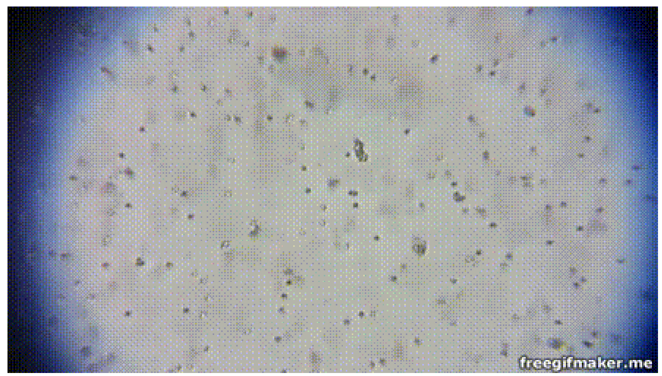
Stochastic Boundary Integral Method for Brownian Suspensions



Changho Kim

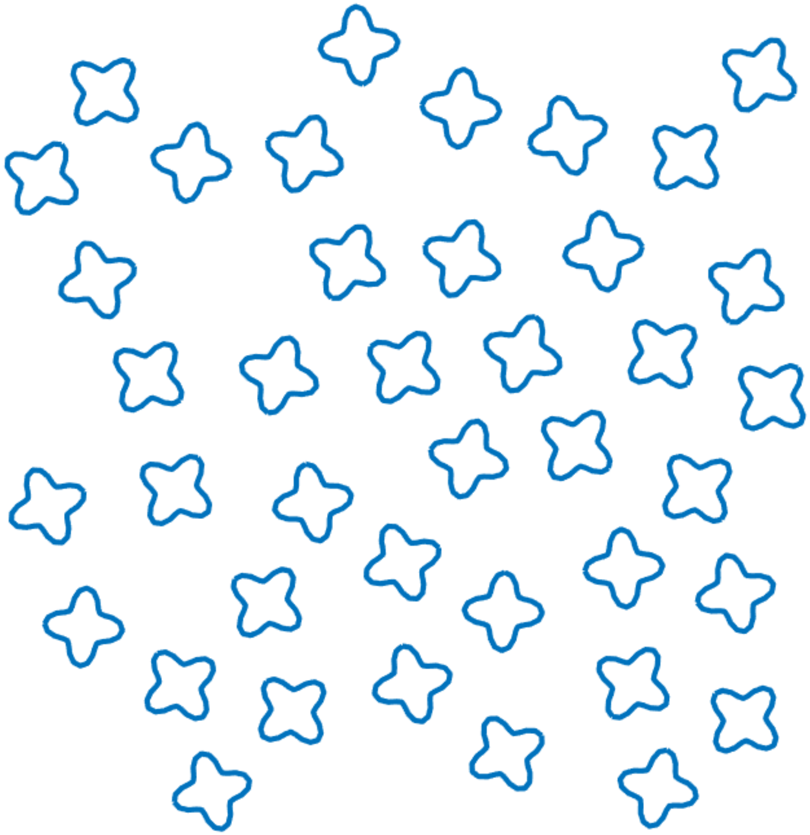
Boundary Integral Equation Research (BIER) Seminar

Main Reference

"A Fluctuating Boundary Integral Method for Brownian Suspensions"

Yuanxun Bao, Manas Rachh, Eric E. Keaveny, Leslie Greengard, Aleksandar Donev

J. Comput. Phys. 374, 1094 (2018)



The first boundary integral method that accounts for Brownian motion of non-spherical particles immersed in a viscous incompressible fluid.

Proof-of-concept example:
Starfish-shaped particles
in a two-dimensional periodic domain

Outline

1. Stochastic dynamics 101

2. Formulations

3. Numerical method

Before We Talk about the FBIM…
(Stochastic Dynamics 101)

1. Langevin description of Brownian motion

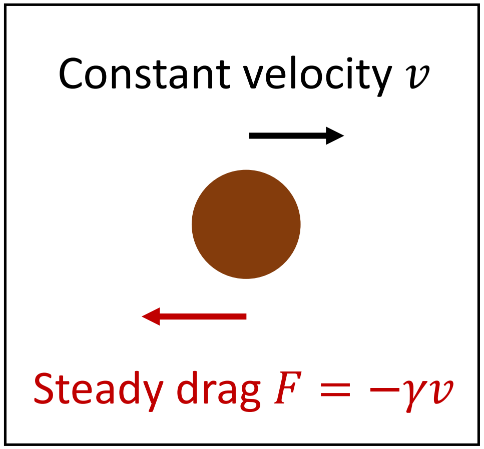
2. Fluctuating hydrodynamics of a homogeneous fluid

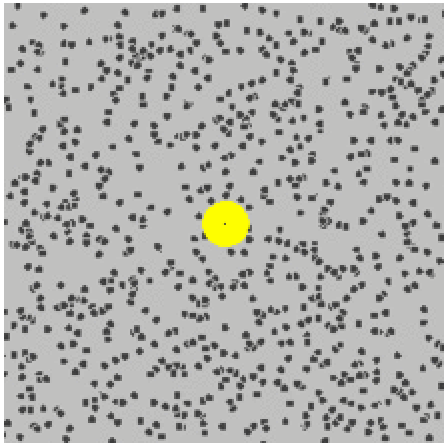
- Basic building blocks for stochastic dynamics
  - Gaussian white noise processes
  - Spatio-temporal Gaussian white noise fields

Langevin Description of Brownian Motion

friction, random force

$$\dot{x} = v \qquad m\dot{v} = -\gamma v + \sqrt{2\gamma k_B T}\,\xi(t)$$





Gaussian white noise process $\xi(t)$: $\langle \xi(t) \rangle = 0 \quad \langle \xi(t)\xi(t') \rangle = \delta(t - t')$

$$\int_0^t \xi(t')dt' \sim \mathcal{N}(\mu = 0, \sigma^2 = t)$$

Hence, $m[v(t + \Delta t) - v(t)] \approx -\gamma v(t)\Delta t + \sqrt{2\gamma k_B T}\,\mathcal{N}(0, \Delta t)$

Fluctuation-Dissipation Balance

$$m\dot{v} = -\gamma v + A\xi(t) \quad \rightarrow \quad v(t) = A\int_{-\infty}^{t} e^{-\frac{\gamma}{m}(t-t')}\xi(t')dt'$$

$A = \sqrt{2\gamma k_B T}$ is chosen so that $\frac{1}{2}\boldsymbol{m}\langle \boldsymbol{v}^2\rangle = \frac{1}{2}\boldsymbol{k_B T}$.

- For each dissipative process, a fluctuating process needs to be incorporated so that the **correct equilibrium** be established.
- The friction and random forces originate from the interactions with the surrounding fluid.

Many Interacting Brownian Particles

Langevin dynamics

$$\dot{\boldsymbol{x}}_i = \boldsymbol{v}_i$$

$$m_i\dot{\boldsymbol{v}}_i = \boldsymbol{f}_{\text{int}} - \gamma_i \boldsymbol{v}_i + \sqrt{2\gamma_i k_B T}\boldsymbol{\xi}_i(t)$$

Brownian dynamics

(overdamped $\rightarrow m_i\dot{\boldsymbol{v}}_i \approx 0$)

$$\dot{\boldsymbol{x}}_i = \frac{\boldsymbol{f}_{\text{int}}}{\gamma_i} + \sqrt{\frac{2k_B T}{\gamma_i}}\boldsymbol{\xi}_i(t) = \frac{D_i}{k_B T}\boldsymbol{f}_{\text{int}} + \sqrt{2D_i}\boldsymbol{\xi}_i(t)$$

- Einstein relation: $D\gamma = k_B T$

Fluctuating Hydrodynamics

momentum dissipation

pressure advection

$$\rho \frac{\partial \boldsymbol{v}}{\partial t} + \boldsymbol{\nabla}\pi = -\rho \boldsymbol{\nabla} \cdot (\boldsymbol{v}\boldsymbol{v}^T) + \eta \nabla^2 \boldsymbol{v} \; + \sqrt{\eta k_B T}\boldsymbol{\nabla} \cdot (\boldsymbol{\mathcal{Z}} + \boldsymbol{\mathcal{Z}}^T)$$

stochastic momentum flux

$$\boldsymbol{\nabla} \cdot \boldsymbol{v} = 0$$

Gaussian white noise field $\langle \mathcal{Z}_{ij}(\boldsymbol{r},t)\mathcal{Z}_{i'j'}(\boldsymbol{r}',t')\rangle = \delta_{ii'}\delta_{jj'}\delta(\boldsymbol{r}-\boldsymbol{r}')\delta(t-t')$

$$\int_{\Delta V} d\boldsymbol{r}' \int_t^{t+\Delta t} dt'\, \mathcal{Z}_{ij}(\boldsymbol{r}',t') \;\sim\; \mathcal{N}(0, \Delta V \Delta t)$$

In the k-space, you can find a similar structure to the Langevin equation:
(i.e. fluctuation-dissipation balance)

$$-(\eta k^2)v_k + \left(\sqrt{2\eta k_B T} ik\right)\mathcal{Z}_k$$

cf. $-\gamma v + \sqrt{2\gamma k_B T}\xi(t)$

Formulations

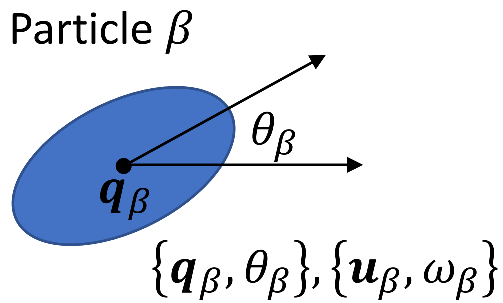
1. Full (=inertial) description

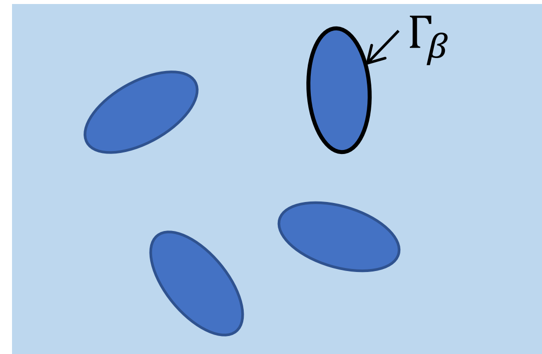
2. Overdamped limit

3. Stokes boundary value problems

4. First-kind integral formulation

Full Fluctuating Hydrodynamics Description





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

$$\rho\, \partial_t \boldsymbol{v} + \boldsymbol{\nabla}\pi = \eta \boldsymbol{\nabla}^2 \boldsymbol{v} + \sqrt{2\eta k_B T}\ \boldsymbol{\nabla} \cdot \boldsymbol{\mathcal{Z}},$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{v} = 0,$$

incompressible Stokes equations

$$\boldsymbol{v}(\boldsymbol{x}, t) = \boldsymbol{u}_\beta + \boldsymbol{\omega}_\beta \times (\boldsymbol{x} - \boldsymbol{q}_\beta), \quad \forall \boldsymbol{x} \in \Gamma_\beta,$$

no-slip boundary condition

traction vectors

$$\boldsymbol{\lambda}_\beta(\boldsymbol{x}) = (\boldsymbol{\sigma} \cdot \boldsymbol{n}_\beta)(\boldsymbol{x})$$

$$\boldsymbol{\lambda}_\beta^{(s)}(\boldsymbol{x}) = \left(\boldsymbol{\sigma}^{(s)} \cdot \boldsymbol{n}_\beta\right)(\boldsymbol{x})$$

stress tensors

$$\boldsymbol{\sigma} = -\pi \boldsymbol{I} + \eta(\boldsymbol{\nabla}\boldsymbol{v} + \boldsymbol{\nabla}^\top \boldsymbol{v}),$$

$$\boldsymbol{\sigma}^{(s)} = \sqrt{2\eta k_B T}\boldsymbol{\mathcal{Z}},$$

$$m_\beta \frac{d\boldsymbol{u}_\beta}{dt} = \boldsymbol{f}_\beta - \int_{\Gamma_\beta} (\boldsymbol{\lambda}_\beta + \boldsymbol{\lambda}_\beta^{(s)})(\boldsymbol{x})\, \mathrm{d}S_{\boldsymbol{x}},$$

$$\mathbf{I}_\beta \cdot \frac{d\boldsymbol{\omega}_\beta}{dt} = \boldsymbol{\tau}_\beta - \int_{\Gamma_\beta} (\boldsymbol{x} - \boldsymbol{x}_\beta) \times (\boldsymbol{\lambda}_\beta + \boldsymbol{\lambda}_\beta^{(s)})(\boldsymbol{x})\, \mathrm{d}S_{\boldsymbol{x}},$$

Overdamped Limit

$$\boldsymbol{Q}_\beta = \{\boldsymbol{q}_\beta, \boldsymbol{\theta}_\beta\} \quad \boldsymbol{Q} = \{\boldsymbol{Q}_\beta\}_{\beta=1}^{N}$$

$$\frac{d\boldsymbol{Q}}{dt} = \boldsymbol{\mathcal{N}}\boldsymbol{F} + \sqrt{2k_BT}\boldsymbol{\mathcal{N}}^{\frac{1}{2}}\boldsymbol{\mathcal{W}} + (k_BT)(\partial_{\boldsymbol{Q}} \cdot \boldsymbol{\mathcal{N}})$$

deterministic case

Body mobility matrix $\boldsymbol{\mathcal{N}} = \boldsymbol{\mathcal{N}}(\boldsymbol{Q})$

$$\boldsymbol{F}(\boldsymbol{Q}) = \{\boldsymbol{f}_\beta(\boldsymbol{Q}), \boldsymbol{\tau}_\beta(\boldsymbol{Q})\}_{\beta=1}^{N} \quad \longleftrightarrow \quad \boldsymbol{U} = \{\boldsymbol{u}_\beta, \boldsymbol{\omega}_\beta\}_{\beta=1}^{N_b}$$

Standard mobility problem

$$-\boldsymbol{\nabla} \cdot \boldsymbol{\sigma} = \boldsymbol{\nabla}\pi - \eta\boldsymbol{\nabla}^2\boldsymbol{v} = \boldsymbol{0},$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{v} = 0,$$

$$\boldsymbol{v}(\boldsymbol{x}) = \boldsymbol{u}_\beta + \boldsymbol{\omega}_\beta \times (\boldsymbol{x} - \boldsymbol{q}_\beta), \quad \forall \boldsymbol{x} \in \Gamma_\beta,$$

$$\int_{\Gamma_\beta} \boldsymbol{\lambda}_\beta(\boldsymbol{x})\, \mathrm{d}S_{\boldsymbol{x}} = \boldsymbol{f}_\beta \quad \text{and} \quad \int_{\Gamma_\beta} (\boldsymbol{x} - \boldsymbol{x}_c) \times \boldsymbol{\lambda}_\beta(\boldsymbol{x})\, \mathrm{d}S_{\boldsymbol{x}} = \boldsymbol{\tau}_\beta.$$

Comparison with Brownian Dynamics

$$\dot{\boldsymbol{x}}_i = \frac{D_i}{k_B T}\boldsymbol{f}_{\mathrm{int}} + \sqrt{2D_i}\boldsymbol{\xi}_i(t)$$

mean velocity   random velocity

$$\frac{d\boldsymbol{Q}}{dt} = \boldsymbol{\mathcal{N}}\boldsymbol{F} + \sqrt{2k_BT}\boldsymbol{\mathcal{N}}^{\frac{1}{2}}\boldsymbol{\mathcal{W}} + (k_BT)(\partial_{\boldsymbol{Q}}\cdot\boldsymbol{\mathcal{N}})$$

$$\boldsymbol{\mathcal{N}}^{\frac{1}{2}}\left(\boldsymbol{\mathcal{N}}^{\frac{1}{2}}\right)^{\top} = \boldsymbol{\mathcal{N}}$$

$$\langle \boldsymbol{\mathcal{W}}(t)\boldsymbol{\mathcal{W}}^T(t')\rangle = \boldsymbol{I}(t-t')$$

$$(\partial_{\boldsymbol{x}}\cdot\boldsymbol{A})_i = \textstyle\sum_j \partial A_{ij}/\partial x_j$$

- Random velocity is multiplicative noise.
  - Third term is stochastic drift due to Ito interpretation.

- How to sample $\int_t^{t+\Delta t}\sqrt{2k_BT}\boldsymbol{\mathcal{N}}^{1/2}\boldsymbol{\mathcal{W}}dt' \approx \widetilde{\boldsymbol{U}}\Delta t$?
  - $\langle \tilde{\boldsymbol{U}}\tilde{\boldsymbol{U}}^{\top}\rangle = \frac{2k_BT}{\Delta t}\boldsymbol{\mathcal{N}},$

Stochastic Stokes Boundary Value Problem

For simplicity, a single particle case is presented.

$$-\boldsymbol{\nabla}\cdot\boldsymbol{\sigma} = \boldsymbol{\nabla}\pi - \eta\boldsymbol{\nabla}^2\boldsymbol{v} = 0, \quad \boldsymbol{r}\in\mathcal{V}\backslash\overline{D},$$

$$\boldsymbol{\nabla}\cdot\boldsymbol{v} = 0,$$

$$\boldsymbol{v}(\boldsymbol{x}) = \boldsymbol{u} + \boldsymbol{\omega}\times(\boldsymbol{x}-\boldsymbol{q}) - \boxed{\breve{\boldsymbol{v}}(\boldsymbol{x})} \quad \boldsymbol{x}\in\Gamma,$$

$$\int_\Gamma \boldsymbol{\lambda}(\boldsymbol{x})\,\mathrm{d}S_{\boldsymbol{x}} = \boldsymbol{f} \quad \text{and} \quad \int_\Gamma (\boldsymbol{x}-\boldsymbol{q})\times\boldsymbol{\lambda}(\boldsymbol{x})\,\mathrm{d}S_{\boldsymbol{x}} = \boldsymbol{\tau}$$

$$\boxed{\langle\breve{\boldsymbol{v}}(\boldsymbol{x})\,\breve{\boldsymbol{v}}(\boldsymbol{y})\rangle = \frac{2k_BT}{\Delta t}\mathbb{G}(\boldsymbol{x}-\boldsymbol{y}), \quad \text{for all} \;\; (\boldsymbol{x}\neq\boldsymbol{y})\in\Gamma}$$

$\mathbb{G}(\boldsymbol{r})$ = Green's function for steady Stokes flow

$$\boldsymbol{v} = \bar{\boldsymbol{v}} + \tilde{\boldsymbol{v}}\;,\;\; \boldsymbol{\sigma} = \bar{\boldsymbol{\sigma}} + \tilde{\boldsymbol{\sigma}}\;,\;\; \boldsymbol{U} = \bar{\boldsymbol{U}} + \tilde{\boldsymbol{U}}, \quad \Rightarrow \quad \langle\tilde{\boldsymbol{U}}\tilde{\boldsymbol{U}}^\top\rangle = \frac{2k_BT}{\Delta t}\boldsymbol{\mathcal{N}},$$

Two BVPs

Stokes BVP without random surface velocity (standard mobility problem)

for $\bar{\boldsymbol{U}} = \boldsymbol{\mathcal{N}}\boldsymbol{F}$

$$-\boldsymbol{\nabla}\cdot\bar{\boldsymbol{\sigma}} = \boldsymbol{\nabla}\bar{\pi} - \eta\boldsymbol{\nabla}^2\bar{\boldsymbol{v}} = \boldsymbol{0},$$

$$\boldsymbol{\nabla}\cdot\bar{\boldsymbol{v}} = 0,$$

$$\bar{\boldsymbol{v}}(\boldsymbol{x}) = \bar{\boldsymbol{u}} + \bar{\boldsymbol{\omega}}\times(\boldsymbol{x}-\boldsymbol{q}), \quad \boldsymbol{x}\in\Gamma$$

$$\int_\Gamma \bar{\boldsymbol{\lambda}}(\boldsymbol{x})\,\mathrm{d}S_{\boldsymbol{x}} = \boldsymbol{f} \quad \text{and} \quad \int_\Gamma (\boldsymbol{x}-\boldsymbol{q})\times\bar{\boldsymbol{\lambda}}(\boldsymbol{x})\,\mathrm{d}S_{\boldsymbol{x}} = \boldsymbol{\tau},$$

A force- and torque-free Stokes BVP with a random surface velocity

for $\widetilde{\boldsymbol{U}} \approx \frac{\mathbf{1}}{\Delta t}\int_t^{t+\Delta t}\sqrt{2k_BT}\boldsymbol{\mathcal{N}}^{1/2}\boldsymbol{\mathcal{W}}dt'$

$$-\boldsymbol{\nabla}\cdot\tilde{\boldsymbol{\sigma}} = \boldsymbol{\nabla}\tilde{\pi} - \eta\boldsymbol{\nabla}^2\tilde{\boldsymbol{v}} = \boldsymbol{0},$$

$$\boldsymbol{\nabla}\cdot\tilde{\boldsymbol{v}} = 0,$$

$$\tilde{\boldsymbol{v}}(\boldsymbol{x}) = \tilde{\boldsymbol{u}} + \tilde{\boldsymbol{\omega}}\times(\boldsymbol{x}-\boldsymbol{q}) - \breve{\boldsymbol{v}}(\boldsymbol{x}), \quad \boldsymbol{x}\in\Gamma,$$

$$\int_\Gamma \tilde{\boldsymbol{\lambda}}(\boldsymbol{x})\,\mathrm{d}S_{\boldsymbol{x}} = \boldsymbol{0} \quad \text{and} \quad \int_\Gamma (\boldsymbol{x}-\boldsymbol{q})\times\tilde{\boldsymbol{\lambda}}(\boldsymbol{x})\,\mathrm{d}S_{\boldsymbol{x}} = \boldsymbol{0}.$$

First-kind Integral Formulation

It is possible to extend the fluid to the entire domain.

$$\boldsymbol{v}(\boldsymbol{x} \in \Gamma) = \boldsymbol{u} + \boldsymbol{\omega} \times (\boldsymbol{x} - \boldsymbol{q}) - \breve{\boldsymbol{v}}(\boldsymbol{x}) = \int_\Gamma \mathbb{G}(\boldsymbol{x} - \boldsymbol{y})\, \boldsymbol{\psi}(\boldsymbol{y})\, \mathrm{d}S_{\boldsymbol{y}},$$

$$\int_\Gamma \boldsymbol{\psi}(\boldsymbol{x})\, \mathrm{d}S_{\boldsymbol{x}} = \boldsymbol{f} \qquad \int_\Gamma (\boldsymbol{x} - \boldsymbol{q}) \times \boldsymbol{\psi}(\boldsymbol{x})\, \mathrm{d}S_{\boldsymbol{x}} = \boldsymbol{\tau}.$$

These equations define a (saddle-point) linear system to be solved for the single-layer density $\boldsymbol{\psi}(\boldsymbol{x} \in \Gamma)$ and particle velocity $\boldsymbol{U} = \{\boldsymbol{u}, \omega\}$

$$(\boldsymbol{\mathcal{M}}\boldsymbol{\psi})(\boldsymbol{x} \in \Gamma) = \int_\Gamma \mathbb{G}(\boldsymbol{x} - \boldsymbol{y})\, \boldsymbol{\psi}(\boldsymbol{y})\, \mathrm{d}S_{\boldsymbol{y}}$$

Compact, self-adjoint, and positive-semidefinite operator in the L^2 sense

⇒

$$\langle \breve{\boldsymbol{v}}\breve{\boldsymbol{v}} \rangle = \frac{2k_BT}{\Delta t}\boldsymbol{\mathcal{M}},$$

$$\breve{\boldsymbol{v}} \overset{\mathrm{d.}}{=} \sum_{i=1}^{\infty} \sqrt{\lambda_i}\, W_i\, \boldsymbol{w}_i,$$

Karhunen-Loeve expansion

cf. $\langle \breve{\boldsymbol{v}}(\boldsymbol{x})\, \breve{\boldsymbol{v}}(\boldsymbol{y}) \rangle = \frac{2k_BT}{\Delta t}\mathbb{G}(\boldsymbol{x} - \boldsymbol{y}), \quad \text{for all } (\boldsymbol{x} \neq \boldsymbol{y}) \in \Gamma$

The most direct way to regularize the singular Green's function is to represent it in Fourier space and then simply truncate the finite-dimensional sum to a finite number of Fourier modes.

Numerical Method

- First-kind formulation → a discrete saddle-point linear system
- Its solution strictly obeys discrete fluctuation-dissipation balance without any approximation
- GMRes
- Inherent ill-conditioning
  - Preconditioning for the iterative solver

❖ Computational cost of FBIM scales linearly with the number of particles.

❖ The Brown displacements of the particles are computed along the way with only a marginal increases in the overall cost.

Summary

Overdamped Brownian dynamics

$$\frac{d\boldsymbol{Q}}{dt} = \boldsymbol{\mathcal{N}}\boldsymbol{F} + \sqrt{2k_BT}\boldsymbol{\mathcal{N}}^{\frac{1}{2}}\boldsymbol{\mathcal{W}} + (k_BT)(\partial_{\boldsymbol{Q}} \cdot \boldsymbol{\mathcal{N}})$$

- $\boldsymbol{\mathcal{N}}\boldsymbol{F}$ and $\sqrt{2k_BT}\boldsymbol{\mathcal{N}}^{1/2}\boldsymbol{\mathcal{W}}$ can be calculated from deterministic and stochastic Stokes BVPs, respectively.
- The first-kind formulation provides a suitable starting point for a finite-dimensional discretization of the random surface velocity (→ discrete fluctuation-dissipation balance).

Thank You!!!