Quelques modèles pour la simulation d'écoulements bi-fluide.

Application à la dynamique des bulles, gouttes et vésicules

Journée MMSN : chaire modélisation mathématique et simulation numérique.

École Polytechnique, *9 octobre 2012*

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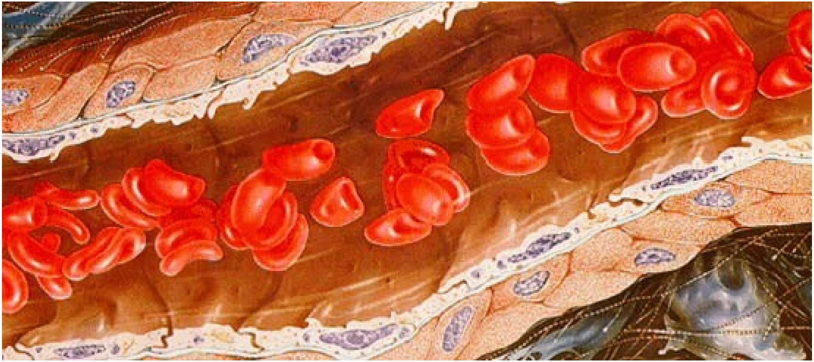
Final Goal

Figure : Photo O. K. Baskurt, from `http://www.rheology.org`



Challenges

- How to take into account the presence of RBCs? which models?
- Complex interactions at different levels :
  - Blood/arteries
  - Plasma/RBCs
  - RBCs/RBCs
- Different kinds of deformations and different scales
  - Dynamic of RBCs in arteries
  - Deformation of RBCs in capillaries

Collaborations

Level Set Models using FEEL++ Library.
http://www.feelpp.org/
Collaboration with

- Vincent Doyeux
- Yann Guyot
- Vincent Chabannes
- Christophe Prud'homme

"Necklace Model". From fluid/rigid particles to vesicles.
Collaboration with

- Aline Lefebvre

using FreeFEM++ software.
http://www.freefem.org/ff++

Outline

dépasser les frontières

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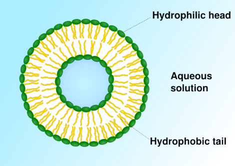
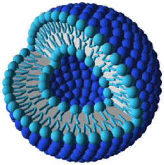
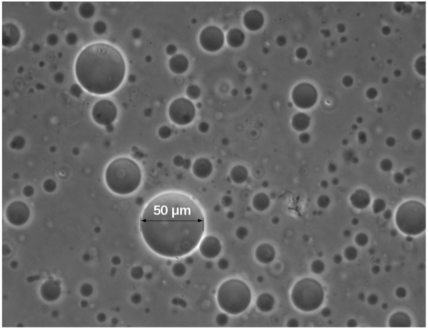
Vesicle : A Simple RBC Model I

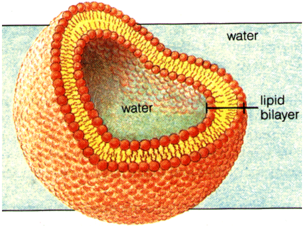


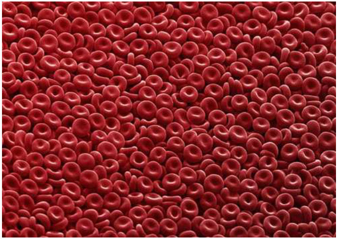


- Unilamellar vesicle : lipid bi-layer membrane
- Easy to produce in the laboratory
- Imitate some behaviors of red blood cells
  ➠ passive mechanical properties
- Properties of the membrane :
  - Nonporous : Conservation of inner fluid's Volume
  - Non extensible : Conservation of the membrane surface (perimeter in 2D)
  - Bending Energy (Helfrich energy)

Vesicle : A Simple RBC Model II

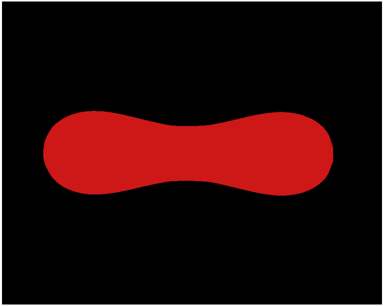




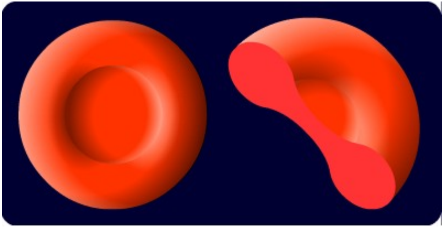


Biconcave shape

Reduce volume of a red blood cell ≈ 0.5
Biconcave shape recovered



Vesicle simulation RV = 0.5

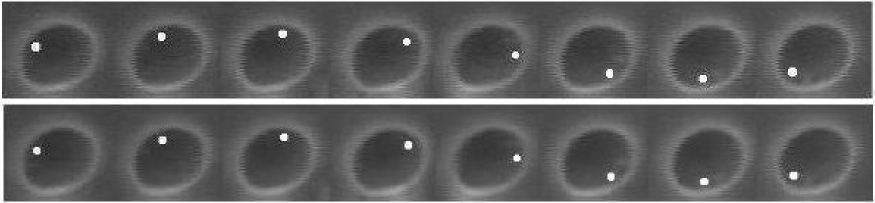


Picture of a red blood cell

Vesicle under shear flow. Tank treading motion

Small Viscosity Contrast ➠ Tank-Treading motion

- vesicle reaches a stationary angle
- rotation of the membrane

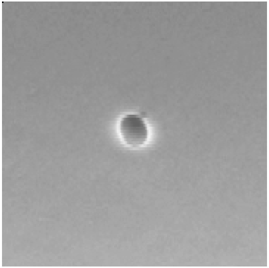


Experimental observation of a Tank-Treading motion [T. Podgorski]

Vesicle under shear flow. Tumbling motion

High viscosity ratio ➠ Tumbling motion

- vesicle in quasi solid rotation
- rotation velocity depends on the angle



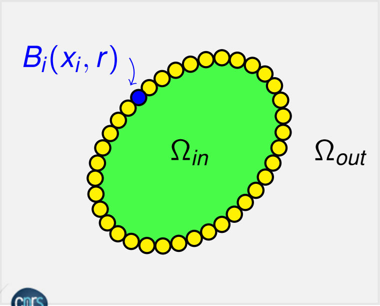
Experimental observation of a tumbling motion [T. Podgorski]

Outline

From Fluid/Rigid Particles model to Vesicles I

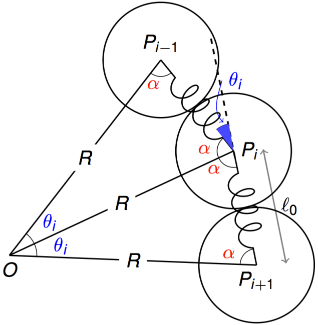
Collaboration with A. Lefebvre. [available on HAL]

Vesicle membrane modeled by a “Necklace" of rigid particles



- Membrane modeled by a Necklace of small rigid particles
- Incompressibility and curvature forces modeled by interaction between rigid particles (springs)
- FEM and Penalty Methods

From Fluid/Rigid Particles model to Vesicles II



- stretch/compression springs f_i^s on B_i and bending springs f_i^b on B_i
- classical energy for strech/compression springs :

$$E_{st} = \sum_i k_{rp_i} \ell_i^2$$

with $k_{rp_i} = cst = k_{rp}$

- bending spring energy :

$$E_b = \sum_i k_{a_i} (u_i \cdot v_i + 1)$$

with $k_{a_i} = cst = k_a$.

Formulation I

- Let

$$K_B = \left\{ \begin{array}{l} v \in H_0^1(\Omega), \ \ \forall i, \ \ \exists (V_i, \omega_i) \in \mathbb{R}^2 \times \mathbb{R}, \\ v = V_i + \omega_i (x - x_i)^\perp \text{ a.e. in } B_i \end{array} \right\}$$
$$= \left\{ v \in H_0^1(\Omega), \ \ \mathrm{D}v = 0 \text{ a.e. in } B \right\}$$

- Find u in K_B and p in $L_0^2(\Omega)$ s.t.

$$(\mathcal{P}) \left\{ \begin{array}{l} 2\mu \int_\Omega \mathrm{D}u : \mathrm{D}\tilde{u} - \int_\Omega p \nabla \cdot \tilde{u} = \int_\Omega f \cdot \tilde{u}, \ \ \forall \tilde{u} \in K_B, \\ \int_\Omega q \nabla \cdot u = 0, \ \ \forall q \in L_0^2(\Omega), \end{array} \right.$$

where $f = \sum_{i=1}^{N} f_i \mathbf{1}_{B_i}$.

Formulation II

- A penalty method is used to approximate the constraint problem $(\mathcal{P})$ by a sequence $(\mathcal{P}^{\varepsilon})$ of unconstrained problems:

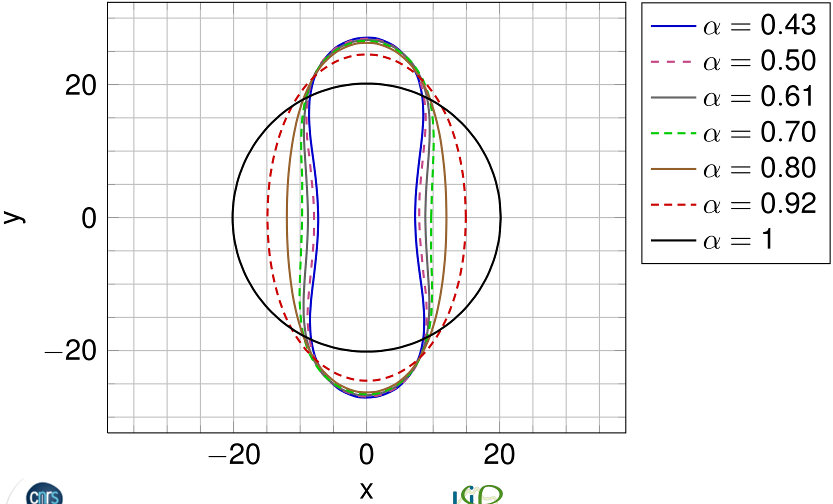
$$
\left\{
\begin{array}{l}
\text{Find } u^{\varepsilon} \text{ in } H_0^1(\Omega) \text{ and } p^{\varepsilon} \text{ in } L_0^2(\Omega) \text{ such that} \\
2\mu \displaystyle\int_{\Omega} \mathrm{D}u^{\varepsilon} : \mathrm{D}\tilde{u} + \frac{2}{\varepsilon}\int_{B} \mathrm{D}u^{\varepsilon} : \mathrm{D}\tilde{u} - \int_{\Omega} p^{\varepsilon}\nabla\cdot\tilde{u} = \displaystyle\int_{\Omega} f\cdot\tilde{u}, \quad \forall \quad \tilde{u} \in H_0^1(\Omega), \\
\displaystyle\int_{\Omega} q\nabla\cdot u^{\varepsilon} = 0, \quad \forall \quad q \in L_0^2(\Omega).
\end{array}
\right.
$$

Algorithm

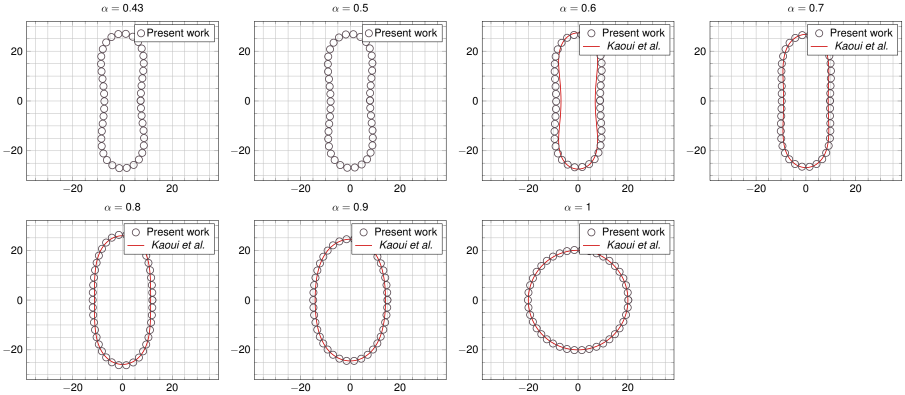
1. Compute (u^n, p^n) solution to $(\mathcal{P}^\varepsilon)$ with $B = B^n$ and $f = f^n$,
2. Compute the corresponding velocities of the particles:
$$\tilde{V}_i^n = \frac{1}{|B_i^n|}\int_{B_i^n} u^n,$$
3. Deal with contacts: $\hat{V}^n = \Pi_{K_c^n}\tilde{V}^n$,
4. Deal with the volume constraint: $V^n = \Pi_{K_v^n}\hat{V}^n$,
5. Compute B^{n+1}: $x_i^{n+1} = x_i^n + hV_i^n$,

where Π_K denotes the projection onto K and is performed using a Uzawa algorithm.

Equilibrium Shapes I

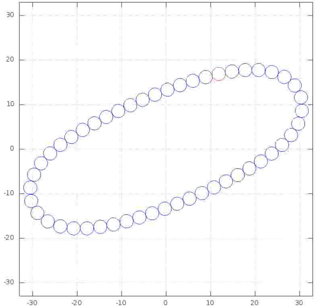


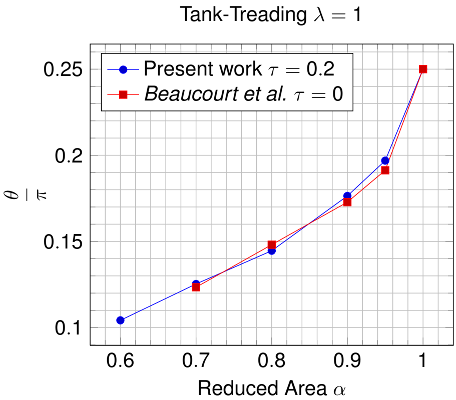
Equilibrium Shapes II



Comparison with results from [Kaoui et al. Phys. Rev. E, 83, 2011]

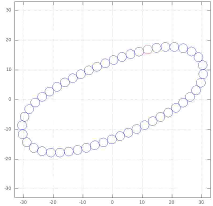
Tank treading angles



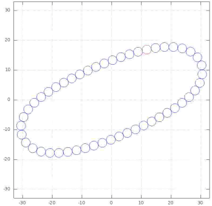


Comparison with results from [Beaucourt et al. Phys. Rev. E, 69, 2004]

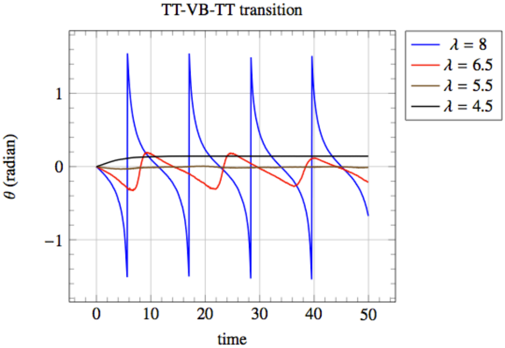
Tumbling and Vacillating-Breathing



TB



VB



Comparison with results from [Beaucourt et al. Phys. Rev. E, 69, 2004]

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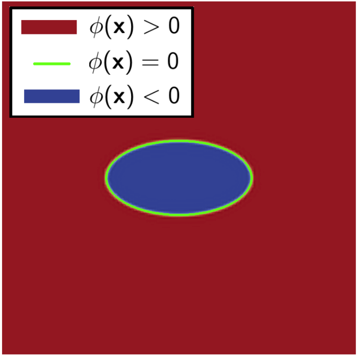
Outline

Level set method

$\phi(\boldsymbol{x})$ used to track an interface

$$\phi(\boldsymbol{x}) = \begin{cases} dist(\boldsymbol{x},\Gamma) & \boldsymbol{x} \in \Omega_1, \\ 0 & \boldsymbol{x} \in \Gamma, \\ -dist(\boldsymbol{x},\Gamma) & \boldsymbol{x} \in \Omega_2, \end{cases}$$



Advection by a divergence-free velocity $\boldsymbol{u}$

$$\frac{D\phi}{Dt} = 0 \qquad \frac{\partial \phi}{\partial t} + \boldsymbol{u} \cdot \nabla \phi = 0$$

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Coupling with Navier Stokes equations

$$\rho_\phi \left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} \right) - \nabla \cdot (2\mu_\phi D(\boldsymbol{u})) + \nabla p = \boldsymbol{F}_\phi$$
$$\nabla \cdot \boldsymbol{u} = 0$$
$$\frac{\partial \phi}{\partial t} + \boldsymbol{u} \cdot \nabla \phi = 0$$

- level set advected by solution of Navier Stokes equations
- fluid quantities depend on level set function ρ_ϕ, μ_ϕ, $\boldsymbol{F}_\phi$

$$\rho_\phi = \rho^- + (\rho^+ - \rho^-) H_\epsilon(\phi)$$
$$\mu_\phi = \mu^- + (\mu^+ - \rho^-) H_\epsilon(\phi)$$
$$\boldsymbol{F}_\phi = \int_\Gamma \boldsymbol{F}_s = \int_\Omega \boldsymbol{F}_s \delta_\epsilon(\phi)$$

Variational formulation

find $(\boldsymbol{u}, p, \phi) \in H^1(\Omega)^2 \times L^2(\Omega) \times H^1(\Omega)$ which verify $\forall(\boldsymbol{v}, q, \psi) \in H_0^1(\Omega)^2 \times L_0^2(\Omega) \times H^1(\Omega)$:

$$\begin{aligned}
\rho_\phi \int_\Omega \left(\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} \right) \cdot \boldsymbol{v} + \mu_\phi \int_{\Omega_f} D(\boldsymbol{u}) : D(\boldsymbol{v}) - \int_\Omega p \nabla \cdot \boldsymbol{v} &= \int_\Omega (\boldsymbol{F}_\phi) \\
\int_{\Omega_f} q \nabla \cdot \boldsymbol{u} &= 0, \\
\int_\Omega \partial_t \phi \psi + \int_\Omega (\boldsymbol{u} \cdot \nabla \phi)\psi + \int_\Omega S(\phi, \psi) &= 0.
\end{aligned}$$

with $S(\phi, \psi)$ a stabilization term (SUPG, GLS, SGS, CIP).

➠ Solved by FEM and using FEEL++ library

[V. Doyeux PhD thesis]

[JCAM 2012, available on HAL]

➠ **Curvature force derived from Helfrich energy**

$$E_h = \int_\Gamma \frac{k_B}{2}\kappa^2$$

$$\boldsymbol{F_b} = \int_\Gamma \frac{k_B}{2}\left[\frac{\kappa^3}{2} + \boldsymbol{t}\cdot\nabla(\boldsymbol{t}\cdot\nabla\kappa)\right]\boldsymbol{n}$$

➠ **Two different approaches to impose membrane inextensibility**

- Write an elastic energy from level set gradient information

$$E_{el} = \int_\Gamma E(|\nabla\phi|)$$

$$\boldsymbol{F_{el}} = \int_\Gamma \{\nabla E'(|\nabla\phi|) - \nabla\cdot[E'(|\nabla\phi|)\boldsymbol{n}]\,\boldsymbol{n}\}$$ [Maitre et al. (2010)]

- Add a Lagrange multiplier

constraint : $\nabla_s\cdot\boldsymbol{u} = \nabla\cdot\boldsymbol{u} - (\nabla\boldsymbol{u}\cdot\boldsymbol{n})\cdot\boldsymbol{n} = 0$ [Laadhari (2011)]

Advantages - Drawbacks - inextensibility force

Add an elastic force $\boldsymbol{F_{el}}$

Advantages

- Do not need to enter in fluid solver (Stokes, Navier-Stokes, or more complex ...)
- Can easily add other forces (surface tension, elasticity...)

Drawbacks

- Bad conservation of surface area
- Need to keep the stretching information $|\nabla\phi|$
- Complexity of the force

$$\boldsymbol{F_{el}} = \int_{\Omega} \left\{ \nabla E'(|\nabla\phi|) - \nabla \cdot \left[E'(|\nabla\phi|) \frac{\nabla\phi}{|\nabla\phi|} \right] \frac{\nabla\phi}{|\nabla\phi|} \right\} \delta_{\epsilon} \left(\frac{\phi}{|\nabla\phi|} \right)$$

Lagrange multiplier

Variational formulation on Stokes equation

$$
\begin{aligned}
-\nabla \cdot (2\mu_\phi D(\boldsymbol{u})) + \nabla p &= \boldsymbol{F}_\phi \ \text{ in } \Omega \\
\nabla \cdot \boldsymbol{u} &= 0 \ \text{ in } \Omega \\
\nabla_s \cdot \boldsymbol{u} &= 0 \ \text{ on } \Gamma
\end{aligned}
$$

find $(\boldsymbol{u}, p, \lambda) \in H^1(\Omega)^2 \times L^2(\Omega) \times L^2(\Gamma)$ which verify $\forall(\boldsymbol{v}, q, \nu) \in H^1_0(\Omega)^2 \times L^2_0(\Omega) \times L^2(\Gamma)$:

$$
\begin{aligned}
\mu_\phi \int_{\Omega_f} D(\boldsymbol{u}) : D(\boldsymbol{v}) - \int_\Omega p \nabla \cdot \boldsymbol{v} + \int_\Gamma \lambda \nabla_s \cdot \boldsymbol{v} &= \int_\Omega \boldsymbol{F}_\phi \cdot \boldsymbol{v} \\
\int_\Omega q \nabla \cdot \boldsymbol{u} &= 0 \\
\int_\Gamma \nu \nabla_s \cdot \boldsymbol{u} &= 0
\end{aligned}
$$

Advantages - Drawbacks - Lagrange multiplier

Add Lagrange multiplier

Advantages

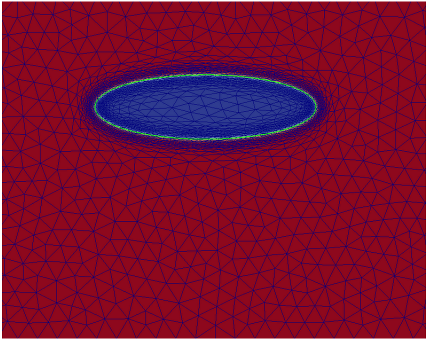
- Good conservation of surface area
- Depend only on level set position

Drawbacks

- Add one more variable in the fluid solver
- More difficult to get $\nabla \cdot \boldsymbol{u} = 0$

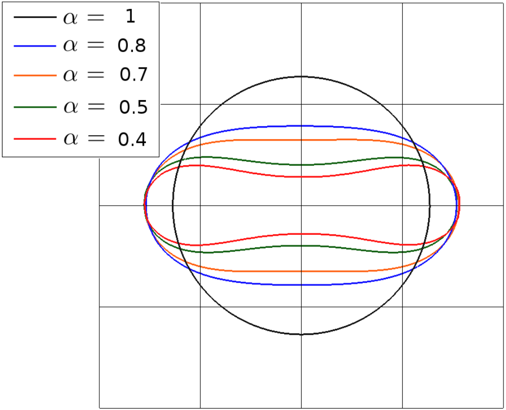
Mesh adaptation

Adapt mesh using GMSH anisotropic refinement



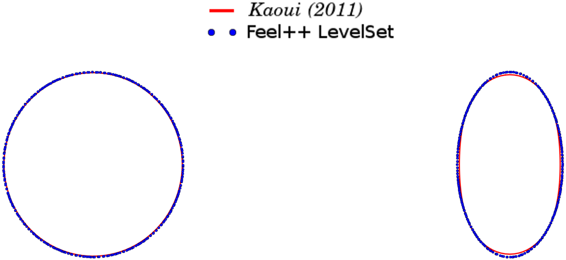
Equilibrium shapes

$$\text{reduce area } \alpha = \frac{\text{area vesicle}}{\text{area circle with same perimeter}}$$



Comparison with another model

Comparison with boundary integral method from [Kaoui et al. 2011]



– Reduce area = 1	– Reduce area = 0.90
·· Reduce area = 1	·· Reduce area = 0.93

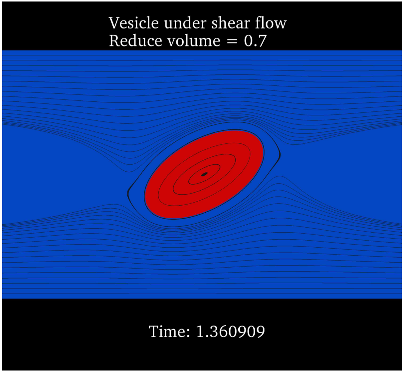
Comparison with another model

Comparison with boundary integral method from [Kaoui et al. 2011]

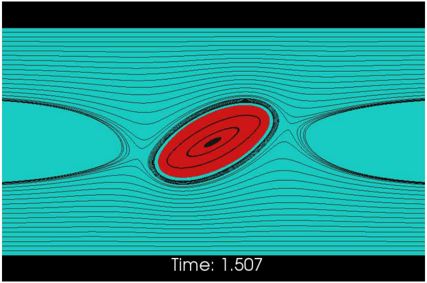
– Reduce area = 0.80
·· Reduce area = 0.78

– Reduce area = 0.60
·· Reduce area = 0.61

Tank treading motion

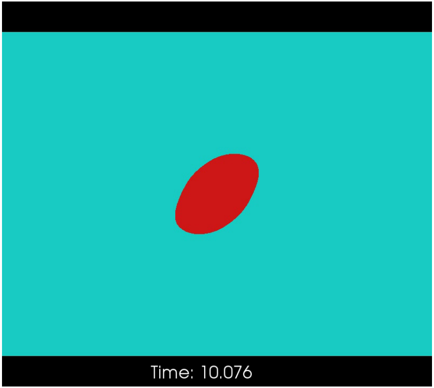


Forces method

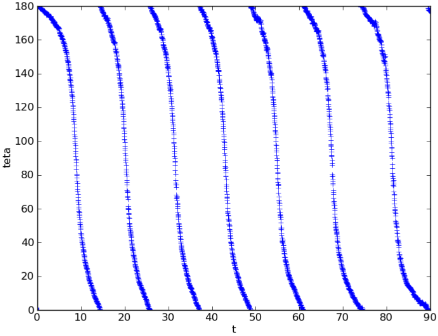


Lagrange Multiplier method

Tumbling motion - Simulation



Lagrange Multiplier method



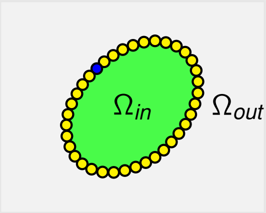
Angle of the vesicle during time

Outline

Conclusions I

First Model

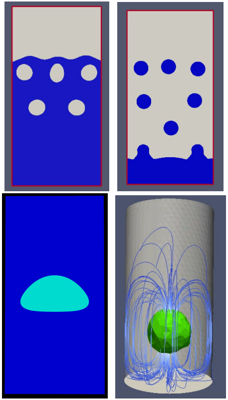
- ✔ A new model to study the dynamics of 2D vesicles
- ✔ VB regime recovered numerically in 2D for the first time
- ✔ Area and perimeter conservation (about 0.5%)
- ✘ Extension to 3D vesicles not easy



Conclusions II

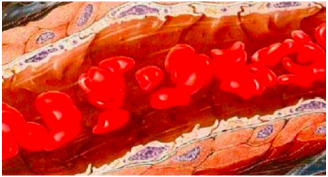
Second Model

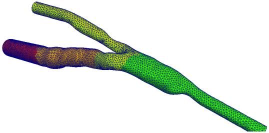
- ✔ Unified framework for two-fluid flows (2D and 3D using `FEEL++` `http://www.feelpp.org/`). Application to bubbles, drops and vesicles
- ✔ Validation using benchmarks

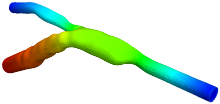


Work in progress

[V. Chabannes and V. Doyeux PhD thesis]







- Parallelism
- Flow in complex geometries
- Multi particles simulation (Effective Viscosity)