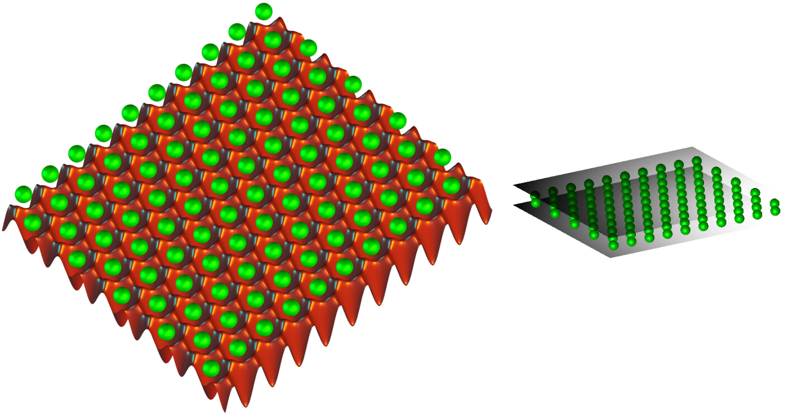
# Large Scale Brownian Dynamics of Confined Suspensions of Rigid Particles

Brennan Sprinkle
**Aleksandar Donev**

Courant Institute, *New York University*

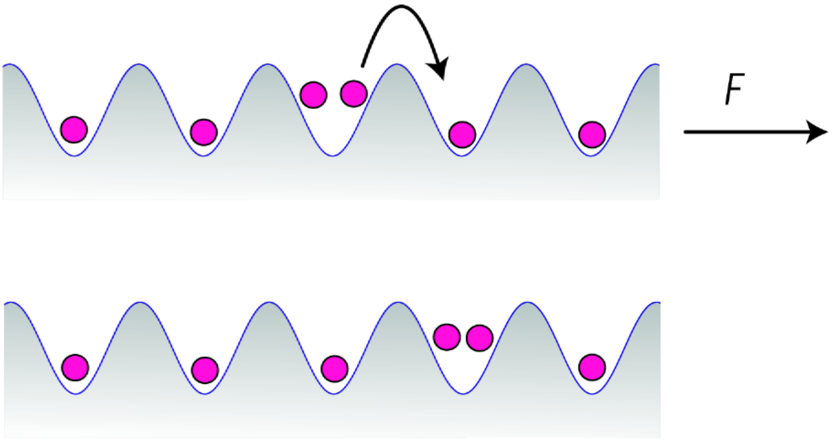
Minisymposium on Complex Fluids at Small Scales
ICIAM, Valencia, Spain, July 17th 2019

# Soliton Kinks in Pinned Colloidal Monolayers



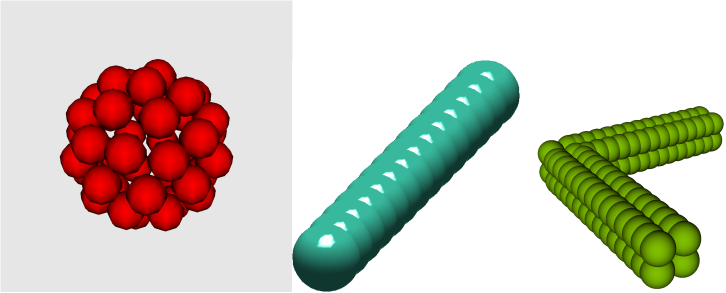
Inspired by experiments on "**kinks and antikinks in colloidal monolayers driven across ordered surfaces**", Bohlein *et al*, Nature Materials 2011.

# Thermal Fluctuations: Brownian Motion




Depinning of the driven monolayer (transition from static to dynamic friction) happens by thermally-activated hops of the colloids.

# Rigid MultiBlob Models



- The rigid body is discretized through a number of "**beads**" or "**blobs**" with hydrodynamic radius *a* [1] connected into a **rigid multiblob**.
- **How to efficiently simulate the active and Brownian motion of the rigid particles in fully confined domains?**
  **Rigid-Body Fluctuating Immersed Boundary (RB-FIB)** [2]

# Fluctuating Hydrodynamics

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

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

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

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

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,

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

with the **inertial body dynamics**

$$m\frac{d\mathbf{u}}{dt}=\mathbf{F}-\int_{\partial\Omega}\boldsymbol{\lambda}\left(\mathbf{q}\right)d\mathbf{q},$$
$$\mathbf{I}\frac{d\boldsymbol{\omega}}{dt}=\boldsymbol{\tau}-\int_{\partial\Omega}\left[\mathbf{q}\times\boldsymbol{\lambda}\left(\mathbf{q}\right)\right]d\mathbf{q}$$

where $\boldsymbol{\lambda}\left(\mathbf{q}\right)$ is the normal component of the stress on the outside of the surface of the body, i.e., the **traction**

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

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**:

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

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

With **force and torque balance**

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

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

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

# 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**

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

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

- "Square root" of mobility matrix given by **fluctuation-dissipation balance**

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

# 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) or microfluidic channels that modify the hydrodynamics strongly.

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**.

# Rough idea of temporal integration

- Temporarily neglecting the stochastic drift, the apparent velocity of the particles over an **Euler-Maruyama** (EM) **time step** $\Delta t$,

$$\mathbf{U}_{\mathrm{EM}} = \mathcal{N}\mathbf{F} + \sqrt{\frac{2k_B T}{\Delta t}}\,\mathcal{N}^{1/2}\mathbf{W},$$

where $\mathbf{W}$ is a standard Gaussian random vector.

- The EM update can be corrected to add the drift by using **random finite differences**,

$$\mathbf{Q}^{n+1} = \mathbf{Q}^{n} + \Delta t \mathbf{U}_{\mathrm{EM}}^{n} + \frac{\Delta t}{\delta}\left(\mathbf{U}^{+} - \mathbf{U}^{-}\right),$$

where, for a small $\delta \to 0$ and a random displacement/rotation $\Delta\mathbf{Q}^{n}$,

$$\mathbf{U}^{\pm} = \mathcal{N}\left(\mathbf{Q}^{n} \pm \frac{\delta}{2}\Delta\mathbf{Q}^{n}\right)\Delta\mathbf{Q}^{n}.$$

- This is too expensive/inaccurate as it requires three mobility solves per step; one can do a bit better [2].

# Immersed Boundary (IB) Re-formulation

Following the IB method we extend the fluid equation over the whole domain $\forall \mathbf{x} \in \Omega$ and use delta functions to evaluate fluid variables on the surfaces of the bodies $\forall p, \forall \mathbf{r} \in \partial \mathcal{B}_p$, to write a system of **semi–continuum** linear equations for $\mathbf{U}_{\text{EM}} = \left[ \mathbf{u}_1^{\text{EM}}, \boldsymbol{\omega}_1^{\text{EM}}, \ldots \mathbf{u}_{N_b}^{\text{EM}}, \boldsymbol{\omega}_{N_b}^{\text{EM}} \right]$,

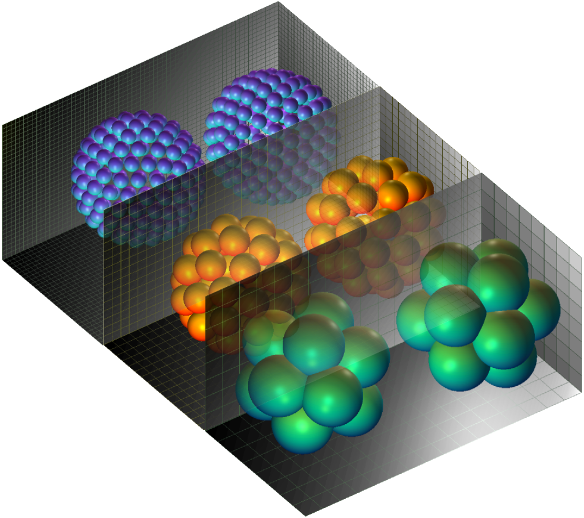
$$-\eta \boldsymbol{\nabla}^2 \mathbf{v} + \boldsymbol{\nabla} \pi = \sqrt{\frac{2 k_B T \eta}{\Delta t}} \boldsymbol{\nabla} \cdot \mathbf{Z}(\mathbf{x}) + \sum_p \int_{\partial \mathcal{B}_p} \delta(\mathbf{x} - \mathbf{r}) \boldsymbol{\lambda}(\mathbf{r}) \, dA(\mathbf{r})$$

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

$$\int_{\Omega} \delta(\mathbf{x} - \mathbf{r}) \mathbf{v}(\mathbf{x}) \, dV(\mathbf{x}) = \mathbf{u}_p^{\text{EM}} + (\mathbf{r} - \mathbf{q}_p) \times \boldsymbol{\omega}_p^{\text{EM}} + \breve{\mathbf{u}}(\mathbf{r}),$$

$$\mathbf{f}_p = \int_{\partial \mathcal{B}_p} \boldsymbol{\lambda}(\mathbf{r}) \, dA(\mathbf{r}), \quad \boldsymbol{\tau}_p = \int_{\partial \mathcal{B}_p} (\mathbf{r} - \mathbf{q}_p) \times \boldsymbol{\lambda}(\mathbf{r}) \, dA(\mathbf{r}).$$

# Rigid Multiblob Discretization



Two tightly confined spheres at different grid resolutions.

# Immersed Boundary Discretization

- Represent body $\mathcal{B}_p$ as a rigid agglomerate of markers or *blobs* with positions $\mathbf{r}_i^p \in \partial\mathcal{B}_p$.
- Discretize $\boldsymbol{\lambda}$ on the Lagrangian grid as a collection of forces $\boldsymbol{\lambda}_i^p \approx \boldsymbol{\lambda}\left(\mathbf{r}_i^p\right) \Delta A \left(\mathbf{r}_i^p\right)$.
- For **fully confined domains, discretize the Stokes equations on a staggered grid**: fluid velocity $\mathbf{v}$ is defined on the face centers $\mathbf{x}_\alpha$.
- Key idea of IB method: Replace delta function with a discrete approximation $\delta_h$ of width several grid cells (Peskin).

# Notation

- Define the *spreading operator* $\mathcal{S}$ and the **adjoint** *interpolation operator* $\mathcal{J} = \Delta V \mathcal{S}^{\star}$ as

$$(\mathcal{J}\mathbf{v})_i^p = \sum_{\mathbf{x}_\alpha \in \Omega} \delta_h \left(\mathbf{x}_\alpha - \mathbf{r}_i^p\right) \mathbf{v}\left(\mathbf{x}_\alpha\right) \approx \int_\Omega \delta\left(\mathbf{x} - \mathbf{r}_i^p\right) \mathbf{v}\left(\mathbf{x}\right) dV(\mathbf{x}),$$

$$(\mathcal{S}\boldsymbol{\lambda})_\alpha = \frac{1}{\Delta V} \sum_p \sum_{\mathbf{r}_i^p} \delta_h \left(\mathbf{x}_\alpha - \mathbf{r}_i^p\right) \boldsymbol{\lambda}_i^p \approx \int_{\partial \mathcal{B}^p} \delta\left(\mathbf{x}_\alpha - \mathbf{r}\right) \boldsymbol{\lambda}\left(\mathbf{r}\right) dA(\mathbf{r}).$$

- Define the geometric matrix $\mathcal{K}(\mathbf{Q})$

$$(\mathcal{K}\mathbf{U})_i^p = \mathbf{u}_p + \left(\mathbf{r}_i^p - \mathbf{q}_p\right) \times \boldsymbol{\omega}_p,$$

$$\left(\mathcal{K}^T\boldsymbol{\lambda}\right)_p = \begin{bmatrix} \sum_{\mathbf{r}_i^p} \boldsymbol{\lambda}_i^p \\ \sum_{\mathbf{r}_i^p} \left(\mathbf{r}_i^p - \mathbf{q}_p\right) \times \boldsymbol{\lambda}_i^p \end{bmatrix} \approx \begin{bmatrix} \int_{\partial \mathcal{B}_p} \boldsymbol{\lambda}\left(\mathbf{r}\right) dA(\mathbf{r}) \\ \int_{\partial \mathcal{B}_p} \left(\mathbf{r} - \mathbf{q}_p\right) \times \boldsymbol{\lambda}\left(\mathbf{r}\right) dA(\mathbf{r}) \end{bmatrix}.$$

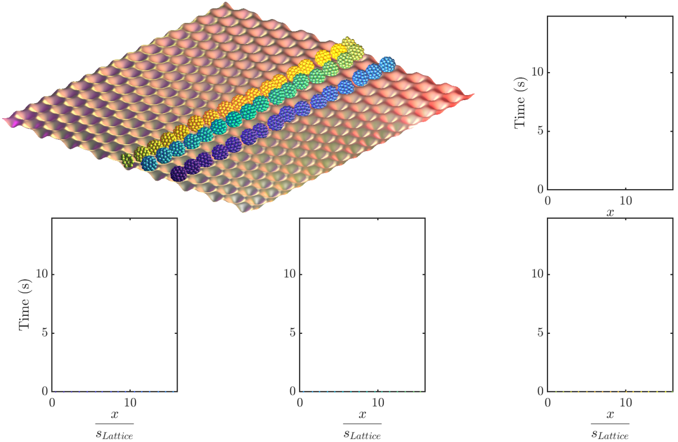
# Spatial Discretization

- We can now compactly write the spatially discretized system for $[\mathbf{v}, \pi, \boldsymbol{\lambda}, \mathbf{U}_{\mathrm{EM}}]$,

$$
\begin{aligned}
-\eta \mathbb{L} \mathbf{v} + \mathbf{G}\pi &= \left(\frac{2k_B T \eta}{\Delta V \Delta t}\right)^{1/2} \mathbb{D}\mathbf{W} + \boldsymbol{\mathcal{S}}\boldsymbol{\lambda}, \\
\mathbf{D}\mathbf{v} &= 0, \\
\mathcal{J}\mathbf{v} &= \mathcal{K}\mathbf{U}_{\mathrm{EM}} + \breve{\mathbf{u}}, \\
\mathcal{K}^T \boldsymbol{\lambda} &= \mathbf{F}.
\end{aligned}
$$

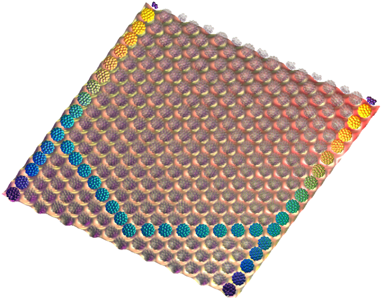
- This is a nested **double saddle-point system** that can be solved efficiently iteratively using **preconditioners** developed for a deterministic rigid-body IB method [3, 1].
- Our **Split–Euler–Maruyama** (SEM) temporal integrator requires solving this kind of system twice, plus solving a fluid-only problem once per time step [2].

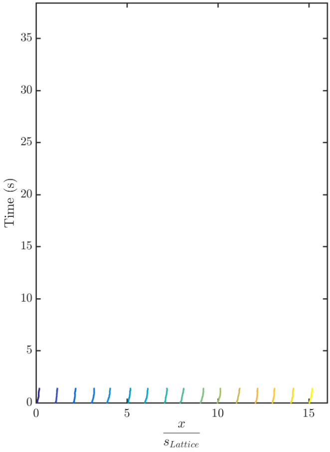
# Kink Soliton Waves




Nearby particles move in a coordinated manner creating "kink solitons."

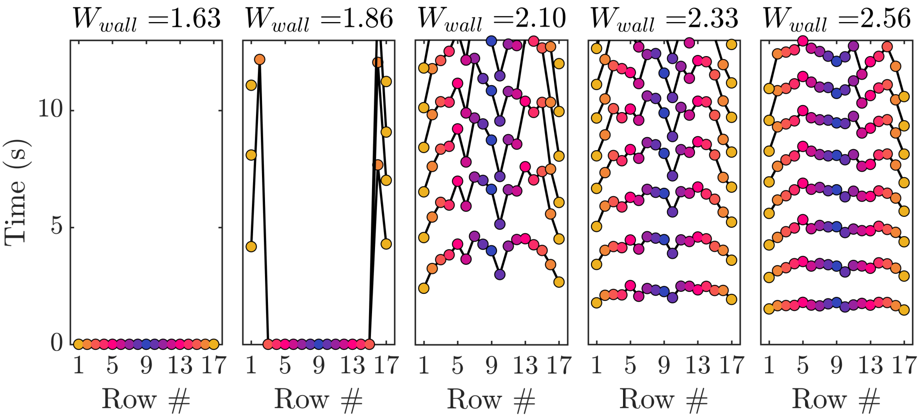
# Effect of Confinement






Depinning starts near the side walls at low driving speeds.

# Effect of Side Boundaries




At moderate driving speeds **particles near the side walls move first but then the middle goes next** and not last.

# Conclusions

- We have constructed a **linear-scaling** algorithm for Brownian dynamics of **nonspherical fully-confined colloids**.
- Key to generating **Brownian increments** efficiently in any **finite domain** is to use **fluctuating hydrodynamics** (Stokes solver using FFTs or multigrid) to handle the far-field hydrodynamic interactions.
- Specialized temporal integrators employing **random finite differences** are required to obtain the correct stochastic drift terms.
- There are related methods for **other boundary conditions**, e.g., triply periodic (Swan talk or RB-FIB) or bottom wall [4] only; currently working on methods for **doubly-periodic domains** (**unbounded** in one direction).
- More accurate but much less flexible is our **Fluctuating Boundary Integral** method [5], right now only works in two dimensions.

# References


F. Balboa Usabiaga, B. Kallemov, B. Delmotte, A. P. S. Bhalla, B. E. Griffith, and A. Donev.
Hydrodynamics of suspensions of passive and active rigid particles: a rigid multiblob approach.
*Communications in Applied Mathematics and Computational Science*, 11(2):217–296, 2016.
Software available at `https://github.com/stochasticHydroTools/RigidMultiblobsWall`.

Brennan Sprinkle, Aleksandar Donev, Amneet Pal Singh Bhalla, and Neelesh Patankar.
Brownian dynamics of fully confined suspensions of rigid particles without Green's functions.
*The Journal of Chemical Physics*, 150(16):164116, 2019.

B. Kallemov, A. Pal Singh Bhalla, B. E. Griffith, and A. Donev.
An immersed boundary method for rigid bodies.
*Communications in Applied Mathematics and Computational Science*, 11(1):79–141, 2016.
Software available at `https://github.com/stochasticHydroTools/RigidBodyIB`.

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`.

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.