Fast Electrostatics and (Brownian) Hydrodynamics in Doubly-Periodic Geometries

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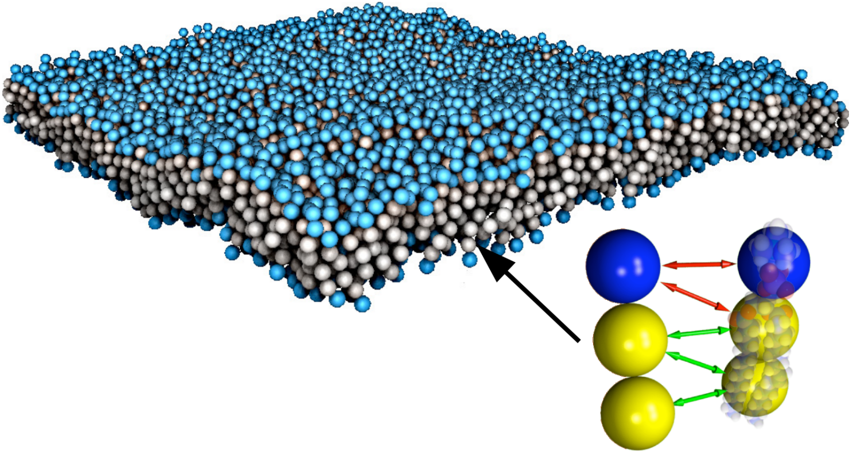
Outline

1. Doubly-Periodic Problems in Soft Matter
2. Doubly periodic problems with smooth forcing
3. Ewald splitting for point-like charges
4. Dielectric boundaries (walls)
5. Results

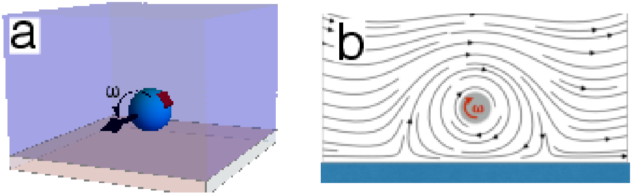
Lipid Membranes

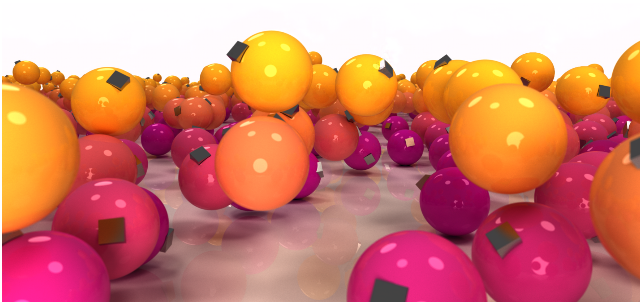
Coarse-grained modeling of lipid membranes using **Brownian HydroDynamics**:



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

Colloids: Microrollers

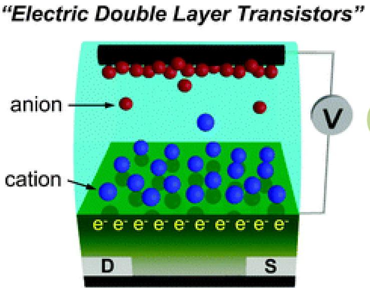


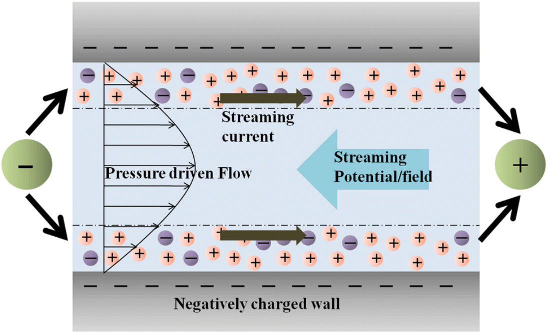


B. Sprinkle, E. B. van der Wee and Y. Luo and M. Driscoll, and A. Donev, *Driven dynamics in dense suspensions of microrollers*, ArXiv:2005.06002.

Electrolytes

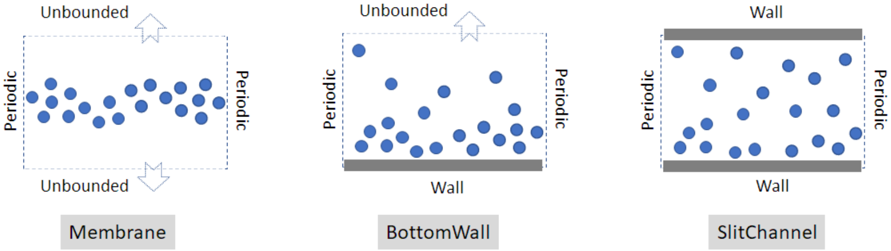
Coarse-grained modeling of electrolyte solutions using **Brownian HydroDynamics** (see LBNL talks in session)





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

Doubly-Periodic Geometries



Poisson preprint at **ArXiv:2101.07088**, code at `https://github.com/stochasticHydroTools/DPPoissonTests`

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Doubly periodic geometry

Poisson's equation for electrostatic potential

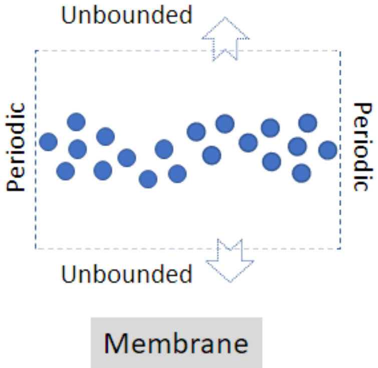
$$\epsilon \Delta \phi = -f$$

Domain *doubly periodic* in $(x, y) \in [-L, L]$ and unbounded in z.

Assuming electroneutral domain

$$\nabla \phi(x, y, z \to \pm\infty) \to 0$$

For now, assume f is a smooth function.



Fourier approach

For quasi-2D systems, f is compactly supported in $[-L, L]^2 \times [0, H]$.

$$\rightarrow \epsilon \Delta \phi = 0 \quad z < 0 \text{ or } z > H$$

Harmonic solve in xy Fourier space $k^2 = k_x^2 + k_y^2$

$$\epsilon \left(\widehat{\phi}_{zz} - k^2 \widehat{\phi} \right) = 0$$

$$\rightarrow \widehat{\phi}(k, z) = \begin{cases} A e^{-kz} & z > H \\ B e^{kz} & z < 0 \end{cases}$$

This implies the boundary conditions

$$\widehat{\phi}_z(k, H) + k \widehat{\phi}(k, H) = 0$$

$$\underbrace{\widehat{\phi}_z(k, 0) - k \widehat{\phi}(k, 0) = 0}_{\text{Dirichlet to Neumann map!}}$$

Solution smooth at $z = 0/H \rightarrow$ same BCs hold for *interior* $\widehat{\phi}$!

Finite problem to solve

For $z \in [0, H]$, we get a simple 2-point BVP for each $\mathbf{k}$:

$$\epsilon \left(\widehat{\phi}_{zz} - k^2 \widehat{\phi} \right) = -\widehat{f}(k, z)$$

$$\widehat{\phi}_z(x, y, H) + k\phi(k, H) = 0$$

$$\widehat{\phi}_z(x, y, 0) - k\widehat{\phi}(x, y, 0) = 0$$

Solve this BVP using spectral integration matrix (Greengard 1991)

- Lay down Chebyshev grid
- Solve for $\hat{\phi}_{zz}$ on the Cheb grid
- Obtain $\hat{\phi}$ by integration

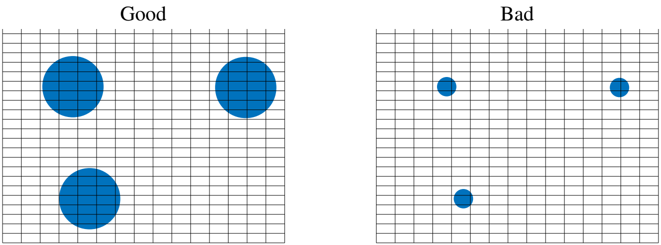
Greengard. *SIAM J. Numer. Anal.* 28 (4), 1991.

Smoothness of f

- For electrolytes, f is the charge density due to collection of **Gaussian charges**

$$f(\mathbf{x}) = \sum_{i=1}^{N} \frac{q_i}{(2\pi g_w^2)^{3/2}} \exp\left(-\frac{\|\mathbf{x}-\mathbf{z}_i\|^2}{2g_w^2}\right)$$

- Can a grid-based method work? Only if $h \sim g_w$.



Need alternative strategy for point-like (narrow) charges

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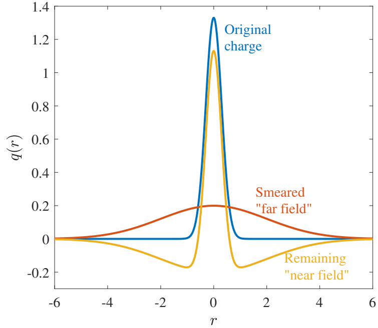
Ewald splitting

- Introduce Gaussian splitting function

$$\gamma(r;\xi) \propto e^{-r^2\xi^2}$$

- *Splitting parameter* ξ has units 1/length optimized for speed
- Split charge = smeared charge + "dipole"

$$f = \underbrace{f * \gamma}_{\text{far field}} + \underbrace{f * (1-\gamma)}_{\text{near field}}$$



Why does Ewald help?

- Near field charge clouds have zero net charge
  - Exponentially-decaying near field interaction
  - Free space BC $\rightarrow$ analytical solution
  - Can be made nonzero at $\mathcal{O}(1)$ **neighbors** per point
- Far field $\epsilon\Delta\phi^{(f)} = \gamma * f$ is smooth
  - **Grid-based solver works**
  - Spread charge density to grid by convolving $f * \gamma^{1/2}$
  - Solve $\epsilon\Delta\psi = (f * \gamma^{1/2})$ on grid
  - Interpolate grid $\gamma^{1/2} * \psi$ to get $\phi^{(f)} = \epsilon^{-1}\Delta^{-1}(f * \gamma)$ at charges.

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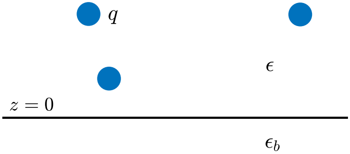
Permittivity jump - single wall

BCs for the potential ϕ at a dielectric interface: continuity of potential and displacement

$$\phi(x, y, 0^+) = \phi(x, y, 0^-)$$
$$\epsilon\phi_z(x, y, 0^+) = \epsilon_b\phi_z(x, y, 0^-)$$



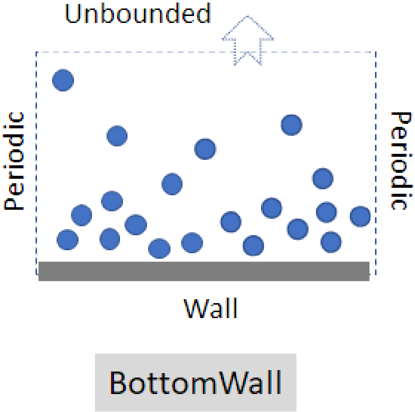
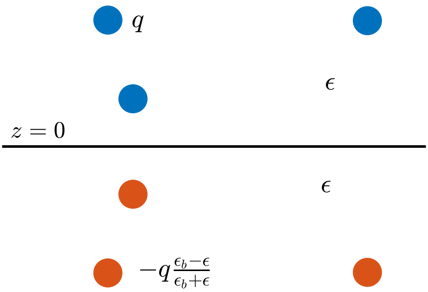


Image construction - single wall

Solution on $z > 0$ same as with uniform permittivity and set of *image charges*

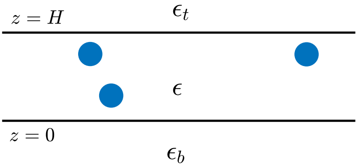


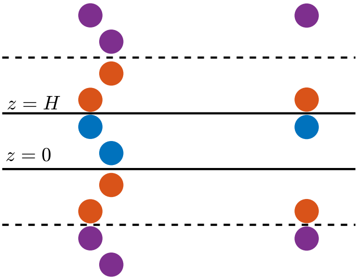
Use DP solver + Ewald splitting on the problem with images

Complications for slab geometry

- Three different permittivities
- We can also add **surface charge**

$$\epsilon\phi_z(x,y,0^+) - \epsilon_b\phi_z(x,y,0^-) = -\sigma_b(x,y)$$
$$\epsilon\phi_z(x,y,H^-) - \epsilon_t\phi_z(x,y,H^+) = \sigma_t(x,y)$$

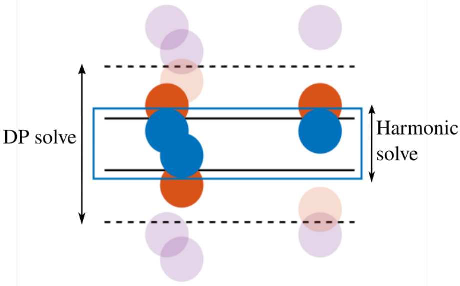




- Infinitely many images in **far-field problem** (near-field easy)

Ewald splitting in slabs

- Spread to grid = smear charges
- We only need potential in a **thicker slab**
- Find images that overlap domain
- Do initial **DP solve** with *only* these images (BCs *not* satisfied)
- Compute potential due to far-away images using a **harmonic solve**



- Uses 3D FFTs + decoupled BVP solves for each wavenumber + neighbor sums (all parallelizable on GPU).
- **UAMMD = Brownian dynamics GPU code** by Raul Perez.

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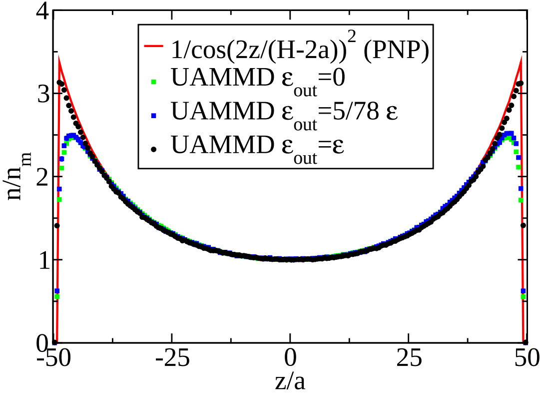
Confined electrolyte

Positively-charged wall with negatively charged ions

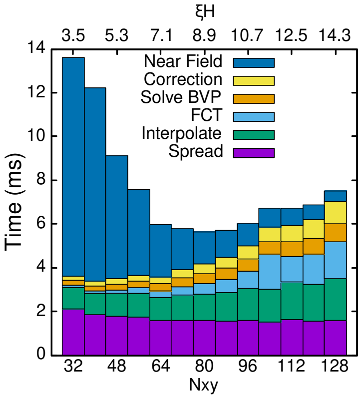
- $\epsilon_{\text{out}} = \epsilon \rightarrow$ no images, matches analytical solution of PNP equations
- $\epsilon_{\text{out}} = 5/78\epsilon \approx 0.06\epsilon \rightarrow$ Images repelled by each other (**not in PNP**!)
- $\epsilon_{\text{out}} = 0 \rightarrow$ field outside irrelevant, close to glass



Speed on the GPU

Splitting parameter ξ chosen to optimize speed

- Smaller ξ: Coarser grid, near field eats up entire cost
- Larger ξ: Finer grid, far field (spread & interpolate, FFT) cost more



- 20K charges = 6 ms per time step!