Fluctuating Hydrodynamics of Suspensions of Rigid Particles

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Outline

Levels of Coarse-Graining

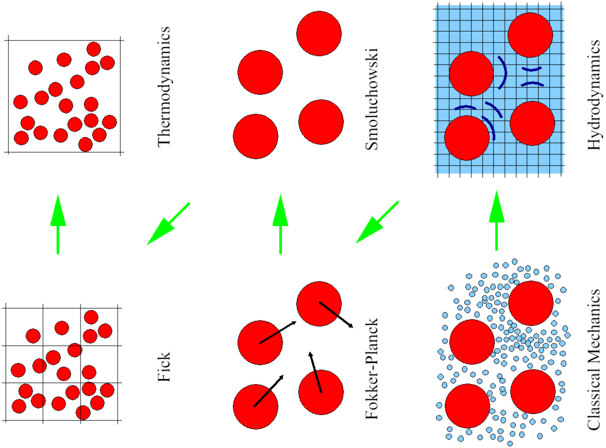

Figure: From Pep Español, “Statistical Mechanics of Coarse-Graining”.

Incompressible Fluctuating Hydrodynamics

- The particles are immersed in an incompressible fluid that we assume can be described by the time-dependent **fluctuating incompressible Stokes** equations for the velocity $\mathbf{v}(\mathbf{r}, t)$,

$$\begin{aligned} \rho\partial_t \mathbf{v} + \boldsymbol{\nabla}\pi &= \eta\boldsymbol{\nabla}^2\mathbf{v} + \mathbf{f} + \sqrt{2\eta k_B T}\,\boldsymbol{\nabla}\cdot\boldsymbol{\mathcal{W}} \\ \boldsymbol{\nabla}\cdot\mathbf{v} &= 0, \end{aligned} \quad (1)$$

  along with appropriate boundary conditions.

- Here the **stochastic momentum flux** is modeled via a random Gaussian tensor field $\boldsymbol{\mathcal{W}}(\mathbf{r}, t)$ whose components are white in space and time with mean zero and covariance

$$\langle \mathcal{W}_{ij}(\mathbf{r}, t)\mathcal{W}_{kl}(\mathbf{r}', t')\rangle = (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\,\delta(t - t')\delta(\mathbf{r} - \mathbf{r}'). \quad (2)$$

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.
- Let $\mathbf{u}$ be the linear and $\boldsymbol{\omega}$ is angular velocity of the body, $\mathbf{F}$ the applied force and $\boldsymbol{\tau}$ is the applied torque, m_e the **excess mass** of the body, and I_e the **excess moment of inertia** over that of the fluid.

Immersed Rigid Bodies

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

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

where the **induced fluid-body force** [1] $\boldsymbol{\lambda}(\mathbf{q})$ is a Lagrange multiplier enforcing the final **no-slip condition** (rigidity).

Overdamped Limit

- Ignoring fluctuations, for **viscous-dominated** flow we can switch to the **steady Stokes** equation.
- The result is a linear mapping or extended **mobility matrix** $\mathcal{M}$,

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

  where the left-hand side collects the linear and angular velocities, and the right hand side collects the applied forces.
- When the inertia-free or overdamped limit is taken carefully, an **overdamped Langevin equation** for the positions $\mathbf{Q}$ and orientations $\boldsymbol{\Theta}$ of the bodies emerge.
- **Fluctuation-dissipation balance** needs to be studied more rigorously, but see Hinch and especially work by Roux [2].
- Problem: **How to compute $\mathcal{M}$ and the simulate the Brownian motion of the particles?**

Brownian Particle Model

- 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*).
- We will call our particles "**blobs**" since they are not really point particles.

Local Averaging and Spreading Operators

- Postulate a **no-slip condition** between the particle and local fluid velocities,

$$\dot{\mathbf{q}} = \mathbf{u} = [\mathbf{J}(\mathbf{q})]\,\mathbf{v} = \int \delta_a(\mathbf{q} - \mathbf{r})\,\mathbf{v}(\mathbf{r}, t)\,d\mathbf{r},$$

  where the *local averaging* linear operator $\mathbf{J}(\mathbf{q})$ averages the fluid velocity inside the particle to estimate a local fluid velocity.

- The **induced force density** in the fluid because of the force $\mathbf{F}$ applied on particle is:

$$\mathbf{f} = -\mathbf{F}\delta_a(\mathbf{q} - \mathbf{r}) = -[\mathbf{S}(\mathbf{q})]\,\mathbf{F},$$

  where the *local spreading* linear operator $\mathbf{S}(\mathbf{q})$ is the reverse (adjoint) of $\mathbf{J}(\mathbf{q})$.

- The physical **volume** of the particle ΔV is related to the shape and width of the kernel function via

$$\Delta V = (\mathbf{J}\mathbf{S})^{-1} = \left[\int \delta_a^2(\mathbf{r})\,d\mathbf{r}\right]^{-1}. \tag{3}$$

Many-Particle Systems

- Denote composite vector of positions $\mathbf{Q} = \{\mathbf{q}_1, \dots, \mathbf{q}_N\}$ and $\mathbf{\Theta} = \{\boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_N\}$ the orientations of all of the N blobs.
- Composite velocity $\boldsymbol{\mathcal{U}} = \{\mathbf{u}_1, \dots, \mathbf{u}_N\}$ and angular velocity $\mathbf{\Omega} = \{\boldsymbol{\omega}_1, \dots, \boldsymbol{\omega}_N\}$.
- Applied forces $\mathcal{F}(\mathbf{Q}) = \{\mathbf{F}_1(\mathbf{Q}), \dots, \mathbf{F}_N(\mathbf{Q})\}$, applied torques $\mathcal{T} = \{\boldsymbol{\tau}_1, \dots, \boldsymbol{\tau}_N\}$.
- Define composite local *averaging* linear operator $\mathcal{J}(\mathbf{Q})$ operator, is the composite *spreading* linear operator, $\mathcal{S}(\mathbf{Q}) = \mathcal{J}^\star(\mathbf{Q})$,

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

$$(\mathcal{S}\mathcal{F})(\mathbf{r}) = \sum_{i=1}^{N} \mathbf{F}_i \delta_a(\mathbf{q}_i - \mathbf{r}).$$

Inertial Equations of Motion

- The momentum equation, $\boldsymbol{\nabla} \cdot \mathbf{v} = 0$ and

$$\rho \partial_t \mathbf{v} + \boldsymbol{\nabla} \pi = \eta \boldsymbol{\nabla}^2 \mathbf{v} + \sqrt{2 \eta k_B T}\, \boldsymbol{\nabla} \cdot \boldsymbol{\mathcal{W}} + \boldsymbol{\mathcal{S}} \boldsymbol{\mathcal{F}} + \frac{1}{2} \boldsymbol{\nabla} \times (\boldsymbol{\mathcal{S}} \boldsymbol{\mathcal{T}}) + \mathbf{f}_{\text{th}}.$$

- The suspended particles are prescribed to follow the local fluid motion, leading to the N **minimally-resolved no-slip conditions**

$$\begin{aligned} \boldsymbol{\mathcal{U}} &= d\mathbf{Q}/dt = \boldsymbol{\mathcal{J}} \mathbf{v}, \\ \boldsymbol{\Omega} &= d\boldsymbol{\Theta}/dt = \boldsymbol{\nabla} \times (\boldsymbol{\mathcal{J}} \mathbf{v})/2. \end{aligned} \tag{4}$$

- Henceforth we will not include rotation and only consider translational DOFs.

Fluctuation-Dissipation Balance

- One must ensure **fluctuation-dissipation balance** in the coupled fluid-particle system: our equations are ergodic with respect to the **Gibbs-Boltzmann distribution** [3]

$$P_{\text{eq}}\left(\mathbf{Q},\mathbf{\Theta}\right)\sim\exp\left(-U\left(\mathbf{Q},\mathbf{\Theta}\right)/k_B T\right),$$

  where $\mathbf{F}=-\partial_{\mathbf{Q}}U$ and $\boldsymbol{\mathcal{T}}=-\partial_{\mathbf{\Theta}}U$.
- No entropic contribution to the coarse-grained free energy because our formulation is isothermal and the particles do not have internal structure.
- In order to ensure that the dynamics is ergodic with respect to an appropriate Gibbs-Boltzmann distribution), add the thermal or **stochastic drift** forcing [4, 3, 5]

$$\mathbf{f}_{\text{th}}=\left(k_B T\right)\partial_{\mathbf{Q}}\cdot\boldsymbol{\mathcal{S}}\left(\mathbf{Q}\right). \tag{5}$$

Overdamped Limit

- Let us assume that the Schmidt number is very large,

$$\text{Sc} = \eta / (\rho\chi) \gg 1,$$

where $\chi \approx k_B T / (6\pi\eta a)$ is a typical value of the diffusion coefficient of the particles.

- To obtain the asymptotic dynamics in the limit $\text{Sc} \to \infty$ heuristically, we delete the inertial term $\rho \partial_t \mathbf{v}$ in (1), $\boldsymbol{\nabla} \cdot \mathbf{v} = 0$ and

$$\begin{aligned} \boldsymbol{\nabla}\pi &= \eta \boldsymbol{\nabla}^2 \mathbf{v} + \boldsymbol{\mathcal{S}}\boldsymbol{\mathcal{F}} + \sqrt{2\eta k_B T}\, \boldsymbol{\nabla} \cdot \boldsymbol{\mathcal{W}} \quad \Rightarrow \\ \mathbf{v} &= \eta^{-1} \boldsymbol{\mathcal{L}}^{-1} \left(\boldsymbol{\mathcal{S}}\boldsymbol{\mathcal{F}} + \sqrt{2\eta k_B T}\, \boldsymbol{\nabla} \cdot \boldsymbol{\mathcal{W}} \right), \end{aligned} \tag{6}$$

where $\boldsymbol{\mathcal{L}}^{-1} \succeq \mathbf{0}$ is the Stokes solution operator.

Overdamped Limit

- A rigorous adiabatic mode elimination procedure informs us that the correct interpretation of the noise term in this equation is the **kinetic stochastic integral**,

$$\frac{d\mathbf{Q}\left(t\right)}{dt}=\mathcal{J}(\mathbf{Q})\mathcal{L}^{-1}\left[\frac{1}{\eta}\mathcal{S}(\mathbf{Q})\mathcal{F}(\mathbf{Q})+\sqrt{\frac{2k_{B}T}{\eta}}\,\boldsymbol{\nabla}\diamond\mathcal{W}\left(\mathbf{r},t\right)\right]. \tag{7}$$

- This is equivalent to the standard equations of **Brownian Dynamics** (BD),

$$\frac{d\mathbf{Q}}{dt}=\mathcal{M}\mathcal{F}+\left(2k_{B}T\mathcal{M}\right)^{\frac{1}{2}}\,\widetilde{\mathcal{W}}(t)+k_{B}T\,\left(\partial_{\mathbf{Q}}\cdot\mathcal{M}\right), \tag{8}$$

where $\mathcal{M}(\mathbf{Q})\succeq\mathbf{0}$ is the symmetric positive semidefinite (SPD) mobility matrix

$$\mathcal{M}=\eta^{-1}\mathcal{J}\mathcal{L}^{-1}\mathcal{S}.$$

Brownian Dynamics via Fluctuating Hydrodynamics

- It is not hard to show that $\mathcal{M}$ is very similar to the **Rotne-Prager mobility** used in BD, for particles i and j,

$$\mathcal{M}_{ij} = \eta^{-1} \int \delta_a(\mathbf{q}_i - \mathbf{r}) \mathbf{K}(\mathbf{r}, \mathbf{r}') \delta_a(\mathbf{q}_j - \mathbf{r}') \, d\mathbf{r} d\mathbf{r}' \tag{9}$$

  where $\mathbf{K}$ is the Green's function for the Stokes problem (**Oseen tensor** for infinite domain).
- The self-mobility defines a consistent **hydrodynamic radius** of a blob,

$$\mathcal{M}_{ii} = \mathcal{M}_{\text{self}} = \frac{1}{6\pi\eta a}\mathbf{I}.$$

- For well-separated particles we get the correct **Faxen correction**,

$$\mathcal{M}_{ij} \approx \eta^{-1} \left(\mathbf{I} + \frac{a^2}{6}\boldsymbol{\nabla}^2_{\mathbf{r}}\right) \left(\mathbf{I} + \frac{a^2}{6}\boldsymbol{\nabla}^2_{\mathbf{r}'}\right) \mathbf{K}(\mathbf{r} - \mathbf{r}')\Big|_{\mathbf{r}'=\mathbf{q}_i}^{\mathbf{r}=\mathbf{q}_j}.$$

- At smaller distances the mobility is **regularized** in a natural way and positive-semidefiniteness ensured automatically.

Numerical Methods

- Both **compressible and incompressible, inertial and overdamped**, numerical methods have been implemented by Florencio Balboa (UAM) on GPUs for periodic BCs (public-domain!), and in the parallel **IBAMR code** of Boyce Griffith by Steven Delong for general boundary conditions (to be made public-domain next fall!).
- Spatial discretization is based on previously-developed **staggered schemes** for fluctuating hydro [6] and the **immersed-boundary method kernel functions** of Charles Peskin.
- Temporal discretization follows a second-order **splitting algorithm** (move particle + update momenta), and is limited in **stability** only by **advective CFL**.
- We have constructed specialized temporal integrators that ensure **discrete fluctuation-dissipation balance**, including for the overdamped case.

(Simple) Midpoint Scheme

Fluctuating Immersed Boundary Method (FIBM) method:

- Solve a **steady-state Stokes problem** (here $\delta \ll 1$)

$$\begin{aligned} \boldsymbol{\nabla}\boldsymbol{\pi}^n &= \eta\boldsymbol{\nabla}^2\mathbf{v}^n + \sqrt{2\eta k_B T}\,\boldsymbol{\nabla}\cdot\boldsymbol{\mathcal{Z}}^n + \boldsymbol{\mathcal{S}}^n\mathbf{F}\left(\mathbf{q}^n\right) \\ &+ \frac{k_B T}{\delta}\left[\boldsymbol{\mathcal{S}}\left(\mathbf{q}^n + \frac{\delta}{2}\widetilde{\mathbf{W}}^n\right) - \boldsymbol{\mathcal{S}}\left(\mathbf{q}^n - \frac{\delta}{2}\widetilde{\mathbf{W}}^n\right)\right]\widetilde{\mathbf{W}}^n \\ \boldsymbol{\nabla}\cdot\mathbf{v}^n &= 0. \end{aligned}$$

- **Predict** particle position:

$$\mathbf{q}^{n+\frac{1}{2}} = \mathbf{q}^n + \frac{\Delta t}{2}\mathcal{J}^n\mathbf{v}$$

- **Correct** particle position,

$$\mathbf{q}^{n+1}. = \mathbf{q}^n + \Delta t\,\mathcal{J}^{n+\frac{1}{2}}\mathbf{v}.$$

Slit Channel

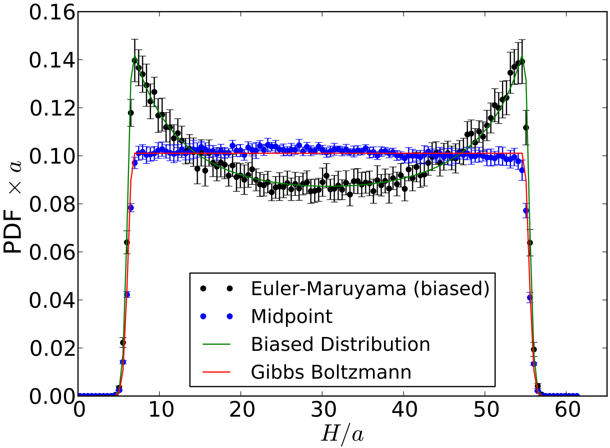

Figure: Probability distribution of the distance H to one of the walls for a freely-diffusing blob in a two dimensional slit channel.

Colloidal Gellation: Cluster collapse

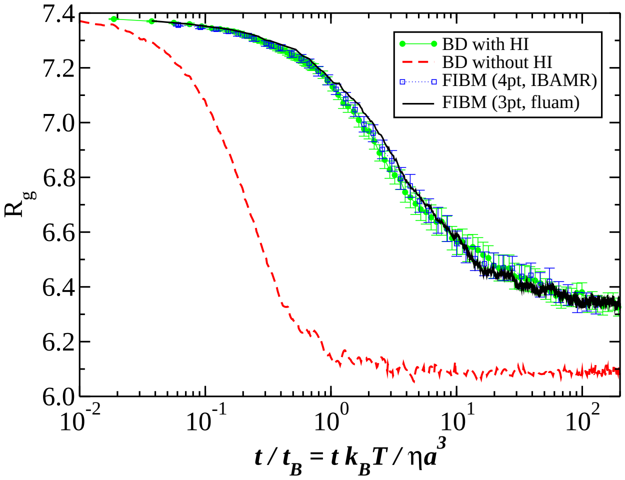

Figure: Relaxation of the radius of gyration of a colloidal cluster of 13 spheres toward equilibrium, taken from Furukawa+Tanaka.

Blob/Bead Models

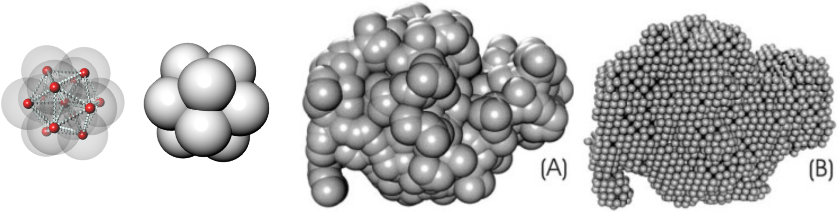

Figure: Blob or "raspberry" models of: a spherical colloid, and a lysozyme [7].

Review: Immersed Rigid Bodies

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

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

where the **induced fluid-body force** [1] $\boldsymbol{\lambda}(\mathbf{q})$ is a Lagrange multiplier enforcing the final **no-slip condition** (rigidity).

Rigid-Body Immersed-Boundary Method

- A **neutrally-buoyant rigid-body** immersed boundary formulation using blobs:

$$\rho \partial_t \mathbf{v} + \boldsymbol{\nabla} \pi = \eta \boldsymbol{\nabla}^2 \mathbf{v} - \boldsymbol{\mathcal{S}} \boldsymbol{\Lambda} + \sqrt{2 \eta k_B T}\ \boldsymbol{\nabla} \cdot \boldsymbol{\mathcal{W}} + \mathbf{f}_{th}$$

$$\boldsymbol{\nabla} \cdot \mathbf{v} = 0 \text{ (Lagrange multiplier is } \pi \text{)}$$

$$\sum_i \boldsymbol{\lambda}_i = \mathbf{F} \text{ (Lagrange multiplier is } \mathbf{u} \text{)} \tag{10}$$

$$\sum \mathbf{q}_i \times \boldsymbol{\lambda}_i = \boldsymbol{\tau} \text{ (Lagrange multiplier is } \boldsymbol{\omega} \text{)}, \tag{11}$$

$$\boldsymbol{\mathcal{J}} \mathbf{v} = \mathbf{u} + \boldsymbol{\omega} \times \mathbf{Q} + \text{slip (activity)}$$

where $\boldsymbol{\Lambda} = \{\boldsymbol{\lambda}_1, \dots, \boldsymbol{\lambda}_N\}$ are the unknown **rigidity forces** on each blob that **need to be solved for** (this is the hard part!).

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).

Rigid-Body Langevin Dynamics

- This system of equations (once $\mathbf{f}_{th}$ is determined) is ergodic wrt the **Gibbs-Boltzmann distribution**.
- The many-body mobility matrix $\mathcal{N}$ takes into account higher-order hydrodynamic interactions,

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

  relating the total applied forces and torques with the resulting linear and angular velocities.
  Here $\mathcal{K}$ is a simple geometric matrix, defined via $\mathcal{K}^{\star}\left[\mathbf{U},\boldsymbol{\Omega}\right]^{T} = \mathbf{U} + \boldsymbol{\Omega} \times \mathbf{Q}$.
- This works for **confined systems**, **non-spherical** particles, and even **active particles**.
  Can also be extended to **semi-rigid structures** (e.g., bead-link polymer chains).

Overdamped Limit

- The overdamped limit can be taken and amounts to (aside from thermal drift terms) to simply deleting $\rho \partial_t \mathbf{v}$, to get

$$\begin{bmatrix} \mathcal{U} \\ \boldsymbol{\Omega} \end{bmatrix} = \mathcal{N} \left(\begin{bmatrix} \mathcal{F} \\ \mathcal{T} \end{bmatrix} + \sqrt{\frac{2k_B T}{\eta}} \mathcal{K} \mathcal{M}^{-1} \mathcal{J} \mathcal{L}^{-1} \boldsymbol{\nabla} \diamond \mathcal{W} \right) = \tag{12}$$

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

- Observe the noise automatically has the right covariance,

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

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

without any approximations and for *all* types of boundary conditions.

Shell-in-Shell Test

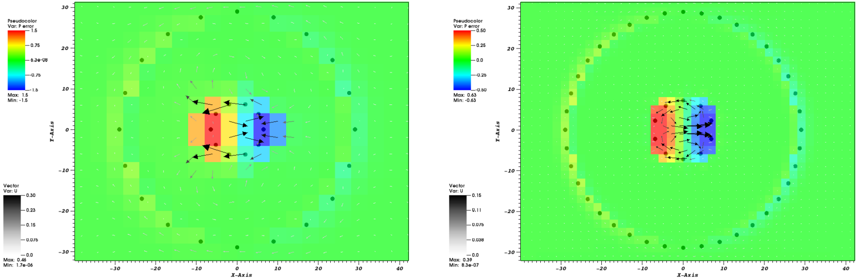

Figure: *Error* in the velocity and pressure for different resolutions. (Left) Outer: 162, Inner: 12 blobs. (Right) Outer: 642, Inner: 42 blobs.

Steady Stokes Test

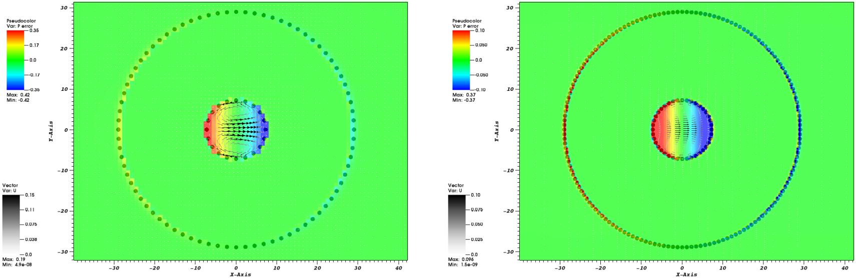

Figure: *Error* in the velocity and pressure for different resolutions. (Left) Outer: 2562, Inner: 162 blobs. (Right) Outer: 10242, Inner: 642 blobs.

Alternative Discretizations

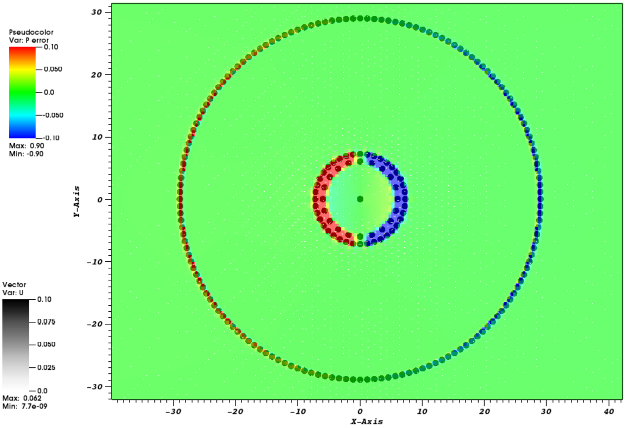

Figure: *Error* in the velocity and pressure for shell-in-shell steady Stokes test with double-shell.

Sphere in Shear Flow

- The **low-order moments** of the fluid-particle stress converge relatively rapidly.
- The total **drag** (zeroth moment) and **torque** (antisymmetric part of the second moment),

$$\mathbf{F} = \sum_i \mathbf{\Lambda}_i \text{ and } \boldsymbol{\tau} = \sum_i \boldsymbol{\lambda}_i \times \mathbf{r}_i.$$

These are nonzero and consistent even for a **single blob**.

- But to get a nonzero **stresslet** (symmetric part of the second moment) we need a raspberry-type model,

$$\mathbf{S} = \text{SymmTraceless}\left\{\sum_i \boldsymbol{\lambda}_i \otimes \mathbf{r}_i\right\}.$$

Accuracy

- Compare to theoretical formulae to derive an effective hydrodynamic radius:

$$\mathbf{T} = 8\pi\mu R^3 \boldsymbol{\omega} \text{ where } \boldsymbol{\omega} = \left(\boldsymbol{\nabla} \times \mathbf{v}\right)/2 \tag{13}$$

$$\mathbf{S} = \frac{10\pi}{3}\eta R^3 \dot{\gamma} \text{ where } \dot{\gamma} = \boldsymbol{\nabla}\mathbf{v} + \boldsymbol{\nabla}^T\mathbf{v}.$$

# blobs	Drag R_h	Torque R_τ	Stresslet R_s	Geom R_g
12	1.4847	1.3774	1.4492	1
42	1.2152	1.1671	1.2474	1
162	1.0864	1.0730	1.0959	1
642	1.0377	1.0343	1.0405	1
2562	1.0172	1.0163	1.0184	1

Table: Hydrodynamic radii for several resolutions of shell sphere models.

Conclusions

- **Fluctuating hydrodynamics** seems to be a very good coarse-grained model for fluids, and coupled to immersed particles to model Brownian suspensions (model can be **justified microscopically**, ongoing work with Pep Espanol).
- The **minimally-resolved blob approach** provides a low-cost but reasonably-accurate representation of rigid particles in flow (has been extended to **reaction-diffusion problems**).
- Particle and fluid **inertia** can be included in the description, or, an **overdamped limit** can be taken if $S_c \gg 1$.
- More **complex particle shapes** can be built out of a collection of blobs to form a **rigid body**.
- A **postdoc position** is available in my group:
  Fluctuating Hydrodynamics of chemically reactive + multiphase + multispecies liquid mixtures

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