Mesoscale Hydrodynamics Simulations of Microswimmers

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Motivation

- Many examples
- Interesting phenomena

Nicolle Rager Fuller, National Science Foundation
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Riedel et al., Science 309, 300 (2005)

Kaupp et al.

Machemer, Cilia and Flagella (1974)
Modelling

- Computer simulations
- Mesoscale hydrodynamics (Multiparticle collision dynamics – MPC)
- Brownian dynamics (BD)
- Internal activity
- Self-propelled rods
- Sperm
Advantages:

- Unconditionally stable
- Galilean invariance
- Boundary conditions easily implemented
  - Curved wall
  - Deformable boundaries
  - Slip / no-slip walls
- Thermal fluctuations naturally included
- High Schmidt numbers

Self-Propelled Rods (Brownian Dynamics)

- Non-propelled rods depleted from surfaces
- Propulsion creates surface adhesion
- Surface excess

\[ s := \frac{1}{p_0} \int_{0}^{\infty} \left[ P(z) - P(\infty) \right] dz \]

J. Elgeti, G. Gompper, EPL 85, 38002 (2009)
Surface excess increases with:

- rod length
- propulsive force
Scaling Theory

Exploit analogy of self-propelled rod with semi-flexible polymers

- Rod trajectory $\leftrightarrow$ polymer conformation
- Rod orientation at time $t$ $\leftrightarrow$ tangent vector to polymer contour at position $s = vt$
- Orientational diffusion constant $D_r \sim l^{-3}$ $\leftrightarrow$ bending rigidity $\kappa$

Persistence length $\xi_p \sim v/D_r \sim v/l^3$
Scaling Theory

- Semi-flexible polymer in the bulk:
  Fluctuations of angle $\Theta$ of tangent vector: $\langle \Theta^2 \rangle \sim \frac{k_B T}{\kappa} s$
  implies vertical positional fluctuations: $\langle z^2 \rangle \sim \frac{k_B T}{\kappa} s^3$
  but $\langle \Theta \rangle = 0$ and $\langle z \rangle = 0$.

- Semi-flexible polymer near surface:
  $\langle \Theta \rangle \sim s^{1/2}$ and $\langle z \rangle \sim s^{3/2}$
Scaling Theory

Estimate $s$ via resting times:

$$P(z < l/2) = \frac{\tau_w}{\tau_w + \tau_b}$$

- Average time at wall
  $$\tau_w \sim l^{5/3} v^{-2/3}$$
- Ballistic bulk time
  $$\tau_b \sim d l^{2/3} v^{-2/3}$$
- Ballistic regime:
  $$p_B = \frac{l}{(l + a_B d)}$$
- Diffusive bulk time
  $$\tau_b \sim d l^{-2/3} v^{-4/3}$$
- Diffusive regime:
  $$p_D = \frac{l}{[l + a_D d v^{-2/3} l^{-4/3}]}$$
Rod-Length Dependence

Surface excess:

- rod length
- propulsive force
- scaling theory

\[ p_B = \frac{l}{l + a_B d} \]
\[ p_D = \frac{l}{l + a_D d} \nu^{-2/3} l^{-4/3} \]

J. Elgeti, G. Gompper, EPL 85, 38002 (2009)
With full hydrodynamics

- $\tau_w$, $\tau_b$ reduced
- surface adhesion reduced
- very similar behavior to Brownian rods

J. Elgeti, G. Gompper, EPL 85, 38002 (2009)
Hydrodynamic Interactions – Squirmers

Squirmers

- colloidal spheres with surface velocity
- expansion in Legendre polynomials, \( B_n \)
- \( B_2/B_1 > 0 \) puller
- \( B_2/B_1 < 0 \) pusher
- \( B_2/B_1 = 0 \) neutral swimmer

- flow field
- hydrodynamic force: very weak for neutral swimmer

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Sperm
Sperm Model

- Axoneme + midpiece + head
- Propulsion: Propagating sine wave

Surface Adhesion

- Sperm adhere to surface (fluid particles not shown)
- **Hydrodynamics** $\Rightarrow$ Midpiece attraction, tail repulsion
- **Repulsion** of the tail $\Rightarrow$ Orientation of sperm
- Directed thrust plus hydrodyn. attraction $\Rightarrow$ Sperm stay at wall
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Circular Motion

- Chirality by bending the midpiece causes circular motion

Multiple Swimmers

- Swarm behaviour
- Vortices
- Sperm trains

Riedel et al., Science 309, 300 (2005)

Hydrodynamic interactions of two swimmers:

Synchronization and aggregation

Kaupp, Alvarez, Dai (2008)
Consider distribution of beat frequencies (variance $\delta_f$)

Average cluster size:

Self Propelled Rods in 2 Dimensions

Simplified model: Self-propelled rods with orientational fluctuations (Brownian Dynamics)

Cluster-size distributions:

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Cluster-size distributions:

Conclusions

- Self-propelled rods – surface excess
- Single sperm dynamics – wall adhesion and circular motion
- Multiple sperm in 2D – synchronization and aggregation