Derivation of a continuum description of sheared jammed soft suspensions from particle dynamics

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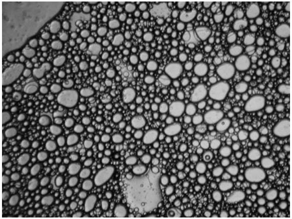
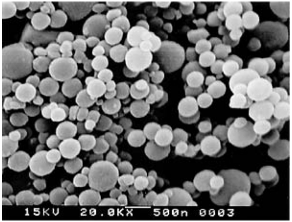
Soft jammed suspensions

Small soft particles packed in a fluid

Concentrated emulsion



Microgel suspensions



[Fréchet lab, UC Berkeley]

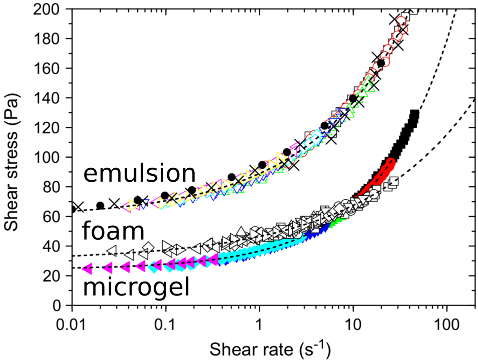
Rheology of yield stress fluids

Stationary flow curve

- Hershel-Bulkley behavior in simple shear (yield stress σ_{y})

$$\sigma = \sigma_{\mathrm{y}} + k\dot{\gamma}^n \qquad (0 < n < 1)$$

- $n = 1$: limit case of a Bingham fluid



[Ovarlez et al., JNNFM 2013]

Rheological models

Phenomenological constitutive models

- Relate stress tensor $\boldsymbol{\Sigma}$ to strain tensor $\mathbf{E} = \frac{1}{2}(\nabla \mathbf{v} + \nabla \mathbf{v}^T)$
- *Viscoelastoplastic* models

$$\frac{\mathcal{D}\boldsymbol{\Sigma}}{\mathcal{D}t} = \frac{2\eta}{\tau_{\mathrm{el}}}\mathbf{E} + f(\boldsymbol{\Sigma}), \qquad f(\boldsymbol{\Sigma}) \text{ to be determined}$$

- Von Mises yield criterion: plastic flow when $|\boldsymbol{\Sigma}'| > \sigma_{\mathrm{y}}$
  ($\boldsymbol{\Sigma}'$ = deviatoric/traceless part of $\boldsymbol{\Sigma}$)
- For a Bingham fluid [Saramito, JNNFM 2007]

$$f(\boldsymbol{\Sigma}) = -\frac{1}{\tau_{\mathrm{el}}} \max\left(0, \frac{|\boldsymbol{\Sigma}'| - \sigma_{\mathrm{y}}}{|\boldsymbol{\Sigma}'|}\right) \boldsymbol{\Sigma}$$

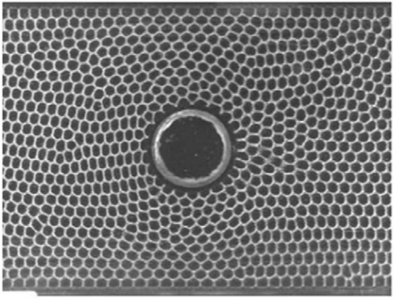
- Can be adapted to provide Hershel-Bulkley [Saramito, 2009]
- No microscopic guidance for $f(\boldsymbol{\Sigma})$, purely phenomenological

Rheological models

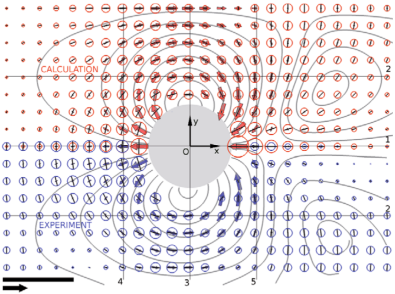
Experimental test of viscoelastoplastic models

$$\frac{\mathcal{D}\boldsymbol{\Sigma}}{\mathcal{D}t} = \frac{2\eta}{\tau_{\rm el}}\mathbf{E} - \frac{1}{\tau_{\rm el}} \max\left(0, \frac{|\boldsymbol{\Sigma}'| - \sigma_{\rm y}}{|\boldsymbol{\Sigma}'|}\right)\boldsymbol{\Sigma}$$

Foam flow around an obstacle under pressure gradient



[Cheddadi et al., EPJE 2011]



Top: theory, bottom: experiment

Open questions

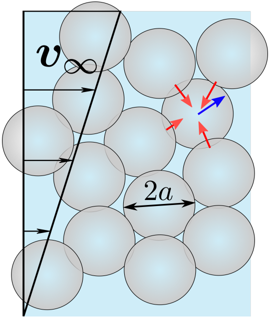
- Microscopic grounding?
- Can one *derive* a viscoelastoplastic constitutive law from a given microscopic dynamics of soft particles?

A minimal suspension model

- Overdamped soft disks, no hydrodynamic interactions
- Equation of motion of particle i (2D, athermal)

$$-\lambda\left(\mathbf{v}_i - \mathbf{v}_\infty(\mathbf{r}_i)\right) + \sum_{j\neq i} \mathbf{F}(\mathbf{r}_j - \mathbf{r}_i) = 0$$

System driven by flow field $\mathbf{v}_\infty(\mathbf{r})$, with uniform gradient $\nabla\mathbf{v}_\infty$



Probabilistic description

Exact evolution equation for the pair correlation function $g(\mathbf{r})$

$$\partial_t g(\mathbf{r}) + \nabla \cdot \mathbf{J}(r) = 0$$

with probability flux

$$\mathbf{J}(r) = \nabla v_\infty \cdot [\mathbf{r} \otimes g(\mathbf{r})] - \mathbf{F}(\mathbf{r}) g(\mathbf{r}) - \rho \int \mathbf{r}' \, g_3(\mathbf{r}, \mathbf{r}') \, d\mathbf{r}'$$

Exact stress dynamics

- Microscopic definition of stress tensor

$$\boldsymbol{\Sigma} = \frac{1}{V}\sum_{j\neq i}(\mathbf{r}_j - \mathbf{r}_i)\otimes\mathbf{F}(\mathbf{r}_j - \mathbf{r}_i) = \frac{\rho^2}{2}\int d\mathbf{r}\,\mathbf{r}\otimes\mathbf{F}(\mathbf{r})\,g(\mathbf{r})$$

- Stress evolution: multiply by $\mathbf{r}\otimes\mathbf{F}(\mathbf{r})$ and integrate over $\mathbf{r}$

$$\partial_t\boldsymbol{\Sigma} = \nabla v_\infty\cdot\boldsymbol{\Sigma} + \boldsymbol{\Sigma}\cdot\nabla v_\infty + \mathbf{S}_2[g(\mathbf{r})] + \mathbf{S}_3[g_3(\mathbf{r},\mathbf{r}')]$$

e.g., $\mathbf{S}_3 = -\frac{\rho^3}{2}\int\left[\mathbf{F}(\mathbf{r}')\otimes\mathbf{F}(\mathbf{r}) + \mathbf{r}\otimes\mathbf{F}(\mathbf{r}')\cdot(\nabla\mathbf{F}(\mathbf{r}))^T\right]g_3(\mathbf{r},\mathbf{r}')d\mathbf{r}d\mathbf{r}'$

- Standard result for colloidal suspensions

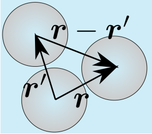
[Batchelor 70s; Russel 80s, 90s; Brady 90s; Morris 2010s,...]

- **Need to close stress dynamics**

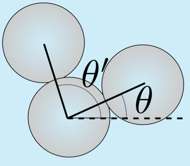
Microstructure closure

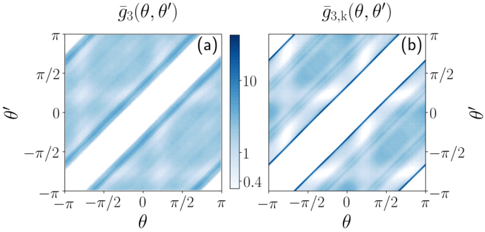
Approximate g_3 in terms of g

- Simplest assumption: Kirkwood closure
  $g_3(\mathbf{r}, \mathbf{r}') \approx g(\mathbf{r})g(\mathbf{r}')g(\mathbf{r}-\mathbf{r}')$



- Numerical test in contact area (LAMMPS simulations, $\phi = 0.875$)



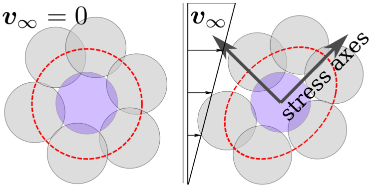


$$\bar{g}_3(\theta, \theta') = \int_{r, r' < 2a} r dr\, r' dr'\, g_3(\mathbf{r}, \mathbf{r}')$$

$$\bar{g}_{3,k}(\theta, \theta') = \int_{r, r' < 2a} r dr\, r' dr'\, g(\mathbf{r})g(\mathbf{r}')g(\mathbf{r}-\mathbf{r}')$$

Stress closure

Parametrize $g(\mathbf{r})$ with Σ'



Anisotropy expansion

$$
\begin{aligned}
g(\mathbf{r}) &= g_{\mathrm{rest}}\left(\frac{|\mathbf{r}|}{1-\alpha\mathbf{r}\cdot\boldsymbol{\Sigma}'\cdot\mathbf{r}/|\mathbf{r}|^2}\right) \\
&= g_{\mathrm{rest}}(|\mathbf{r}|)+\alpha g'_{\mathrm{rest}}(|\mathbf{r}|)\,\frac{\mathbf{r}\cdot\boldsymbol{\Sigma}'\cdot\mathbf{r}}{|\mathbf{r}|}
\end{aligned}
$$

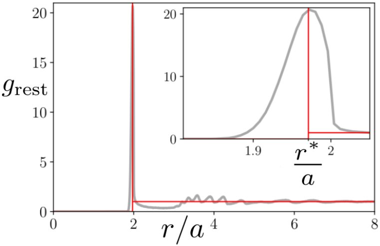
α is determined self-consistently

Stress closure

Minimal model for $g_{\mathrm{rest}}(r)$

$$g_{\mathrm{rest}}(r) \approx \frac{3}{\pi \rho r^*}\,\delta(r - r^*) + H(r - r^*)$$

- Dirac weight such that 6 nearest neighbors [$H(r)$ Heaviside function]
- Nearest neighbor peak location $r^*(p)$, with pressure $p = -\frac{1}{2}\mathrm{Tr}(\mathbf{\Sigma})$



Stress evolution equation

Lowest order approximation: $p = p(\phi)$

$$\partial_t \boldsymbol{\Sigma}' = \kappa(\phi)\mathbf{E}_\infty + \boldsymbol{\Omega}_\infty \cdot \boldsymbol{\Sigma}' - \boldsymbol{\Sigma}' \cdot \boldsymbol{\Omega}_\infty + \big(\beta(\phi) - \xi(\phi)\, \boldsymbol{\Sigma}' : \boldsymbol{\Sigma}'\big)\boldsymbol{\Sigma}'$$

- Minimal form of the stress evolution equation

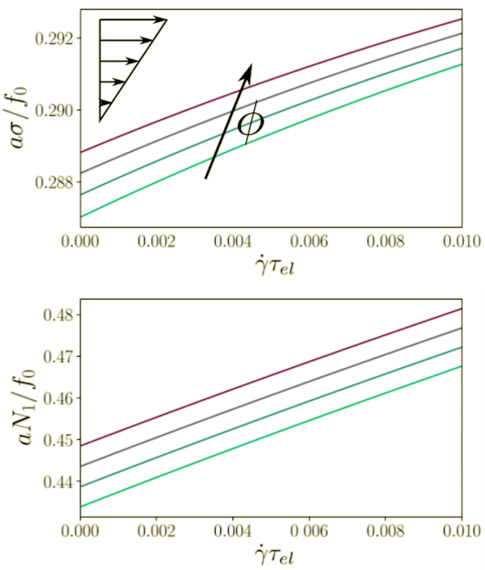
  All coefficients κ, β, ξ,... have **known** (but complicated) **expressions** in terms of packing fraction ϕ and microscopic parameters

[Cuny, Mari, **EB**, PRL **127**, 218003 (2021); JSTAT 033206 (2022)]

Yield stress behavior

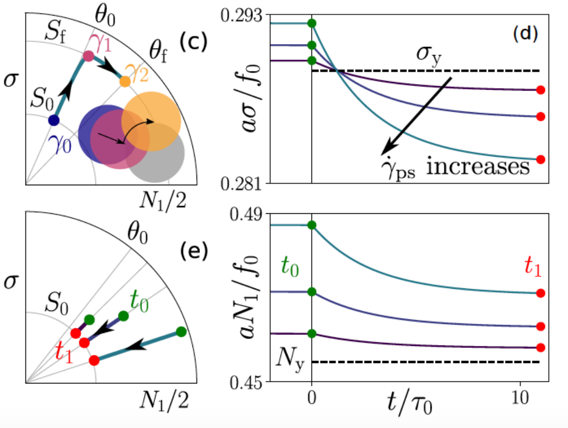
Bingham-like yield stress behavior for both shear stress σ and normal stress difference N_1

$$\boldsymbol{\Sigma}' = \begin{pmatrix} N_1/2 & \sigma \\ \sigma & -N_1/2 \end{pmatrix}$$



[Cuny, Mari, **EB**, PRL (2021)]

Relaxation after a preshear



Polar representation (S, θ): $N_1 = 2S\cos\theta, \quad \sigma = S\sin\theta$

S fast variable, θ slow variable for low shear rate $\dot\gamma$

[Cuny, Mari, **EB**, PRL (2021); Soft Matter (2022)]

Conclusion

- A constitutive model for jammed soft suspensions *derived from microscopics*
- **Reproduces important qualitative features:** yield stress, stress overshoot on step increase of shear rate, power-law decay in creep, etc.
  [Cuny, Mari, **EB**, Soft Matter (2022)]
- **Outlook:** Try to improve closure approximations to get Hershel-Bulkley behavior and solid elastic branch