Practical Brownian Dynamics

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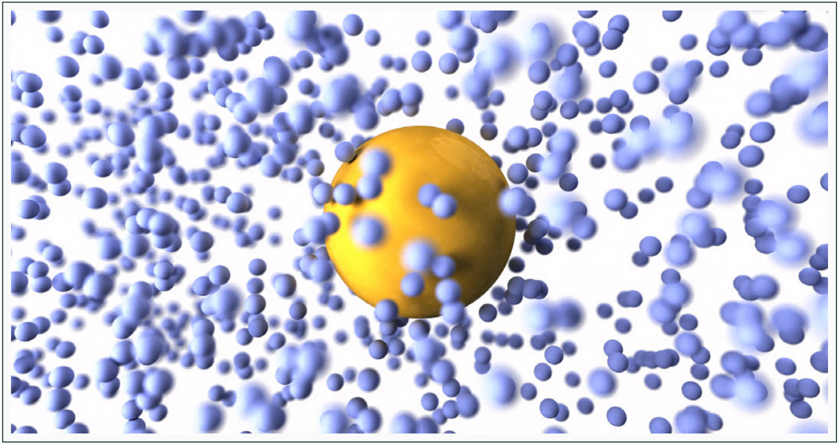
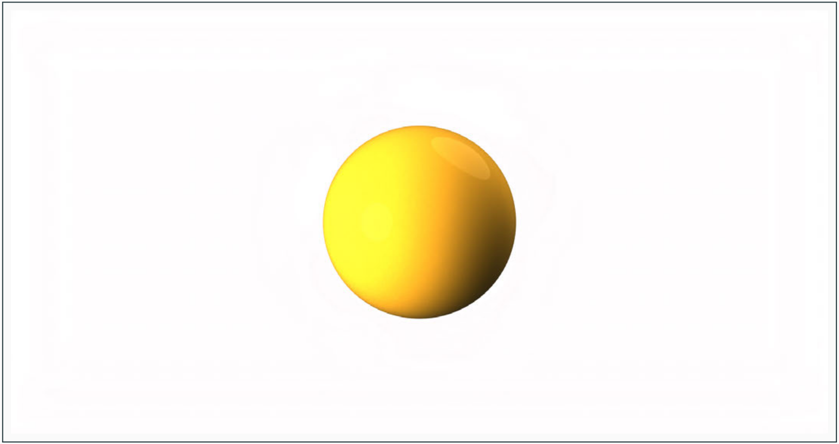
A Sense of Scale

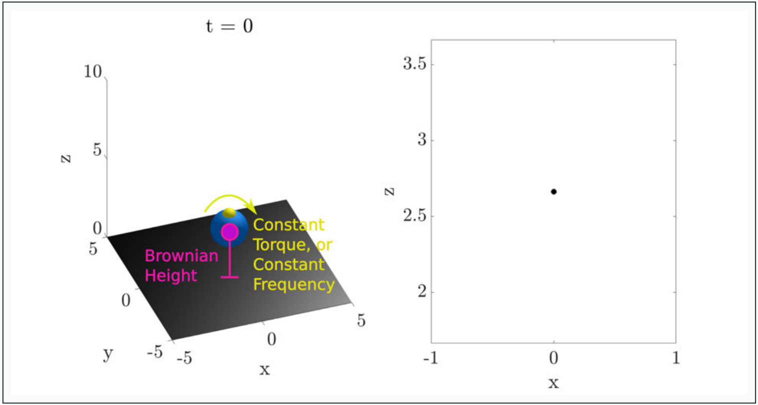
Brownian motion



Brownian motion



Active Particles



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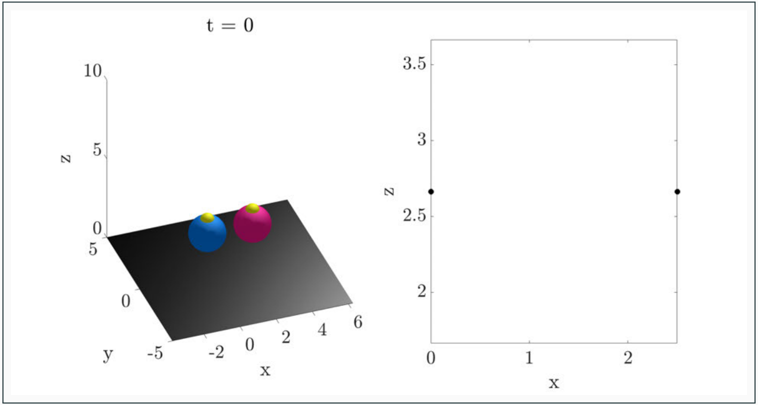


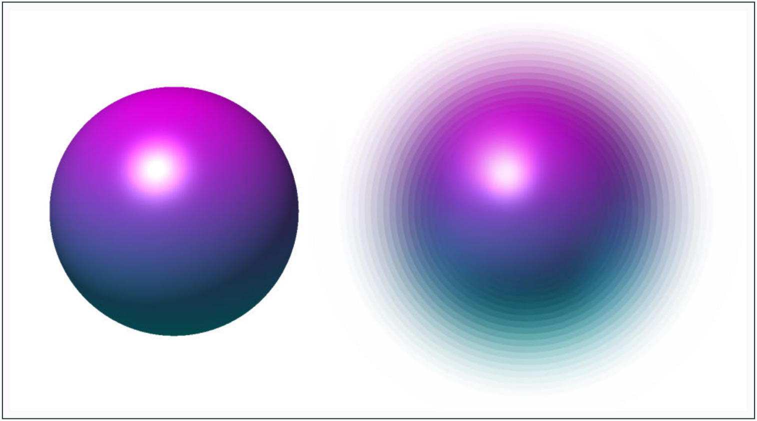
Active Particles

We need fast methods for Brownian Dynamics to study collective behavior

Blobs

A hydrodynamic blob

The building block of every method I'll talk about is a **blob**.
Which is hydrodynamically *similar* to a sphere



Equation of motion

Ignoring fluctuations for a moment, to simulate a hydrodynamic blob we solve

$$\nabla P - \eta \nabla^2 \mathbf{v} = F \tag{1}$$

$$\nabla \cdot \mathbf{v} = 0 \tag{2}$$

$$\tag{3}$$

- Stokes Equations

Equation of motion

Ignoring fluctuations for a moment, to simulate a hydrodynamic blob we solve

$$\nabla P - \eta \nabla^2 \mathbf{v} = \sum_i \mathsf{F}_i \, \delta_a (\mathsf{x} - \mathsf{r}_i) \tag{1}$$

$$\nabla \cdot \mathbf{v} = 0 \tag{2}$$

$$\frac{d\mathsf{r}_i}{dt} = \mathsf{V}_i = \int_V \mathbf{v}(\mathsf{x}) \, \delta_a (\mathsf{x} - \mathsf{r}_i) \, dV_x \tag{3}$$

- Stokes Equations
- $\mathbf{r}_i$ are the positions of blobs

Equation of motion

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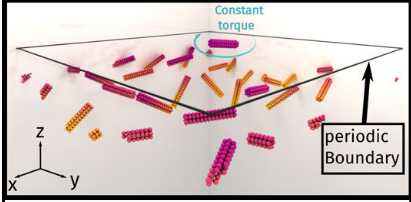
- Stokes Equations
- $\mathbf{r}_i$ are the positions of blobs
- δ_a is a regularized delta function that gives the blobs their ‘blurry’

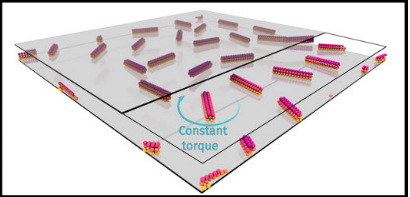
Equation of motion

We can solve these equations very efficiently in the following geometries:

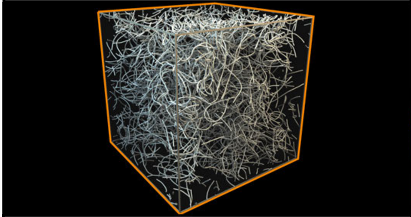
doubly periodic free space



doubly periodic slit channel



triply periodic



doubly periodic single wall

free space

free space with single wall

The 'blob' stokes equations are linear so we can write the solution using a hydrodynamic *Mobility Operator*

$$\frac{d\mathrm{r}}{dt} = \mathrm{V} = \boldsymbol{\mathcal{M}}\left(\mathrm{r}\right)\mathrm{F}$$

Bring back the thermal fluctuations, we want to solve

$$\frac{d\mathrm{r}}{dt} = \mathrm{V} = \boldsymbol{\mathcal{M}}\mathrm{F} + k_B T \left(\boldsymbol{\nabla}_{\mathrm{r}} \cdot \boldsymbol{\mathcal{M}}\right) + \sqrt{2 k_B T}\,\boldsymbol{\mathcal{M}}^{1/2}\boldsymbol{\mathcal{W}}(t)$$

which is time reversible with respect to the Gibbs-Boltzmann distribution

$$\mathrm{U}_{\mathrm{GB}}(\mathrm{r}) \sim \exp\left(-\frac{E(\mathrm{r})}{k_B T}\right)$$

where

$$\mathrm{F} = -\frac{\delta E\left(\mathrm{r}\right)}{\delta \mathrm{r}}$$

Challenges

We know how to compute $\mathsf{U} = \mathcal{M}\mathsf{F}$ in linear time in different geometries, but $\cdots$

Key Challenges

1. How do we adjust $\mathcal{M}$ to account for constrained particles like: rigid bodies or inextensible fibers
2. How do we compute the Stochastic Drift $k_B T \left(\boldsymbol{\nabla}_{\mathsf{q}} \cdot \mathcal{M} \right)$ in linear time.
3. How do we compute the Brownian Increment $\sqrt{2 k_B T} \mathcal{M}^{1/2} \mathcal{W}(t)$ in linear time.

Spherical Particles

Sphere Hydrodynamics

We can correct the hydrodynamics for a single blob using lubrication corrections in the mobility [1]

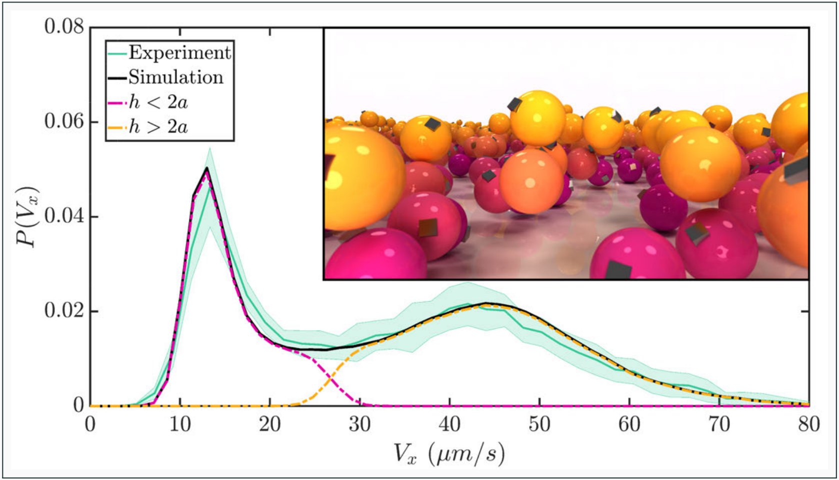
$$\mathcal{N} = \left(\mathcal{M}^{-1} - \mathcal{M}^{-1}_{\text{close surfaces}} + \left(\mathcal{M}^{\text{asymptotics}}_{\text{close surfaces}} \right)^{-1} \right)^{-1}$$

Introduced for *Stokesian Dynamics* in (Brady et al., 1988) but only in free space and very slow to compute. **We can do it fast**

[1] B. Sprinkle, E. B. van der Wee, Y. Luo, M. Driscoll, and A. Donev, “Driven dynamics in dense suspensions of microrollers,” Soft Matter, vol. 16, pp. 7982–8001, 2020.

First Example

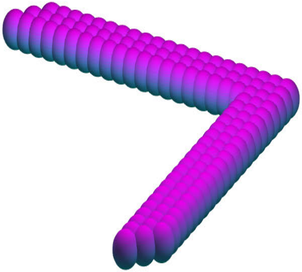
Results



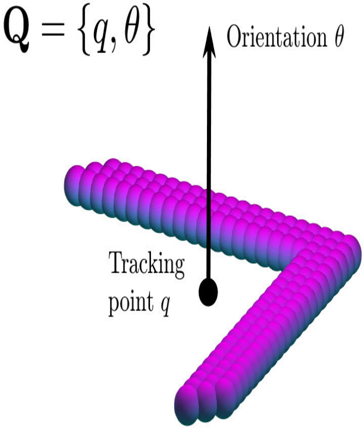
Experiment
Simulation
$h < 2a$
$h > 2a$
$P(V_x)$
0.08
0.06
0.04
0.02
0
0
10
20
30
40
50
60
70
80
$V_x\ (\mu m/s)$

Brownian Dynamics for Rigid Bodies

Rigid Multiblob Model

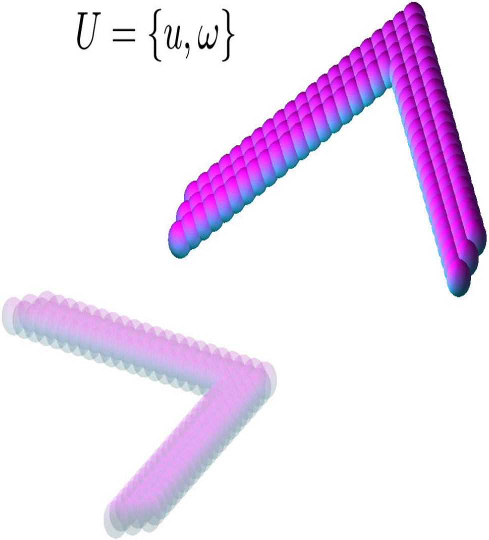


notation



notation

$$U = \{u, \omega\}$$



Equation of motion

A rigid body is held rigid by constraint forces λ so that:

$$\mathsf{V}_i = \boldsymbol{\mathcal{M}}_{ij}\boldsymbol{\lambda}_j \tag{4}$$

But also a rigid body velocity related to blob velocity according to:

$$\mathsf{V}_i = \mathsf{u} + (\mathbf{r}_i - \mathbf{q}) \times \boldsymbol{\omega} \equiv \mathcal{K}\begin{bmatrix} \mathsf{u} \\ \boldsymbol{\omega} \end{bmatrix} = \mathcal{K}\mathsf{U} \tag{5}$$

$$\boxed{\boldsymbol{\mathcal{M}}\boldsymbol{\lambda} = \mathsf{V} = \mathcal{K}\mathsf{U}}$$

Equation of motion

Using the principle of virtual work

$$\begin{bmatrix} \mathcal{M} & -\mathcal{K} \\ -\mathcal{K}^T & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda} \\ \mathrm{U} \end{bmatrix} = \begin{bmatrix} 0 \\ \mathrm{F} \end{bmatrix}$$

which we know how to solve in linear time! using preconditioned GMRES.

But for easy notation we can write

$$\mathrm{U} = \left(\mathcal{K}^T \mathcal{M}^{-1} \mathcal{K}\right)^{-1} \mathrm{F} \equiv \mathcal{N} \mathrm{F}$$

so that

$$\frac{\mathrm{q}}{dt} = \mathrm{U} = \mathcal{N}\mathrm{F} + k_B T \left(\boldsymbol{\nabla}_{\mathrm{q}} \cdot \mathcal{N}\right) + \sqrt{2 k_B T}\, \mathcal{N}^{1/2} \mathcal{W}(t)$$

Some notes

1. Since we solve for the stochastic rigid velocity U, we can update the rigid body directly by translating and rotating

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2. Solving

$$\begin{bmatrix} \boldsymbol{\mathcal{M}} & -\boldsymbol{\mathcal{K}} \\ -\boldsymbol{\mathcal{K}}^T & \mathbf{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda} \\ \mathsf{U} \end{bmatrix} = \begin{bmatrix} \sqrt{2k_BT/dt}\boldsymbol{\mathcal{M}}^{1/2}\boldsymbol{\mathcal{W}} \\ \mathsf{F} \end{bmatrix}$$

   gives

$$\boldsymbol{\mathcal{N}}\mathsf{F} + \sqrt{2k_BT/dt}\boldsymbol{\mathcal{N}}^{1/2}\boldsymbol{\mathcal{W}}(t)$$

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3. The thermal drift term $k_BT\ \boldsymbol{\nabla}_{\mathrm{q}} \cdot \mathcal{N}$ is captured through time integration.

Some notes

The most expensive pieces in each time step are:

1. Computing[2]

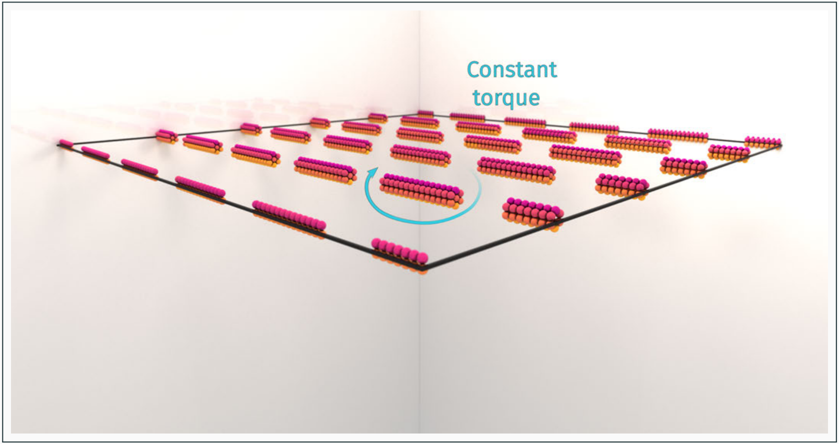
$$\sqrt{\frac{2k_BT}{\Delta t}}\mathcal{M}^{1/2}\mathcal{W}$$

2. Solving

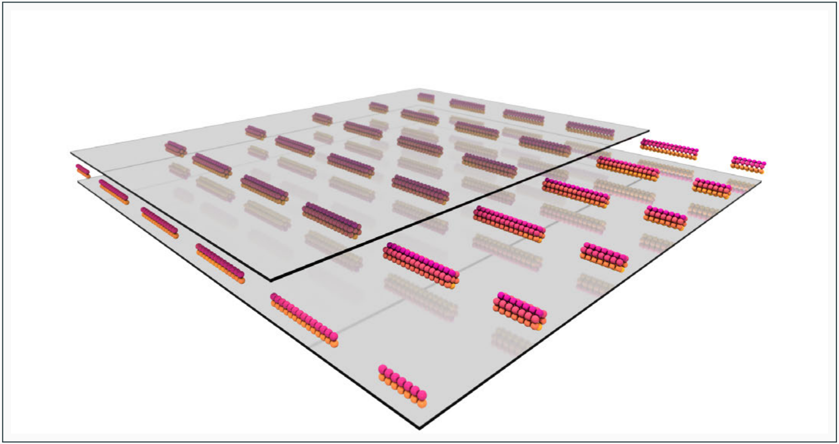
$$\begin{bmatrix} \mathcal{M} & -\mathcal{K} \\ -\mathcal{K}^T & \mathbf{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda} \\ \mathrm{U} \end{bmatrix} = \begin{bmatrix} \mathrm{RHS}_1 \\ \mathrm{RHS}_2 \end{bmatrix}$$

[2] We can use PSE (Swan, 2017) or Lanczos

Example 2

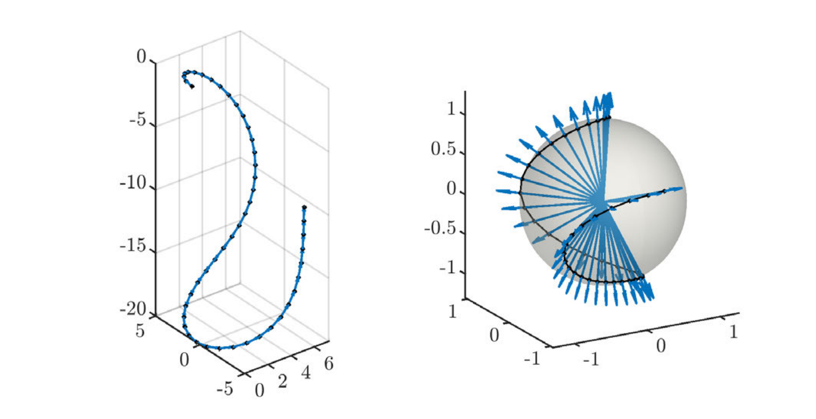


Example 2



Flexible Fibers

We represent **inextensible** fibers as chains of blobs and describe the chains using their unit tangent vectors $\boldsymbol{\tau}_i$ which point from blob to blob.



New Coordinates

Given a set of unit tangent vectors

$$\underline{\boldsymbol{\tau}} = \{\boldsymbol{\tau}_1, \boldsymbol{\tau}_2, \cdots, \boldsymbol{\tau}_N\}$$

we can find

$$\underbrace{\mathrm{x}_i = \mathrm{x}_0 + \Delta s \sum_{j=1}^{i-1} \boldsymbol{\tau}_i}_{\boldsymbol{\mathcal{S}}_{\underline{\boldsymbol{\tau}}}} \approx \mathrm{x}_0 + \int_0^s \boldsymbol{\tau}(s')ds'$$

as a map from

$$\boldsymbol{\tau} \in S^2 \to \mathrm{x} \in \mathbb{R}^3$$

Evolving the fiber in time

We have two ways to update the fiber

$$\frac{\partial \underline{\boldsymbol{\tau}}}{\partial t} = \boldsymbol{\Omega} \times \underline{\boldsymbol{\tau}}$$

and

$$\mathsf{V} = \frac{\partial \underline{\mathsf{X}}}{\partial t}$$

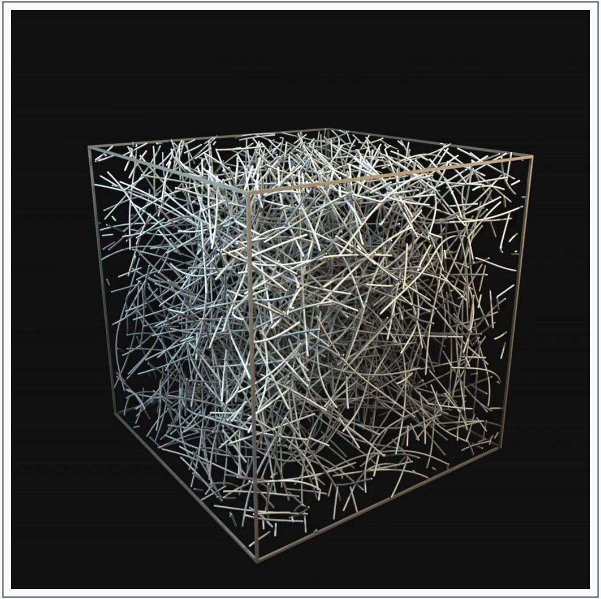
so using

$$\mathsf{X}_i = \Delta s \sum_{j=1}^{i-1} \boldsymbol{\tau}_j \Rightarrow \underline{\mathsf{X}} = \boldsymbol{\mathcal{S}} \underline{\boldsymbol{\tau}}$$

we can write

$$\boxed{\mathsf{V} = \boldsymbol{\mathcal{S}} \left[\boldsymbol{\Omega} \times \underline{\boldsymbol{\tau}} \right] = \boldsymbol{\mathcal{K}} \boldsymbol{\Omega}} \tag{6}$$

Example 3



Questions