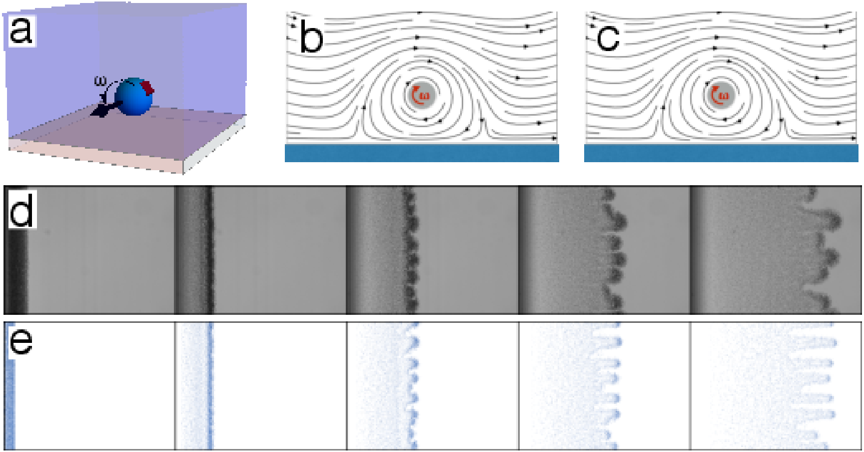
Dynamics of Colloids Above a Bottom Wall Driven by Active Torques and Forces

Aleksandar Donev, CIMS
Blaise Delmotte (Ladhyx, Paris), Florencio Balboa (Flatiron), Brennan Sprinkle (CIMS)

Courant Institute, *New York University*

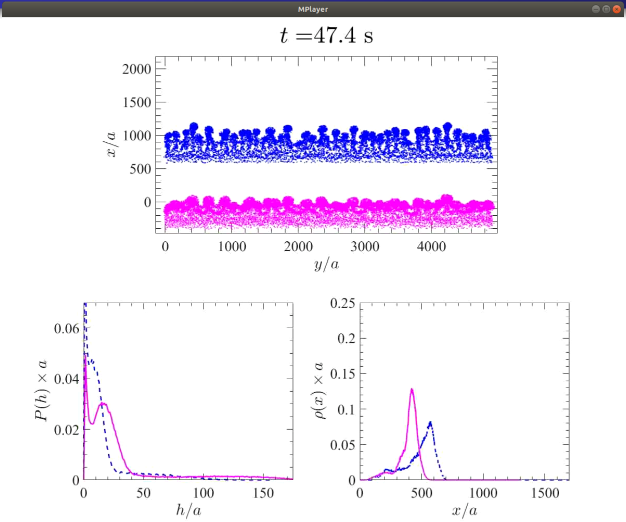
Math Colloquium, Drexel University
April 10th 2019

Microrollers: Fingering Instability



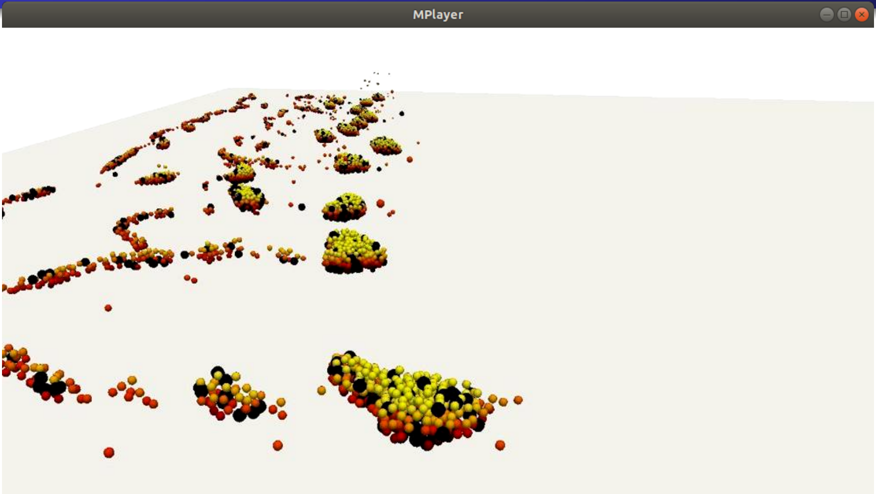
Experiments by Michelle Driscoll (lab of Paul Chaikin, NYU Physics, now at Northwestern), simulations by **Blaise Delmotte** [1, 2].

Role of Brownian Motion



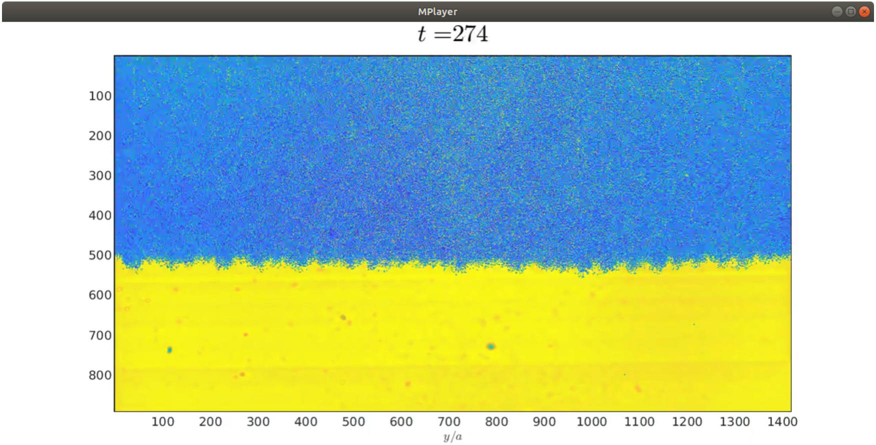
Simulations show that thermal fluctuation are quantitatively important because they set the **gravitational height**.[2].

Critters



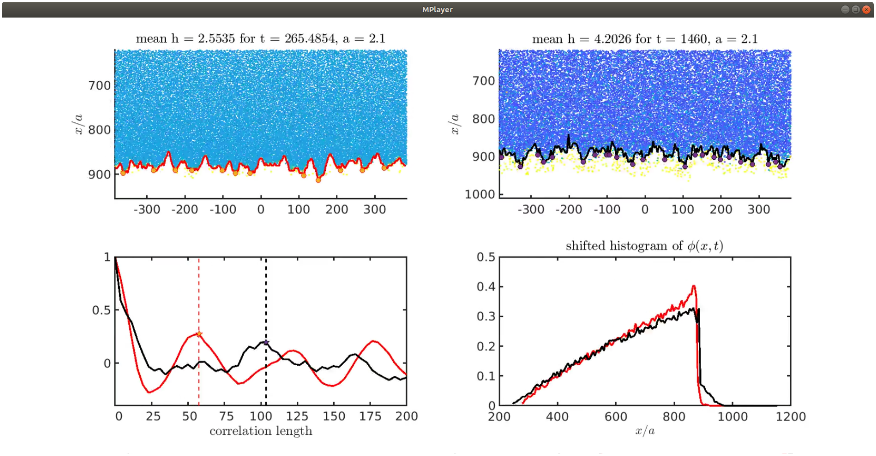
Simulations by **Blaise Delmotte** revealed that stable motile clusters termed **critters can form purely by hydrodynamic interactions** [1]. Still trying to create critters that don't shed particles in the lab...

Sedimentation of colloidal monolayer



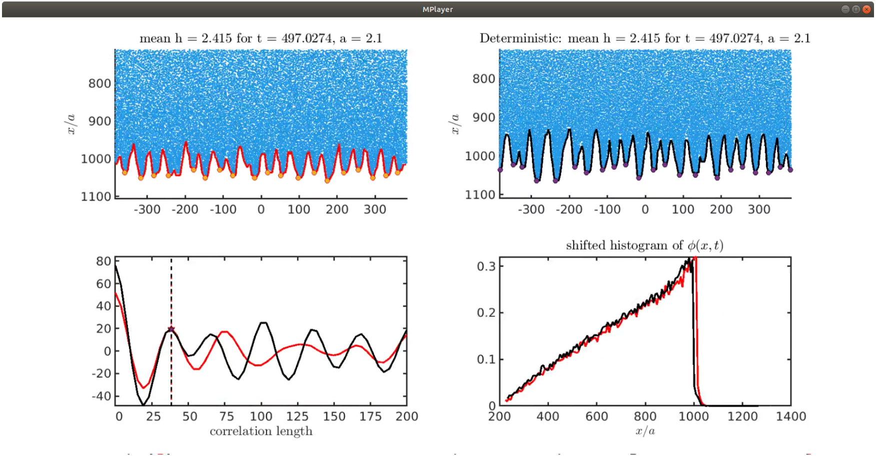
Experiments in lab of Paul Chaikin show that a sedimenting front roughens due to a sort of "instability".

3D simulations of sedimentation



Simulations of **Brennan Sprinkle** show the gravitational height matters, but no precise explanation yet.

2D simulations of sedimentation



Quasi-2D simulations of **Brennan Sprinkle** show that Brownian motion in the plane don't matter that much.

Fluctuating Hydrodynamics

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

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

with **no-slip BCs** on the bottom wall, and the fluid stress tensor

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

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,

$$\mathbf{v}(\mathbf{q}) = \mathbf{u} + \boldsymbol{\omega} \times \mathbf{q} - \breve{\mathbf{u}}(\mathbf{q}) \text{ for all } \mathbf{q} \in \partial\Omega, \tag{2}$$

with the **inertial body dynamics**

$$m\frac{d\mathbf{u}}{dt} = \mathbf{F} - \int_{\partial\Omega} \boldsymbol{\lambda}(\mathbf{q})\, d\mathbf{q}, \tag{3}$$

$$\mathbf{I}\frac{d\boldsymbol{\omega}}{dt} = \boldsymbol{\tau} - \int_{\partial\Omega} [\mathbf{q} \times \boldsymbol{\lambda}(\mathbf{q})]\, d\mathbf{q} \tag{4}$$

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, or consider external forces/torques.

Mobility Problem

From linearity, the rigid-body motion is defined by a linear mapping $\mathbf{U} = \boldsymbol{\mathcal{N}}\mathbf{F}$ via the deterministic **mobility problem**:

$$\boldsymbol{\nabla}\pi = \eta\boldsymbol{\nabla}^2\mathbf{v} \quad \text{and} \quad \boldsymbol{\nabla}\cdot\mathbf{v}{=}0 \quad +\text{BCs}$$

$$\mathbf{v}\left(\mathbf{q}\right) = \mathbf{u} + \boldsymbol{\omega}\times\mathbf{q} - \breve{\mathbf{u}}\left(\mathbf{q}\right) \;\text{ for all } \mathbf{q}\in\partial\Omega, \tag{5}$$

With **force and torque balance**

$$\int_{\partial\Omega}\boldsymbol{\lambda}\left(\mathbf{q}\right)d\mathbf{q} = \mathbf{F} \quad \text{and} \quad \int_{\partial\Omega}\left[\mathbf{q}\times\boldsymbol{\lambda}\left(\mathbf{q}\right)\right]d\mathbf{q} = \boldsymbol{\tau}, \tag{6}$$

where $\boldsymbol{\lambda}\left(\mathbf{q}\right) = \boldsymbol{\sigma}\cdot\mathbf{n}\left(\mathbf{q}\right)$ with

$$\boldsymbol{\sigma} = -\pi\mathbf{I} + \eta\left(\boldsymbol{\nabla}\mathbf{v} + \boldsymbol{\nabla}^T\mathbf{v}\right). \tag{7}$$

Overdamped 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**, with "square root" given by **fluctuation-dissipation balance**

$$\mathcal{N}^{\frac{1}{2}}\left(\mathcal{N}^{\frac{1}{2}}\right)^{T} = \mathcal{N}.$$

$\mathbf{U} = \{\mathbf{u}, \boldsymbol{\omega}\}$ collects the **linear and angular velocities**
$\mathbf{F}(\mathbf{Q}) = \{\mathbf{f}, \boldsymbol{\tau}\}$ collects the **applied forces and torques**.

Difficulties/Goals

Complex shapes We want to stay away from analytical approximations that only work for spherical particles.

Boundary conditions Whenever observed experimentally there are microscope slips (glass plates) that modify the hydrodynamics strongly. Because of **gravity** the particles sediment **close to the bottom wall** ($\sim$ 100nm).

Many-body hydrodynamics Want to be able to scale the algorithms to suspensions of **many particles**.

Brownian increments How to generate $\boldsymbol{\mathcal{N}}^{\frac{1}{2}}\mathbf{W}$, i.e., Gaussian random variables with covariance $\boldsymbol{\mathcal{N}}$.

Stochastic drift How to include the $(k_B T)\,\partial_{\mathbf{Q}} \cdot \boldsymbol{\mathcal{N}}$ term in **temporal integrators**.

Minimally-Resolved Simulations

- Represent each spherical particle by a **single blob**, and solve the Ito equations of **Brownian HydroDynamics** for the (correlated) positions of the N spherical microrollers $\mathbf{Q}(t) = \{\mathbf{q}_1(t), \dots, \mathbf{q}_N(t)\}$,

$$d\mathbf{Q} = \boldsymbol{\mathcal{M}}\mathbf{F}dt + \boldsymbol{\mathcal{M}}_c\mathbf{T} + (2k_B T\,\boldsymbol{\mathcal{M}})^{\frac{1}{2}}\,d\boldsymbol{\mathcal{B}} + k_B T\,(\partial_{\mathbf{Q}} \cdot \boldsymbol{\mathcal{M}})\,dt, \quad (8)$$

  where $\boldsymbol{\mathcal{B}}(t)$ is a vector of Brownian motions, and $\mathbf{F}(\mathbf{Q})$ are applied forces, and $\mathbf{T}$ the external magnetic torques.
- How to compute **deterministic velocities** $\boldsymbol{\mathcal{M}}\mathbf{F}$ efficiently?
- How to generate **Brownian increments** $(2k_B T\,\boldsymbol{\mathcal{M}})^{\frac{1}{2}}\,\Delta\boldsymbol{\mathcal{B}}$ efficiently?
- How to generate **stochastic drift** $k_B T\,(\partial_{\mathbf{Q}} \cdot \boldsymbol{\mathcal{M}})$ efficiently by only solving mobility problems?

Blobs in Stokes Flow

- The symmetric positive semidefinite (SPD) **blob-blob mobility matrix** $\mathcal{M}$ encodes the hydrodynamics:
  3×3 block $\mathbf{M}_{ij}$ maps a force on blob j to a velocity of blob i.
- The mobility is approximated to have a far-field **pairwise approximation**

$$\mathbf{M}_{ij}\left(\mathbf{Q}\right) \equiv \mathbf{M}_{ij}\left(\mathbf{q}_i, \mathbf{q}_j\right) = \mathcal{R}\left(\mathbf{q}_i, \mathbf{q}_j\right),$$

where the **hydrodynamic kernel** $\mathcal{R}$ for spheres of radius a is

$$\mathcal{R}\left(\mathbf{q}_i, \mathbf{q}_j\right) \approx \eta^{-1}\left(\mathbf{I} + \frac{a^2}{6}\boldsymbol{\nabla}^2_{\mathbf{r}'}\right)\left(\mathbf{I} + \frac{a^2}{6}\boldsymbol{\nabla}^2_{\mathbf{r}''}\right)\mathbb{G}(\mathbf{r}', \mathbf{r}'')\Big|_{\mathbf{r}''=\mathbf{q}_i}^{\mathbf{r}'=\mathbf{q}_j} \qquad (9)$$

where $\mathbb{G}$ is the **Green's function** for steady Stokes flow, *given* the appropriate boundary conditions.

Confined Geometries

- The Green's function is only known explicitly in some very special circumstances, e.g., for a **single no-slip boundary** $\mathbb{G}$ is the **Oseen-Blake** tensor.
- For blobs next to a wall the **Rotne-Prager-Blake** tensor has been computed by Swan (MIT) and Brady (Caltech) and we will use it here. It is still missing corrections when the blobs overlap the wall so we have made a heuristic fix [2].
- We compute $\boldsymbol{\mathcal{M}\lambda}$ using **GPU-accelerated** $O(N_b^2)$ sum.
  Often faster than Fast Multipole Methods for up to 10^5 blobs.
- For slit channels we can use a grid-based **fluid Stokes solver** to compute the (action of the) **Green's functions on the fly** [3]
  In the triply periodic case [4] or explicit Stokes solver [3] approach adding thermal fluctuations (Brownian motion) can be done using **fluctuating hydrodynamics**.

Generating Brownian increments

- We need a fast way to compute the **Brownian velocities**

$$\mathbf{U}_b = \sqrt{\frac{2k_B T}{\Delta t}}\, \mathcal{M}^{\frac{1}{2}} \mathbf{W}$$

  where $\mathbf{W}$ is a vector of Gaussian random variables.
- The product $\mathcal{M}^{\frac{1}{2}} \mathbf{W}$ can be computed iteratively by **repeated multiplication** of a vector by $\mathcal{M}$ using (preconditioned) Krylov subspace **Lanczos methods**.
- When particles are sedimented close to a bottom wall, pairwise hydrodynamic interactions decay rapidly like $1/r^3$, which appears to be enough to make the Krylov method converge in a **small constant number of iterations**, without any preconditioning.

Periodic suspensions

- Because of the long-ranged $1/r$ nature of the Oseen kernel in free space, the number of iterations is found to grow with the number of particles, leading to an overall complexity of at least $O\left(N^{4/3}\right)$.
- More precisely, we want to sample Gaussian random variables with mean zero and covariance $\boldsymbol{\mathcal{M}}$:

$$\langle \mathbf{U}_b \mathbf{U}_b^T \rangle = \boldsymbol{\mathcal{M}}$$

- This is **easier** than computing some specific square roots, since there is a **lot of freedom**! For example, if $\boldsymbol{\mathcal{M}} = \boldsymbol{\mathcal{M}}_1 + \boldsymbol{\mathcal{M}}_2$, where $\boldsymbol{\mathcal{M}}_{1/2}$ are **both SPD**, then in law

$$\boldsymbol{\mathcal{M}}^{\frac{1}{2}} \mathbf{W} \equiv \boldsymbol{\mathcal{M}}_1^{\frac{1}{2}} \mathbf{W}_1 + \boldsymbol{\mathcal{M}}_2^{\frac{1}{2}} \mathbf{W}_2.$$

- With the group of James Swan (MIT ChemE), we have combined this with fluctuating hydrodynamics in our **Positively Split Ewald** (PSE) method [4]: $\boldsymbol{\mathcal{M}}^{\frac{1}{2}} \mathbf{W}$ with only a few **FFTs** in **linear time** for periodic suspensions (also works with **multigrid**).

Stochastic drift term

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

- Key idea to get $\left(\partial_{\mathbf{Q}} \cdot \mathcal{M}\right)_i = \partial \mathcal{M}_{ij} / \partial Q_j$ is to use **random finite differences (RFD)** [2]: If $\langle \Delta\mathbf{P}\Delta\mathbf{Q}^T = \mathbf{I} \rangle$,

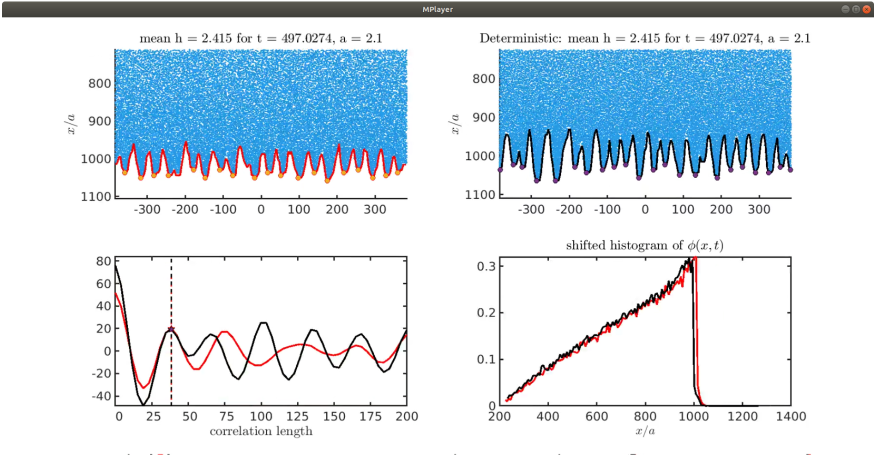
$$\lim_{\delta \to 0} \frac{1}{\delta} \langle \left\{ \mathcal{M}\left(\mathbf{Q} + \frac{\delta}{2}\Delta\mathbf{Q}\right) - \mathcal{M}\left(\mathbf{Q} - \frac{\delta}{2}\Delta\mathbf{Q}\right) \right\} \Delta\mathbf{P} \rangle = \tag{10}$$

$$\left\{ \partial_{\mathbf{Q}} \mathcal{M}(\mathbf{Q}) \right\} : \langle \Delta\mathbf{P}\Delta\mathbf{Q}^T \rangle = k_B T\, \partial_{\mathbf{Q}} \cdot \mathcal{M}(\mathbf{Q}). \tag{11}$$

- This leads to a **stochastic Adams-Bashforth** temporal integrator [2],

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

2D simulations of sedimentation



Quasi-2D simulations of **Brennan Sprinkle** show that Brownian motion in the plane don't matter that much.

Continuum Models of Sedimentation

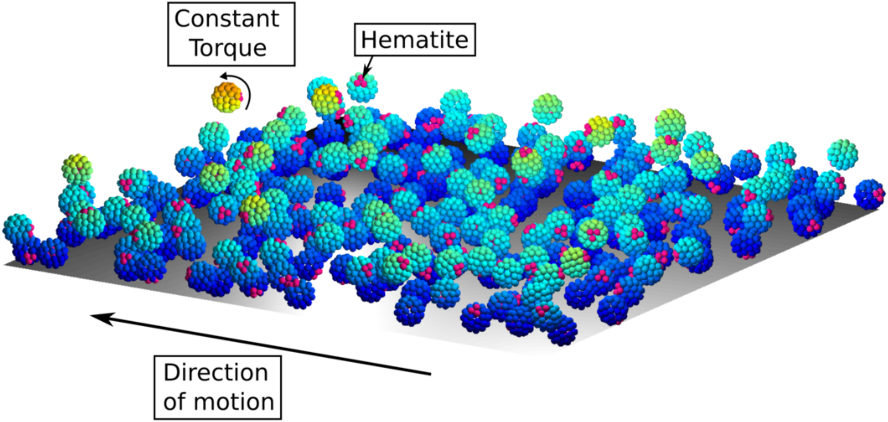
- Instead of particle-based simulations, we can also try to write a **mean field continuum model** where we represent density of particles $\rho(\mathbf{r}, t)$ either in 3D or in the xy plane.
- Ignoring Brownian motion, for sedimentation down an inclined plane of angle θ this gives a **nonlocal conservation law** [5]

$$\partial_t \rho + \boldsymbol{\nabla} \cdot (\rho \mathbf{v}) = 0$$

$$\mathbf{v}(\mathbf{r};\, \rho) = m_e g \sin\theta \int d\mathbf{r}'\; \rho(\mathbf{r}')\, \boldsymbol{\mathcal{R}}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{e}_x$$

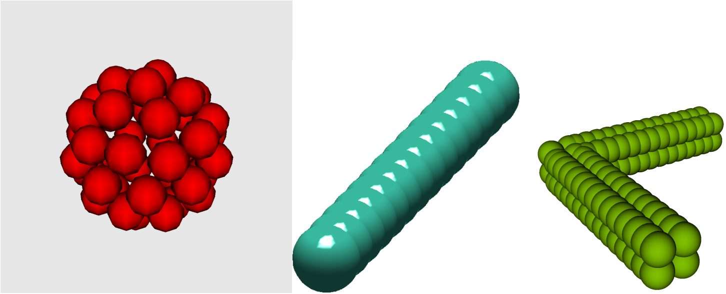
- Currently developing numerical methods to solve PDEs in 2D (the xy plane, keeping $z = h$ fixed for all particles):
  Use **FFT-based aperiodic convolution** to compute advective velocity $\mathbf{v}$, then use **BDS advection** scheme for conservation law.

Microrollers: Uniform Suspension



Simulations by **Brennan Sprinkle**+Blaise Delmotte [3] of a uniform suspension of microrollers at packing fraction $\phi = 0.4$ (GIF). Compare to experiments (AVI) by **Michelle Driscoll**.

Rigid MultiBlob Models



- The rigid body is discretized through a number of "**beads**" or "**blobs**" with hydrodynamic radius *a*.
- Standard is **stiff springs** but we want **rigid multiblobs**.
- Equivalent to a **(smartly!) regularized first-kind boundary integral formulation**.
- **We can efficiently simulate the driven and Brownian motion of the rigid multiblobs.**

Rigid MultiBlobs

- We add **rigidity forces** as Lagrange multipliers $\boldsymbol{\lambda} = \{\boldsymbol{\lambda}_1, \ldots, \boldsymbol{\lambda}_n\}$ to constrain a group of blobs forming body p to move rigidly,

$$\begin{aligned}\sum_j \mathcal{M}_{ij}\boldsymbol{\lambda}_j =& \mathbf{u}_p + \boldsymbol{\omega}_p \times \left(\mathbf{r}_i - \mathbf{q}_p\right) \\ \sum_{i\in\mathcal{B}_p} \boldsymbol{\lambda}_i =& \mathbf{f}_p \\ \sum_{i\in\mathcal{B}_p} (\mathbf{r}_i - \mathbf{q}_p) \times \boldsymbol{\lambda}_i =& \boldsymbol{\tau}_p.\end{aligned} \tag{12}$$

  where $\mathbf{u}$ is the velocity of the tracking point $\mathbf{q}$, $\boldsymbol{\omega}$ is the angular velocity of the body around $\mathbf{q}$, $\mathbf{f}$ is the total force applied on the body, $\boldsymbol{\tau}$ is the total torque applied to the body about point $\mathbf{q}$, and $\mathbf{r}_i$ is the position of blob i.
- This can be a **very large linear system** for suspensions of many bodies discretized with many blobs:
  Use **iterative solvers** with a **good preconditioner**.

Suspensions of Rigid Bodies

- In matrix notation we have a **saddle-point** linear system of equations for the rigidity forces $\boldsymbol{\lambda}$ and unknown motion $\mathbf{U}$,

$$\begin{bmatrix} \mathcal{M} & -\mathcal{K} \\ \mathcal{K}^T & \mathbf{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda} \\ \mathbf{U} \end{bmatrix} = \begin{bmatrix} \breve{\mathbf{u}} \\ \mathbf{F} \end{bmatrix}. \tag{13}$$

  Same as **first-kind boundary integral methods**!
- The **surface velocity** $\breve{\mathbf{u}}$ can be used to model **active slip** or to generate **Brownian velocities** [3].
- Solution gives the **mobility matrix**

$$\mathcal{N} = \left(\mathcal{K}^T \mathcal{M}^{-1} \mathcal{K}\right)^{-1} \tag{14}$$

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

Lubrication for **spherical colloids**

- Use **Stokesian Dynamics** approach introduced by Brady, but with more accurate rigid multiblob "far-field" mobility:

$$\begin{pmatrix} \mathcal{M} & -\mathcal{K} \\ \mathcal{K}^T & \boldsymbol{\Delta}_{MB} \end{pmatrix} \begin{pmatrix} \boldsymbol{\lambda} \\ \mathbf{U} \end{pmatrix} = \begin{pmatrix} -\breve{\mathbf{u}} \\ \mathbf{F} \end{pmatrix}, \tag{15}$$

- $\boldsymbol{\Delta}_{MB}$ is a **lubrication correction to the resistance matrix** formed by adding **pairwise** contributions for each pair of nearby surfaces (either particle-particle or particle-wall).
- The pairwise terms in $\boldsymbol{\Delta}_{MB}$ can be computed analytically using asymptotic expansion (for very close particles) or tabulated by using a more accurate reference method (e.g., boundary integral).
- Lubrication-corrected mobility matrix

$$\overline{\mathcal{N}} = \left[\mathcal{N}^{-1} + \boldsymbol{\Delta}_{MB}\right]^{-1} = \mathcal{N} \cdot \left[\mathbf{I} + \boldsymbol{\Delta}_{MB} \cdot \mathcal{N}\right]^{-1}.$$

Linear Algebra

- Without lubrication corrections, we have had great success with the indefinite **block-diagonal preconditioner**

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

  where we neglect all hydrodynamic interactions between blobs on distinct bodies in the preconditioner.
- For the **mobility problem**, we find a **small constant number of GMRES iterations** independent of the number of rigid multiblobs.
- For minimally-resolved single blob models we get the saddle-point system

$$\begin{pmatrix} \mathcal{N}_{\mathrm{min}} & -I \\ I & \boldsymbol{\Delta}_{\mathrm{min}} \end{pmatrix} \begin{pmatrix} \boldsymbol{\lambda} \\ \mathbf{U} \end{pmatrix} = \begin{pmatrix} -\breve{\mathbf{u}} \\ \mathbf{F} \end{pmatrix},$$

  where $\mathcal{N}_{\mathrm{min}}$ is the generalized RPY mobility **including rotation**. Brennan Sprinkle is working on preconditioners.

Generating Brownian Displacements $\sim \mathcal{N}^{\frac{1}{2}}\mathbf{W}$

- Assume that we knew how to efficiently generate Brownian blob velocities $\mathcal{M}^{\frac{1}{2}}\mathbf{W}$ (PSE for periodic, Lancsoz for sedimented suspensions, fluctuating Stokes solver for slit channels).
  For rigid multiblobs use the **block-diagonal preconditioner** in the Lancsoz iteration.
- *Key idea*: Solve the mobility problem with random slip $\breve{\mathbf{u}}$,

$$\begin{bmatrix} \mathcal{M} & -\mathcal{K} \\ -\mathcal{K}^T & \mathbf{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda} \\ \mathbf{U} \end{bmatrix} = - \begin{bmatrix} \breve{\mathbf{u}} = (2k_B T)^{1/2} \mathcal{M}^{\frac{1}{2}}\mathbf{W} \\ \mathbf{F} \end{bmatrix}, \tag{17}$$

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

which defines a $\mathcal{N}^{\frac{1}{2}} = \mathcal{N}\mathcal{K}^T\mathcal{M}^{-1}\mathcal{M}^{\frac{1}{2}}$:

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

Random Traction Euler-Maruyuama

- One can use the RFD idea to make more efficient temporal integrators for Brownian rigid multiblobs [3], such as 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**:

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

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

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:

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

3. Move the particles (rotate for orientation)

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

Conclusions

- It is possible to construct **efficient algorithms** for Brownian HydroDynamics of **nonspherical colloids in the presence of boundaries**.
- *Collective dynamics of active colloidal suspensions above a wall is strongly affected by the bottom wall!*
- Specialized temporal integrators employing **random finite differences** are required to obtain the correct stochastic drift terms.
- Higher accuracy can be reached by using our recently-developed **fluctuating boundary integral method (FBIM)** [6], which uses the same ideas I described here for rigid multiblobs but replaces the RPY tensor with a **high-order singular quadrature**.

References

Michelle Driscoll, Blaise Delmotte, Mena Youssef, Stefano Sacanna, Aleksandar Donev, and Paul Chaikin.
Unstable fronts and motile structures formed by microrollers.
Nature Physics, 13:375–379, 2017.

Florencio Balboa Usabiaga, Blaise Delmotte, and Aleksandar Donev.
Brownian dynamics of confined suspensions of active microrollers.
J. Chem. Phys., 146(13):134104, 2017.
Software available at https://github.com/stochasticHydroTools/RigidMultiblobsWall.

Brennan Sprinkle, Florencio Balboa Usabiaga, Neelesh A. Patankar, and Aleksandar Donev.
Large scale Brownian dynamics of confined suspensions of rigid particles.
The Journal of Chemical Physics, 147(24):244103, 2017.
Software available at https://github.com/stochasticHydroTools/RigidMultiblobsWall.

A. M. Fiore, F. Balboa Usabiaga, A. Donev, and J. W. Swan.
Rapid sampling of stochastic displacements in brownian dynamics simulations.
J. Chem. Phys., 146(12):124116, 2017.
Software available at https://github.com/stochasticHydroTools/PSE.

Blaise Delmotte, Michelle Driscoll, Paul Chaikin, and Aleksandar Donev.
Hydrodynamic shocks in microroller suspensions.
Phys. Rev. Fluids, 2:092301, 2017.

Y. Bao, M. Rachh, E. E. Keaveny, L. Greengard, and A. Donev.
A fluctuating boundary integral method for Brownian suspensions.
J. Comp. Phys., 374:1094 – 1119, 2018.