A Fluctuating Immersed Boundary Method for Brownian Suspensions of Rigid Particles

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Bent Active Nanorods

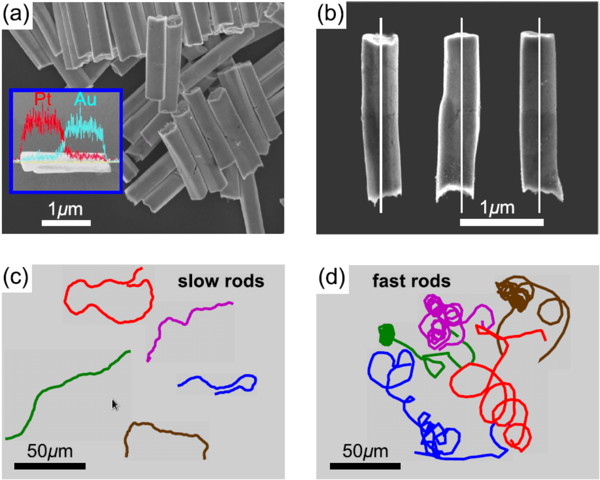
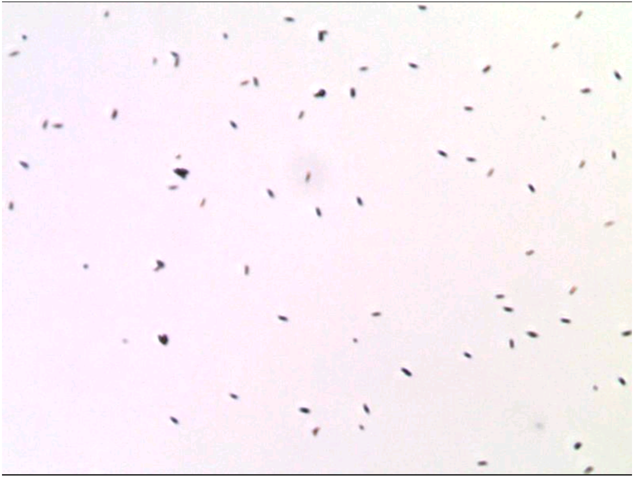


Figure: From the Courant Applied Math Lab of Zhang and Shelley [1]

Thermal Fluctuation Flips



QuickTime

Blob/Bead Models

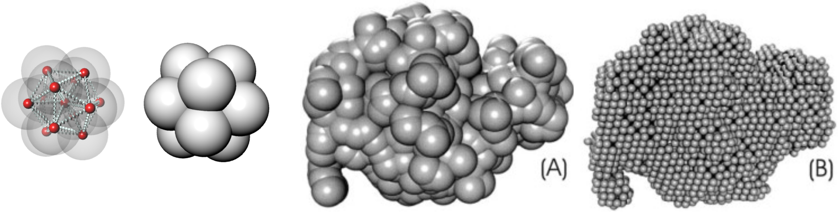


Figure: Blob or "raspberry" models of: a spherical colloid, and a lysozyme [2].

Immersed Rigid Bodies

- In the **immersed boundary method** we extend the fluid velocity everywhere in the domain,

$$
\begin{aligned}
\rho \partial_t \mathbf{v} + \boldsymbol{\nabla} \pi &= \eta \boldsymbol{\nabla}^2 \mathbf{v} - \int_\Omega \boldsymbol{\lambda}(\mathbf{q})\, \delta(\mathbf{r} - \mathbf{q})\, d\mathbf{q} + \boldsymbol{\nabla} \cdot \left(\sqrt{2 \eta k_B T}\, \boldsymbol{\mathcal{W}} \right) \\
\boldsymbol{\nabla} \cdot \mathbf{v} &= 0 \text{ everywhere} \\
m_e \dot{\mathbf{u}} &= \mathbf{F} + \int_\Omega \boldsymbol{\lambda}(\mathbf{q})\, d\mathbf{q} \\
I_e \dot{\boldsymbol{\omega}} &= \boldsymbol{\tau} + \int_\Omega [\mathbf{q} \times \boldsymbol{\lambda}(\mathbf{q})]\, d\mathbf{q} \\
\mathbf{v}(\mathbf{q}, t) &= \mathbf{u} + \mathbf{q} \times \boldsymbol{\omega} \\
&= \int \mathbf{v}(\mathbf{r}, t)\, \delta(\mathbf{r} - \mathbf{q})\, d\mathbf{r} \text{ for all } \mathbf{q} \in \Omega,
\end{aligned}
$$

where the **induced fluid-body force** [3] $\boldsymbol{\lambda}(\mathbf{q})$ is a Lagrange multiplier enforcing the final **no-slip condition** (rigidity).

Body Mobility Matrix

- Ignoring fluctuations, for **viscous-dominated** flow we can switch to the **steady Stokes** equation.
- For a suspension of rigid bodies define the **body mobility matrix** $\mathcal{N}$,

$$[\mathcal{U}, \Omega]^T = \mathcal{N} [\mathcal{F}, \mathcal{T}]^T ,$$

  where the left-hand side collects the **linear and angular velocities**, and the right hand side collects the **applied forces and torques**.
- The **Brownian dynamics** of the rigid bodies is given by the overdamped Langevin equation

$$\begin{bmatrix} \mathcal{U} \\ \Omega \end{bmatrix} = \mathcal{N} \begin{bmatrix} \mathcal{F} \\ \mathcal{T} \end{bmatrix} + (2k_B T \mathcal{N})^{\frac{1}{2}} \boldsymbol{\nabla} \diamond \mathcal{W}.$$

- Problem: **How to compute $\mathcal{N}$ and $\mathcal{N}^{\frac{1}{2}}$ and simulate the Brownian motion of the bodies?**

Immersed-Boundary Method

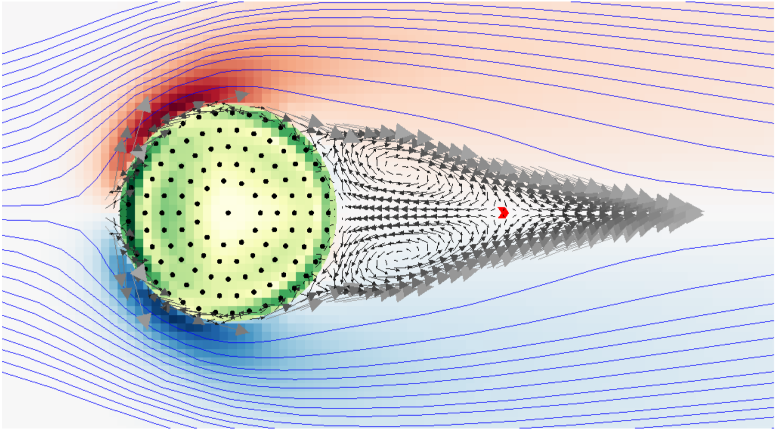


Figure: Flow past a rigid cylinder computed using our rigid-body immersed-boundary method at $Re = 20$. The cylinder is discretized using 121 markers/blobs.

Blob Model

- The rigid body is discretized through a number of "**markers**" or "**blobs**" [4] with positions $\mathbf{Q} = \{\mathbf{q}_1, \ldots, \mathbf{q}_N\}$.
- 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 (regularized delta function).
- Our methods:
  - Work for the steady Stokes regime ($\mathrm{Re} = 0$) as well as finite Reynolds numbers because there is **no time splitting**.
  - **Strictly** enforce the **rigidity** constraint.
  - Ensure **fluctuation-dissipation balance** even in the presence of **nontrivial boundary conditions**.
  - Involve **no Green's functions**, but rather, use a finite-volume staggered-grid **fluid solver** to include hydrodynamics.

Rigid-Body Immersed-Boundary Method

- **Rigidly-constrained Stokes** linear system

$$\begin{aligned} \boldsymbol{\nabla}\pi - \eta\boldsymbol{\nabla}^2\mathbf{v} &= -\sum \boldsymbol{\lambda}_i \delta_a(\mathbf{q}_i - \mathbf{r}) + \sqrt{2\eta k_B T}\,\boldsymbol{\nabla}\cdot\boldsymbol{\mathcal{W}} \\ \boldsymbol{\nabla}\cdot\mathbf{v} &= 0 \text{ (Lagrange multiplier is } \pi) \\ \sum_i \boldsymbol{\lambda}_i &= \mathbf{F} \text{ (Lagrange multiplier is } \mathbf{u}) \\ \sum \mathbf{q}_i \times \boldsymbol{\lambda}_i &= \boldsymbol{\tau} \text{ (Lagrange multiplier is } \boldsymbol{\omega}), \\ \int \delta_a(\mathbf{q}_i - \mathbf{r})\,\mathbf{v}(\mathbf{r},t)\,d\mathbf{r} &= \mathbf{u}_i + \boldsymbol{\omega}_i \times \mathbf{q}_i + \text{slip (Multiplier is } \boldsymbol{\lambda}_i) \end{aligned} \tag{1}$$

where $\boldsymbol{\Lambda} = \{\boldsymbol{\lambda}_1, \ldots, \boldsymbol{\lambda}_N\}$ are the unknown **rigidity forces**.

1. **Specified kinematics** (e.g., swimming object): Unknowns are $\mathbf{v}$, π and $\boldsymbol{\Lambda}$, while $\mathbf{F}$ and $\boldsymbol{\tau}$ are outputs (easier).
2. **Free bodies** (e.g., colloidal suspension): Unknowns are $\mathbf{v}$, π and $\boldsymbol{\Lambda}$, $\mathbf{u}$ and $\boldsymbol{\omega}$, while $\mathbf{F}$ and $\boldsymbol{\tau}$ are inputs (harder).

Suspensions of Rigid Bodies

$$[\mathcal{U},\, \boldsymbol{\Omega}]^T = \mathcal{N}\, [\mathcal{F},\, \mathcal{T}]^T \,,$$

- The many-body mobility matrix $\mathcal{N}$ takes into account higher-order hydrodynamic interactions,

$$\mathcal{N} = \left(\mathcal{K}\mathcal{M}^{-1}\mathcal{K}^{\star}\right)^{-1},$$

where the **blob mobility matrix** $\mathcal{M}$ is defined by

$$\mathcal{M}_{ij} = \eta^{-1} \int \delta_a(\mathbf{q}_i - \mathbf{r})\mathbf{G}(\mathbf{r},\mathbf{r}')\delta_a(\mathbf{q}_j - \mathbf{r}')\; d\mathbf{r}d\mathbf{r}' \qquad (2)$$

where $\mathbf{G}$ is the Green's function for the Stokes problem (**Oseen tensor** for infinite domain), and $\mathcal{K}$ is a simple geometric matrix, defined via

$$\mathcal{K}^{\star}\,[\mathbf{U},\boldsymbol{\Omega}]^T = \mathbf{U} + \boldsymbol{\Omega} \times \mathbf{Q}.$$

Numerical Method

- The difficulty is in the numerical method for solving the rigidity-constrained Stokes problem: **large saddle-point system**.
- We use an iterative method based on a **Schur complement** in which we approximate the blob mobility matrix analytically relying on **near translational-invariance** of the Peskin IB method [5].
- **Fast direct solvers** (related to FMMs) are required to approximately compute the action of $\boldsymbol{\mathcal{M}}^{-1}$.
- This works for **confined systems**, **non-spherical** particles, **finite-Reynolds numbers** and even **active particles**.
  Can also be extended to **semi-rigid structures** (e.g., bead-link polymer chains).

References

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