Brownian Suspensions of Rigid Particles

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Non-Spherical Colloids near Boundaries

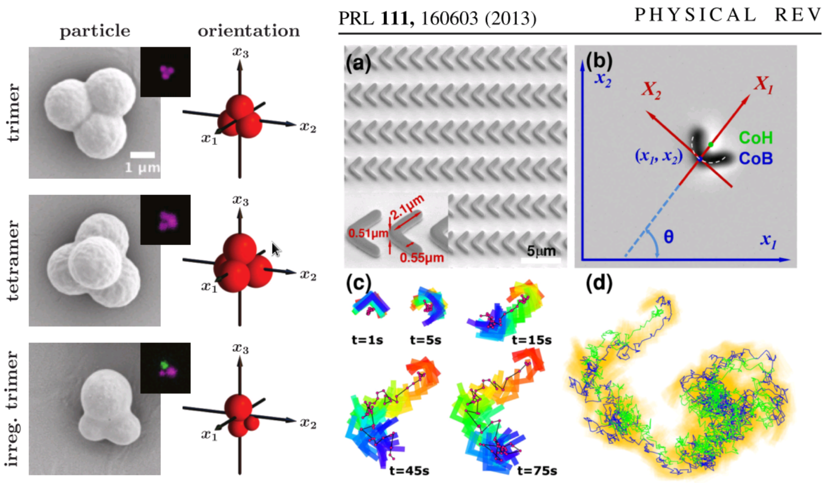


Figure: (Left) Cross-linked spheres; Kraft et al. [1]. (Right) Lithographed boomerangs; Chakrabarty et al. [2].

Bent Active Nanorods

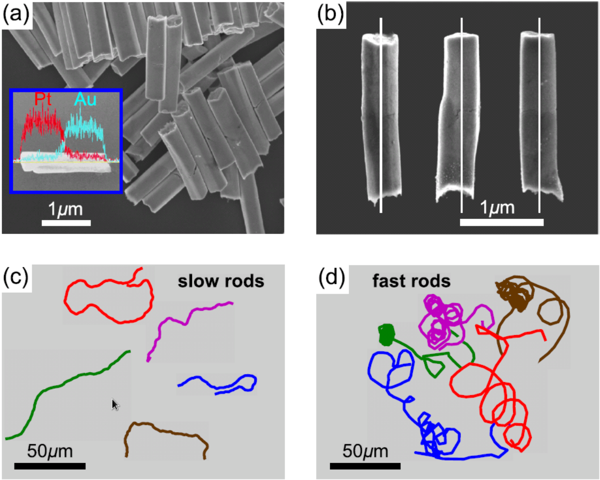
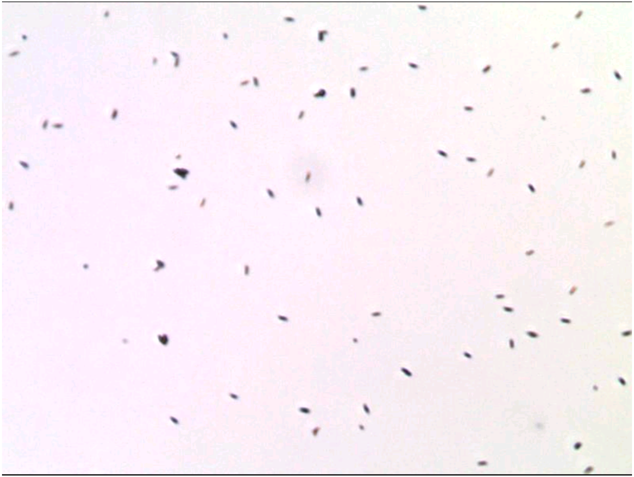


Figure: From the Courant Applied Math Lab of Zhang and Shelley [3]

Thermal Fluctuation Flips



QuickTime

Steady Stokes Flow (Re $\to$ 0)

- Consider a **suspension of N_b rigid bodies** with positions $\mathcal{Q} = \left\{ \varrho_1, \ldots, \varrho_{N_b} \right\}$ and orientations $\boldsymbol{\Theta} = \{\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_{N_b}\}$. We describe orientations using **quaternions**.

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- For viscous-dominated flows we can assume **steady Stokes flow** and define the **body mobility matrix** $\mathcal{N}(\mathcal{Q}, \boldsymbol{\Theta})$,

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

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and the right hand side collects the **applied forces** $\mathcal{F}(\mathcal{Q}, \boldsymbol{\Theta}) = \{\mathbf{F}_1, \ldots, \mathbf{F}_{N_b}\}$ and **torques** $\mathcal{T}(\mathcal{Q}, \boldsymbol{\Theta}) = \{\boldsymbol{\tau}_1, \ldots, \boldsymbol{\tau}_{N_b}\}$.

Brownian Motion

- The Brownian motion of the rigid bodies is described by the **overdamped Langevin equation**, symbolically:

$$\begin{bmatrix} d\mathcal{Q}/dt \\ d\boldsymbol{\Theta}/dt \end{bmatrix} = \begin{bmatrix} \mathcal{U} \\ \boldsymbol{\Omega} \end{bmatrix} = \mathcal{N} \begin{bmatrix} \mathcal{F} \\ \mathcal{T} \end{bmatrix} + (2k_B T \mathcal{N})^{\frac{1}{2}} \diamond \mathcal{W}(t) .$$

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- What is the correct thermal drift (i.e., what does $\diamond$ mean)?
- **How to compute (the action of) $\mathcal{N}$ and $\mathcal{N}^{\frac{1}{2}}$ and simulate the Brownian motion of the bodies?**

Difficulties/Goals

Stochastic drift It is crucial to handle stochastic calculus issues carefully for **overdamped Langevin** dynamics. Since diffusion is slow we also want to be able to take **large time step sizes**.

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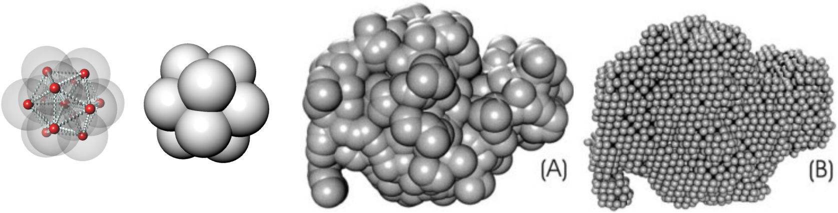

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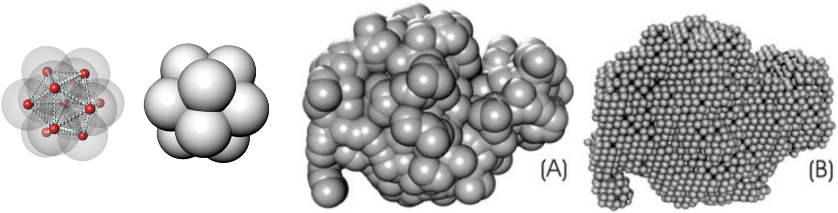

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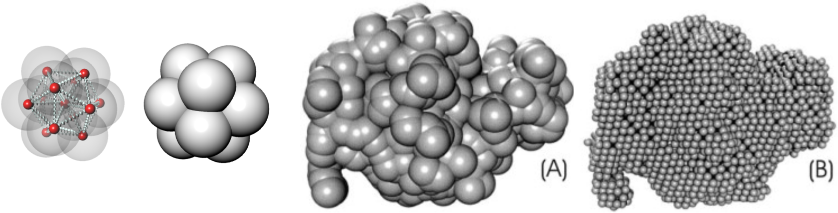

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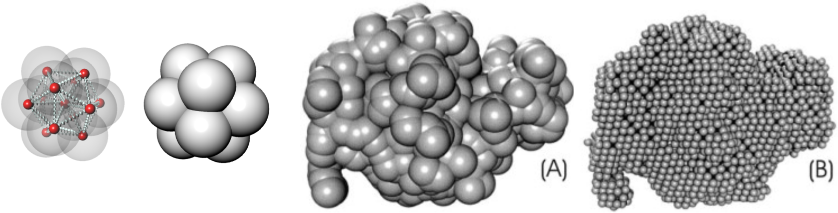

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- Describe the fluid-blob interaction using a localized smooth **kernel** $\delta_a(r)$ with compact support of size a giving the effective hydrodynamic radius of the blob (diffuse sphere).
- Standard in fluctuating/stochastic immersed boundary methods but with **stiff springs** instead of **truly rigid agglomerates**.

Rigidly-Constrained Blobs

$$
\begin{aligned}
\boldsymbol{\nabla}\pi - \eta\boldsymbol{\nabla}^2\mathbf{v} &= \sum_{i=1}^{N} \boldsymbol{\lambda}_i \delta_a\left(\mathbf{q}_i - \mathbf{r}\right) + \sqrt{2\eta k_B T}\;\boldsymbol{\nabla}\cdot\boldsymbol{\mathcal{W}} \\
\boldsymbol{\nabla}\cdot\mathbf{v} &= 0 \text{ (Lagrange multiplier is } \pi) \\
\sum_{i=1}^{N} \boldsymbol{\lambda}_i &= \mathbf{F} \text{ (Lagrange multiplier is } \boldsymbol{\upsilon}) \\
\sum_{i=1}^{N} \left(\mathbf{q}_i - \boldsymbol{\varrho}^0\right) \times \boldsymbol{\lambda}_i &= \boldsymbol{\tau} \text{ (Lagrange multiplier is } \boldsymbol{\omega}), \\
\forall i: \quad \int \delta_a\left(\mathbf{q}_i - \mathbf{r}\right)\mathbf{v}\left(\mathbf{r}, t\right)\, d\mathbf{r} &= \boldsymbol{\upsilon} + \boldsymbol{\omega} \times \left(\mathbf{q}_i - \boldsymbol{\varrho}^0\right) + \textbf{slip} \text{ (Multiplier is } \boldsymbol{\lambda}_i)
\end{aligned} \tag{1}
$$

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- Define the composite local **averaging** linear operator $\mathcal{J}(\mathbf{Q})$ operator, and the composite **spreading** linear operator, $\mathcal{S}(\mathbf{Q}) = \mathcal{J}^{\star}(\mathbf{Q})$,

$$\mathbf{u}_i = (\mathcal{J}\mathbf{v})_i = \int \delta_a(\mathbf{q}_i - \mathbf{r})\, \mathbf{v}(\mathbf{r}, t)\, d\mathbf{r}$$

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- Denote the (potentially discrete) operators scalar gradient $\mathbf{G} \equiv \boldsymbol{\nabla}$, vector divergence $\mathbf{D} = -\mathbf{G}^\star \equiv \boldsymbol{\nabla}\cdot$, tensor divergence $\mathbf{D}_\mathbf{v}$, and vector Laplacian $\mathbf{L} = -\mathbf{D}_\mathbf{v}\mathbf{D}_\mathbf{v}^\star \equiv \boldsymbol{\nabla}^2$.

Saddle-Point Problem

- Define the geometric matrix $\mathcal{K}$ that converts body kinematics to blob kinematics,

$$\mathbf{U} = \mathcal{K}\mathcal{Y} = \mathcal{K}\left[\mathcal{U}, \boldsymbol{\Omega}\right]^T = \mathcal{U} + \boldsymbol{\Omega} \times \left(\mathbf{Q} - \mathcal{Q}^0\right).$$

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- We get the symmetric **constrained Stokes saddle-point problem**,

$$\begin{bmatrix} -\eta\mathbf{L} & \mathbf{G} & -\mathcal{S} & \mathbf{0} \\ -\mathbf{D} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ -\mathcal{J} & \mathbf{0} & \mathbf{0} & \mathcal{K} \\ \mathbf{0} & \mathbf{0} & \mathcal{K}^\star & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{v} \\ \pi \\ \boldsymbol{\Lambda} \\ \mathcal{Y} \end{bmatrix} = \begin{bmatrix} \boldsymbol{\nabla} \cdot \left(\sqrt{2\eta k_B T}\,\mathcal{W}\right) \\ 0 \\ 0 \\ \mathcal{R} \end{bmatrix},$$

where $\mathcal{Y} = \left[\mathcal{U}, \, \boldsymbol{\Omega}\right]^T$ and $\mathcal{R} = \left[\mathcal{F}, \, \mathcal{T}\right]^T$, and recall that $\mathcal{S} = \mathcal{J}^\star$.

Mobility Matrix

- Eliminate velocity and pressure using the Schur complement

$$\begin{bmatrix} \mathcal{M} & -\mathcal{K} \\ -\mathcal{K}^\star & \mathbf{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{\Lambda} \\ \mathcal{Y} \end{bmatrix} = \begin{bmatrix} \text{slip} \\ -\left(\mathcal{R} + \widetilde{\mathcal{R}}\right) \end{bmatrix},$$

where $\widetilde{\mathcal{R}} = \sqrt{2\eta k_B T}\, \mathcal{K}^\star \mathcal{M}^{-1} \mathcal{J} \mathcal{L}^{-1} \mathbf{D}_v \mathcal{W}$ are the random (stochastic) forces and torques.

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- Here the all-important $3N \times 3N$ blob **mobility matrix** $\boldsymbol{\mathcal{M}}$ is

$$\boldsymbol{\mathcal{M}}=\boldsymbol{\mathcal{J}}\boldsymbol{\mathcal{L}}^{-1}\boldsymbol{\mathcal{S}},$$

where $\boldsymbol{\mathcal{L}}^{-1}=-\mathbf{L}^{-1}+\mathbf{L}^{-1}\mathbf{G}\left(\mathbf{D}\mathbf{L}^{-1}\mathbf{G}\right)^{-1}\mathbf{D}\mathbf{L}^{-1}$ denotes the Stokes solution operator.

Rigidly-Constrained Blobs

- The physical interpretation is simple:

$$\mathcal{M}\boldsymbol{\Lambda} = \mathcal{K}\mathcal{Y} + \text{slip}$$
$$\mathcal{K}^{\star}\boldsymbol{\Lambda} = \mathcal{R} + \widetilde{\mathcal{R}},$$

where the unknown $\mathcal{Y} = [\mathcal{U}, \boldsymbol{\Omega}]^T$ are the body kinematics, $\mathcal{R} = [\mathcal{F}, \mathcal{T}]^T$ are the applied forces and torques and $\widetilde{\mathcal{R}}$ are the random (stochastic) forces and torques.

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- Here $\boldsymbol{\Lambda}$ are the *unknown* rigidity forces (Lagrange multipliers) acting on the blobs that needs to be solved for.
- The $3N \times 3N$ block **mobility matrix** $\mathcal{M}$ has a **simple pairwise physical interpretation**:
  The 3×3 block $\mathbf{M}_{ij}$ maps a force on blob j to a velocity of blob i,

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

  where $\mathbf{G}$ is the Green's function (**Oseen tensor** for unbounded).

Suspensions of Rigid Bodies

- Taking yet one more Schur complement we get

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

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- If a fluctuating fluid solver is used it gives an **explicit square root** of

$$\mathcal{N}^{\frac{1}{2}} = \sqrt{2k_B T}\, \mathcal{N} \mathcal{K}^{\star} \mathcal{M}^{-1} \mathcal{J} \mathcal{L}^{-1} \mathbf{D}_v \mathcal{W}.$$

  Observe that **discrete fluctuation-dissipation balance** is guaranteed,

$$\mathcal{N}^{\frac{1}{2}} \left(\mathcal{N}^{\frac{1}{2}}\right)^{\star} = \mathcal{N} \mathcal{K}^{\star} \mathcal{M}^{-1} \left(\mathcal{J} \mathcal{L}^{-1} \mathbf{L} \mathcal{L}^{-1} \mathcal{S}\right) \mathcal{M}^{-1} \mathcal{K} \mathcal{N} =$$

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  - In more general cases we can use a fluctuating **FEM/FVM fluid Stokes solver** [6, 7].

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- We add gravity which makes the equilibrium **Gibbs-Boltzmann distribution** be

$$P_{GB}\left(\mathcal{Q},\boldsymbol{\Theta}\right)\sim\exp\left[-\frac{mgh+U_{\text{steric}}}{k_B T}\right],$$

where h is the center-of-mass height and U_{steric} is a Yukawa-type repulsion with the wall.

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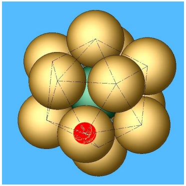
  Is it true for non-spherical particles?

MSD for a sphere



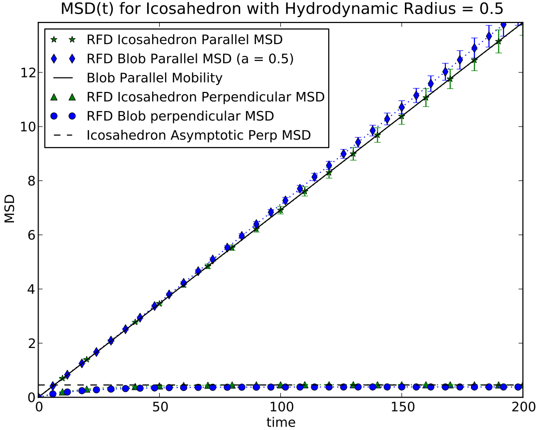
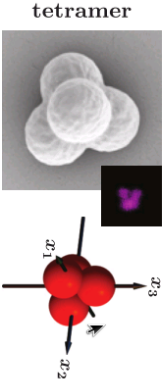


Figure: Mean square displacement (MSD) for a non-uniform **spherical particle** of unit diameter discretized as an icosahedron of 12 blobs or just a single blob.

MSD for a tetrahedron



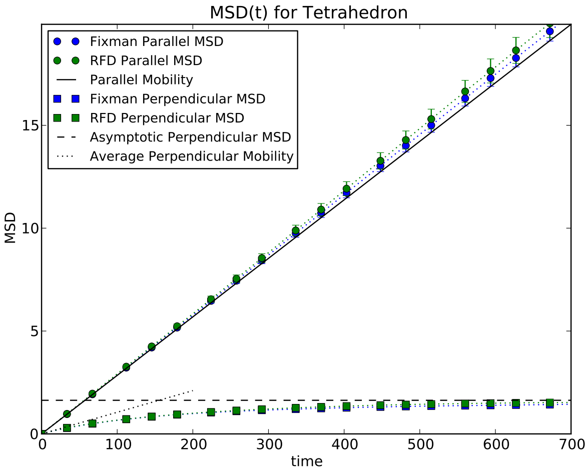
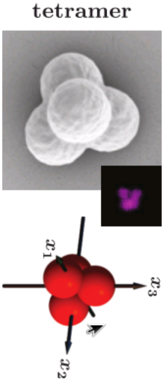
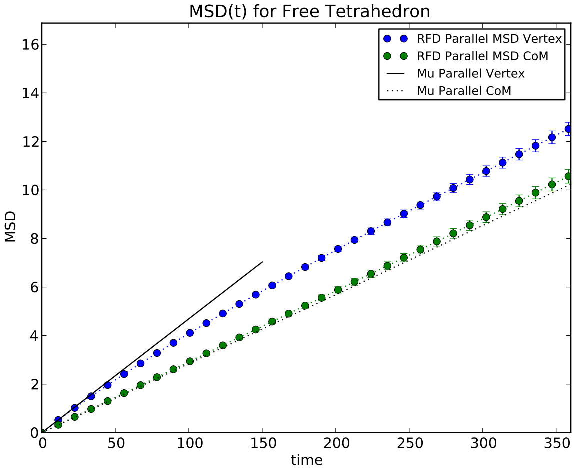


Figure: MSD for a **non-spherical particle** (tetrahedron/tetramer).

The choice of tracking point matters





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Resolving lubrication forces

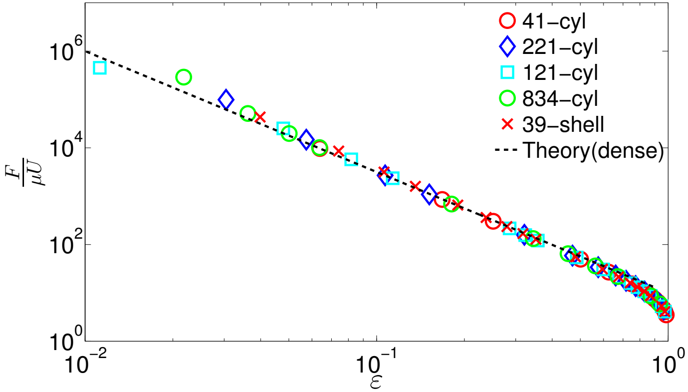

Figure: The drag coefficient for a periodic array of cylinders in steady Stokes flow for close-packed arrays with inter-particle gap ε, showing the correct asymptotic $\varepsilon^{-\frac{5}{2}}$ lubrication force divergence.

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