Minimally-Resolved Simulations of Suspensions of Active Brownian Particles

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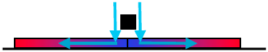
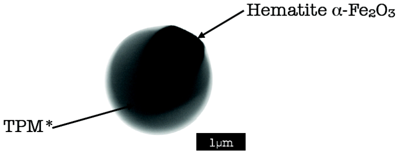
Outline

Light-Activated Diffusio/Osmophoresis

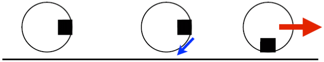


An Osmotic Flow at the Glass

Light activated H_2O_2 decomposition



Attraction to the glass



Colloidal "Surfers":
set-up a gradient and displace on the osmotic flow

Symmetric Flow but unstable
=> Self-Propulsion

Figure: From Jeremie Palacci, Paul Chaikin lab (NYU Physics) [1]

Light-Activated Colloidal Surfers

QuickTime

Bent Active Nanorods

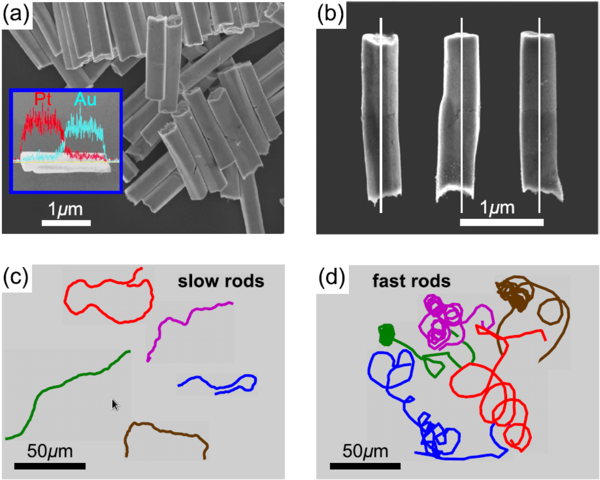
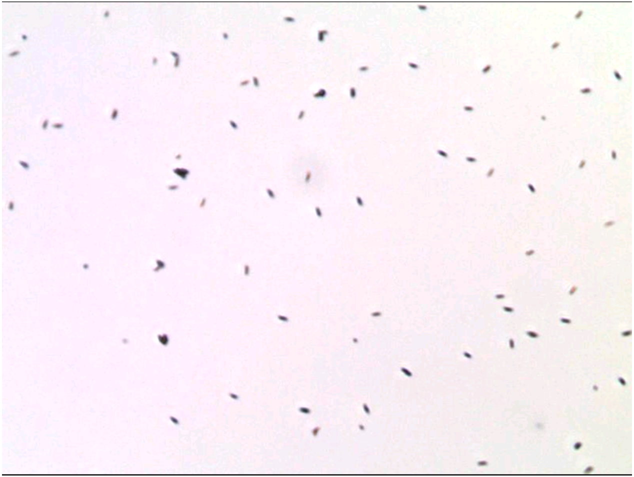


Figure: From the Courant Applied Math Lab of Zhang and Shelley [2]

Thermal Fluctuation Flips



QuickTime

Fluid-Structure Coupling

- We want to construct a **bidirectional coupling** between a fluctuating fluid and a small spherical **Brownian particle (blob)**.
- Macroscopic coupling between flow and a rigid sphere:
  - **No-slip** boundary condition at the surface of the Brownian particle.
  - Force on the bead is the integral of the (fluctuating) stress tensor over the surface.
- The above two conditions are **questionable at nanoscales**, but even worse, they are very hard to implement numerically in an efficient and stable manner.
- We need to include **thermal fluctuations** (Brownian motion) into the fluid dynamics.

Blob Model of a Brownian Particle

- Consider a **Brownian particle** of size a with position $\mathbf{q}(t)$ and velocity $\mathbf{u} = \dot{\mathbf{q}}$, and the velocity field for the fluid is $\mathbf{v}(\mathbf{r}, t)$.
- We do not care about the fine details of the flow around a particle, which is nothing like a hard sphere with stick boundaries in reality anyway.
- Take an **Immersed Boundary Method** (IBM) approach and describe the fluid-blob interaction using a localized smooth **kernel** $\delta_a(\Delta\mathbf{r})$ with compact support of size a (integrates to unity).
- Often presented as an interpolation function for point Lagrangian particles but here a is a **physical size** of the particle (as in the **Force Coupling Method** (FCM) of Maxey *et al.* [8]).
- We will call our particles "**blobs**" since they are not really point particles.

Fluctuating Hydrodynamics

- The incompressible Navier-Stokes equation for the fluid velocity $\mathbf{v}(\mathbf{r}, t)$ with N immersed **neutrally-buoyant** blobs is

$$\rho \partial_t \mathbf{v} + \boldsymbol{\nabla} \pi = \eta \boldsymbol{\nabla}^2 \mathbf{v} + \boldsymbol{\nabla} \cdot \left[\left(k_B T \eta \right)^{\frac{1}{2}} \left(\mathcal{W} + \mathcal{W}^T \right) \right] \tag{1}$$

$$+ \sum_{i=1}^{N} \left\{ \mathbf{F}_i \delta_a \left(\mathbf{q}_i - \mathbf{r} \right) + \frac{1}{2} \boldsymbol{\nabla} \times \left[\boldsymbol{\tau}_i \delta_a \left(\mathbf{q}_i - \mathbf{r} \right) \right] \right\}, \tag{2}$$

  subject to $\boldsymbol{\nabla} \cdot \mathbf{v} = 0$. Since the Reynolds number is very small ($\sim 10^{-6}$), we have **linearized**.
- $\mathbf{F}_i$ is the force and $\boldsymbol{\tau}_i$ is the torque applied on particle i externally, or via interactions with boundaries and other particles.
  They are **spread locally** to the fluid as a smooth force/torque density.
- The stochastic momentum flux (inducing the translational and rotational **Brownian motion**) is modeled using a white-noise random Gaussian tensor field $\mathcal{W}(\mathbf{r}, t)$.

Particle Motion

- The particles are advected by the **locally-averaged velocity/vorticity**, as encoded in the **no-slip condition [3]**

$$\mathbf{u}_i = \frac{d\mathbf{q}_i}{dt} = \int \delta_a(\mathbf{q}_i - \mathbf{r})\, \mathbf{v}(\mathbf{r}, t)\; d\mathbf{r}$$
$$\boldsymbol{\omega}_i \equiv \frac{d\boldsymbol{\theta}_i}{dt} = \frac{1}{2} \int \delta_a(\mathbf{q} - \mathbf{r})\, \boldsymbol{\nabla} \times \mathbf{v}(\mathbf{r}, t)\; d\mathbf{r}.$$

- In practice the particle Schmidt number is very large, and we take the **overdamped (inertia-less) limit** $\rho \to 0$ (fluctuations have to be handled with care [4]).
- In the overdamped limit, without fluctuations, the particle motion follows

$$\mathbf{v} = \boldsymbol{\mathcal{L}}^{-1} \sum_{i=1}^{N} \left\{ \mathbf{F}_i \delta_a(\mathbf{q}_i - \mathbf{r}) + \frac{1}{2} \boldsymbol{\nabla} \times \left[\boldsymbol{\tau}_i \delta_a(\mathbf{q}_i - \mathbf{r}) \right] \right\},$$

where $\boldsymbol{\mathcal{L}}^{-1}$ is the solution operator for the **steady Stokes equation**.

Reactive Blobs

- **Advection-diffusion-reaction** equation for the concentration of the species $c(\mathbf{r}, t)$ in the **diffusion-limited regime**,

$$\partial_t c + \mathbf{v} \cdot \boldsymbol{\nabla} c = \chi \boldsymbol{\nabla}^2 c \text{ in } \Omega \setminus \mathcal{S}, \quad (3)$$

$$c = 0 \text{ on } \partial \mathcal{S}, \quad (4)$$

where $\mathcal{S}$ is the reactive sphere. Typically Peclet number is small and one can ignore $\mathbf{v} \cdot \boldsymbol{\nabla} c$.

- **Reactive-blob** model leads to **saddle-point problem**

$$\partial_t c + \mathbf{v} \cdot \boldsymbol{\nabla} c = \chi \boldsymbol{\nabla}^2 c - \sum_{i=1}^{N} r_i \delta_a (\mathbf{q}_i - \mathbf{r}),$$

$$\text{s.t.} \quad \int \delta_a (\mathbf{q}_i - \mathbf{r}) \, c(\mathbf{r}, t) \, d\mathbf{r} = 0 \text{ for all } i. \quad (5)$$

Here r_i is an unknown (Lagrange multiplier) reactive **sink strength** that has to be solved for [5].

Versatility

- The concentration and velocity equations can be coupled via boundary conditions, e.g., **osmotic/phoretic slip** at boundaries

$$v_n = 0, \quad \mathbf{v}_{\boldsymbol{\tau}} = -\mu \frac{\partial c}{\partial \boldsymbol{\tau}},$$

  where μ is a constant, n denotes the normal direction at the boundary and $\boldsymbol{\tau}$ the tangential direction.
- Note that this sort of coupling cannot be handled by **Green's function-based** approaches such as Stokesian/Brownian dynamics.
- We have **low accuracy due to minimal resolution but** gain **efficiency** (thousands of particles) and **flexibility**:
  - More complicated particle shapes (rods, ellipses, etc.) can be constructed from many blobs, with some caveats.
  - Additional physical processes, nonlinearities, more complicated boundaries, etc., can be included using standard numerical techniques.

Numerical Scheme

- Spatial discretization of fluid equations is based on second-order **staggered schemes** for **fluctuating hydrodynamics** [6].
- For blobs we use **Immersed Boundary kernel functions** of Charles Peskin (these ensure excellent translational invariance despite minimal resolution!).
- Computational scheme implemented in the **IBAMR library** (Boyce Griffith, NYU). Stokes solver uses a projection-based preconditioner [7] and iterative reaction-diffusion solver uses an approximate Schur complement **preconditioner** [5].
- Temporal discretization is implicit and limited in **stability** only by **advective CFL**.

  Let $\mathbf{J}$ denote the discrete **local averaging operator** $\int d\mathbf{r}\, \delta_a(\mathbf{q}_i - \mathbf{r})$ and $\mathbf{S}$ its adjoint discrete **spreading operator** $\delta_a(\mathbf{q}_i - \mathbf{r})$.

Example Temporal Discretization

1. Solve concentration equation using backward Euler:

$$\frac{c^{n+1}-c^{n}}{\Delta t} = \chi \boldsymbol{\nabla}^{2} c^{n+1} - \mathbf{S}^{n} \lambda^{n+1} \quad (6)$$

$$\mathbf{J}^{n} c^{n+1} = 0 \quad (7)$$

and evaluate slip velocity $\mathbf{v}_{\boldsymbol{\tau}}^{n+1} = -\mu \frac{\partial c^{n+1}}{\partial \boldsymbol{\tau}}$ at boundaries.

2. Solve steady Stokes fluid equation using $\mathbf{v}_{\boldsymbol{\tau}}^{n+1}$ as the boundary condition,

$$\boldsymbol{\nabla} \pi^{n+1} = \eta \boldsymbol{\nabla}^{2} \mathbf{v}^{n+1} + \mathbf{S}^{n} \mathbf{F}^{n} + \frac{1}{2} \boldsymbol{\nabla} \times \mathbf{S}^{n} \boldsymbol{\tau}^{n} + \text{thermal} \quad (8)$$

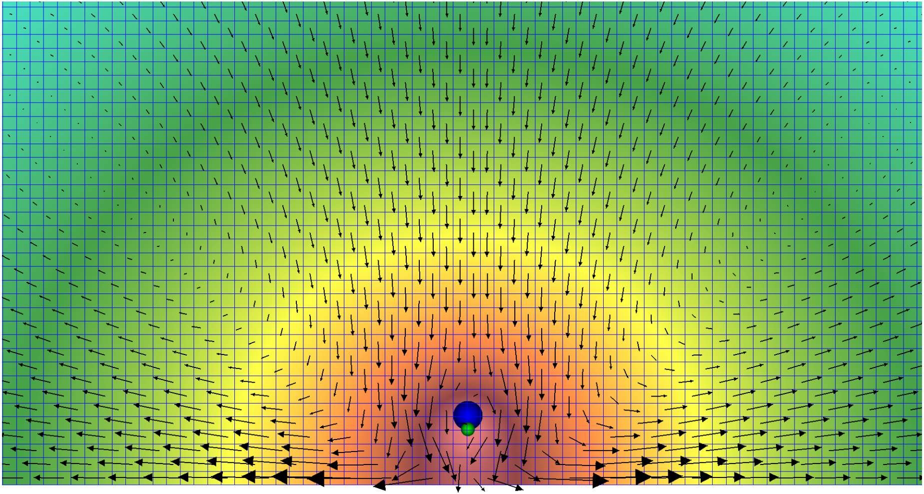
$$\boldsymbol{\nabla} \cdot \mathbf{v}^{n+1} = 0, \quad (9)$$

3. Update particle positions and orientations,

$$\mathbf{q}^{n+1} = \mathbf{q}^{n} + \Delta t \, \mathbf{J}^{n} \mathbf{v}^{n+1}.$$

$$\boldsymbol{\theta}^{n+1} = \boldsymbol{\theta}^{n} + \frac{\Delta t}{2} \mathbf{J}^{n} \boldsymbol{\nabla} \times \mathbf{v}^{n+1}.$$

Osmophoretic Colloidal Surfers



MPEG

Immersed Rigid Blobs

- Unlike a **rigid sphere**, a blob particle would not perturb a pure shear flow.
- In the far field our blob particle looks like a force monopole (**stokeset**), and does not exert a symmetric force dipole (**stresslet**) on the fluid, only an anti-symmetric dipole (**rotlet**) via the torque.
- One can, however, construct more **complex rigid body shapes** (rods, ellipsoids) from blobs (work with Boyce Griffith and Neelesh Patankar).
- This is similar to what is done in the **regularized Stokeslet methods** (Cortez *et al.*) but discretization of fluid equations is direct, not based on Green's functions.

Immersed Rigid Bodies

- This approach can be extended to an **immersed rigid body** Ω:

$$\begin{aligned}
\rho D_t \mathbf{v} + \boldsymbol{\nabla} \pi &= \eta \boldsymbol{\nabla}^2 \mathbf{v} + \int_\Omega \mathbf{S}(\mathbf{q})\, \boldsymbol{\lambda}(\mathbf{q})\, d\mathbf{q} + \text{thermal} \\
\int_\Omega \boldsymbol{\lambda}(\mathbf{q})\, d\mathbf{q} &= \mathbf{F} \quad \text{(force balance)} \\
\int_\Omega [\mathbf{q} \times \boldsymbol{\lambda}(\mathbf{q})]\, d\mathbf{q} &= \boldsymbol{\tau} \quad \text{(torque balance)} \\
\int \delta_a(\mathbf{q} - \mathbf{r})\, \mathbf{v}(\mathbf{r}, t)\; d\mathbf{r} &= \mathbf{u} + \mathbf{q} \times \boldsymbol{\omega} \text{ for all } \mathbf{q} \in \Omega \quad \text{(no slip)} \\
\boldsymbol{\nabla} \cdot \mathbf{v} &= 0 \text{ everywhere,}
\end{aligned}$$

  where $\mathbf{u}$ is the linear and $\boldsymbol{\omega}$ is the angular velocity of the body, and $\boldsymbol{\lambda}(\mathbf{q} \in \Omega)$ is an Lagrange multiplier internal stress field.
- This can be discretized using blobs but effectively **preconditioning** the linear solvers is hard (saddle-point systems).
- **Fluctuation-dissipation balance** needs to be studied carefully...

Conclusions

- **Fluctuating hydrodynamics** is a very good coarse-grained model for fluids, and can be coupled to immersed particles to model **Brownian suspensions**.
- The **minimally-resolved blob approach** provides a low-cost but reasonably-accurate representation Brownian particles in flow.
- One can construct **reactive blobs**, in either the diffusion-limited or reaction-limited cases.
- **Active particles** can be created from combinations of reactive and non-reactive blobs.
- **No Green's functions** are used: fluid equations solved using staggered finite-volume methods.
- More **complex particle shapes** can be built out of a collection of blobs.

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