Brownian HydroDynamics of Colloidal Suspensions

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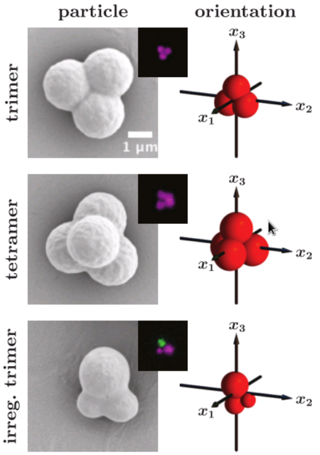
Brownian Motion

Experiments: Non-Spherical Designer Colloids



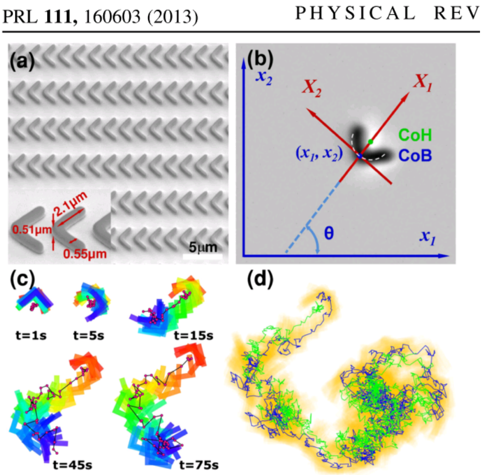
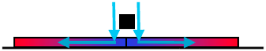


Figure: (Left) Cross-linked spheres; Kraft et al. PRE 2013. (Right) Lithographed boomerangs; Chakrabarty et al. PRL 2013.

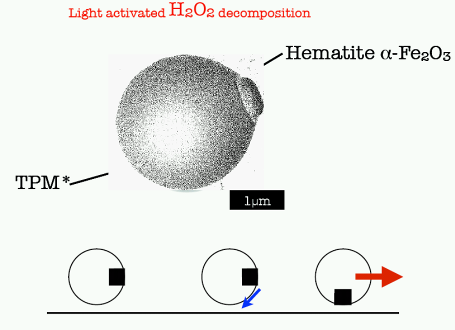
Simulations: Dense Boomerang Suspension

Figure: (Left) Lithographed boomerang colloids. (Right) Brownian dynamics of boomerangs above a bottom wall [1].

Light-Activated Diffusio/Osmophoresis



An Osmotic Flow at the Glass



Attraction to the glass

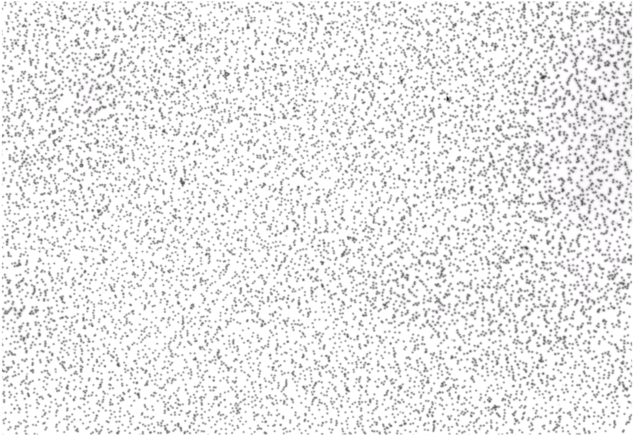
Symmetric Flow but unstable
=> Self-Propulsion

Figure: From Jeremie Palacci and Paul Chaikin (Science 2013)

Light-Activated Colloidal Surfers

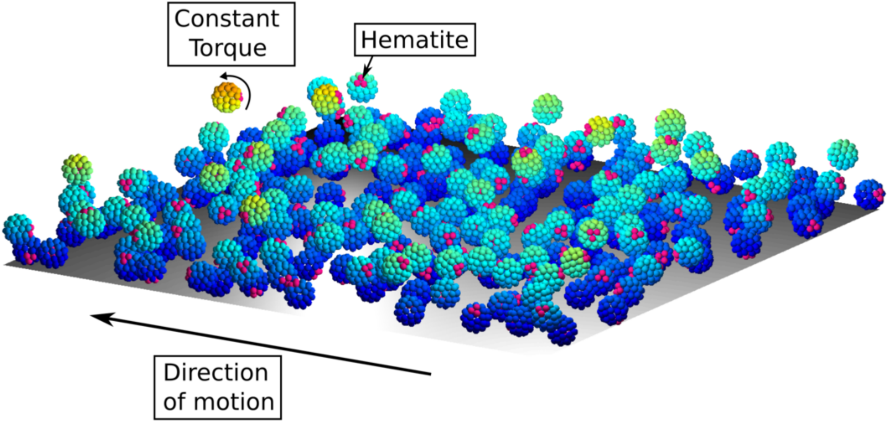
QuickTime

Uniform Suspension of Microrollers: Simulation



Experiments on uniform suspensions by Michelle Driscoll (in progress).

Uniform Suspension of Microrollers: Simulation



Simulations by **Brennan Sprinkle** [1] of a uniform suspension of microrollers at packing fraction $\phi = 0.4$ (MP4).

Bent Active Nanorods

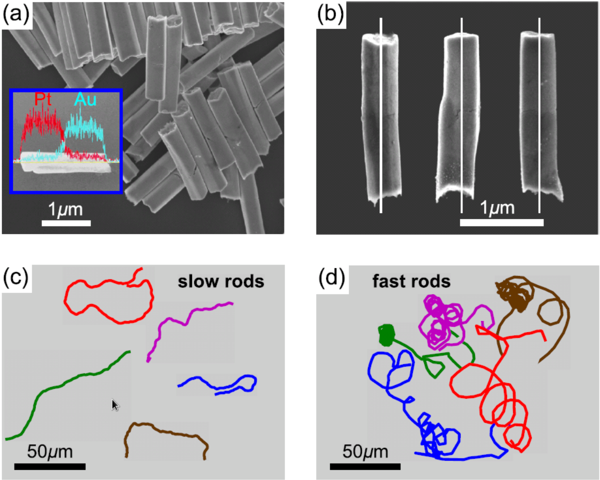


Figure: From the Courant Applied Math Lab of Michael Shelley

Thermal Fluctuation Flips

QuickTime

Brownian Motion

- Consider a **single spherical particle** of radius a with position $\mathbf{q}(t)$ diffusing **in an unbounded domain** with the fluid at rest at infinity.
- If there are no forces applied on the particle, the displacement of the particle in each direction over a time interval Δt has a normal (Gaussian) probability distribution with mean zero and variance (**mean square displacement**)

$$\langle (q_\alpha (t + \Delta t) - q_\alpha (t))^2 \rangle = 2D\Delta t, \quad \alpha = x, y, z$$

  where D is the **diffusion coefficient** in units of m^2/s.
- Therefore, we can write the recurrence relationship

$$q_\alpha (t + \Delta t) = q_\alpha (t) + \mathcal{N} (0, 2D\Delta t),$$

  where $\mathcal{N}(m, \sigma^2)$ denotes a Gaussian random variable (pseudo-random number on a computer) with mean m and variance σ^2 (standard deviation σ).

The simplest SDE

- If we take the **time step size** $\Delta t \to 0$ the trajectory $\mathbf{q}(t)$ converges to a continuous-time stochastic process with (almost surely) continuous trajectories that we call **Brownian Motion**.
- In this limit we formally write this as a **stochastic differential equation** (SDE)

$$\frac{d}{dt} q_\alpha(t) = \sqrt{2D}\, \mathcal{W}_\alpha(t) \quad \text{(physics notation)}$$

$$dq_\alpha(t) = \sqrt{2D}\, d\mathcal{B}_\alpha(t) \quad \text{(math notation)},$$

  where $\mathcal{W}(t) \equiv d\mathcal{B}(t)/dt$ is a **white noise process**, and $\mathcal{B}(t)$ is the **standard Wiener process** or standard Brownian motion.
- I will employ heavily vector/matrix (physics) notation,

$$\frac{d\mathbf{q}(t)}{dt} = \sqrt{2D}\, \boldsymbol{\mathcal{W}}(t).$$

Classical Fluid Dynamics

- Now imagine that the sphere was large (macroscopic) so that Brownian motion did not play a role (more on this soon).
- If we apply a force **F** on the sphere (e.g. gravity), small enough so that **Reynolds number** **Re** $\ll 1$, hydrodynamics (steady Stokes equations) says that the velocity of the particle (e.g., sedimenting sphere) is

$$\mathbf{u} = \frac{d\mathbf{q}}{dt} = \frac{1}{6\pi\eta a}\mathbf{F} = \mu\mathbf{F},$$

  where μ is the **mobility** of the sphere.
- We also have the following fundamental **Einstein relationship** between diffusion and mobility:

$$D = (k_B T)\,\mu.$$

- Understanding where this comes from requires a whole class on **nonequilibrium statistical mechanics**.

Single Colloidal Sphere

- Assuming we can combine these gives the Stokes-Einstein relation (approximate but nearly exact)

$$D \approx \frac{k_B T}{6\pi\eta a} \quad \Rightarrow \quad \frac{d\mathbf{q}(t)}{dt} = \mu\mathbf{F} + \sqrt{2k_B T\mu}\,\boldsymbol{\mathcal{W}}(t).$$

- When the particle is **confined near walls** (no-slip boundaries) the diffusion coefficient depends on how far the particle is from the wall. Different directions are also different – mobility is in general a 3×3 matrix, i.e., a **mobility tensor**.
- The more general SDE for Brownian motion is then

$$\frac{d\mathbf{q}(t)}{dt} = \left(\boldsymbol{\mu}(\mathbf{q})\,\mathbf{F} + (k_B T)\frac{\partial}{\partial\mathbf{q}} \cdot \boldsymbol{\mu}(\mathbf{q})\right) + \sqrt{2k_B T\boldsymbol{\mu}(\mathbf{q})}\,\boldsymbol{\mathcal{W}}(t).$$

Note that $\displaystyle \frac{dx(t)}{dt} = a(x,t) + \sqrt{b(x)}\,\mathcal{W}(t)$

is notation for the limit as $\Delta t \to 0$ of

$$x(t + \Delta t) = x(t) + a(x(t), t)\,\Delta t + \mathcal{N}\left(0,\; b(x(t))\,\Delta t\right).$$

When is Brownian motion "important"

- The **diffusion time** is the time it takes a particle to diffuse one radius,

$$\tau = \frac{a^2}{D} = \frac{6\pi\eta a^3}{k_B T} \approx \frac{\left(a/\left(1\mu\mathrm{m}\right)\right)^3}{0.2} s.$$

- If $a \sim 1$mm then $\tau \sim 10^6$s which is quite long: We don't see sand particles diffusing.
- But if $a = 1\mu$m, a typical colloidal particle made in the lab, then $\tau \approx 5s$ which is observable by microscopes.
- Now what if there was also convective/advective flow carrying the particles with speed v? We define the dimensionless **Péclet number**

$$\mathrm{Pe} = \frac{va}{D}.$$

- If Pe $\lesssim 1$, then diffusion is "important" and must be included.
- But importantly, we see that deterministic and random motions are intimately linked and given by the same **hydrodynamic mobility**.

Two Spheres Far Away

- Now what if there were two spheres and we applied a force on one of them? The force would create a fluid flow velocity $\mathbf{v}(\mathbf{r})$ and the other particle would move also; this is called **hydrodynamic interaction** although this is a misnomer.
  Recall Re $\ll 1$ and we assume steady Stokes, so not $\mathbf{v}(\mathbf{r}, t)$.
- Since the steady Stokes equations are linear, we have that
  $$\mathbf{u}_2 \approx \mathbf{v}(\mathbf{q}_2) = \boldsymbol{\mu}_{12}(\mathbf{q}_1, \mathbf{q}_2)\,\mathbf{F}_1,$$
  where $\boldsymbol{\mu}_{12}$ is the 3×3 **pair mobility tensor**.
- The Einstein relationship tells us that the Brownian motions of the two spheres would become correlated. So one can call this **hydrodynamic correlations**.
- If the spheres were far apart at a distance $r \gg a$, then they would look like "point particles."

Point singularity approximation

- A force applied at a point $\mathbf{q}$ is called a Stokeslet. The flow it creates is the solution to the steady Stokes equation
$$\nabla\pi(\mathbf{r}) = \eta\nabla^2\mathbf{v}(\mathbf{r}) + \mathbf{F}\delta(\mathbf{r}-\mathbf{q})$$
$$\nabla\cdot\mathbf{v} = 0 \quad + \text{boundary conditions},$$
which is also called the Green's function for Stokes flow,
$$\mathbf{v}(\mathbf{r}) = \mathbb{G}(\mathbf{r},\mathbf{q}).$$
- For a three dimensional unbounded domain, the Green's function is the so-called **Oseen tensor**, with $\mathbf{r} = \mathbf{r}' - \mathbf{r}''$:
$$\mathbb{G}(\mathbf{r}',\mathbf{r}'') \equiv \mathbb{O}(\mathbf{r}'-\mathbf{r}'') = \frac{1}{8\pi\eta r}\left(\mathbf{I} + \frac{\mathbf{r}\otimes\mathbf{r}}{r^2}\right). \tag{1}$$
- So for two spheres far away with applied forces we can add all the pieces together because of the linearity of Stokes equations, and ignore for now Brownian motion,
$$\mathbf{u}_{1/2} = \frac{d\mathbf{q}_{1/2}}{dt} \approx \frac{1}{6\pi\eta a}\mathbf{F}_{1/2} + \mathbb{O}(\mathbf{q}_1-\mathbf{q}_2)\,\mathbf{F}_{2/1}.$$

Mobility matrix

- For a collection of spheres we can very generally write in matrix notation
$$d\mathbf{Q}/dt = \mathcal{M}(\mathbf{Q})\,\mathbf{F},$$
where $\mathbf{Q}(t) = \{\mathbf{q}_1(t), \ldots, \mathbf{q}_N(t)\}$ collects the particle positions and $\mathbf{F}$ collects the forces applied on the particles.
- The **mobility matrix** $\mathcal{M}(\mathbf{Q})$ is symmetric and has all positive eigenvalues (is positive definite) – it encodes the hydrodynamic interactions/correlations.
- If there are applied torques on the particles, this will induce translational motion, especially near boundaries, and we have
$$d\mathbf{Q}/dt = \mathcal{M}\mathbf{F} + \mathcal{M}_c\mathbf{T},$$
- But we can only analytically compute $\mathcal{M}(\mathbf{Q})$ or $\mathcal{M}_c(\mathbf{Q})$ approximately for low-density or **dilute suspensions**.

Blob-blob pairwise mobility

- Now, if the particles are not exactly points, there will be corrections to this. The next order of approximation gives that the pairwise mobility is the so-called **Rotne-Prager mobility** $\boldsymbol{\mathcal{R}}$,

$$\boldsymbol{\mu}_{12} \approx \boldsymbol{\mathcal{R}}\left(\mathbf{q}_1, \mathbf{q}_2\right) \text{ where}$$

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

- For an unbounded domain we call $\boldsymbol{\mathcal{R}}\left(\mathbf{r}', \mathbf{r}''\right) = \boldsymbol{\mathcal{R}}\left(\mathbf{r}' - \mathbf{r}''\right) = \boldsymbol{\mathcal{R}}\left(\mathbf{r}\right)$ the **Rotne-Prager-Yamakawa (RPY) tensor**, but this can be generalized to confined domains [2].
- When the two spheres overlap we need to define the RPY tensor differently, but this can be done in a way such that [2]

$$\boldsymbol{\mathcal{R}}\left(\mathbf{r}, \mathbf{r}\right) = \frac{1}{6\pi\eta a}\mathbf{I}.$$

Blob-bob mobility matrix

- The 3×3 block $\mathbf{M}_{ij}$ of mobility matrix $\boldsymbol{\mathcal{M}}(\mathbf{Q})$ maps a force on particle j to a velocity of particle i.
- For dilute suspensions we might at first assume that each pair of particles is not affected by the other particles, and just add over all pairs by linearity, giving the **pairwise approximation**:

$$\mathbf{M}_{ij}(\mathbf{Q}) \equiv \mathbf{M}_{ij}\left(\mathbf{q}_i, \mathbf{q}_j\right) = \boldsymbol{\mathcal{R}}\left(\mathbf{q}_i, \mathbf{q}_j\right) \quad \text{for all } (i,j).$$

- We will call spherically-symmetric particles that interact/correlate through the RPY mobility **"blobs"**.
- Even if the suspension is not dilute we may approximate the particles as blobs without violating basic physics laws!

Brownian Hydrodynamics with blobs

- 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 $\mathbf{Q}(t) = \{\mathbf{q}_1(t), \ldots, \mathbf{q}_N(t)\}$,
$$d\mathbf{Q}/dt = \boldsymbol{\mathcal{M}}\mathbf{F} + \boldsymbol{\mathcal{M}}_c\mathbf{T} + k_B T\left(\partial_{\mathbf{Q}} \cdot \boldsymbol{\mathcal{M}}\right) + \left(2k_B T\,\boldsymbol{\mathcal{M}}\right)^{\frac{1}{2}}\boldsymbol{\mathcal{W}}(t).$$
- Computational issues (not discussed here heavily but very important to my research group):
  - How to compute **deterministic velocities** $\boldsymbol{\mathcal{M}}\mathbf{F}$ (matrix-vector product) efficiently?
  - How to generate **Brownian increments** $\mathcal{N}\left(\mathbf{0},\, 2k_B T \Delta t\,\boldsymbol{\mathcal{M}}\right)$ or, equivalently, **Brownian velocities** $\mathcal{N}\left(\mathbf{0},\, (2k_B T/\Delta t)\,\boldsymbol{\mathcal{M}}\right)$ efficiently?
  - How to generate **stochastic drift** $k_B T\left(\partial_{\mathbf{Q}} \cdot \boldsymbol{\mathcal{M}}\right)$ efficiently by only multiplying vectors by $\boldsymbol{\mathcal{M}}$, without derivatives.

Generating Brownian increments

- We need a fast way to compute the **Brownian velocities**
$$\mathbf{U}_b = \sqrt{\frac{2k_B T}{\Delta t}}\, \boldsymbol{\mathcal{M}}^{\frac{1}{2}}\mathbf{W} = \mathcal{N}\left(\mathbf{0}, 2k_B T/\Delta t\, \boldsymbol{\mathcal{M}}\right)$$
where $\mathbf{W}$ is a vector of Gaussian random variables.
- The product $\boldsymbol{\mathcal{M}}^{\frac{1}{2}}\mathbf{W}$ can be computed iteratively by **repeated multiplication** of a vector by $\boldsymbol{\mathcal{M}}$ 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.

Stochastic drift term

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

- Key idea to get $(\partial_{\mathbf{Q}} \cdot \mathcal{M})_i = \partial \mathcal{M}_{ij} / \partial Q_j$ is to use **random finite differences (RFD)** [3]: If $\langle \Delta\mathbf{P}\Delta\mathbf{Q}^T = \mathbf{I} \rangle$,

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

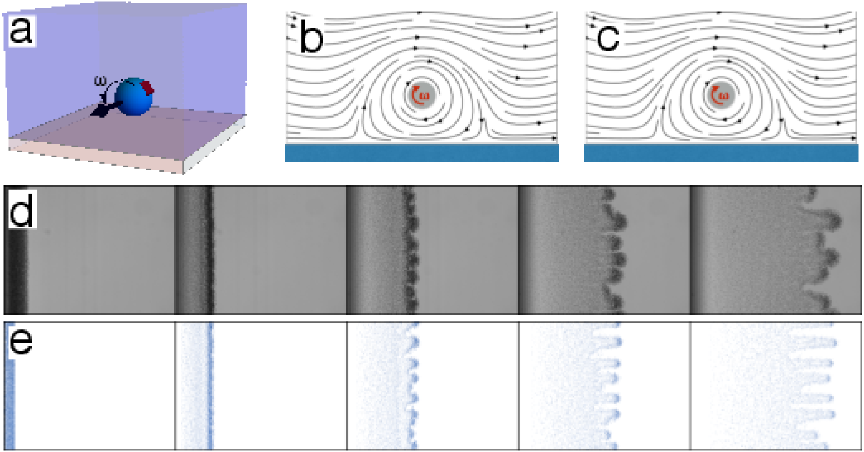
$$\{\partial_{\mathbf{Q}}\mathcal{M}(\mathbf{Q})\} : \langle \Delta\mathbf{P}\Delta\mathbf{Q}^T \rangle = k_B T\,\partial_{\mathbf{Q}} \cdot \mathcal{M}(\mathbf{Q}).$$

- This leads to a **stochastic Adams-Bashforth** temporal integrator [3],

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

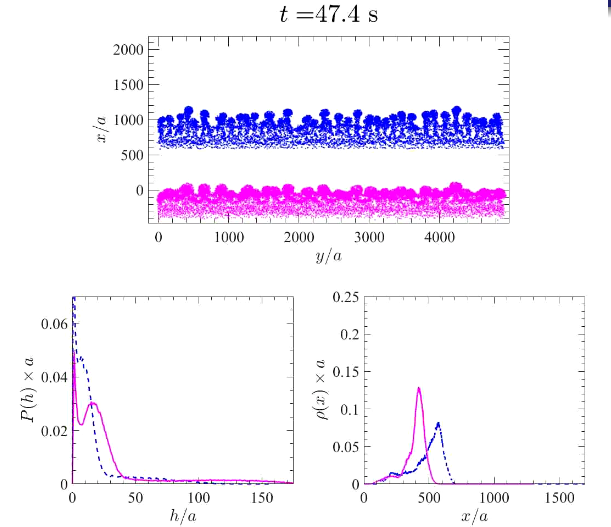
$$+ \frac{k_B T}{\delta}\left(\mathcal{M}\left(\mathbf{Q} + \frac{\delta}{2}\widetilde{\mathbf{W}}^n\right) - \mathcal{M}\left(\mathbf{Q} - \frac{\delta}{2}\widetilde{\mathbf{W}}^n\right)\right)\widetilde{\mathbf{W}}^n.$$

Microrollers: Fingering Instability



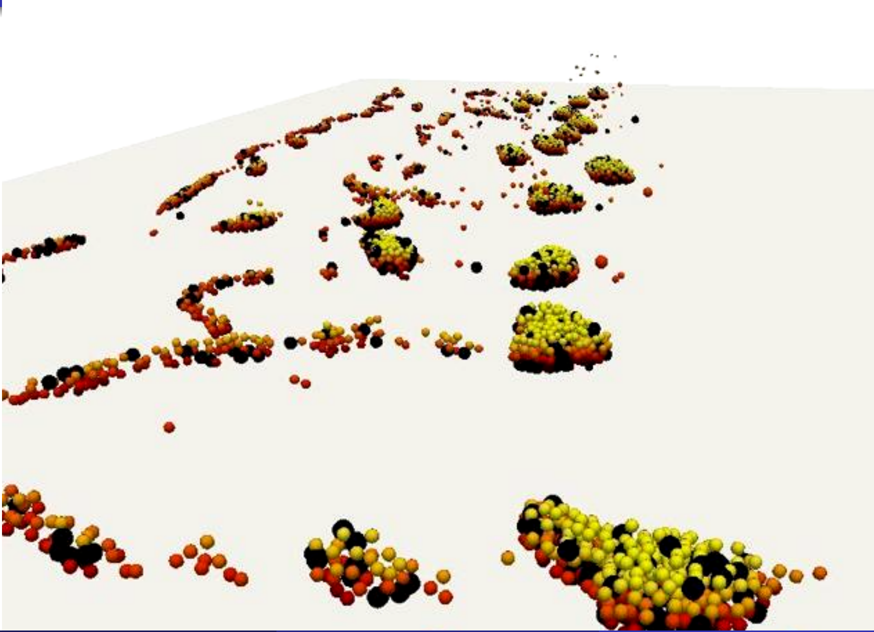
Experiments by Michelle Driscoll (lab of Paul Chaikin, NYU Physics, now at Northwestern), simulations by **Blaise Delmotte** [4, 3].

Role of Brownian Motion

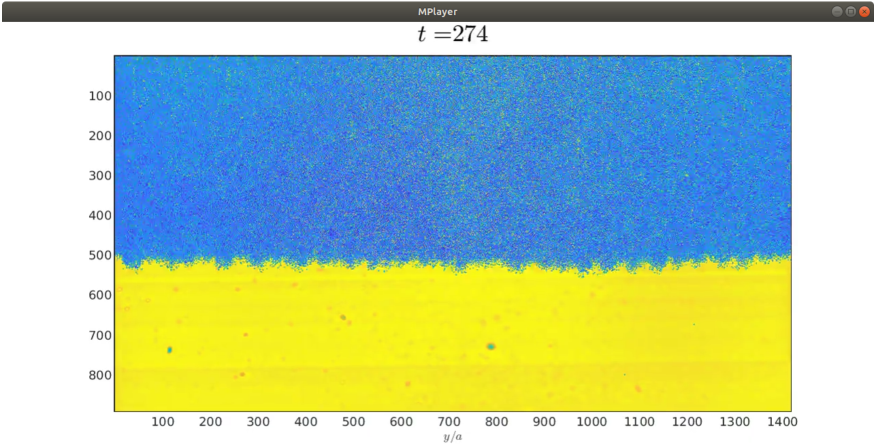


Simulations show that thermal fluctuation are quantitatively important because they set the **gravitational height**.[3].

Critters

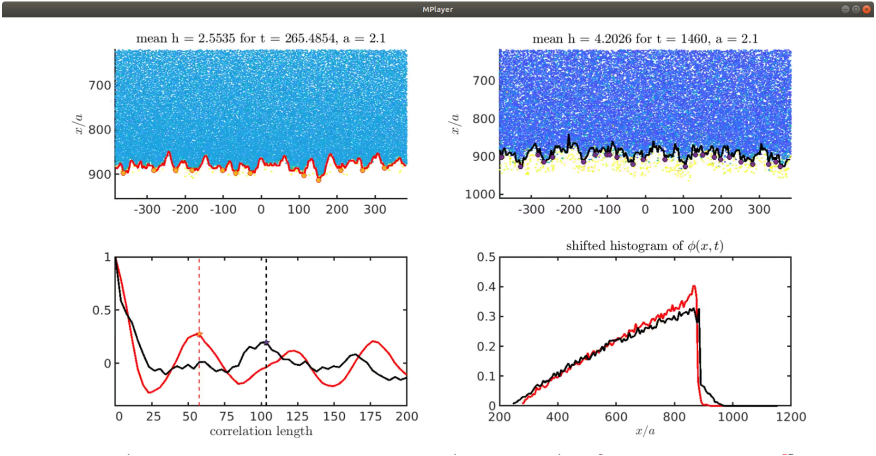


Sedimentation of colloidal monolayer



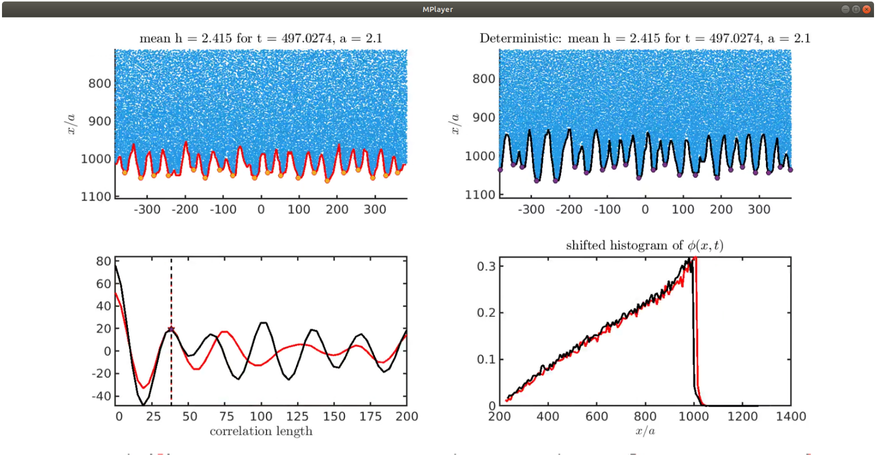
Experiments in lab of Paul Chaikin show that a sedimenting front roughens due to a sort of "instability".

3D simulations of sedimentation



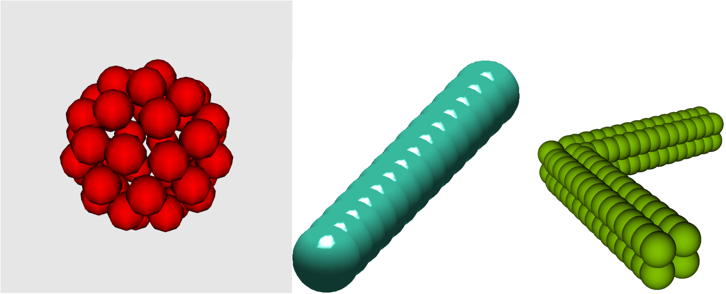
Simulations of **Brennan Sprinkle** show the gravitational height matters, but no precise explanation yet.

2D simulations of sedimentation



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

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** [5].
- **We can efficiently simulate the driven and Brownian motion of the rigid multiblobs.**

Nonspherical Rigid Multiblobs

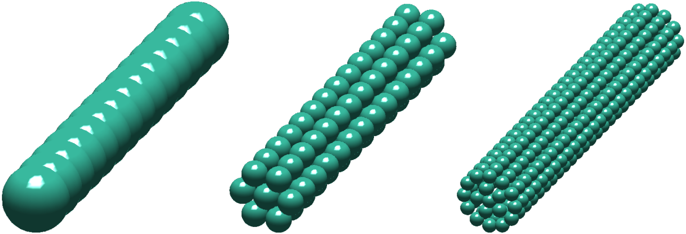


Figure: Rigid multiblob models of a rigid cylinder (rod) going from **minimally resolved** (left) to **well-resolved** (right).

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,

$$\begin{aligned} \sum_j \mathcal{M}_{ij}\boldsymbol{\lambda}_j &= \mathbf{u}_p + \boldsymbol{\omega}_p \times \left(\mathbf{r}_i - \mathbf{q}_p\right) + \breve{u}_p \qquad (2) \\ \sum_{i \in \mathcal{B}_p} \boldsymbol{\lambda}_i &= \mathbf{f}_p \\ \sum_{i \in \mathcal{B}_p} (\mathbf{r}_i - \mathbf{q}_p) \times \boldsymbol{\lambda}_i &= \boldsymbol{\tau}_p. \end{aligned}$$

  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 $\mathbf{U} = (\mathbf{u}, \boldsymbol{\omega})$,

$$\begin{bmatrix} \mathcal{M} & -\mathcal{K} \\ \mathcal{K}^T & \mathbf{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda} \\ \mathbf{U} \end{bmatrix} = \begin{bmatrix} \breve{\mathbf{u}} \\ \mathbf{F} \end{bmatrix}, \tag{3}$$

where $\mathbf{F} = (\mathbf{f}, \boldsymbol{\tau})$ are the applied forces and torques.

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

gives the **multiblob mobility matrix** [sorry for change of notation of letter $\mathcal{N}$]

$$\mathcal{N} = \left(\mathcal{K}^T\mathcal{M}^{-1}\mathcal{K}\right)^{-1} \tag{4}$$

- The inverse of the mobility matrix is called the **resistance matrix**, $\mathcal{R} = \mathcal{N}^{-1} = \mathcal{K}^T\mathcal{M}^{-1}\mathcal{K}$.
- The **surface velocity $\breve{\mathbf{u}}$** can be used to model **active slip** or to generate **Brownian velocities** [1].

Lubrication for **spherical colloids**

- Use **Stokesian Dynamics** approach introduced by Brady to account for the strong lubrication for thin gaps by adding lubrication forces:
$$\begin{pmatrix} \mathcal{M} & -\mathcal{K} \\ \mathcal{K}^T & \boldsymbol{\Delta}_{MB} \end{pmatrix} \begin{pmatrix} \boldsymbol{\lambda} \\ \mathbf{U} \end{pmatrix} = \begin{pmatrix} -\breve{\mathbf{u}} \\ \mathbf{F} \end{pmatrix}, \tag{5}$$
- $\boldsymbol{\Delta}_{MB}$ 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) — can be computed semi-analytically or tabulated by using an expensive but accurate reference method (e.g., boundary integral).
- Lubrication-corrected mobility matrix
$$\overline{\mathcal{N}} = \left[\mathcal{N}^{-1} + \boldsymbol{\Delta}_{MB}\right]^{-1} = \mathcal{N} \cdot \left[\mathbf{I} + \boldsymbol{\Delta}_{MB} \cdot \mathcal{N}\right]^{-1}.$$
- One can even use a single blob per sphere (**minimally-resolved**) by adding rotation/torque to the RPY tensor, and setting $\mathcal{K} = \mathbf{I}$.

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

- Assume that we knew how to efficiently generate Brownian blob velocities $\mathcal{M}^{\frac{1}{2}}\mathbf{W}$.
- *Key idea*: Solve the mobility problem with random slip $\breve{\mathbf{u}}$,

$$\begin{bmatrix} \mathcal{M} & -\mathcal{K} \\ -\mathcal{K}^T & \mathbf{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda} \\ \mathbf{U} \end{bmatrix} = - \begin{bmatrix} \breve{\mathbf{u}} = (2k_B T)^{1/2} \mathcal{M}^{\frac{1}{2}}\mathbf{W} \\ \mathbf{F} \end{bmatrix}, \qquad (6)$$

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

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 [1], such as the following **Euler scheme**:

1. Solve a mobility problem with a **random force+torque**:
$$\begin{bmatrix} \mathcal{M} & -\mathcal{K} \\ -\mathcal{K}^T & \mathbf{0} \end{bmatrix}^n \begin{bmatrix} \lambda^{RFD} \\ \mathbf{U}^{RFD} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ -\widetilde{\mathbf{W}} \end{bmatrix}. \tag{7}$$
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:

$$\begin{bmatrix} \mathcal{M} & -\mathcal{K} \\ -\mathcal{K}^T & \mathbf{0} \end{bmatrix}^n \begin{bmatrix} \boldsymbol{\lambda}^n \\ \mathbf{U}^n \end{bmatrix} = - \begin{bmatrix} \breve{\mathbf{u}}^n + \breve{\mathbf{u}}^{RFD} \\ \mathbf{F}^n - \mathbf{F}^{RFD} \end{bmatrix}. \tag{8}$$

3. Move the particles (rotate for orientation)

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

Fluctuating Hydrodynamics

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

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

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

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

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

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,

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

with the **inertial body dynamics**

$$m\frac{d\mathbf{u}}{dt} = \mathbf{F} - \int_{\partial\Omega} \boldsymbol{\lambda}(\mathbf{q})\, d\mathbf{q}, \tag{11}$$

$$\mathbf{I}\frac{d\boldsymbol{\omega}}{dt} = \boldsymbol{\tau} - \int_{\partial\Omega} [\mathbf{q} \times \boldsymbol{\lambda}(\mathbf{q})]\, d\mathbf{q} \tag{12}$$

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 $\mathbf{U} = \mathcal{N}\mathbf{F}$ via the deterministic **mobility problem**:

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

$$\mathbf{v}(\mathbf{q}) = \mathbf{u} + \boldsymbol{\omega}\times\mathbf{q} - \breve{\mathbf{u}}(\mathbf{q}) \;\; \text{for all } \mathbf{q}\in\partial\Omega, \tag{13}$$

With **force and torque balance**

$$\int_{\partial\Omega}\boldsymbol{\lambda}(\mathbf{q})\,d\mathbf{q} = \mathbf{F} \quad \text{and} \quad \int_{\partial\Omega}\left[\mathbf{q}\times\boldsymbol{\lambda}(\mathbf{q})\right]d\mathbf{q} = \boldsymbol{\tau}, \tag{14}$$

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

$$\boldsymbol{\sigma} = -\pi\mathbf{I} + \eta\left(\boldsymbol{\nabla}\mathbf{v} + \boldsymbol{\nabla}^T\mathbf{v}\right). \tag{15}$$

Overdamped Brownian Dynamics

- Consider a suspension of N_b rigid bodies with **configuration** $\mathbf{Q} = \{\mathbf{q}, \theta\}$ 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**

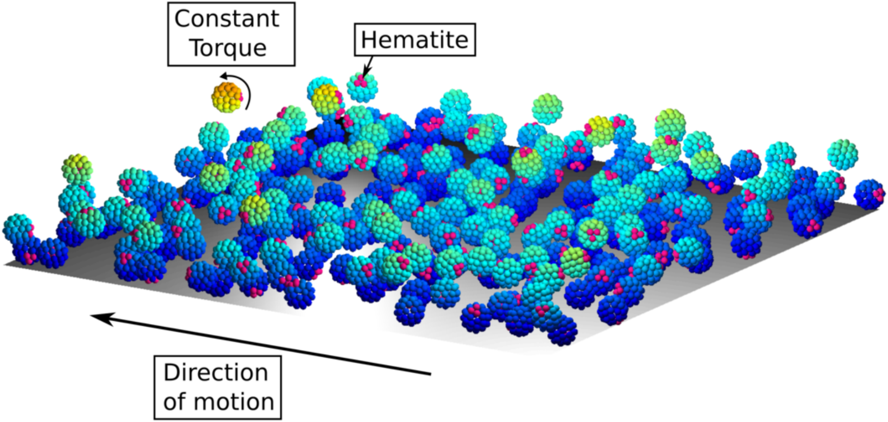
$$\frac{d\mathbf{Q}(t)}{dt} = \mathbf{U} = \mathcal{N}\mathbf{F} + (2k_B T \mathcal{N})^{\frac{1}{2}} \mathcal{W}(t) + (k_B T)\,\partial_{\mathbf{Q}} \cdot \mathcal{N},$$

where $\mathcal{N}(\mathbf{Q})$ is the **body mobility matrix**, with "square root" given by **fluctuation-dissipation balance**

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

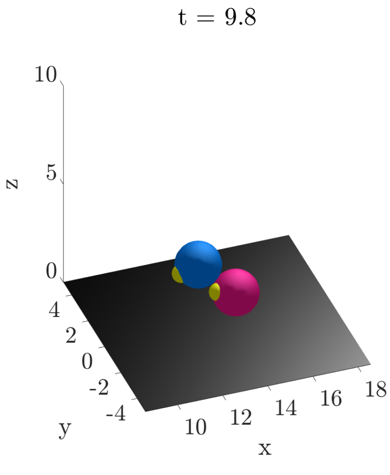
$\mathbf{U} = \{\mathbf{u}, \omega\}$ collects the **linear and angular velocities**
$\mathbf{F}(\mathbf{Q}) = \{\mathbf{f}, \tau\}$ collects the **applied forces and torques**.

Microrollers: Uniform Suspension

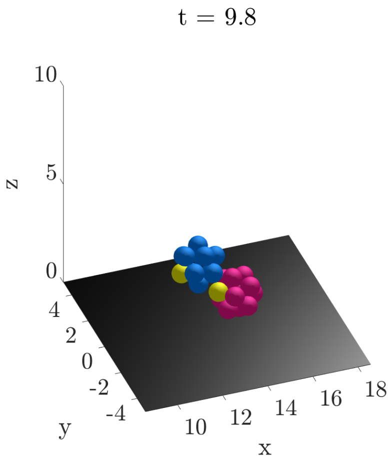


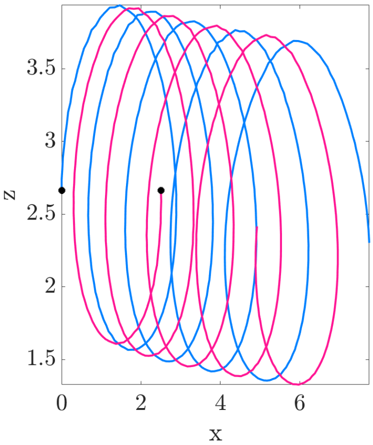
Simulations by **Brennan Sprinkle**+Blaise Delmotte [1] of a uniform suspension of microrollers at packing fraction $\phi = 0.4$ (GIF). Compare to experiments (AVI) by **Michelle Driscoll**.

Example 1: Bound Roller Dimer

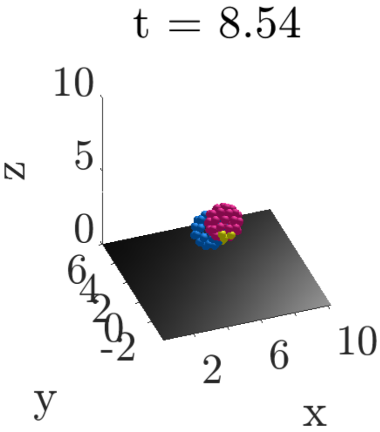


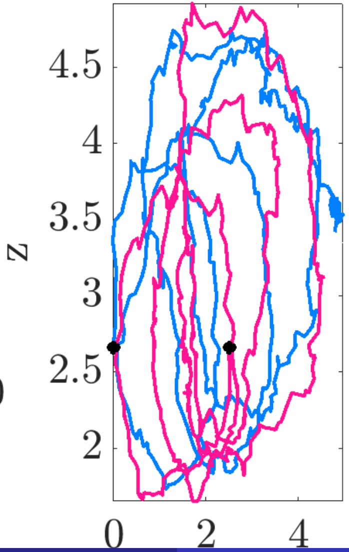
Example 1: Deterministic 12 blobs



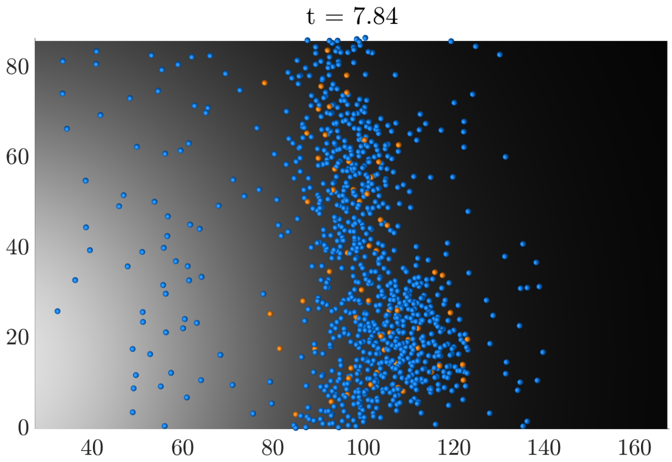


Example 1: Bound Roller Dimer





Example 2: Formation of Critters



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