Microscopic modeling and direct simulation of active suspensions

A. Decoene, S. Martin, B. Maury

Laboratoire de Mathématiques
Université Paris - Sud

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Outline

Introduction : from individual to collective dynamics

A simple microscopic model : pointlike particles

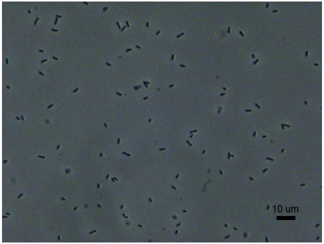
A model for chemotaxis

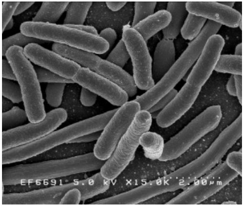
An accurate microscopic model : rigid particles

Ongoing work and perspectives

Active suspensions

Bacteria : E. Coli *[Berg, 1983]* ($\sim$ 2 μm x 0.5 μm)





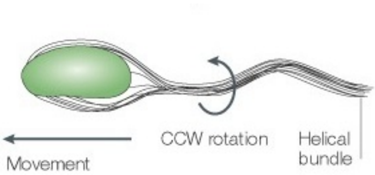
Green algae : Chlamydomonas (radius $\sim$ 10 μm)

life at low Reynolds number ($Re \ll 1$) : viscous forces dominate !

Self-propulsion in Stokes flow

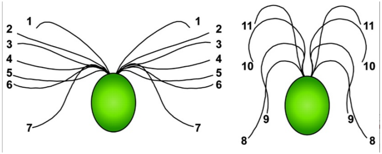
Pushers : bacteria *E. coli*, *B. Subtilis*

- helical flagella localized on the surface, responsible of propulsion



Pullers : *Chlamydomonas*

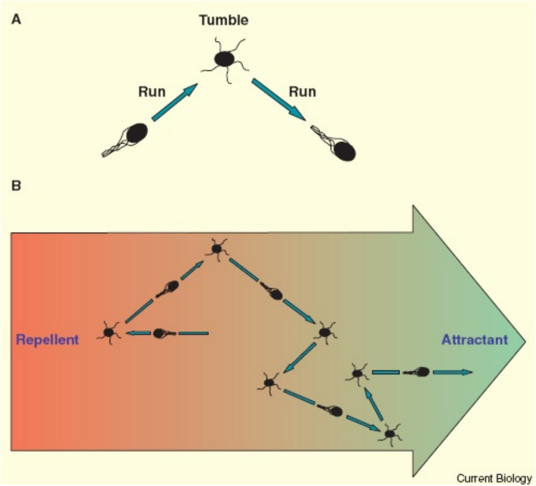
- two cilia performing non-reversible breast stroke



$\longrightarrow$ capable of swimming many cell-lengths per second

$\longrightarrow$ long-range perturbation of the flow (decreases as $O(\frac{1}{r})$ in $2D$, $O(\frac{1}{r^2})$ in $3D$)

Chemotaxis



⟶ on a long time scale each swimmer performs a **random walk with a bias towards favorable direction**

Coherent structures [Cisneros *et al.* '07], [Aranson *et al.* '07], ...

- self-organized coherent structures with the spatial scale exceeding the size of an individual swimmer
- collective velocity greater than the individual velocity
- weakly turbulent appearance of the flow: recirculations, vortices...

$\longrightarrow$ enhanced transport and mixing of particles, can be essential for nutriments resupplying

Impact of active particles on the viscosity of the suspension

- experiments [Sokolov & Aranson '07], [Rafaï *et al.*'10]
- analytical and numerical studies [Pedley '07], [Berlyand *et al.*'08], [Shelley *et al.*'09]

  Motility can strongly modify the effective viscosity of a suspension

Chemotaxis [Tuval *et al.*'05]

- bioconvection ▶|
- hydrodynamic instabilities ▶|

A simple model (1)

Swimmers are modelled as point particles $i_{i=1\ldots N}$ in a fluid domain Ω,

$\boldsymbol{u}$ and p velocity and pressure in the fluid

$\boldsymbol{x}_i$ and θ_i position and orientation of swimmer i

- Equilibrium of forces and torque on each body :

$$\begin{aligned} \boldsymbol{F}_{drag} + \boldsymbol{F}_{prop} + \boldsymbol{F}_{buoy} &= 0 \\ \boldsymbol{G} &= 0 \end{aligned}$$

- Stokes flow :

$$\begin{aligned} -\mu\Delta\boldsymbol{u} + \boldsymbol{\nabla} p &= \sum_{i=1\ldots N} - \boldsymbol{F}_{drag,i}\,\delta_{x_i} - \boldsymbol{F}_{prop,i}\,\delta_{y_i} \\ &= \sum_{i=1\ldots N} \boldsymbol{F}_{buoy}\delta_{x_i} + \boldsymbol{F}_{prop}(\delta_{x_i} - \delta_{y_i}) \end{aligned}$$

A simple model (2)

- Fluid :

$$\begin{cases} -\mu\Delta \boldsymbol{u} + \boldsymbol{\nabla} p = \boldsymbol{f}_f & \text{in } \Omega \\ \boldsymbol{\nabla}\cdot \boldsymbol{u} = 0 & \text{in } \Omega \end{cases}$$

with $\boldsymbol{f}_f = \sum_{i=1\dots N} \boldsymbol{F}_{buoy}\chi_i$ (only first order contributions,

regularization of dirac)

- Particle dynamics :

Faxen's law for spherical rigid bodies (radius a)

$$(\dot{\boldsymbol{x}}_i - \boldsymbol{u}(\boldsymbol{x}_i)) = \frac{1}{6\pi\mu a}\left(-\pi\mu a^3 \, \Delta \boldsymbol{u}(x_i) + \boldsymbol{F}_{buoy} + \boldsymbol{F}_p\right)$$

$$\dot{\theta}_i = \frac{1}{2}\,(\boldsymbol{\nabla} \times \boldsymbol{u})(\boldsymbol{x}_i)$$

- Dealing with congestion :

Finite size of particles is taken into account in order to compute non-elastic collisions.

A model for chemotaxis

Tumbling : Poisson process

T_{run} = duration of a Run $\sim \exp(\lambda)$

λ = Tumbling frequency : variable !

θ = new orientation $\sim U(0, 2\pi)$

- first model :

$$\lambda(c) \ = \ 1 \ - \ \epsilon \text{ Signe} \left(\frac{Dc}{Dt} \right), \quad \epsilon < 1$$

- a finer model ("memory" of the swimmer) :
[Locsei, 2007] :

$$\lambda(c) \ = \ 1 \ - \ \epsilon \text{ Signe} \left(\int_{t-\Delta t}^{t} c(s)\, g(t-s)\, ds \right)$$

where $g(s) = 1$ si $s \leq \Delta t/4$ et $g(s) = -1/3$ si $s > \Delta t/4$

A model for chemotaxis

Interaction with oxygen (oxygentaxis)

1. Convection-diffusion equation for oxygen :

$$\partial_t c \; + \; \boldsymbol{u} \cdot \nabla c \; - \; D_c \, \Delta c \; = \; - \, \kappa \, f(c) \, \chi_B \quad dans \; \Omega \, .$$

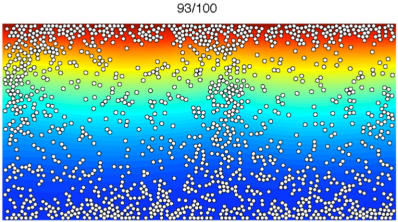
   c : oxygen concentration in the fluid,
   κ : consuming rate
   $f(c)$: modulation of the rate ($\rightarrow$ 0 when $c \rightarrow 0$, $\rightarrow 1$ when $c \rightarrow +\infty$).

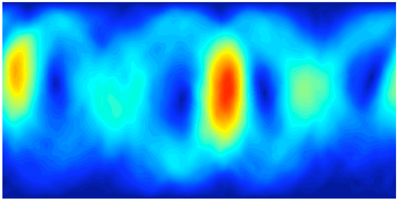
2. Modulation of the propulsion force intensity :

   $f_p \longrightarrow 0$ when $c \longrightarrow 0$

Simulating bioconvective phenomena

mise en évidence d'instabilités hydrodynamiques dues au gradient de densité





Simulating bioconvective phenomena

in a droplet (after the experiment by *Goldstein e.a., 2005*) :

boycott effect + hydrodynamic instabilities

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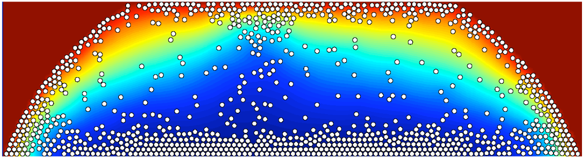
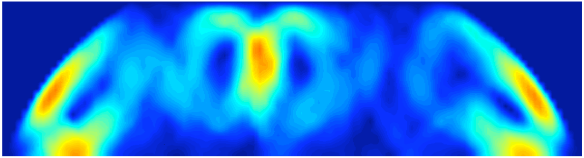




Introduction : from individual to collective dynamics

A simple microscopic model : pointlike particles

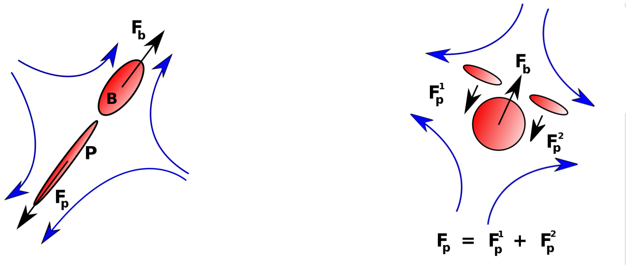
A model for chemotaxis

An accurate microscopic model : rigid particles

Ongoing work and perspectives

Full microscopic model

- Each swimmer = rigid ellipsoidal particle B + associated region in the fluid P (representing cilia or flagellar bundle) (not rigid !)
- Selfpropulsion : force of magnitude f_P and direction $\boldsymbol{\tau}$ acting on the fluid in region P and on the cell in B (in opposite direction !)



Isolated swimmer (force-free) : $\boldsymbol{F}_p = -f_p \boldsymbol{\tau} = -\boldsymbol{F}_b$

Volumic forces : $\boldsymbol{F}_p = \int_P \boldsymbol{f}_p \, d\boldsymbol{x}, \quad \boldsymbol{F}_b = \int_B \boldsymbol{f}_b \, d\boldsymbol{x}$

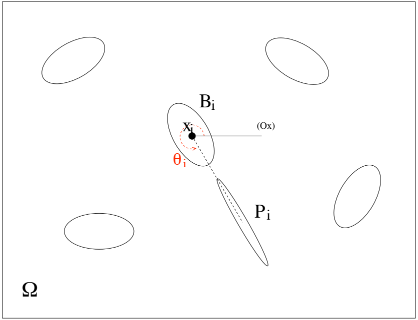
Fluid-structure interaction problem

Notations:

$\Omega \subset \mathbb{R}^2$: bounded and regular domain,

$(B_i)_{i=1...N}$: rigid inclusions in Ω, denoting the bodies of the swimmers,

$B = \bigcup_{i=1...N} B_i$ rigid domain,



$\boldsymbol{x}_i$ coordinates of the center of mass of B_i,

θ_i angle defining the position of the flagellum of B_i,

$\boldsymbol{V} = (\boldsymbol{V}_i = \dot{\boldsymbol{x}}_i) \in \mathbb{R}^{2N}$,

$\omega = (\omega_i = \dot{\theta}_i) \in \mathbb{R}^N$.

Fluid-structure interaction problem

- **Notations:**

$(\boldsymbol{u}, p)$	velocity and pressure fields defined in $\Omega \setminus \bar{B}$
$(\boldsymbol{V}, \omega)$	translational and rotational velocities of swimmers

- **Stokes fluid:**

$$\begin{cases} -\mu\Delta\boldsymbol{u} + \boldsymbol{\nabla} p = \boldsymbol{f}_f := \sum_{i=1}^{N} \boldsymbol{f}_{p_i}\, \chi_{P_i} & \text{in } \Omega \setminus \bar{B}, \\ \boldsymbol{\nabla}\cdot\boldsymbol{u} = 0 & \text{in } \Omega \setminus \bar{B}, \\ \boldsymbol{u} = 0 & \text{on } \partial\Omega, \\ \boldsymbol{u} = \boldsymbol{V}_i + \omega_i\,(\boldsymbol{x} - \boldsymbol{x}_i)^{\perp} & \text{on } \partial B_i,\ \forall i. \end{cases}$$

- **Forces equilibrium** (Newton's second law of motion)**:**

$$\begin{cases} \displaystyle\int_{B_i} \boldsymbol{f}_{b_i} - \int_{\partial B_i} \boldsymbol{\sigma}\cdot\boldsymbol{n} = 0, & \forall i, \\ \displaystyle\int_{B_i} (\boldsymbol{x} - \boldsymbol{x}_i)^{\perp}\cdot\boldsymbol{f}_{b_i} - \int_{\partial B_i} (\boldsymbol{x} - \boldsymbol{x}_i)^{\perp}\cdot(\boldsymbol{\sigma}\cdot\boldsymbol{n}) = 0, & \forall i. \end{cases}$$

The problem comes to **minimize the functional**

$$J(\tilde{\boldsymbol{u}}) \; = \; \mu \int_\Omega |\mathbb{D}(\tilde{\boldsymbol{u}})|^2 \; - \; \int_\Omega \boldsymbol{f} \cdot \tilde{\boldsymbol{u}}$$

on the subspace :

$$K_0 \cap K_\nabla = \left\{ \boldsymbol{u} \in H_0^1(\Omega) \; / \; \boldsymbol{\nabla} \cdot \boldsymbol{u} = 0, \; \mathbb{D}(\boldsymbol{u}) = 0 \; a.e. \; on \; B \right\}$$

with

$$\boldsymbol{f} = \sum_{i=1}^{N} \left(\boldsymbol{f}_{b_i} \chi_{B_i} + \boldsymbol{f}_{p_i} \chi_{P_i} \right).$$

$\rightarrow$ strong coupling of the problems on fluid and particles, without direct estimation of $\boldsymbol{\sigma} \cdot \boldsymbol{n}$.

Numerical method

Fictitious domain approach, in order to work with fixed cartesian meshes

- In 2D : **Penalty method** ([Peyla '04], [Lefebvre '05], ...) leads to unconstrained spaces:

Let $\varepsilon > 0$ be small (inverse of the "viscosity" of the solid phase)

Minimization problem is approached by a modified minimization problem :

$$\left\{ \begin{array}{l} \boldsymbol{u} \in K_{\nabla} \cap K_{\theta} \\ J(\boldsymbol{u}) \;=\; \min_{\tilde{\boldsymbol{u}} \in K_{\nabla} \cap K_{\theta}} J(\tilde{\boldsymbol{u}}) \end{array} \right. \approx \left\{ \begin{array}{l} \boldsymbol{u}_{\epsilon} \in K_{\nabla} \\ J_{\epsilon}(\boldsymbol{u}_{\epsilon}) \;=\; \min_{\tilde{\boldsymbol{u}} \in K_{\nabla}} J_{\epsilon}(\tilde{\boldsymbol{u}}) \end{array} \right.$$

where

$$J_{\epsilon}(\tilde{\boldsymbol{u}}) \;=\; J(\tilde{\boldsymbol{u}}) \;+\; \frac{1}{\epsilon} \int_{B} |\mathbb{D}(\tilde{\boldsymbol{u}})|^2$$

Proposition.

$$\boldsymbol{u}_{\epsilon} \longrightarrow \boldsymbol{u} \textit{ when } \epsilon \longrightarrow 0 \quad \textit{and} \quad \exists C > 0 \textit{ such that } \mid \boldsymbol{u}_{\epsilon} - \boldsymbol{u} \mid \leq C\epsilon$$

Numerical method

Fictitious domain approach, in order to work with fixed cartesian meshes

- In 2D : **Penalty method**

- In 3D : this **penalty method** is not efficient : bad conditioning of matrix so that only direct methods can be used + non-optimal convergence rate.

  Ongoing work (B. Fabrèges and B. Maury) :
  fast 3D solver for fluid - rigid particles interaction based on an optimal order fictitious domain method.

Particle dynamics and contact

Updating positions and orientations by evaluating $\boldsymbol{V}_i$ and ω_i and solving :

$$\boldsymbol{x}_i^{n+1} = \boldsymbol{x}_i^n + \Delta t\, \boldsymbol{V}_i, \qquad \theta_i^{n+1} = \theta_i^n + \Delta t\, \omega_i.$$

Contacts :
In principle no contact in finite time.
In practice (time discretization, inexact estimate of lubrication forces) : contact or overlapping between bodies may occur.

Contact algorithm : robust handling relying on purely non-elastic collisions.

= **projection of the velocities on a space of "admissible velocities"** (based on a granular flow approach [Maury '06])

Algorithm | Contact handling

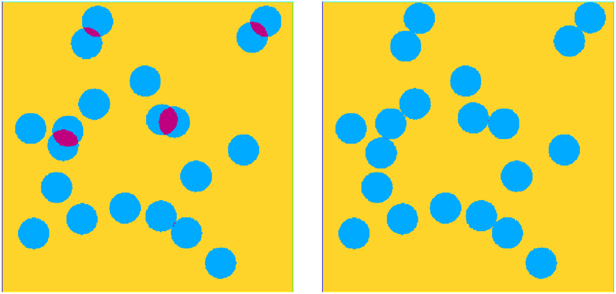


Figure: The contact algorithm applied to a set of circles

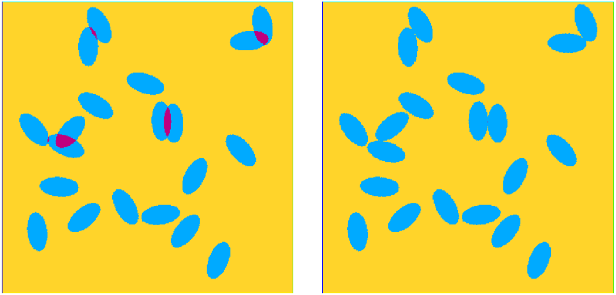


Figure: The contact algorithm applied to a set of ellipses

Hydrodynamics: individual dynamics

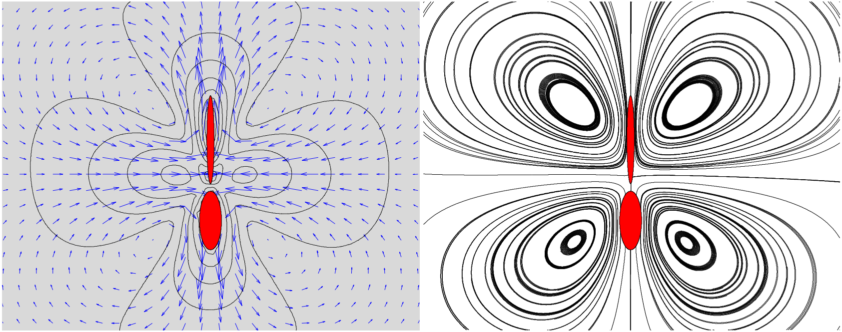


Figure: Pusher in a fluid at rest

Hydrodynamics: individual dynamics

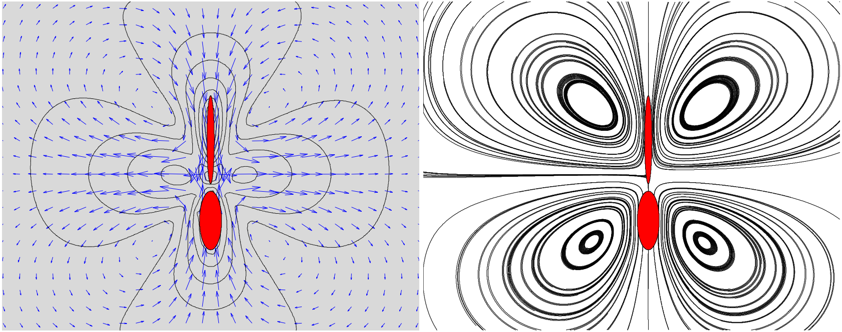


Figure: Puller in a fluid at rest

Hydrodynamics: individual dynamics

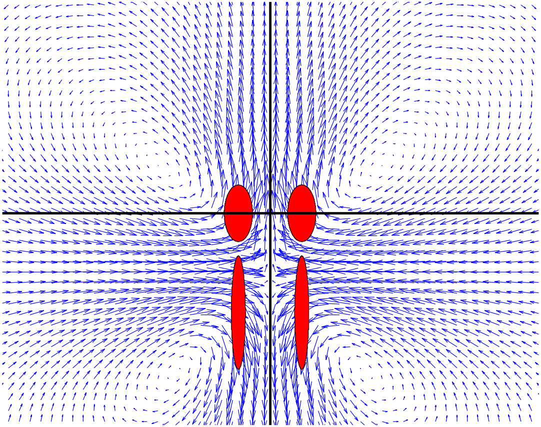


Figure: ▶| Two pusher side by side

Hydrodynamics: individual dynamics

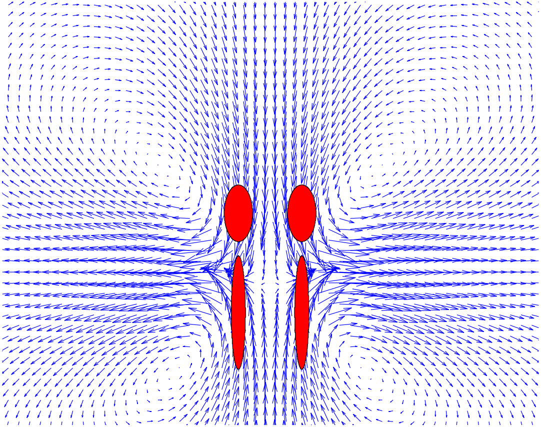


Figure: ▶|Two puller side by side

Hydrodynamics: collective dynamics

PUSHER

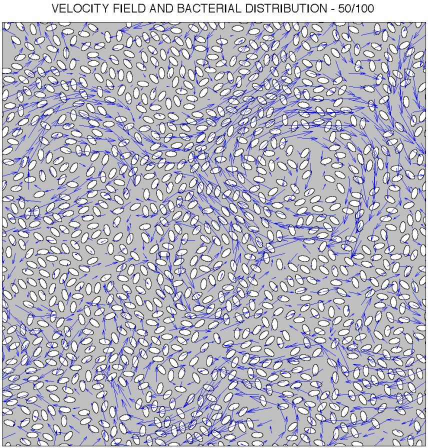
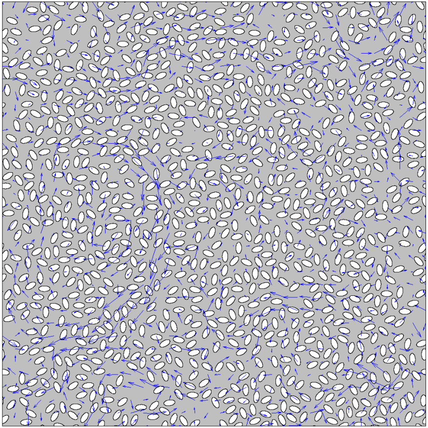


Figure: Dense suspension (solid fraction : 30%)

PULLER



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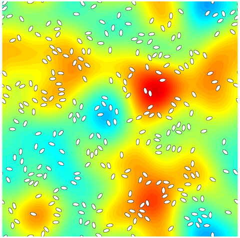


Correlation length of collective motion can exceed the size of individual cells by more than an order of magnitude.

- weak turbulence
- persistence of coherent structures
- ▶|

Velocity correlation

$$\mathcal{I}(r,t) \quad := \quad \frac{\left\langle \boldsymbol{u}(\boldsymbol{x},t)\cdot\boldsymbol{u}(\boldsymbol{x}+re^{i\theta},t)\right\rangle_{\boldsymbol{x},\theta} - \langle \boldsymbol{u}(\boldsymbol{x},t)\rangle_{\boldsymbol{x}}^2}{\langle \boldsymbol{u}(\boldsymbol{x},t)^2\rangle_{\boldsymbol{x}} - \langle \boldsymbol{u}(\boldsymbol{x},t)\rangle_{\boldsymbol{x}}^2}$$

$$\mathcal{J}(\boldsymbol{x},t) \quad := \quad \frac{\langle \boldsymbol{u}(\boldsymbol{x},s)\cdot\boldsymbol{u}(\boldsymbol{x},s+t)\rangle_s}{\langle \boldsymbol{u}(\boldsymbol{x},s)^2\rangle_s}$$

Hydrodynamics: collective dynamics

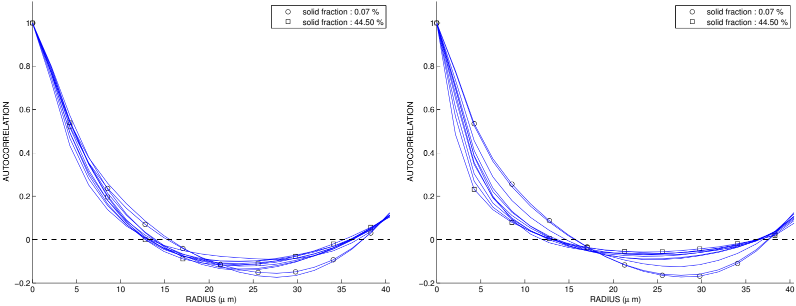


Figure: Space correlation functions for suspensions of pushers (left) and pullers (right)

- constant size of coherent structures already reached for $\phi = 8\%$
- typical size $\sim$ 5 times particle size

Hydrodynamics: collective dynamics

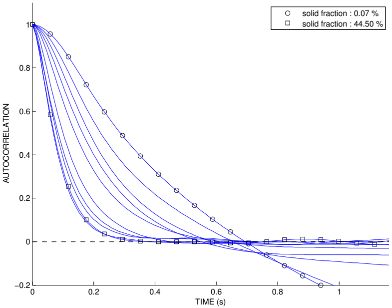
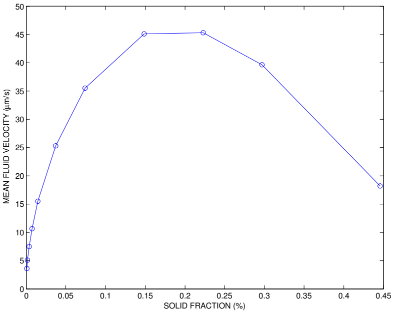
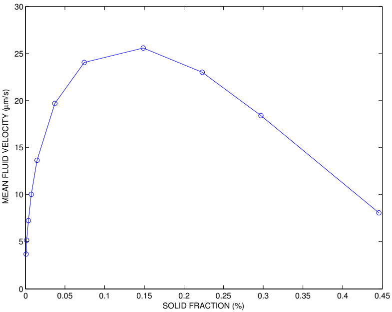


Figure: Time correlation functions for suspensions of pushers (left) and pullers (right)

Numerical results (2/4) | Hydrodynamics: collective dynamics



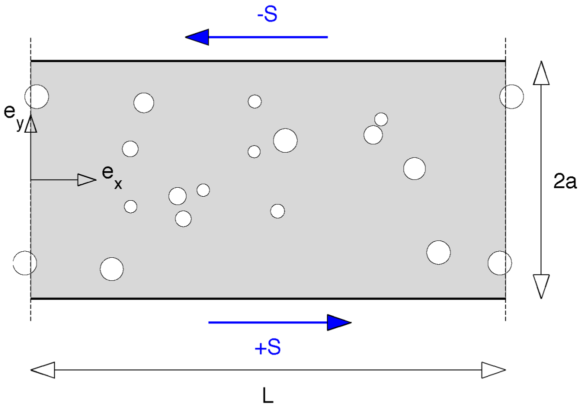


- average velocity increases with the solid fraction
  above a critical concentration it decreases, due to congestion.

Rheology

Effective viscosity:

- resistance of a fluid which is being deformed by a shear stress
- macroscopic observable quantity measured by a rheometer:



Effective viscosity

- Forces exerted by the fluid on the walls:

$$F_{|y=+a} = \int_{y=+a} \mathbf{e}_x \cdot \sigma \cdot (-\mathbf{e}_y), \quad F_{|y=-a} = \int_{y=-a} \mathbf{e}_x \cdot \sigma \cdot (+\mathbf{e}_y)$$

- In case of a Newtonian fluid, the exact solution is

$$\boldsymbol{u}(x,y) = -S\frac{y}{a}\mathbf{e}_x, \qquad p(x,y) = 0,$$

  we have

$$F_0 := F_{|y=+a} - F_{|y=-a} = 2\mu\frac{S}{a}L.$$

- Therefore, the effective viscosity can be defined as

$$\mu_{\mathrm{eff}} = \frac{a}{2LS}F_0, \quad \text{with } F_0 := \int_{\{y=+a\}\cup\{y=-a\}} \mathbf{e}_x \cdot \sigma \cdot (-\mathbf{e}_y)$$

Effective viscosity : PUSHERS

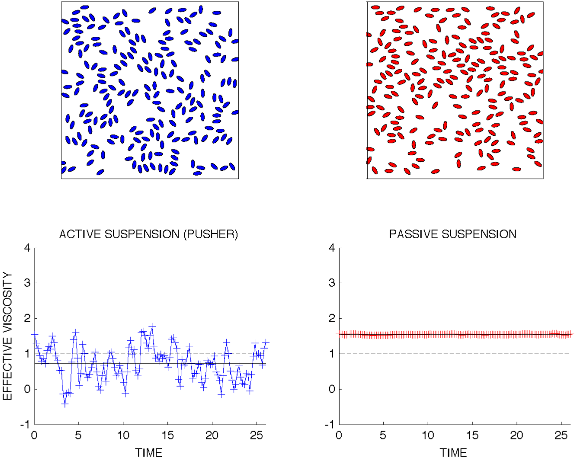
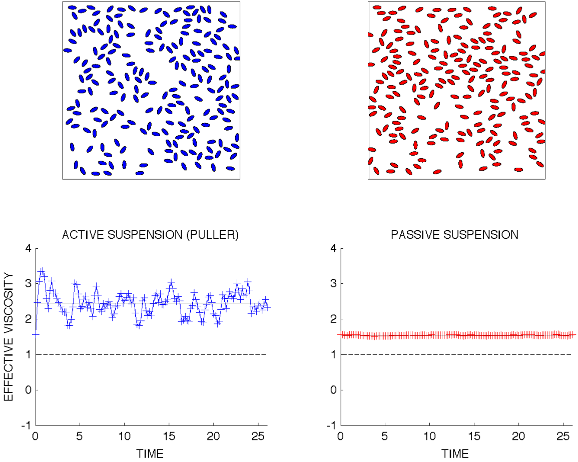


Figure: Active suspension (l.) vs passive suspension (r.)

Effective viscosity : PULLERS



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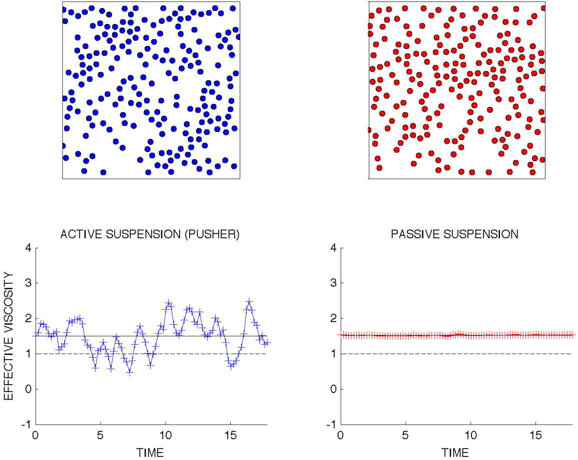
Effective viscosity : PULLERS



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Effective viscosity : PULLERS

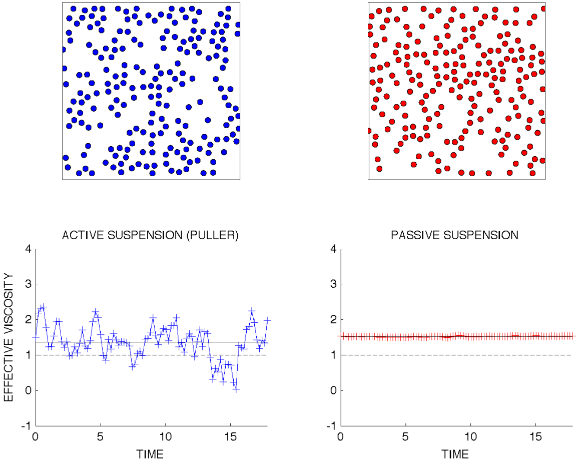


Figure: Active suspension (l.) vs passive suspension (r.)

Effective viscosity

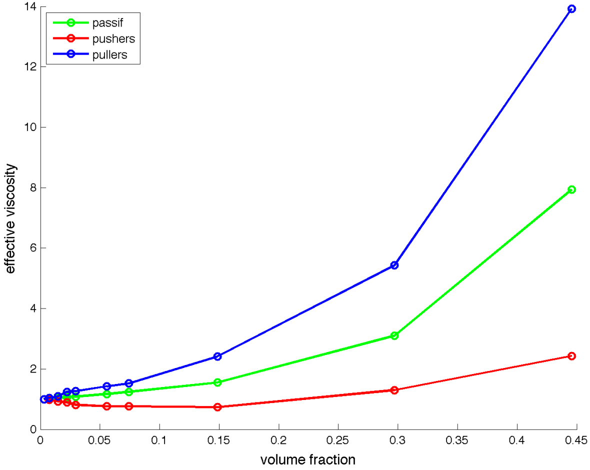


Figure: Effective viscosity η/η_0 with respect to the solid fraction

Representing cilia and flagella

Phd work by Loic Lacouture (Paris Sud)

- Numerical analysis of the FE solution of elliptic problems with singular source term :
  - Solution of Stokes equations with dirac mass source term (2d and 3d) $\rightarrow$ **singular solution** $\rightarrow$ does not enter in the classical framework of finite element solutions for elliptic problems.
  - Numerical analysis shows that the convergence rate is not optimal.
  - Development of a **numerical method allowing to recover the optimal convergence rate** by extracting the singularity.

- Application to the micro-swimmer model :
  - Cilia and flagella can be seen as one-dimensional (infinitely thin) structures in a 3d flow in the asymptotic : thickness $\epsilon \rightarrow 0$ while the resultant force $\boldsymbol{F}_{hydro}$ they apply on the fluid remains constant.

Representing cilia and flagella

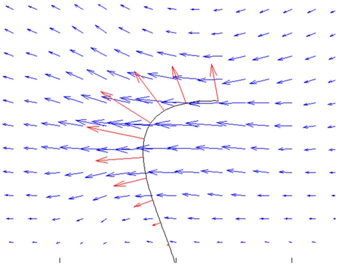
Prescribed description of the position of the cilium → hydrodynamic force $\boldsymbol{f}$ deduced using slender body theory

Here : mathematical formulation of the tracheal cilium beat cycle given by Fulford and Blake (1986)

We solve :

$$\left\{ \begin{array}{rcl} -\mu\Delta\boldsymbol{u} + \nabla p & = & \boldsymbol{f}\delta_S \\ \nabla\cdot\boldsymbol{u} & = & 0 \end{array} \right.$$

with $\boldsymbol{f}$ density of force distributed over the cilium.



Towards 3D simulations

3D simulations (B. Fabreges, PhD supervised by B. Maury) ▶|

Thank you for your attention