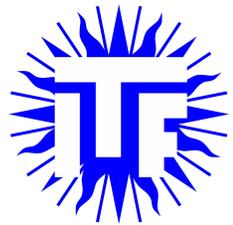# Hydrodynamic Modeling of Sheared Capillary Suspensions

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Introduction

Capillary suspensions are ternary systems, wherein solid particles are dispersed in two immiscible liquids, one of which preferentially wets the particles. Diverse structures are obtained based on the liquid ratio. Adding a minor amount of the wetting liquid to a particle-liquid mixture significantly alters its rheological behavior, transforming it from fluid-like to gel-like and greatly increasing yield stress and viscosity. This transition, driven by capillary forces acting between the particles, enables the creation of tunable and stable mixtures for applications ranging from low-fat foods to advanced materials like pastes for printed electronics [1].
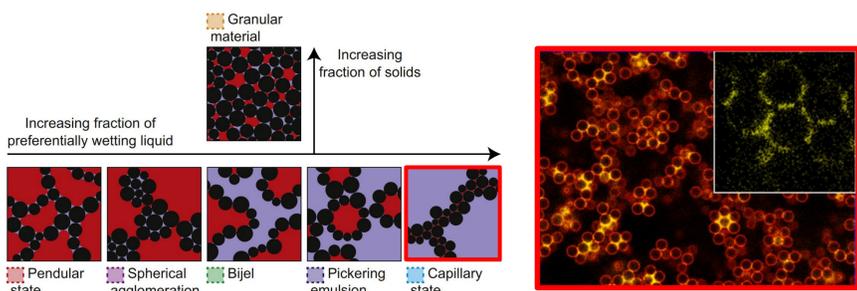
(Left) Adapted from [1], pictographs of particle-liquid-liquid systems in various states. (Right) Adapted from [2], confocal micrographs (82 μm x 55 μm) of capillary suspensions with $\phi_{solid} = 20\%$, $\phi_{sec} = 1\%$. The particles are shown as red rings and the secondary fluid is colored yellow.

Simulation Method

We perform particle-based simulations using Jax-based Fast Stokesian Dynamics algorithm [3]. This is a Python implementation of the original method developed by the Brady and Swan groups [4,5].
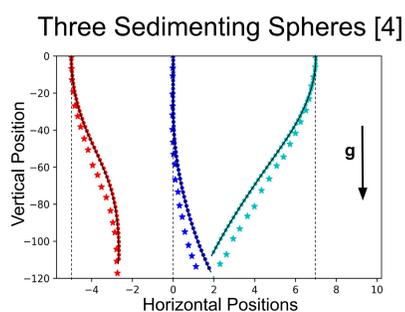
Monodisperse Spherical Particles

$$\underbrace{U - U^\infty}_{\text{Velocity}} = \underbrace{R_{FU}^{-1}}_{\substack{\text{Hydrodynamic}\\\text{Resistance}}} \cdot (\underbrace{F^P}_{\text{Applied Force}} + \underbrace{R_{FE} \cdot E^\infty}_{\text{Applied Shear}})$$

$$R_{FU} = \underbrace{\mathcal{B}^T \cdot \mathcal{M}^{-1} \cdot \mathcal{B}}_{\text{Far-Field (many-body)}} + \underbrace{R_{FU}^{nf}}_{\text{Near-Field (two-body)}}$$

Three Sedimenting Spheres [4]

Potential Free Hard-Spheres [6]

$$F_i^{hs} = -\sum_j k(r_{ij} - \sigma)\,\hat{r}_{ij}$$

Testing Simple Shear

$$v_\infty \,//\, \hat{x}$$

Box Size $= 10\sigma$
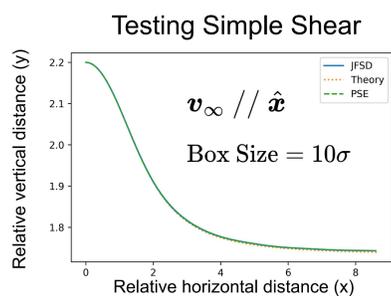
Particles Initial Configuration

Experimental particle positions are refined for simulation using gradient descent, effectively eliminating overlaps introduced by mapping a (slightly) polydisperse system with tracking errors to a monodisperse system.
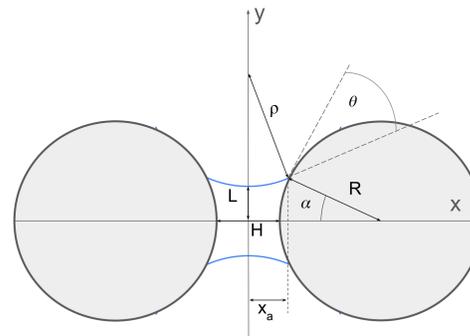
$$V = \begin{cases} \sum_{i,j} \frac{1}{2}(\Delta r_{i,j})^2 & \Delta r < \sigma \\ 0 & \Delta r \geq \sigma \end{cases} \qquad r_{\text{new}} = -\epsilon\,\nabla V$$
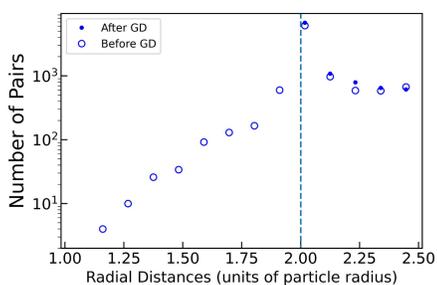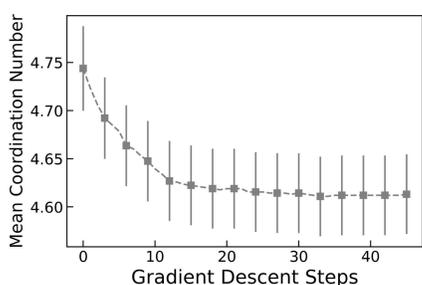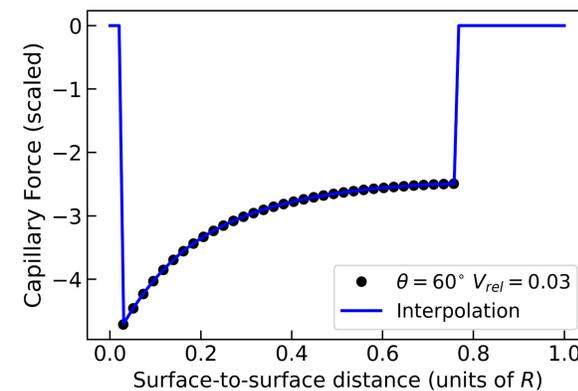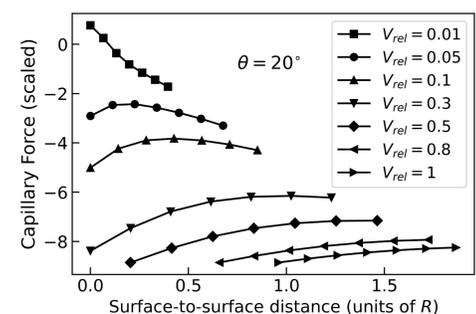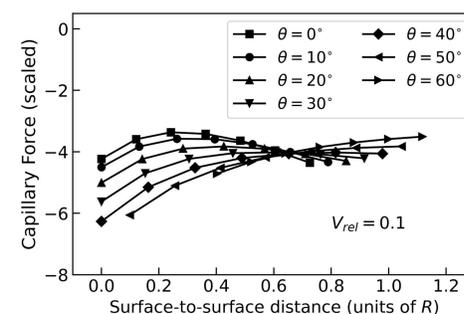

Capillary Bridges

Assuming constant bridge volume and a toroidal shape for the bridges, forces can be computed as functions of surface-to-surface distance between particle pairs [7]:

$$\frac{F_{cap}}{T\sigma} = -\pi \sin\alpha \sin(\alpha + \theta) - \frac{\pi\sigma}{4}\sin^2\alpha\left(\frac{1}{L} - \frac{1}{\rho}\right)$$
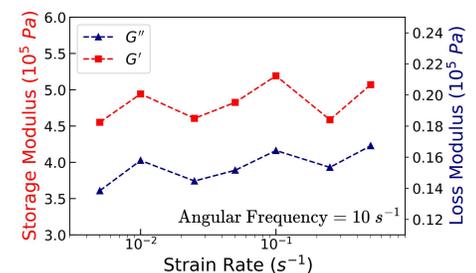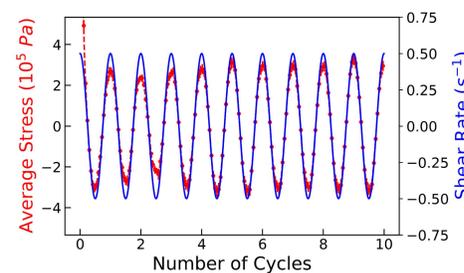

$$\text{Mason number} = \frac{3\pi\eta\sigma\dot{\gamma}}{T} \ll 1$$

$$\begin{cases} \eta = \text{Dynamic Viscosity} \\ \dot{\gamma} = \text{Shear Rate Amplitude} \\ T = \text{Surface Tension} \end{cases}$$

Forces are computed numerically and tabulated. Interpolated values are used in simulations.

Preliminary Results

Outlook and Future Direction

- Mason number not small enough
- Small amount of shear cycles
- Tuning capillary forces

→ Computationally challenging (longer simulations)

References and Funding

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[3] Torre, Jax-Fast Stokesian Dynamics, GitHub repository, https://github.com/torrewk/Python-Jax-Fast-Stokesian-Dynamics
[4] Brady *et al.*, J. Fluid Mech., **180** (1987)
[5] Fiore, Swan, J. Fluid Mech., **878** (2019)
[6] Heyes, Melrose, J. Nonnewton. Fluid Mech., **46** (1993)
[7] Megias-Alguacil *et al.*, AIChE journal **55** (2009)

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