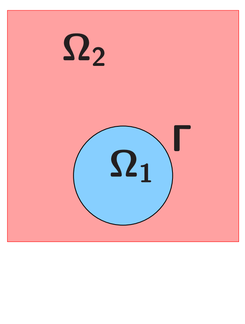
  - Kinematic interface condition:

$$\mathbf{V}_\Gamma = \mathbf{u}\cdot\mathbf{n}_\Gamma \qquad \text{on } \Gamma.$$

  - A viscous interface condition:

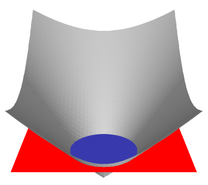
$$[\sigma\mathbf{n}_\Gamma] = \operatorname{div}_\Gamma(\sigma_\Gamma) \qquad \text{on } \Gamma,$$

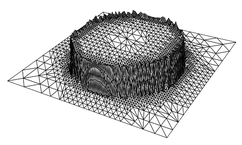
where the surface stress tensor $\sigma_\Gamma = \tau\mathbf{P} + (\lambda_\Gamma - \mu_\Gamma)(\operatorname{div}_\Gamma\mathbf{u})\,\mathbf{P} + \mu_\Gamma\mathbf{D}_\Gamma(\mathbf{u})$ is according to the *Boussinesq-Scriven* law.

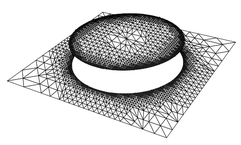


Numerical methods - DROPS package

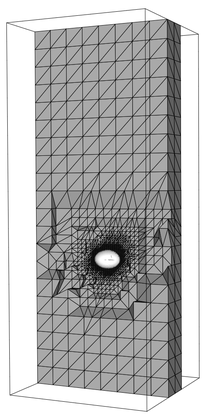
- Aims:
  - Parallel simulation of coupled fluid dynamics, mass- and surfactant-transport with variable surface properties.
  - Simulation of real physical systems; validation of numerical methods.
  - Development and analysis of numerical methods.
- Key components:
  - Adaptive multilevel hierarchy of tetrahedral triangulations. Local refinement / coarsening.
  - Level set method for interface representation.
  - Finite element methods. Extended-FEM (XFEM) for discretization of discontinuous quantities.

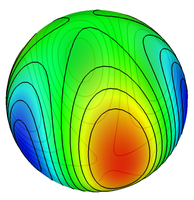


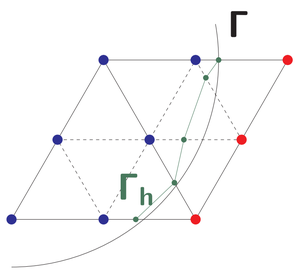




  - Special Laplace-Beltrami method for surface tension force discretization.
  - Implicit time discretization method with strong coupling of fluid dynamics and interface dynamics.
  - New FE method for discretization of surfactant transport equation.
  - Method for treatment of variable surface tension coefficients.
  - Fast iterative solvers.
  - Parallelization with MPI.







Numerical treatment of viscous surface stress tensor

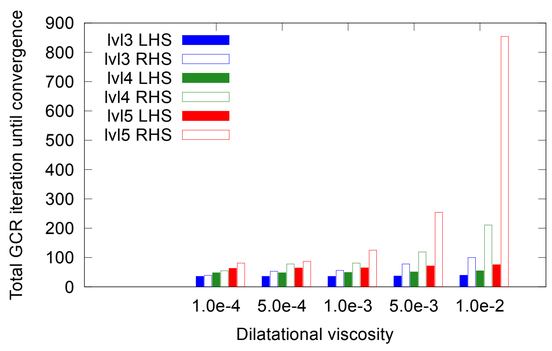
- Introduction of localized force term in weak formulation:

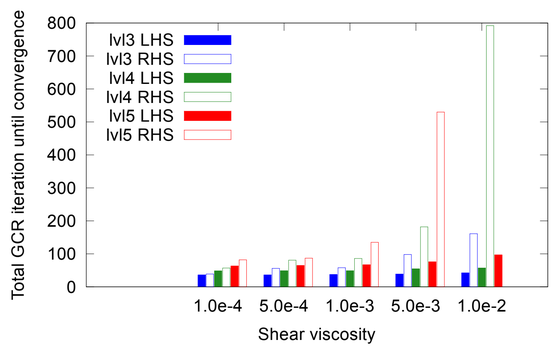
$$\mathbf{f}_\Gamma(\mathbf{v}) = \int_\Gamma (\operatorname{div}_\Gamma\sigma_\Gamma)\cdot\mathbf{v}\,ds$$

  Accurate discretization of $\mathbf{f}_\Gamma$ is *essential* !
- Decoupling of level set function and fluid dynamics.
- Convergence acceleration :
  - Linearization of $\mathbf{f}_\Gamma(\mathbf{v})$ term accelerates the convergence rate[1].

Δt	no acceleration	LinST
10^{-3}	4 (18)	4 (20)
10^{-2}	> 250	17 (70)
10^{-1}	> 250	214 (1578)

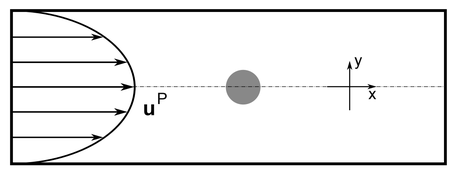
  - Implicit treatment of viscous terms.





Validation[2]

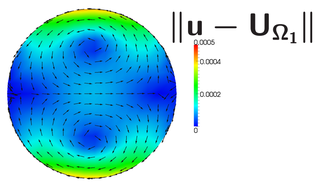
- Test case: a droplet in a plane Poiseuille flow

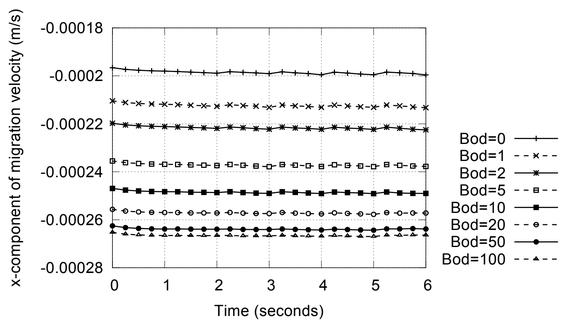


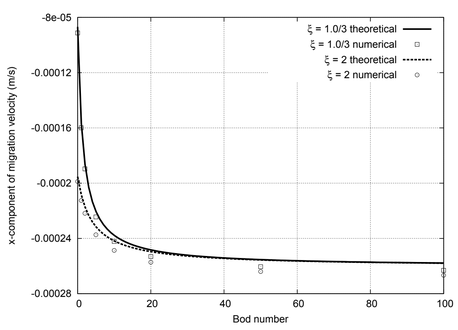
- Theoretical analysis[3]:
  - A *spherical* droplet with viscous interface in an *unbounded* domain.
  - Creeping flow condition.
  - Predication for migration velocities.

$$\mathbf{U}_{\text{mig}} = -\frac{2\text{Bo}^{\text{d}} + 3\xi}{3(2 + 2\text{Bo}^{\text{d}} + 3\xi)}\alpha r^2\vec{\mathbf{e}}_x.$$

- Numerical experiments:
  - *Enough* surface tension is needed for a spherical shape.
  - *Bounded* domain, restrictions of flow numbers (**Re**, **We**, **Ca**).
  - Calculated migration velocities are compared to theoretical results for validation.







Conclusion

- We choose a simple Newtonian droplet model with a viscous interface to simulate a biological cell in blood vessels.
- Numerical methods for solving the model problem have been introduced.
- We validate our numerical results by considering a simple test problem and comparing with theoretical analysis.
- More complicated is the *viscoelastic* behavior of biointerfaces.

Literature

[1] Gross S, Reusken A. *Numerical Methods for Two-Phase Incompressible Flows*, Volume 40 of Springer Series in Computational Mathematics. Springer:Heidelberg, 2011.

[2] Reusken A, Zhang Y. Numerical simulation of incompressible two-phase flows with a Boussinesq-Scriven interface stress tensor. *Int. J. Numer. Meth. Fluids*, 2013.

[3] Schwalbe JT, Phelan FR Jr., Vlahovska PM, Hudson SD. Interfacial effects on droplet dynamics in poiseuille flow. *Soft Matter* 2011; 7:7797-7804.

[4] DROPS package for simulation of two-phase flows. (Available from: http://www.igpm.rwth-aachen.de/forschung/DROPS)

[5] Kamm RD. Cellular fluid mechanics. *Annu. Rev. Fluid Mech.* 2002; 34:211-32.

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