A fluctuating boundary integral method for Brownian suspensions

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Colloidal Gelation

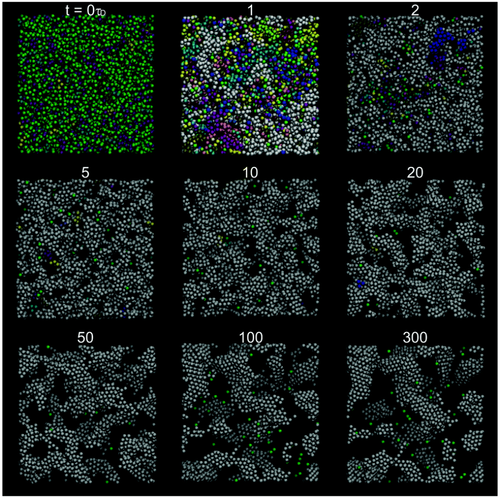

Figure : Colloidal gelation simulated using Brownian Dynamics with Hydrodynamic Interactions (from work of James Swan, MIT Chemical

Non-Spherical Colloids

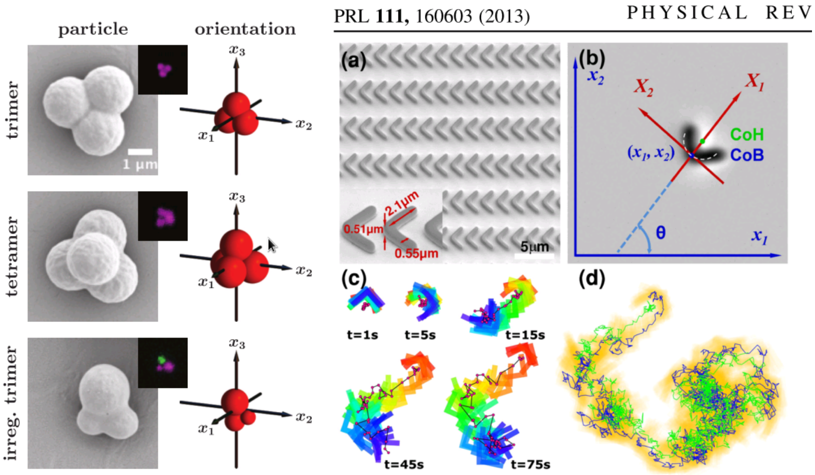

Figure : (Left) Cross-linked spheres from Kraft et al. (Right) Lithographed boomerangs in a microchannel from Chakrabarty et al.

Motivation

- Part 1 on **Brownian Dynamics with Hydrodynamic Interactions**: **How to efficiently capture the effect of long-ranged hydrodynamic correlations (interactions) in the Brownian motion of 10^6 spherical colloids?**
- Because we want to simulate huge numbers of particles we have to sacrifice accuracy and use a very low-resolution (far-field) approximation for the hydrodynamics: "**long-ranged hydrodynamic interactions** are sufficient for establishing the gel boundary, structure and coarsening kinetics observed in experiments..."
- Note: The problem of generating Gaussian variates with a covariance specified by a long-ranged kernel has many **other applications** as well, e.g., in data science, not discussed here.
- Part 2 on a **Fluctuating Boundary Element Method** (FBEM): **How to accurately (yet efficiently) model the Brownian motion of complex-shaped colloids including near-field hydrodynamics?**

Brownian Dynamics with Hydrodynamic Interactions (BD-HI)

- The Ito equations of **Brownian Dynamics** (BD) for the (correlated) positions of the N particles $\mathbf{Q}(t) = \{\mathbf{q}_1(t), \ldots, \mathbf{q}_N(t)\}$ are

$$d\mathbf{Q} = \mathbf{M} \cdot \mathbf{F}(\mathbf{Q})\, dt + (2k_B T\, \mathbf{M})^{\frac{1}{2}}\, d\boldsymbol{\mathcal{B}} + k_B T\, (\partial_{\mathbf{Q}} \cdot \mathbf{M})\, dt, \qquad (1)$$

  where $\boldsymbol{\mathcal{B}}(t)$ is a vector of Brownian motions, and $\mathbf{F}(\mathbf{Q})$ are forces.
- Here $\mathbf{M}(\mathbf{Q}) \succeq \mathbf{0}$ is a symmetric positive semidefinite (SPD) **mobility matrix**, assumed to have a far-field **pairwise approximation**

$$\mathbf{M}_{ij}(\mathbf{Q}) \equiv \mathbf{M}_{ij}(\mathbf{q}_i, \mathbf{q}_j) = \boldsymbol{\mathcal{R}}(\mathbf{q}_i - \mathbf{q}_j).$$

- Here we use the **Rotne-Prager-Yamakawa (RPY) kernel**:

$$\boldsymbol{\mathcal{R}}(\mathbf{r}) = \frac{k_B T}{6\pi\eta a} \begin{cases} \left(\frac{3a}{4r} + \frac{a^3}{2r^3}\right)\mathbf{I} + \left(\frac{3a}{4r} - \frac{3a^3}{2r^3}\right)\frac{\mathbf{r}\otimes\mathbf{r}}{r^2}, & r > 2a \\ \left(1 - \frac{9r}{32a}\right)\mathbf{I} + \left(\frac{3r}{32a}\right)\frac{\mathbf{r}\otimes\mathbf{r}}{r^2}, & r \leq 2a \end{cases}$$

  where a is the radius of the colloidal particles.

Hydrodynamic Correlations

- Observe that in the far-field, $r \gg a$, the RPY tensor becomes the **long-ranged** Oseen tensor

$$\mathcal{R}\left(r \gg a\right) \to \frac{1}{8\pi r}\left(\mathbf{I} + \frac{\mathbf{r} \otimes \mathbf{r}}{r^2}\right). \tag{2}$$

- To solve the equations of BD numerically (*not* the subject of this talk), one needs two fast routines:
  - A fast matrix-vector product to compute **MF**.
    This can be done using **Fast Multipole Methods (FMM)** [1] (Greengard) in an unbounded domain or using the **Spectral Ewald (SE) Method** [2] (Tornberg) for periodic domains.
  - A fast method to compute $\mathbf{M}^{\frac{1}{2}}\mathbf{W}$, where $\mathbf{W}$ is a vector of Gaussian random variables. More precisely, we want to sample Gaussian random variables with mean zero and covariance $\mathbf{M}$.
    First part of this talk: **How to compute $\mathbf{M}^{\frac{1}{2}}\mathbf{W}$ using a fast method.**

Existing Approaches

- The product $\mathbf{M}^{\frac{1}{2}}\mathbf{W}$ is usually computed iteratively by **repeated multiplication** of a vector by $\mathbf{M}$.
- Traditionally chemical engineers have used an approach by **Fixman** based on a Chebyshev polynomial approximation to the square root.
- Recently, Chow and Saad have developed Krylov subspace **Lanczos methods** [3] for multiplying a vector with the principal square root of $\mathbf{M} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$,

$$\mathbf{M}^{\frac{1}{2}}\mathbf{W} \equiv \mathbf{U}\mathbf{\Lambda}^{\frac{1}{2}}\mathbf{U}^T\mathbf{W} \approx \left\|\mathbf{W}\right\|_2 \mathbf{V}_m \mathbf{H}_m^{1/2}\mathbf{e}_1,$$

  where $\mathbf{V}_m$ is an orthonormal basis for the Krylov subspace of order m, and $\mathbf{H}_m = \mathbf{V}_m^T\mathbf{M}\mathbf{V}_m$ is a tridiagonal matrix, both computed in the course of a Lanczos iteration through m matrix-vector multiplies.
- The Krylov method is vastly superior, but, because of the long-ranged nature of the Oseen kernel the number of iterations is found to grow with the number of particles, leading to an overall complexity of at least $O\left(N^{4/3}\right)$.

Near-Far field decomposition

- Work done by **Andrew Fiore and James Swan** (MIT Chemical Engineering), with help from **Florencio Balboa** (Courant).
- We don't really need to multiply any particular matrix "square root" by $\mathbf{W}$, rather, we want to generate a Gaussian random vector $\delta\mathbf{U}$ with specified covariance, $\langle(\delta\mathbf{U})(\delta\mathbf{U})^T\rangle = \mathbf{M}$.
- *First key idea*: Use (Spectral) Ewald approach to decompose $\mathbf{M} = \mathbf{M}^{(w)} + \mathbf{M}^{(r)}$ into a **far-field wave-space part** $\mathbf{M}^{(w)}$ and a **near-field real space part** $\mathbf{M}^{(r)}$, then in law,

$$\mathbf{M}^{\frac{1}{2}}\mathbf{W} \overset{\mathrm{d}}{=} \left(\mathbf{M}^{(w)}\right)^{\frac{1}{2}}\mathbf{W}^{(w)} + \left(\mathbf{M}^{(r)}\right)^{\frac{1}{2}}\mathbf{W}^{(r)},$$

  if **both** $\mathbf{M}^{(w)}$ **and** $\mathbf{M}^{(r)}$ **are SPD** and $\langle\mathbf{W}^{(w)}\mathbf{W}^{(r)}\rangle = \mathbf{0}$.
- For the real-space part, use the Krylov Lanczos method to compute $\left(\mathbf{M}^{(r)}\right)^{\frac{1}{2}}\mathbf{W}^{(r)}$ since $\mathbf{M}^{(r)}$ is **sparse and well-conditioned**.
- *Second key idea*: Compute $\mathbf{M}^{(w)}\mathbf{F}$ and $\left(\mathbf{M}^{(w)}\right)^{\frac{1}{2}}\mathbf{W}^{(w)}$ in **Fourier space (using FFTs)** as in fluctuating hydrodynamics.

Spectral RPY

- We need to find an Ewald-like decomposition where both the real space and wave space kernels decay exponentially and are SPD.
- The most physically-relevant and simplest definition of RPY is the integral representation:

$$\mathcal{R}(\mathbf{r}_1, \mathbf{r}_2) = \mathcal{R}(\mathbf{r}_1 - \mathbf{r}_2) = \int \delta_a(\mathbf{r}_1 - \mathbf{r}') \, \mathbb{G}(\mathbf{r}', \mathbf{r}'') \, \delta_a(\mathbf{r}_2 - \mathbf{r}'') \, d\mathbf{r}' d\mathbf{r}'',$$

  where δ_a denotes a surface delta function on a sphere of radius a.
- In other $O(N)$ methods for BD other regularized delta functions have been used (Peskin's in fluctuating immersed boundary methods and Gaussians in the fluctuating force coupling method).
- Here the Green's function for periodic Stokes flow is given by

$$\mathbb{G}(\mathbf{x}, \mathbf{y}) = \frac{1}{\mu V} \sum_{\mathbf{k} \neq 0} e^{i\mathbf{k} \cdot (\mathbf{x} - \mathbf{y})} \frac{1}{k^2} \left(\mathbf{I} - \hat{\mathbf{k}}\hat{\mathbf{k}} \right).$$

- The surface delta functions in Fourier space give us a sinc factor.

Positively Split Ewald RPY

- This gives us a previously-unappreciated simple spectral representation of the periodic RPY tensor:

$$\boldsymbol{\mathcal{R}}(\mathbf{r}) = \frac{1}{\mu V} \sum_{\mathbf{k} \neq 0} e^{i \mathbf{k} \cdot \mathbf{r}} \frac{1}{k^2} \operatorname{sinc}^2(ka) \left(\mathbf{I} - \hat{\mathbf{k}}\hat{\mathbf{k}} \right). \tag{3}$$

- We can now directly apply Hasimoto's Ewald-like decomposition [2] to RPY to get the desired **Positively Split Ewald (PSE) RPY tensor**, $\boldsymbol{\mathcal{R}} = \boldsymbol{\mathcal{R}}_\xi^{(w)} + \boldsymbol{\mathcal{R}}_\xi^{(r)}$,

$$\boldsymbol{\mathcal{R}}_\xi^{(w)}(\mathbf{r}) = \frac{1}{\mu V} \sum_{\mathbf{k} \neq 0} e^{i \mathbf{k} \cdot \mathbf{r}} \frac{\operatorname{sinc}^2(ka)}{k^2} H(k, \xi) \left(\mathbf{I} - \hat{\mathbf{k}}\hat{\mathbf{k}} \right), \tag{4}$$

  where the Hasimoto splitting function is determined by the **splitting parameter** ξ,

$$H(k, \xi) = \left(1 + \frac{k^2}{4\xi^2} \right) e^{-k^2/4\xi^2}. \tag{5}$$

Real-space part

- Converting back to real space we get

$$\mathcal{R}_{\xi}^{(r)}(\mathbf{r}) = F(r,\xi)\left(\mathbf{I} - \hat{\mathbf{r}}\hat{\mathbf{r}}\right) + G(r,\xi)\,\hat{\mathbf{r}}\hat{\mathbf{r}}, \tag{6}$$

  where and $F(r,\xi)$ and $G(r,\xi)$ are scalar functions that **both decay exponentially** in $r^2\xi^2$.
  Analytical formulas are complicated but these can easily be **tabulated** for fast evaluation.

- Diagonal part is well-defined,

$$\mathbf{M}_{ii}^{(r)} = \mathcal{R}^{(r)}(\mathbf{0}) = \frac{1}{24\pi^{3/2}\mu\xi a^2}\left(1 - e^{-4a^2\xi^2} + 4\pi^{1/2}a\xi\,\mathrm{erfc}\,(2a\xi)\right)\mathbf{I}.$$

- If we choose $0 \leq H(k,\xi) \leq 1$ (satisfied by Hasimoto but not Beenakker) we obtain SPD real and wave space parts.

Conditioning

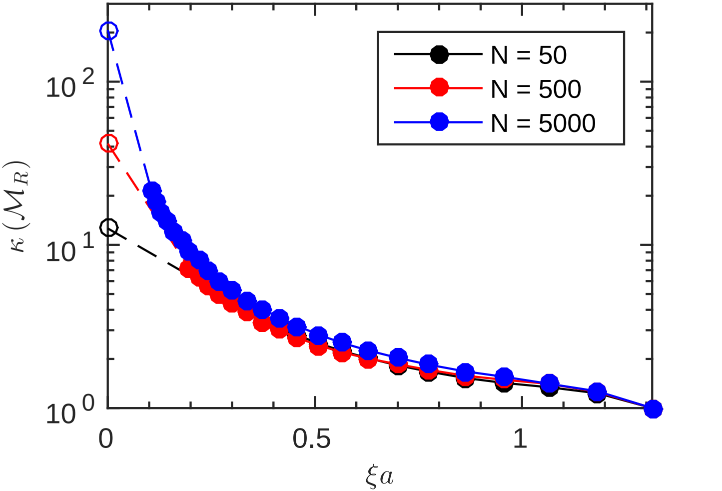

Figure : Condition number of $\mathbf{M}^{(r)}$ for varying number of particles N.

Fourier-space part

- The wave space component of the mobility can be applied efficiently using FFTs as

$$\mathbf{M}^{(w)} = \mathbf{D}^{-1}\mathbf{B}\mathbf{D} = \left(\mathbf{D}^{\dagger}\mathbf{B}^{1/2}\right)\left(\mathbf{D}^{\dagger}\mathbf{B}^{1/2}\right)^{\dagger}, \qquad (7)$$

where **D** is the non-uniform FFT (NUFFT) of Greengard/Lee [2] and

$$\mathbf{B}^{1/2} = \mathrm{Diag}\left(\frac{1}{\mu V}\frac{\mathrm{sinc}^2\left(ka\right)}{k^2}H(k,\xi)\right)^{1/2}.$$

- This shows that the wave space Brownian displacement can be calculated with a single call to the NUFFT,

$$\left(\mathbf{M}^{(w)}\right)^{\frac{1}{2}}\mathbf{W}^{(w)} \equiv \mathbf{D}^{\dagger}\mathbf{B}^{1/2}\mathbf{W}^{(w)}. \qquad (8)$$

- This is basically **equivalent to fluctuating hydrodynamics** (putting stochastic forcing on fluid rather than on particles) as in existing methods, but now corrected in the near field.

Efficiency

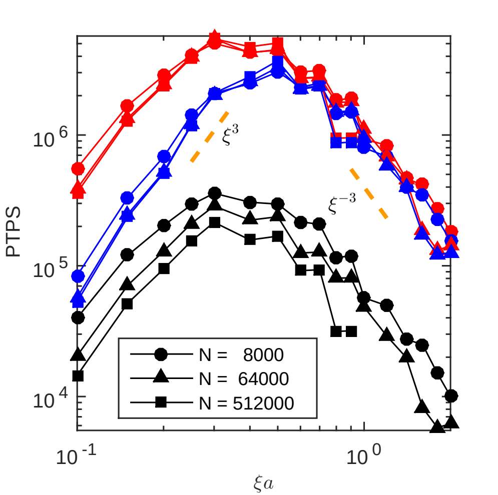

Figure : Particle timesteps per second (PTPS) for a random suspension of hard spheres ($\phi = 0.1$) implemented as a plugin to the HOOMD **GPU framework**. Red=**MF**, blue=$\mathbf{M}^{\frac{1}{2}}\mathbf{W}$ using PSE, black=$\mathbf{M}^{\frac{1}{2}}\mathbf{W}$ without PSE.

Brownian Motion via Fluctuating Hydrodynamics

We consider a rigid body Ω immersed in a fluctuating fluid. In the fluid domain, we have the **fluctuating Stokes equation**

$$\rho \partial_t \mathbf{v} = -\boldsymbol{\nabla} \cdot \boldsymbol{\sigma} = \boldsymbol{\nabla} \pi - \eta \boldsymbol{\nabla}^2 \mathbf{v} - (2 k_B T \eta)^{\frac{1}{2}} \boldsymbol{\nabla} \cdot \boldsymbol{\mathcal{Z}}$$
$$\boldsymbol{\nabla} \cdot \mathbf{v} = 0,$$

with **periodic BCs**, and the fluid stress tensor

$$\boldsymbol{\sigma} = -\pi \mathbf{I} + \eta \left(\boldsymbol{\nabla} \mathbf{v} + \boldsymbol{\nabla}^T \mathbf{v} \right) + (2 k_B T \eta)^{\frac{1}{2}} \boldsymbol{\mathcal{Z}} \tag{9}$$

consists of the usual **viscous stress** as well as a **stochastic stress** modeled by a symmetric **white-noise** tensor $\boldsymbol{\mathcal{Z}}(\mathbf{r}, t)$, i.e., a Gaussian random field with mean zero and covariance

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

Fluid-Body Coupling

At the fluid-body interface the **no-slip boundary condition** is assumed to apply,

$$\mathbf{v}(\mathbf{q}) = \mathbf{u} + \boldsymbol{\omega} \times \mathbf{q} \text{ for all } \mathbf{q} \in \partial\Omega, \tag{10}$$

with the **force and torque balance**

$$\int_{\partial\Omega} \boldsymbol{\lambda}(\mathbf{q})\, d\mathbf{q} = \mathbf{F} \quad \text{and} \quad \int_{\partial\Omega} [\mathbf{q} \times \boldsymbol{\lambda}(\mathbf{q})]\, d\mathbf{q} = \boldsymbol{\tau}, \tag{11}$$

where $\boldsymbol{\lambda}(\mathbf{q})$ is the normal component of the stress on the outside of the surface of the body, i.e., the **traction**

$$\boldsymbol{\lambda}(\mathbf{q}) = \boldsymbol{\sigma} \cdot \mathbf{n}(\mathbf{q}).$$

To model activity we can add **active slip** $\breve{\mathbf{u}}$ due to active boundary layers, without any difficulties (not done here).

Resolved Brownian Dynamics

- Consider a suspension of N_b rigid bodies with **configuration** $\mathbf{Q} = \{\mathbf{q}, \boldsymbol{\theta}\}$ consisting of **positions and orientations** (described using **quaternions**) immersed in a Stokes fluid.
- By eliminating the fluid from the equations in the **overdamped limit** (infinite Schmidt number) we get the equations of **Brownian Dynamics**

$$\frac{d\mathbf{Q}(t)}{dt} = \mathbf{U} = \mathcal{N}\mathbf{F} + \left(2k_B T\,\mathcal{N}\right)^{\frac{1}{2}} \mathcal{W}(t) + \left(k_B T\right) \partial_{\mathbf{Q}} \cdot \mathcal{N},$$

  where $\mathcal{N}(\mathbf{Q})$ is the **body mobility matrix**,
  $\mathbf{U} = \{\mathbf{u}, \omega\}$ collects the **linear and angular velocities**
  $\mathbf{F}(\mathbf{Q}) = \{\mathbf{f}, \boldsymbol{\tau}\}$ collects the **applied forces and torques**.
- **How to compute (the action of) $\mathcal{N}$ and $\mathcal{N}^{\frac{1}{2}}$ and simulate the Brownian motion of the bodies?**

First Kind Boundary Integral Formulation

- Let us first ignore the Brownian motion and compute $\mathcal{N}\mathbf{F}$.
- We can write down an equivalent **first-kind boundary integral equation** for the surface traction $\boldsymbol{\lambda}\,(\mathbf{q} \in \partial\Omega)$,

$$\mathbf{v}\,(\mathbf{q}) = \mathbf{u} + \boldsymbol{\omega} \times \mathbf{q} = \int_{\partial\Omega} \mathbb{G}\left(\mathbf{q}, \mathbf{q}'\right) \boldsymbol{\lambda}\left(\mathbf{q}'\right) d\mathbf{q}' \text{ for all } \mathbf{q} \in \partial\Omega, \quad (12)$$

  along with the force and torque balance condition (11).
  Here $\mathbb{G}$ is the **periodic Stokeslet** (Oseen tensor).
- Note that one can also use a **completed second-kind** or a mixed first-second kind formulation for improved conditioning.
  We only know how to generate Brownian terms efficiently in the first-kind formulation!
- In 2D only the second-kind layer is non-singular and can be discretized spectrally using a simple trapezoidal rule (but nearby bodies interact with a singular $1/r$ kernel, worse than the *log r* for first kind).

Suspensions of Rigid Bodies

- Assume that the surface of the body is discretized in some manner and the **single-layer operator** is computed using some quadrature,

$$\int_{\partial\Omega} \mathbb{G}\left(\mathbf{q},\mathbf{q}'\right) \boldsymbol{\lambda}\left(\mathbf{q}'\right) d\mathbf{q}' \equiv \boldsymbol{\mathcal{M}}\boldsymbol{\lambda} \rightarrow \mathbf{M}\boldsymbol{\lambda},$$

  where $\boldsymbol{\mathcal{M}}$ is an SPD operator given by a kernel that decays like r^{-1}, **discretized as an SPD mobility matrix M**.
- In matrix/operator notation the **mobility problem** is a **saddle-point** linear system for the tractions $\boldsymbol{\lambda}$ and rigid-body motion $\mathbf{U}$,

$$\begin{bmatrix} \boldsymbol{\mathcal{M}} & -\boldsymbol{\mathcal{K}} \\ -\boldsymbol{\mathcal{K}}^T & \mathbf{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda} \\ \mathbf{U} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ -\mathbf{F} \end{bmatrix}, \qquad (13)$$

  where $\boldsymbol{\mathcal{K}}$ is a simple geometric matrix.
- Solve formally using Schur complements to get

$$\mathbf{U} = \boldsymbol{\mathcal{N}}\mathbf{F} = \left(\boldsymbol{\mathcal{K}}^T\boldsymbol{\mathcal{M}}^{-1}\boldsymbol{\mathcal{K}}\right)^{-1}\mathbf{F}.$$

- How do we generate a Gaussian random vector with covariance $\boldsymbol{\mathcal{N}}$?

Brownian motion

- Assume that we knew how to generate a Gaussian random vector with covariance $\mathcal{M}$, i.e., to **generate a random "slip" velocity $\breve{\mathbf{u}}$ with covariance given by the (periodic) Stokeslet**, $\langle \breve{\mathbf{u}} \breve{\mathbf{u}}^T \rangle = \mathcal{M}$.
- *Key idea*: Solve the mobility problem with random slip $\breve{\mathbf{u}}$,

$$\begin{bmatrix} \mathcal{M} & -\mathcal{K} \\ -\mathcal{K}^T & \mathbf{0} \end{bmatrix} \begin{bmatrix} \lambda \\ \mathbf{U} \end{bmatrix} = - \begin{bmatrix} \breve{\mathbf{u}} = (2k_B T)^{1/2} \mathcal{M}^{\frac{1}{2}} \mathbf{W} \\ \mathbf{F} \end{bmatrix}, \qquad (14)$$

$$\mathbf{U} = \mathcal{N}\mathbf{F} + (2k_B T)^{\frac{1}{2}} \mathcal{N}\mathcal{K}^T \mathcal{M}^{-1} \mathcal{M}^{\frac{1}{2}} \mathbf{W} = \mathcal{N}\mathbf{F} + (2k_B T)^{\frac{1}{2}} \mathcal{N}^{\frac{1}{2}} \mathbf{W}.$$

which defines a $\mathcal{N}^{\frac{1}{2}}$ with the correct covariance:

$$\mathcal{N}^{\frac{1}{2}} \left(\mathcal{N}^{\frac{1}{2}} \right)^{\dagger} = \mathcal{N}\mathcal{K}^T \mathcal{M}^{-1} \mathcal{M}^{\frac{1}{2}} \left(\mathcal{M}^{\frac{1}{2}} \right)^{\dagger} \mathcal{M}^{-1} \mathcal{K} \mathcal{N}$$
$$= \mathcal{N} \left(\mathcal{K}^T \mathcal{M}^{-1} \mathcal{K} \right) \mathcal{N} = \mathcal{N} \mathcal{N}^{-1} \mathcal{N} = \mathcal{N}. \qquad (15)$$

- This **works for a number of different discretizations** including our rigid multiblob or immersed boundary methods [4].

Block-Diagonal Preconditioner

- We have had great success with the indefinite **block-diagonal preconditioner** [4]

$$\mathcal{P} = \begin{bmatrix} \widetilde{\mathcal{M}} & -\mathcal{K} \\ -\mathcal{K}^T & \mathbf{0} \end{bmatrix} \tag{16}$$

where we neglect all hydrodynamic interactions between distinct bodies in the preconditioner,

$$\widetilde{\mathcal{M}}^{(pq)} = \delta_{pq} \mathcal{M}^{(pp)}. \tag{17}$$

- This takes care of the inherent ill-conditioning of first-kind integral methods so we don't really need second-kind formulations, except for unreasonably tight error tolerances (highly-resolved problems).
- For the **mobility problem**, we find a **constant number of GMRES iterations** independent of the number of particles, growing only weakly with density.

Fluctuating Boundary Integral method

- The **FBEM method** is the core of **Bill Bao**'s Ph.D. thesis (May 2017), with help from **Manas Rachh**, **Leslie Greengard**, and **Eric Keaveny**.
- This proof-of-concept algorithm/implementation is in **2D only**, but the basic ideas can be carried over to 3D *in principle* (but with many technical difficulties that need to be overcome!).
- First, we follow the Spectral Ewald method of Lindbo and Tornberg [2] and apply the same **Hasimoto splitting** of the Stokeslet into far-field and near-field pieces,

$$\mathbb{G} = \mathbb{G}_{\xi}^{(w)} + \mathbb{G}_{\xi}^{(r)},$$

with the same formulas as for RPY but now without the (regularizing) sinc factors,

$$\mathbb{G}_{\xi}^{(w)}(\mathbf{x}, \mathbf{y}) = \frac{1}{\mu V} \sum_{\mathbf{k} \neq 0} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} \frac{H(k,\xi)}{k^2} \left(\mathbf{I} - \hat{\mathbf{k}}\hat{\mathbf{k}} \right).$$

Boundary element discretization

- Recall that $(\boldsymbol{\mathcal{M}}\boldsymbol{\lambda})(\mathbf{q}) \equiv \int_{\partial\Omega} \mathbb{G}\left(\mathbf{q},\mathbf{q}'\right)\boldsymbol{\lambda}\left(\mathbf{q}'\right) d\mathbf{q}'$.
- This splitting of $\mathbb{G}$ induces a corresponding splitting of the mobility operator where **both pieces are SPD**

$$\boldsymbol{\mathcal{M}} = \boldsymbol{\mathcal{M}}_{\xi}^{(w)} + \boldsymbol{\mathcal{M}}_{\xi}^{(r)}.$$

- Observe that the wave-space kernel $\mathbb{G}^{(w)}$ is smooth and regular, so that in 2D we can discretize $\boldsymbol{\mathcal{M}}^{(w)}$ with a trapezoidal rule with spectral accuracy,

$$\mathbf{M}_{ij}^{(w)} = \mathbb{G}_{\xi}^{(w)}\left(\mathbf{r}_i, \mathbf{r}_j\right).$$

- Both $\mathbf{M}^{(w)}$ and $\left(\mathbf{M}^{(w)}\right)^{\frac{1}{2}}$ can be applied efficiently in Fourier space using the FFT, just as for the RPY kernel in the first part of the talk.

Singular quadrature

- Because of the lack of the RPY regularization, here $\mathbb{G}_{\xi}^{(r)}$ is not smooth and it is **singular** just like the Stokeslet (Oseen tensor), i.e., as $\log r$ in 2D and r^{-1} in 3D.
- A higher-order discretization of the singular integrals against $\mathbb{G}_{\xi}^{(r)}$ in 2D can be obtained by using **Alpert quadrature**,

$$\mathbf{M}^{(r)} = \mathbf{M}_{\text{trap}}^{(r)} + \mathbf{M}_{\text{Alpert}}^{(r)},$$

where $\left(\mathbf{M}_{\text{trap}}^{(r)}\right)_{ij} = \mathbb{G}_{\xi}^{(r)}(\mathbf{r}_i, \mathbf{r}_j)$ for $i \neq j$ is a trapezoidal rule for off-diagonal entries, and $\mathbf{M}_{\text{Alpert}}^{(r)}$ is a **block-diagonal banded correction** to obtain singular corrections to the trapezoidal rule.
- The question now is whether $\mathbf{M}^{(r)}$ is SPD and whether we can compute $\left(\mathbf{M}^{(r)}\right)^{\frac{1}{2}} \mathbf{W}^{(r)}$ efficiently.

Near-field part of random slip

- In general $\mathbf{M}^{(r)}_{\text{Alpert}}$ is neither symmetric nor positive semidefinite and so $\mathbf{M}^{(r)}$ is not SPD strictly speaking.
- Nevertheless, we find that symmetrizing $\mathbf{M}^{(r)}_{\text{Alpert}}$ preserves the order of accuracy of Alpert quadrature, and that the Krylov method for computing $\left(\mathbf{M}^{(r)}\right)^{\frac{1}{2}}\mathbf{W}^{(r)}$ is rather insensitive to any small negative eigenvalues of $\mathbf{M}^{(r)}$.
- The Lanczos method converges in a **modest number of iterations** if a block-diagonal **preconditioner** [3] neglecting hydrodynamic interactions among bodies is used.
- Note that for rigid bodies the preconditioner can be obtained by **pre-computing the eigenvalue decomposition** of $\mathbf{M}^{(r)}$ for each body (modest-size matrices).

Numerical Tests

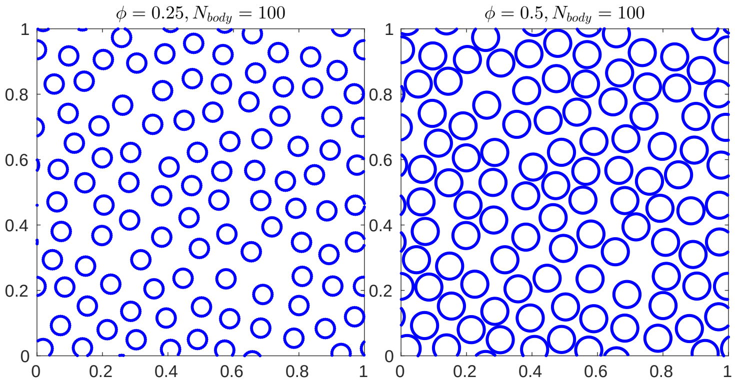

Figure : Random configurations of 100 disks with packing ratio $\phi = 0.25$ (low density) and $\phi = 0.5$ (moderately high density).

Accuracy

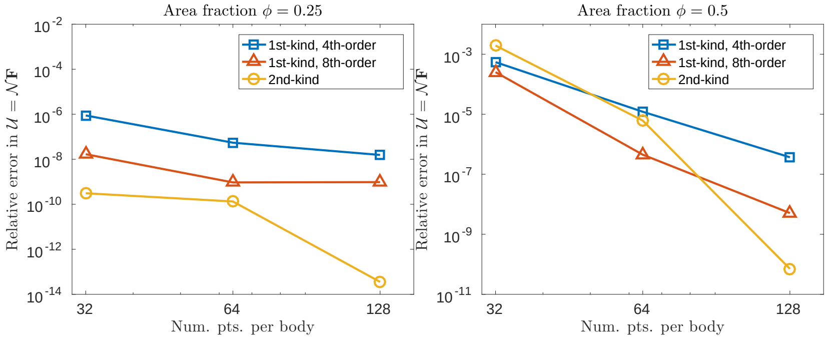

Figure : Accuracy of 1st- and 2nd-kind (spectral in 2D!) mobility solvers for dilute and dense hard-disk suspensions. While the 2nd kind gives spectral accuracy and converges faster with number of DOFs, the first-kind is more accurate for low resolutions especially at higher densities (but what about 3D?).

Convergence and robustness (2D specific!)

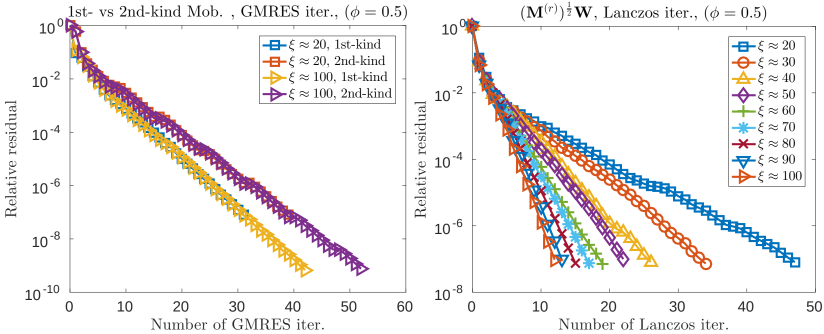

Figure : We expect much better scaling in 3D due to faster decay of Oseen tensor!

Efficiency and Scaling

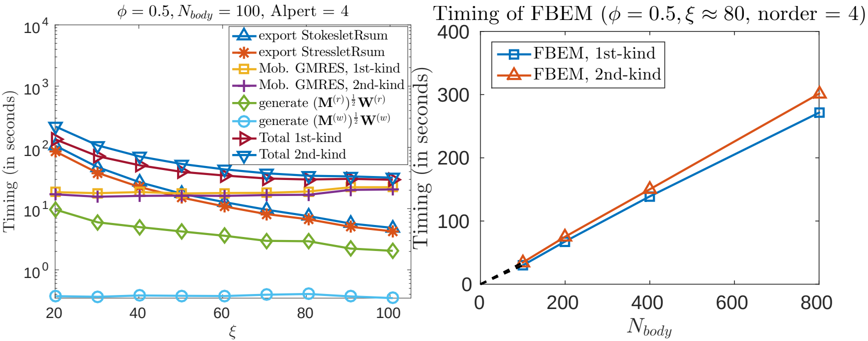

Figure : Optimal splitting parameters and linear scaling.

Brownian Dynamics using FBEM

$$\frac{d\mathbf{Q}(t)}{dt} = \mathbf{U} = \mathcal{N}\mathbf{F} + (2k_B T\mathcal{N})^{\frac{1}{2}}\,\mathcal{W}(t) + (k_B T)\,\partial_{\mathbf{Q}} \cdot \mathcal{N}$$

- We can use a stochastic Adams-Bashforth method [5],

$$\mathbf{Q}^{n+1} = \mathbf{Q}^n + \Delta t\left(\frac{3}{2}\mathbf{N}^n\mathbf{F}^n - \frac{1}{2}\mathbf{N}^{n-1}\mathbf{F}^{n-1}\right) + \sqrt{2k_B T\Delta t}(\mathbf{N}^n)^{\frac{1}{2}}\mathbf{W}^n$$
$$+\Delta t\frac{k_B T}{\delta}\left[\mathbf{N}\left(\mathbf{Q}^n + \frac{\delta}{2}\widetilde{\mathbf{W}}^n\right)\widetilde{\mathbf{W}}^n - \mathbf{N}\left(\mathbf{Q}^n - \frac{\delta}{2}\widetilde{\mathbf{W}}^n\right)\widetilde{\mathbf{W}}^n\right].$$

- The red terms can be computed using the **FBEM method**.
- The magenta terms (here $\delta \to 0$ is a numerical parameter) are a **random finite difference (RFD) technique** that we have developed over the past few years [5].
- This method is **expensive** because it requires 4 GMRES solves per time step.

Stochastic Drift via RFD

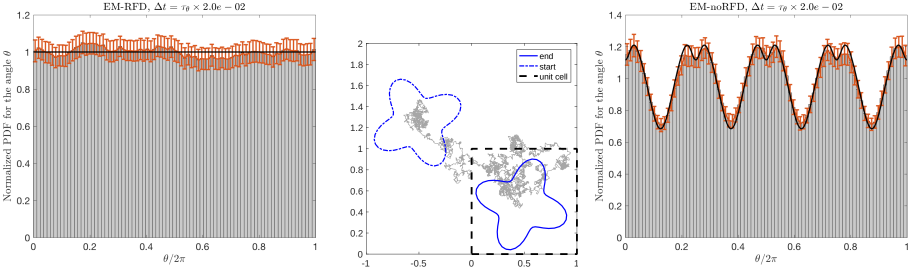

Figure : Equilibrium distributions of θ of a 4-fold starfish diffusing in a periodic domain. (Left) EM with RFD (correct!). (Right) EM without RFD (wrong).

Multi-Body Test

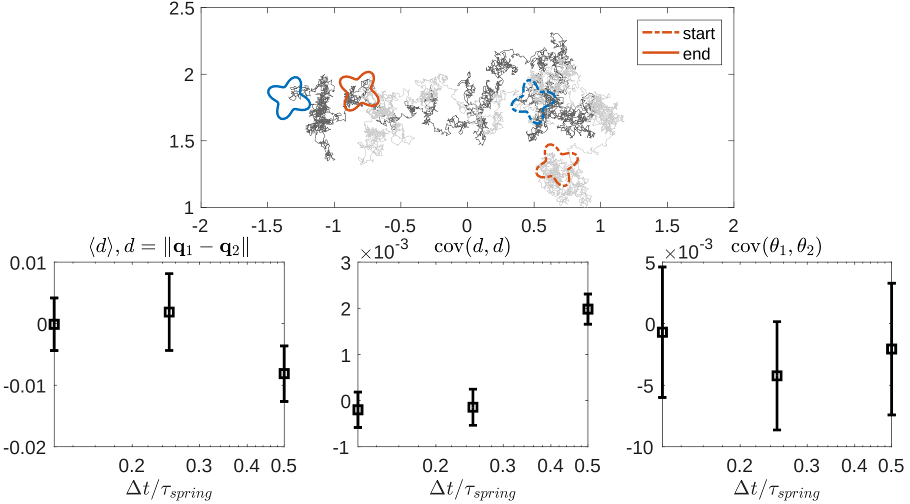

Figure : $U(\mathbf{q}_1, \theta_1, \mathbf{q}_2, \theta_2) = \frac{k_s}{2}(|\mathbf{q}_1 - \mathbf{q}_2| - l_s)^2 + \frac{k_\theta}{2}(\theta_1 - \frac{\pi}{4})^2 + \frac{k_\theta}{2}(\theta_2 - \frac{\pi}{2})^2$

Random Traction Euler-Maruyuama

- One can make more efficient temporal integrators (work by Brennan Sprinkle and Florencio Balboa) that are more accurate and require less GMRES solves per time step, for example, the following **Euler scheme**:

1. Solve a mobility problem with a **random force+torque**:

$$\begin{bmatrix} \mathcal{M} & -\mathcal{K} \\ -\mathcal{K}^T & \mathbf{0} \end{bmatrix}^n \begin{bmatrix} \lambda^{RFD} \\ \mathbf{U}^{RFD} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ -\widetilde{\mathbf{W}} \end{bmatrix}. \tag{18}$$

2. Compute **random finite differences**:

$$\begin{aligned} \mathbf{F}^{RFD} &= \frac{k_B T}{\delta} \left(\mathcal{K}^T \left(\mathbf{Q}^n + \delta \widetilde{\mathbf{W}} \right) - \left(\mathcal{K}^n \right)^T \right) \lambda^{RFD} \\ \breve{\mathbf{u}}^{RFD} &= \frac{k_B T}{\delta} \left(\mathcal{M} \left(\mathbf{Q}^n + \delta \widetilde{\mathbf{W}} \right) - \mathcal{M}^n \right) \lambda^{RFD} + \\ &- \frac{k_B T}{\delta} \left(\mathcal{K} \left(\mathbf{Q}^n + \delta \widetilde{\mathbf{W}} \right) - \mathcal{K}^n \right) \mathbf{U}^{RFD}. \end{aligned}$$

Random Traction EM contd.

1. Compute **correlated random slip**:

$$\breve{\mathbf{u}}^n = \left(\frac{2k_B T}{\Delta t}\right)^{1/2} (\mathcal{M}^n)^{\frac{1}{2}} \mathbf{W}^n$$

2. Solve the saddle-point system:

$$\begin{bmatrix} \mathcal{M} & -\mathcal{K} \\ -\mathcal{K}^T & \mathbf{0} \end{bmatrix}^n \begin{bmatrix} \boldsymbol{\lambda}^n \\ \mathbf{U}^n \end{bmatrix} = -\begin{bmatrix} \breve{\mathbf{u}}^n + \breve{\mathbf{u}}^{RFD} \\ \mathbf{F}^n - \mathbf{F}^{RFD} \end{bmatrix}. \tag{19}$$

3. Move the particles (rotate for orientation)

$$\mathbf{Q}^{n+1} = \mathbf{Q}^n + \Delta t\, \mathbf{U}^n$$

.

Random Slip Trapezoidal Scheme

- One can make more efficient temporal integrators (work by Brennan Sprinkle and Florencio Balboa) that are more accurate and require less GMRES solves per time step, for example, the following **trapezoidal scheme**:

1. Solve a mobility problem with an **uncorrelated random slip**:

$$\begin{bmatrix} \mathcal{M} & -\mathcal{K} \\ -\mathcal{K}^T & \mathbf{0} \end{bmatrix}^n \begin{bmatrix} \boldsymbol{\lambda}^{RFD} \\ \mathbf{U}^{RFD} \end{bmatrix} = \begin{bmatrix} -\widetilde{\mathbf{W}} \in \text{Range}\left(\mathcal{M}^n\right) \\ 0 \end{bmatrix}. \qquad (20)$$

2. Compute **random finite differences**:

$$\mathbf{F}^{RFD} = \frac{k_B T}{\delta} \left(\mathcal{K}^T \left(\mathbf{Q}^n + \delta \mathbf{U}^{RFD} \right) - \left(\mathcal{K}^n \right)^T \right) \widetilde{\mathbf{W}}$$

$$\breve{\mathbf{u}}^{RFD} = \frac{k_B T}{\delta} \left(\mathcal{M} \left(\mathbf{Q}^n + \delta \mathbf{U}^{RFD} \right) - \mathcal{M}^n \right) \widetilde{\mathbf{W}}$$

Random Slip Trapezoidal Scheme contd.

1. Compute **correlated random slip**:

$$\breve{\mathbf{u}}^n = \left(\frac{2k_B T}{\Delta t}\right)^{1/2} (\mathcal{M}^n)^{\frac{1}{2}} \mathbf{W}^n$$

2. Take a **predictor FBEM** step:

$$\begin{bmatrix} \mathcal{M} & -\mathcal{K} \\ -\mathcal{K}^T & \mathbf{0} \end{bmatrix}^n \begin{bmatrix} \boldsymbol{\lambda}^p \\ \mathbf{U}^p \end{bmatrix} = - \begin{bmatrix} \breve{\mathbf{u}}^n \\ \mathbf{F}^n \end{bmatrix}. \tag{21}$$

3. Compute predicted $\mathbf{Q}^p = \mathbf{Q}^n + \Delta t\, \mathbf{U}^n$.
4. Take a **trapezoidal corrector FBEM** step:

$$\begin{bmatrix} \mathcal{M} & -\mathcal{K} \\ -\mathcal{K}^T & \mathbf{0} \end{bmatrix}^p \begin{bmatrix} \boldsymbol{\lambda}^c \\ \mathbf{U}^c \end{bmatrix} = - \begin{bmatrix} \breve{\mathbf{u}}^n + 2\breve{\mathbf{u}}^{RFD} \\ \mathbf{F}^p - 2\mathbf{F}^{RFD} \end{bmatrix}. \tag{22}$$

5. Complete the update, $\mathbf{Q}^{n+1} = \mathbf{Q}^n + \frac{\Delta t}{2} (\mathbf{U}^p + \mathbf{U}^c)$.

Rigid Multiblob Models

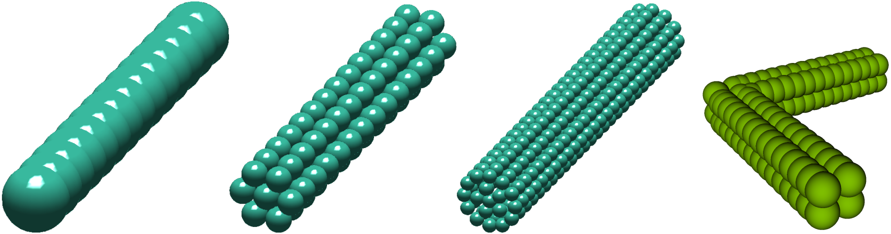

Figure : Blob or "raspberry" models of a spherical colloid.

- The rigid body is discretized through a number of spherical "**beads**" or "**blobs**" which interact via the **Rotne-Prager-Yamakawa** tensor.
- The mathematics is the same as in FBEM, except that $\mathcal{M}$ is now given by the RPY mobility, which is equivalent to a **(smartly!) regularized first-kind boundary integral formulation** [4].

Example: Confined Boomerang Suspension

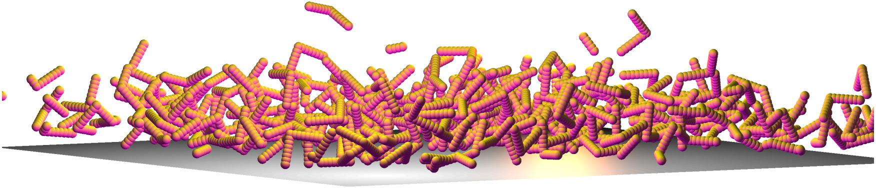

Figure : Quasi-periodic suspension of sedimented colloidal boomerangs using slip trapezoidal scheme and rigid multiblobs (Brennan Sprinkle).

Conclusions

- **Ewald (Hasimoto) splitting** can be used to accelerate both deterministic and stochastic colloidal simulations in periodic domains.
- Key is to ensure that **both the near-field and far-field are (essentially) SPD** so one piece of the noise is generated using FFTs and the other using an iterative method.
- Using these principles we have constructed a **linear-scaling** fluctuating boundary element method.
- Specialized temporal integrators employing **random finite differences** are required to do BD correctly and efficiently.
- The far-field can be done in **non-periodic but finite domains** using a discrete Stokes solver and fluctuating hydrodynamics.
- **Can a similar idea be used with grid-free fast multipole methods?**

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