

What simulations tell us about granular suspension rheology ?

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A bit of hydrodynamics

- Hydrodynamic interaction matrices

- Mean suspension stress

- Some numerical methods

Contacting particles

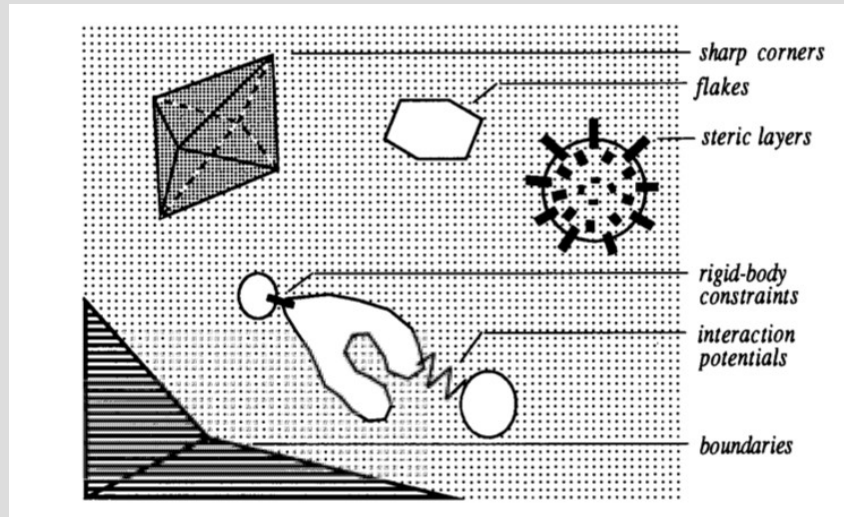
- Historical perspective

- Roughness and friction

- Shear reversal

- Shear thickening as a lubricated-to-frictional transition

- Shear thinning in frictional non-Brownian suspensions



Suspensions / emulsions / foams

Particles

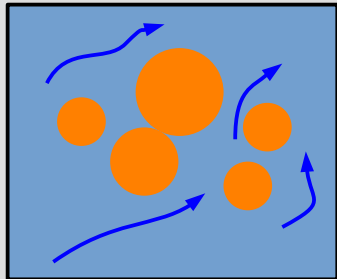
- Fluid, solid, visco-elastic
- Size, shape, surface properties and interactions
- Buoyancy

Suspending fluid

- Non-Newtonian

Brownian motion

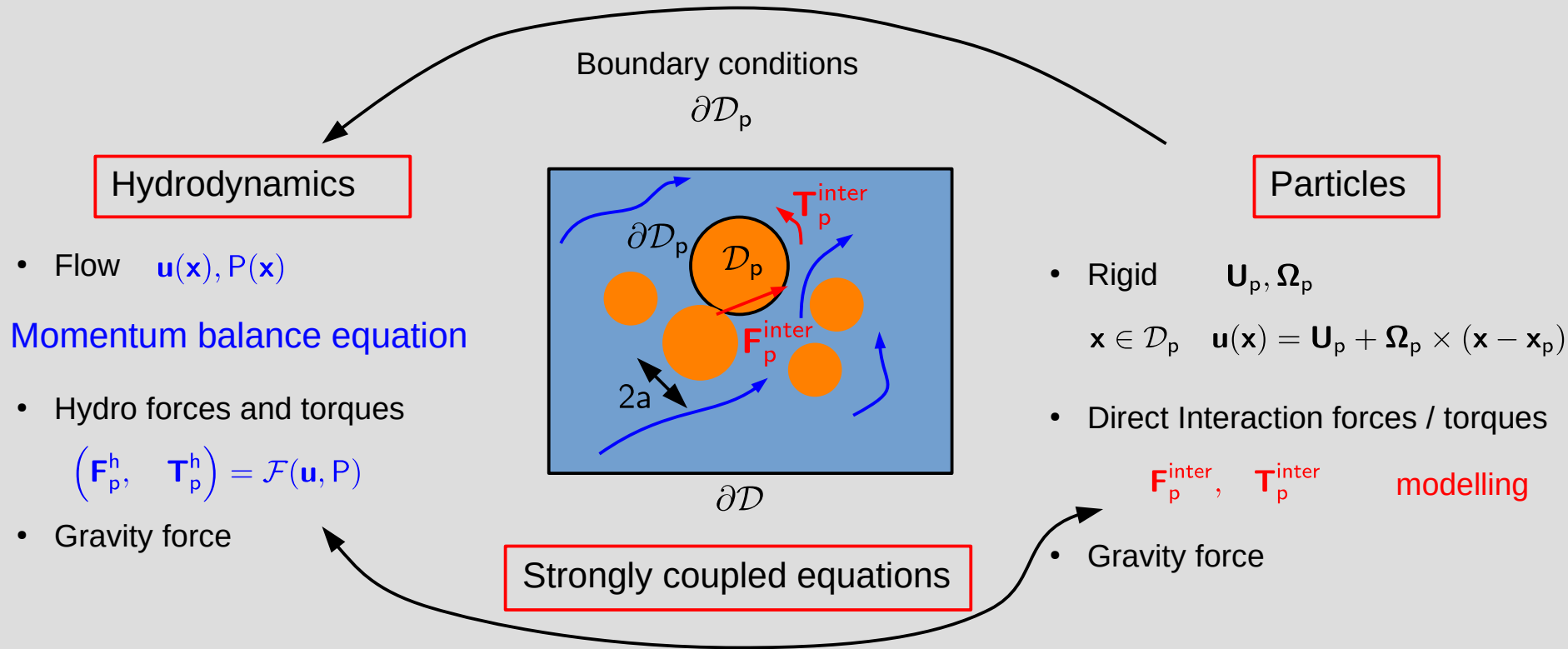
S. Kim and S.J. Karrila. *Microhydrodynamics: principles and selected applications*. Dover (2005).



Here

- "rigid" particles = no vesicle, droplet ...
- Short range ("contact") interactions (solid-solid, grafted polymer chains, double-layer ...)
- Newtonian liquid
- No Brownian motion
- No particle nor fluid inertia

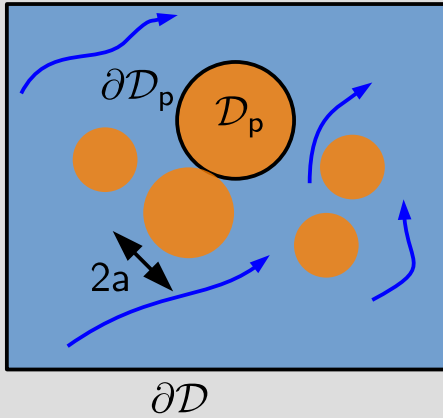
What's left?



Particle linear / angular momentum balance equations

$$\mathbf{F}_p^h + \mathbf{F}_p^{\text{inter}} + (\rho_p - \rho_f)V_p\mathbf{g} = M_p \frac{d\mathbf{U}_p}{dt}$$

$$\mathbf{T}_p^h + \mathbf{T}_p^{\text{inter}} = I_p \frac{d\boldsymbol{\Omega}_p}{dt}$$



Newtonian liquid

$$\boldsymbol{\sigma}_m = -P_m \mathbf{I} + \eta (\nabla \mathbf{u} + \nabla \mathbf{u}^\dagger)$$

$$P_m = P - (\rho_0 - \rho)gz$$

Momentum balance equation

$$\eta \Delta \mathbf{u} - \nabla P_m = \rho \frac{d\mathbf{u}}{dt}$$

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

$$Re = \frac{\rho U a}{\eta} \ll 1$$

$$St = \frac{a^2 \rho}{T \eta} \ll 1$$

Stokes equations

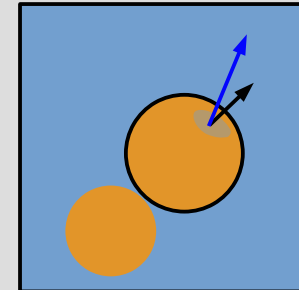
Boundary conditions

- Particles $\mathbf{x} \in \mathcal{D}_p$ $\mathbf{u}(\mathbf{x}) = \mathbf{U}_p + \boldsymbol{\Omega}_p \times (\mathbf{x} - \mathbf{x}_p)$
- External boundaries $\mathbf{x} \in \partial \mathcal{D}$ $\mathbf{u}(\mathbf{x}) = \mathbf{U}(\mathbf{x})$

Forces and torques

$$\mathbf{F}_p^h = \iint_{\partial \mathcal{D}_p} \boldsymbol{\sigma}_m \cdot \mathbf{n} \, dS$$

$$\mathbf{T}_p^h = \iint_{\partial \mathcal{D}_p} (\mathbf{x} - \mathbf{x}_p) \times \boldsymbol{\sigma}_m \cdot \mathbf{n} \, dS$$

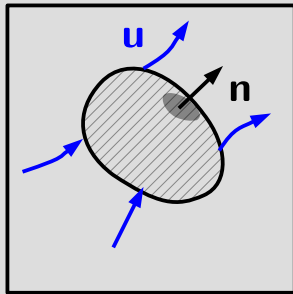


Stokes equations : some fundamental properties

$$\eta \Delta \mathbf{u} - \nabla P_m = 0$$

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

• No inertia \iff



Any fluid volume
 $\mathbf{F}^h = 0$

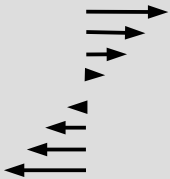
• Flow instantaneously driven by the B.C.

• Linear equations for $(\mathbf{u}(\mathbf{x}), P_m(\mathbf{x})) \implies$ Linear relation **Hydrodynamic forces / Velocities**

N particles in a **linear** flow

$$\mathbf{x} \in \partial \mathcal{D} \quad \mathbf{u}(\mathbf{x}) = \mathbf{u}_\infty(\mathbf{x}) = \mathbf{U}_0 + \boldsymbol{\Omega}_\infty \times \mathbf{x} + \mathbf{E}_\infty \cdot \mathbf{x}$$

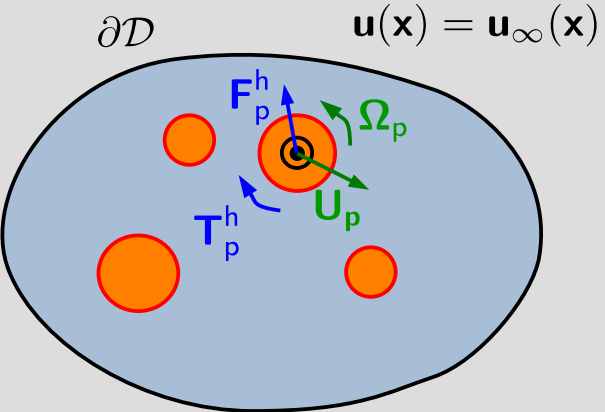
Simple shear
Extensional flow ...



$$\mathcal{F} = (\mathbf{F}_1, \mathbf{F}_2, \dots, \mathbf{T}_1, \mathbf{T}_2, \dots)$$

$$\mathcal{U} = (\mathbf{U}_1, \mathbf{U}_2, \dots, \boldsymbol{\Omega}_1, \boldsymbol{\Omega}_2, \dots)$$

$$\mathcal{U}_\infty = (\mathbf{u}_\infty(\mathbf{x}_1), \mathbf{u}_\infty(\mathbf{x}_2), \dots, \boldsymbol{\Omega}_\infty, \boldsymbol{\Omega}_\infty, \dots)$$



$$\mathcal{F} = -\mathcal{R}_{FU} \cdot (\mathcal{U} - \mathcal{U}_\infty) + \mathcal{R}_{FE} : \mathbf{E}_\infty$$


\mathcal{R}_{XY} Resistance tensors

$(\mathcal{R}_{FU}, \mathcal{R}_{FE}) = f(\mathbf{x}_1, \mathbf{x}_2, \dots)$ Not to be computed exactly (in general)

Two-particle grand resistance matrix

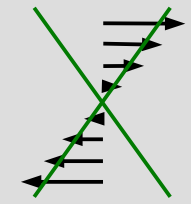
Jeffrey, D. J., & Onishi, Y. (1984). *Journal of Fluid Mechanics*
 Jeffrey, D. J. (1992). *Physics of Fluids A: Fluid Dynamics*
 Jeffrey, D., Morris, J., & Brady, J. (1993). *Phys. Fluids A*.

- Known exactly (= analytical / semi-analytical) for any particle distance

Stresslet : later 

$$\begin{pmatrix} \mathbf{F}_1 \\ \mathbf{F}_2 \\ \mathbf{T}_1 \\ \mathbf{T}_2 \\ \mathbf{S}_1 \\ \mathbf{S}_2 \end{pmatrix} = -\eta \underbrace{\begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} & \tilde{\mathbf{B}}_{11} & \tilde{\mathbf{B}}_{12} & \tilde{\mathbf{G}}_{11} & \tilde{\mathbf{G}}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} & \tilde{\mathbf{B}}_{21} & \tilde{\mathbf{B}}_{22} & \tilde{\mathbf{G}}_{21} & \tilde{\mathbf{G}}_{22} \\ \mathbf{B}_{11} & \mathbf{B}_{12} & \mathbf{C}_{11} & \mathbf{C}_{12} & \tilde{\mathbf{H}}_{11} & \tilde{\mathbf{H}}_{12} \\ \mathbf{B}_{21} & \mathbf{B}_{22} & \mathbf{C}_{21} & \mathbf{C}_{22} & \tilde{\mathbf{H}}_{21} & \tilde{\mathbf{H}}_{22} \\ \mathbf{G}_{11} & \mathbf{G}_{12} & \mathbf{H}_{11} & \mathbf{H}_{12} & \mathbf{M}_{11} & \mathbf{M}_{12} \\ \mathbf{G}_{21} & \mathbf{G}_{22} & \mathbf{H}_{21} & \mathbf{H}_{22} & \mathbf{M}_{21} & \mathbf{M}_{22} \end{pmatrix}}_{\text{Tensors of order 2 to 4}} \cdot \begin{pmatrix} \mathbf{U}_1 - \mathbf{u}_\infty(\mathbf{x}_1) \\ \mathbf{U}_2 - \mathbf{u}_\infty(\mathbf{x}_2) \\ \Omega_1 - \Omega_\infty \\ \Omega_2 - \Omega_\infty \\ -\mathbf{E}_\infty \\ -\mathbf{E}_\infty \end{pmatrix}$$

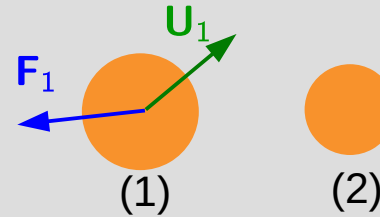
= $f(\mathbf{x}_1, \mathbf{x}_2, \dots)$



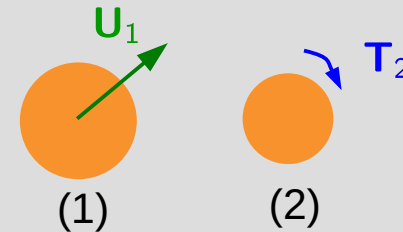
Example

$$\begin{aligned}
 \mathbf{u}_\infty &= 0 \\
 \mathbf{U}_2 &= 0 \\
 \Omega_1 &= \Omega_2 = 0
 \end{aligned}$$

$$\mathbf{F}_1 = -\eta \mathbf{A}_{11} \cdot \mathbf{U}_1$$

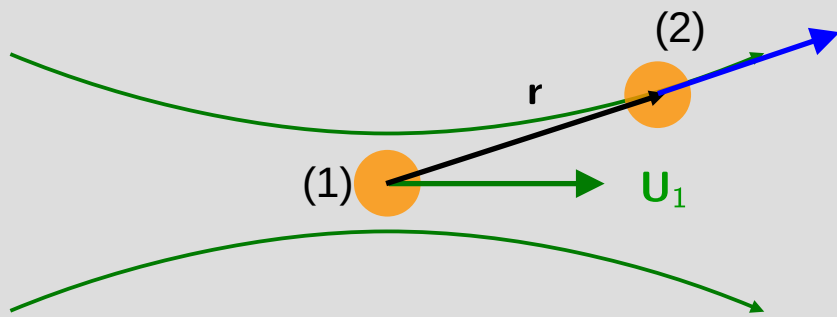


$$\mathbf{T}_2 = -\eta \mathbf{B}_{21} \cdot \mathbf{U}_1$$



Hydrodynamic interactions : both long and short range

- $r \gg a_1, a_2$



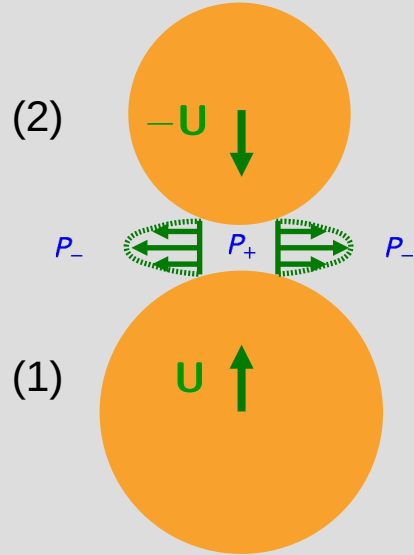
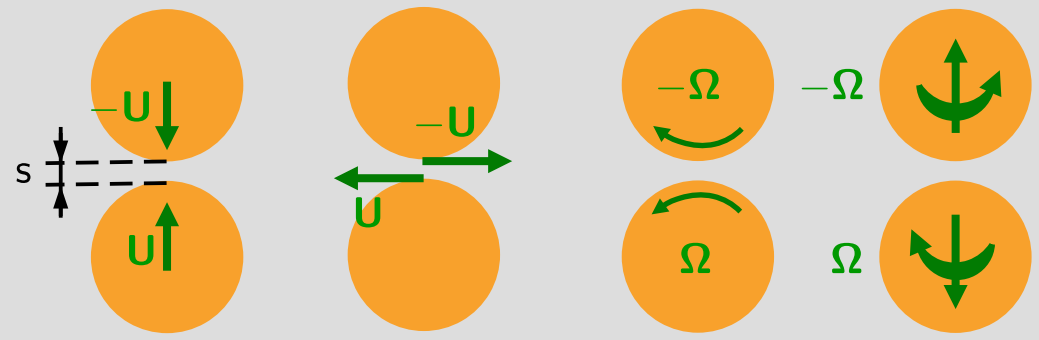
$$u(r) \propto \frac{a_1}{r} U_1$$

$$F_2 \propto 6\pi\eta a_2 \frac{a_1}{r} U_1$$

- Very long range ($1/r$)
- Primary role when external forces are considered (sedimentation ...)

- $s = r - (a_1 + a_2) \ll a_1, a_2$

Lubrication approximation

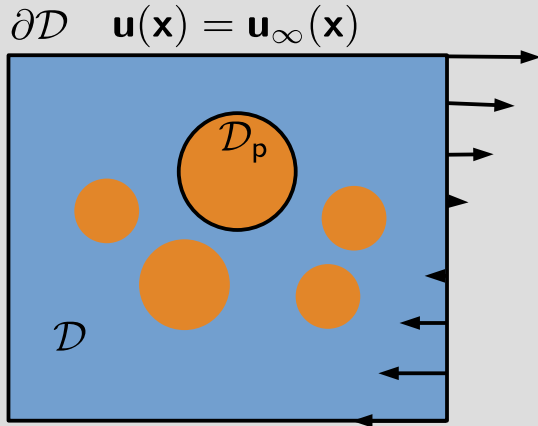


$$\xi = \frac{s}{(a_1 + a_2)/2} \ll 1$$

- Squeeze
 $F_1, F_2 \propto 1/\xi$
- Other terms
 $\propto \log(\xi)$
 or smaller

Mean suspension stress

Batchelor, G. K. (1970). Journal of fluid mechanics, 41(3), 545-570.



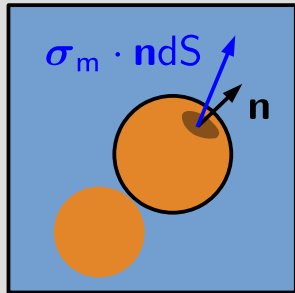
Mean stress $\Sigma_{ij} = \frac{1}{V} \iiint_{\mathcal{D}} \sigma_{ij} dV$

$$\Sigma_{ij} = -(1 - \phi) \langle P \rangle_f \delta_{ij} + \eta \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \frac{1}{V} \sum_{p=1}^N D_{ij}^p$$

Mean fluid pressure

Mean fluid deformation rate

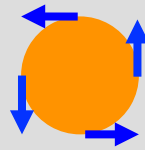
Particle contribution



$$\mathbf{D}_p = \iint_{\partial \mathcal{D}_p} \boldsymbol{\sigma}_m \cdot \mathbf{n} \otimes (\mathbf{x} - \mathbf{x}_p) dS = \mathcal{T}_p + \mathbf{S}_p$$

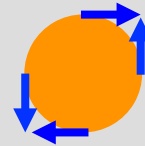
Second moment of the force distribution = **Force dipole**

\mathcal{T}_p Antisymmetric part
 \longleftrightarrow torque



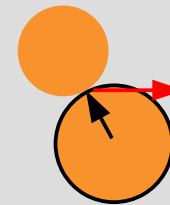
Induces particle rotation

\mathbf{S}_p Symmetric part
 = stresslet



Induces particle deformation

Stress = hydro contribution + point contact forces



$$\mathcal{T}_p = \mathcal{T}_p^c + \mathcal{T}_p^h = 0 \quad \text{No inertia}$$

$$\mathbf{S}_p = \mathbf{S}_p^c + \mathbf{S}_p^h$$

$$\mathbf{S}_p^c = \frac{1}{2} (\Delta \mathbf{r} \otimes \mathbf{F}^c + \mathbf{F}^c \otimes \Delta \mathbf{r})$$

N.B. Another splitting hydro / contact is possible (next slide)

Hydrodynamic and contact contributions

Two different ways of separating contact and hydrodynamic contributions :

- The « Stokesian dynamics » way Phung et al. (1996). . JFM, 313, 181-207. Mari et al. (2015). Phys. Rev. E, 91(5), 052302.
Banchio and Brady, J. Chem. Phys. 118, 10323 (2003).

Hydro. in nature (viscous stress)

$$\mathcal{S} = \underbrace{\left[-\mathcal{R}_{SU} \cdot \mathcal{R}_{FU}^{-1} \cdot \mathcal{R}_{FE} + \mathcal{R}_{SE} \right] : \mathbf{E}_\infty}_{\text{Produced by the external shear w/o forces = hydro}} - \underbrace{\mathcal{R}_{SU} \cdot \mathcal{R}_{FU}^{-1} \cdot \mathbf{F}^c + \frac{1}{2} (\Delta \mathbf{r} \otimes \mathbf{F}^c + \mathbf{F}^c \otimes \Delta \mathbf{r})}_{\text{Produced by the forces w/o external shear = contact}}$$

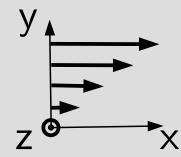
Physical meaning in shear reversal (Peters et al. 2016 J.O.R) and shear rotation (Blanc et al. 2023 PRL)

More about this on Wednesday 11h15 : Romain Mari

- The « direct » way

$$\Sigma = -(1 - \phi) \langle P \rangle_f \delta + \eta (\nabla \otimes \mathbf{u} + \nabla \otimes \mathbf{u}^\dagger) + \underbrace{\frac{1}{V} \sum_{p=1}^N \mathbf{s}_p^h}_{\Sigma^h} + \underbrace{\frac{1}{V} \sum_{p=1}^N \mathbf{s}_p^c}_{\Sigma^c}$$

- Shear flow



Reduced Viscosity

$$\eta_r = \frac{\Sigma_{xy}}{\eta \dot{\gamma}} = 1 + \frac{\Sigma_{xy}^h + \Sigma_{xy}^c}{\eta \dot{\gamma}} = \eta^h + \eta^c$$

Normal stresses

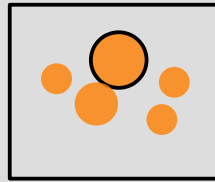
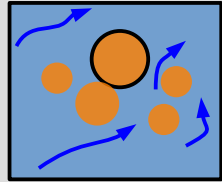
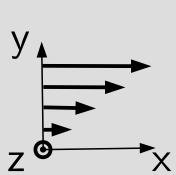
$$N_1 = \Sigma_{xx} - \Sigma_{yy}$$

$$N_2 = \Sigma_{yy} - \Sigma_{zz}$$

- Stokesian dynamics

Brady, J. F., & Bossis, G. (1988). Annual Review of Fluid Mechanics

Sierou, A., & Brady, J. F. (2001). Journal of Fluid Mechanics



No flow is computed

$$\mathcal{F}^h + \mathcal{F}^c = 0 \quad \begin{pmatrix} \mathcal{F}^h \\ \mathcal{S}^h \end{pmatrix} = -\mathcal{R} \cdot \begin{pmatrix} \mathbf{u} - \mathbf{u}_\infty \\ \boldsymbol{\varepsilon}_\infty \end{pmatrix}$$

$$\mathbf{u} = \mathbf{u}_\infty + \mathcal{R}_{FU}^{-1} \cdot \mathcal{R}_{FE} : \mathbf{E}_\infty + \mathcal{R}_{FU}^{-1} \cdot \mathcal{F}^c \implies \text{Particle motion}$$

$$\mathcal{S} = [-\mathcal{R}_{SU} \cdot \mathcal{R}_{FU}^{-1} \cdot \mathcal{R}_{FE} + \mathcal{R}_{SE}] : \mathbf{E}_\infty - \mathcal{R}_{SU} \cdot \mathcal{R}_{FU}^{-1} \cdot \mathcal{F}^c + \frac{1}{2} (\Delta \mathbf{r} \otimes \mathcal{F}^c + \mathcal{F}^c \otimes \Delta \mathbf{r}) \implies \text{Stress}$$

$$\mathcal{R} = \mathcal{M}_{ff}^{-1} + \mathcal{R}_{2B}^{th} - \mathcal{M}_{ff,2B}^{-1}$$

\mathcal{M}_{ff} Far field multipole expansion (pairwise-additive construction of the mobility tensor)

\mathcal{R}_{2B}^{th}

Theoretical 2-body lubrication resistance (pairwise-additive construction \implies sparse matrices)

→ Original method : \mathcal{M}_{ff} is dense \implies building $O(N^2)$, inverting $O(N^3)$

→ Accelerated SD : $O(N \ln(N))$

Pros

- accurate (long range and lub.)
- quite fast Ouaknin et al (2021). JCP

Cons

- for spheres only (and maybe spheroids)
- for Newtonian liquid only
- Re = 0 only
- method quite involved

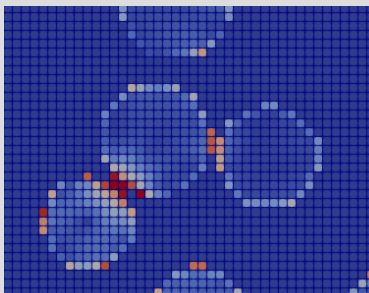
Fictitious Domain Methods : actual flow computation

- Fluid flow computed over the whole domain
- Particles accounted for using force density λ

$$\eta \Delta \mathbf{u} - \nabla p - \nabla P_0 + \rho_f \lambda = 0$$

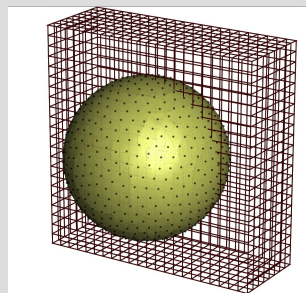
$$\nabla \cdot \mathbf{u} = 0$$

Immersed body



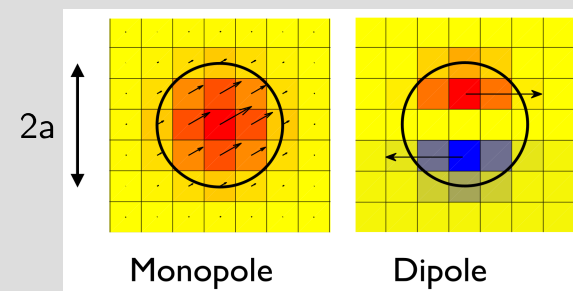
Gallier et al. (2014) JCP.
Orsi et al. (2023) JCP.

Immersed boundary method (IBM)



Uhlmann (2008) Phys. Fluids
Breugem (2012) JCP.

Force coupling method (FCM)

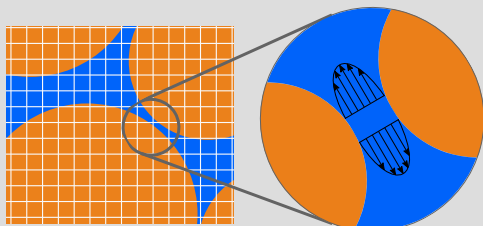


Maxey & Patel (2001) Int. J. Multiphase Flow
Yeo & Maxey (2011) JCP.

- Constraints $\mathbf{x} \in \mathcal{D}_p \quad \mathbf{u}(\mathbf{x}) = \mathbf{U}_p + \boldsymbol{\Omega}_p \times \mathbf{x} \quad \mathbf{F}^{\text{FDM},p} + \mathbf{F}^{\text{SG},p} + \mathbf{F}^{\text{C},p} = 0$

$$\mathbf{T}^{\text{FDM},p} + \mathbf{T}^{\text{SG},p} + \mathbf{T}^{\text{C},p} = 0$$

- Subgrid corrections



$$\begin{pmatrix} \mathcal{F}^{\text{SG}} \\ \mathcal{S}^{\text{SG}} \end{pmatrix} = -\mathcal{R}^{\text{SG}} \cdot \begin{pmatrix} \mathbf{u} - \mathbf{u}_\infty(\mathbf{x}_p) \\ -\boldsymbol{\varepsilon}_\infty \end{pmatrix}$$

pairwise-additive construction

Pros

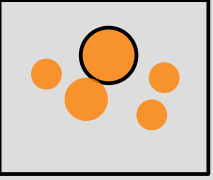
- Hydrodynamics : short and long range interactions included, few restrictive assumptions.
- Sedimentation allowed (long range interactions)
- Extension to any particle shape or liquid
- Extension to $Re, St \neq 0$
- Some open CFD toolboxes (OpenFOAM, Basilisk) with native MPI integration

Cons

- **Not that fast**
- Parallelized particle sub-problem implementation quite difficult

Distinct (or discrete) elements methods (DEM)

- From granular physics Cundall, P. A., & Strack, O. D. L. (1980). Géotechnique, 29(1), 47-65.
- Molecular dynamics w/o thermal forces, no fluid flow computed
- Different versions (not a comprehensive list)

$$M_p \frac{d\mathbf{U}_p}{dt} = \mathbf{F}_p^c + \mathbf{F}^h$$


→ No inertia, 2-particle lubrication interactions and drag

Seto et al. (2013) PRL
Mari et al. (2014) JOR

$$\mathbf{F}_p^{\text{drag}} = -6\pi\eta a (\mathbf{U}_p - \mathbf{u}_\infty(\mathbf{x}_p))$$

$$\mathbf{T}_p^{\text{drag}} = -8\pi\eta a^3 (\boldsymbol{\Omega}_p - \boldsymbol{\Omega}_\infty)$$

$$\mathcal{F} = \mathcal{F}_{\text{drag}} - \mathcal{R}_{\text{lub}} \cdot (\mathbf{U} - \mathbf{U}_\infty) + \mathcal{R}'_{\text{lub}} : \mathbf{E}_\infty$$

Pairwise additive lubrication



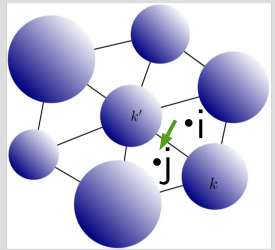
→ Inertia, 2-particle lubrication interactions, drag or no drag (depending on the papers)

Ness & Sun (2015) PRE
Cheal & Ness (2016) JOR

$$\mathcal{F} = -\mathcal{R} \cdot \mathbf{U} + (\mathcal{F}_{\text{drag}})$$

→ Inertia, 2-particle lubrication interactions, poromechanical coupling

Chareyre et al. (2012] Transp. in porous media
Marzougui et al. (2015) Granular Matter
Chevremont (2019) Phys.rev. Fluids



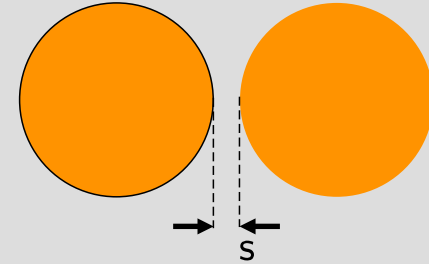
$$q_{ij} \propto P_i - P_j$$

→ Pressure velocity coupling $\frac{dV_i}{dt} = \sum_j q_{ji}$

→ Viscous force $\mathcal{F}_{\text{Pore P.}} = \mathbf{l}^f \cdot \mathcal{P}$

Adapted from
Marzougui et al. (2015)
Granular Matter

- All versions : cutoff distance for lubrication interactions $s/a \gtrsim 0.1 \Rightarrow \mathcal{F} = 0$



Pros

- **Fast** (meaning large size systems, large volume fractions ...)
- Some open codes, **easy to use** (LAMMPS (Ness), YADE (Chareyre et al.)...)

Cons

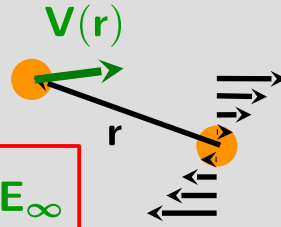
- Only lubrication interactions :
 - Better for high volume fraction
 - Not suitable for sedimentation
 - Specific strategies for some problems involving heterogeneous flow, e.g. migration (Kolmogorov flow = external force on the particles), resuspension...
 - Data to be checked against method with more comprehensive hydrodynamics (migration, velocity fluctuations etc.)

A force free particle pair in simple shear flow

- Resistance matrices known exactly (semi-analytical)
- Direct integration of the momentum balance equation

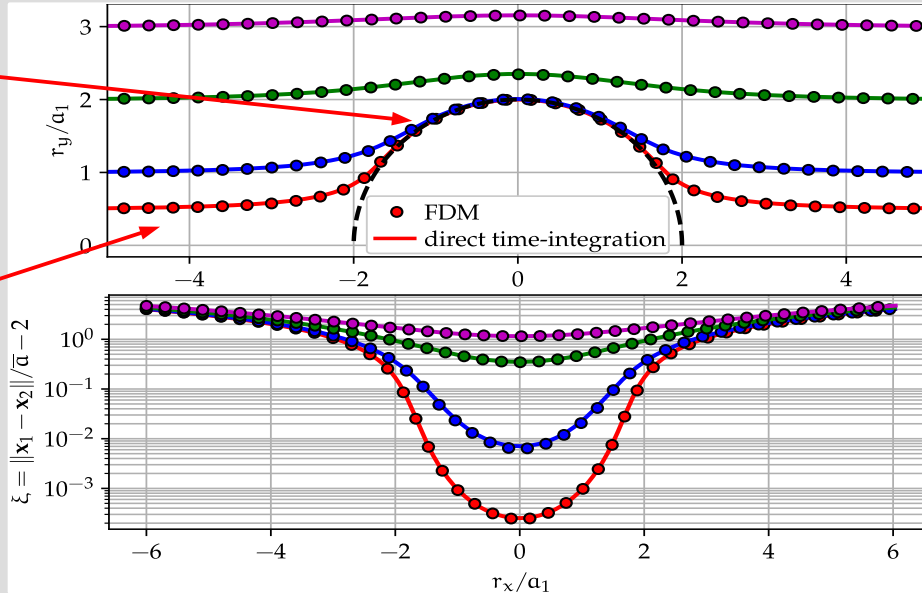
$$0 = -\mathcal{R}_{FU} \cdot (\mathbf{U} - \mathbf{U}_\infty) + \mathcal{R}_{FE} : \mathbf{E}_\infty$$

$$(\mathbf{U}_1, \mathbf{U}_2, \Omega_1, \Omega_2) = \mathbf{U}_\infty + \mathcal{R}_{FU}^{-1}(\mathbf{r}) \cdot \mathcal{R}_{FE}(\mathbf{r}) : \mathbf{E}_\infty$$



Short range Interactions (lubrication)

Long range interactions



Orsi, M. (2022) Doctoral dissertation, Université Côte d'Azur.

Lubrication



No contact but

$$\frac{r_{\min}}{a} \approx 4 \cdot 10^{-5}$$

Arp, P. A. & Mason, S. G. (1977).
J. Colloid Interface Sc.

$$a = 40 \mu\text{m} \Rightarrow r_{\min} \approx 1.6 \cdot 10^{-9} \text{m}$$

Asperities = contact !

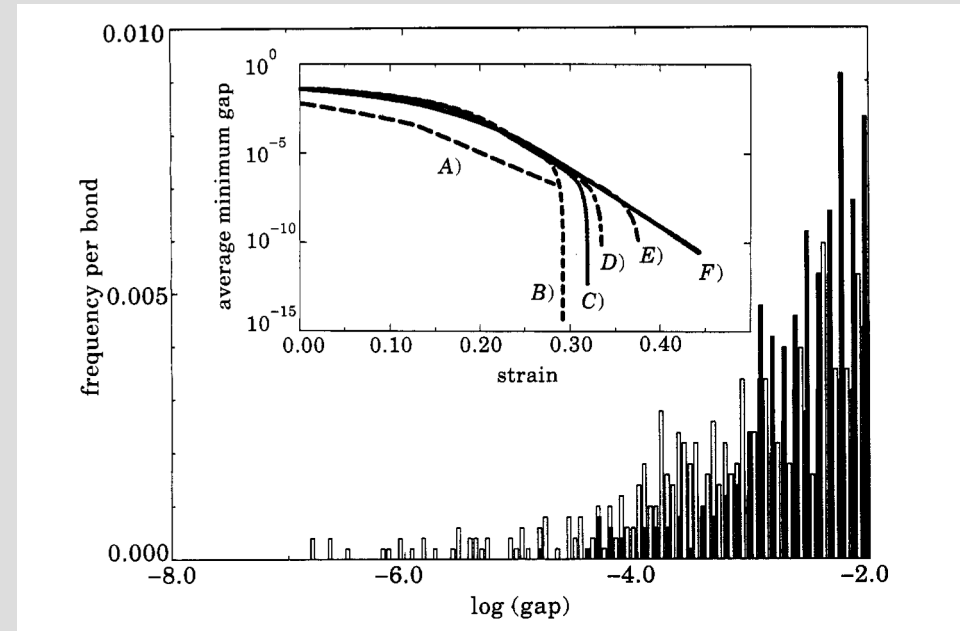
No direct interaction force in NB suspensions: lubrication breakdown

Melrose, J. R., & Ball, R. C. (1995). The pathological behaviour of sheared hard spheres with hydrodynamic interactions. *Europhysics letters*, 32(6), 535.

Ball, R. C., & Melrose, J. R. (1995). Lubrication breakdown in hydrodynamic simulations of concentrated colloids. *Advances in colloid and interface science*, 59, 19-30.

- Simplified Stokesian dynamics (DEM, no far field)
- Various time schemes (4th order RK, 2nd order predictor corrector) and time steps
- Unphysical value of the gap
 $d = 40\mu\text{m} \Rightarrow s = 4.10^{-15}\text{m}$
- No steady state (viscosity)
- Simulation stops (too long, gap collapse)
- Also observed in full SD

Dratler, D. I., & Schowalter, W. R. (1996). *Journal of Fluid Mechanics*



Melrose, J. R., & Ball, R. C. (1995). *Europhysics letters*, 32(6), 535.

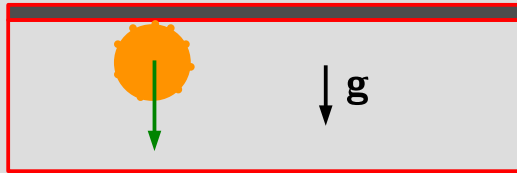
RK. $N_p=700$ (A), $N_p=50$ (F)

PC. $N_p=50$. $dt = 5.10^{-4}$ (B), $dt = 5.10^{-4}$ (C), $dt = 5.10^{-5}$ (D), $dt = 1.10^{-5}$ (E)

Unphysical
Computationally Intractable

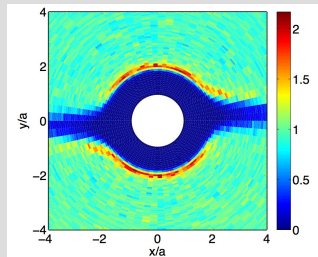
Contact due to roughness in NB suspensions : quite an old idea (1980-1990)

- Breaking of periodic orbit of a particle pair in shear flow Arp, P. A. & Mason, S. G. (1977) J. Colloid Interface Sci.
- Proposed to explain particle migration Leighton, D., & Acrivos, A. (1987) Journal of Fluid Mechanics
- Measured via particle-wall hydro interactions Smart & Leighton (1989). Physics of Fluids A: Fluid Dynamics



Time for separation = $f(h_r)$ \longleftrightarrow Lubrication cutoff

- Roughness connected to asymmetric pair distribution function Rampall et al. (1997). Journal of Fluid Mechanics



Blanc, F. et al. (2011). Physical review letters, 107(20), 208302.

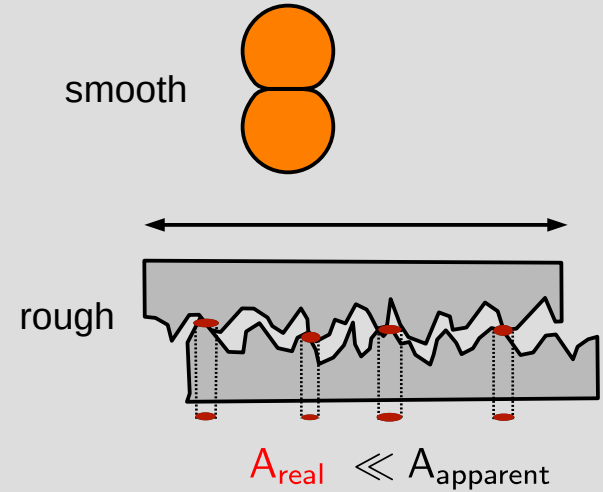
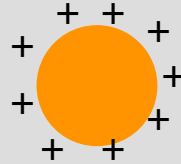
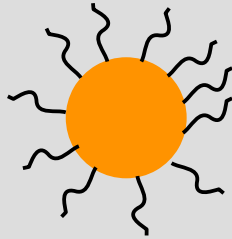
Contact force modelling

- Contact between solid bodies : complicated matter

Johnson, K. L. (1987). Contact mechanics. Cambridge university press.

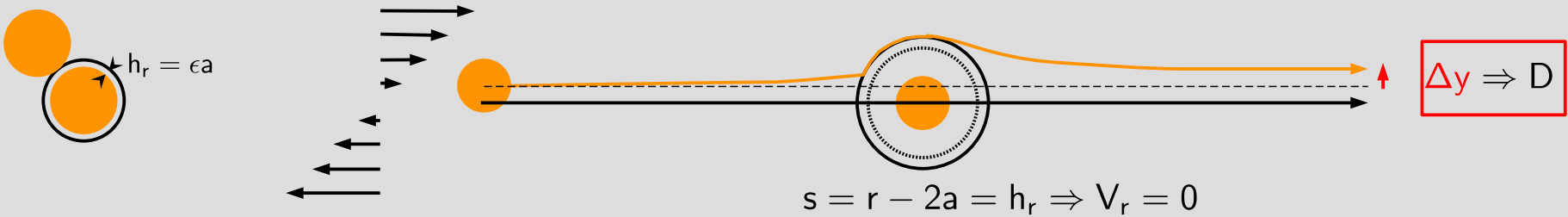
- Suspensions: many parameters (Jean Comtet lecture)

- Smooth / rough surface
- Elastic / plastic / viscoelastic solids
- Adhesion
- Surface physico-chemistry (grafted polymers, electric charge)

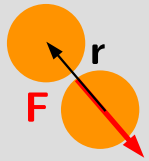


Contact forces in simulations (NB suspensions) : the early days

- Roughness (contact) induces irreversibility Da Cunha, F. R., & Hinch, E. J. (1996). J.F.M
 - Shear-induced diffusivity in dilute suspensions (2 particles)
 - Simple model of roughness : modification of the mobility functions equivalent to a radial force



- Repulsive spherical potential
 - Avoid lubrication breakdown
 - Weak influence of the specific form if short range (w.r.t radius a)



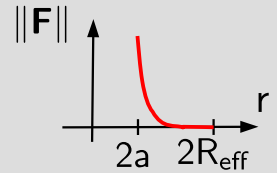
Double layer-like $\mathbf{F} = 2f_0\tau \frac{e^{-\tau s}}{1 + e^{-\tau s}} \frac{\mathbf{r}}{\|\mathbf{r}\|}$ Dratler, D. I., & Schowalter, W. R. (1996). J.F.M, 325, 53-77.

$h_r \sim 1/\tau$

$\mathbf{F} = f_0\tau \frac{e^{-\tau s}}{1 - e^{-\tau s}} \frac{\mathbf{r}}{\|\mathbf{r}\|}$ Sierou, A., & Brady, J. F. (2002). J. Rheol. 46(5), 1031-1056.

Arbitrary $r < R_{\text{eff}} \Rightarrow \mathbf{F} = -6\pi\eta a V_{\text{ref}} \left(\frac{R_{\text{ref}}^2 - \|\mathbf{r}\|^2}{R_{\text{ref}}^2 - a^2} \right)^6 \frac{\mathbf{r}}{\|\mathbf{r}\|}$

Yeo, K., & Maxey, M. R. (2010). Journal of Fluid Mechanics, 649, 205-231.



Cut off distance
 $R_{\text{eff}}/a = 2.002$
 $h_r = R_{\text{eff}} - 2a = 0.002a$

Further modelling : elasto-frictional contact

- Standard in dry granular physics

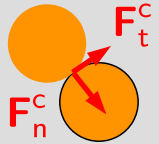
Cundall, P. A., & Strack, O. D. L. (1980). Géotechnique

Shäfer, J., Dippel, S., & Wolf, D. E. (1996). Journal de physique I

- More recently in suspensions

Seto, R., Mari, R., Morris, J. F., & Denn, M. M. (2013) PRL

Gallier, S., Lemaire, E., Peters, F., & Lobry, L. (2014). JFM



Point forces

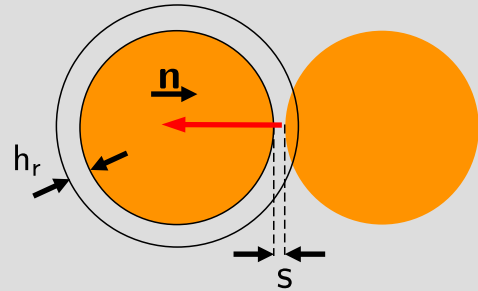
- Elastic normal force

Compression $\delta = h_r - s$

$$s < h_r \Rightarrow \mathbf{F}_n^c = -k_n \delta \mathbf{n} \quad \text{Linear spring}$$

(Hertz $k_n \propto \sqrt{\delta}$)

No need for dissipative terms $-\gamma_n \dot{\delta}$
if lubrication is kept $-\gamma_t \dot{\mathcal{Y}}$



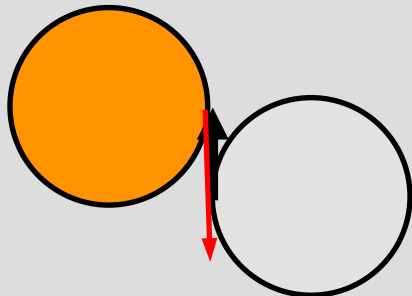
- Elastic tangential force

Slip velocity $\mathbf{U}_s = \mathbf{U}_i - \mathbf{U}_j - [(\mathbf{U}_i - \mathbf{U}_j) \cdot \mathbf{n}] \cdot \mathbf{n} + (a_i \boldsymbol{\Omega}_i + a_j \boldsymbol{\Omega}_j) \times \mathbf{n}$

Accumulated slip $\mathcal{Y} = \int_0^t \mathbf{U}_s dt$

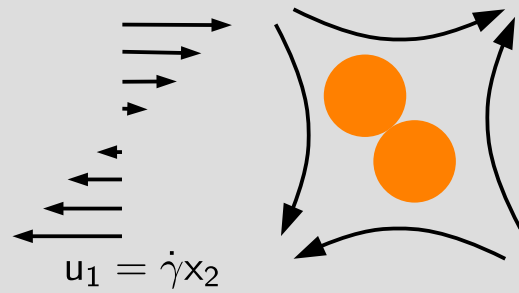
Elastic force (stick phase) $\mathbf{F}_t^c = -k_t \mathcal{Y}$ (Hertz-Mindlin $k_t \propto \sqrt{\delta}$)

Slip condition (Amontons-Coulomb) $\|\mathbf{F}_t^c\| \geq \mu_s \|\mathbf{F}_n^c\| \Rightarrow \mathbf{F}_t^c = \mu_s \|\mathbf{F}_n^c\| \frac{\mathbf{F}_t^c}{\|\mathbf{F}_t^c\|}$



Dimensionless numbers

- Equations made dimensionless
 - Length : radius a
 - Time : $\dot{\gamma}^{-1}$
 - Force : $6\pi\eta a^2 \dot{\gamma}$



Two particles
= dilute suspension
 $F \sim 6\pi\eta a^2 \dot{\gamma} = 6\pi \Sigma_{12} a^2$
Nir, A., & Acrivos, A. (1973). JFM

Volume fraction $\phi = \frac{V_s}{V_{tot}}$

Roughness $h_r/a \sim 10^{-3} - 10^{-2}$ Experiments with model spheres

Shear rate $\dot{\Gamma}_L = \frac{6\pi\eta a^2 \dot{\gamma}}{k_n h_r}$
 $\dot{\Gamma}_H = \frac{6\pi\eta a^2 \dot{\gamma}}{k_n h_r^{3/2}}$

$F_n^c(\bar{\delta}) \sim 6\pi a^2 \Sigma_{12} \iff \left(\frac{\bar{\delta}}{h_r} \right)_L \sim \dot{\Gamma}_L$
 $\left(\frac{\bar{\delta}}{h_r} \right)_H \sim \dot{\Gamma}_H^{2/3}$

Increases with
volume fraction or stress

N.B. Shear stress : $\eta_r \dot{\Gamma}$

Typical compression (dilute case)

Tangential stiffness k_t/k_n

Friction coefficient μ_s

Stiffnesses

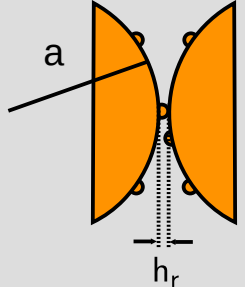
- A simple estimation: a sphere (a) against an asperities ($h_r \ll a$) $F_n^c = \frac{2}{3} \frac{E}{1-\nu^2} h_r^{1/2} \delta^{3/2}$

Peters et al. (2016). Journal of rheology,

PMMA $E \sim 3\text{GPa}$ $a \sim 20\mu\text{m}$
 $\nu \sim 0.4$ $h_r/a \sim 10^{-2}$
 $\eta \sim 1\text{Pa}\cdot\text{s}$
 $\dot{\gamma} \sim 100\text{s}^{-1}$

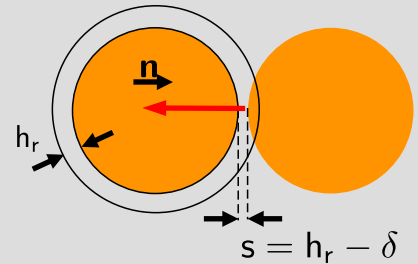
$$\dot{\Gamma} \sim 8.10^{-3}$$

$$\bar{\delta}/h_r \sim 4.10^{-2}$$



- $\dot{\Gamma} \leq 10^{-1}$ Mostly Newtonian
- $\dot{\Gamma} > 10^{-1}$ Weak shear thickening behaviour

Gallier et al. (2014). Journal of Fluid Mechanics



$\Sigma_{12} \nearrow \Rightarrow \delta \nearrow$
 \Rightarrow lubrication \nearrow

- One strategy : keeping $\langle \delta/a \rangle \leq \delta_{\text{max}}/a \sim 5\%$ and $k_n/k_t \propto \dot{\gamma}$ $\eta_s(\phi, h_r, 6\pi a^2 \eta \dot{\gamma} / F_n^c(h_r))$
- $\langle \mathcal{Y}/a \rangle \leq \mathcal{Y}_{\text{max}}/a \sim 5\%$

Mari et al. (2014). J. Rheol.

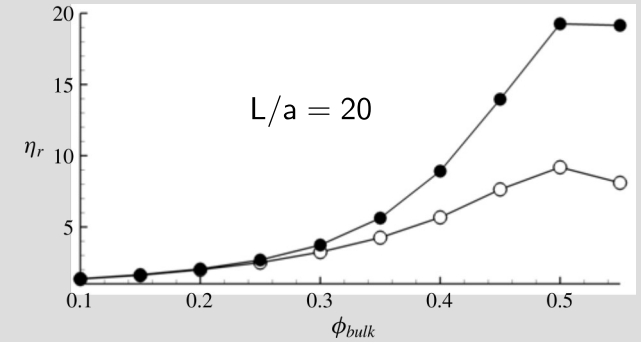
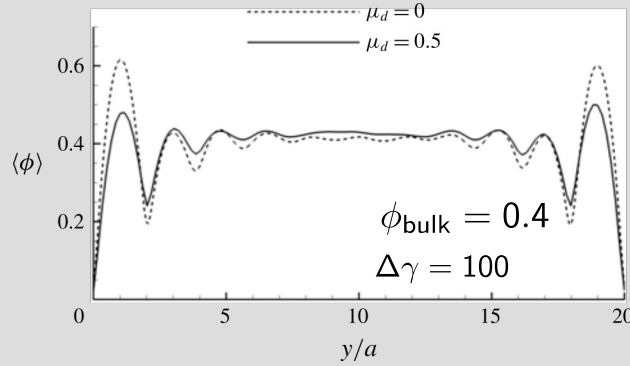
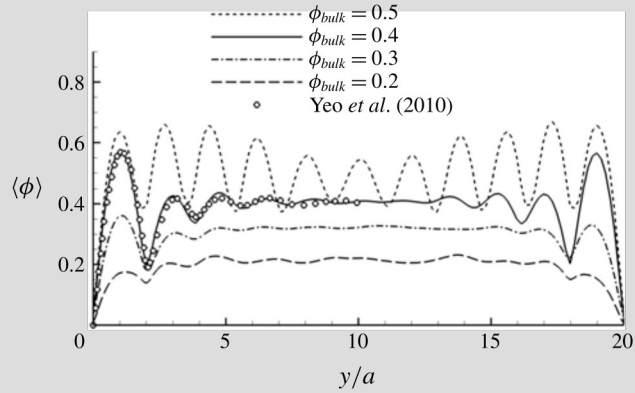
No stress scale other than $\eta \dot{\gamma} \Rightarrow \approx$ Newtonian behavior

$$\dot{\Gamma} = \text{cst} \iff \bar{\delta} \sim \text{cst}$$

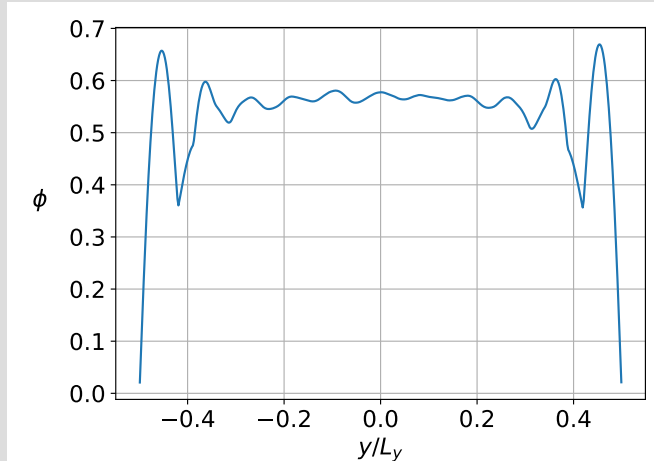
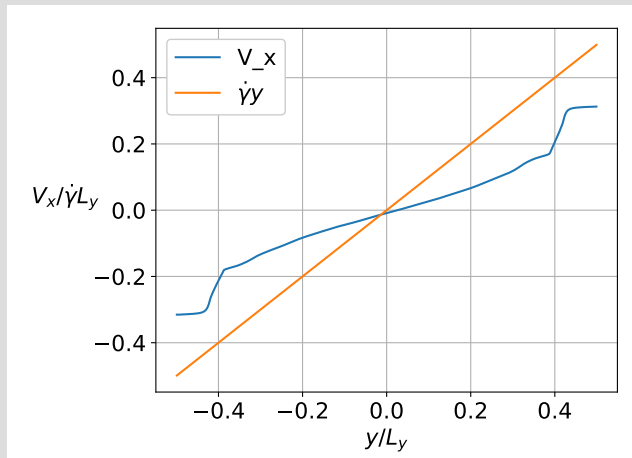
- Usually $k_t/k_n = 2/7$

Monodisperse suspensions

Gallier et al. (2016). J. Fluid Mech.



Slight bidispersity



$$\mu_s = 0.5$$

$$\bar{\phi} = 0.54$$

$$a_2/a_1 = 1.4$$

$$\bar{\phi}_1 = \bar{\phi}_2 = \bar{\phi}/2$$

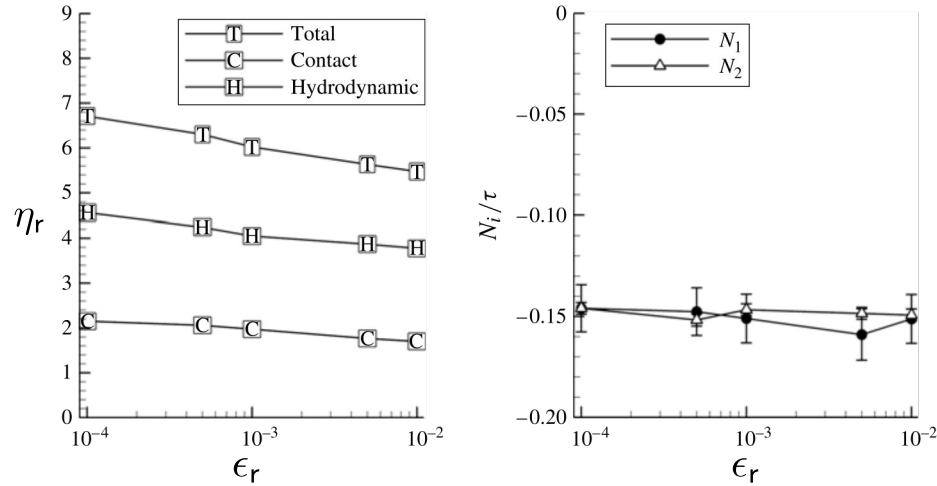
Same Data as in
Michel Orsi (2023) JCP.

Roughness

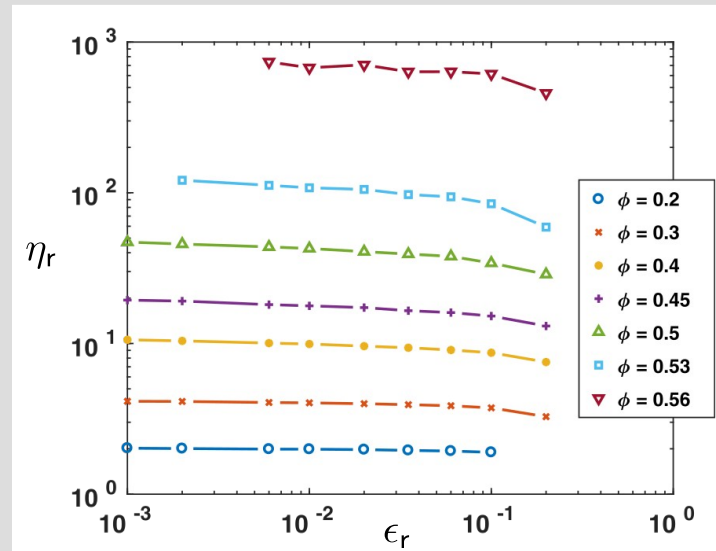
$$\epsilon_r = h_r/a$$

$$\mu_s = 0$$

$$\phi = 0.4$$



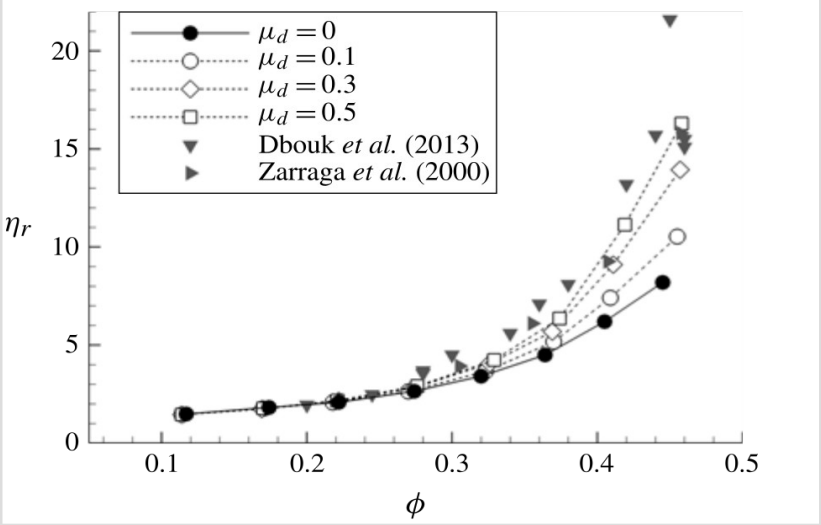
Gallier et al. (2014). J. Fluid Mech.



- h_r as such : weak influence
- $h_r \searrow \Rightarrow$ lubrication \nearrow
 $\Rightarrow \eta_r \nearrow$
- h_r acts as a lubrication cut-off

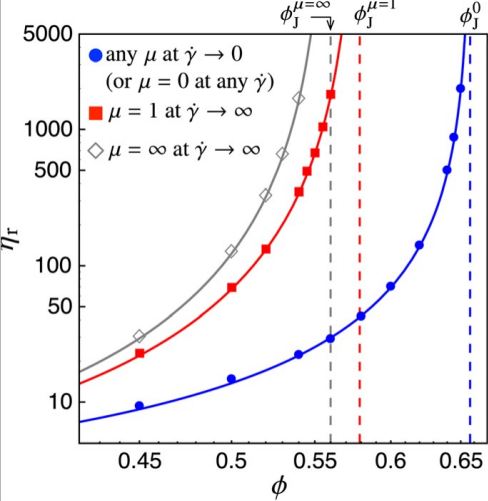
Chevremont et al. (2019). Phys. Rev. Fluids

Friction coefficient



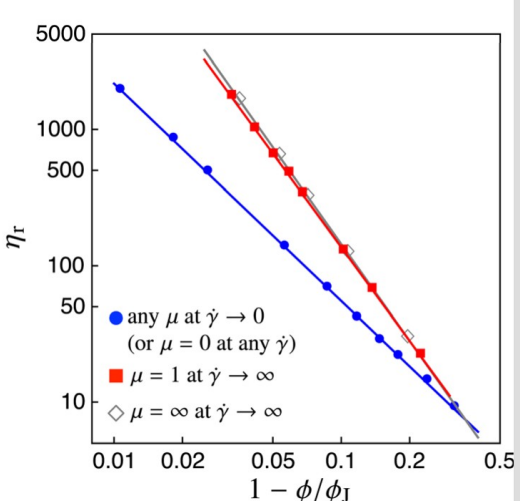
Gallier et al. (2014). J. Fluid Mech.

$$\mu_s = 0, 5 \Rightarrow \eta_r^{\text{simulation}} \approx \eta_r^{\text{exp}}$$



Mari et al. (2014). J. Rheol.

$$\mu_s \nearrow \Rightarrow \phi_J \searrow \Rightarrow \eta_r \nearrow$$

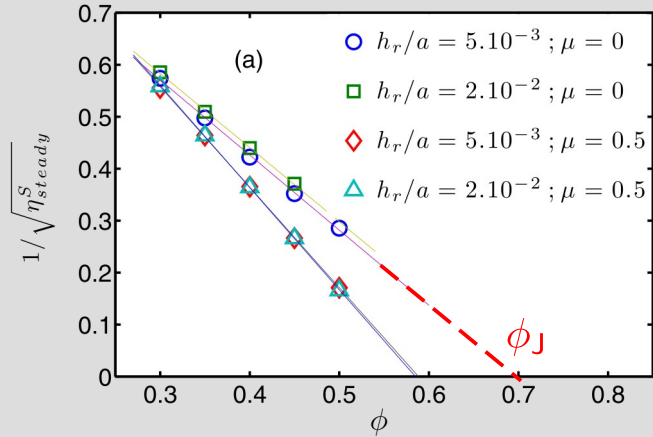


Close to jamming

$$\eta_r(\mu_s = 0) \propto (1 - \phi/\phi_J)^{-1.6} \quad \phi_J \approx 0.66$$

$$\eta_r(\mu_s = 1) \propto (1 - \phi/\phi_J)^{-2.3} \quad \phi_J \approx 0.58$$

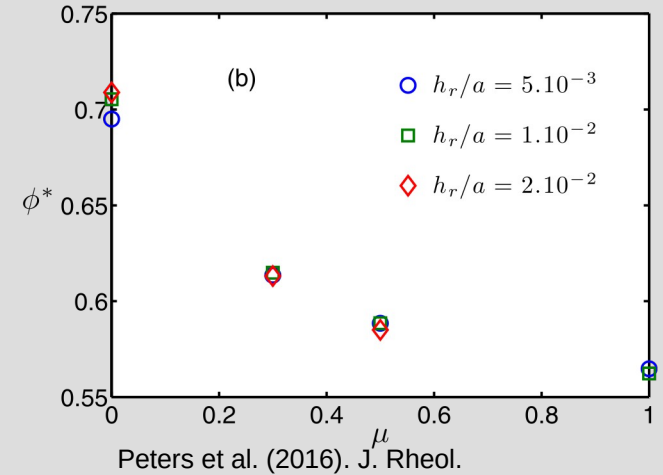
Correlation laws



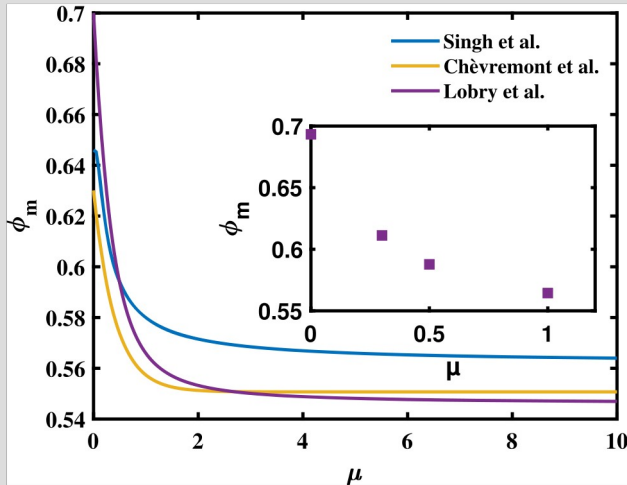
$$\eta_r = \frac{\alpha}{(1 - \phi/\phi_J)^2}$$

Maron-Pierce

- $\mu_s \nearrow \Rightarrow \phi_J \searrow \Rightarrow \eta_r \nearrow$
- $\phi_J(\mu_s = 0) \approx 0.7$ too large



Peters et al. (2016). J. Rheol.

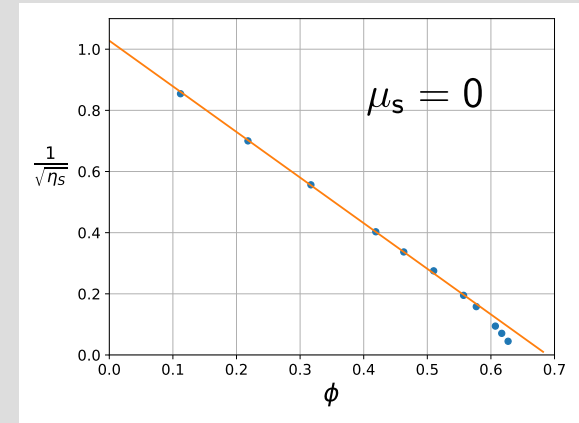


Singh et al. (2018). JOR

Chèvremont et al. (2019). Phys. Rev. Fluids

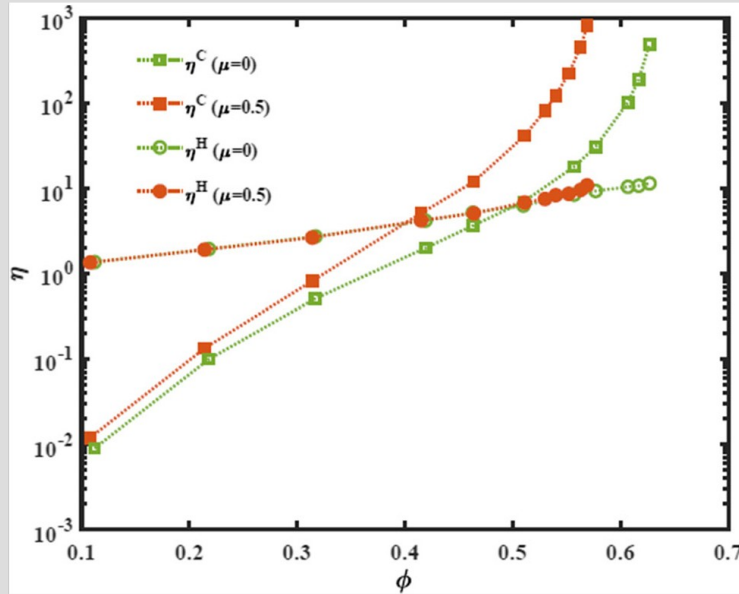
Lobry et al. (2019). JFM

Lemaire et al. (2023) Rheologica Acta



data from Gallier al. (2018). Phys. Rev. Fluids

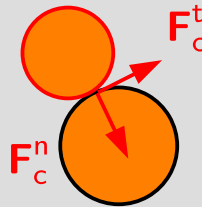
Contact vs. hydrodynamics



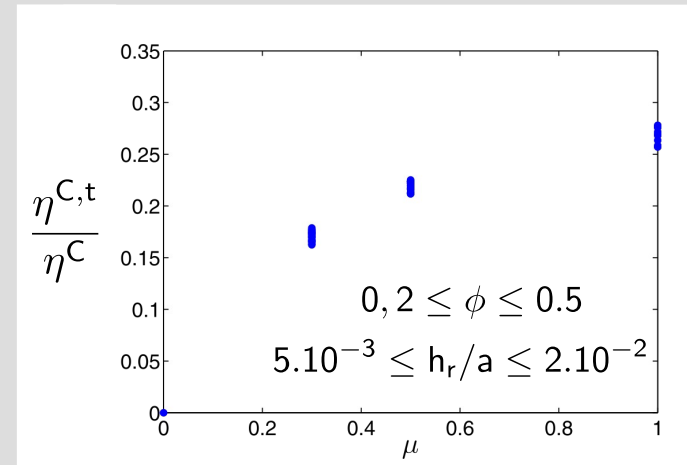
Lemaire et al. (2023). Rheologica Acta.

data from Gallier al. (2018). Phys. Rev. Fluids

- $\mu_s \nearrow \Rightarrow \eta^{C,n} \nearrow$
 $\eta^{C,t} \nearrow$
- $\frac{\eta^{C,t}}{\eta^C} = f(\mu_s)$

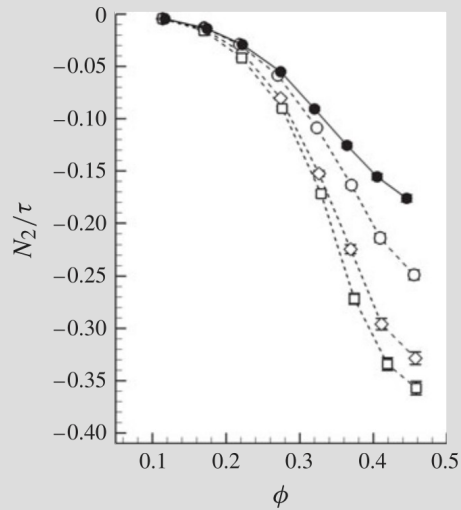
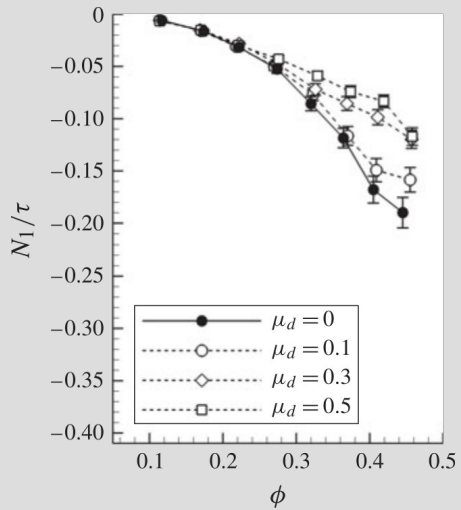


- $\eta^H = f(\phi, \mu_s)$
- $\mu_s \nearrow \Rightarrow \eta^C \nearrow$
- $\mu_s = 0 \quad \eta^c = \eta^h \text{ at } \phi \approx 0.5$
 $\mu_s = 0.5 \quad \eta^c = \eta^h \text{ at } \phi \approx 0.4$



Peters et al. (2016). J. Rheol.

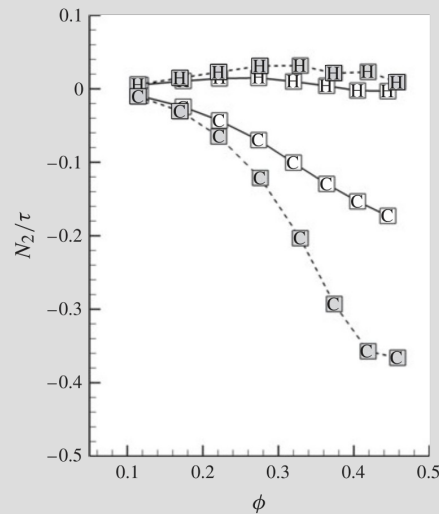
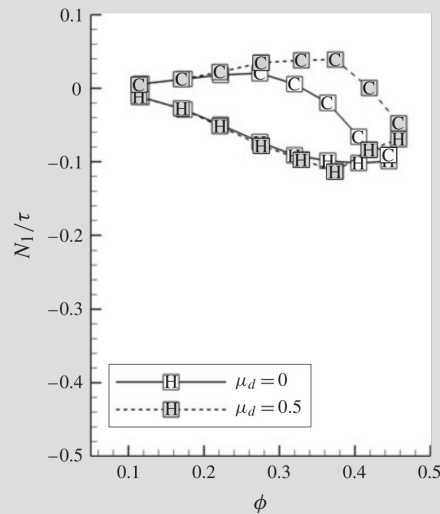
Normal stresses



Gallier et al. (2014). J. Fluid Mech.

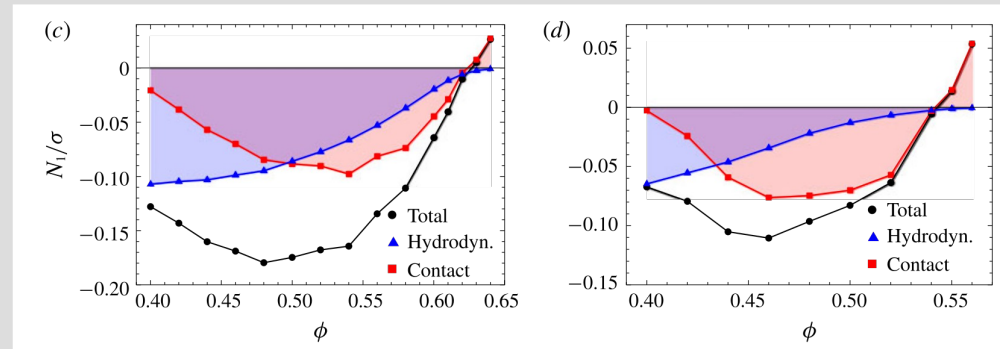
- $\mu_S = 0 \Rightarrow \frac{N_1}{\tau} \approx \frac{N_2}{\tau} \leq 0$
- $\mu_S \nearrow \Rightarrow \left| \frac{N_1}{\tau} \right| \searrow$
- $\mu_S \nearrow \Rightarrow \left| \frac{N_2}{\tau} \right| \nearrow$

Seto & Giusteri (2018). J. Fluid Mech.

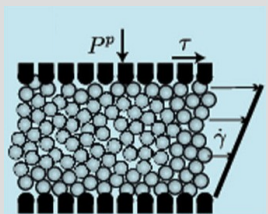


$\mu = 0$

$\mu = 1$

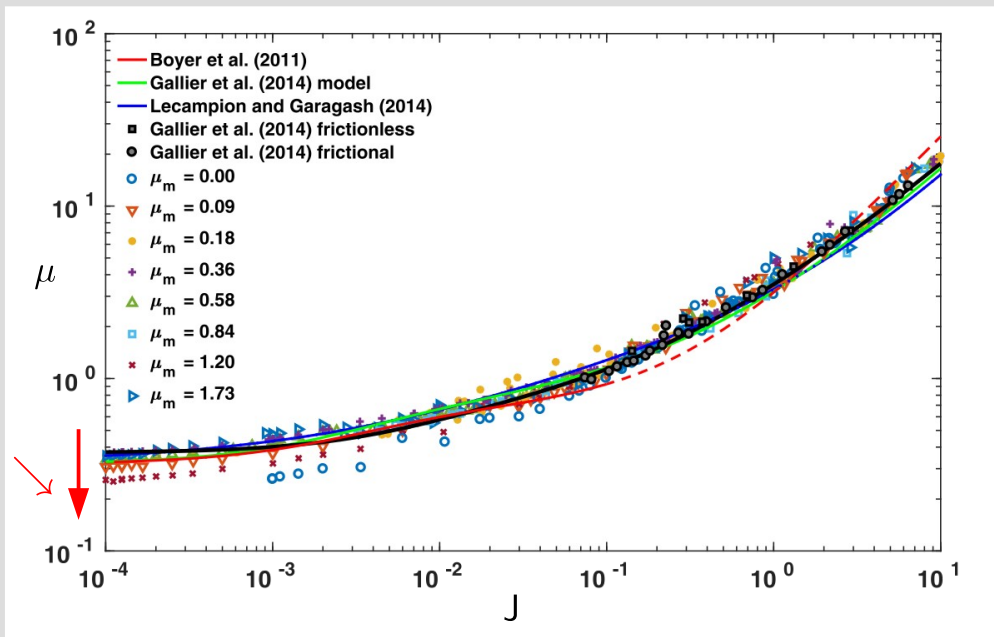


$N_1 > 0$: finite particle stiffness



$$J = \frac{\eta \dot{\gamma}}{\Sigma_{22}^c} \quad \mu = \frac{\Sigma_{12}}{\Sigma_{22}^c} = \mu(J, \mu_s)$$

$$\phi / \phi_J = f(J, \mu_s) \approx f(J)$$



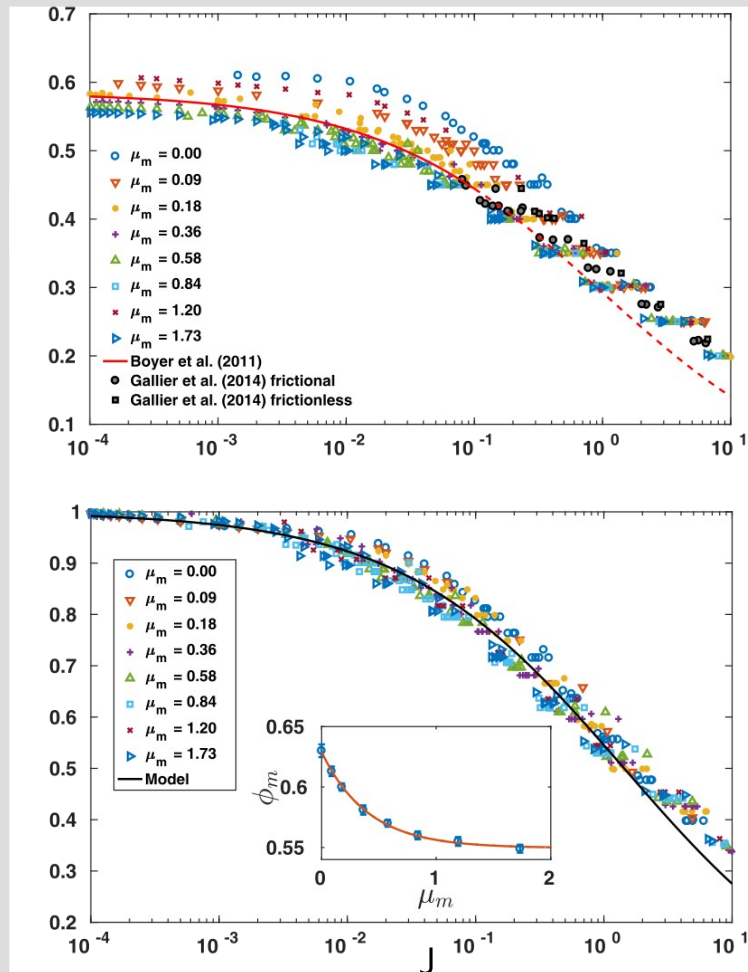
Chevremont et al. (2019). Phys. Rev. Fluids

$\mu_c = \lim_{J \rightarrow 0} \mu \sim 0.3 - 0.4$ Independent of μ_m if $\mu_m \gtrsim 0.3 - 0.4$

$\mu_c(\mu_m = 0) \sim 0.1$

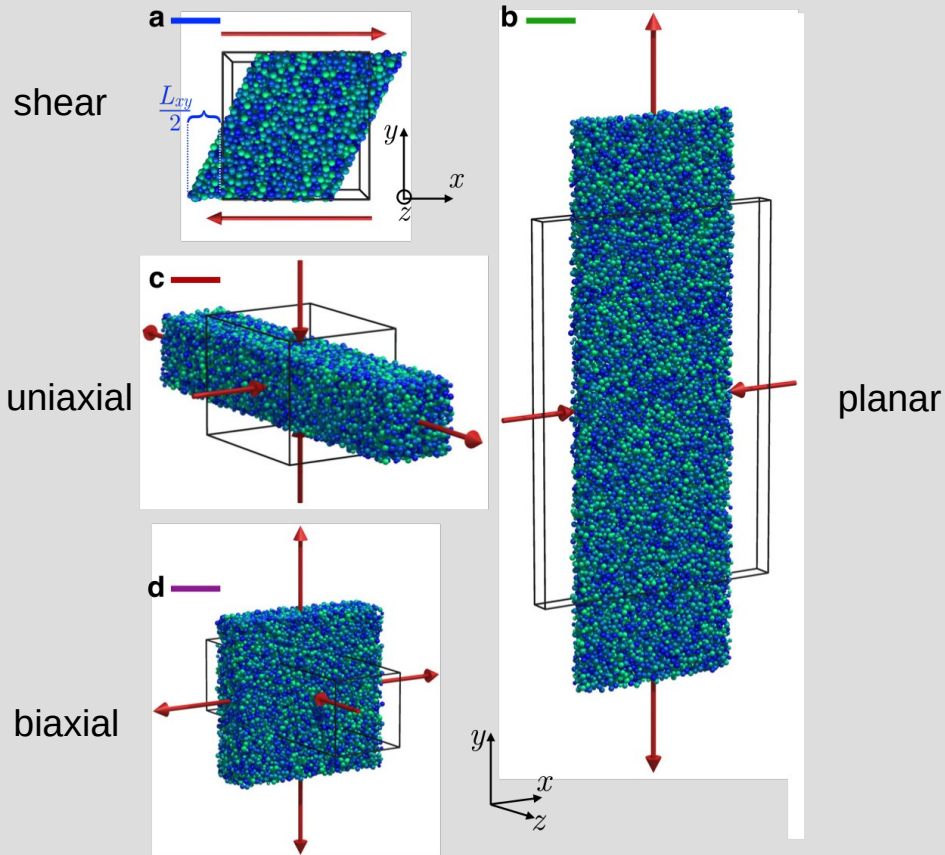
ϕ

ϕ / ϕ_J



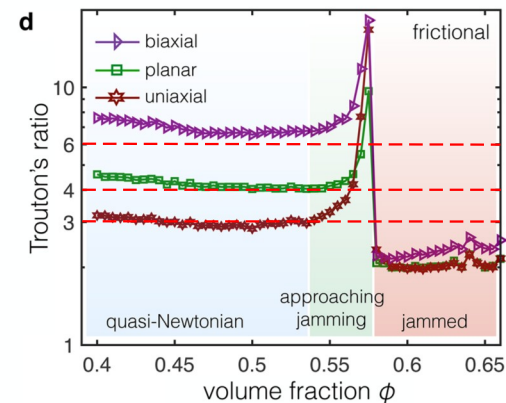
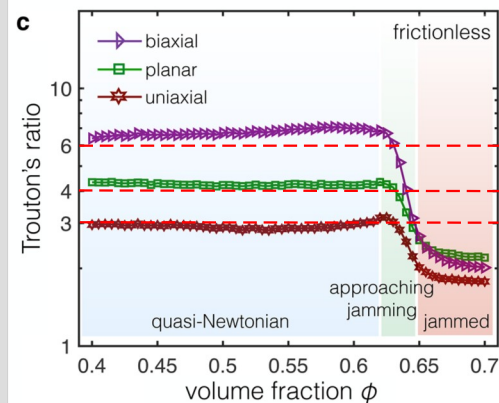
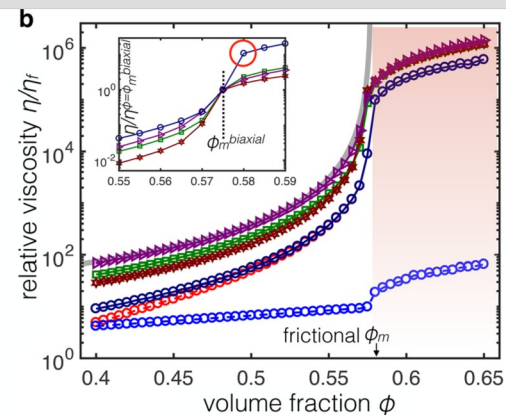
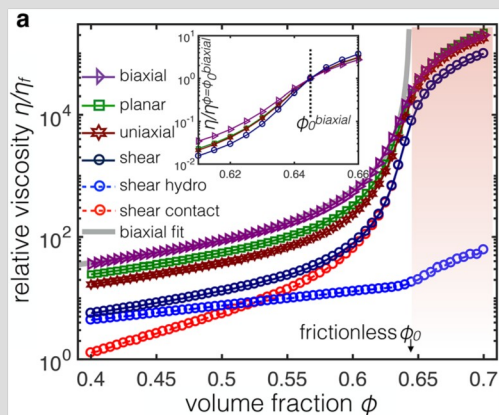
Extensional rheology

Cheal, O., & Ness, C. (2018). J. Rheol.



$$\eta_E = \frac{\Sigma_{\text{ext}} - \Sigma_{\text{dilat}}}{\dot{\epsilon}_{\text{ext}}}$$

Seto



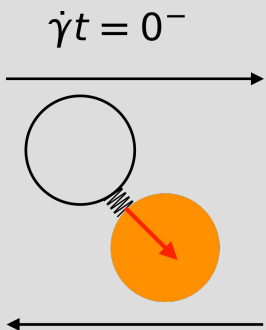
Trouton's ratio

$$\text{Tr} = \frac{\eta_E}{\eta_S}$$

Newtonian ---

Shear reversal

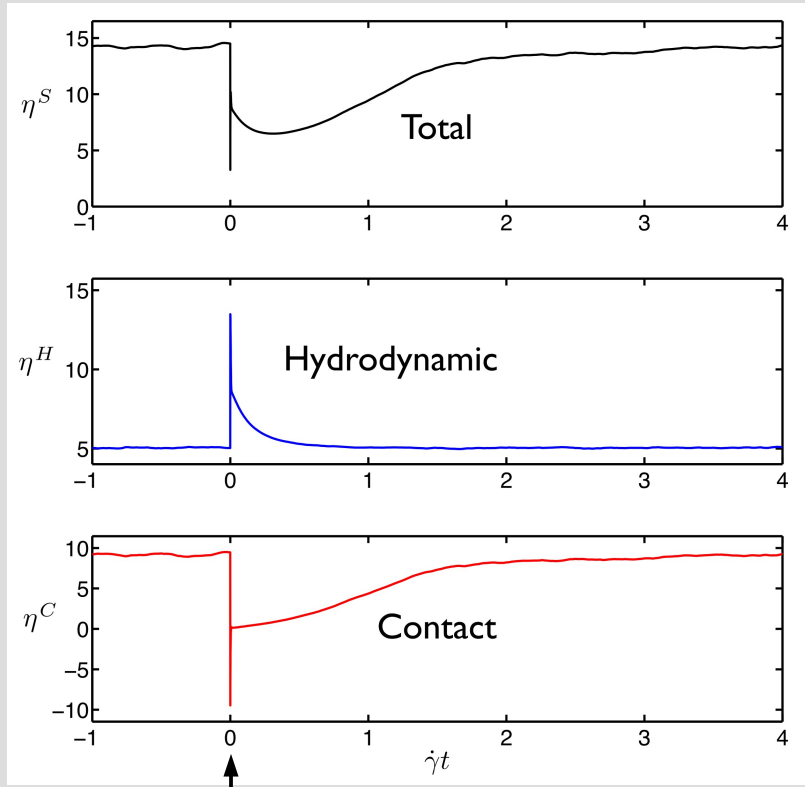
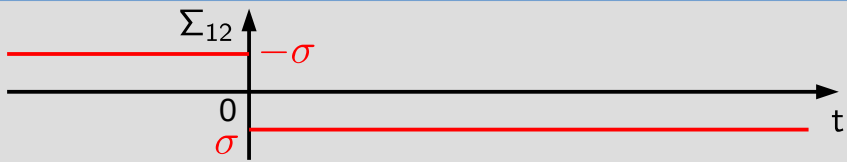
Standard splitting H/C



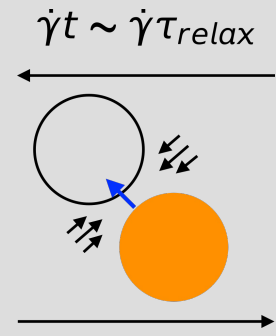
Positive contact contribution

Low lubrication contribution

$\phi = 0.45$
 $h_r/a = 5.10^{-3}$
 $\mu_s = 0.5$



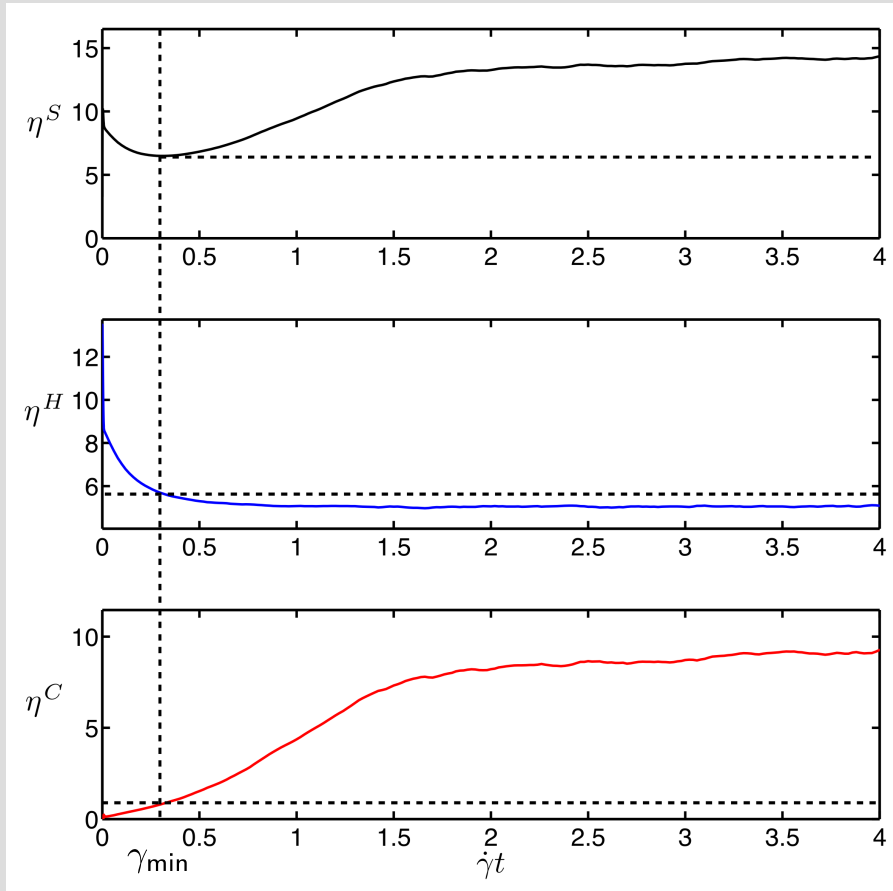
Steady shear | « Slow » transient
 Fast force relaxation



Contact contribution ≈ 0

High and positive lubrication contribution

Shear reversal : measuring η^C



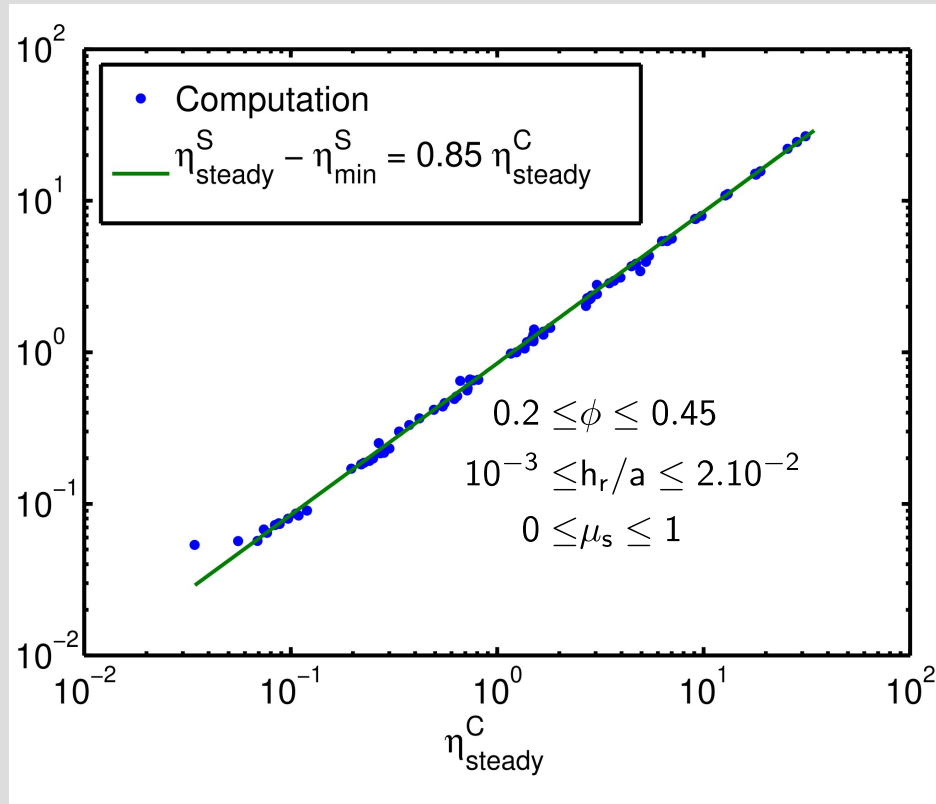
$$\uparrow \eta_{\text{steady}}^S - \eta_{\text{min}}^S$$

$$\gamma = \gamma_{\text{min}} \quad \begin{aligned} \eta^H &\approx \eta_{\text{steady}}^H \\ \eta^C &\approx 0 \end{aligned} \Rightarrow \boxed{\eta_{\text{min}}^S \approx \eta_{\text{steady}}^H}$$

$$\boxed{\eta_{\text{steady}}^S - \eta_{\text{min}}^S \approx \eta_{\text{steady}}^S - \eta_{\text{steady}}^H = \eta_{\text{steady}}^C}$$

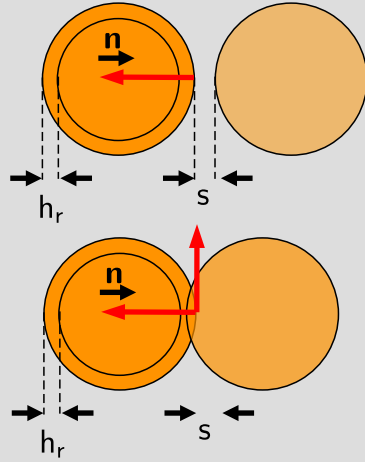
Shear reversal : measuring η^C

$$\eta_{\text{steady}}^S - \eta_{\text{min}}^S = f(\eta_{\text{steady}}^C)$$



Peters et al. (2016) JOR

- Direct interaction forces : short range repulsive + contact



Double layer-like frictionless

$$s > 0 \Rightarrow \mathbf{F}_n = -F^* e^{-\kappa s} \mathbf{n}$$

$$\mathbf{F}_t = 0$$

Contact frictional

$$s < 0 \Rightarrow \mathbf{F}_n = (k_n s - F^*) \mathbf{n}$$

$$\mathbf{F}_t = -k_t \mathcal{Y}$$

→ Sliding criteria

$$\frac{\|\mathbf{F}_t\|}{\|\mathbf{F}_n\| - F^*} \geq \mu_s$$

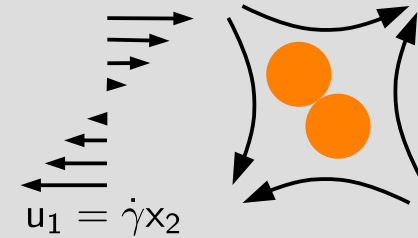
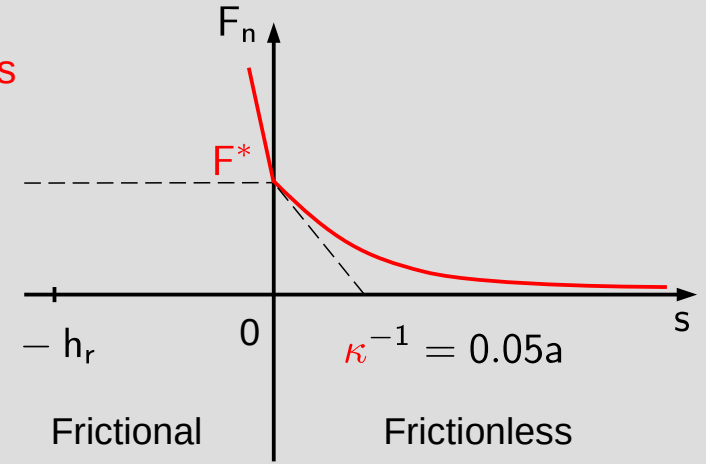
• Stress scale

$$\sigma_0 = \frac{F^*}{6\pi a^2}$$

$$\dot{\gamma}_0 = \frac{\sigma_0}{\eta_0}$$

Contact if $6\pi a^2 \Sigma_{12} \gtrsim F^*$

$$\Sigma_{12} \gtrsim \sigma_0$$

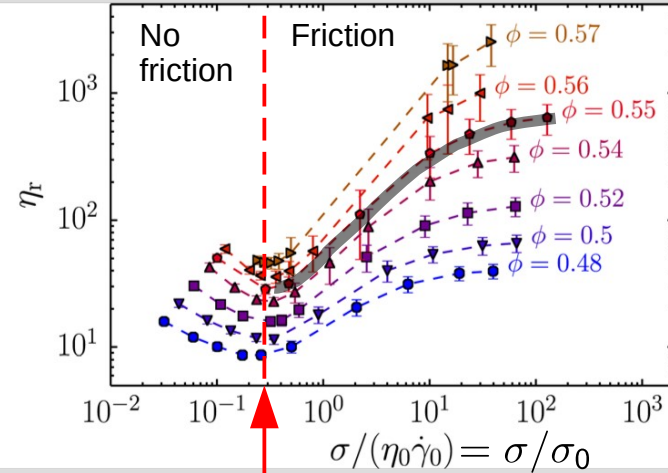
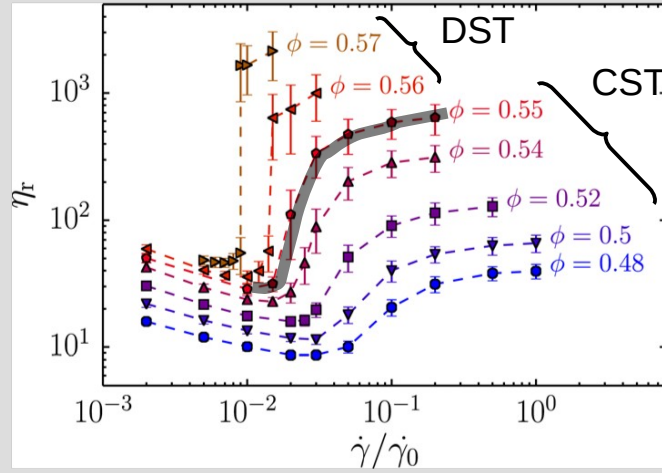
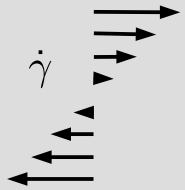


- Roughness = lubrication cut-off $h_r/a = 10^{-3}$

- DEM (high ϕ), bidisperse $a_2/a_1 = 1.4$

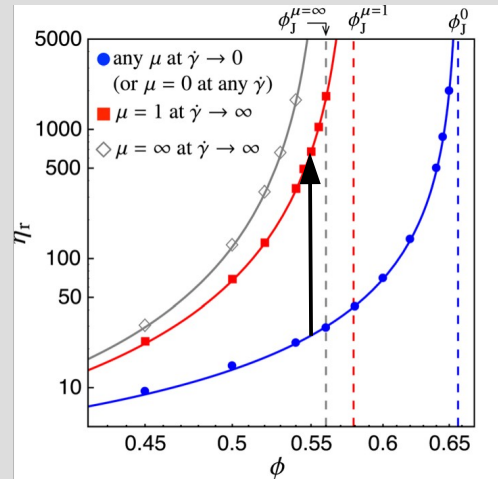
Continuous / discontinuous shear thickening : lubricated to frictional transition

Controlled shear rate

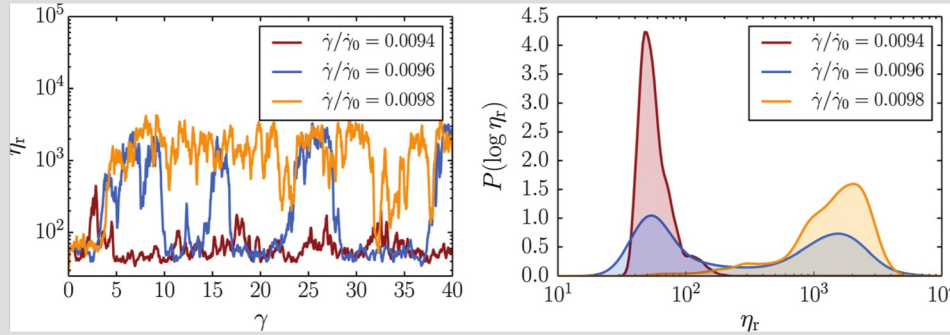


Mari et al. (2014). J. Rheol.

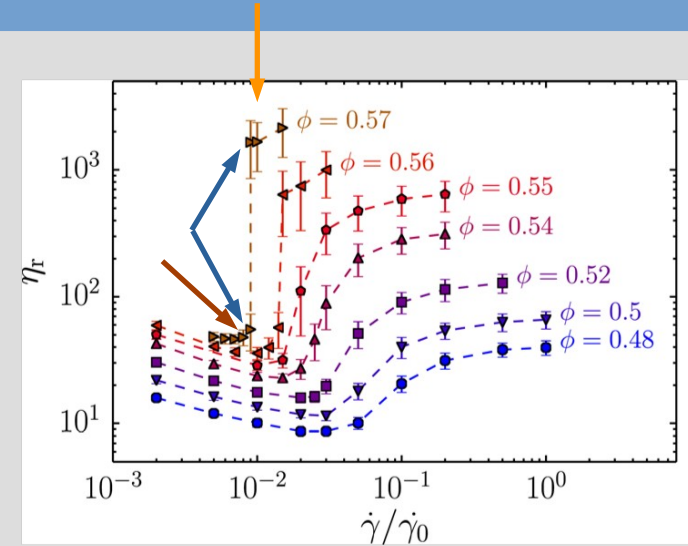
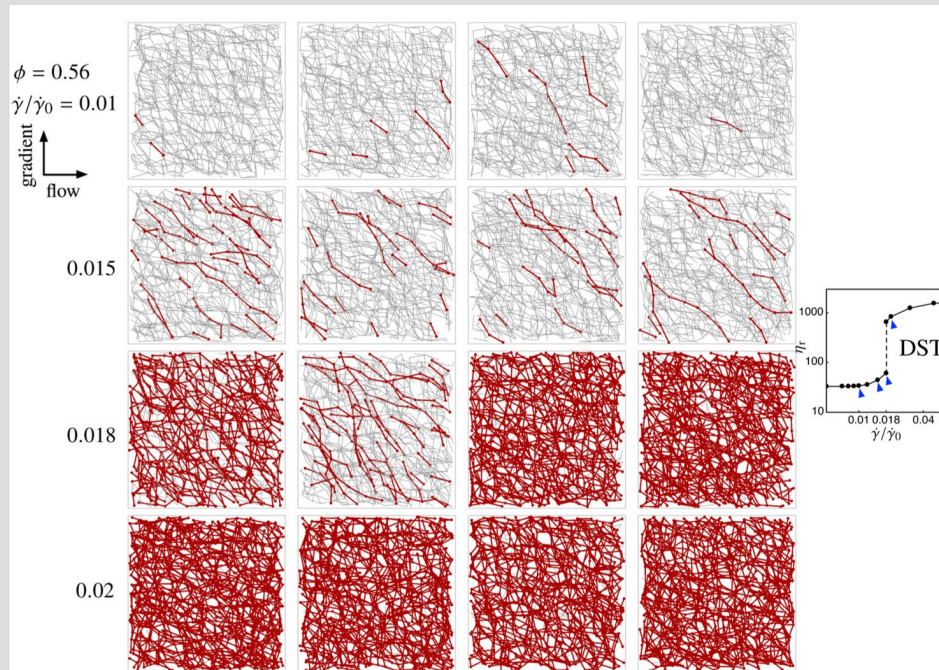
ST inception $\sigma \sim 0.3\sigma_0$



Intermittency in DST transition (controlled rate)

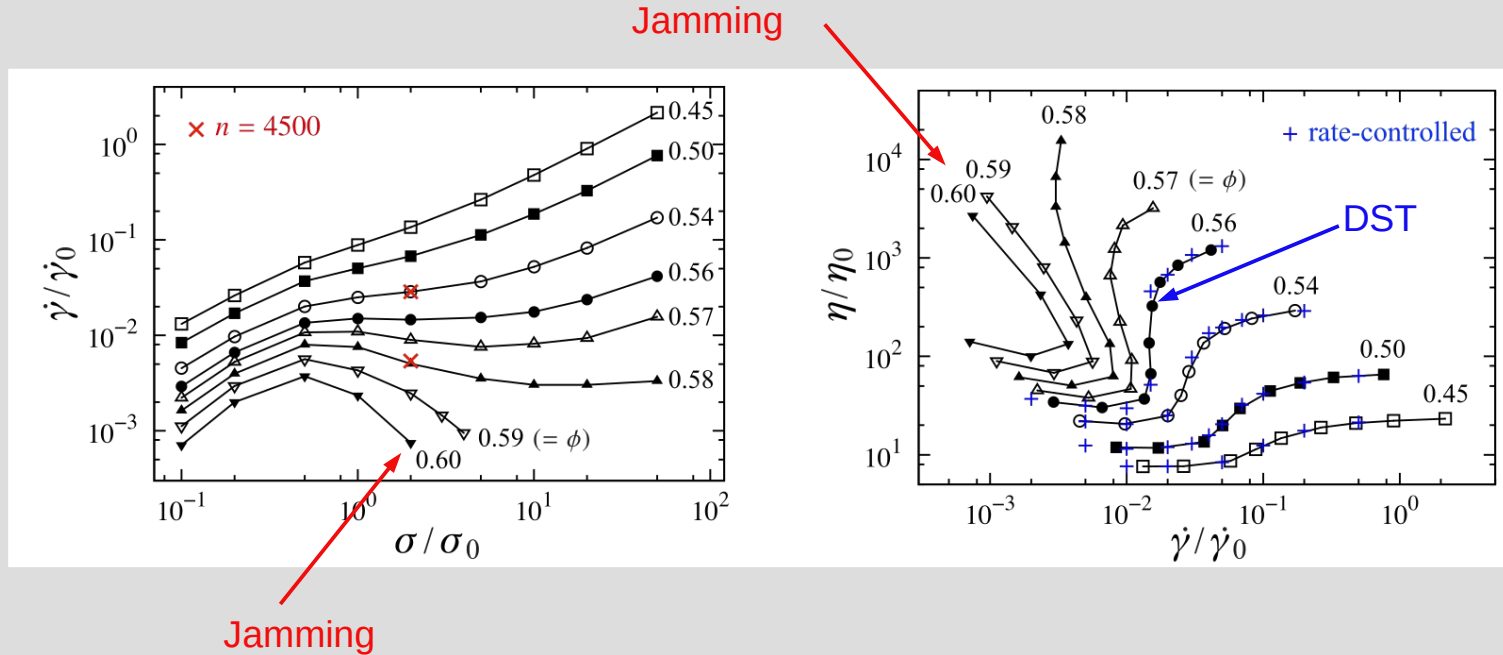


Mari et al. (2014). J. Rheol.



- Intermittency at DST transition (not CST)
- Intermittent contact network
- No influence of the system size

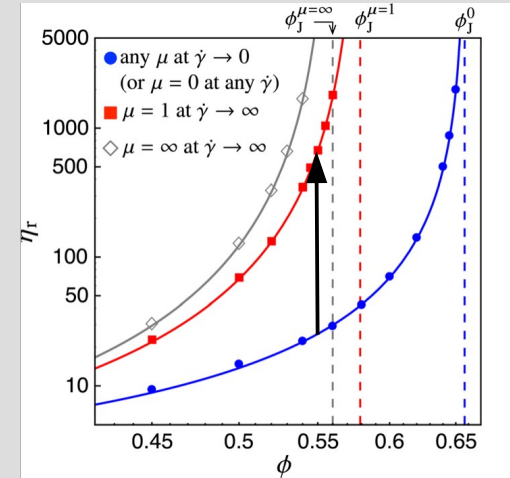
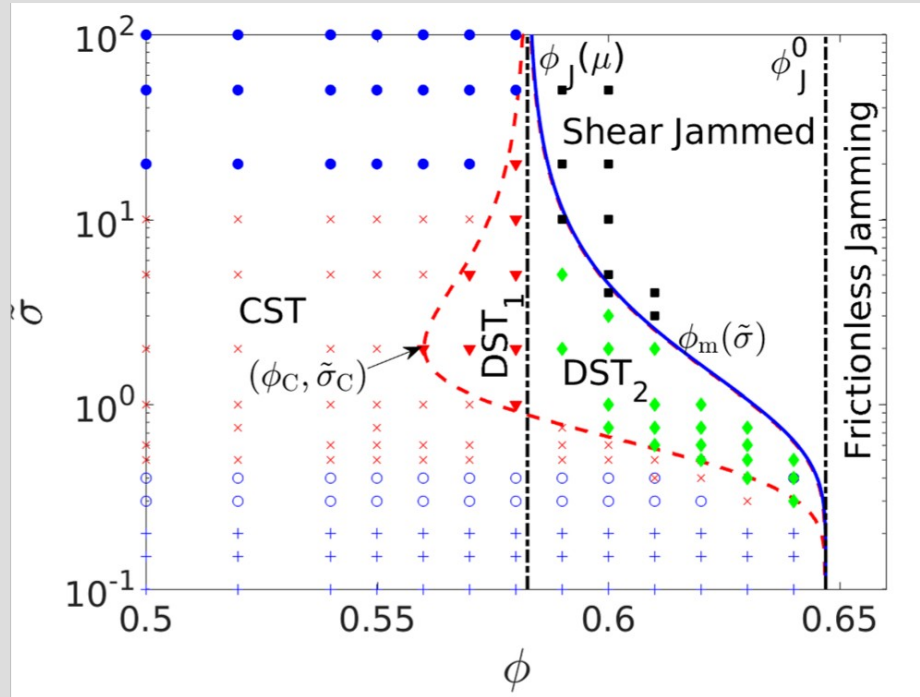
- Controlling stress is easy (using DEM w/o inertia) \implies Mari et al. (2015). Phys. Rev. E.
- S-shape flow curve include DST at controlled rate \implies Wyart & Cates (2014). Phys. Rev. Lett.



- $\phi \leq 0.54$ rate controlled = stress controlled
- $\phi \geq 0.56$ DST in rate controlled
S-shape in stress controlled $\dot{\gamma}(\sigma)$
- $\phi \leq 0.59$ (i.e. $\phi \leq \phi_j^{mu}$) Shear jamming

- Homogeneous shear flow in the S-shape part, no phase separation
- No size effect

Shear thickening suspensions : phase diagram



- + Thinning
- o Frictionless rate independent
- Frictional rate independent
- x CST
- ▼ DST low viscosity \rightarrow high viscosity
- ◆ DST low viscosity \rightarrow shear jammed
- Shear jammed

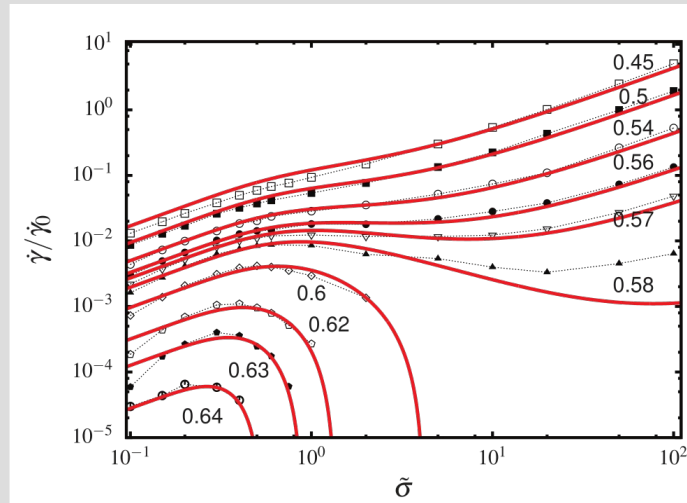
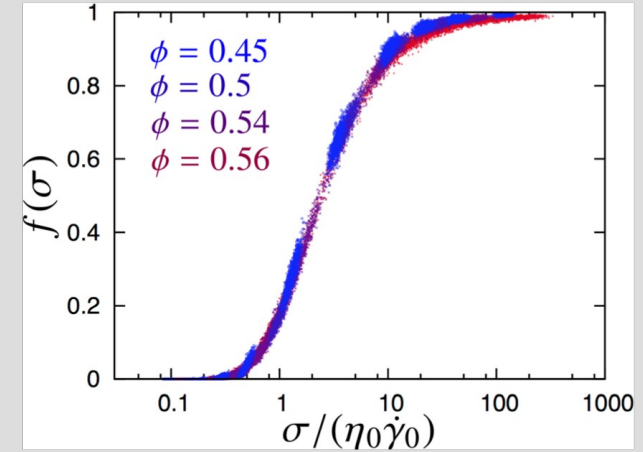
$$\phi_m(\tilde{\sigma}) = f(\tilde{\sigma})\phi_J^\mu + [1 - f(\tilde{\sigma})]\phi_J^0 \quad \text{cf. Wyart \& Cates (2014) PRL}$$

$$\alpha_m(\tilde{\sigma}) = f(\tilde{\sigma})\alpha^\mu + [1 - f(\tilde{\sigma})]\alpha^0$$

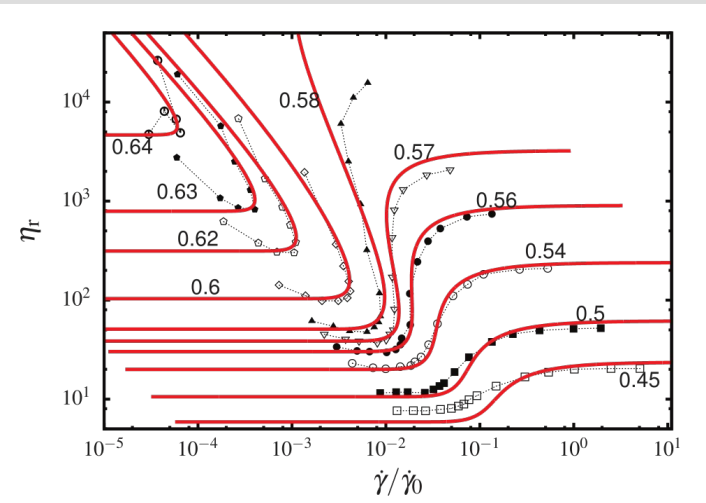
$$f(\tilde{\sigma}) = \exp(-\tilde{\sigma}^*/\tilde{\sigma})$$

$$\eta_r(\phi, \tilde{\sigma}) = \frac{\alpha_m(\tilde{\sigma})}{[\phi_m(\tilde{\sigma}) - \phi]^2}$$

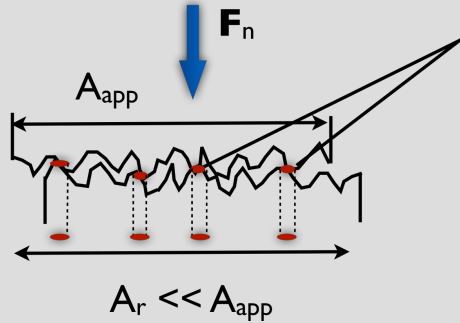
Mari et al (2014) JOR



Singh et al (2018) JOR



- Amontons-Coulomb law : Greenwood & Williamson (1966)

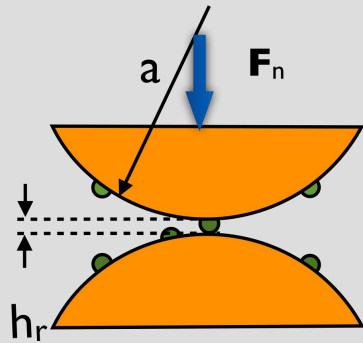


- Statistical distribution of asperity height $\longrightarrow A_r \propto F_n$

- Sliding if $F_t = \sigma_s A_r \propto F_n$

$$\mu = \frac{F_t}{F_n} = \text{constant}$$

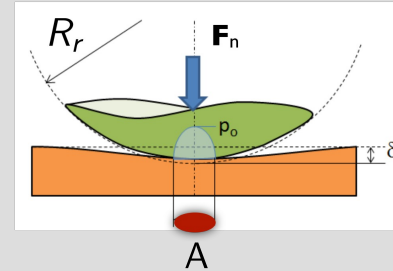
- Single asperity model : a first course



- Elastic regime ($F_n < F_c$) :

Hertz : $A \propto F_n^{2/3}$ $F_t = \sigma_s A \propto F_n^{2/3}$

$$\mu = \frac{F_t}{F_n} \propto F_n^{-1/3}$$



- Plastic regime ($F_n > F_c$) :

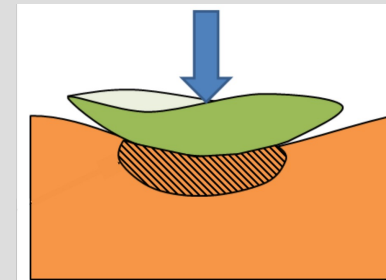
$$F_c \propto \frac{Y^3}{E^2} R_r^2$$

E : Young modulus

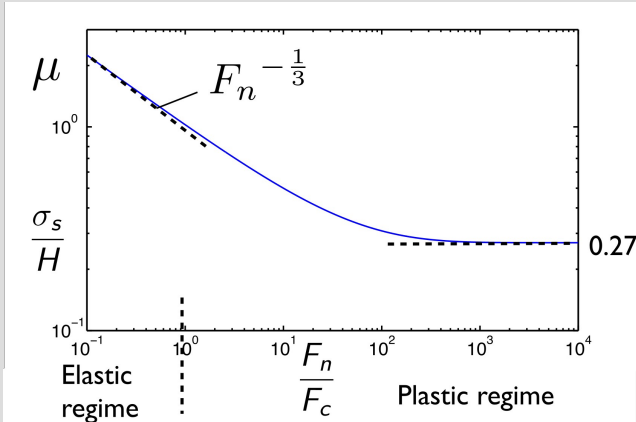
Y : yield strength

$$\bar{p} = \frac{F_n}{A} \longrightarrow H \Rightarrow \mu = \frac{\sigma_s}{H} = \text{constant}$$

H = hardness



Brizmer model of elasto-plastic contact



1

Elastic-plastic contact model



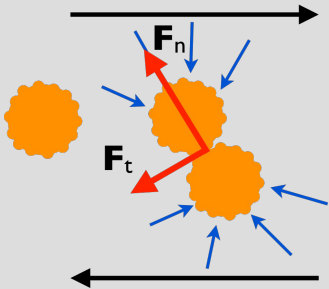
FEM simulations (Brizmer et al. Tribology Letters 2007)

$$\mu = 0.27 \coth \left[0.27 \left(\frac{F_n}{F_c} \right)^{0.35} \right]$$

$$F_c \propto \frac{Y^3}{E^2} R_r^2$$

F_c : force scale for the variation of μ

Stress scale



$$F_n \sim 6\pi a^2 \Sigma \rightarrow \frac{F_n}{F_c} \sim \frac{6\pi a^2 \Sigma}{F_c} = \frac{\Sigma}{\Sigma_c}$$

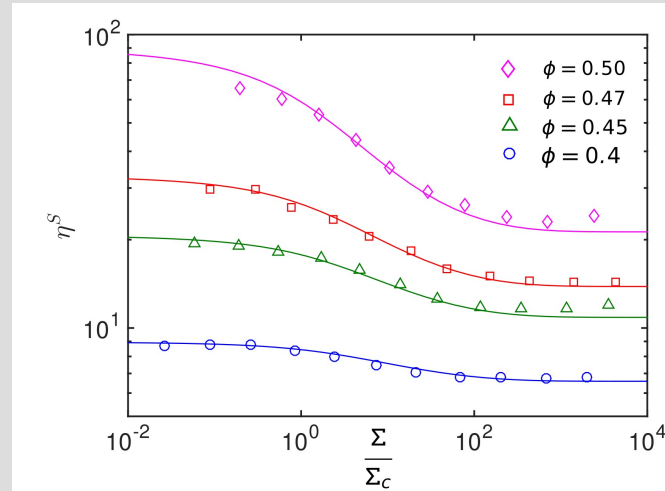
$$\Sigma_c = \frac{F_c a}{6\pi a^2}$$

Simulations and model

$$\frac{\Sigma}{\Sigma_c} \rightarrow 0 \quad \mu \rightarrow \infty$$

$$\eta^s \rightarrow \eta_0^s = \frac{\alpha_0(\mu = \infty)}{\left(1 - \frac{\phi}{\phi_m(\mu = \infty)}\right)^2}$$

$$\phi_m(\mu = \infty) \approx 0.545$$



$$\frac{\Sigma}{\Sigma_c} \rightarrow \infty \quad \mu \rightarrow 0.27$$

$$\eta^s \rightarrow \eta_\infty^s = \frac{\alpha(\mu = 0.27)}{\left(1 - \frac{\phi}{\phi_m(\mu = 0.27)}\right)^2}$$

$$\phi_m(\mu = 0.27) \approx 0.622$$

Simple model $\frac{F_n}{F_c} \sim \frac{\Sigma}{\Sigma_c}$

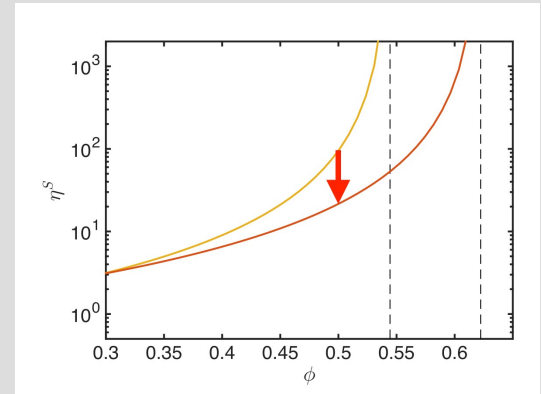
$$\mu^{eff} = 0.27 \coth \left[0.27 \left(a_{fit} \frac{\Sigma}{\Sigma_c} \right)^{0.35} \right] \approx \langle \mu \rangle$$

$$\eta^s \left(\frac{\Sigma}{\Sigma_c}, \phi \right) = \frac{\alpha_0(\mu^{eff})}{\left[1 - \frac{\phi}{\phi_m(\mu^{eff})} \right]^2}$$

$\alpha_0(\mu), \phi_m(\mu) \leftarrow$ Simulations at constant μ

$$a_{fit} = 0.59$$

$$\frac{\bar{F}_n}{F_c} = 0.59 \frac{\Sigma}{\Sigma_c}$$



μ from experiments : Arshad, et al. (2021). Soft Matter

Microscopic measurements

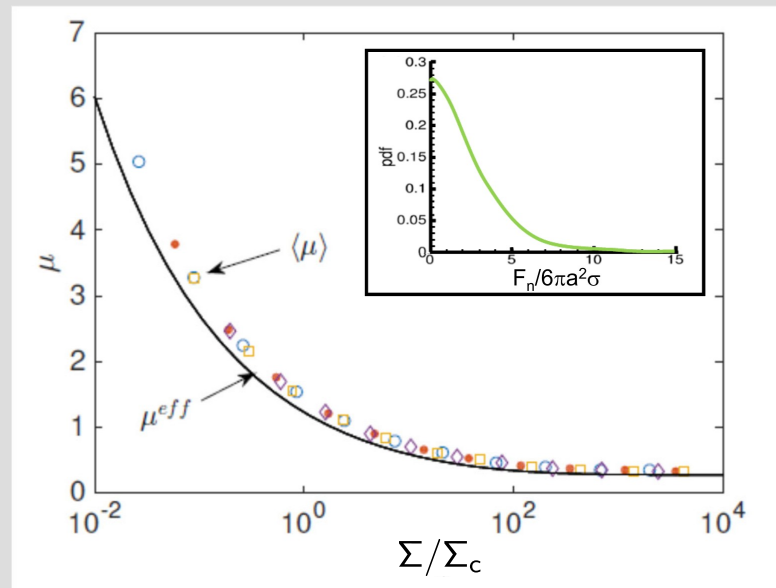
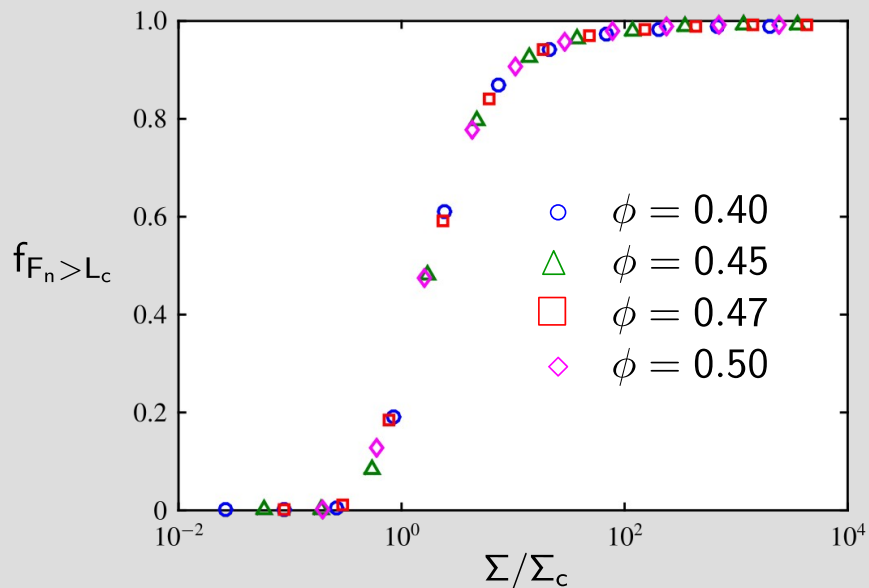
- Mean friction coefficient

Model

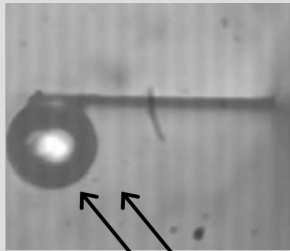
Simulations

$$\mu^{eff} = 0.27 \coth \left[0.27 \left(a_{fit} \frac{\Sigma}{\Sigma_c} \right)^{0.35} \right] \approx \langle \mu \rangle_{\text{contacting particles}}$$

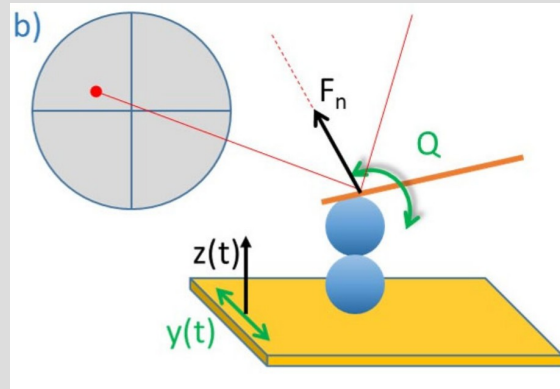
- Fraction of plastic contacts



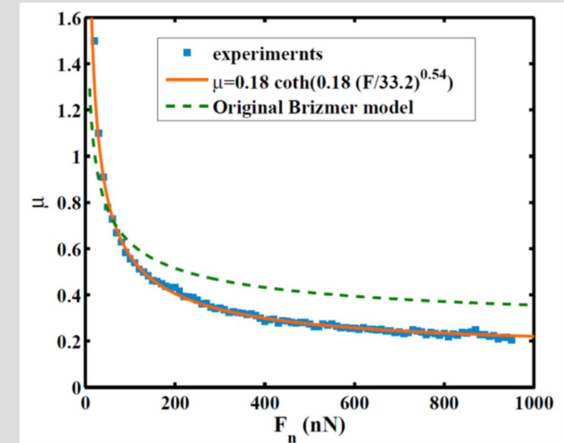
- $\phi = 0.40$
- $\phi = 0.45$
- $\phi = 0.47$
- ◇ $\phi = 0.50$



Polystyrene particle $2a=40\mu\text{m}$
(Dynoseeds TS40)

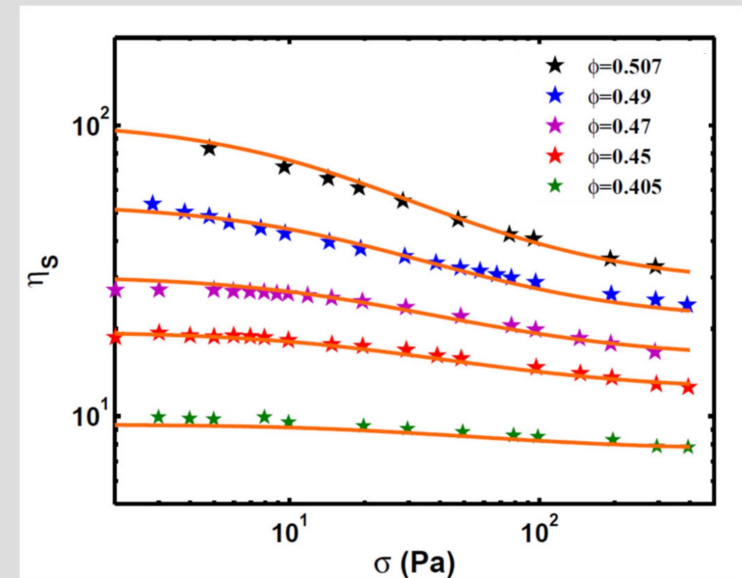


Liquid : water+ Ucon oil



$$\left. \begin{array}{l} \mu(F_N) \text{ or } \mu(\sigma) \\ + \\ \eta_s(\mu) \end{array} \right\} \rightarrow \eta_s(\sigma)$$

Lobry et al. JFM 2019



- Not enough time to talk about :
 - Heterogeneous flows (migration / sedimentation, resuspension)
 - Other interactions (adhesion, rolling friction...).
- Primary interest : microscopic measurements (AFM, SFA) for relevant modelling
- Beyond rigid particles ? Very soft particles, elasto-hydrodynamics ...

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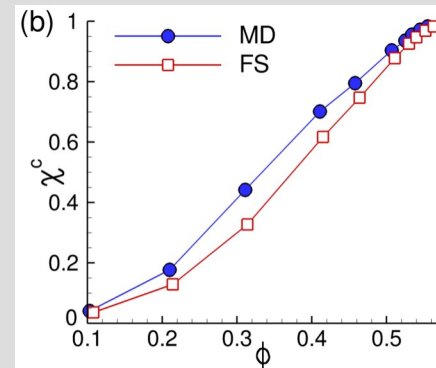
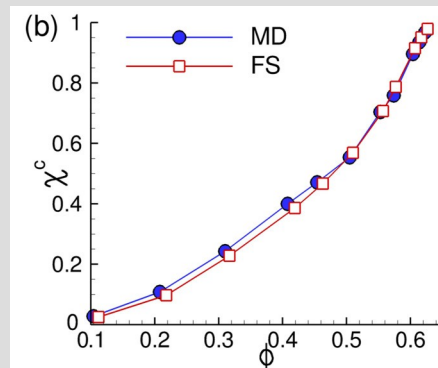
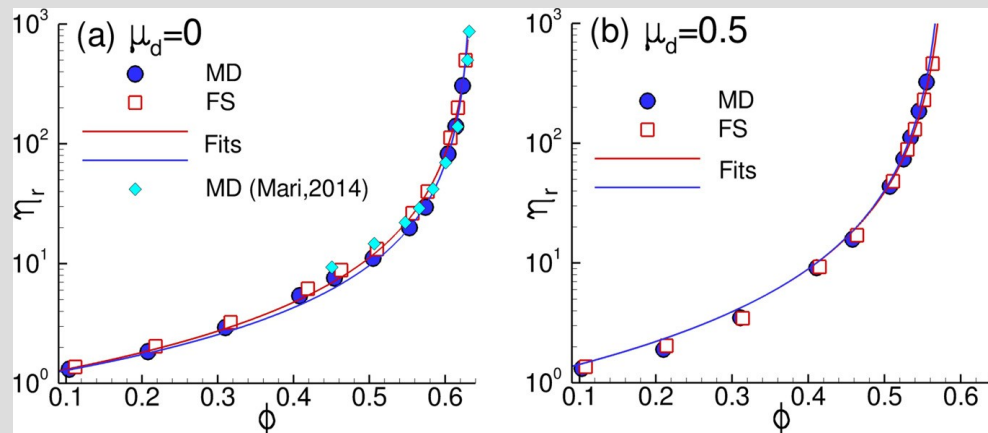
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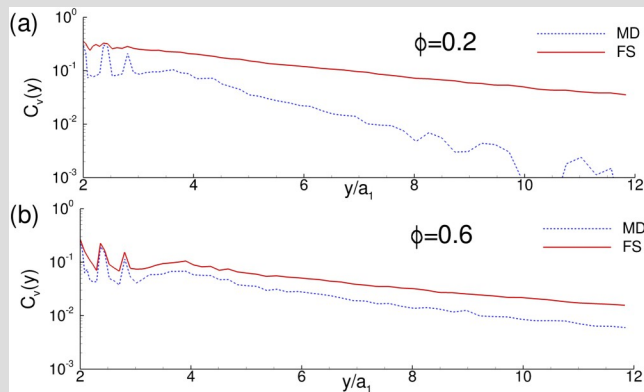
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Long range hydrodynamic interactions ?



Gallier et al. (2018). Phys. Rev. Fluids



Moments de la contrainte

Force totale sur la sphère

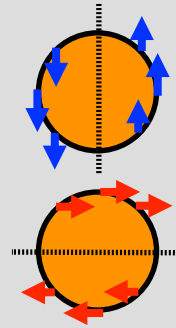
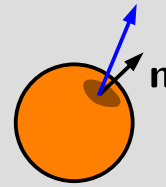
$$\vec{F} = \iint_{(\partial\Omega)} \vec{\sigma} \cdot \vec{n} dS = 0 \quad \Sigma = \sigma \cdot n dS$$

Couple total sur la sphère

$$\vec{T} = \iint_{(\partial\Omega)} \vec{r} \times \vec{\sigma} \cdot \vec{n} dS = 0$$

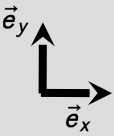
$$T_z = \iint_{(\partial\Omega)} (\Sigma_y x - \Sigma_x y) dS = 0$$

$$T_z = D_{yx} - D_{xy}$$



$$D_{yx} = \iint_{(\partial\Omega)} \Sigma_y x dS \neq 0$$

$$D_{xy} = \iint_{(\partial\Omega)} \Sigma_x y dS \neq 0$$



D_{xy} et D_{yz} considérés séparément : efficacité de la distribution de contrainte pour cisailer la particule

Moment d'ordre 2 de la distribution de contrainte = moment **dipolaire** (de force)

$$D_{ij} = \iint_{(\partial\Omega)} \sigma_{ik} n_k x_j dS$$

$$\bar{D} = \iint_{(\partial\Omega)} (\vec{\sigma} \cdot \vec{n}) \vec{x} dS$$

9 composantes

$$\bar{D} = \bar{S} + \bar{T}$$

$$T_{ij} = \frac{1}{2} \iint_{(\partial\Omega)} [\sigma_{ik} n_k x_j - \sigma_{jk} n_k x_i] dS$$

$$\bar{T} = \frac{1}{2} \iint_{(\partial\Omega)} [(\vec{\sigma} \cdot \vec{n}) \vec{x} - \vec{x} (\vec{\sigma} \cdot \vec{n})] dS$$

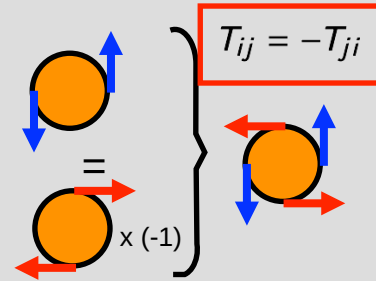
Rotlet

$$S_{ij} = \frac{1}{2} \iint_{(\partial\Omega)} [\sigma_{ik} n_k x_j + \sigma_{jk} n_k x_i] dS$$

$$\bar{S} = \frac{1}{2} \iint_{(\partial\Omega)} [(\vec{\sigma} \cdot \vec{n}) \vec{x} + \vec{x} (\vec{\sigma} \cdot \vec{n})] dS$$

Stresslet

Partie anti-symétrique
 \iff
 couple sur la particule



Partie symétrique

