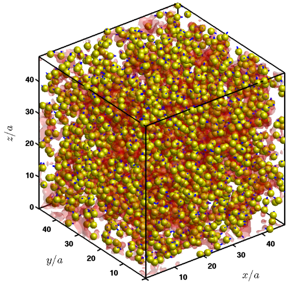
Large populations of swimming micro-organisms and individual modelling



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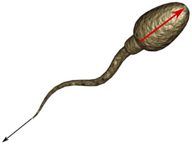
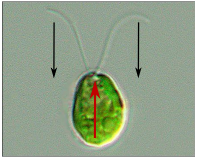
motimo

Université de Toulouse

Contents

What is a microswimmer ?

- Self-locomoting microorganism,
- Characteristic length $L \sim \mu$m
- Two types of swimming gaits:

Pushers	Pullers
propulsion from the aft part	traction from the fore part
	
Spermatozoa	*Chlamidomonas Reinhardtii*

Swimming dynamics

Example for a spermatozoon (pusher)

Low Reynolds number: $\text{Re} = \dfrac{\text{Inertial force}}{\text{Viscous force}} = \dfrac{\rho U L}{\eta}$

ρ	η	U	L
Density of semen	Vicosity of semen	Swimming velocity	Length
$10^3 kg.m^{-3}$	$10^{-3} N.s.m^{-2}$ at 37°C	$\approx 100\mu m.s^{-1}$	$\approx 60\mu m$

$$\Rightarrow \mathbf{Re} = 10^{-3} \approx 0$$

$$\sum \mathbf{F} = \mathbf{0}$$

Swimming dynamics

Example for a spermatozoon

$$\sum \mathbf{F} = \mathbf{0}$$

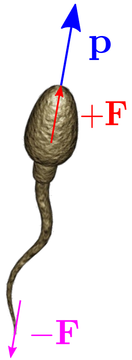
$$\Downarrow$$

$$\text{Head drag} + \text{Flagellum thrust} = \mathbf{0}$$

$$\Downarrow$$

Microswimmer =Moving symmetric force dipole (Stresslet)

$$\mathbf{D}_{sw} = \underbrace{-\frac{L}{2}F}_{S_{push}}\left(\mathbf{p}\otimes\mathbf{p} - \frac{1}{3}\mathbf{I}\right)$$



Swimming dynamics

Example for a puller

$$\sum \mathbf{F} = \mathbf{0}$$

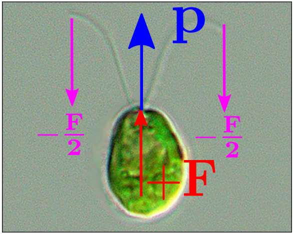
$$\Downarrow$$

$$\text{Head drag} + \text{Cilia thrust} = \mathbf{0}$$

$$\Downarrow$$

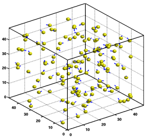
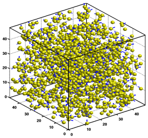
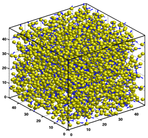
Microswimmer =Moving symmetric force dipole (Stresslet)

$$\mathbf{D}_{sw} = \underbrace{+\frac{L}{2}F}_{S_{pull}} \left(\mathbf{p} \otimes \mathbf{p} - \frac{1}{3}\mathbf{I} \right)$$



Interactions between swimmers

- Present work : **steric** and **hydrodynamic interactions**,
- Effects of hydrodynamic interactions depend on :
  - the swimming gait,
  - swimmer's geometry,
  - swimmer volumic fraction c.

Dilute	Semi-dilute	Concentrated
$c < 0.05$	$c \approx 0.05 - 0.15$	$c > 0.15$
		

Suspension dynamics

Swimmers provide extra-stress contribution to the fluid

$$\mathbf{\Sigma} = \frac{N_p}{V} S \left(\langle \mathbf{p} \otimes \mathbf{p} \rangle - \frac{1}{3}\mathbf{I} \right)$$

where S depends on their size/swimming gait

$\frac{N_p}{V}$ depends on their concentration

↓

Fluid disturbances

↙ ↘

Reorientations ↔ Concentration fluctuations

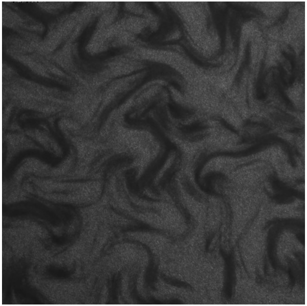
↕ ↕

Orientation correlations — Position correlations

Coherent motion / Suspension instability

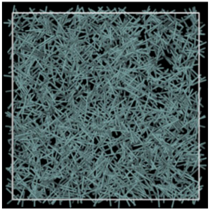
Examples of coherent motion

Mammal Semen:

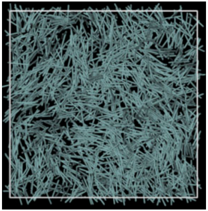


Highly concentrated $2000 \times 2000 \times 150 \mu m^3$ ram sperm sample, observed with phase contrast microscopy.

Computer simulations:



t = 0



t = 50

3D periodic simulations of active rods in the semi-dilute regime $(c \approx 0.05)$. Birth of collective motion from isotropic random state. [Saintillan et Shelley 2012]

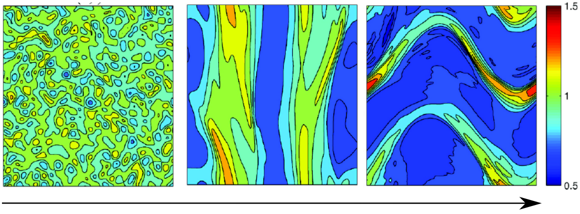
Macroscopic parameters to characterize coherent motion

1. density parameter

[Saintillan & Shelley PRL 2008, Baskaran & Marchetti PNAS 2009, Ezhilan *et al.* POF 2013]

$$c(\mathbf{x}, t) = \sum_{\alpha=1}^{N_p} \delta(\mathbf{x} - \mathbf{Y}^{\alpha}(t)) / N_p .$$

$c(\mathbf{x}, t)$



Concentration fluctuations: isotropy → unsteady ordered state [Saintillan & Shelley PRL 2008].

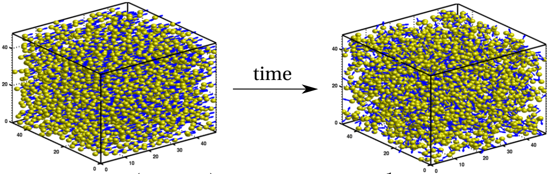
Macroscopic parameters to characterize coherent motion

1. density parameter,
2. polar order parameter

[Saintillan & Shelley PRL 2007, Ishikawa *et al.* JFM 2008, Baskaran & Marchetti 2009, Evans *et al.* PRL 2011]

$$P(t) = \left| \sum_{\alpha=1}^{N_p} \mathbf{p}^{\alpha}(t) \right| / N_p \quad \text{or} \quad \bar{\mathbf{p}}(t) = \sum_{\alpha=1}^{N_p} \mathbf{p}^{\alpha}(t) / N_p .$$

Polar order | Isotropy



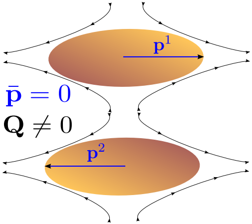
$P = 1, \bar{\mathbf{p}} = (1,\ 0,\ 0)$ | $P \sim \frac{1}{\sqrt{N_p}}, \bar{\mathbf{p}} = (0,\ 0,\ 0)$

Macroscopic parameters to characterize coherent motion

1. density parameter,
2. polar order parameter,
3. nematic order parameter (same structure as swimming dipole $\boldsymbol{\Sigma}$)

[Simha & Ramaswamy PRL 2002, Saintillan & Shelley PRL 2007-2008 JRSI 2012, Baskaran & Marchetti PNAS 2009]

$$Q_{ij}(t) = \sum_{\alpha=1}^{N_p} \left(p_i^\alpha p_j^\alpha - \frac{1}{3}\delta_{ij} \right) / N_p .$$



The Force Coupling Method

Force coupling method (FCM) validated for **passive particles** :

- Designed by Maxey & Patel 2001
  [Maxey & Patel IJMF 2001]
- Validations for suspensions of passive particles up to $c = 0.5$
  [Lomholt IJMF 2002, Climent IJMF 2003, Abbas POF 2006, Yeo JCP 2010]
- Include particle-wall interactions
  [Lomholt JCP 2003, Dance JCP 2003, Yeo JFM 2012]
- Suited for large populations $\sim \mathcal{O}(10^3)$
  [Yeo JCP 2010]
- Detailed short-range hydrodynamic interactions: finite size effects + lubrication
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What about active particles ?

Governing Equations

Stokes equations (Re $\approx$ 0) :

$$\begin{cases} \nabla \cdot \mathbf{u}(\mathbf{x},t) & = & 0 \\ 0 & = & -\nabla p(\mathbf{x},t) + \mu \triangle \mathbf{u}(\mathbf{x},t) + \mathbf{f}(\mathbf{x},t) \end{cases}$$

whith

- $\mathbf{u}(\mathbf{x},t)$: fluid velocity field,
- $p(\mathbf{x},t)$: pressure field,
- $\mathbf{f}(\mathbf{x},t)$: forcing term, account for the presence of swimmers in the fluid,
- μ : fluid viscosity,

Forcing ?

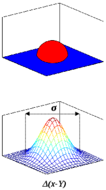
Question :

How to correctly model the forcing term $\mathbf{f}(\mathbf{x}, t)$ due the presence of swimmers ?

Method (1/5)

- 3D Gaussian enveloppe,

$$\Delta(\mathbf{x}, \sigma) = \frac{1}{2\pi\sigma^2} \exp\left(-\frac{|\mathbf{x}|^2}{2\sigma^2}\right),$$



- Distribution of forces **F** and dipoles **D**

$$f_i(\mathbf{x}, t) = \sum_{\alpha=1}^{N_p} \left(F_i^\alpha \Delta_F \left(\mathbf{x} - \mathbf{Y}^\alpha(t), \sigma_F\right) + D_{ij}^\alpha \frac{\partial}{\partial x_j} \Delta_D \left(\mathbf{x} - \mathbf{Y}^\alpha(t), \sigma_D\right) \right)$$

  - $\mathbf{Y}^\alpha$: position of particle α,
  - $\mathbf{F}^\alpha = \mathbf{F}^\alpha_{lub} + \mathbf{F}^\alpha_{steric}$: lubrication + steric forces,
  - $\mathbf{D}^\alpha = \mathbf{D}^\alpha_r + \mathbf{D}^\alpha{}_{sw}$: dipole to resist strain + swimming dipole.

Method (2/5)

- $\mathbf{D}^{\alpha} = \mathbf{D}_r^{\alpha} + \mathbf{D}^{\alpha}{}_{sw}$: dipole to resist strain + swimming dipole.
- $\mathbf{D}_r^{\alpha}$ ensures no deformation within the particle:

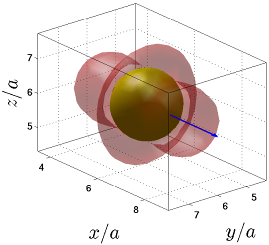
$$\int_{\mathbb{R}^3} \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \Delta_D \left(\mathbf{x} - \mathbf{Y}^{\alpha}(t)\right) d^3\mathbf{x} = 0$$

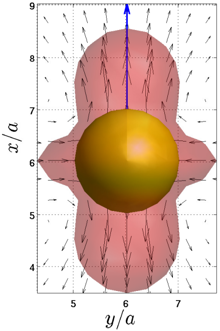
- Iteratively solved linear system

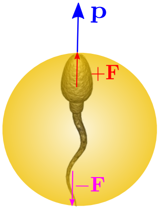
$$\mathcal{L}\mathbf{D}_r = \mathcal{E}.$$

Method (3/5)

- Velocity perturbations $\mathbf{u}(\mathbf{x}, t)$ induced by $f_i(\mathbf{x}, t)$







Method (4/5)

- Swimmer induced velocity $\mathbf{V}^{\alpha}_{ind}$ and rotations Ω^{α}: averaging $\mathbf{u}(\mathbf{x}, t)$

$$\mathbf{V}^{\alpha}_{ind}(t) = \int_{\mathbb{R}^3} \mathbf{u}(\mathbf{x}, t)\Delta_M \left(\mathbf{x} - \mathbf{Y}^{\alpha}(t)\right) d^3\mathbf{x}$$

$$\Omega^{\alpha}_i(t) = \int_{\mathbb{R}^3} \epsilon_{ijk} \frac{\partial u_k}{\partial x_j}(\mathbf{x}, t)\Delta_D \left(\mathbf{x} - \mathbf{Y}^{\alpha}(t)\right) d^3\mathbf{x}$$

- Total swimmer translational velocity

$$\mathbf{V}^{\alpha}_{tot} = \mathbf{V}^{\alpha}_{ind} + \mathbf{V}^{\alpha}_{sw}$$

$\mathbf{V}^{\alpha}_{sw}$: intrinsic swimming velocity

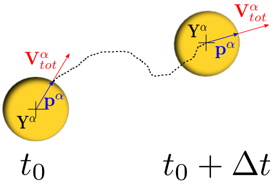
$$\mathbf{V}^{\alpha}_{sw} = V^{\alpha}_{sw}\mathbf{p}^{\alpha}.$$

Method (5/5)

- Swimmers trajectories and orientations time-integrated (Adam-Bashforth 4 scheme)

$$\frac{d\mathbf{Y}^{\alpha}}{dt} = \mathbf{V}^{\alpha}_{tot}$$

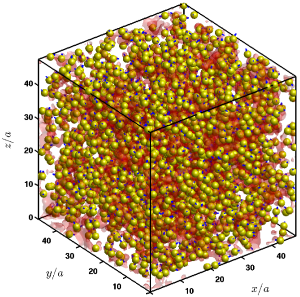
$$\frac{d\mathbf{p}^{\alpha}}{dt} = \Omega^{\alpha} \times \mathbf{p}^{\alpha}$$



- New set of forces and dipoles distributed over the new positionned Gaussian enveloppes.

Simulation configurations

- Spherical pushers or pullers with radius a,
- Periodic box $V \approx (48a)^3$,
- Concentrations $c = 0.05 - 0.3 \rightarrow N_p = 1132 - 7992$,
- Stokes solver: P3DFFT (FFTW3) parallelized with MPI.



$N_p = 2664$, $c = 0.1$.

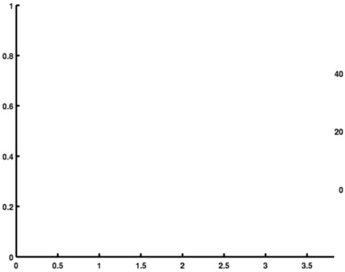
Stability of polar order

Goal

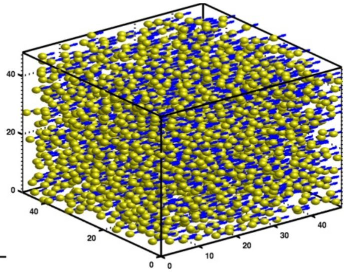
Reach isotropic state from polar order as pedicted by theories and previous computations:

$$P = 1 \rightarrow P \sim {}^{1}/\sqrt{N_p} \quad \text{or} \quad \bar{\mathbf{p}} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \rightarrow \bar{\mathbf{p}} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$P(t)$

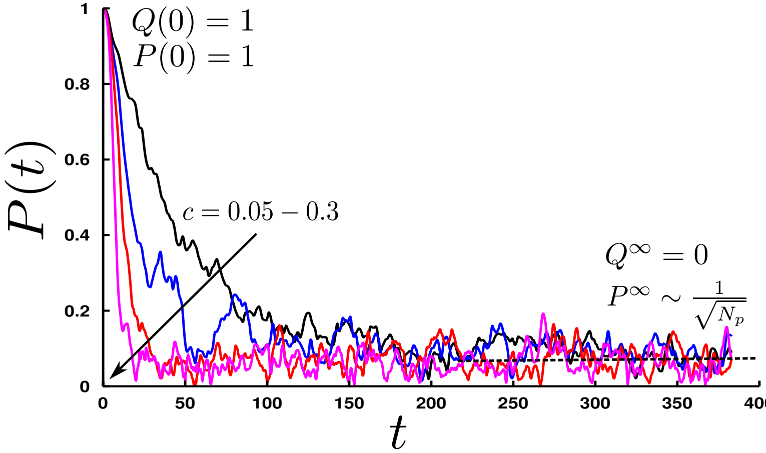


(a) $P(t)$, $c = 0.1$, $N_p = 2664$.

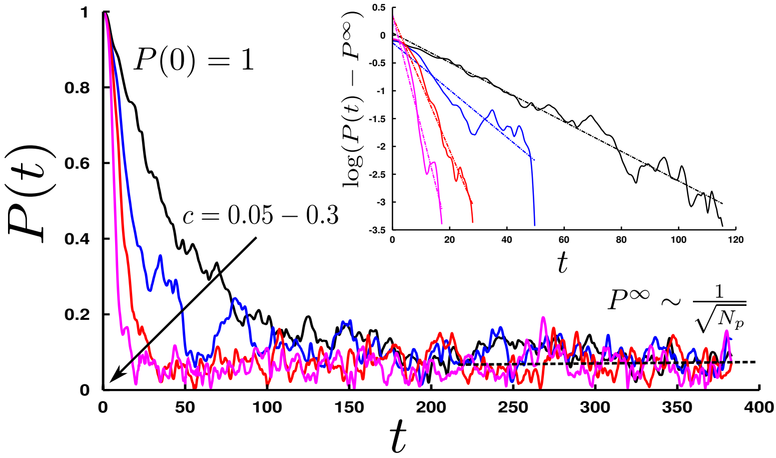


(b) Visualisation

Stability of polar order



Stability of polar order



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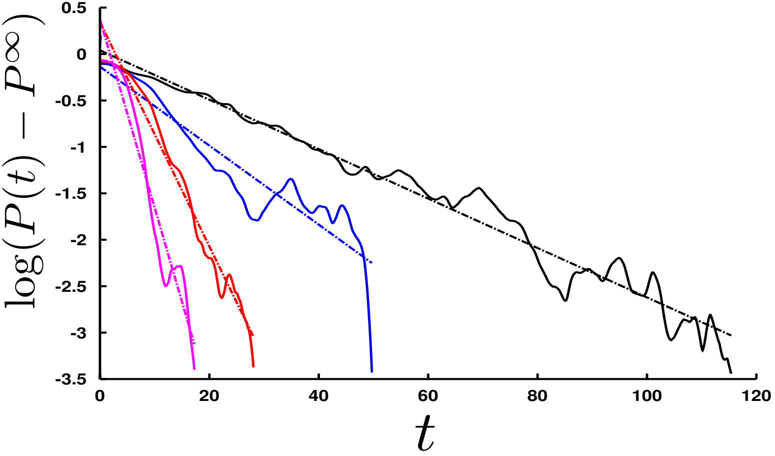
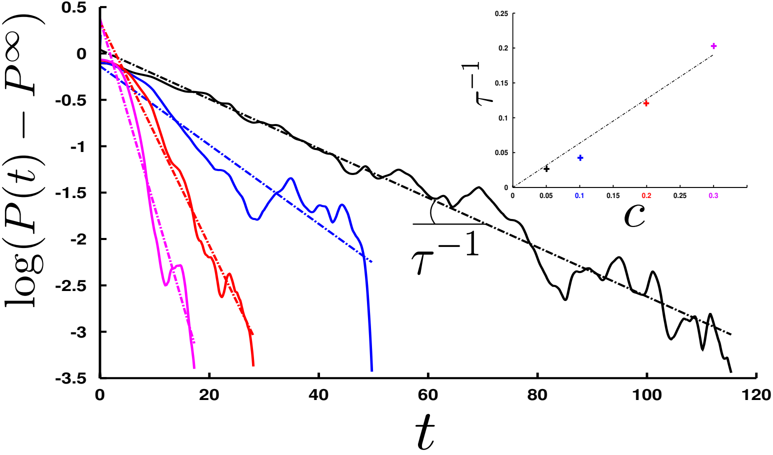
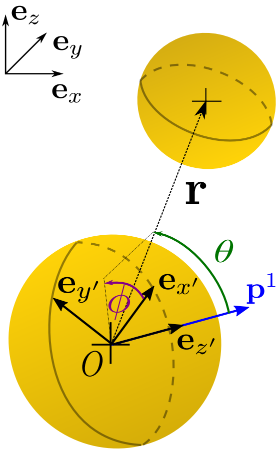


Stability of polar order

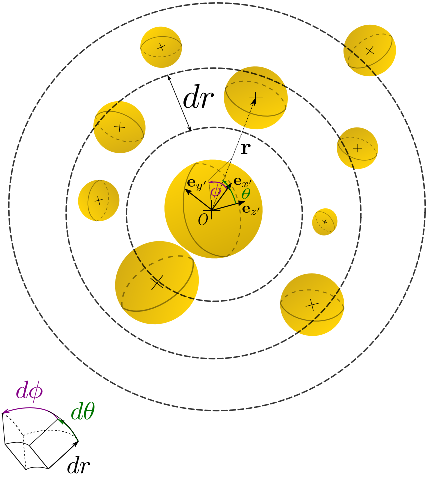


Correlations



- (r, θ, ϕ),
- $\mathbf{r}$: neighbour position relative to local origin,

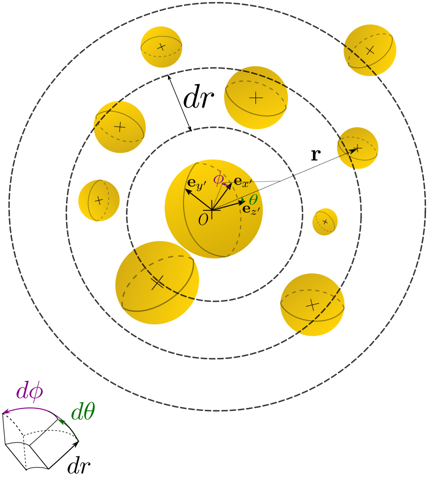
Correlations



Pair distribution function $\mathcal{P}(r, \theta, \phi)$:

likelihood of finding a neighbour at the position (r, θ, ϕ), with a swimmer of radius a at the local origin.

Correlations



Pair distribution function $\mathcal{P}(r, \theta, \phi)$:

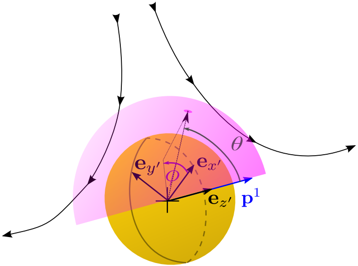
likelihood of finding a neighbour at the position (r, θ, ϕ), with a swimmer of radius a at the local origin.

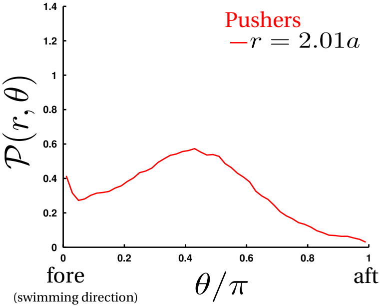
$$\mathcal{P}(r, \theta) = \int_0^{2\pi} \mathcal{P}(r, \theta, \phi) d\phi$$

Position correlations, $c = 0.2$

Pushers:

- Near field ($r = 2.01a$):

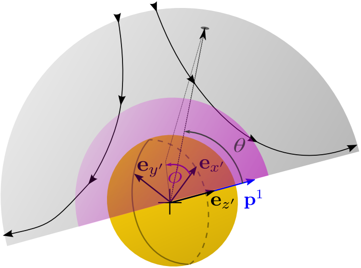


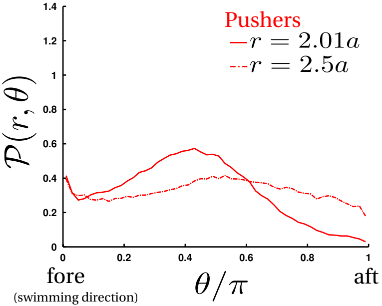


Position correlations, $c = 0.2$

Pushers:

- Far field ($r = 2.5a$):

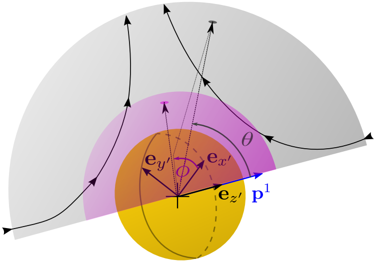


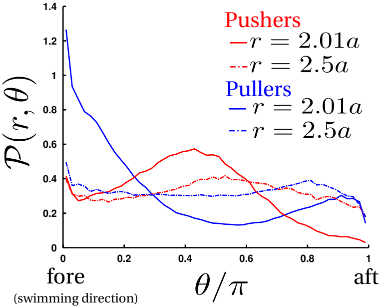


Position correlations, $c = 0.2$

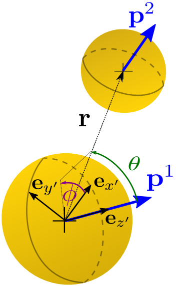
Pullers:

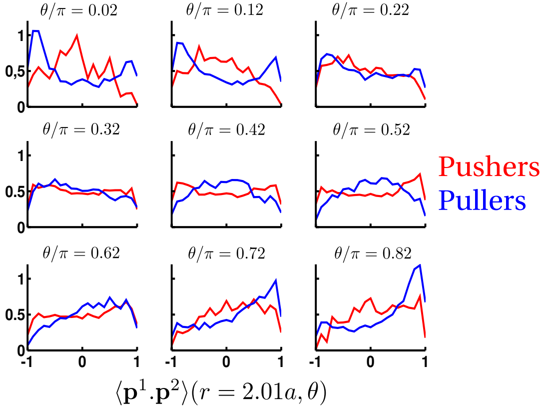
- Near and far field.



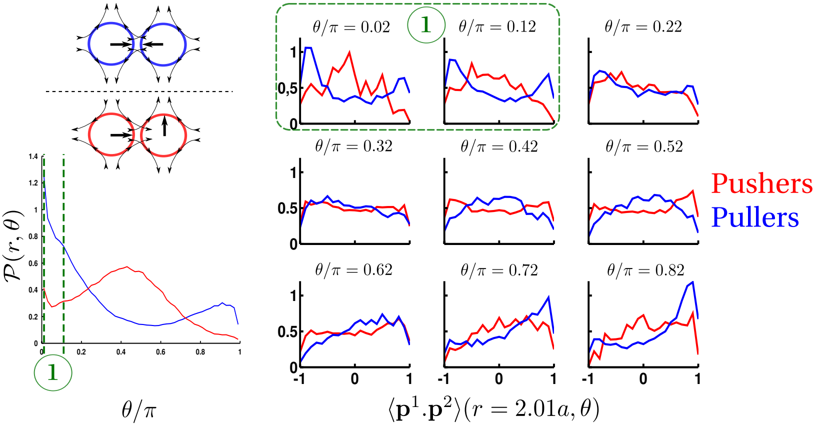


Orientation correlations, $c = 0.2$

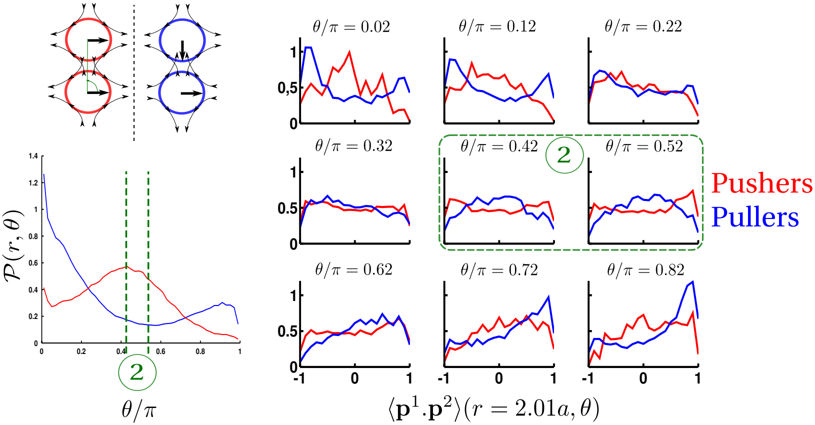




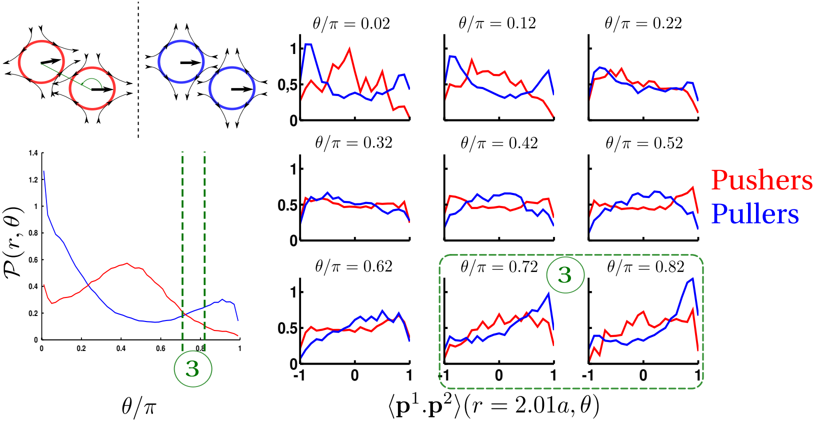
Orientation correlations, $c = 0.2$



Orientation correlations, $c = 0.2$



Orientation correlations, $c = 0.2$

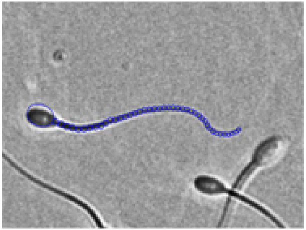


Major Insights

- Extension of FCM to active suspensions,
- Up to 7992 swimmers,
- No large scale coherent motion for spherical swimmers,
- Polar order relaxation time scales with c^{-1},
- Position and orientation correlations on individual scale,
- Correlations highly depend on swimming gait.

Goals

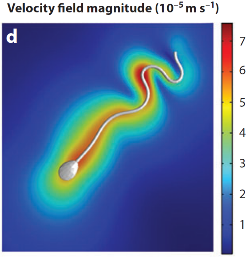
- Build a simple model to reproduce sperm swimming gait depending on its internal properties,
- Understand impact of chemical substrates on flagellum mechanical properties,
  - Comparison with I3S/INRA segmented images,
  - Flagellum mechanical parameter calibration using inverse modelling,



(c) I3S segmentation

How to proceed ?

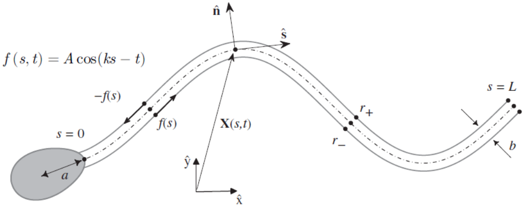
- Modelling approach:
  - fluid/structure interactions,



[Smith *et al.* JFM 2009]

How to proceed ?

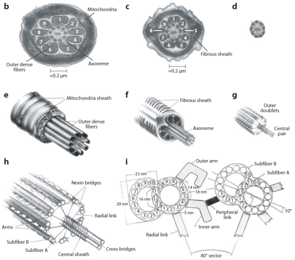
- Modelling approach:
  - fluid/structure interactions,
  - flagellum dynamics (i.e. active mechanical forcing),



[Gadhela *et al.* JRSI 2010]

How to proceed ?

- Modelling approach:
    - fluid/structure interactions,
    - flagellum dynamics (i.e. active mechanical forcing),
    - elastic properties (Young's Modulus E [Pa], shear modulus G [Pa]).



[Gaffney *et al.* ARFM 2011]

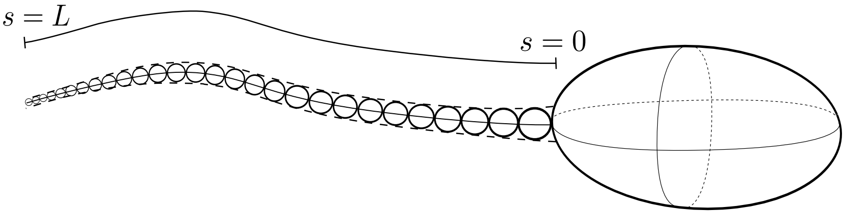
How to proceed ?

- Modelling approach:
  - fluid/structure interactions,
  - flagellum dynamics (i.e. active mechanical forcing),
  - elastic properties (Young's Modulus E [Pa], shear modulus G [Pa]).

Bead Model

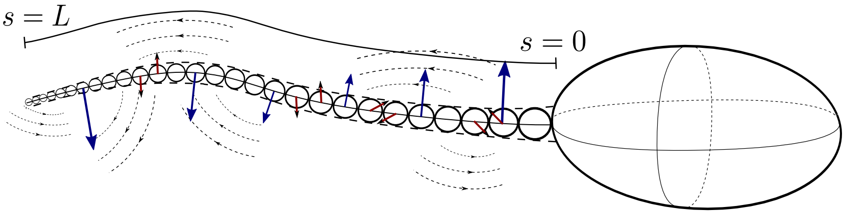
Principle

- Rigid/flexible body made up of N_b bonded spheres,



Principle

- Rigid/flexible body made up of N_b bonded spheres,
- Fluid/structure interaction uncoupled:
  - fluid: hydrodynamic interactions between beads,
  - body: internal contact and elastic forces/torques.



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$$\underbrace{\mathbf{V}}_{\text{Velocities}} = \underbrace{M}_{\text{Hydro}} \left(\underbrace{\mathcal{F}}_{\text{Elastic}} + \underbrace{\mathcal{F}^c}_{\text{Contact}} \right) \tag{1}$$

Principle

- Rigid/flexible body made up of N_b bonded spheres,
- Fluid/structure interaction uncoupled:
  - fluid: hydrodynamic interactions between beads,
  - body: internal contact and elastic forces/torques.
- Flexible:
  - any geometry,
  - adjustable precision on body mechanics or hydrodynamics.

Applications

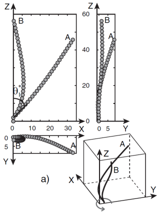
- Bead model applications:
  - Fibers/Polymers,

    [Yamamoto & Matsuoka JChemPhys 1992,

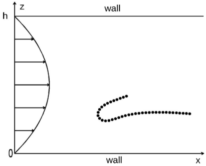
    Skjetne *et al.* JChemPhys 1997,

    Joung *et al.* JNonNewtonianFM 2001,

    Yamanoi *et al.* JNonNewtonianFM 2011]



Rotating filament [Manghi *et al.* PRL 2006].



Sheared fiber [Slowicka *et al.* JChemPhys 2012].

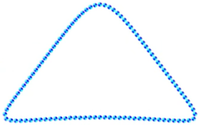
Applications

- Bead model applications:
  - Fibers/Polymers,
  - Microorganisms,

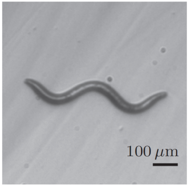
    [Lowe JRSI 2003,

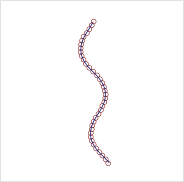
    Swan *et al.* POF 2011,

    Bilbao *et al.* POF 2013]



Amoeba [Swan *et al.* POF 2011].





Nematode [Bilbao *et al.* POF 2013].

Applications

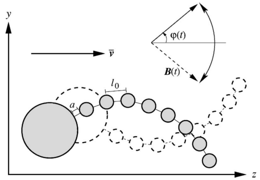
- Bead model applications:
  - Fibers/Polymers,
  - Microorganisms,
  - Artificial microswimmers,

    [Gauger and Stark PRE 2006,

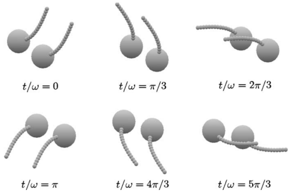
    Keaveny and Maxey JFM 2008,

    Keaveny and Maxey PRE 2008,

    Swan *et al.* POF 2011].



Magnetic swimmer [Gauger and Stark PRE 2006].

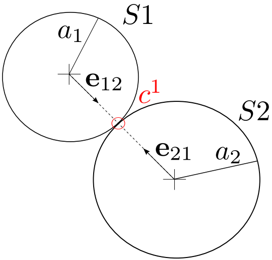


Comoving magnetic swimmers [Keaveny and Maxey PRE 2008].

Kinematic Constraints: Gears Model

- Connectivity and the no-slip condition between beads.
- Kinematic vectorial constraint

$$\mathbf{C}^1(\underbrace{\dot{\mathbf{r}}_1,\omega_1}_{\mathbf{V}_1},\underbrace{\dot{\mathbf{r}}_2,\omega_2}_{\mathbf{V}_2}) = \dot{\mathbf{r}}_1 - a_1\mathbf{e}_{12}\times\omega_1 - \dot{\mathbf{r}}_2 - a_2\mathbf{e}_{21}\times\omega_2 = 0, \quad (2)$$



Kinematic Constraints: Gears Model

- $\mathbf{C}^1$ is linear in $\dot{\mathbf{r}}_1,\ \omega_1,\ \dot{\mathbf{r}}_2$ and ω_2

$$\mathbf{C}^1(\underbrace{\mathbf{V}_1,\mathbf{V}_2}_{\mathbf{V}}) = \mathbf{J}^1\mathbf{V} \tag{3}$$

$\mathbf{J}^1$ is the Jacobian matrix of $\mathbf{C}^1$:

$$J^1_{kl} = \frac{\partial C^1_k}{\partial V_l},\ \ k = 1..3,\ \ l = 1..6 \tag{4}$$

$$\begin{aligned} \mathbf{J}^1 &= \begin{bmatrix} \mathbf{I}_3 & -a_1\mathbf{e}^{\times}_{12} & -\mathbf{I}_3 & a_2\mathbf{e}^{\times}_{21} \end{bmatrix} \\ &= \begin{bmatrix} \mathbf{J}^1_1 & \mathbf{J}^1_2 \end{bmatrix} \end{aligned} \tag{5}$$

where

$$\mathbf{e}^{\times} = \begin{pmatrix} 0 & -e_3 & e_2 \\ e_3 & 0 & -e_1 \\ -e_2 & e_1 & 0 \end{pmatrix} \tag{6}$$

Kinematic Constraints: Gears Model

- Total Jacobian matrix $\mathbf{J}_{tot}$, block bi-diagonal

$$\mathbf{J}_{tot} = \begin{pmatrix} \mathbf{J}_1^1 & \mathbf{J}_2^1 & & & \\ & \mathbf{J}_2^2 & \mathbf{J}_3^2 & & \\ & & \ddots & \ddots & \\ & & & \mathbf{J}_{N_p-1}^{N_p-1} & \mathbf{J}_{N_p}^{N_p-1} \end{pmatrix} \quad (7)$$

$\mathbf{J}_\beta^\alpha$: 3×6 Jacobian of vectorial constraint α for bead β.

- Kinematic constraints for the whole assembly:

$$\mathbf{J}_{tot}\mathbf{V} = \mathbf{0} \quad (8)$$

$\mathbf{V}$: generalized velocities of each bead.

Contact Forces

- Euler-Lagrange formalism:

$$\mathcal{F}^c = \begin{pmatrix} \mathbf{F}_1^c \\ \mathbf{T}_1^c \\ \vdots \\ \mathbf{F}_{N_p}^c \\ \mathbf{T}_{N_p}^c \end{pmatrix} = -\mathbf{J}_{tot}^T \lambda \tag{9}$$

λ contains the $3 \times (N_b - 1)$ Lagrange mutipliers associated to the $N_b - 1$ vectorial constraints.

Contact Forces

- Including contact forces and torques

$$\underbrace{\mathbf{V}}_{\text{Velocities}} = \underbrace{M}_{\text{Hydro}} \left(\underbrace{\mathcal{F}}_{\text{Elastic}} + \underbrace{\mathcal{F}^c}_{\text{Contact}} \right) \tag{10}$$

$$= \mathbf{M} \left(\mathcal{F} - \mathbf{J}_{tot}^T \lambda \right)$$

- adding kinematic constraints

$$\left\{ \begin{array}{rcl} \mathbf{V} & = & \mathbf{M} \left(\mathcal{F} - \mathbf{J}_{tot}^T \lambda \right) \\ \mathbf{J}_{tot} \mathbf{V} & = & 0 \end{array} \right. \tag{11}$$

Contact Forces

- λ obtained by inverting

$$\mathbf{J}_{tot}\mathbf{M}\mathbf{J}_{tot}^{T}\lambda = \mathbf{J}_{tot}\mathbf{M}\mathcal{F} \tag{12}$$

- resulting bead velocities are computed

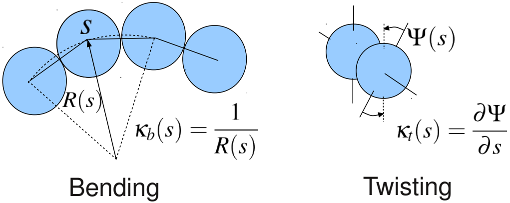
$$\mathbf{V} = \mathbf{M}\left(\mathcal{F} - \mathbf{J}_{tot}^{T}\lambda\right). \tag{13}$$

Flagellum Elasticity

- Bending stiffness $k_b(s) \propto E$ / torsional rigidity $k_t(s) \propto G$,
- Elastic responses to bending / twisting:

$$\mathbf{T}_{bend}(s) = k_b(s)\,(\kappa_b(s) - \kappa_{b,0}(s)) \;\;/\;\; \mathbf{T}_{twist}(s) = k_t(s)\,(\kappa_t(s) - \kappa_{t,0}(s))$$

- κ_b: local curvature, ($\kappa_{b,0}$ equilibrium value),
- κ_t: local twist rate, ($\kappa_{t,0}$equilibrium value).



Hydrodynamic interactions: mobility operator M

- Far-field model: Rotne-Prager-Yamakawa (RPY) tensor
  - matrix formulations M,
  - bead pairwise interactions,
  - frequently used in physics

    [Manghi *et al.* PRL 2006,

    Gauger and Stark PRE 2006,

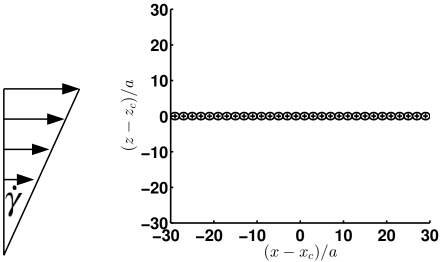
    Wada and Netz EurPhysLett 2006,
    Gao *et al.* PRE 2012]

Sheared rigid fiber

- Rigid spheroid in shear flow $\dot{\gamma}$ with aspect ratio r,
- Rotation orbit and period T analytically known : Jeffery's orbits [Jeffery Proc. Royal Soc. 1922]

$$T = \frac{2\pi}{\dot{\gamma}} \left(r_{eff} + r_{eff}^{-1} \right)$$

- Elongated body $r_{eff} = f(r)$. ($r = N_b$ for bonded spheres)



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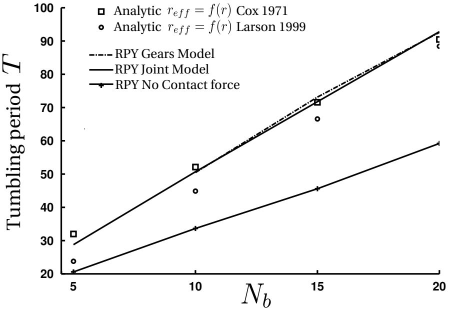

Buckling

- Fibre with small intrinsic curvature:

$$\kappa_{b,0} \ll 1$$

- Shape instability (buckling) due to flow compression
[Forgacs & Mason JColloidSc 1959, Skjetne *et al.* JChemPhys 1997, Becker & Shelley PRL 2001, Tornberg & Shelley JCP 2004, Li *et al.* (JFM) 2013,...]

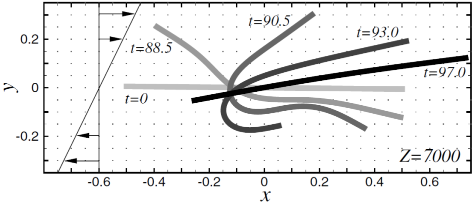

FIG. 3. Nonlinear dynamics vs time of an elastic rod in the plane of shear at flow strength $Z = 7000$.

[Becker & Shelley 2001]

Buckling

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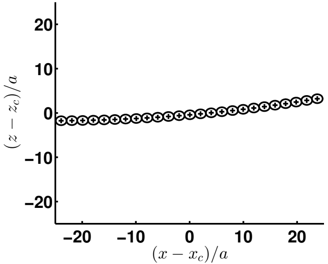


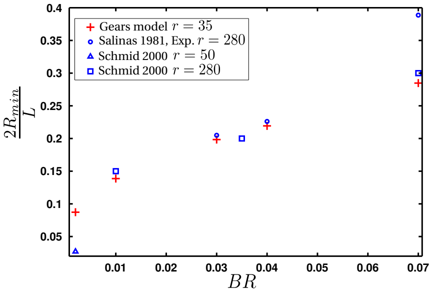
Buckling observed for $BR = 0.01$ and $\kappa_{b,0} = 0.004$

Max curvature

- Maximal curvature of sheared flexible fibers

$$\kappa_{max} = \frac{1}{R_{min}}$$

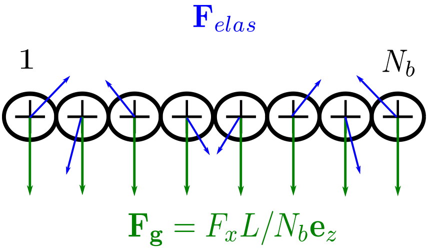
- Depends on bending rigidity BR,
- Experiments and simulations
  [Salinas & Pittman PolymEngSc 1981, Schmid et al JRheo 2000, Lindstrom & Uesaka POF 2007]



Settling fiber

- Elastic settling fiber: $\mathbf{F} = \mathbf{F}_{elas} + F_x L/N_b \mathbf{e}_z$,
- Elasto-gravitation number:

$$B = \frac{L^3 F_x}{k_b}$$



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- Nonlinearities observed for $B \gg 1$.

Settling fiber

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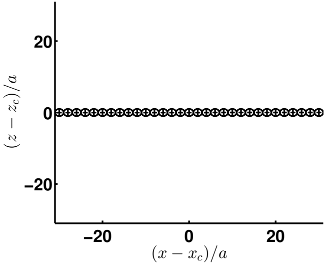
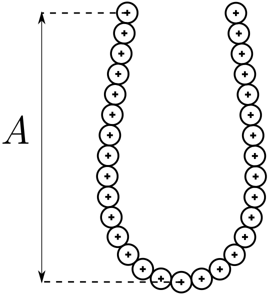


Nonlinear shape, $B = 5000$

Settling fiber

- Nonlinearity quantification:
  - vertical deflection A between central bead and fiber extremity,



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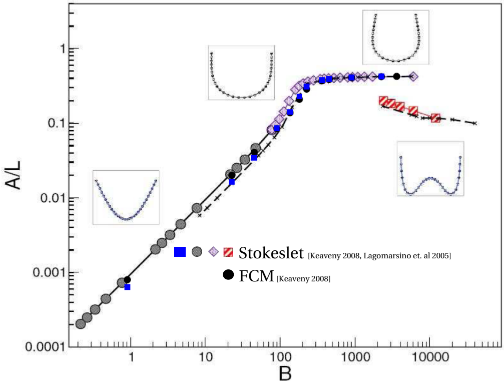

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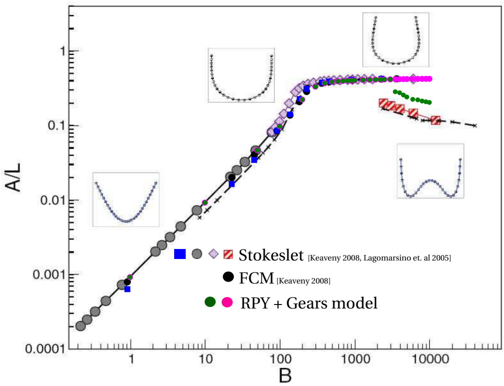

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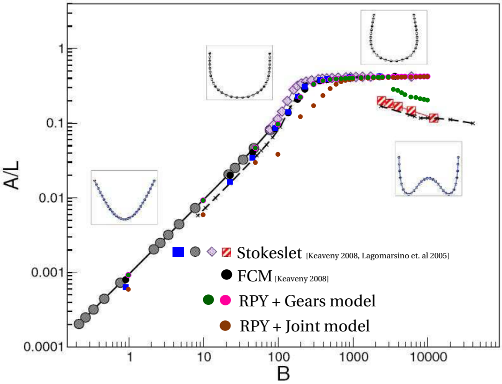
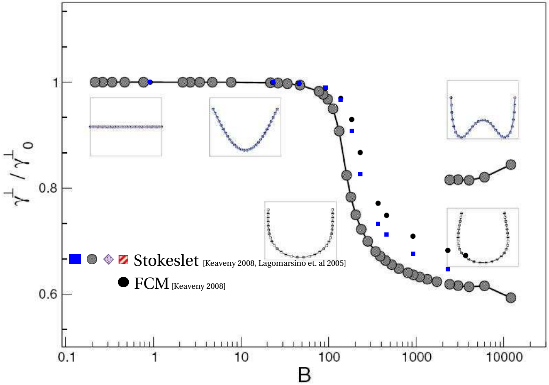


Settling fiber

- Nonlinearity quantification:
  - vertical deflection A between central bead and fiber extremity,
  - net drag coefficient $\gamma^{\perp}/\gamma^{0}$.



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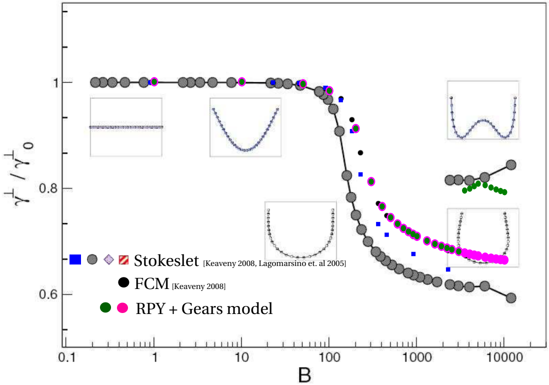

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  - vertical deflection A between central bead and fiber extremity,
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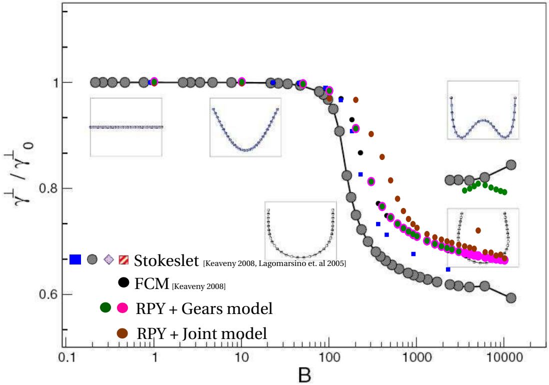
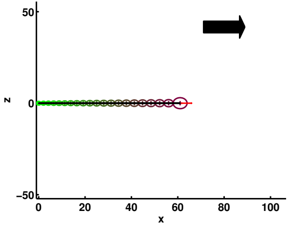
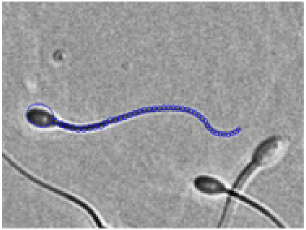


Next Step

- Active forcing validation.



(d) Preliminar simulation



(e) I3S segmentation

The End

Thank you for your attention,
any question ?

Isotropic value of Polar Order $P(t)$

$$
\begin{aligned}
P &= |\bar{\mathbf{p}}| \\
&= \frac{1}{N_p}\sqrt{\left(\sum_{i=1}^{N_p} p_{i,1}\right)^2 + \left(\sum_{i=1}^{N_p} p_{i,2}\right)^2 + \left(\sum_{i=1}^{N_p} p_{i,2}\right)^2} \\
&= \frac{1}{N_p}\sqrt{\underbrace{\sum_{i=1}^{N_p}\left(p_{i,1}^2 + p_{i,2}^2 + p_{i,3}^2\right)}_{=1} + \sum_{i=1}^{N_p}\sum_{j\neq i}\left(p_{i,1}p_{j,1} + p_{i,2}p_{j,2} + p_{i,3}p_{j,3}\right)}
\end{aligned}
$$

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&= \frac{1}{N_p}\sqrt{\underbrace{\sum_{i=1}^{N_p}\left(p_{i,1}^2 + p_{i,2}^2 + p_{i,3}^2\right)}_{=1} + \sum_{i=1}^{N_p}\sum_{j\neq i}\left(p_{i,1}p_{j,1} + p_{i,2}p_{j,2} + p_{i,3}p_{j,3}\right)}
\end{aligned}
$$

$p_{i,k}$, $i = 1 \ldots N_p$, $k = 1..3$, are independent and identically distributed (i.i.d.) with $\mathbb{E}(p_{i,k}) = 0$, and $\mathbb{V}(p_{i,k}) = \sigma^2$.
Thus,

$$\sum_{i=1}^{N_p}\sum_{j\neq i}\left(p_{i,1}p_{j,1} + p_{i,2}p_{j,2} + p_{i,3}p_{j,3}\right) = \sum_{k=1}^{3N_p}\sum_{l\neq k}\left(p_k p_l\right)$$

and

$$\sum_{k=1}^{3N_p}\sum_{l\neq k}\left(p_k p_l\right) \underset{N_p\to\infty}{\longrightarrow} 0$$

because

$$\mathbb{E}(p_k p_l) = \mathbb{E}(p_k)\mathbb{E}(p_l) = 0.$$

Isotropic value of Polar Order $P(t)$

$$P = \frac{1}{N_p}\sqrt{\underbrace{\sum_{i=1}^{N_p}\left(p_{i,1}^2 + p_{i,2}^2 + p_{i,3}^2\right)}_{=1} + \sum_{i=1}^{N_p}\sum_{j\neq i}\left(p_{i,1}p_{j,1} + p_{i,2}p_{j,2} + p_{i,3}p_{j,3}\right)}$$

Hence

$$P(t) \sim \frac{1}{N_p}\sqrt{N_p + 0} \sim \frac{1}{\sqrt{N_p}}$$

How fast does it converge with N_p ?

Isotropic value of Polar Order $P(t)$

$$X = P - \frac{1}{\sqrt{N_p}},$$

$$\mathbb{E}(X) = 0,$$

$$\mathbb{V}(X) = ?$$

$$\begin{aligned}\mathbb{V}(X) &= \mathbb{E}(X^2) - \mathbb{E}(X)\mathbb{E}(X)\\ &= \mathbb{E}(X^2)\end{aligned}$$

with

$$\begin{aligned}X^2 &= \left(\frac{1}{N_p}\sqrt{N_p + \sum_{k=1}^{3N_p}\sum_{l\neq k}(p_k p_l)} - \frac{1}{\sqrt{N_p}}\right)^2\\ &= \frac{1}{N_p^2}\sum_{k=1}^{3N_p}\sum_{l\neq k}(p_k p_l) - \frac{2}{N_p\sqrt{N_p}}\sqrt{N_p + \sum_{k=1}^{3N_p}\sum_{l\neq k}(p_k p_l)} + \frac{2}{N_p}\end{aligned}$$

Isotropic value of Polar Order $P(t)$

$$\begin{aligned}
\mathbb{E}(X^2) &= \frac{3N_p}{N_p^2}\mathbb{E}\left(p_k p_l\right) - \frac{2}{N_p\sqrt{N_p}}\mathbb{E}\left(\sqrt{N_p}\sqrt{1+\frac{1}{N_p}\sum_{k=1}^{3N_p}\sum_{l\neq k}\left(p_k p_l\right)}\right) + \frac{2}{N_p} \\
&= 0 - \frac{2}{N_p}\mathbb{E}\left(\sqrt{1+\frac{1}{N_p}\sum_{k=1}^{3N_p}\sum_{l\neq k}\left(p_k p_l\right)}\right) + \frac{2}{N_p}
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Isotropic value of Polar Order $P(t)$

$$\begin{aligned}\mathbb{E}(X^2) &= \frac{3N_p}{N_p^2}\mathbb{E}\left(p_k p_l\right) - \frac{2}{N_p\sqrt{N_p}}\mathbb{E}\left(\sqrt{N_p}\sqrt{1+\frac{1}{N_p}\sum_{k=1}^{3N_p}\sum_{l\neq k}\left(p_k p_l\right)}\right) + \frac{2}{N_p} \\ &= 0 - \frac{2}{N_p}\mathbb{E}\left(\sqrt{1+\frac{1}{N_p}\sum_{k=1}^{3N_p}\sum_{l\neq k}\left(p_k p_l\right)}\right) + \frac{2}{N_p}\end{aligned}$$

2^{nd} order Taylor expansion of $(1+x)^{\alpha} = 1 + \alpha x + \frac{\alpha(\alpha-1)}{2!}x^2 + o(x^2)$

$$\begin{aligned}\sqrt{1+\frac{1}{N_p}\sum_{k=1}^{3N_p}\sum_{l\neq k}\left(p_k p_l\right)} &= 1 + \frac{1}{2N_p}\sum_{k=1}^{3N_p}\sum_{l\neq k}\left(p_k p_l\right)\dots \\ &\dots - \frac{1}{8N_p^2}\sum_{k=1}^{3N_p}\sum_{l\neq k}\left(p_k p_l\right)\sum_{k=1}^{3N_p}\sum_{l\neq k}\left(p_k p_l\right)\dots \\ &\dots + o\left(\left(\frac{1}{N_p}\sum_{k=1}^{3N_p}\sum_{l\neq k}\left(p_k p_l\right)\right)^2\right)\end{aligned}$$

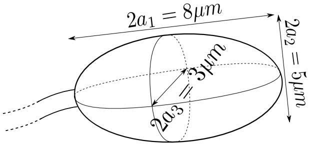
Isotropic value of Polar Order $P(t)$

Hence

$$\begin{aligned}
\mathbb{E}(X^2) &= -\frac{2}{N_p}\mathbb{E}\left(1+\frac{1}{2N_p}\sum_{k=1}^{3N_p}\sum_{l\neq k}(p_k p_l)-\frac{1}{8N_p^2}\sum_{k=1}^{3N_p}\sum_{l\neq k}(p_k p_l)\sum_{k=1}^{3N_p}\sum_{l\neq k}(p_k p_l)\right)\dots \\
&\quad \dots+\frac{2}{N_p} \\
&= -\frac{2}{N_p}\left(1+0-\frac{1}{8N_p^2}\mathbb{E}\left(\sum_{k=1}^{3N_p}\sum_{l\neq k}(p_k p_l)\sum_{k=1}^{3N_p}\sum_{l\neq k}(p_k p_l)\right)\right)+\frac{2}{N_p} \\
&= \frac{1}{4N_p^3}\mathbb{E}\left(2\sum_{k=1}^{3N_p}\sum_{l\neq k}\left(p_k^2 p_l^2\right)+2\sum_{k=1}^{3N_p}\sum_{l\neq k}\sum_{\substack{i=1\\ i\neq k}}^{3N_p}\sum_{\substack{j\neq i\\ j\neq l}}\left(p_k p_l p_i p_j\right)\dots\right. \\
&\quad \left.\dots+2\sum_{k=1}^{3N_p}\sum_{l\neq k}\sum_{\substack{i=1\\ i\neq l}}^{3N_p}\left(p_k^2 p_l p_i\right)\right) \\
&= \frac{1}{4N_p^3}\left(2\sum_{k=1}^{3N_p}\sum_{l\neq k}\mathbb{E}\left(p_k^2\right)\mathbb{E}\left(p_l^2\right)+0+0\right) \\
&= \frac{1}{2N_p^3}3N_p(3N_p-1)\sigma^4 \\
\mathbb{E}(X^2) &= \left(\frac{9}{2N_p}-\frac{3}{2N_p^2}\right)\sigma^4
\end{aligned}$$

Prospects

- Simulations of ellipsoidal swimmers (similar to sperm head)



- Large scale coherent motion should appear (nematic order)
- Microstructure should reveal anisotropic correlations as steric interactions are not.

Main stability results

Parameter	Instability	Characteristics	References
Polar	Polar $\rightarrow$ Isotropy $P = 1 \rightarrow P = 1/\sqrt{N_p}$ $\mathbf{p} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \rightarrow \mathbf{p} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$	Generic instability: all type of swimmers.	[?]^{Num} [?]Th [?]Th
Nematic	Isotropy $\rightarrow$ Nematic $\mathbf{p} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \rightarrow \mathbf{p} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$ $\underline{\underline{Q}} = 0 \rightarrow \underline{\underline{Q}} \neq 0$ $c_0 \rightarrow c(\mathbf{x}, t)$	Spheroidal or rod-like shaped swimmers. - Pullers: above a threshold concentration c_{pull}. - Pushers: always unstable.	[?]^{Num} [?]^{Num} [?]$^{Th,\,Num}$ [?]Th [?]^{Num} [?]^{Num}

Table: Characteristics of identified instabilities in dilute swimmer suspensions. Superscript "Th" : results obtained from theoretical stability analysis. Superscript "Num" : results obtained from numerical simulations.

Pros and cons of simulation methods

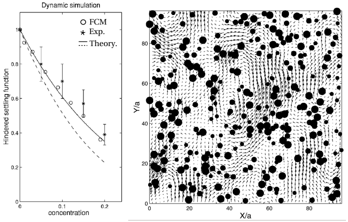
	Pros	Cons
Continuum theories	Computationally cheap	Only for (semi-)dilute suspensions
"Fast" numerical simulations	Reliable Statistics	Coarse hydrodynamics
Detailed numerical simulations	Short range hydrodynamics	Small amount of swimmers $\sim \mathcal{O}(10^2)$
	Steric interactions	Slow statistical convergence
	Concentrated regime	Costly

Need of an efficient, accurate numerical investigation on large ($\mathcal{O}(10^3)$) concentrated ($c \geq 0.1$) populations.

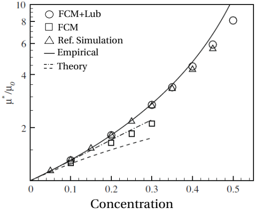
Brief description

Force coupling method (FCM) validated for passive particles :

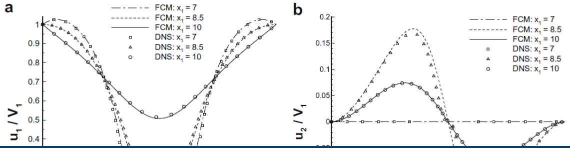
- Designed by Maxey Patel 2001,
- numerous validations for suspensions of passive particles up to $c = 0.5$,
- suited for large populations $\sim \mathcal{O}(10^3)$,
- detailed short-range hydrodynamic interactions: finite size effects + lubrication.



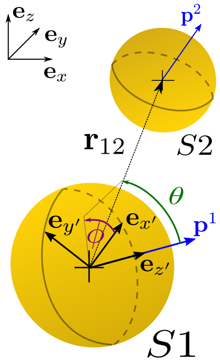
Validations for settling suspensions (Abbas POF 2006, Climent IJMF 2003).



Viscosity of sheared suspension depending on concentration c (Yeo JCP 2010).



Correlations



- Consider a swimmer denoted $S1$ with local frame $(\mathbf{e}_{x'}, \mathbf{e}_{y'}, \mathbf{e}_{z'})$, $\mathbf{e}_{z'} \parallel \mathbf{p}^1$,
- one of its neighbours $S2$, with orientation $\mathbf{p}^2$,
- defining spherical coordinates (r, θ, ϕ), one can compute pair correlations,
- to quantify near field interaction impact.