A fluctuating boundary integral method for Brownian suspensions

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Complex Creeping Fluids: Numerical Methods and Theory
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Brownian Particles of Complex Shape

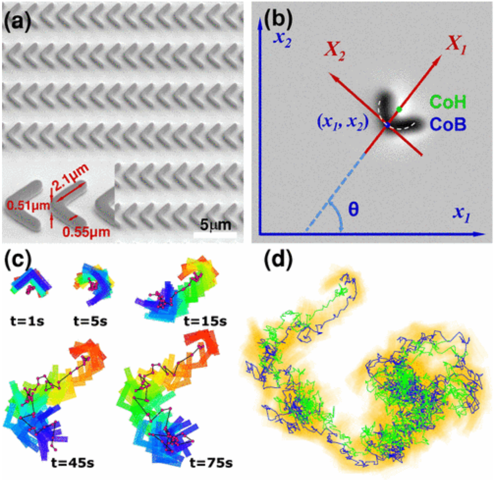

Figure: Brownian motion of *passive* boomerang colloidal particles from Chakrabarty et al. 2013

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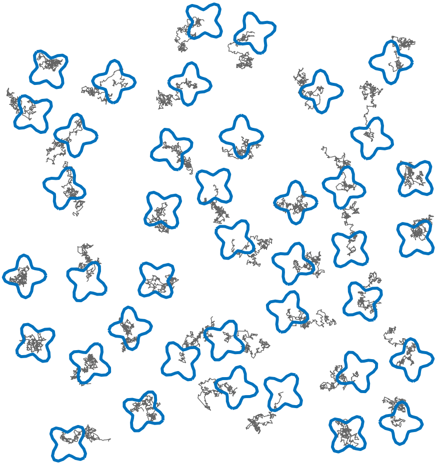


Figure: Brownian suspension of 40 starfish-shaped particles.

Brownian Dynamics with Hydrodynamic Interactions
(BD-HI)

- Consider a suspension of N rigid bodies with configuration $\mathbf{Q} = \{\mathbf{q}_\beta, \boldsymbol{\theta}_\beta\}_{\beta=1}^{N}$ consisting of **positions** and **orientations** immersed in a Stokes fluid.
- The Ito stochastic equation of **Brownian Dynamics** (BD) is

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

  where $\boldsymbol{\mathcal{N}}(\mathbf{Q})$ is the **body mobility matrix**, $\mathbf{F} = \{\mathbf{f}_\beta, \boldsymbol{\tau}_\beta\}_{\beta=1}^{N}$ is the applied **forces** and **torques**, $k_B T$ is the temperature, and $\boldsymbol{\mathcal{W}}(t)$ is a vector of independent white noise processes.
- The stochastic noise amplitude satisfies the **fluctuation-dissipation balance**: $\boldsymbol{\mathcal{N}}^{\frac{1}{2}} \left(\boldsymbol{\mathcal{N}}^{\frac{1}{2}}\right)^{*} = \boldsymbol{\mathcal{N}}$.
- The **stochastic drift** term $\partial_{\mathbf{Q}} \cdot \boldsymbol{\mathcal{N}} = \sum_j \partial_j \mathcal{N}_{ij}$ is related to the Ito interpretation of the noise.

Hydrodynamic Body Mobility Matrix

- The **body mobility matrix** $\mathcal{N}(\mathbf{Q}) \succ \mathbf{0}$ is a **symmetric positive definite** (SPD) and it includes **hydrodynamic interactions** and (periodic) **boundary conditions**.
- For viscous-dominated flows ($Re \to 0$), we can assume **steady Stokes flow** and solve the deterministic **Stokes mobility problem**,

$$\mathbf{U} = \mathcal{N}\mathbf{F},$$

where $\mathbf{U} = \{\mathbf{u}_\beta, \boldsymbol{\omega}_\beta\}_{\beta=1}^{N}$ collects the linear and angular velocities.

- At every time step of BD simulation, we need to generate particle velocity in the form of (dropping $k_B T$),

$$\widetilde{\mathbf{U}} = \mathcal{N}\mathbf{F} + \mathcal{N}^{\frac{1}{2}}\mathbf{W}.$$

- This talk: How to accurately and efficiently compute **the action of** $\mathcal{N}$ and $\mathcal{N}^{\frac{1}{2}}$?

Motivations

The majority of BD-HI methods in chemical engineering:

- are limited to spherical particles;
- use an *uncontrolled* truncation of multipole expansion $\Longrightarrow$ low accuracy in the near field;
- scale super-linearly for generating $\mathcal{N}^{\frac{1}{2}}\mathbf{W}$.

We combine ideas from **Positively Split Ewald** (Fiore et al. 2017) and boundary integral methods to develop methods that

- handle particles of nonspherical, *complex shape*;
- have *controlled* accuracy for dense suspensions;
- achieve *linear-scaling* with the number of particles.

$\Longrightarrow$ *1st* boundary integral method that accounts for Brownian motion of nonspherical particles immersed in a viscous incompressible fluid.
Bao et al. 2017, submitted to JCP [arXiv:1709.01480].

First-Kind Boundary Integral Formulation

- Let us first ignore Brownian terms $\mathcal{N}^{\frac{1}{2}}\mathbf{W}$ and solve a **mobility problem** to compute $\mathcal{N}\mathbf{F}$.
- For simplicity, consider only a single body Ω. The **first-kind boundary integral equation** for the mobility problem,

$$\mathbf{u} + \boldsymbol{\omega} \times (\mathbf{x} - \mathbf{q}) = \mathbf{v}(\mathbf{x} \in \partial\Omega) = \int_{\partial\Omega} \mathbb{G}(\mathbf{x} - \mathbf{y})\ \boldsymbol{\psi}(\mathbf{y}) dS_{\mathbf{y}}, \quad (1)$$

  along with **force and torque balance** conditions,

$$\int_{\partial\Omega} \boldsymbol{\psi}(\mathbf{x})\ dS_{\mathbf{x}} = \mathbf{f} \quad \text{and} \quad \int_{\partial\Omega} (\mathbf{x} - \mathbf{q}) \times \boldsymbol{\psi}(\mathbf{x})\ dS_{\mathbf{x}} = \boldsymbol{\tau}, \quad (2)$$

  where $\boldsymbol{\psi}(\mathbf{x} \in \partial\Omega)$ is the **traction** and $\mathbb{G}$ is the (periodic) Green's function for the Stokes flow (Stokeslet).
- Note that one can alternatively use a **completed second-kind** or a mixed first-second kind formulation for improved conditioning. We only know how to generate Brownian displacements efficiently in the first-kind formulation.

First-Kind Boundary Integral Formulation

- Assume that the surface of the body $\partial\Omega$ is discretized in some manner, and the **single-layer operator** $\mathcal{M}$ is approximated by some quadrature,

$$\int_{\partial\Omega} \mathbb{G}(\mathbf{x}-\mathbf{y})\, \psi(\mathbf{y}) dS_{\mathbf{y}} \equiv \mathcal{M}\psi \to \mathbf{M}\boldsymbol{\mu},$$

  where $\mathcal{M}$ is a SPD operator with kernel $\mathbb{G}$ with r^{-1} singularity in 3D ($\log r$ in 2D), discretized as a SPD *single-layer matrix* $\mathbf{M}$.
- In matrix notation the **mobility problem** can be written as a **saddle-point** linear system for the surface forces $\boldsymbol{\mu}$ and rigid-body motion $\mathbf{U} = \{\mathbf{u}, \boldsymbol{\omega}\}$,

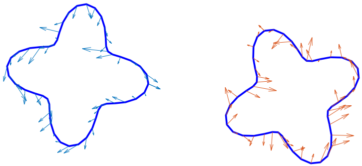
$$\begin{bmatrix} \mathbf{M} & -\mathbf{K} \\ -\mathbf{K}^\top & \mathbf{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{\mu} \\ \mathbf{U} \end{bmatrix} = - \begin{bmatrix} \mathbf{0} \\ \mathbf{F} \end{bmatrix}, \tag{3}$$

  where $\mathbf{K}^\top\boldsymbol{\mu}$ is the discrete force and torque balances.
- Using Schur complement to eliminate $\boldsymbol{\mu}$, we get

$$\mathbf{U} = \mathcal{N}\mathbf{F} = (\mathbf{K}^\top\mathbf{M}^{-1}\mathbf{K})^{-1}\mathbf{F}.$$

Brownian Displacements

- How do we compute the action of $\mathcal{N}^{\frac{1}{2}}$?
  More precisely, how to generate a Gaussian random vector with covariance $\mathcal{N}$?
- Assume for now we knew how to generate a random surface velocity $\breve{\mathbf{v}}(\mathbf{x} \in \partial\Omega)$ with covariance $\mathbf{M}$ (periodic Stokeslet).



- In the continuum setting, $\breve{\boldsymbol{v}}$ is a **distribution**, not a function. Formally,

$$\langle \breve{\boldsymbol{v}} \breve{\boldsymbol{v}} \rangle = \boldsymbol{\mathcal{M}}.$$

Brownian Displacements

- *Key idea 1*: solve the **mobility problem** with $\check{\mathbf{v}} = \mathbf{M}^{\frac{1}{2}}\mathbf{W}$,

$$\begin{bmatrix} \mathbf{M} & -\mathbf{K} \\ -\mathbf{K}^\top & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mu \\ \mathbf{U} \end{bmatrix} = - \begin{bmatrix} \check{\mathbf{v}} \\ \mathbf{F} \end{bmatrix}, \tag{4}$$

$$\Longrightarrow \mathbf{U} = \mathcal{N}\mathbf{F} + \mathcal{N}\mathbf{K}^\top\mathbf{M}^{-1}\mathbf{M}^{\frac{1}{2}}\mathbf{W} = \mathcal{N}\mathbf{F} + \mathcal{N}^{\frac{1}{2}}\mathbf{W},$$

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

$$\begin{aligned} \mathcal{N}^{\frac{1}{2}}\left(\mathcal{N}^{\frac{1}{2}}\right)^* &= \mathcal{N}\ \mathbf{K}^\top\mathbf{M}^{-1}\mathbf{M}^{\frac{1}{2}}\left(\mathbf{M}^{\frac{1}{2}}\right)^*\mathbf{M}^{-1}\mathbf{K}\ \mathcal{N} \\ &= \mathcal{N}(\mathbf{K}^\top\mathbf{M}^{-1}\mathbf{K})\mathcal{N} = \mathcal{N}(\mathcal{N})^{-1}\mathcal{N} = \mathcal{N}. \end{aligned} \tag{5}$$

- $\check{\mathbf{v}}$ comes from the stochastic stress tensor in **fluctuating hydrodynamics** after eliminating the fluid velocity and pressure from the fluid+body equations of motion.

Ewald Splitting of $\mathbf{M}$

- We need accurate and fast algorithms for $\mathbf{M}\boldsymbol{\mu}$ and $\mathbf{M}^{\frac{1}{2}}\mathbf{W}$.
- *Key idea 2*: split the Stokeslet into **SPD** kernels:

$$\mathbb{G} = \underbrace{H * \mathbb{G}}_{\substack{\text{singular}\\ \text{near-field}}} + \underbrace{(\mathbb{G} - H * \mathbb{G})}_{\substack{\text{smooth}\\ \text{far-field}}} \equiv \mathbb{G}_{\xi}^{(r)} + \mathbb{G}_{\xi}^{(w)}, \tag{6}$$

where the Hasimoto function is $\widehat{H}(k;\xi) = \left(1 + \frac{k^2}{4\xi^2}\right) e^{-k^2/4\xi^2}$.
This is the key idea of **Positively Split Ewald** (Fiore et al., J. Chem. Phys., 2017).

- Recall that

$$\int_{\partial\Omega} \mathbb{G}(\mathbf{x}-\mathbf{y})\psi(\mathbf{y})dS_{\mathbf{y}} \equiv \boldsymbol{\mathcal{M}}\psi \approx \mathbf{M}\boldsymbol{\mu}.$$

The splitting of $\mathbb{G}$ naturally induces the splitting of $\boldsymbol{\mathcal{M}}$, and subsequently the splitting of $\mathbf{M}$ into **SPD matrices**,

$$\mathbf{M} = \mathbf{M}^{(r)} + \mathbf{M}^{(w)}. \tag{7}$$

Fast Algorithm for $\mathbf{M}\boldsymbol{\mu}$

▷ $\mathbf{M}^{(r)}\boldsymbol{\mu}$:

- To handle the singularity of $\mathbb{G}_\xi^{(r)}$, we need to employ **singular quadrature** (e.g., Alpert quadrature in 2D).
- Since $\mathbb{G}_\xi^{(r)}$ decays as $\exp(-\xi^2 r^2)$, the mat-vec product $\mathbf{M}^{(r)}\boldsymbol{\mu}$ can be computed rapidly with linear-scaling in the real space.

▷ $\mathbf{M}^{(w)}\boldsymbol{\mu}$:

- The far-field sum can be accelerated by the **Spectral Ewald** method (Lindbo/Tornberg) in Fouier space,

$$\mathbf{M}^{(w)} = \mathbf{D}^\dagger \mathbf{B} \mathbf{D}, \tag{8}$$

where $\mathbf{D}$ is the non-uniform FFT (Greengard/Lee), and $\mathbf{B}$ is a SPD block-diagonal matrix (in Fourier space),

$$\mathbf{B}(k,\xi) = \frac{\widehat{H}(k,\xi)}{k^2}(\mathbf{I} - \hat{\mathbf{k}}\hat{\mathbf{k}}).$$

Splitting of $\mathbf{M}^{1/2}\mathbf{W}$

- *Key Idea 3*: generate random surface velocity with covariance $\mathbf{M}$ by

$$\mathbf{M}^{\frac{1}{2}}\mathbf{W} \overset{\mathrm{d.}}{=} \left(\mathbf{M}^{(w)}\right)^{\frac{1}{2}}\mathbf{W}^{(w)} + \left(\mathbf{M}^{(r)}\right)^{\frac{1}{2}}\mathbf{W}^{(r)}, \tag{9}$$

  if both $\mathbf{M}^{(w)}$ and $\mathbf{M}^{(r)}$ are SPD and $\langle \mathbf{W}^{(w)}\mathbf{W}^{(r)}\rangle = \mathbf{0}$.
- The far-field matrix $\mathbf{M}^{(w)}$ is SPD by construction, and we can write

$$\mathbf{M}^{(w)} = \mathbf{D}^{\dagger}\mathbf{B}\mathbf{D} = \left(\mathbf{D}^{\dagger}\mathbf{B}^{\frac{1}{2}}\right)\left(\mathbf{D}^{\dagger}\mathbf{B}^{\frac{1}{2}}\right)^{\dagger}, \tag{10}$$

  so that the wave-space random surface velocity can be generated with a single call to the NUFFT,

$$\left(\mathbf{M}^{(w)}\right)^{\frac{1}{2}}\mathbf{W}^{(w)} = \mathbf{D}^{\dagger}\mathbf{B}^{\frac{1}{2}}\mathbf{W}^{(w)}. \tag{11}$$

Near-Field Contribution of $\mathbf{M}^{1/2}\mathbf{W}$

- The near-field random surface velocity $\left(\mathbf{M}^{(\mathbf{r})}\right)^{\frac{1}{2}} \mathbf{W}^{(r)}$ can be generated by a **Krylov Lanczos method** of Chow/Saad.
- Because of the **short-ranged** nature of $\mathbf{M}^{(r)}$, the Lanczos method converges in a reasonable amount of iterations.
- However, in general, $\mathbf{M}^{(r)}$ is *not* symmetric, so $\mathbf{M}^{(r)}$ is not SPD strictly speaking, because the Alpert quadrature does not enforce the SPD of $\boldsymbol{\mathcal{M}}$.
- Nevertheless, we find that symmetrizing $\frac{1}{2}\left(\mathbf{M}^{(r)} + \left(\mathbf{M}^{(r)}\right)^{\top}\right)$ preserves the order of accuracy of Alpert quadrature, and the Krylov Lanczos iteration is rather **insensitive** to any small negative eigenvalues.

Block-Diagonal Preconditioners

$$\begin{bmatrix} \mathbf{M} & -\mathbf{K} \\ -\mathbf{K}^\top & \mathbf{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{\mu} \\ \mathbf{U} \end{bmatrix} = - \begin{bmatrix} \mathbf{M}^{\frac{1}{2}}\mathbf{W} \\ \mathbf{F} \end{bmatrix}.$$

- To mitigate the inherent ill-conditioning of $\mathbf{M}$ due to the use of a first-kind boundary integral formulation, we apply a **block-diagonal preconditioner**, *i.e.*, we simply neglect all hydrodynamic interactions between distinct bodies in the preconditioner, both when solving the saddle-point mobility problem using GMRES, and in the Lanczos iteration for generating $\left(\mathbf{M}^{(r)}\right)^{\frac{1}{2}} \mathbf{W}^{(r)}$.
- Both preconditioners can be **precomputed** using LAPACK for a single body, and then applied to many bodies via two fast vector **rotations** per body.
- GMRES and Lanczos converge in a **constant** number of iterations, growing only weakly with packing fraction.

Summary

FBIM provides the key ingredients for BD simulations of complex-shaped particle: $\mathcal{N}\mathbf{F} + \mathcal{N}^{\frac{1}{2}}\mathbf{W}$.

- Solve the **mobility problem** with a random surface velocity:

$$\begin{bmatrix} \mathbf{M} & -\mathbf{K} \\ -\mathbf{K}^\top & \mathbf{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{\mu} \\ \mathbf{U} \end{bmatrix} = - \begin{bmatrix} \mathbf{M}^{\frac{1}{2}}\mathbf{W} \\ \mathbf{F} \end{bmatrix}, \tag{12}$$

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

- Fast methods for $\mathbf{M}\boldsymbol{\mu}$ and $\mathbf{M}^{\frac{1}{2}}\mathbf{W}$.
  - $\mathbf{M} = \mathbf{M}^{(r)} + \mathbf{M}^{(w)}$: sparse mat-vec + Spectral Ewald
  - $\mathbf{M}^{\frac{1}{2}}\mathbf{W} \stackrel{\mathrm{d.}}{=} \left(\mathbf{M}^{(r)}\right)^{\frac{1}{2}}\mathbf{W}^{(r)} + \left(\mathbf{M}^{(w)}\right)^{\frac{1}{2}}\mathbf{W}^{(w)}$: Lanczos + NUFFT.
  - Block-diagonal preconditioner for GMRES and Lanczos.
- An **efficient, accurate, linear-scaling** algorithm for generating deterministic and stochastic particle velocities of Brownian suspensions.

Results

- This proof-of-concept algorithm/implementation is in **2D only**, but the main ideas can be carried over to 3D in principle (but with some technical difficulties that need to be overcome!).

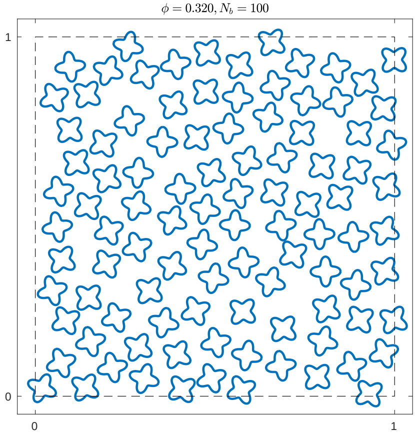


Figure: Random configurations of 100 starfish-shaped particles with packing fraction $\phi = 0.32$ (moderately high density)

Accuracy of $\mathcal{N}$F

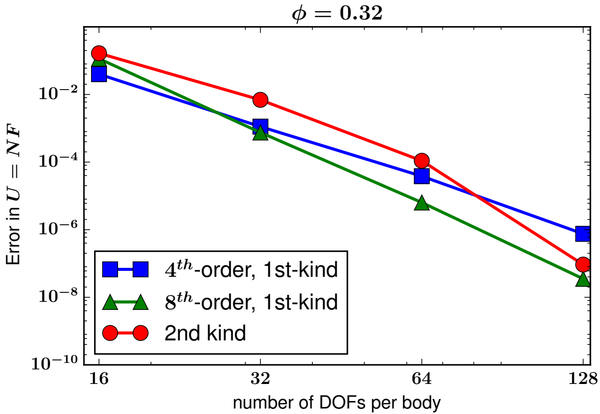


Figure: Accuracy of 1st- and 2nd-kind (spectral in 2D!) deterministic mobility solvers for the dense suspensions. While the 2nd-kind solver gives spectral accuracy and converges faster with number of DOFs, the first kind is more accurate for low resolutions especially at higher densities (but what about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

Convergence and robustness (2D specific!)

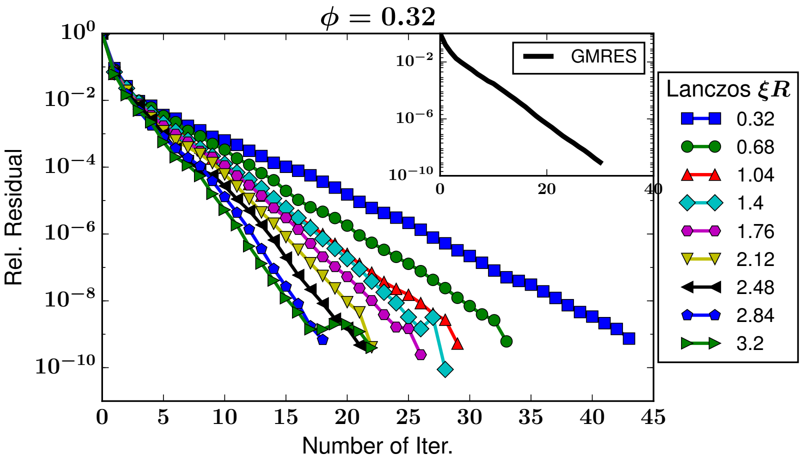


Figure: We expect much better scaling in 3D due to faster decay of Stokeslet.

Scaling

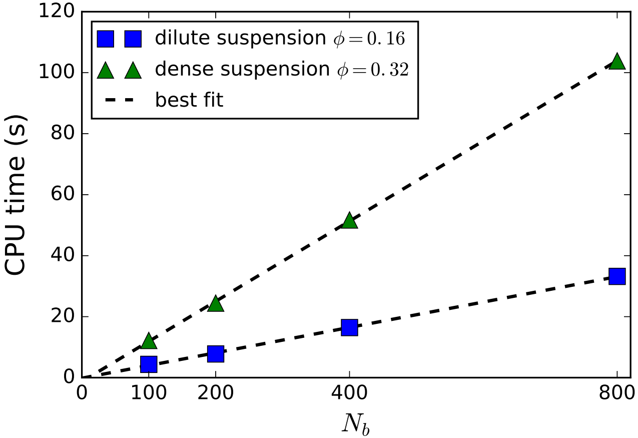


Figure: Linear scaling of the algorithm with the number of bodies.

Conclusion

- **Ewald (Hasimoto) splitting** can be used to accelerate both deterministic and stochastic simulations in periodic domains.
- Key is to ensure both **far-field** and **near-field are (essentially) SPD** so one piece is generated using FFTs and the other using iterative methods.
- Using these principles we have constructed a **linear-scaling** fluctuating boundary integral method (FBIM) for Brownian suspensions of complex-shaped particles.

Future Work

- Generalization to 3D involves several technical difficulties:
  - discretization of particle surfaces (e.g., high-order triangular elements).
  - a suitable choice of quadrature, in particular, one that preserves SPD of the single-layer operator.
- Efficient stochastic temporal integrators that
  - account for the Ito stochastic drift term solving as few as possible mobility problems per time step (see Sprinkle et al., 2017, ArXiv:1709.02410)
  - handle particle collision for denser suspensions.
- Extending FBIM to other domains (e.g., unbounded, confined).
- **Can a similar idea be combined with (grid-free) the Fast Multipole Method for unbounded domains?**