A fluctuating boundary integral method for Brownian suspensions

Aleksandar Donev, CIMS
and collaborators:
CIMS: Bill Bao, Florencio Balboa,
Leslie Greengard, Manas Rachh
External: Andrew Fiore and James Swan (MIT),
Eric Keaveny (Imperial)
Brennan Sprinkle (Northwestern)

Courant Institute, New York University

Simons Foundation Seminar
May 15th 2017
Motivation

Colloidal Gelation

Figure: Colloidal gelation simulated using Brownian Dynamics with Hydrodynamic Interactions (from work of James Swan, MIT Chemical Engineering).
Non-Spherical Colloids

Figure: (Left) Cross-linked spheres from Kraft et al. (Right) Lithographed boomerangs in a microchannel from Chakrabarty et al.
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?
The Ito equations of **Brownian Dynamics** (BD) for the (correlated) positions of the \( N \) particles \( \mathbf{Q}(t) = \{q_1(t), \ldots, q_N(t)\} \) are

\[
d\mathbf{Q} = \mathbf{M} \cdot \mathbf{F}(\mathbf{Q}) \, dt + (2k_B T \mathbf{M})^{1/2} \, d\mathbf{B} + k_B T (\partial \mathbf{Q} \cdot \mathbf{M}) \, dt, \tag{1}
\]

where \( \mathbf{B}(t) \) is a vector of Brownian motions, and \( \mathbf{F}(\mathbf{Q}) \) are forces.

Here \( \mathbf{M}(\mathbf{Q}) \geq 0 \) is a symmetric positive semidefinite (SPD) mobility matrix, assumed to have a far-field pairwise approximation

\[
M_{ij}(\mathbf{Q}) \equiv M_{ij}(q_i, q_j) = \mathcal{R}(q_i - q_j).
\]

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

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

where \( a \) is the radius of the colloidal particles.
Observe that in the far-field, \( r \gg a \), the RPY tensor becomes the long-ranged Oseen tensor

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

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 \( \mathbf{M}_F \).
  - 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 $M^{1/2}W$ is usually computed iteratively by repeated multiplication of a vector by $M$.
- 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 $M = U\Lambda U^T$,

$$M^{1/2}W \equiv U\Lambda^{1/2}U^T W \approx \|W\|_2 V_m H_m^{1/2} e_1,$$

where $V_m$ is an orthonormal basis for the Krylov subspace of order $m$, and $H_m = V_m^T M V_m$ 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 \( W \), rather, we want to generate a Gaussian random vector \( \delta U \) with specified covariance, \( \langle (\delta U)(\delta U)^T \rangle = M \).

- **First key idea:** Use (Spectral) Ewald approach to decompose \( M = M^{(w)} + M^{(r)} \) into a far-field wave-space part \( M^{(w)} \) and a near-field real space part \( M^{(r)} \), then in law,

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

if both \( M^{(w)} \) and \( M^{(r)} \) are SPD and \( \langle W^{(w)}W^{(r)} \rangle = 0 \).

- For the real-space part, use the Krylov Lanczos method to compute \( \left( M^{(r)} \right)^{\frac{1}{2}} W^{(r)} \) since \( M^{(r)} \) is sparse and well-conditioned.

- **Second key idea:** Compute \( M^{(w)}F \) and \( \left( M^{(w)} \right)^{\frac{1}{2}} W^{(w)} \) in Fourier space (using FFTs) as in fluctuating hydrodynamics.
Spectral Ewald approach to Brownian Dynamics

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:

\[ \mathcal{R} (r_1, r_2) = \mathcal{R} (r_1 - r_2) = \int \delta_a (r_1 - r') \mathcal{G} (r', r'') \delta_a (r_2 - r'') \, dr' \, dr'', \]

where \( \delta_a \) 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

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

- The surface delta functions in Fourier space give us a sinc factor.
This gives us a previously-unappreciated simple spectral representation of the periodic RPY tensor:

\[ \mathcal{R}(r) = \frac{1}{\mu V} \sum_{k \neq 0} e^{ik \cdot r} \frac{1}{k^2} \text{sinc}^2 (ka) \left( I - \hat{k}\hat{k} \right). \]  

(3)

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

\[ \mathcal{R}_\xi^{(w)}(r) = \frac{1}{\mu V} \sum_{k \neq 0} e^{ik \cdot r} \frac{\text{sinc}^2 (ka)}{k^2} H(k, \xi) \left( I - \hat{k}\hat{k} \right), \]  

(4)

where the Hasimoto splitting function is determined by the **splitting parameter** \( \xi \),

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

(5)
Real-space part

- Converting back to real space we get

\[
\mathcal{R}_{\xi}^{(r)}(r) = F(r, \xi) (1 - \hat{r}\hat{r}) + G(r, \xi) \hat{r}\hat{r},
\]

(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,

\[
M_{ii}^{(r)} = \mathcal{R}^{(r)}(0) = \frac{1}{24\pi^{3/2} \mu \xi a^2} \left( 1 - e^{-4a^2 \xi^2} + 4\pi^{1/2} a\xi \text{erfc}(2a\xi) \right) I.
\]

- If we choose \( 0 \leq H(k, \xi) \leq 1 \) (satisfied by Hasimoto but not Beenakker) we obtain SPD real and wave space parts.
Figure: Condition number of $M^{(r)}$ for varying number of particles $N$. 
The wave space component of the mobility can be applied efficiently using FFTs as

\[ M^{(w)} = D^{-1} BD = \left( D^\dagger B^{1/2} \right) \left( D^\dagger B^{1/2} \right)^\dagger, \]  

(7)

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

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

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

\[ \left( M^{(w)} \right)^{1/2} W^{(w)} \equiv D^\dagger B^{1/2} W^{(w)}. \]  

(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 = $\text{MF}$, blue = $\text{M}^{1/2} \text{W}$ using PSE, black = $\text{M}^{1/2} \text{W}$ without PSE.
We consider a rigid body $\Omega$ immersed in a fluctuating fluid. In the fluid domain, we have the **fluctuating Stokes equation**

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

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

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

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

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

$$\langle \mathcal{Z}_{ij}(\mathbf{r}, t) \mathcal{Z}_{kl}(\mathbf{r}', t') \rangle = (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \delta(t - t') \delta(\mathbf{r} - \mathbf{r'}).$$
At the fluid-body interface the **no-slip boundary condition** is assumed to apply,

\[ \mathbf{v}(q) = \mathbf{u} + \mathbf{\omega} \times q \text{ for all } q \in \partial \Omega, \]

with the **force and torque balance**

\[ \int_{\partial \Omega} \lambda(q) \, dq = F \quad \text{and} \quad \int_{\partial \Omega} [q \times \lambda(q)] \, dq = \tau, \]

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

\[ \lambda(q) = \mathbf{\sigma} \cdot \mathbf{n}(q). \]

To model activity we can add **active slip** \( \mathbf{u} \) due to active boundary layers, without any difficulties (not done here).
Consider a suspension of $N_b$ rigid bodies with configuration $Q = \{q, \theta\}$ 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

$$\frac{dQ(t)}{dt} = U = \mathcal{N} F + (2k_B T \mathcal{N}')^{1/2} \mathcal{W}(t) + (k_B T) \partial_Q \cdot \mathcal{N'},$$

where $\mathcal{N}'(Q)$ is the body mobility matrix, $U = \{u, \omega\}$ collects the linear and angular velocities, $F(Q) = \{f, \tau\}$ collects the applied forces and torques.

How to compute (the action of) $\mathcal{N}$ and $\mathcal{N}^{1/2}$ and simulate the Brownian motion of the bodies?
Let us first ignore the Brownian motion and compute $\nabla F$.

We can write down an equivalent first-kind boundary integral equation for the surface traction $\lambda (q \in \partial \Omega)$,

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

along with the force and torque balance condition (11). Here $\mathbf{G}$ 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).
Assume that the surface of the body is discretized in some manner and the **single-layer operator** is computed using some quadrature,

\[
\int_{\partial \Omega} G(q, q') \lambda(q') \, dq' \equiv M \lambda \rightarrow M \lambda,
\]

where \( M \) 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 \( \lambda \) and rigid-body motion \( U \),

\[
\begin{bmatrix}
M & -K \\
-K^T & 0
\end{bmatrix}
\begin{bmatrix}
\lambda \\
U
\end{bmatrix} =
\begin{bmatrix}
0 \\
-F
\end{bmatrix},
\]

where \( K \) is a simple geometric matrix.

Solve formally using Schur complements to get

\[
U = N F = (K^T M^{-1} K)^{-1} F.
\]

How do we generate a Gaussian random vector with covariance \( N \)?
Assume that we knew how to generate a Gaussian random vector with covariance $\mathcal{M}$, i.e., to generate a random “slip” velocity $\mathbf{\tilde{u}}$ with covariance given by the (periodic) Stokeslet, $\langle \mathbf{\tilde{u}} \mathbf{\tilde{u}}^T \rangle = \mathcal{M}$.

Key idea: Solve the mobility problem with random slip $\mathbf{\tilde{u}}$,

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

(14)

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

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

$$
\mathcal{N}_{1/2} \left( \mathcal{N}_{1/2} \right)^\dagger = \mathcal{N} \mathcal{K}^T \mathcal{M}^{-1} \mathcal{M}^{1/2} \left( \mathcal{M}^{1/2} \right)^\dagger \mathcal{M}^{-1} \mathcal{K} \mathcal{N}
$$

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

(15)

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

Block-Diagonal Preconditioner

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

\[ P = \begin{bmatrix} \tilde{\mathcal{M}} & -\mathcal{K} \\ -\mathcal{K}^T & 0 \end{bmatrix} \]  

(16)

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

\[ \tilde{\mathcal{M}}^{(pq)} = \delta_{pq} \mathcal{M}^{(pp)}. \]  

(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.
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,

\[ G = G^{(w)} + G^{(r)}, \]

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

\[ G^{(w)}_{\xi}(x, y) = \frac{1}{\mu V} \sum_{k \neq 0} e^{ik \cdot (x-y)} \frac{H(k, \xi)}{k^2} \left( I - \hat{k}\hat{k} \right). \]
Recall that \((M\lambda)(q) \equiv \int_{\partial \Omega} G(q, q') \lambda(q') \, dq'.\)

This splitting of \(G\) induces a corresponding splitting of the mobility operator where both pieces are SPD

\[
M = M^{(w)} + M^{(r)}.
\]

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

\[
M^{(w)}_{ij} = G^{(w)}_{\xi}(r_i, r_j).
\]

Both \(M^{(w)}\) and \(\left(M^{(w)}\right)^{1/2}\) can be applied efficiently in Fourier space using the FFT, just as for the RPY kernel in the first part of the talk.
Because of the lack of the RPY regularization, here $G_\xi^{(r)}$ 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 $G_\xi^{(r)}$ in 2D can be obtained by using **Alpert quadrature**, 

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

where $(M^{(r)}_{\text{trap}})_{ij} = G_\xi^{(r)}(r_i, r_j)$ for $i \neq j$ is a trapezoidal rule for off-diagonal entries, and $M^{(r)}_{\text{Alpert}}$ is a **block-diagonal banded correction** to obtain singular corrections to the trapezoidal rule.

The question now is whether $M^{(r)}$ is SPD and whether we can compute $\left( M^{(r)} \right)^{1/2} W^{(r)}$ efficiently.
In general $M_{\text{Alpert}}^{(r)}$ is neither symmetric nor positive semidefinite and so $M^{(r)}$ is not SPD strictly speaking.

Nevertheless, we find that symmetrizing $M_{\text{Alpert}}^{(r)}$ preserves the order of accuracy of Alpert quadrature, and that the Krylov method for computing $\left(M^{(r)}\right)^{\frac{1}{2}} W^{(r)}$ is rather insensitive to any small negative eigenvalues of $M^{(r)}$.

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 $M^{(r)}$ for each body (modest-size matrices).
Fluctuating Boundary Integral method

Numerical Tests

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

Efficiency and Scaling

Figure: Optimal splitting parameters and linear scaling.
Brownian Dynamics using FBEM

\[
\frac{dQ(t)}{dt} = U = \mathcal{N} F + (2k_B T \mathcal{N})^{1/2} \mathcal{W}(t) + (k_B T) \partial Q \cdot \mathcal{N}
\]

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

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

- The red terms can be computed using the FBEM method.
- The magenta terms (here $\delta \rightarrow 0$ 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.
**Figure**: Equilibrium distributions of $\theta$ of a 4-fold starfish diffusing in a periodic domain. (Left) EM with RFD (correct!). (Right) EM without RFD (wrong).
Figure: \[ U(q_1, \theta_1, q_2, \theta_2) = \frac{k_s}{2} (|q_1 - q_2| - l_s)^2 + \frac{k_\theta}{2} (\theta_1 - \frac{\pi}{4})^2 + \frac{k_\theta}{2} (\theta_2 - \frac{\pi}{2})^2 \]
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:

\[
\begin{bmatrix}
M & -K \\
-K^T & 0
\end{bmatrix}^n
\begin{bmatrix}
\lambda^{RFD} \\
U^{RFD}
\end{bmatrix} =
\begin{bmatrix}
0 \\
-\tilde{W}
\end{bmatrix}. \tag{18}
\]

2. Compute random finite differences:

\[
F^{RFD} = \frac{k_B T}{\delta} \left( K^T \left( Q^n + \delta \tilde{W} \right) - (K^n)^T \right) \lambda^{RFD}
\]

\[
\dot{u}^{RFD} = \frac{k_B T}{\delta} \left( M \left( Q^n + \delta \tilde{W} \right) - M^n \right) \lambda^{RFD} +
- \frac{k_B T}{\delta} \left( K \left( Q^n + \delta \tilde{W} \right) - K^n \right) U^{RFD}.
\]
1. Compute correlated random slip:

\[ \ddot{u}^n = \left( \frac{2k_BT}{\Delta t} \right)^{1/2} (M^n)^{1/2} W^n \]

2. Solve the saddle-point system:

\[
\begin{bmatrix}
M & -K \\
-K^T & 0
\end{bmatrix}^n \begin{bmatrix}
\lambda^n \\
U^n
\end{bmatrix} = - \begin{bmatrix}
\ddot{u}^n + \ddot{u}^{RFD} \\
F^n - F^{RFD}
\end{bmatrix}.
\]

3. Move the particles (rotate for orientation)

\[ Q^{n+1} = Q^n + \Delta t U^n \]
Temporal Integration

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:

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

2. Compute random finite differences:

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

\[
\ddot{\mathbf{u}}^{RFD} = \frac{k_B T}{\delta} \left( \mathbf{M} (\mathbf{Q}^n + \delta \mathbf{U}^{RFD}) - \mathbf{M}^n \right) \mathbf{W}
\]
1. **Compute correlated random slip:**

\[
\tilde{u}^n = \left( \frac{2k_BT}{\Delta t} \right)^{1/2} (\mathcal{M}^n)^{1/2} \mathbf{W}^n
\]

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

\[
\begin{bmatrix}
\mathcal{M} & -\mathcal{K} \\
-\mathcal{K}^T & 0
\end{bmatrix}^n
\begin{bmatrix}
\lambda^p \\
\mathbf{U}^p
\end{bmatrix}
= - \begin{bmatrix}
\tilde{u}^n \\
\mathbf{F}^n
\end{bmatrix}.
\]

3. **Compute predicted** \(Q^p = Q^n + \Delta t \mathbf{U}^n\).

4. **Take a trapezoidal corrector FBEM step:**

\[
\begin{bmatrix}
\mathcal{M} & -\mathcal{K} \\
-\mathcal{K}^T & 0
\end{bmatrix}^p
\begin{bmatrix}
\lambda^c \\
\mathbf{U}^c
\end{bmatrix}
= - \begin{bmatrix}
\tilde{u}^n + 2\tilde{u}^{RFD} \\
\mathbf{F}^p - 2\mathbf{F}^{RFD}
\end{bmatrix}.
\]

5. **Complete the update,** \(Q^{n+1} = Q^n + \frac{\Delta t}{2} (\mathbf{U}^p + \mathbf{U}^c)\).
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).
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?
Zhi Liang, Zydrunas Gimbutas, Leslie Greengard, Jingfang Huang, and Shidong Jiang.
A fast multipole method for the rotne–prager–yamakawa tensor and its applications.

Dag Lindbo and Anna-Karin Tornberg.
Spectrally accurate fast summation for periodic stokes potentials.

Edmond Chow and Yousef Saad.
Preconditioned krylov subspace methods for sampling multivariate gaussian distributions.

Hydrodynamics of suspensions of passive and active rigid particles: a rigid multiblob approach.
Software available at https://github.com/stochasticHydroTools/RigidMultiblobsWall.

Florencio Balboa Usabiaga, Blaise Delmotte, and Aleksandar Donev.
Brownian dynamics of confined suspensions of active microrollers.
Software available at https://github.com/stochasticHydroTools/RigidMultiblobsWall.