Active dynamics in dense suspensions of microrollers

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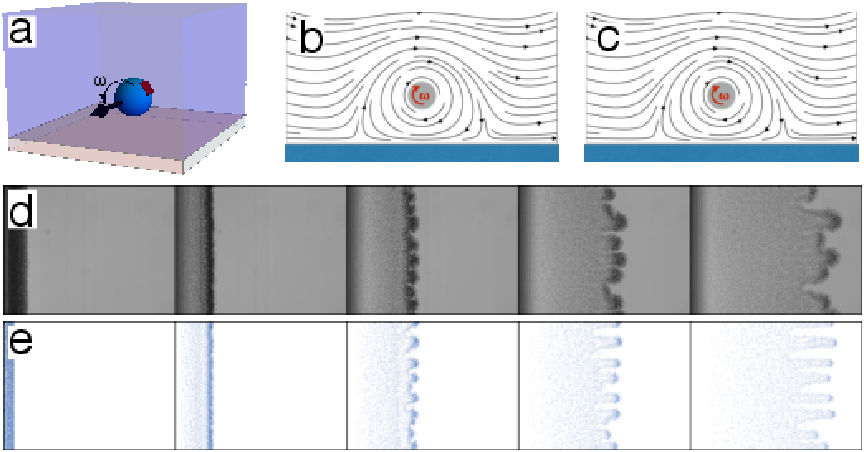
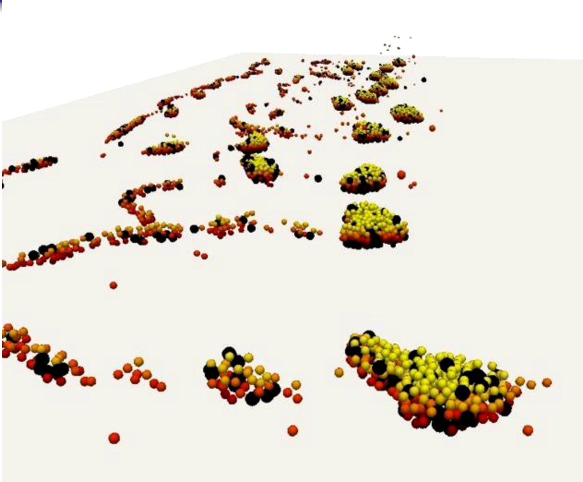
Fingering Instability



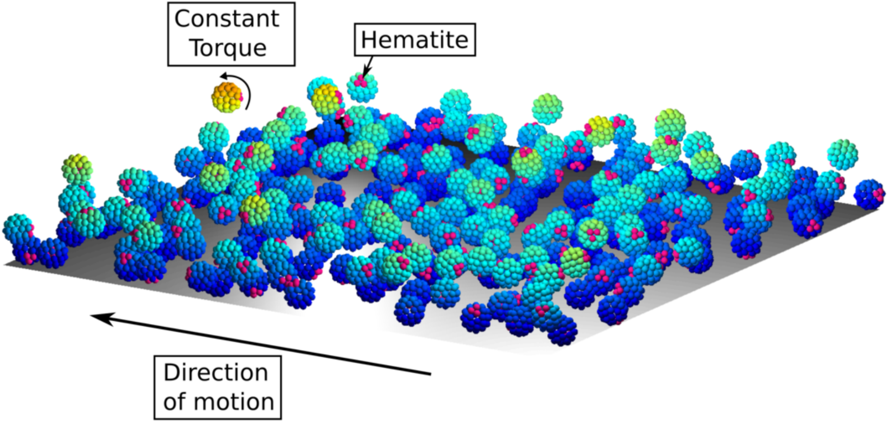
Experiments by Michelle Driscoll (was in the Chaikin lab at NYU Physics, now at Northwestern Physics), simulations by **Blaise Delmotte** (was at Courant, now at LadHyX Paris) [1, 2].

Critters



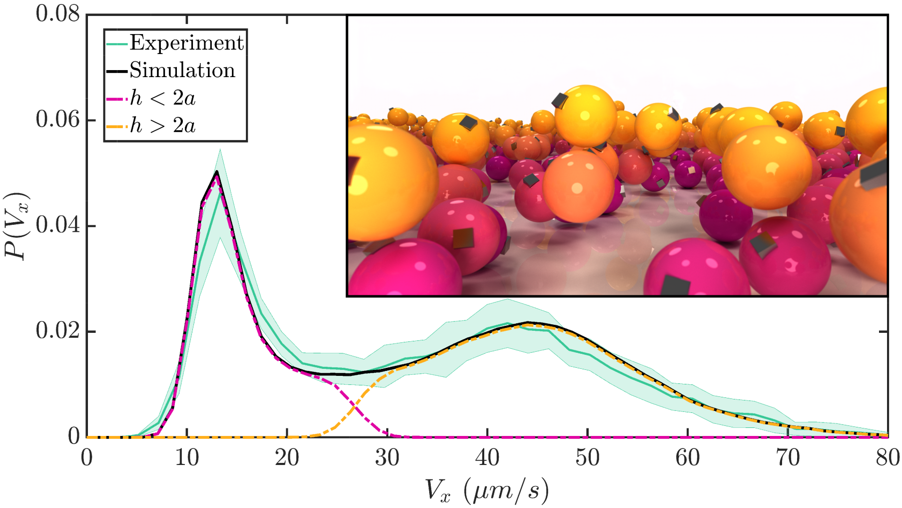
Simulations by **Blaise Delmotte** revealed that stable motile clusters termed **critters can form purely by hydrodynamic interactions** [1]. Still trying to create critters that don't shed particles in the lab...

Uniform Suspension: Rigid multiblobs



Simulations by **Brennan Sprinkle**+Blaise Delmotte [3] of a uniform suspension of microrollers at packing fraction $\phi = 0.4$ (GIF). Compare to experiments (AVI) by **Michelle Driscoll**.

Uniform suspension: Lubrication-corrected



B. Sprinkle, E. B. van der Wee and Y. Luo and M. Driscoll, and A. Donev, **ArXiv:2005.06002** [4].

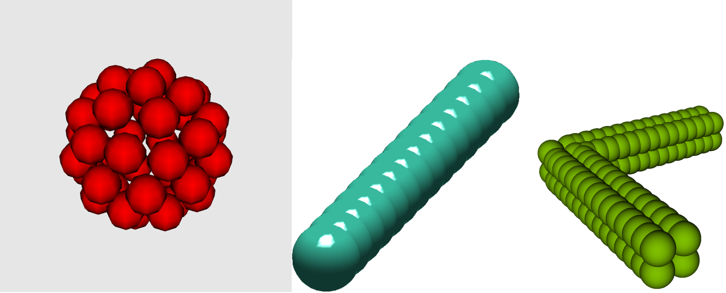
Minimally-Resolved Simulations

- The Ito equations of **Brownian HydroDynamics** for the (correlated) positions of the N spherical microrollers $\mathbf{Q}(t) = \{\mathbf{q}_1(t), \dots, \mathbf{q}_N(t)\}$ are
$$d\mathbf{Q} = \boldsymbol{\mathcal{M}}\mathbf{F}dt + \boldsymbol{\mathcal{M}}_c\mathbf{T}dt + (2k_BT\,\boldsymbol{\mathcal{M}})^{\frac{1}{2}}\,d\boldsymbol{\mathcal{B}} + k_BT\,(\partial_{\mathbf{Q}} \cdot \boldsymbol{\mathcal{M}})\,dt, \quad (1)$$
where $\boldsymbol{\mathcal{B}}(t)$ is a vector of Brownian motions, and $\mathbf{F}(\mathbf{Q})$ are applied forces, and $\mathbf{T}$ the external magnetic torques.
- The symmetric positive semidefinite (SPD) **blob-blob mobility matrix** $\boldsymbol{\mathcal{M}}$ encodes the hydrodynamics:
3×3 block $\mathbf{M}_{ij}$ maps a force on blob j to a velocity of blob i.
- Computing $\boldsymbol{\mathcal{M}}\mathbf{F} + \boldsymbol{\mathcal{M}}_c\mathbf{T}$ means solving a **mobility problem** and is too computationally intensive for dense suspensions of many colloids.

Blobs in Stokes Flow

- In the approach of **Rotne-Prager-Yamakawa (RPY)** the mobility is approximated to have a far-field **pairwise approximation**
$$\mathbf{M}_{ij}\left(\mathbf{Q}\right) \equiv \mathbf{M}_{ij}\left(\mathbf{q}_i, \mathbf{q}_j\right) = \boldsymbol{\mathcal{R}}\left(\mathbf{q}_i, \mathbf{q}_j\right).$$
- The **hydrodynamic kernel** $\mathcal{R}$ for spheres of radius a is
$$\boldsymbol{\mathcal{R}}\left(\mathbf{q}_i, \mathbf{q}_j\right) \approx \eta^{-1}\left(\mathbf{I} + \frac{a^2}{6}\boldsymbol{\nabla}^2_{\mathbf{r}'}\right)\left(\mathbf{I} + \frac{a^2}{6}\boldsymbol{\nabla}^2_{\mathbf{r}''}\right)\mathbb{G}(\mathbf{r}', \mathbf{r}'')\Big|^{\mathbf{r}'=\mathbf{q}_j}_{\mathbf{r}''=\mathbf{q}_i} \qquad (2)$$
where $\mathbb{G}$ is the **Green's function** for steady Stokes flow, *given* the appropriate boundary conditions.
- For particles next to a wall the **Rotne-Prager-Blake** tensor has been computed by Swan (MIT) and Brady (Caltech) [2].
- We compute $\boldsymbol{\mathcal{M}}\boldsymbol{\lambda}$ using **GPU-accelerated** sum; linear-scaling methods exist and new ones are being developed in my group.

Rigid MultiBlob Method



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

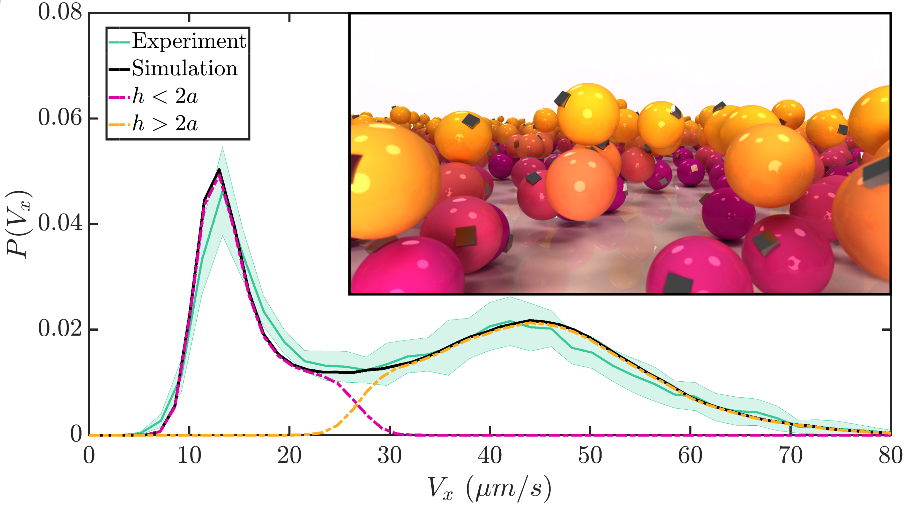
Lubrication for spherical colloids

- Following the **Stokesian Dynamics** approach, but omitting stresslets, we use the **lubrication-corrected mobility matrix**
$$\boldsymbol{\mathcal{M}} = \left[\boldsymbol{\mathcal{M}}_{\text{RPY}}^{-1} + \boldsymbol{\Delta}\mathbf{R}_{\text{lub}}\right]^{-1} = \boldsymbol{\mathcal{M}}_{\text{RPY}} \cdot \left[\mathbf{I} + \boldsymbol{\Delta}\mathbf{R}_{\text{lub}} \cdot \boldsymbol{\mathcal{M}}_{\text{RPY}}\right]^{-1}.$$
- $\boldsymbol{\Delta}\mathbf{R}_{\text{lub}}$ 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).
- The pairwise terms in $\boldsymbol{\Delta}\mathbf{R}_{\text{lub}}$ can be computed analytically using asymptotic expansion (for very close particles) or tabulated by using a more accurate reference method (e.g., boundary integral).
- Lubrication-corrected Brownian Dynamics algorithm described in Sprinkle et al. in **ArXiv:2005.06002**.

Experiments: Fluorescence tracking

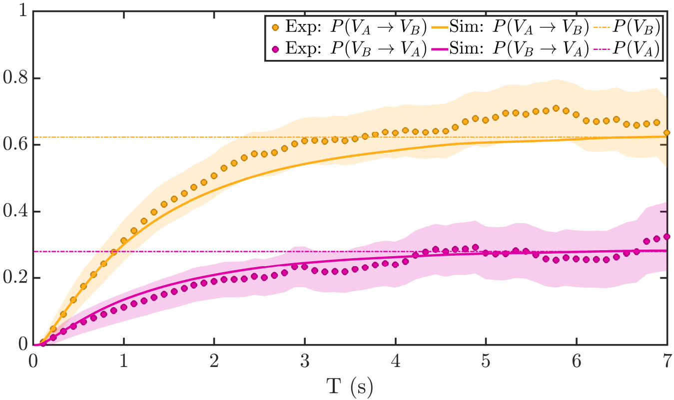
- New experiments performed by Ernest B. van der Wee in the lab of Michelle Driscoll at Northwestern on uniform suspensions with in-plane packing fraction $\phi \approx 0.4$.
- Details: colloid diameter 2.03 ± 0.04 μm, Debye length of $\sim$25 nm, with rotating magnetic field (40 G, 9 Hz).
- To follow the dynamics of single rollers in a crowded layer using particle tracking, they mixed together particles with and without **fluorescent labeling** in a 1:1200 number ratio.
- Calibration of simulation parameters (particle mass, repulsion from bottom wall) against diffusion coefficient and propulsion velocity for a single colloid.

Experiment vs Simulation



Histogram of velocities measured over 1s, showing a **bimodal distribution** due to two layers (yellow=fast=high and magenta=slow=low).

Lane-switching dynamics



Estimate the rate of switching from slow (bottom=A, $9.37 < V < 17.4\mu\text{m/s}$) to fast (top=B, $19.9 < V < 62.6\mu\text{m/s}$) lane based on particle speed (large or small), giving waiting time $\tau_{AB} \approx 1.5\text{s}$.

Lubrication and MIPS

- The group of Denis Bartolo studies experimentally and models in continuum Motility-Induced Phase Separation (MIPS) in monolayers of Quincke rollers [Phys. Rev. X 9, 031043 (2019)]
- "We conjecture a possible microscopic mechanism to explain the arrest of the Quincke rotation at high area fraction: the frustration of rolling motion by **lubrication** interactions."
- We simulate a **monolayer of microrollers** confined to stay close to the wall by a stiff spring in the normal direction.

Lubrication in monolayers

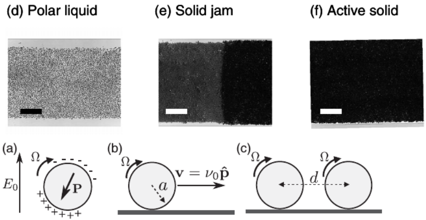
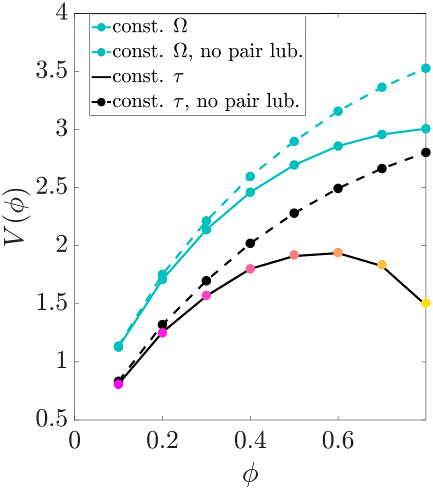


FIG. 6. Quincke rollers. (a) When applying a dc electric field $\mathbf{E_0}$ to an insulating sphere immersed in a conducting fluid, a charge dipole forms at the sphere surface. When $E_0 > E_Q$, the electric dipole makes a finite angle with the electric field causing the steady rotation of the sphere at constant angular speed Ω. (b) The rotation is converted into translation by allowing the sphere to sediment on one electrode. When isolated, the resulting Quincke rotor rolls without sliding at constant speed: $\nu_0(0) = a\Omega$. (c) When two colloids rolling in the same direction are close to each other, the lubrication torque acting on the two spheres separated by a distance d scales as $\log(d - 2a)$ and hinders their rolling motion.



Left: Geyer *et al*, Phys. Rev. X 9, 031043 (2019)

Conclusions

- It is possible to construct **efficient algorithms** for Brownian HydroDynamics of **colloids in the presence of boundaries**.
- **Lubrication friction** with the bottom wall and between neighboring particles in dense suspensions plays a role in collective dynamics and can be captured efficiently using a lubrication-corrected mobility matrix.
- **Microrollers** exhibit rich collective dynamics and are easier to control and simulate since their activity is **externally driven**.
- *Collective dynamics of active colloidal suspensions above a wall is strongly affected by the bottom wall!*

References

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