Institut de Recherche Mathématique Avancée
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FEEL++ developments for micro-swimming simulation

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FEEL++

Finite Element Embedded Library in C++

- Open source library → github.com/feelpp
- Galerkin methods
- Domain Specific Embedded Language (DSEL) in C++
- Scaling : from laptops to supercomputers
- Easy deployment → Docker, Singularity
- (Multi)Physics toolboxes: Heat Transfer, Aerothermics, CFD, CSM, **FSI**, Maxwell

Outline

1. Introduction to micro-swimming
2. Articulated swimmers
3. Deformable swimmers
4. Other fluid models

Introduction to micro-swimming

Context

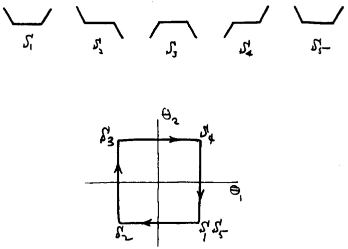
Micro-swimming $\rightleftarrows$ swimming at low Reynolds number

Reynolds number

$$Re = \frac{Inertia}{Viscosity} \propto \frac{\rho L^3 U}{\mu L^2}$$

ρ: Density L: Length
μ: Viscosity U: Speed

Micro-swimming $\rightleftarrows$ swimming at low Reynolds number



Source: "Life at low Reynolds Number", AJP 45.1 (1977)

Figure: Purcell 3-links swimmer

Reynolds number

$$Re = \frac{\rho L U}{\mu} \approx 10^{-4} \text{ (for spermatozoon)}$$

ρ: Density L: Length
μ: Viscosity U: Speed

Context

Micro-swimming $\rightleftarrows$ swimming at low Reynolds number

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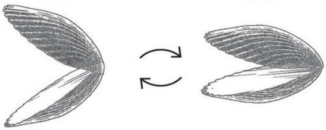


Source: Nat Commun 5, 5119 (2014)

Figure: Scallop theorem

Examples of microswimmers

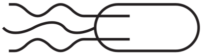


Figure: E. Coli

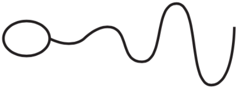


Figure: Sperm cell

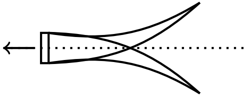


Figure: Artificial microswimmer

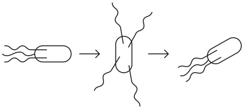


Figure: Run and tumble

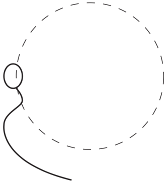


Figure: Motion in proximity of a surface

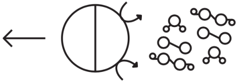


Figure: Functionalised particle

Numerical description

Particle solvers → collective motion

Yang, Yingzi et al. *Cooperation of sperm in two dimensions: Synchronization, attraction, and aggregation through hydrodynamic interactions*. Phys. Rev. E, 78, 6, 2008.

ODE solvers - RFT → solving Newton 2nd law $\sum F = 0$

F. Alouges, L. Giraldi et al. *Self-propulsion of slender micro-swimmers by curvature control: N-link swimmers*. International Journal of Non-Linear Mechanics, 56, 2013.

PDE solvers → solving the flow field

- Differential equations → Finite Element method

  Bergmann, Iollo. *Bioinspired swimming simulations*. (2016). Journal of Computational Physics.

- Integral equations → Boundary Element method

  Kenta Ishimoto. *Bacterial spinning top*, Journal of Fluid Mechanics, 880, 2019.

Scientific positioning: Numerical simulation of micro-swimmers under partial differential equation description. Interplay with optimization and control.

Goal: Simulate and control a magnetically actuated micro-robot

Articulated swimmers

Microswimming problem - Stokes equations

Let $\mathcal{F}_t$ be the fluid domain, S_t the domain occupied by the swimmer.

$$\begin{cases} \nabla p - \mu \Delta u = 0, & \text{on } \mathcal{F}_t, \\ \nabla \cdot u = 0, & \text{on } \mathcal{F}_t, \\ u = \mathbf{U} + \boldsymbol{\omega} \wedge (x - x^{CM}) + u_d(x), & \text{on } \partial S_t \cap \partial \mathcal{F}_t, \end{cases}$$

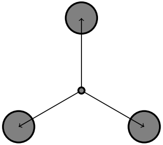
Kinematic coupling:

$\mathbf{U}$ and $\boldsymbol{\omega}$ are the translational and rotational speeds of the swimmer. $\mathbf{u}_d(x)$ is the imposed displacement on the boundary of the swimmer.

Dynamic coupling:

Balance of forces that fluid and swimmer exchange.

Articulated swimmers - Translational constraints



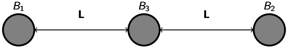


Figure: Example of articulated swimmers with translational constraints

- Analytical computations and benchmarking
- Non-reciprocal strokes can be imposed
- Slight modification of independent rigid bodies formulation

Procedure:

- Identify B_n as the reference body
- $\mathbf{U}_i$ of all the other bodies B_i, $i = 1 \dots n-1$, are expressed as functions of $\mathbf{U}_n$ via constraints of the form

$$\mathbf{U}_i = \mathbf{U}_n + \mathbf{W}_{in}(t), \quad i = 1 \dots n-1,$$

where $\mathbf{W}_{in}(t)$ represents the relative velocity between B_i and B_n.

Coupling with several rigid bodies

$$
\begin{cases}
-\mu\Delta u + \nabla p = f, & \text{on } \mathcal{F}_t, \\
\nabla \cdot u = 0, & \text{on } \mathcal{F}_t, \\
u = \mathbf{U}_i + \boldsymbol{\omega}_i \times (x - x_i^{CM}(t)), \quad i = 1 \dots n, & \text{on } \partial B_i, \\
m_i \dot{\mathbf{U}}_i = -F_{fluid}, & i = 1 \dots n, \\
J_i \dot{\boldsymbol{\omega}}_i = -M_{fluid}, & i = 1 \dots n.
\end{cases}
$$

Weak formulation $\rightarrow$ test functions $(\tilde{u}, \tilde{p}, \tilde{\mathbf{U}}, \tilde{\boldsymbol{\omega}})$ such that $\tilde{u} = \tilde{\mathbf{U}}_i + \tilde{\boldsymbol{\omega}}_i \times (x - x_i^{CM})$ on ∂B_i

$$
2\mu \int_{\mathcal{F}} D(u) : D(\tilde{u})\, dx - \int_{\mathcal{F}} p \nabla \cdot \tilde{u}\, dx + m\mathbf{U} \cdot \tilde{\mathbf{U}} + J\boldsymbol{\omega} \cdot \tilde{\boldsymbol{\omega}} = 0.
$$

B. Maury, *Direct Simulations of 2D Fluid-Particle Flows in Biperiodic Domains*. Journal of Computational Physics, 156, 1999.

Coupling with several rigid bodies

$$\begin{cases} -\mu\Delta u + \nabla p = f, & \text{on } \mathcal{F}_t, \\ \nabla \cdot u = 0, & \text{on } \mathcal{F}_t, \\ u = \mathbf{U}_i + \boldsymbol{\omega}_i \times (x - x_i^{CM}(t)), & i = 1 \dots n, \quad \text{on } \partial B_i, \\ \dot{\mathbf{U}}_i = 0, & i = 1 \dots n, \\ \dot{\boldsymbol{\omega}}_i = 0, & i = 1 \dots n. \end{cases}$$

Weak formulation $\rightarrow$ test functions $(\tilde{u}, \tilde{p}, \tilde{\mathbf{U}}, \tilde{\boldsymbol{\omega}})$ such that $\tilde{u} = \tilde{\mathbf{U}}_i + \tilde{\boldsymbol{\omega}}_i \times (x - x_i^{CM})$ on ∂B_i

$$2\mu \int_{\mathcal{F}} D(u) : D(\tilde{u})\, dx - \int_{\mathcal{F}} p \nabla \cdot \tilde{u}\, dx + \mathbf{U} \cdot \tilde{\mathbf{U}} + \boldsymbol{\omega} \cdot \tilde{\boldsymbol{\omega}} = 0.$$

B. Maury, *Direct Simulations of 2D Fluid-Particle Flows in Biperiodic Domains*. Journal of Computational Physics, 156, 1999.

Algebraic form

Enforcing the condition $\tilde{u} = \tilde{\mathbf{U}}_i + \tilde{\boldsymbol{\omega}}_i \times (x - x_i^{CM})$ on $\partial \mathbf{B_i}$ is done by

- First, building the system matrix A. No coupling for the moment is enforced between fluid and swimmer.

$$A = \begin{bmatrix} A_{II} & A_{I\Gamma} & 0 & 0 & B_I^T \\ A_{\Gamma I} & A_{\Gamma\Gamma} & 0 & 0 & B_\Gamma^T \\ 0 & 0 & T & 0 & 0 \\ 0 & 0 & 0 & R & 0 \\ B_I & B_\Gamma & 0 & 0 & 0 \end{bmatrix}$$

- Second, building a coupling matrix $\mathcal{P}$ such that $(u_I, u_{\partial B_i}, \mathbf{U}_i, \boldsymbol{\omega}_i, p)^T = \mathcal{P}(u_I, \mathbf{U}_i, \boldsymbol{\omega}_i, p)^T$

$$\mathcal{P} = \begin{bmatrix} I & 0 & 0 & 0 \\ 0 & \tilde{P}_{\mathbf{U}_i} & \tilde{P}_{\boldsymbol{\omega}_i} & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & I & 0 \\ 0 & 0 & 0 & I \end{bmatrix} \qquad \rightarrow \qquad \mathcal{P}^T A \mathcal{P} X = \mathcal{P}^T F$$

Fluid toolbox: the interface for rigid-body motion

In the fluid toolbox, an interface for rigid body motion has been introduced. One needs to specify in the *json*:

Materials section

```
"Materials":
{"Fluid":{
"physics":"fluid",
"rho":"1.0e-6",
"mu":"1"
},
"Solid":{
"markers":["Swimmer"],
"physics":"body",
"rho":"1.0e-6"
}}
```

Fluid BC

```
"BoundaryConditions":
{"fluid":{"body":
{"swimmer_markers":
{"markers":["Sphere1"],
"materials":{"names":"Solid"},
//"translational-velocity"
"elastic-velocity":
{"onTail":{
"expr":"{f(x,t),g(x,t)}:x:t",
"markers":"Sphere1"
}}}}
```

Translational constraints - Lagrange multipliers

Lagrange multipliers:

$$\dot{\mathbf{U}}_i \cdot \tilde{\mathbf{U}}_i + \alpha_i \cdot \tilde{\mathbf{U}}_i = 0 \quad i = 1 \dots n-1,$$

$$\dot{\mathbf{U}}_n \cdot \tilde{\mathbf{U}}_n - \sum_{i=1}^{n-1} \alpha_i \cdot \tilde{\mathbf{U}}_n = 0$$

$$\alpha_i \cdot (\mathbf{U}_i - \mathbf{U}_n) = \alpha_i \cdot \mathbf{W}_{in}, \quad i = 1 \dots n-1.$$

The addition of Lagrange multipliers entails the modification of $\mathcal{P}$ by providing an additional identity matrix of size $d(n-1) \times d(n-1)$ on the diagonal.

Translational constraints - Modification of $\mathcal{P}$

$$(u_I, u_{\partial B_i}, \mathbf{U}_i, \boldsymbol{\omega}_i, p)^T = \tilde{\mathcal{P}}(u_I, \mathbf{U}_n, \boldsymbol{\omega}_i, p)^T$$

$$\tilde{\mathcal{P}} = \begin{bmatrix} I & 0 & 0 & 0 \\ 0 & \tilde{\tilde{P}}_{\mathbf{U}} & \tilde{P}_{\boldsymbol{\omega}_i} & 0 \\ 0 & E & 0 & 0 \\ 0 & 0 & I & 0 \\ 0 & 0 & 0 & I \end{bmatrix} \qquad E = \begin{bmatrix} I_d \\ \vdots \\ I_d \\ \vdots \\ I_d \end{bmatrix} \qquad \tilde{\tilde{P}}_{\mathbf{U}} = \begin{bmatrix} \tilde{P}_{\mathbf{U}_1} \\ \vdots \\ \tilde{P}_{\mathbf{U}_i} \\ \vdots \\ \tilde{P}_{\mathbf{U}_n} \end{bmatrix}$$

It constrains further the FEM space to functions satisfying

$$u = \mathbf{U}_n + \boldsymbol{\omega}_i \times (x - x_i^{CM}) + \mathbf{W}_{in}(t), \quad \text{on } \partial B_i$$

The moving domain

The computational domain is transformed in time via ALE maps $\mathcal{A}_t : \mathcal{F}_0 \to \mathcal{F}_t$. It associates the points x in the fluid domain $\mathcal{F}_t$ at time t to their position x^* in the reference domain $\mathcal{F}_0$. In other words $\mathcal{A}_t(x^*) = x$.
ALE maps are computed by solving an extension problem of the displacement $d(x,t)$ on the boundary of the domain

$$\begin{aligned} \Delta\phi_t &= 0 && \text{in } \mathcal{F}_0 \\ \phi_t(x) &= d(t,x) && \text{in } \partial\mathcal{F}_0 \end{aligned}$$

and $\mathcal{A}_t(x^*) = x^* + \phi_t(x^*)$.

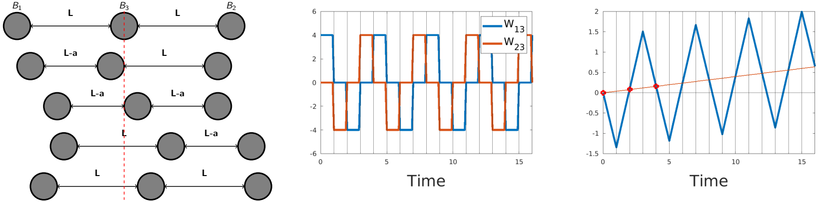
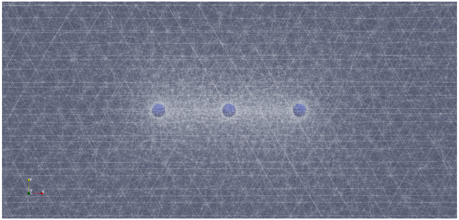


Figure: Three-sphere swimmer and its swimming gait.



Fitted mesh and remeshing

Using ALE to handle moving domains is possible under the condition that movements are not too large.

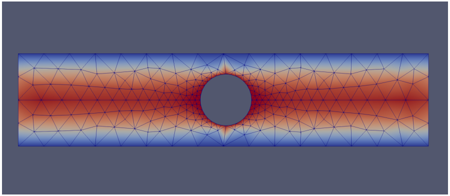
Remeshing depending on mesh quality indices

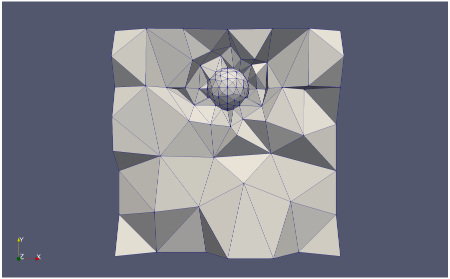
$$\eta_2 = \frac{2r}{R}\,(2D) \qquad \eta_3 = \frac{3r}{R}\,(3D)$$

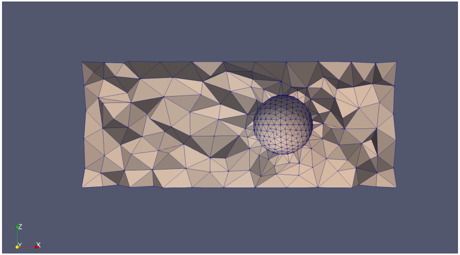
We set constraints:

- Interfaces, that must be kept,
- Interface discretization, that should be remain unvaried as well (in order to maintain all the properties linked to areas and volumes of the enclosed region),
- Interpolating the solution from the old to the new mesh, in order to restart computations.

Simulations with remeshing in Feel++ using (Par)MMG







- Edge split
- Edge collapse
- Edge swap
- Node relocation
- Local size function h

Three-dimensional adaptive domain remeshing, implicit domain meshing, and applications to free and moving boundary problems - C. Dapogny, C. Dobrzynski and P. Frey - April 1, 2014 - JCP

Deformable swimmers

Recall the problem and notation

$$\begin{cases} \nabla p - \mu \Delta u = 0, & \text{on } \mathcal{F}_t, \\ \nabla \cdot u = 0, & \text{on } \mathcal{F}_t, \\ u = \mathbf{U} + \boldsymbol{\omega} \wedge (x - x^{CM}) + u_d(x), & \text{on } \partial S_t \cap \partial \mathcal{F}_t, \end{cases}$$

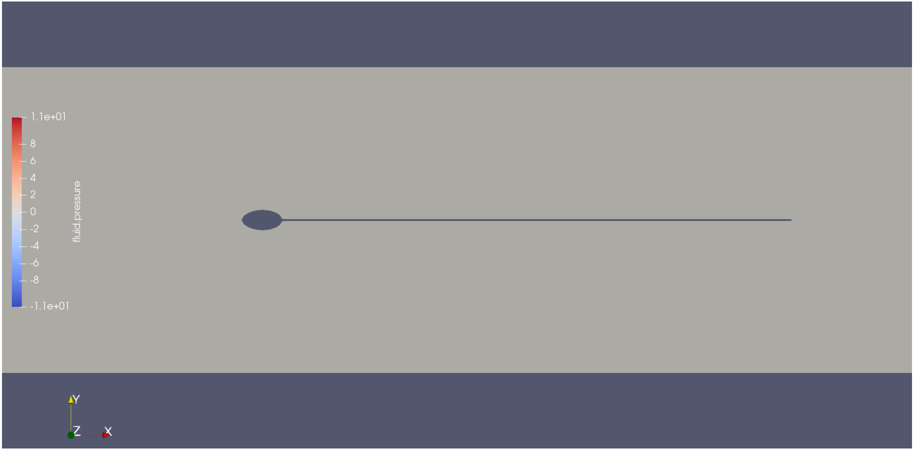
The expression of $u_d(x)$ is often given in the reference frame, and via the ALE map $\mathcal{A}_t$, gives the velocity in the current frame

$$u_d(x) = u_d(\mathcal{A}_t(x^*))$$

For example,

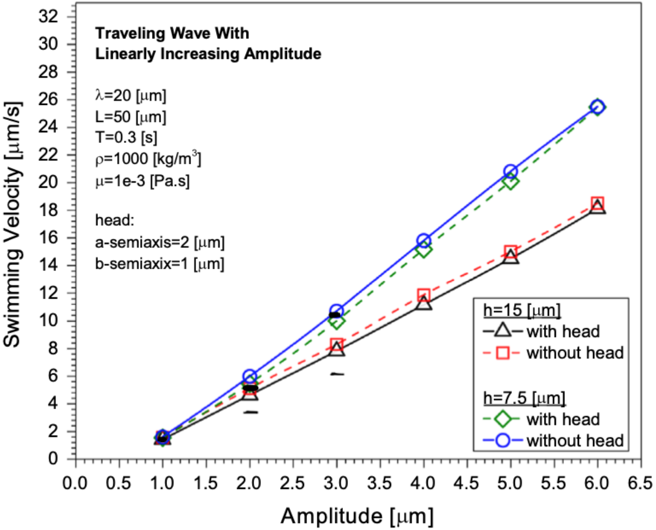
$$u_d^*(x^*) = (A(x^*)\cos(2B_t t - 2B_x x^*), C(x^*)\cos(B_t t - B_x x^*))$$

Spermatozoon simulation



$$u_d^*(x^*) = (A(x^*)\cos(2B_t t - 2B_x x^*), C(x^*)\cos(B_t t - B_x x^*))$$

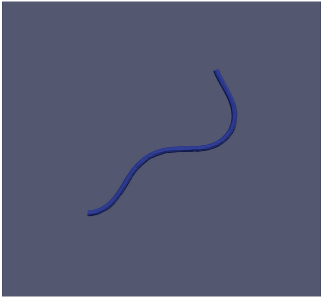
Spermatozoon simulation



$$u_d^*(x^*) = (A(x^*)\cos(2B_t t - 2B_x x^*), C(x^*)\cos(B_t t - B_x x^*))$$

Tail centerline described by ODEs

- Spermatozoon with ellipsoidal head (3D)
- ODE system describing the tail's centerline beating $\frac{dX}{d\ell}(t,\ell) = F(t,\ell)$
- Imposition of the centerline shape onto the meshed tail:
  - Solution of the 1d ODE giving the centerline coordinates, $\forall t$
  - Interpolation of the tail's shape
  - Transfer of the displacement onto the mesh nodes



Jikeli Jan F., Friedrich Benjamin M. et al. *Sperm navigation along helical paths in 3D chemoattractant landscapes*. Nature Communications 6, 2015.

Hyperelasticity equations

Let Ω^* be the intial position of the solid body, $x^* \in \Omega^*$. We take this as the reference position.

Let $\eta(t, x^*) = x(t, x^*) - x^*$ be the solid displacement, i.e. the difference between the current and initial position of the points in the domain.

Let $F(t, x^*) = \mathbb{I} + \nabla\eta$ be the deformation gradient.

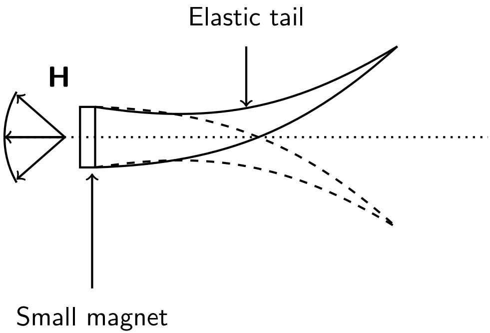
Let $\Sigma(t, x^*)$ be the second Piola-Kirkhhoff tensor of the elastic material, a function of the elastic properties of the material and of the displacement gradient.

They satisfy

$$\rho \frac{\partial^2 \eta}{\partial t^2} - \nabla \cdot (F\Sigma) = 0$$

ISIR robot

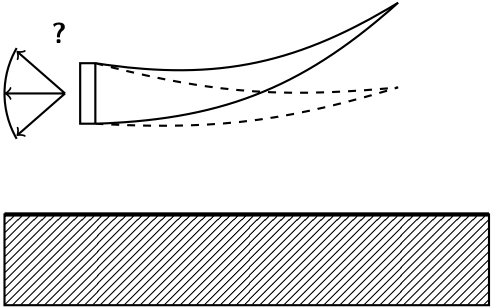
The swimmer we want to simulate is



It swims under the external magnetic field **H**, uniform in space, that produces a torque on the magnet.

Objective

The final objective is analyzing swimming close to solid boundaries.



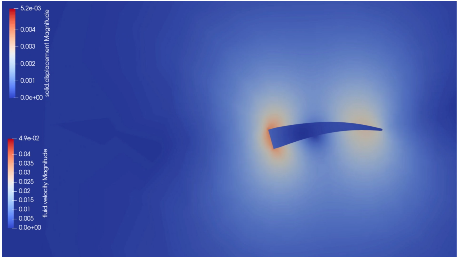
Coupled problem

Let $\mathcal{F}$ be the fluid domain, T the domain occupied by the elastic tail, H the domain occupied by the magnetic head. Let $S = H \cup T$.

$$\begin{cases} -\mu\Delta u + \nabla p = 0, & \text{in } \mathcal{F} \setminus S, \\ \nabla \cdot u = 0, & \text{in } \mathcal{F} \setminus S, \\ \rho \dfrac{\partial^2 \eta}{\partial t^2} - \nabla \cdot (F\Sigma) = 0, & \\ u = U + \Omega \times (x - x^{CM}) + \partial_t \eta(x), & \text{on } \partial S, \\ m\dot{U} = F = F_{ext} - F_{fluid}, & \\ J\dot{\Omega} = M = M_{ext} - M_{fluid}. & \end{cases}$$

Coupled problem

In this simulation, the swimmer is dragged on its magnetic head



Other fluid models

Other fluid models: Brinkman model

$$-\nabla p + \mu \Delta u = \mu \alpha^2 u$$
$$\nabla \cdot u = 0$$

$\alpha^2 = \frac{9\phi}{2a^2}$ for a network of spheres of radius a and volume fraction ϕ

- Variation of Darcy equations for heterogeneous media with sparse solid matrix
- Models relevant fluids, like mucus, where the volume fraction of solid obstacles is low
- Recent publications applied to microswimming

Other fluid models: quasi-Newtonian

$$\sigma(p, u) = -pI + 2\mu(\dot{\gamma})D(u)$$

where $\dot{\gamma} = \sqrt{2tr(D(u))}$ measures the deformation rate of the fluid

- Different expressions for $\mu(\dot{\gamma})$ (power law, Carreau-Yasuda)
- Blood can be modeled via these fluids (when size of vessels is less than 1mm)
- Parameters have been fitted in the literature

Other fluid models: viscoelastic fluids

$$Re(\partial_t u + u \cdot \nabla u) = -\nabla p + (1-\varepsilon)\Delta u + \frac{\varepsilon}{W_i}\nabla \cdot \sigma$$

$$\nabla \cdot u = 0$$

$$\partial_t \sigma + (u \cdot \nabla)\sigma = \nabla u \cdot \sigma + \sigma(\nabla u)^T - \frac{1}{W_i}(\sigma - I)$$

$\sigma = I + \frac{W_i}{\varepsilon}\tau \rightarrow$ conformation tensor
$W_i = \frac{\lambda U}{L}$ Weissemberg number $\rightarrow$ polymer relaxation time vs. flow timescale
$\varepsilon = \frac{\mu_p}{\mu_f + \mu_p}$ effective elastic viscosity

- Oldroyd-B viscoelastic model
- Models swimming in fluids with elastic suspended matrices (polymers for instance)

Perspectives

- Interface swimming simulations with remeshing
- Test the available swimmers in non-Newtonian fluid models presented before
- Control of the elastic swimmer

Thank you for your attention!