Fast (Brownian) HydroDynamics in Doubly-Periodic Geometries

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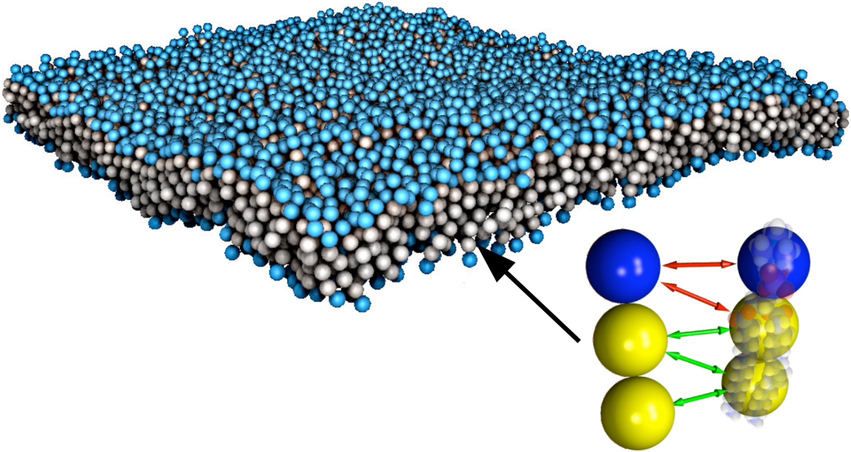
Work done at **Courant Institute**, *New York University*

In honor of Martin Maxey
Brown University, May 2023

Outline

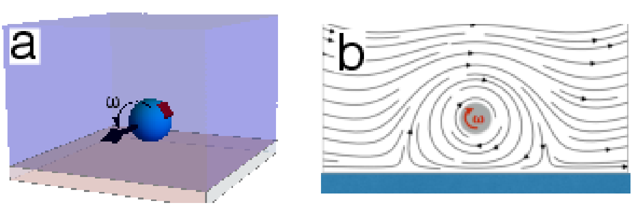
Lipid Membranes

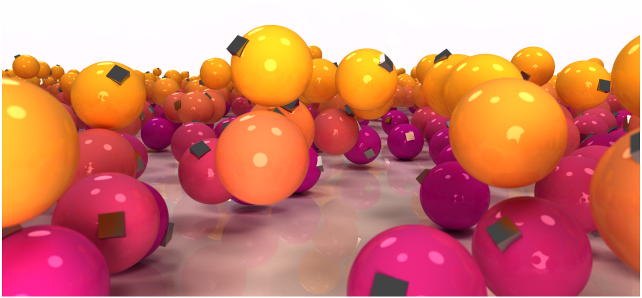
Coarse-grained modeling of lipid membranes using **Brownian HydroDynamics**:



Lateral (collective) **diffusion of lipids** and inclusions (Saffman?).

Colloids: Microrollers



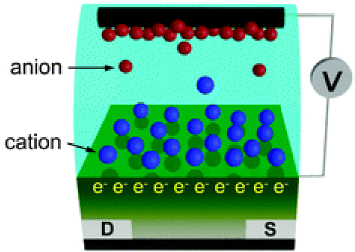


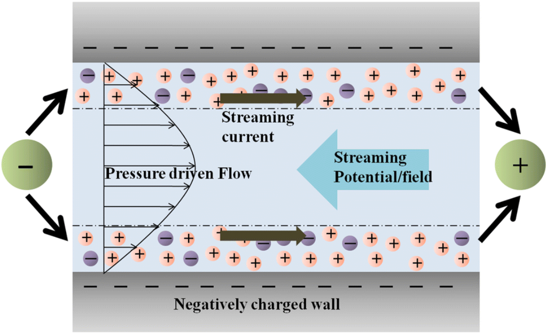
B. Sprinkle, E. B. van der Wee and Y. Luo and M. Driscoll, and A. Donev, *Driven dynamics in dense suspensions of microrollers,* ArXiv:2005.06002.

Electrolytes

Coarse-grained modeling of electrolyte solutions using **Brownian HydroDynamics** (see LBNL talks in session)

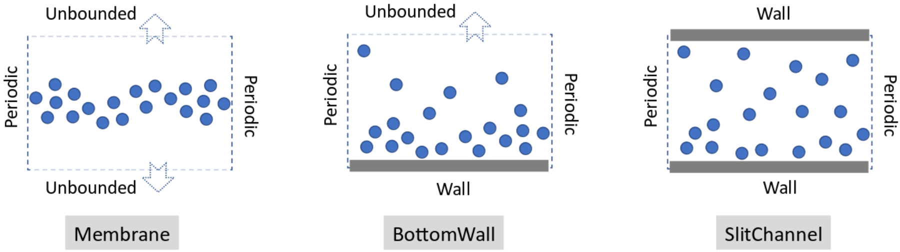
"Electric Double Layer Transistors"





Electrohydrodynamics, conduction in nano channels, battery electrodes, **ion channels** (in lipid membranes!).

Doubly-Periodic Geometries



Poisson ArXiv:2101.07088 [1], code at
`github.com/stochasticHydroTools/DPPoissonTests`
Stokes FCM ArXiv:2210.01837 [2], code at
`github.com/stochasticHydroTools/DoublyPeriodicStokes`

Outline

Force Coupling Method

- The **Force Coupling Method** (FCM) was created by Martin Maxey and collaborators, and has been used to study suspensions for a couple of decades.
- One can think of it as an **alternative to Stokesian Dynamics** that uses grid-based fluid solvers instead of Oseen/RPY tensors.
- Same formulation/idea as immersed boundary method but **smooth kernel** $\Delta(\mathbf{x})$ **is specified** *a priori* and is **grid-independent**:

$$-\eta\boldsymbol{\nabla}^2\mathbf{u}+\boldsymbol{\nabla}p=\mathbf{f}(\mathbf{x})=\sum_{j=1}^{N}\left[\mathbf{F}^{(j)}\Delta_M(\mathbf{x}-\mathbf{r}^{(j)})+\frac{1}{2}\boldsymbol{\nabla}\times(\boldsymbol{\tau}^{(j)}\Delta_D(\mathbf{x}-\mathbf{r}^{(j)}))\right],$$

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

- In classical FCM, the envelopes are (truncated) Gaussians with std $g_M=R_h/\sqrt{\pi}$ and $g_D=R_h/\left(6\sqrt{\pi}\right)^{\frac{1}{3}}$, with R_h as the effective **hydrodynamic radius of a particle/blob**.

No-slip walls

- Linear and angular velocities of the particles:

$$\mathbf{U}^{(j)} = \int_{\mathbf{x}} \mathbf{u}(\mathbf{x}) \Delta_M(\mathbf{x} - \mathbf{r}^{(j)}) d\mathbf{x},$$

$$\Omega^{(j)} = \frac{1}{2} \int_{\mathbf{x}} (\boldsymbol{\nabla} \times \mathbf{u}(\mathbf{x}))\, \Delta_D(\mathbf{x} - \mathbf{r}^{(j)}) d\mathbf{x},$$

- Following Yeo and Maxey [3], if the kernel overlaps a single wall then use

$$\Delta_M \to \Delta^W_{M/D}\left(\mathbf{x} - \mathbf{r}^{(j)}\right) = \Delta_{M/D}\left(\mathbf{x} - \mathbf{r}^{(j)}\right) - \Delta_{M/D}\left(\mathbf{x} - \mathbf{r}^{(j)}_{\text{im}}\right),$$

where $\mathbf{r}^{(j)}_{\text{im}} = \mathbf{r}^{(j)} - 2\hat{\mathbf{z}}(\hat{\mathbf{z}} \cdot \mathbf{r}^{(j)})$ is the **image blob**.

- This only *approximately* implements no-slip, but it ensures that **mobility goes to zero at the wall** ($z = 0$).

Exponential of semicircle kernel

- For improved efficiency, we use the **exponential of a semicircle (ES) kernel** (Alex Barnett) [4]:

$$\Delta_{M/D}\left(\mathbf{x}; \alpha_{M/D}, \beta_{M/D}\right) = \prod_{i=1}^{3} \phi\left(x_i; \alpha_{M/D}, \beta_{M/D}\right),$$

where ES kernel ϕ is **compactly supported** on $[-\alpha, \alpha]$:

$$\phi(z; \alpha, \beta) = Z^{-1} \begin{cases} e^{\beta\left(\sqrt{1-\left(\frac{z}{\alpha}\right)^2}-1\right)}, & \left|\frac{z}{\alpha}\right| \le 1 \\ 0, & \text{otherwise.} \end{cases}$$

- Effective hydrodynamic radius of blob (grid spacing is h)

$$R_h(\alpha, \beta) = 2\alpha\ c(\beta) = (hw)\ c(\beta).$$

- Value of β chosen to **maximize translational invariance**, for $w \ge 4$ **grid cells**: $\beta_M/m \approx 1.75$ and $\beta_D/m \approx 1.6$ (Barnett suggests $\beta/m \approx 2.7$ for the NUFFT [5]), giving translational invariance (accuracy) to **at least 2 digits**.

Outline

Doubly-periodic Stokes solver

- An obvious difficulty in solving the Stokes problem is that the **domain is unbounded** in z for Membrane and BottomWall geometry.
- Assume force density $\mathbf{f}$ is smooth on and vanishes outside of $z \in [-H/2, H/2]$.
- Key idea: The open boundary condition can be reduced to $z \in [-H/2, H/2]$ through the **Dirichlet-to-Neumann map**, as we previously did for Poisson (suggested by Leslie Greengard) [1].
- The D-to-N map is easy to figure out analytically due to the **double-periodicity in** xy; our method doesn't work otherwise!

BVP for pressure

- Split into Membrane (DP) + correction due to wall(s)

$$\mathbf{u} = \mathbf{u}_{\text{DP}} + \mathbf{u}_{\text{corr}}, \quad \text{and} \quad p = p_{\text{DP}} + p_{\text{corr}}.$$

- For **DP** we have **unbounded in** z, periodic in xy,

$$\eta \boldsymbol{\nabla}^2 \mathbf{u}_{\text{DP}} - \boldsymbol{\nabla} p_{\text{DP}} = -\mathbf{f},$$
$$\boldsymbol{\nabla} \cdot \mathbf{u}_{\text{DP}} = 0.$$

- First solve a 2nd order two-point **BVP for pressure**:

$$\boldsymbol{\nabla}^2 p_{\text{DP}} = \boldsymbol{\nabla} \cdot \mathbf{f} \quad \Rightarrow \quad \left(\partial_z^2 - k^2\right) \hat{p}_{\text{DP}}(\mathbf{k}, z) = \begin{bmatrix} i\mathbf{k} \\ \partial_z \end{bmatrix} \cdot \hat{\mathbf{f}}(\mathbf{k}, z).$$

For $z \notin [0, H], \mathbf{f} = \mathbf{0} \quad \Rightarrow \quad \hat{p}_{\text{DP}}(\mathbf{k}, |z| \geq H/2) = C_1 e^{\pm kz}$.

- Pressure is continuously differentiable at $z = \pm H/2 \quad \Rightarrow$

$$\text{BCs:} \;\; \left(\partial_z \pm k\right) \hat{p}_{\text{DP}}(\mathbf{k}, z = \pm H/2) = 0.$$

BVP for velocity

$$-\eta\left(\partial_z^2 - k^2\right)\hat{\mathbf{u}}_{\mathrm{DP}}(\mathbf{k},z) + \begin{bmatrix} i\mathbf{k} \\ \partial_z \end{bmatrix}\hat{p}_{\mathrm{DP}}(\mathbf{k},z) = \hat{\mathbf{f}}(\mathbf{k},z).$$

- The D-to-N map for velocities becomes

$$(\partial_z \pm k)\,\hat{\mathbf{u}}_{\mathrm{DP}}^{\parallel}(\mathbf{k},\pm H/2) = \mp\frac{i\mathbf{k}}{2k\eta}\hat{p}_{\mathrm{DP}}(\mathbf{k},\pm H/2)$$

$$(\partial_z \pm k)\,\hat{\mathbf{u}}_{\mathrm{DP}}^{\perp}(\mathbf{k},\pm H/2) = \frac{1}{2\eta}\hat{p}_{\mathrm{DP}}(\mathbf{k},\pm H/2)$$

- We use a **pentadiagonal** Chebyshev solver by L. Greengard to solve these BVPs:
  trivially parallelizable (each $\mathbf{k} = (k_x, k_y)$ is an independent solve) and requires **low memory** of $O(N_z)$ (**good for GPUs**).

Correction "solve"

$$\begin{aligned} \eta \boldsymbol{\nabla}^2 \mathbf{u}_{\text{corr}} - \boldsymbol{\nabla} p_{\text{corr}} &= 0, \\ \boldsymbol{\nabla} \cdot \mathbf{u}_{\text{corr}} &= 0, \\ \mathbf{u}_{\text{corr}}\big|_{z=0} = -\mathbf{u}_{\text{DP}}\big|_{z=0}. \end{aligned}$$

- Since this is homogeneous Stokes, we can **solve it analytically**!
- Note that the $k = 0$ **mode** *cannot* be separated into a DP+correction, but it can still be handled analytically when there is at least one wall present.
- If there are no walls one must somehow account for the **backflow**.
- Algorithm uses a Fourier-Chebyshev 3D transform, implemented using **3D FFTs**, with oversampling factor of 2 (in z).

Outline

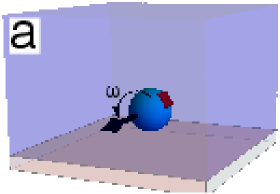
Quick intro to BD-HI

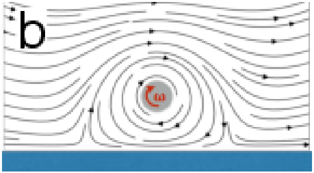
- The Ito equations of **Brownian HydroDynamics** for the (correlated) positions of N particles $\mathbf{Q}(t) = \{\mathbf{q}_1(t), \dots, \mathbf{q}_N(t)\}$ are

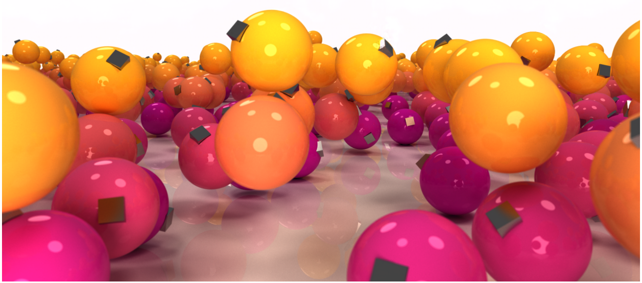
$$d\mathbf{Q} = \boldsymbol{\mathcal{M}}\mathbf{F}dt + (2k_BT\,\boldsymbol{\mathcal{M}})^{\frac{1}{2}}\,d\boldsymbol{\mathcal{B}} + k_BT\,(\partial_{\mathbf{Q}} \cdot \boldsymbol{\mathcal{M}})\,dt,$$

where $\boldsymbol{\mathcal{B}}(t)$ is a vector of Brownian motions, and $\mathbf{F}(\mathbf{Q})$ are electrostatic+steric+external forces.
- The symmetric positive semidefinite (SPD) **hydrodynamic mobility matrix** $\boldsymbol{\mathcal{M}}$ has 3×3 block $\mathbf{M}_{ij}$ that maps a force on particle j to a velocity of particle i.
- Key challenges for fast **linear-scaling**:
  - Long-ranged hydrodynamics ($\boldsymbol{\mathcal{M}}\mathbf{F}$); "solved" with DP-FCM
  - Generating **Brownian displacements** with covariance $\sim \boldsymbol{\mathcal{M}}$
  - Generating stochastic drift $\sim \partial_{\mathbf{Q}} \cdot \boldsymbol{\mathcal{M}}$ (temporal integrators)

Colloidal microrollers







B. Sprinkle, E. B. van der Wee, Y. Luo, M. Driscoll, and A. Donev,
Driven dynamics in dense suspensions of microrollers, **ArXiv:2005.06002** [6].

Microrollers: FCM+lubrication+Brownian motion

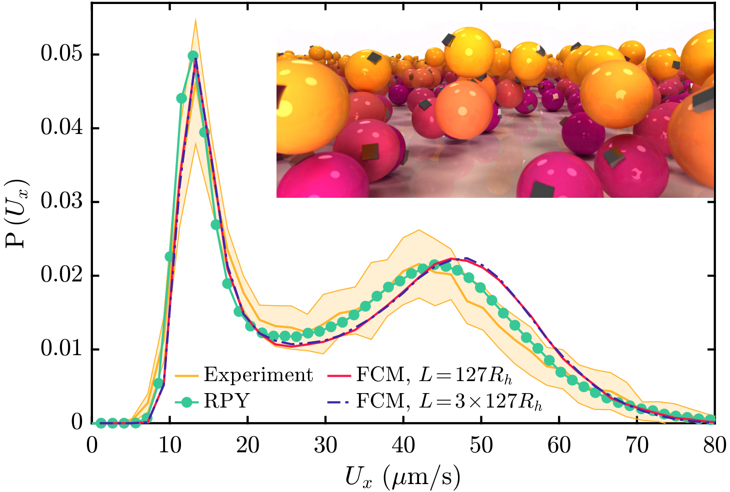


Figure: Experimentally measured and numerically computed distributions of particle velocities for a suspension of microrollers above a bottom wall.

GPU efficiency in UAMMD

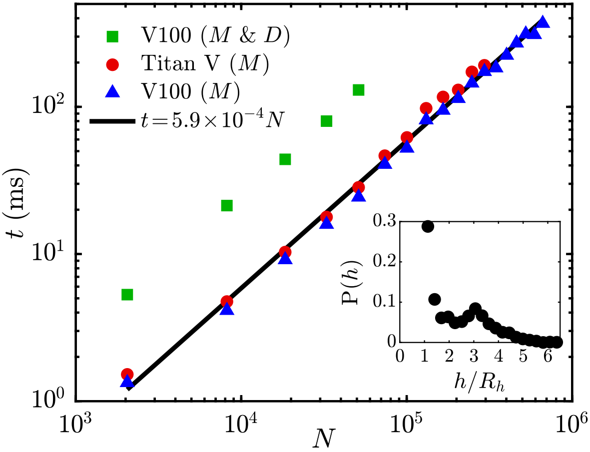


Figure: Time per mobility solve versus number of particles on V100 and Titan V NVIDIA GPUs (area packing fraction of $\phi = 0.4$). Biggest system $663,552$ particles (370 ms) to compute with **UAMMD** (**Raul Perez**).

Fully confined microrollers

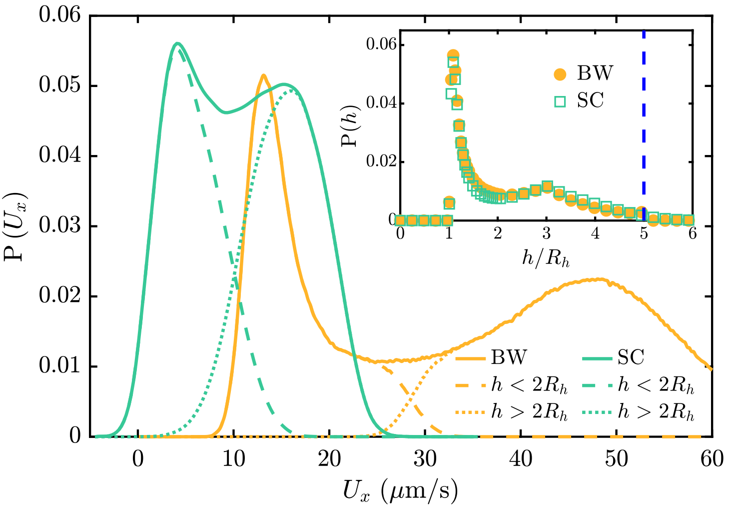


Figure: Distributions of particle height (inset) and velocity (main figure) for microrollers above a single wall (BW), and a slit channel with $H = 6R_h$ (SC).

Generating Brownian increments

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

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

  where **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.

Lanczos for generating $\mathcal{M}^{\frac{1}{2}}\mathbf{W}$

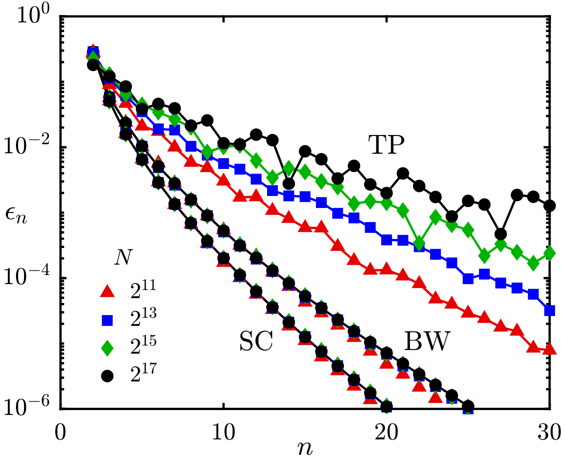


Figure: Relative error ϵ_n vs number of iterations n of the Lanczos algorithm for a suspension of particles ($H = 7.5R_h$); the TP result is for height of the (periodic) domain set to $H = 130R_h$.

Conclusions

- It is possible to construct **linear-scaling algorithms** for Brownian HydroDynamics of **colloids in the presence of boundaries**.
- **Missing: Ewald splitting** — right now too fine FFT grid required at low densities or for the rigid multiblob method at higher resolutions.
- **Image systems** for walls + correction solve required to enable efficient Ewald splitting in the presence of boundaries [1].

References

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