Anisotropy of sheared dense suspensions: normal stress differences and microstructure

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Seto and Giusteri, arXiv:1806.09423

科研費
KAKENHI

Newtonian fluids…



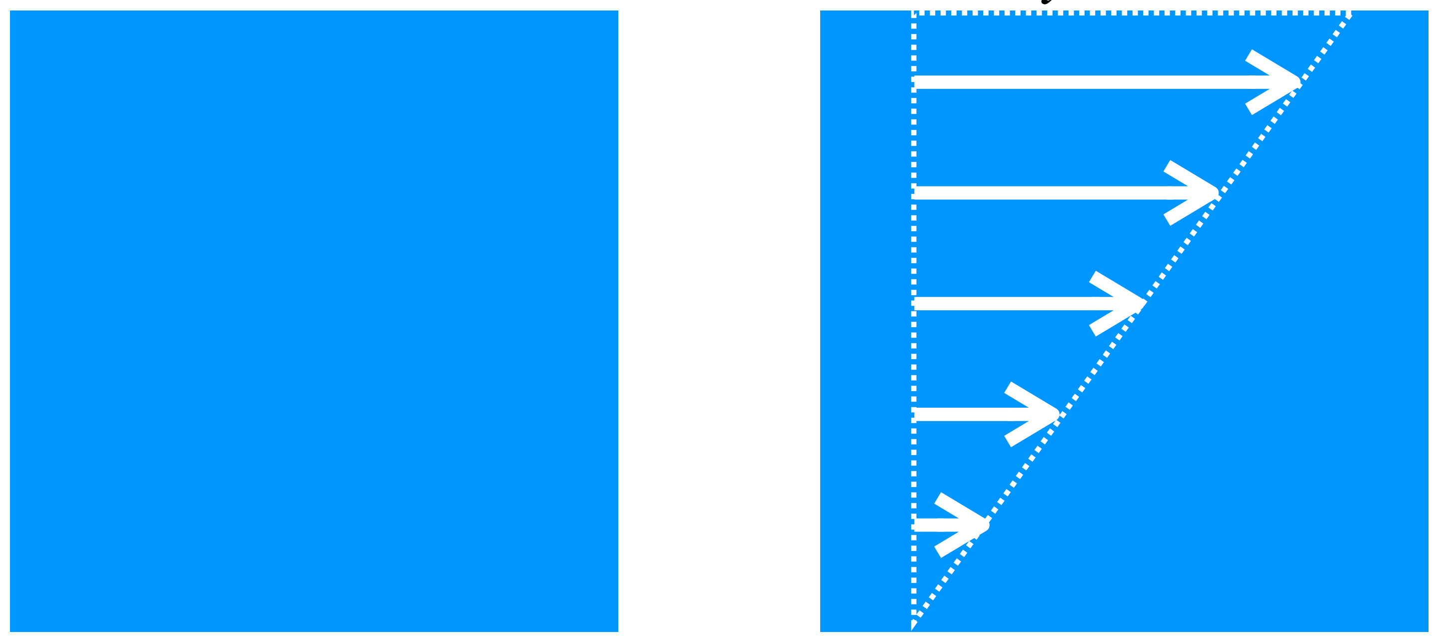


$$\rho \left[\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} \right] = \nabla \cdot \boldsymbol{\sigma} \textbf{ with } \nabla \cdot \boldsymbol{u} = 0$$

$$\boldsymbol{\sigma} = -p\mathrm{I} + 2\eta \mathsf{D} \qquad \mathsf{D} \equiv \frac{1}{2}\left(\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^{\top} \right)$$

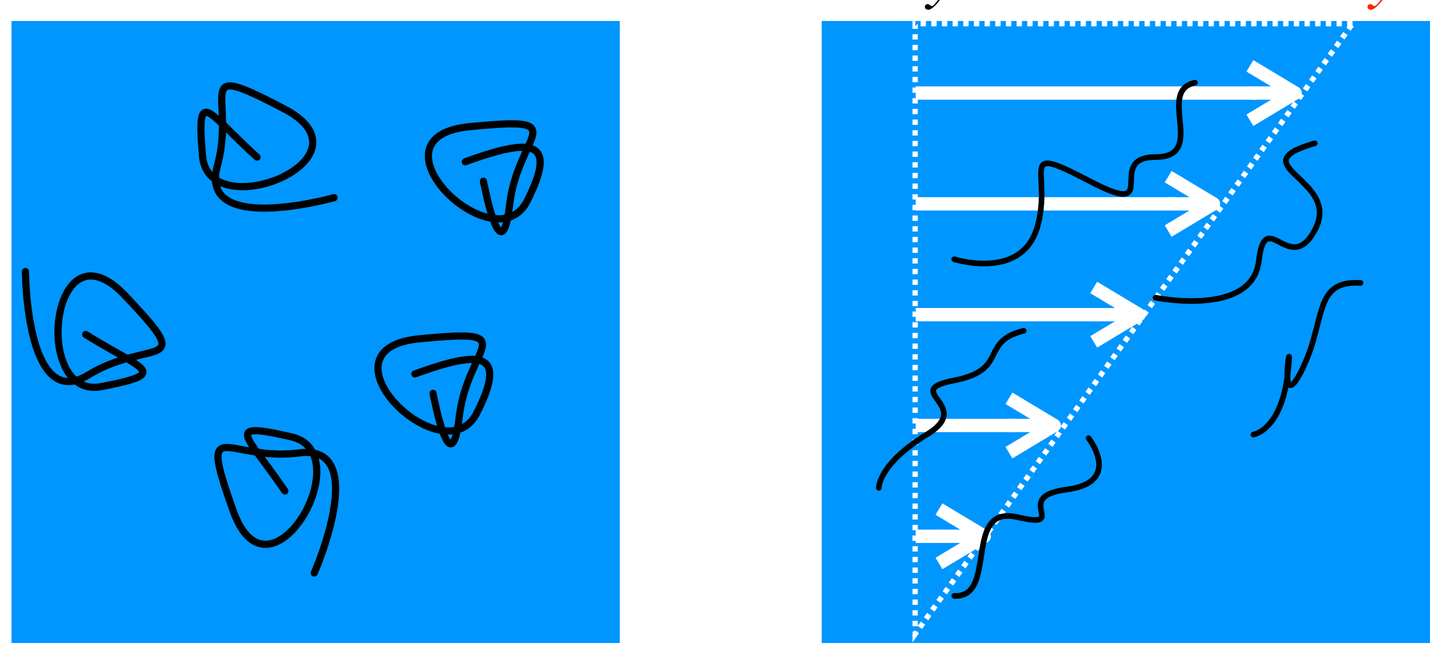
Newtonian liquid

$$\sigma_{xy} = \eta\dot{\gamma}$$

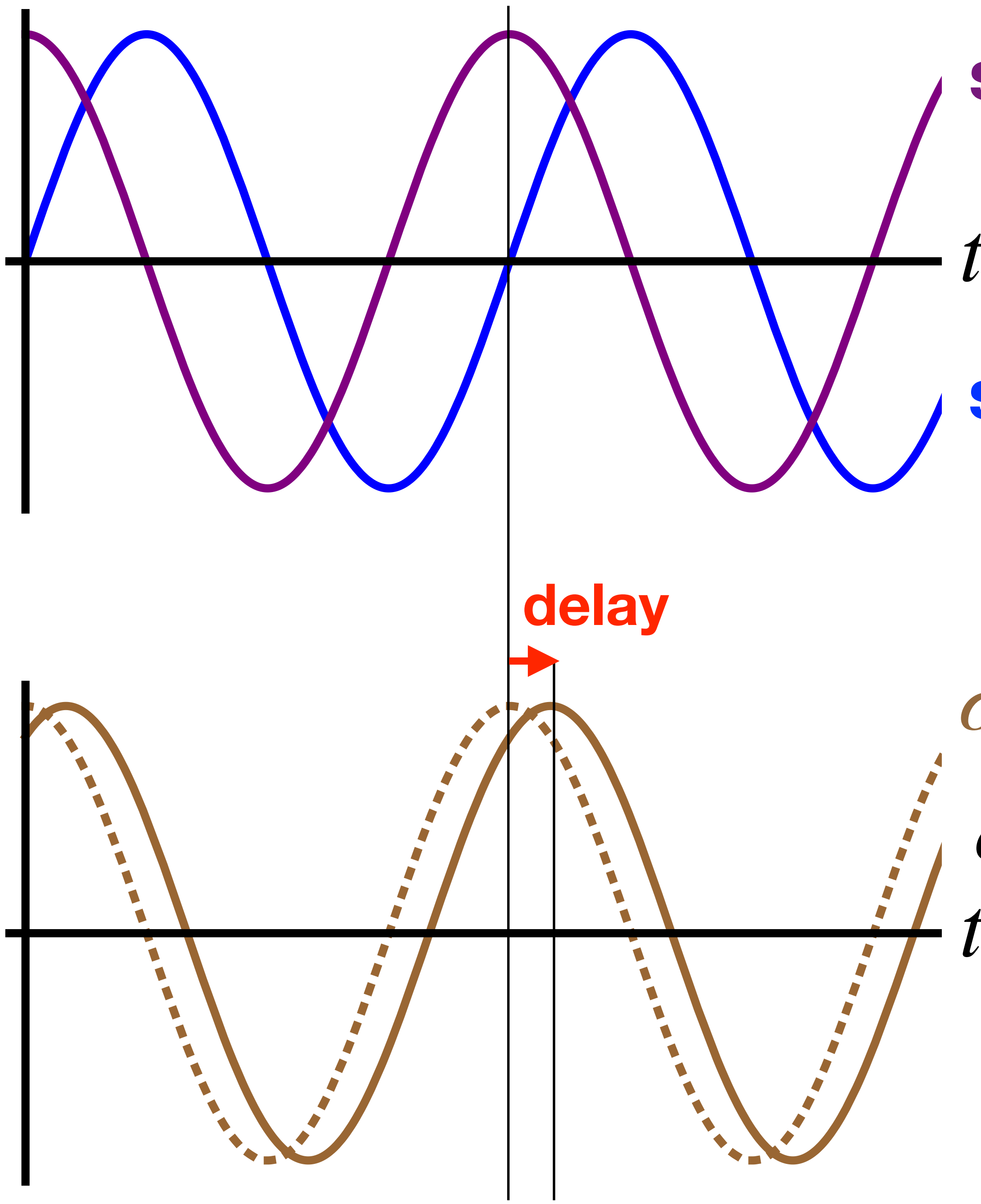


Newtonian liquid
+ elastic chains

$$\sigma_{xy} = \eta\dot{\gamma} + \tau_{xy}$$



Oscillatory rheology



shear rate $\dot{\gamma}(t) = \cos \omega t$

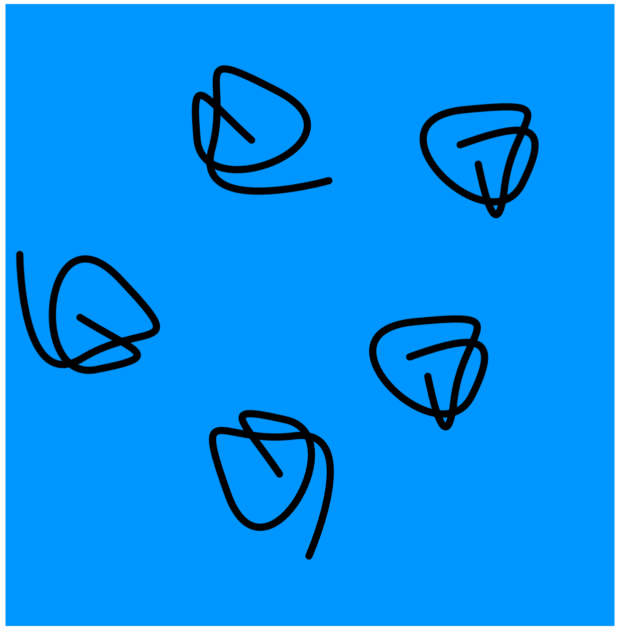
shear strain $\gamma(t) = \sin \omega t$

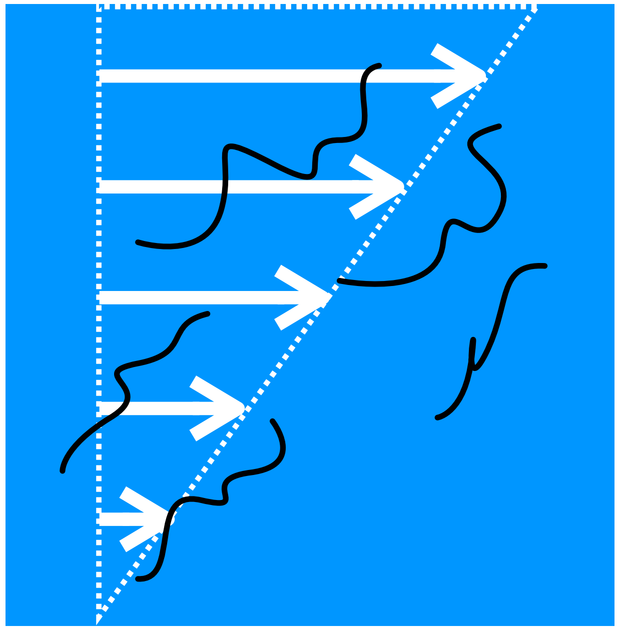
$\sigma_{xy}(t) = \eta \dot{\gamma}(t)$ **viscous**

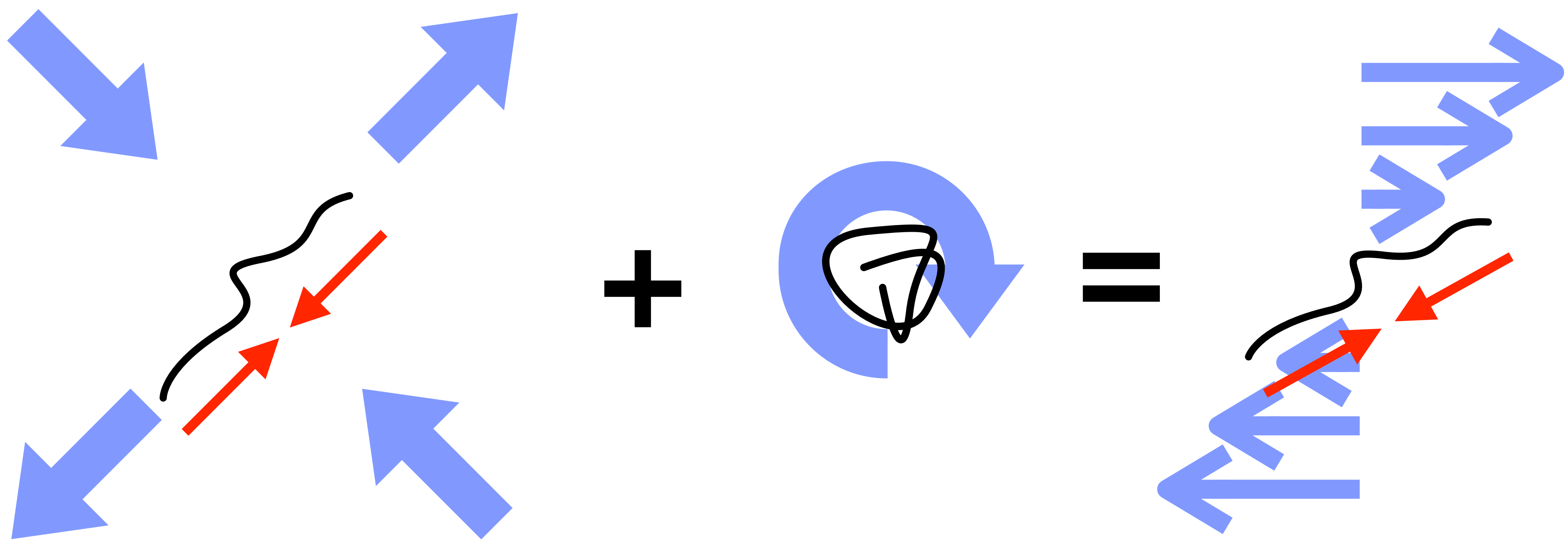
$\sigma_{xy}(t) = \eta \dot{\gamma}(t) + \tau_{xy}(t)$ **viscoelastic**

Can we distinguish them by ***steady shear*** rheology?

$$\sigma_{xy} = \eta\dot{\gamma} + \tau_{xy}$$







Stress "tensor" (not only σ_{xy})

$$\boldsymbol{\sigma} = -p\mathrm{I} + 2\eta\mathrm{D} + \boldsymbol{\tau}_{\mathrm{elastic}}$$

$$\sigma_{xx} > \sigma_{yy}$$

i.e. $N_1 \equiv \sigma_{xx} - \sigma_{yy} > 0$

note: Contributions from stretched chains are positive: $\sigma_{xx} > 0,\ \sigma_{yy} > 0$

Viscometric functions

simple shear flow → **stress tensor**

$$\nabla \boldsymbol{u} = \begin{pmatrix} 0 & \dot{\gamma} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \mathsf{D} + \mathsf{W}$$

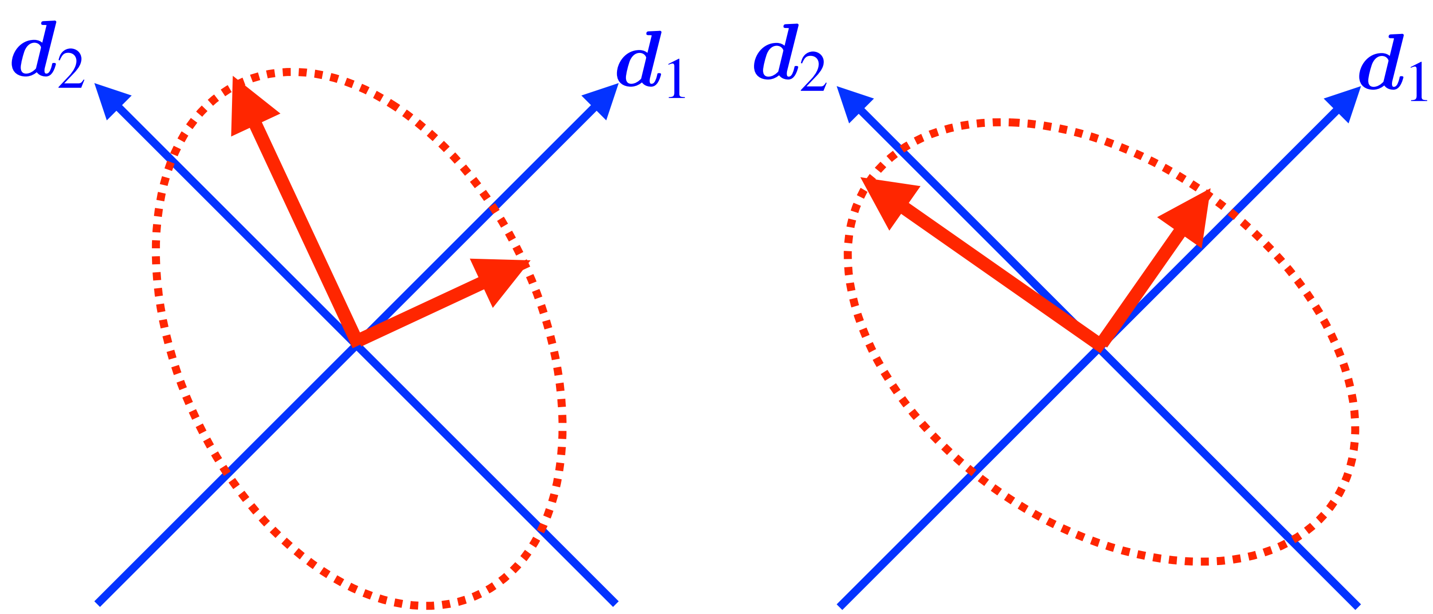
$$\mathsf{D} = \begin{pmatrix} 0 & \dot{\gamma}/2 & 0 \\ \dot{\gamma}/2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \mathsf{W} = \begin{pmatrix} 0 & \dot{\gamma}/2 & 0 \\ -\dot{\gamma}/2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ \sigma_{xy} & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$$

viscometric functions

$$\begin{cases} \eta \equiv \sigma_{xy}/\dot{\gamma} \\ N_1 \equiv \sigma_{xx} - \sigma_{yy} \\ N_2 \equiv \sigma_{yy} - \sigma_{zz} \end{cases}$$

$$p \equiv -\frac{1}{3}\mathrm{Tr}\,\boldsymbol{\sigma}$$



$N_1 > 0$ $\qquad$ $N_1 < 0$

Characterization with different flows

(Fluids may behave differently in different flows)

planar extensional flow → **stress tensor**

$$\nabla \boldsymbol{u} = \begin{pmatrix} \dot{\varepsilon} & 0 & 0 \\ 0 & -\dot{\varepsilon} & 0 \\ 0 & 0 & 0 \end{pmatrix} = \mathrm{D}$$

$$\boldsymbol{\sigma} = \begin{pmatrix} -p+A & 0 & 0 \\ 0 & -p+B & 0 \\ 0 & 0 & -p-(A+B) \end{pmatrix}$$

2 components:
viscosity
+ anisotropy due to the planarity of the flow

uniaxial extensional flow → **stress tensor**

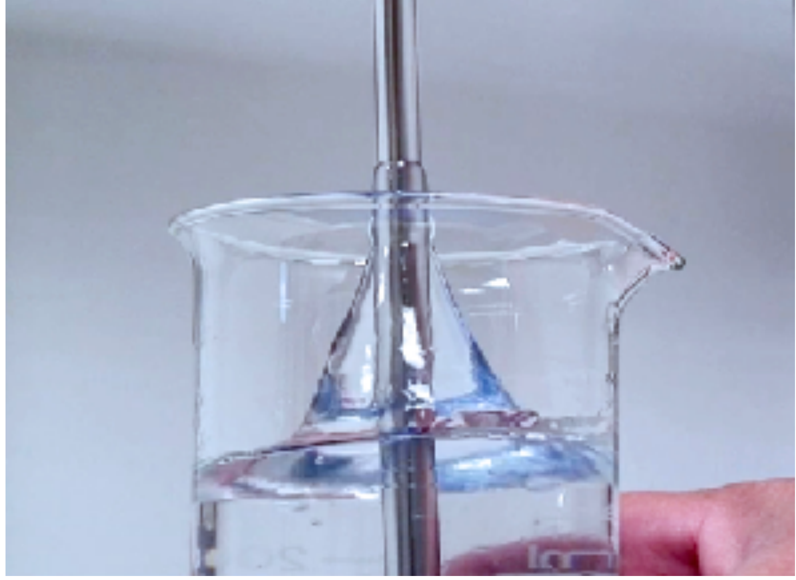
$$\nabla \boldsymbol{u} = \begin{pmatrix} -\dot{\varepsilon}/2 & 0 & 0 \\ 0 & -\dot{\varepsilon}/2 & 0 \\ 0 & 0 & \dot{\varepsilon} \end{pmatrix} = \mathrm{D}$$

$$\boldsymbol{\sigma} = \begin{pmatrix} -p-A & 0 & 0 \\ 0 & -p-A & 0 \\ 0 & 0 & -p+2A \end{pmatrix}$$

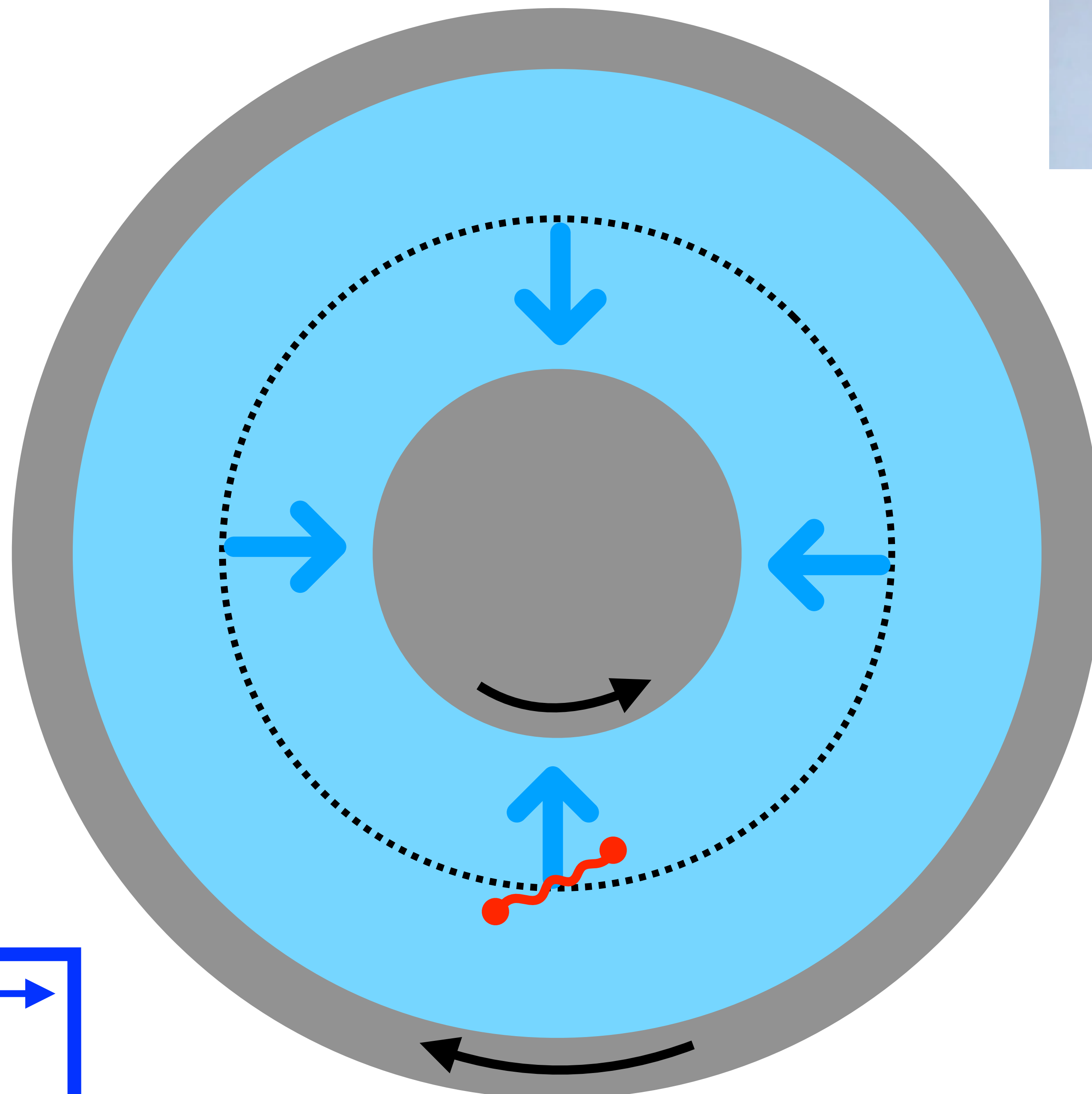
1 component:
only viscosity

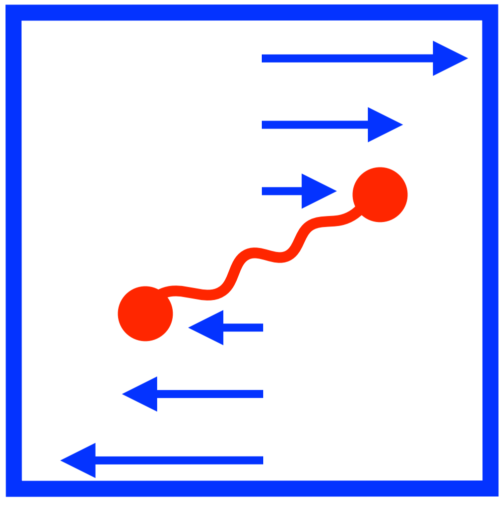
Giusteri and Seto (2018) J. Rheol.

Weissenberg effect



wikipedia





Newtonian liquid

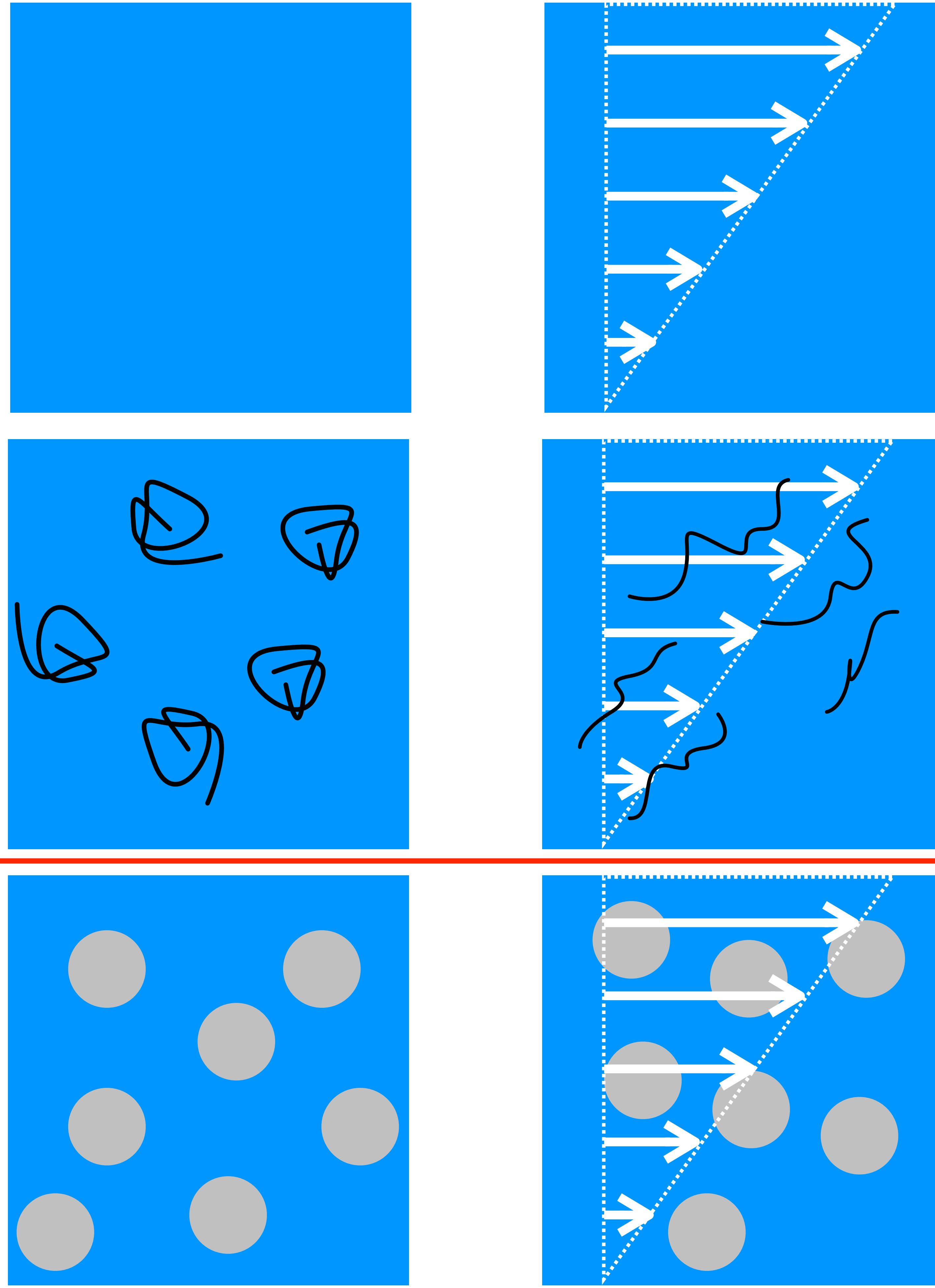
$$\sigma_{xy} = \eta\dot{\gamma}$$

Newtonian liquid
+ elastic chains

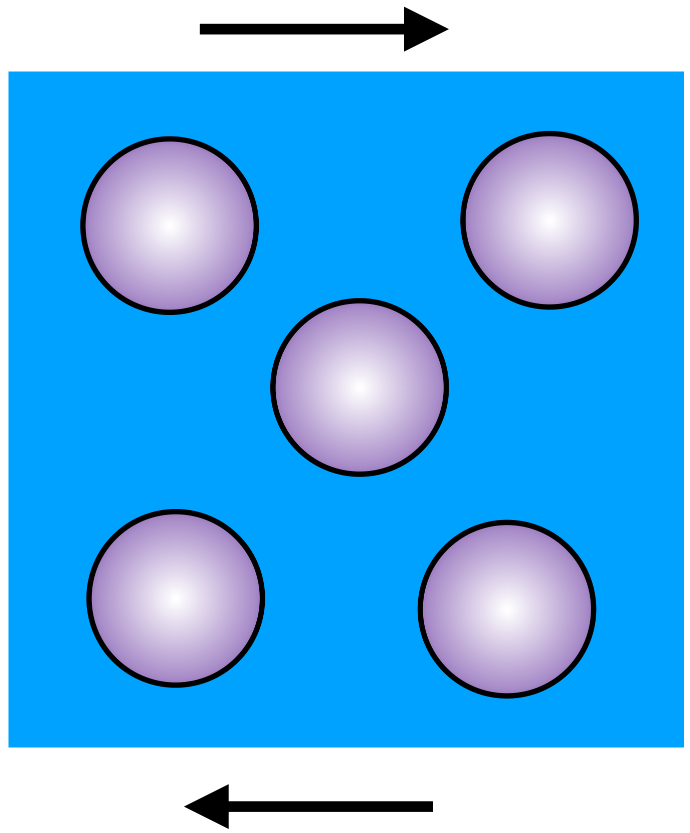
$$\sigma_{xy} = \eta\dot{\gamma} + \tau_{xy}$$

Newtonian liquid
+ rigid balls

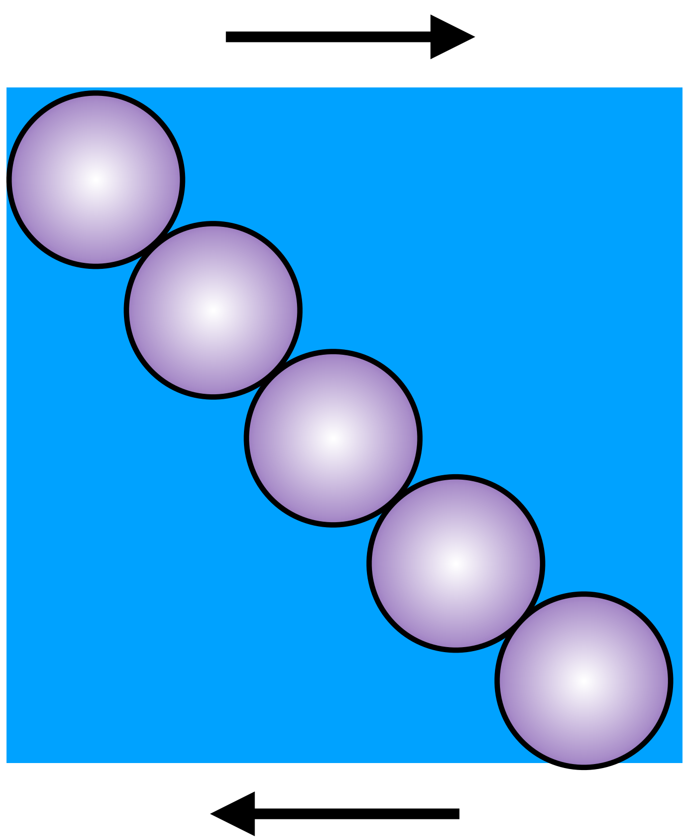
$$\sigma_{xy} = \eta\dot{\gamma} + \tau_{xy}$$

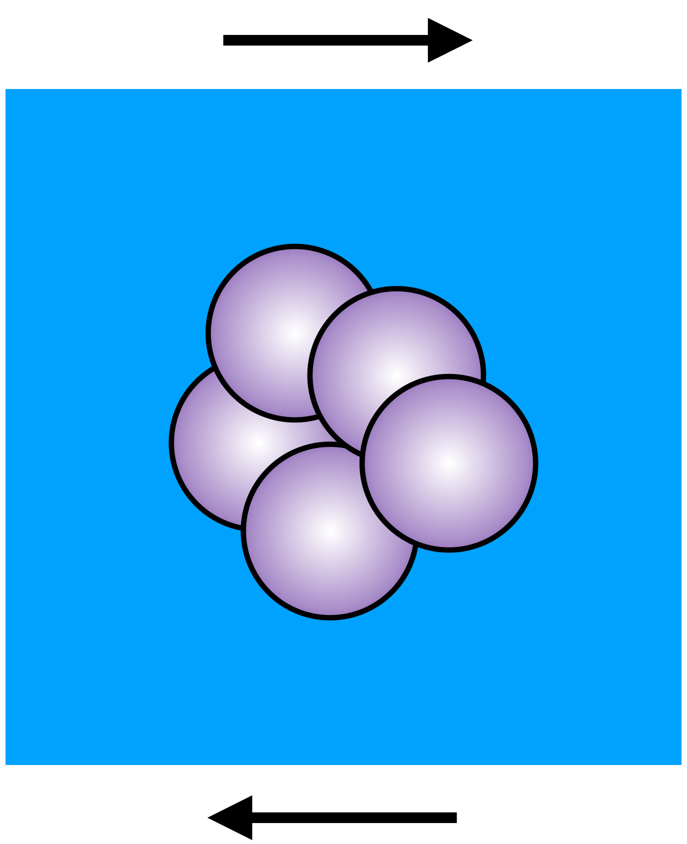


Negligible inertia…



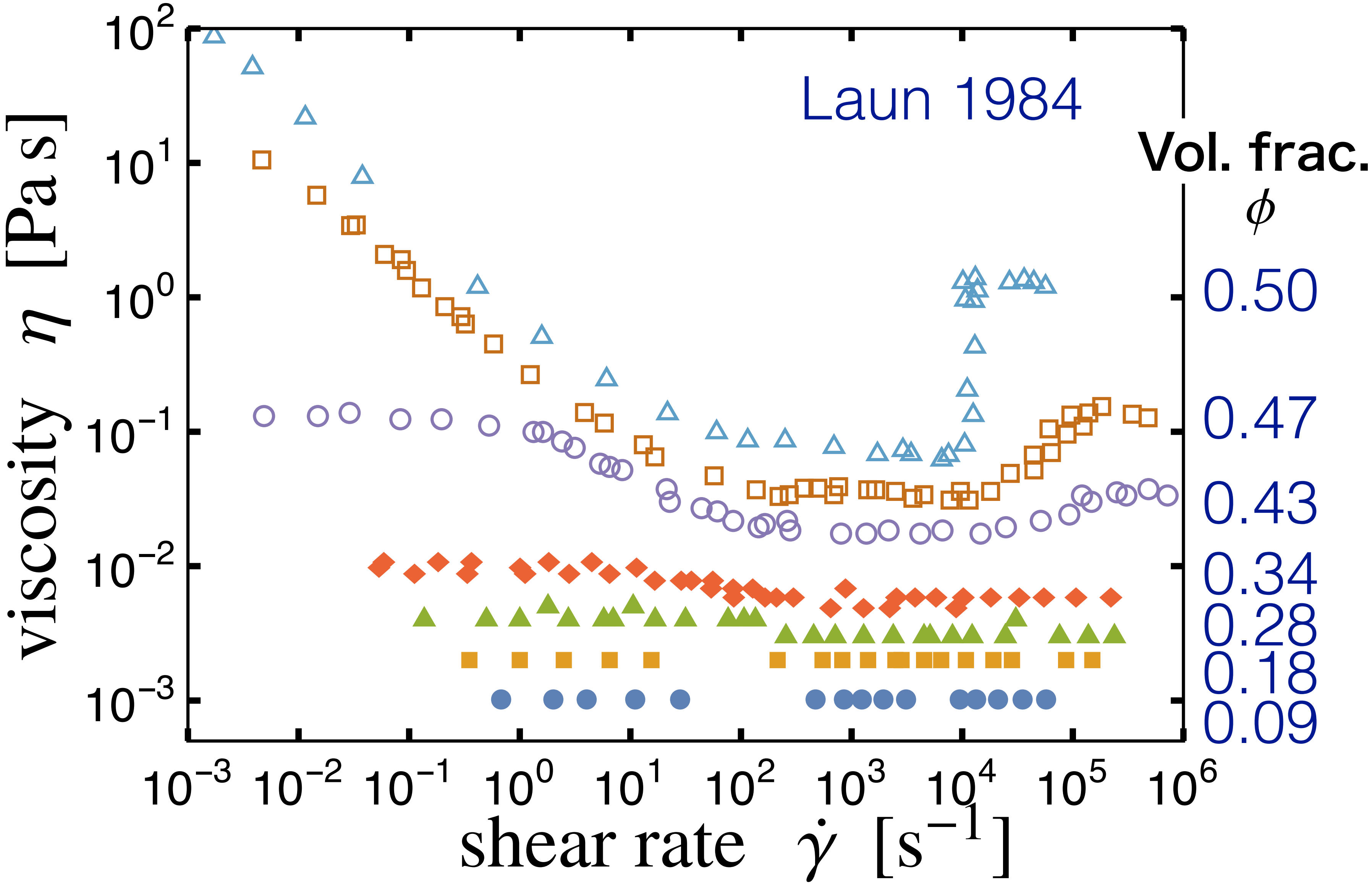
Microstructure determines the rheology!

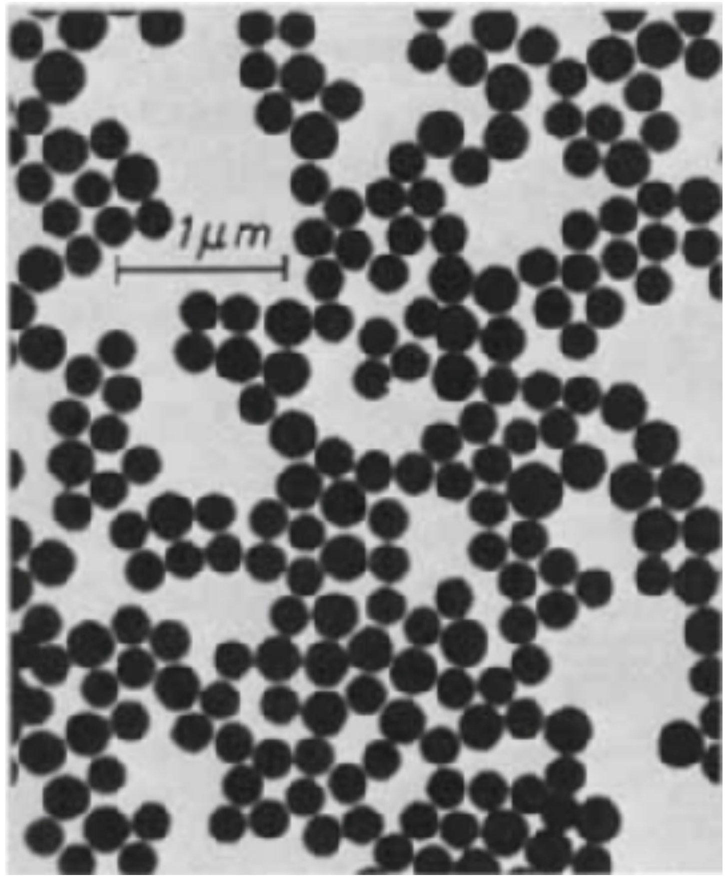




Non-Newtonian behavior in steady-shear rheology

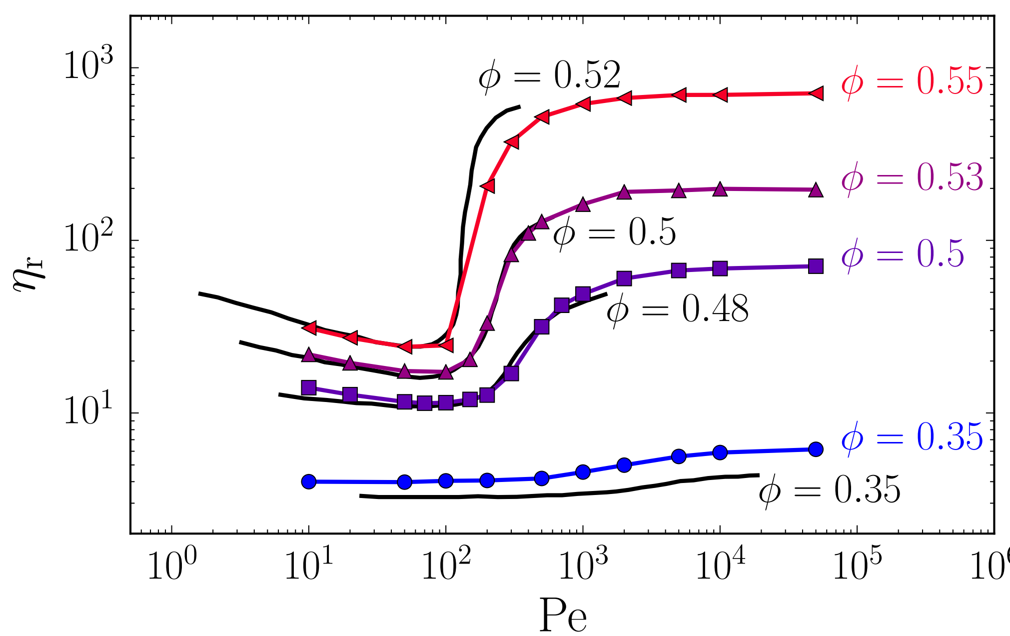
$$\eta(\dot{\gamma})$$





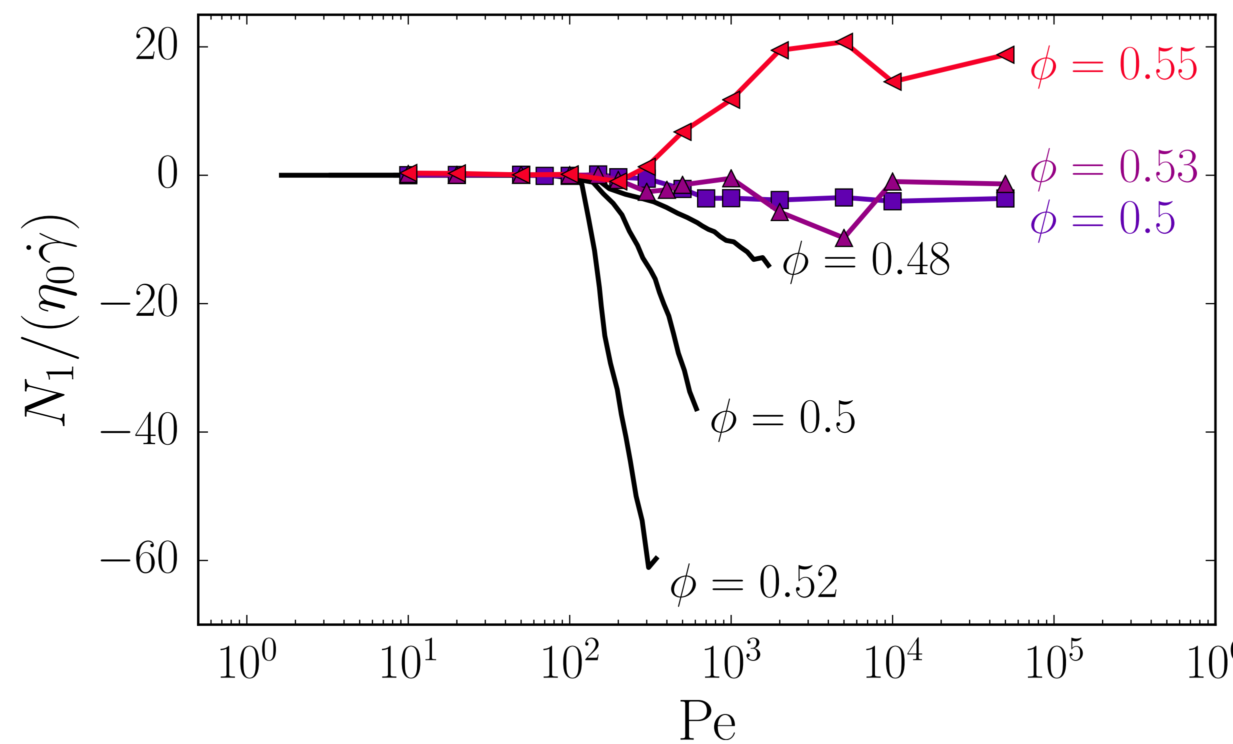
We could reproduce two of the three.

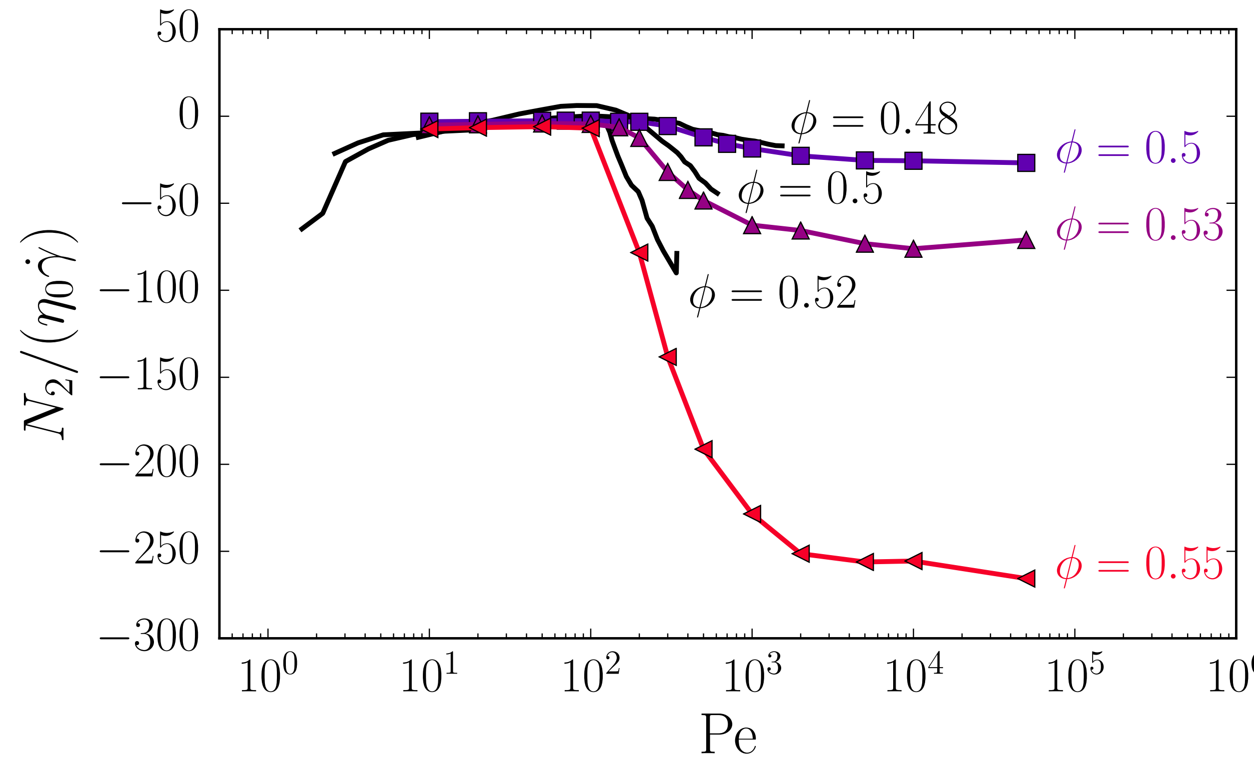
Mari, Seto, Morris, Denn PNAS (2015)



Experimental data black-solid lines

Cwalina and Wagner, JOR (2014)





liquid

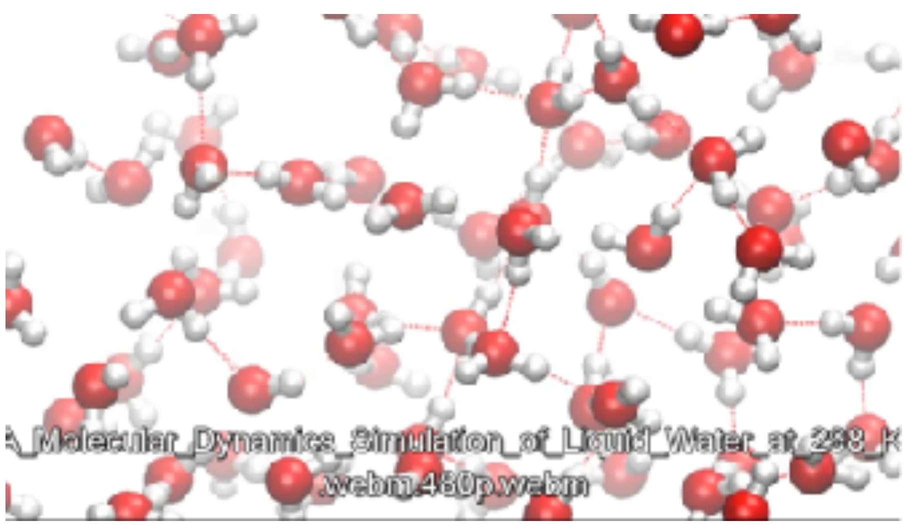
Newtonian fluid

$$\boldsymbol{\sigma} = -p\mathrm{I} + 2\eta \mathrm{D}$$

time scale $1/\dot{\gamma}$

↕ **macro** / **micro**

Molecular dynamics



$$\frac{\text{mean free path}}{\text{velocity}} \sim 10^{-11}\,\mathrm{s}$$

Colloidal suspension

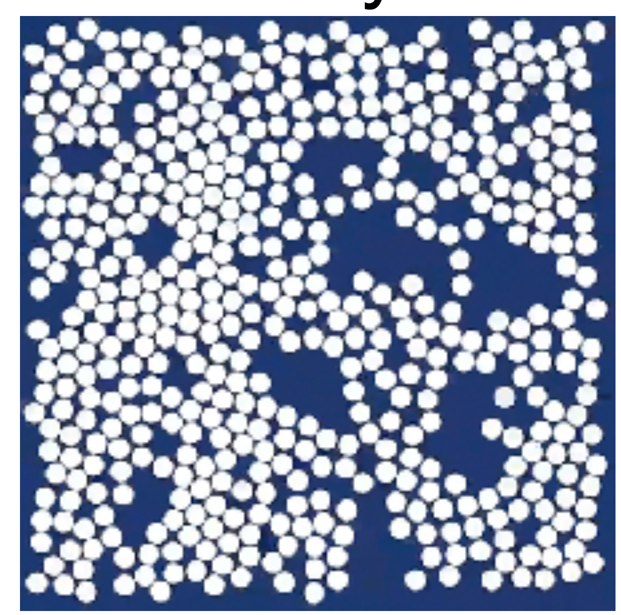
Non-Newtonian fluid

?

time scale $1/\dot{\gamma}$

↕ **macro** / **micro**

Colloidal dynamics



$$\frac{\text{radius}^2}{\text{diffusion constant}} \sim 1\,\mathrm{s}$$

Stokesian Dynamics

Brady & Bossis 1985

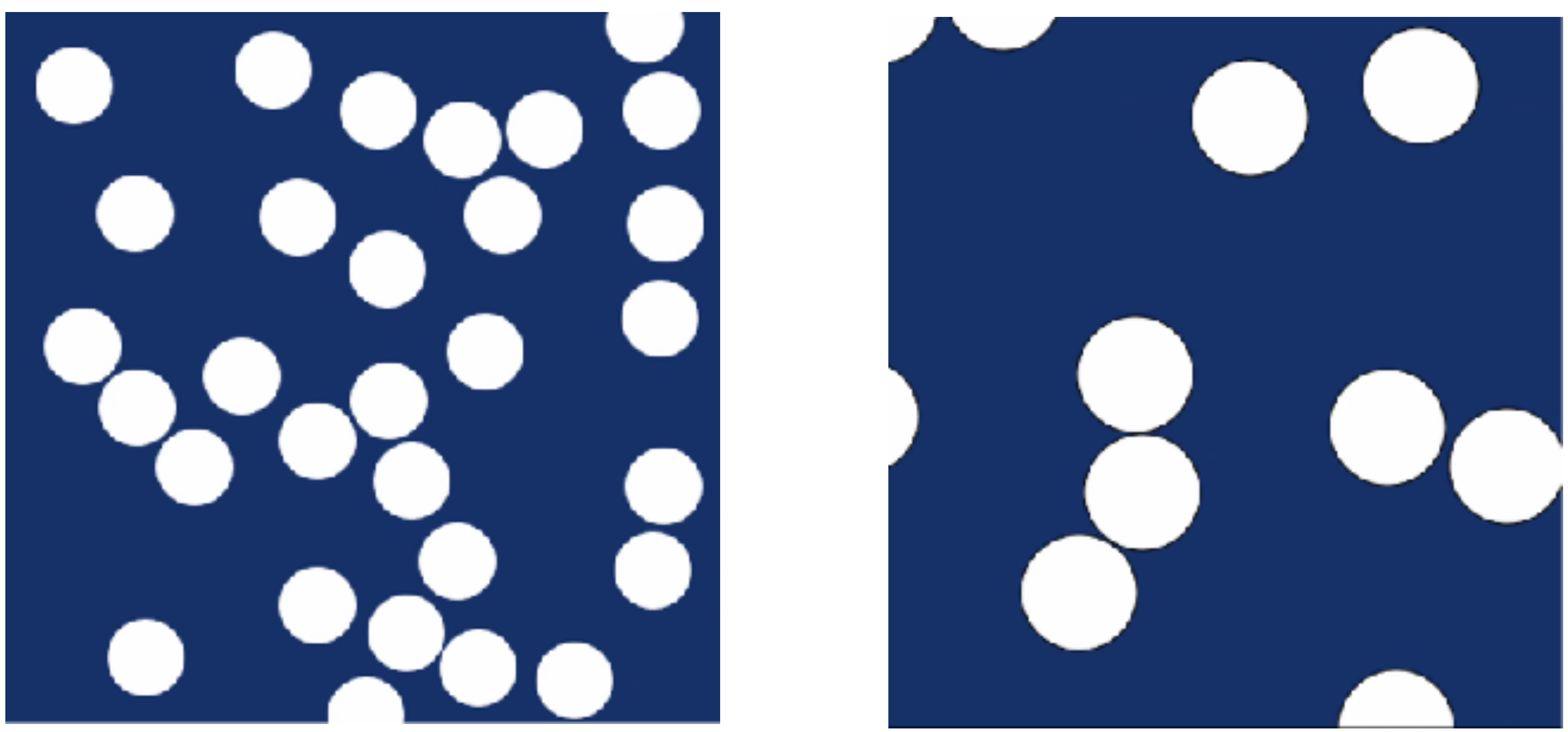
6N-dimensional overdamped Langevin eq. with hydrodynamic interaction

$$\boldsymbol{F}_{\mathrm{B}} + \boldsymbol{F}_{\mathrm{H}} = \boldsymbol{0}$$

Hydrodynamic force $\boldsymbol{F}_{\mathrm{H}} = -\mathsf{R}\cdot(\boldsymbol{U}-\boldsymbol{u}) + \mathsf{R}' : \mathsf{D}$

Brownian force $\langle \boldsymbol{F}_{\mathrm{B}} \rangle = 0, \quad \langle \boldsymbol{F}_{\mathrm{B}}(t_1)\boldsymbol{F}_{\mathrm{B}}(t_2)\rangle = 2k_{\mathrm{B}}T\mathsf{R}\delta(t_1 - t_2)$

$$\boldsymbol{u}(\boldsymbol{r}) = \nabla\boldsymbol{u}\cdot\boldsymbol{r} = \mathsf{D}\cdot\boldsymbol{r} + (\boldsymbol{\omega}/2)\times\boldsymbol{r}$$



Brownian >> Flow → equilibrium

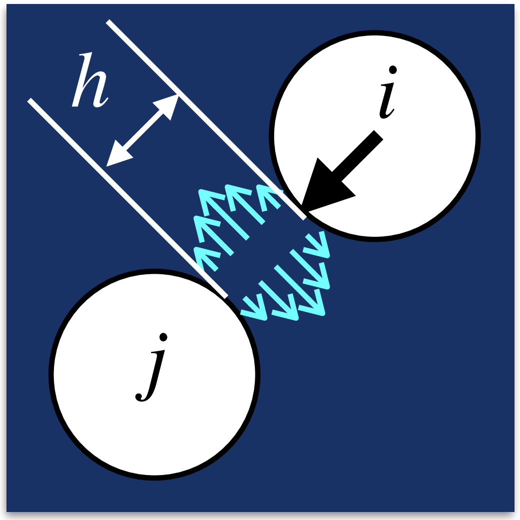
Brownian << Flow → non-equilibrium

“Divergence-free” Stokesian Dynamics

lubrication force

$$\boldsymbol{F} \sim -\frac{1}{h}(\boldsymbol{U}^i - \boldsymbol{U}^j)\cdot\boldsymbol{nn}$$

$$\frac{1}{h} \to \frac{1}{h+\delta}$$

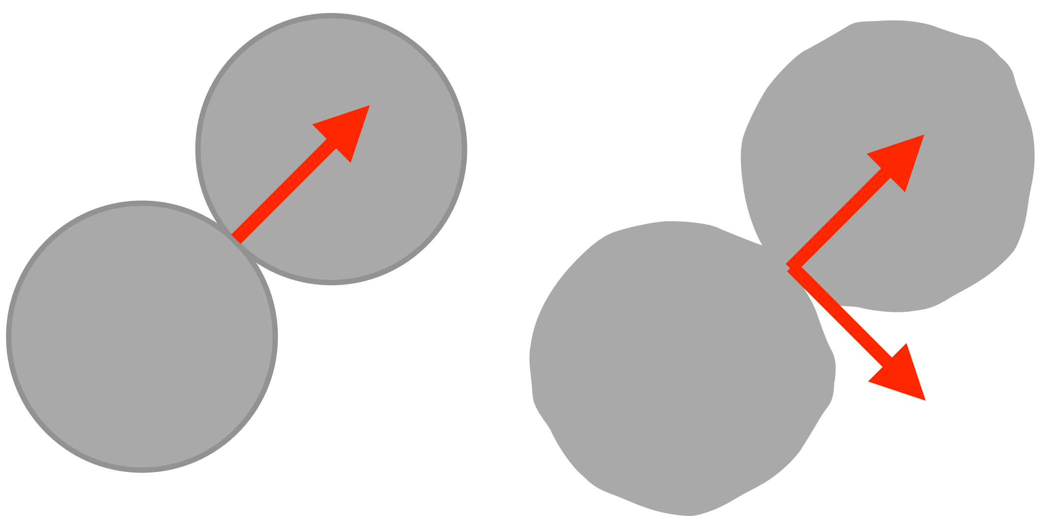


One important consequence
→ Particle contacts are no longer forbidden…

We *must* include a contact force model

$$\boldsymbol{F}_{\mathrm{H}} + \boldsymbol{F}_{\mathrm{B}} + \boldsymbol{F}_{\mathrm{C}} = \mathbf{0}$$

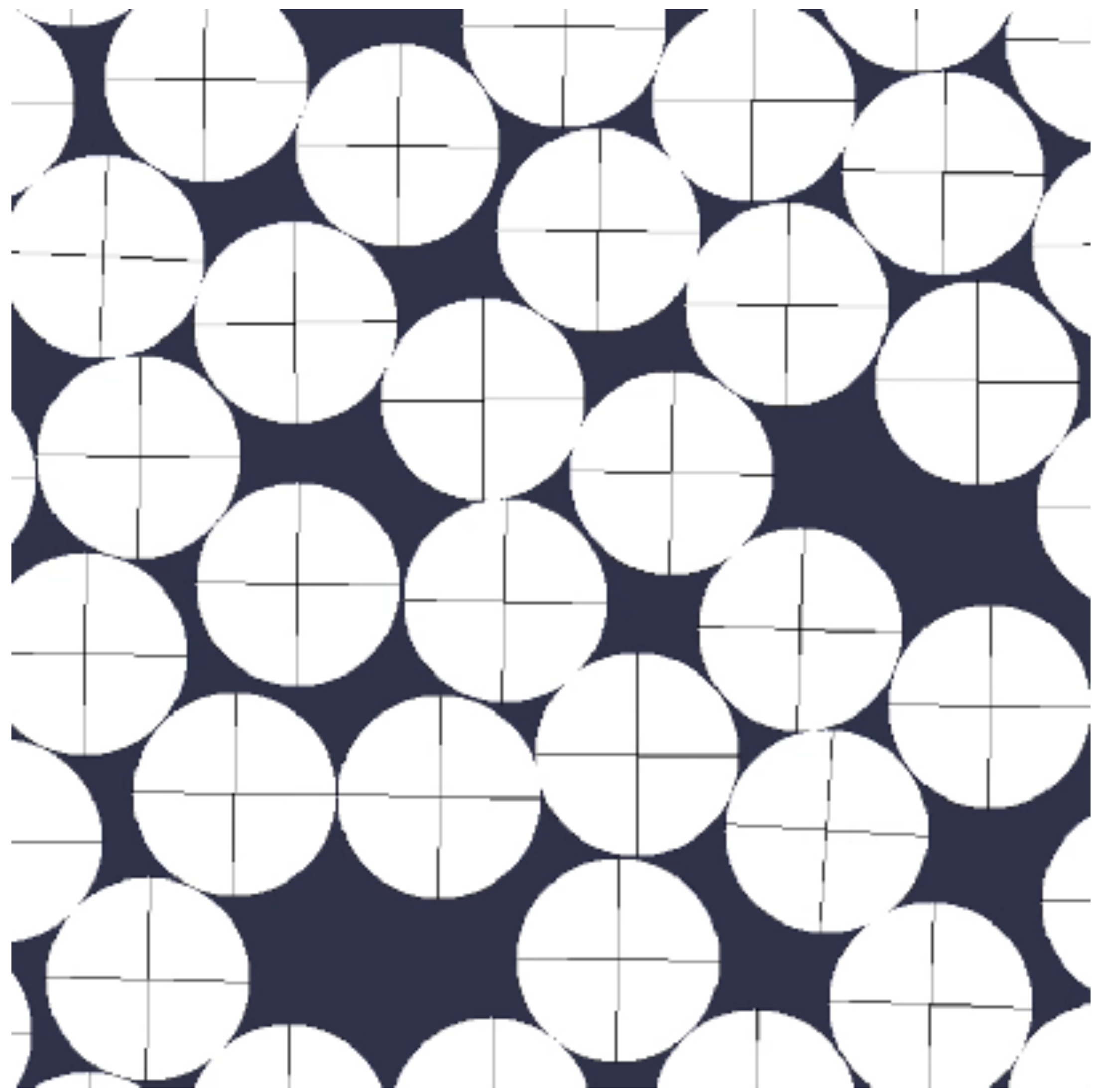
$$\boldsymbol{F}_{\mathrm{H}} = -\,\mathsf{R} \cdot (\boldsymbol{U} - \boldsymbol{u}) + \mathsf{R}' : \mathsf{D}$$



$$|\boldsymbol{F}_{\mathrm{C}}^{tan}| < \mu\,|\boldsymbol{F}_{\mathrm{C}}^{nor}|$$

$$\left(\boldsymbol{F}_{\mathrm{C}}^{ij}\right)^{nor} = k_{\mathrm{n}}(r_{ij} - 2a)\boldsymbol{n}^{ij}$$

$$\left(\boldsymbol{F}_{\mathrm{C}}^{ij}\right)^{tan} = -\,k_{\mathrm{t}}\boldsymbol{\xi}^{ij}$$



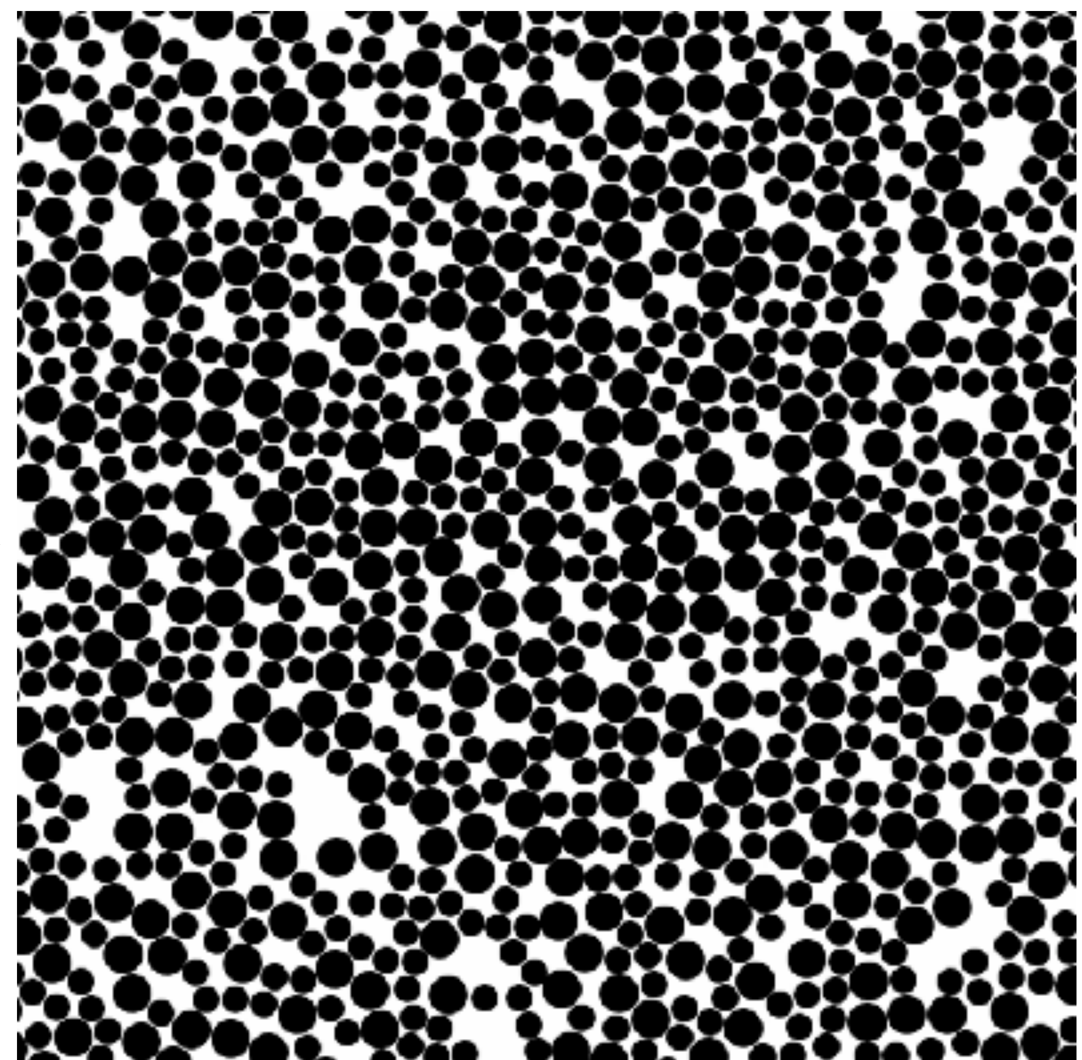
We can simulate the non-equlibiwrum limit (thanks to these two modifications)

$$Pe \to \infty \quad \longrightarrow \quad \boldsymbol{F}_{\mathrm{H}} + \cancel{\boldsymbol{F}_{\mathrm{B}}} + \boldsymbol{F}_{\mathrm{C}} = \mathbf{0}$$

cf. Brady 1995: Perturbation theory for the small Pe regime (Shear distorts isotropic microstructures)

$$\boldsymbol{F}_{\mathrm{H}} + \boldsymbol{F}_{\mathrm{C}} = \mathbf{0}$$

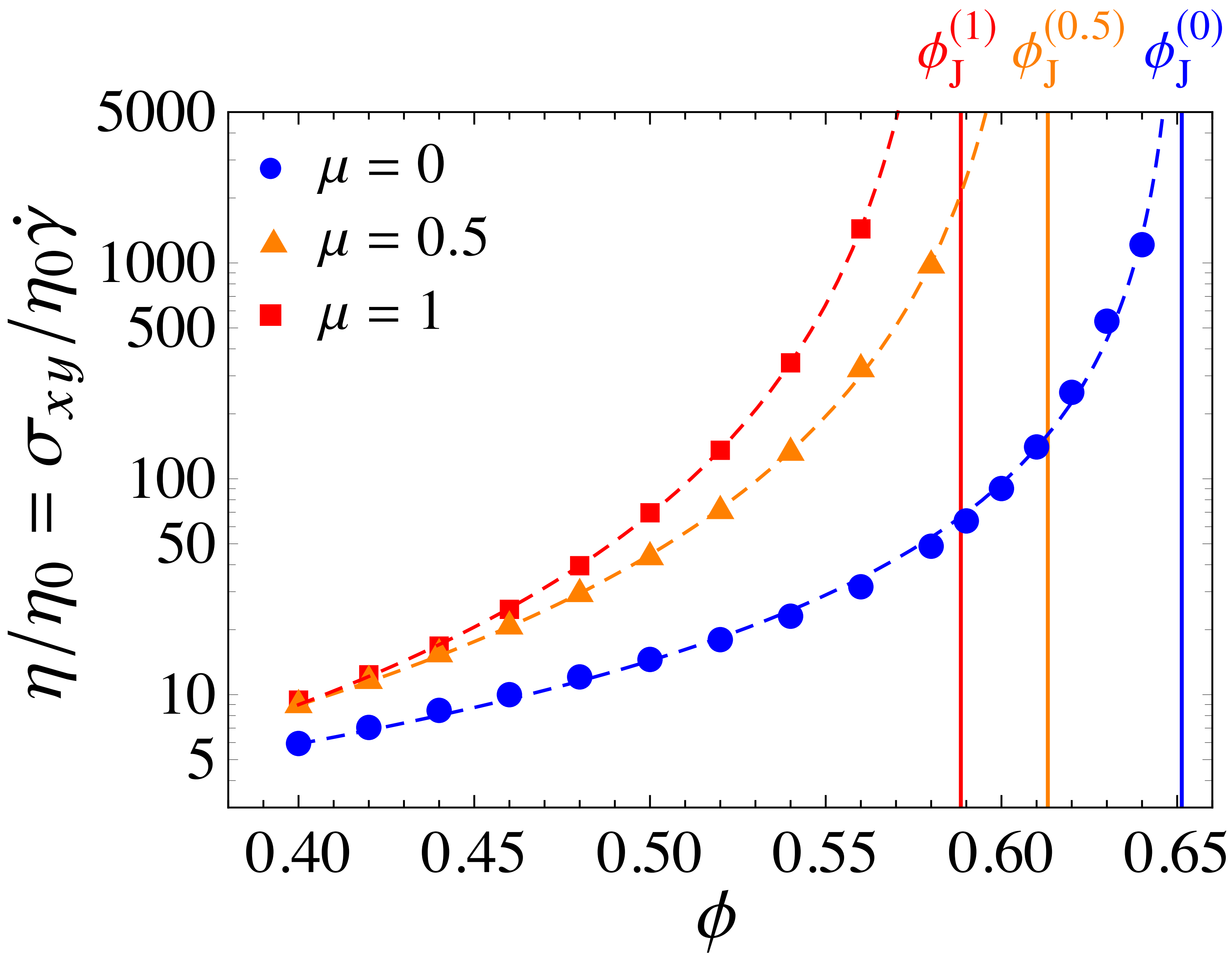
$$\boldsymbol{F}_{\mathrm{H}} = -\,\mathsf{R}\cdot(\boldsymbol{U} - \boldsymbol{u}) + \mathsf{R}' : \mathsf{D}$$



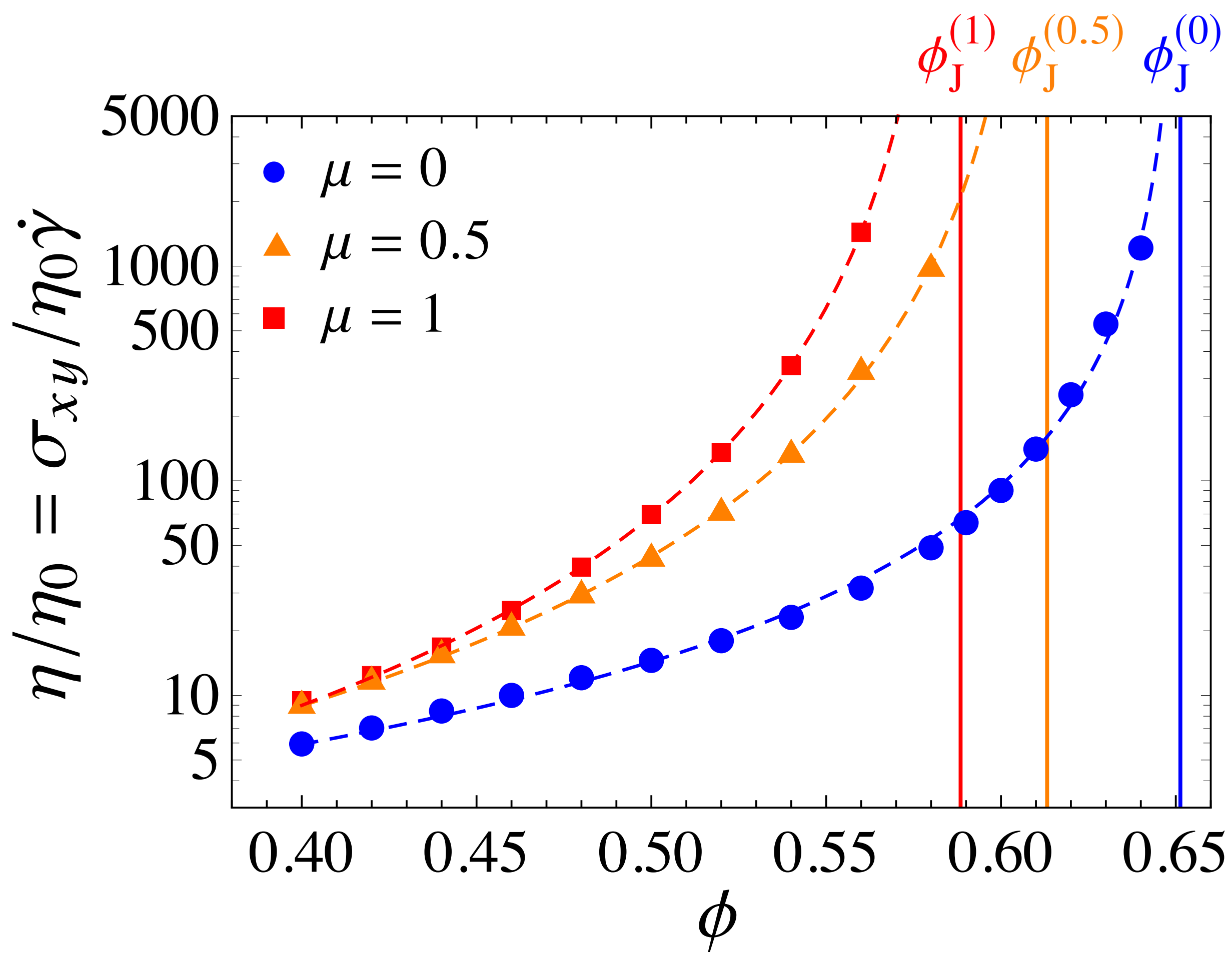
(2D demo)

Monotonic increase of viscosity

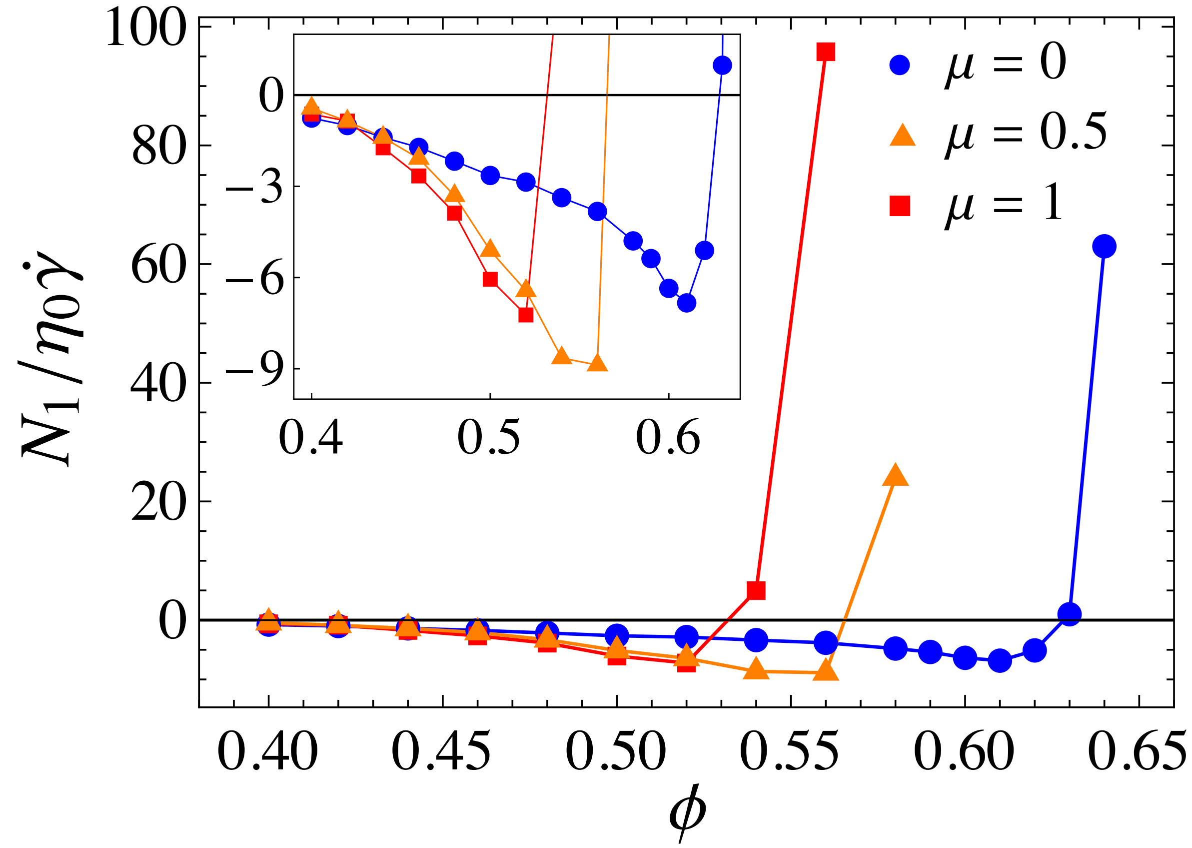
$$\eta(\phi)/\eta_0 = c(\phi_\mathrm{J} - \phi)^{-\lambda}$$



Non-monotonic ϕ dependence of N_1



monotonic dependence



abrupt change…

Steady shear rheology

$$\sigma_{xy} = \eta\dot{\gamma}$$
$$N_1 = \sigma_{xx} - \sigma_{yy}$$
$$N_2 = \sigma_{yy} - \sigma_{zz}$$
$$p = -\frac{1}{3}\operatorname{Tr}\boldsymbol{\sigma}$$

$$\longleftrightarrow \quad \boldsymbol{\sigma} = \begin{pmatrix} -p + \frac{2}{3}N_1 + \frac{1}{3}N_2 & \sigma_{xy} & 0 \\ \sigma_{xy} & -p - \frac{1}{3}N_1 + \frac{1}{3}N_2 & 0 \\ 0 & 0 & -p - \frac{1}{3}N_1 - \frac{2}{3}N_2 \end{pmatrix}$$

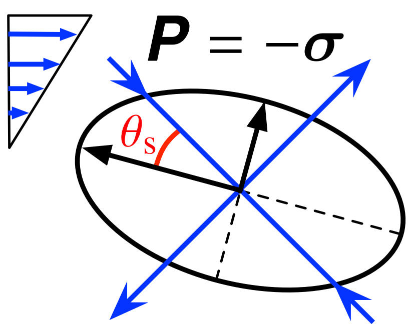
$$N_0 \equiv \sigma_{zz} - \frac{\sigma_{xx} + \sigma_{yy}}{2} = -N_2 - 0.5N_1$$

Eigenvalues

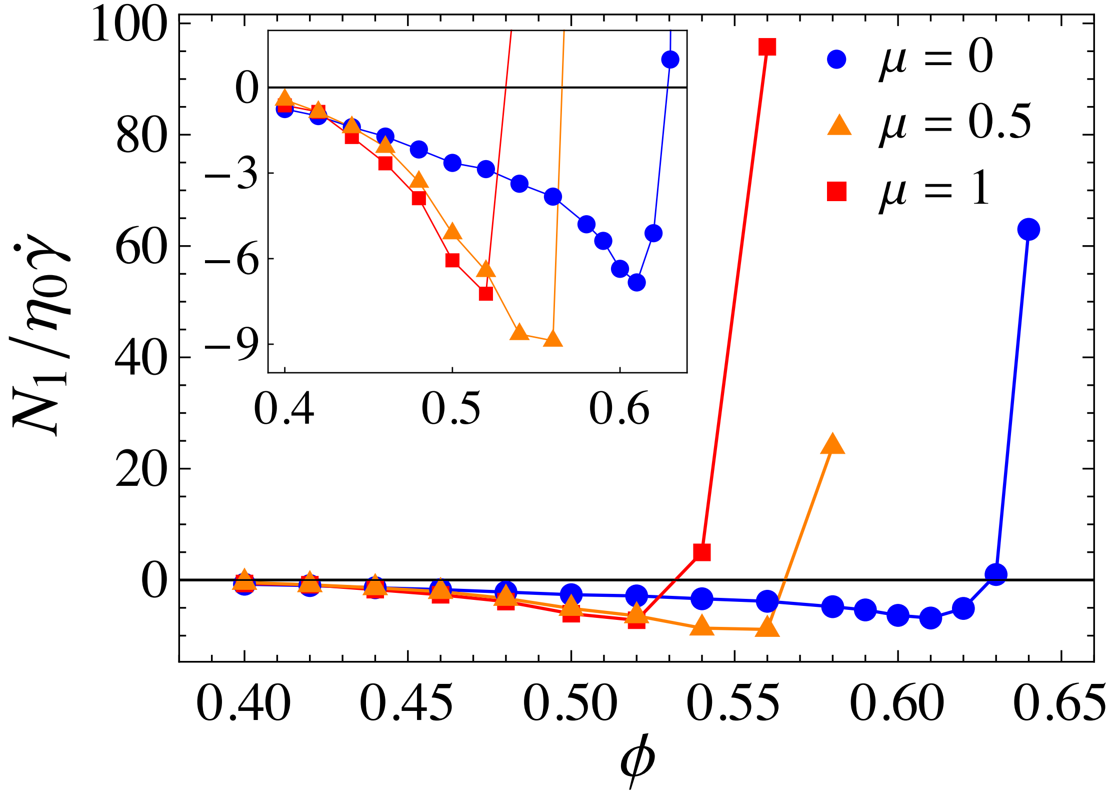
$$\begin{cases} P_1 = p\left(1 + \dfrac{N_0}{3p}\right) + \dfrac{\sigma_{xy}}{2}\sqrt{4 + (N_1/\sigma_{xy})^2} \\ P_2 = p\left(1 + \dfrac{N_0}{3p}\right) - \dfrac{\sigma_{xy}}{2}\sqrt{4 + (N_1/\sigma_{xy})^2} \\ P_3 = p\left(1 - 2\dfrac{N_0}{3p}\right) \end{cases}$$

Eigenvectors

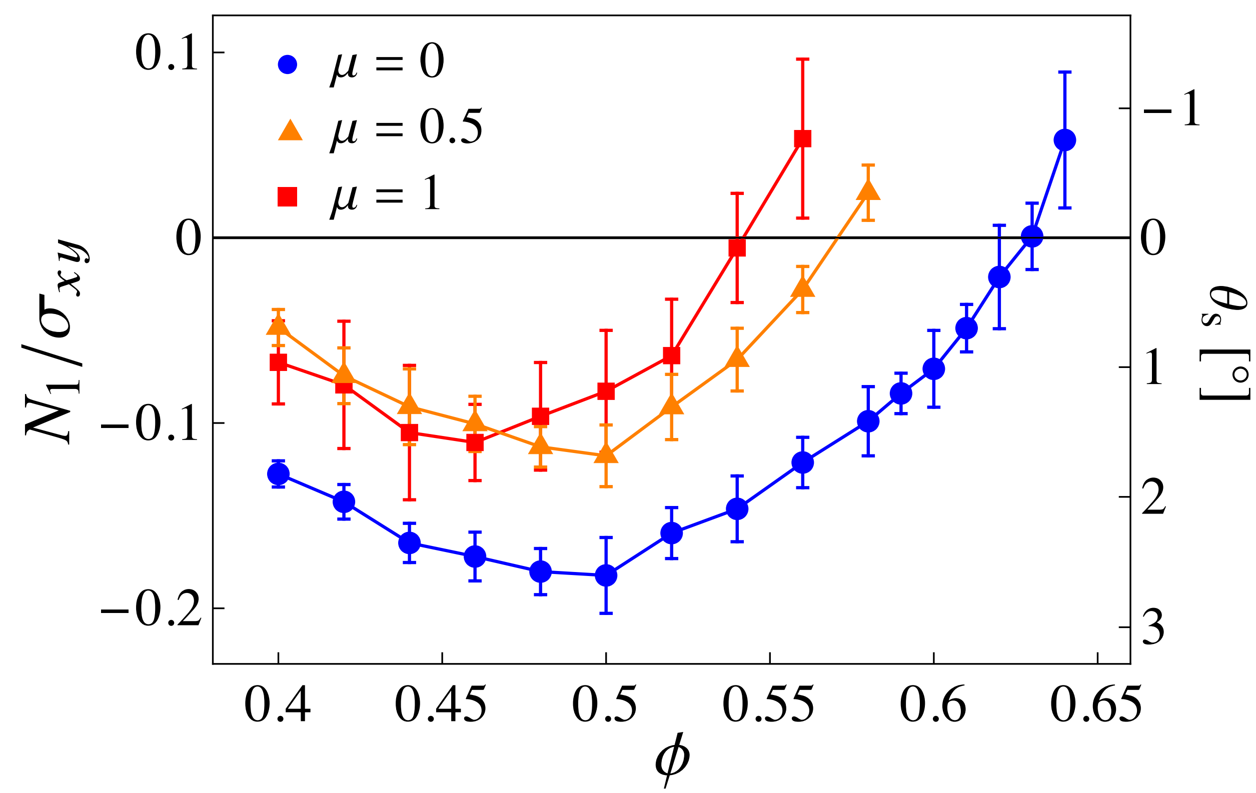
$$\begin{cases} \hat{\boldsymbol{n}}_1 = \begin{pmatrix} \cos(\theta_s + 3\pi/4) \\ \sin(\theta_s + 3\pi/4) \\ 0 \end{pmatrix}, \quad \hat{\boldsymbol{n}}_2 = \begin{pmatrix} \cos(\theta_s + \pi/4) \\ \sin(\theta_s + \pi/4) \\ 0 \end{pmatrix}, \quad \hat{\boldsymbol{n}}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \\ \theta_s \equiv \tan^{-1}\left(\dfrac{-N_1/\sigma_{xy}}{2 + \sqrt{4 + (N_1/\sigma_{xy})^2}}\right) \approx -\dfrac{N_1}{4\sigma_{xy}} \end{cases}$$

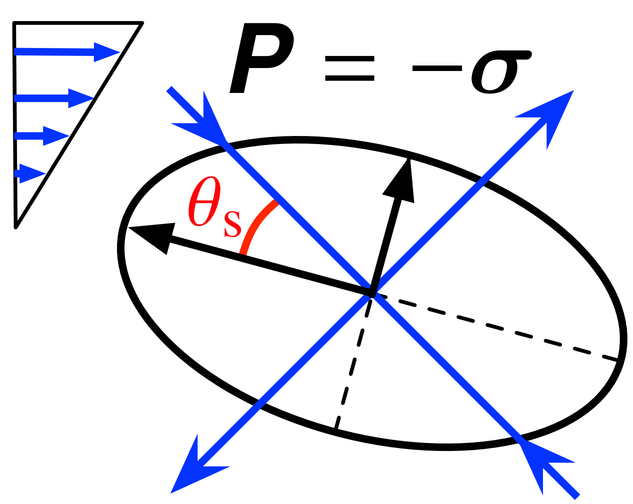


abrupt change



rather smooth sign change



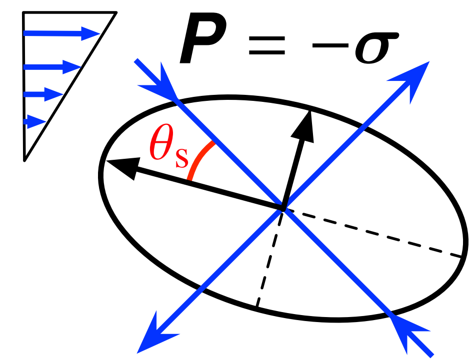


$$\theta_s \equiv \tan^{-1}\left(\frac{-N_1/\sigma_{xy}}{2+\sqrt{4+(N_1/\sigma_{xy})^2}}\right) \approx -\frac{N_1}{4\sigma_{xy}}$$

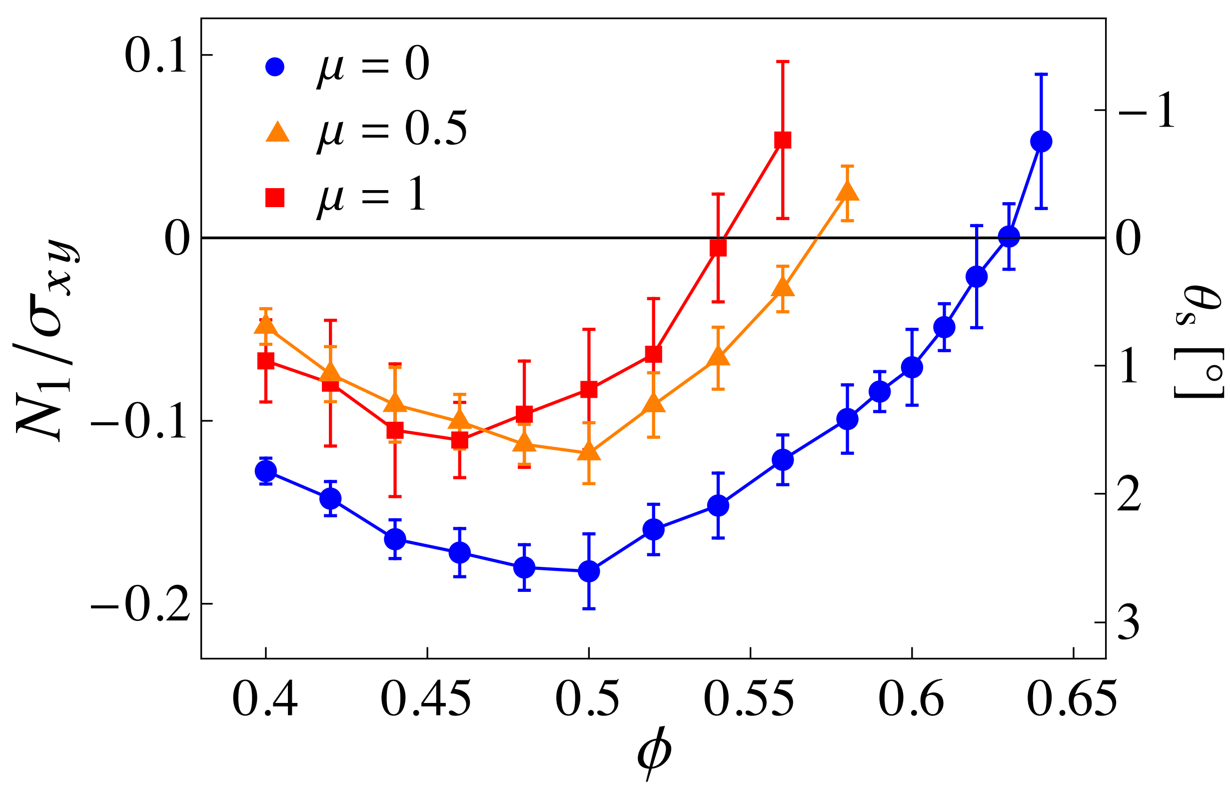
$$N_0 \equiv \sigma_{zz} - \frac{\sigma_{xx} + \sigma_{yy}}{2} = -N_2 - 0.5N_1$$

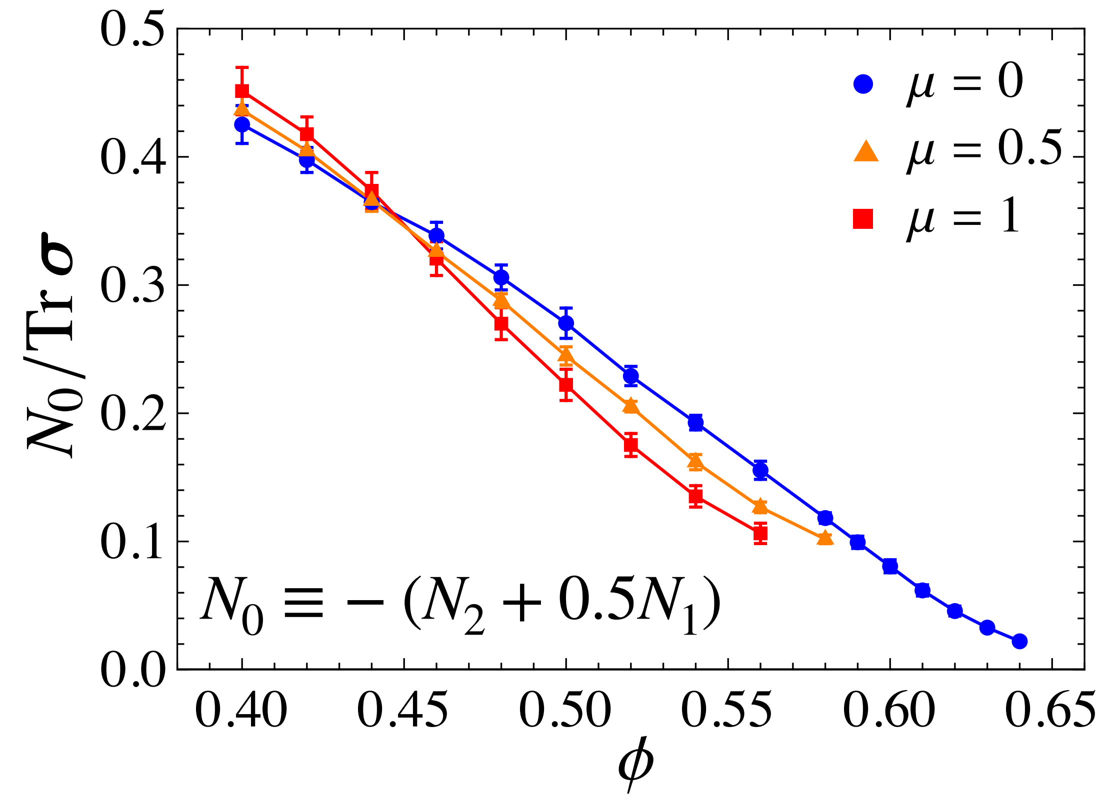
Eigenvalues

$$\begin{cases} P_1 = p\left(1 + \frac{N_0}{3p}\right) + \frac{\sigma_{xy}}{2}\sqrt{4 + (N_1/\sigma_{xy})^2} \\ P_2 = p\left(1 + \frac{N_0}{3p}\right) - \frac{\sigma_{xy}}{2}\sqrt{4 + (N_1/\sigma_{xy})^2} \\ P_3 = p\left(1 - 2\frac{N_0}{3p}\right) \end{cases}$$

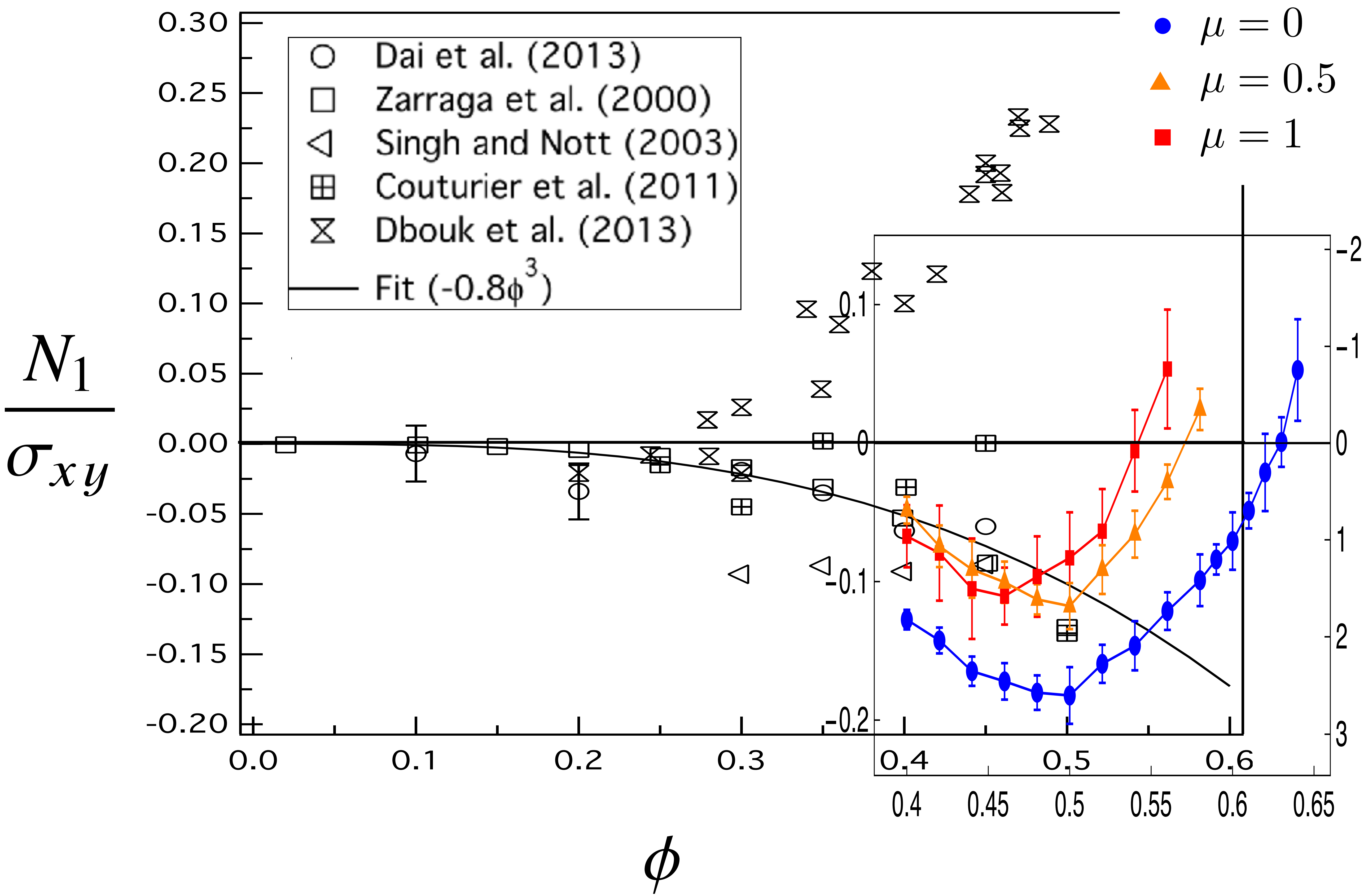


$$\theta_s \equiv \tan^{-1}\left(\frac{-N_1/\sigma_{xy}}{2 + \sqrt{4 + (N_1/\sigma_{xy})^2}}\right) \approx -\frac{N_1}{4\sigma_{xy}}$$

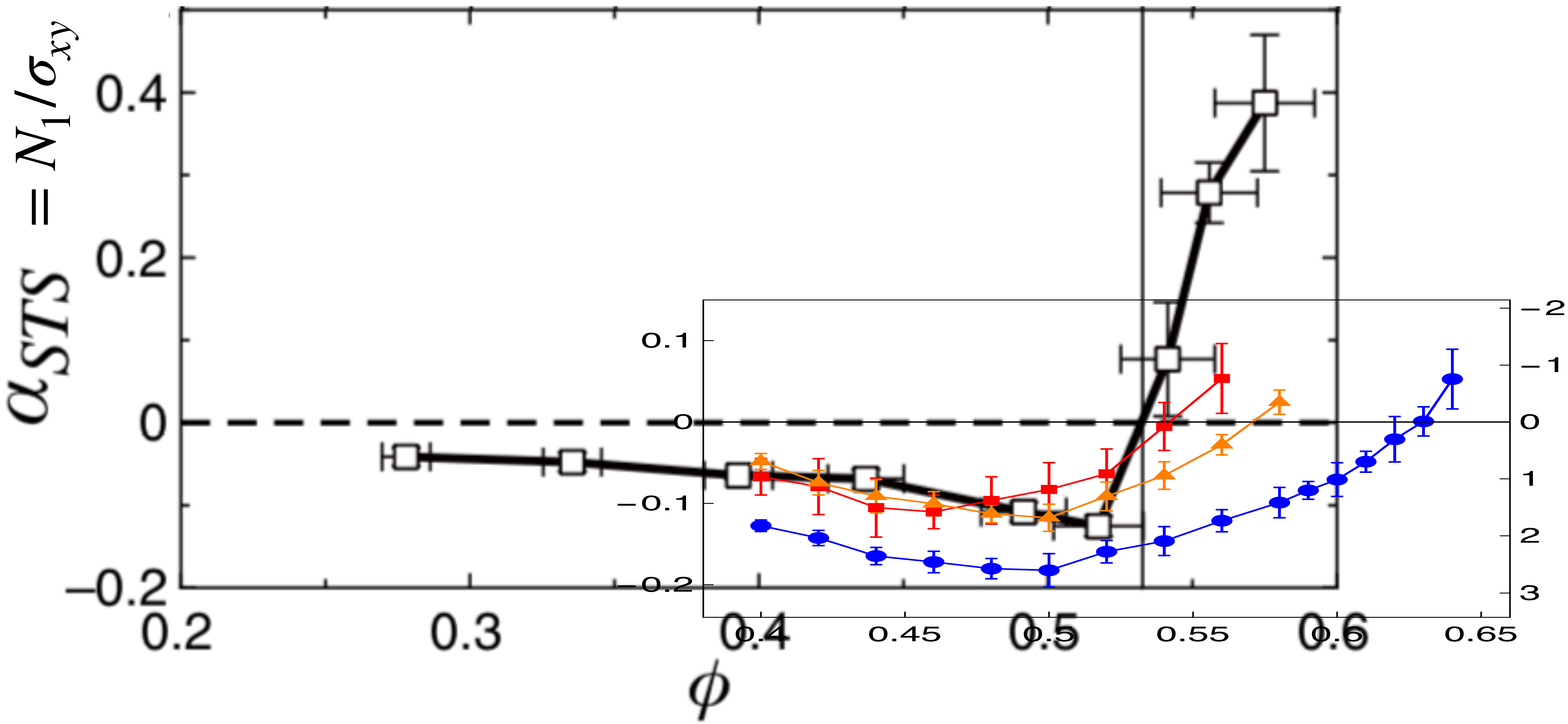




Experimental data



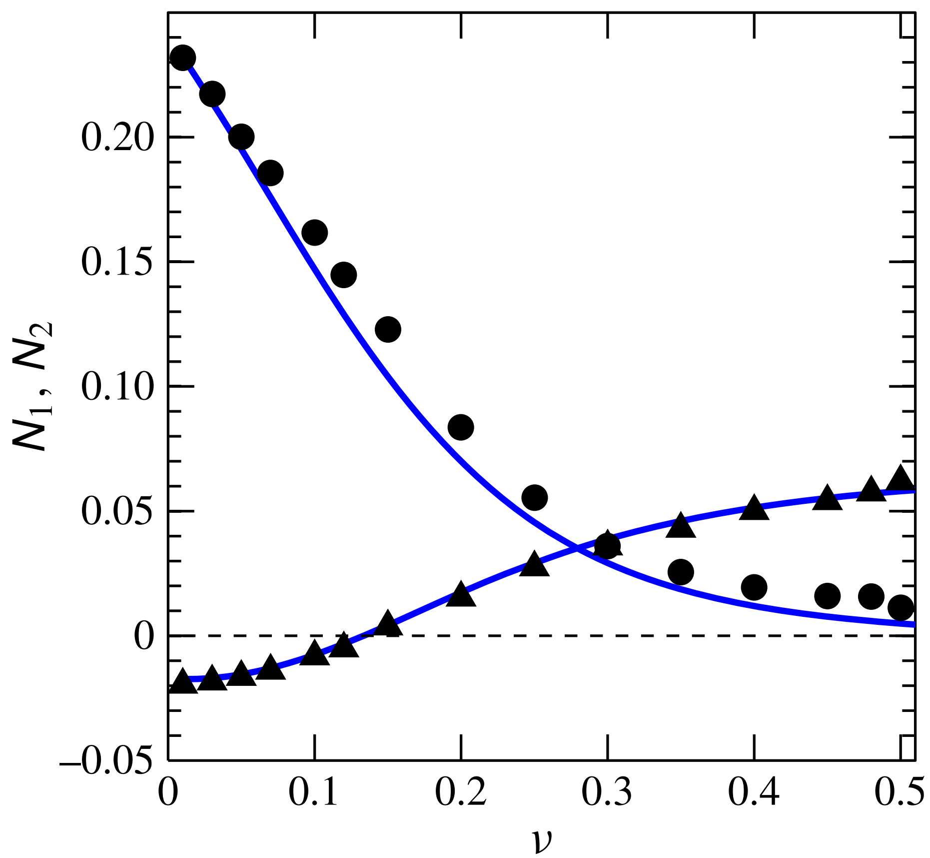
Experimental data



Royer, Blair, and Hudson
Phys. Rev. Lett., 116:188301, 2016.

Simulation of collisional granular systems

Alam and Luding (2005)



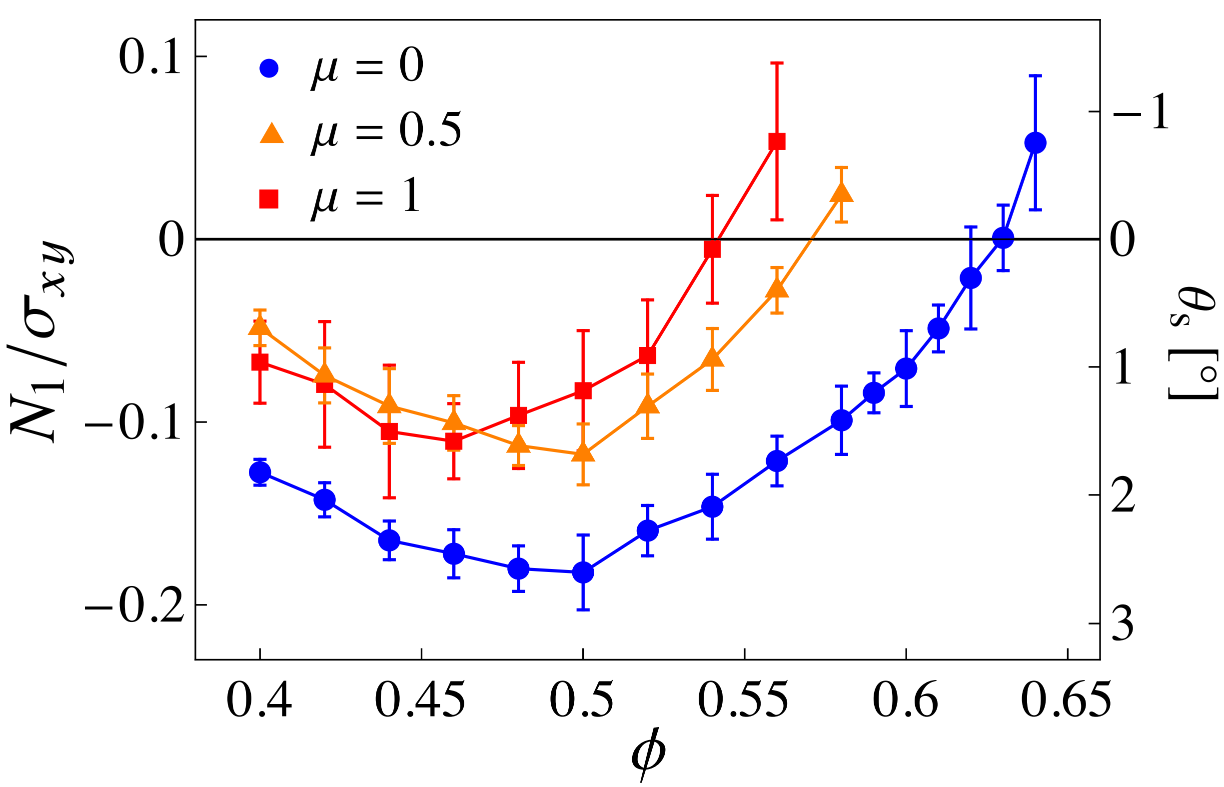
$\tilde{N}_2 \equiv (P_{yy} - P_{zz})/p$

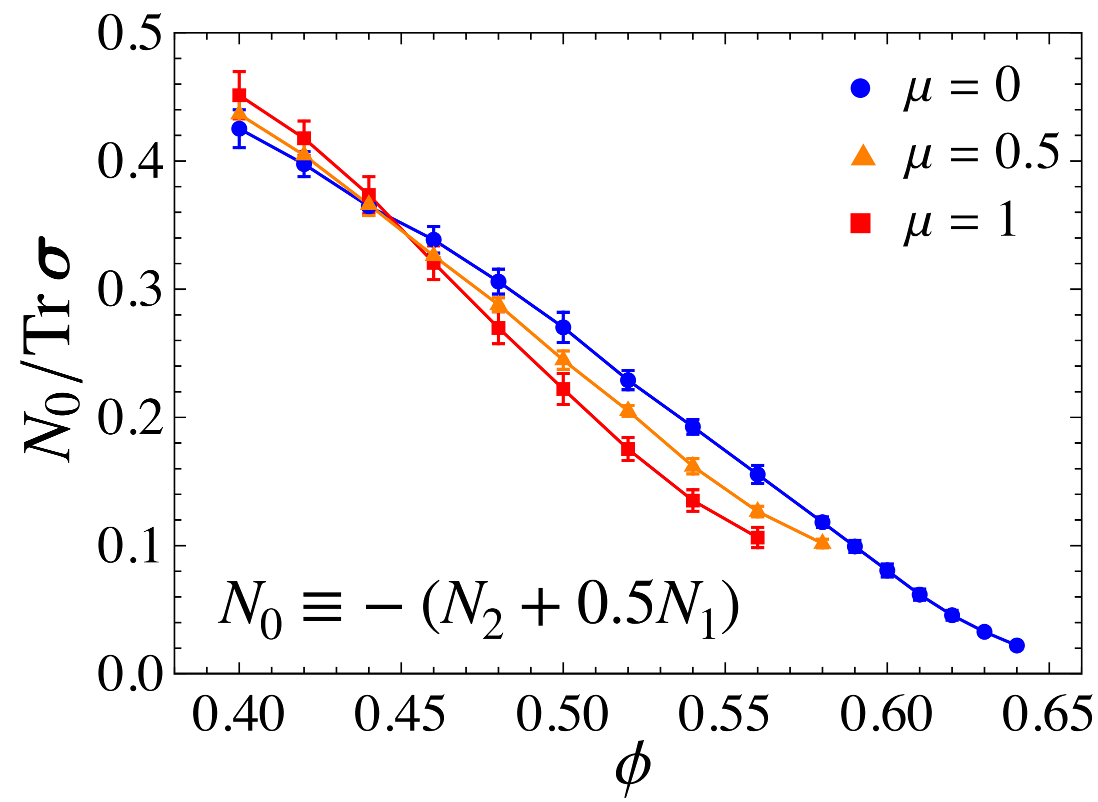
$\tilde{N}_1 \equiv (P_{xx} - P_{yy})/p$

note: opposite signs in the definitions of NSD.

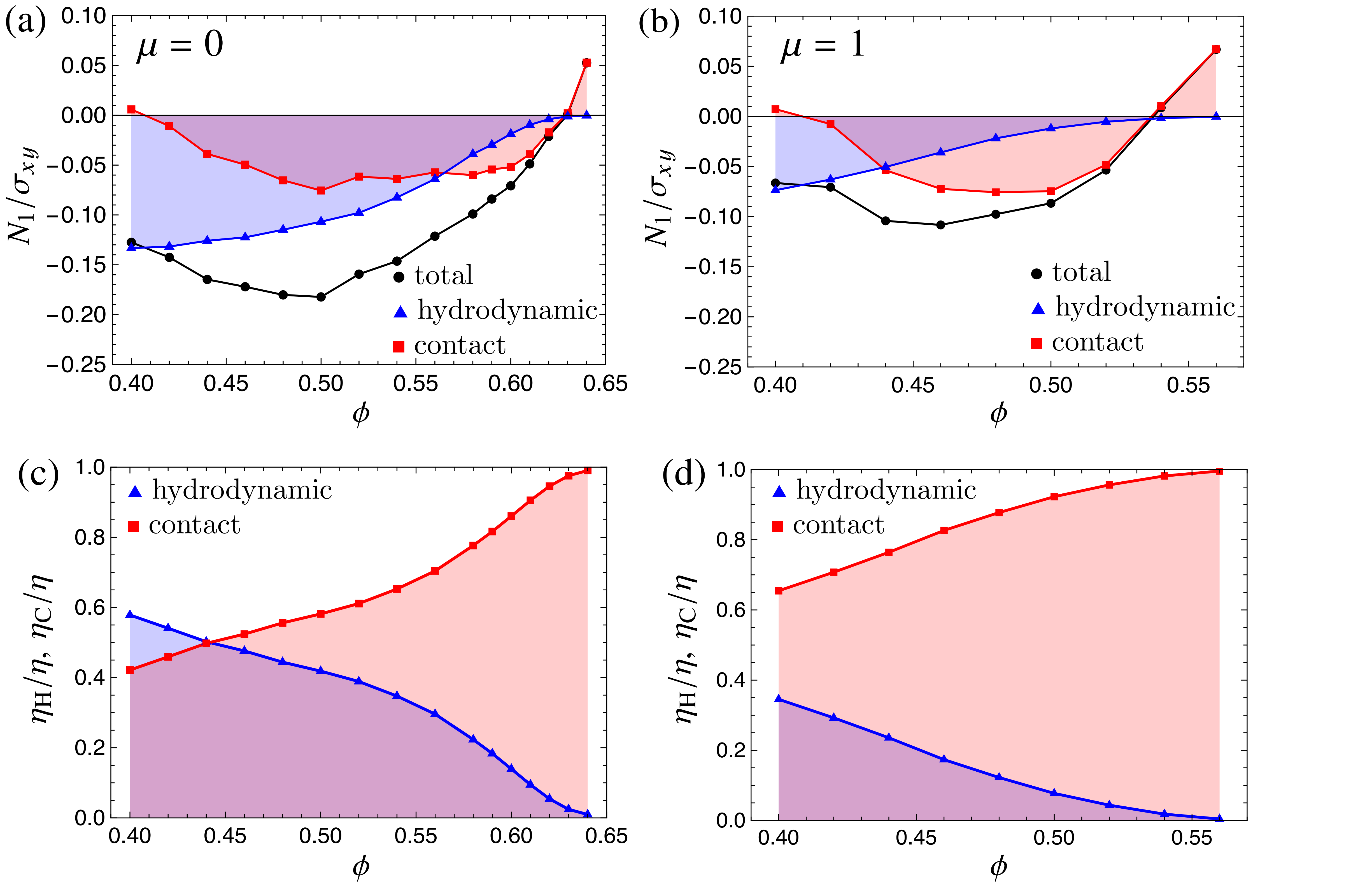
$N_1 \equiv \sigma_{xx} - \sigma_{yy}$

$N_2 \equiv \sigma_{yy} - \sigma_{zz}$

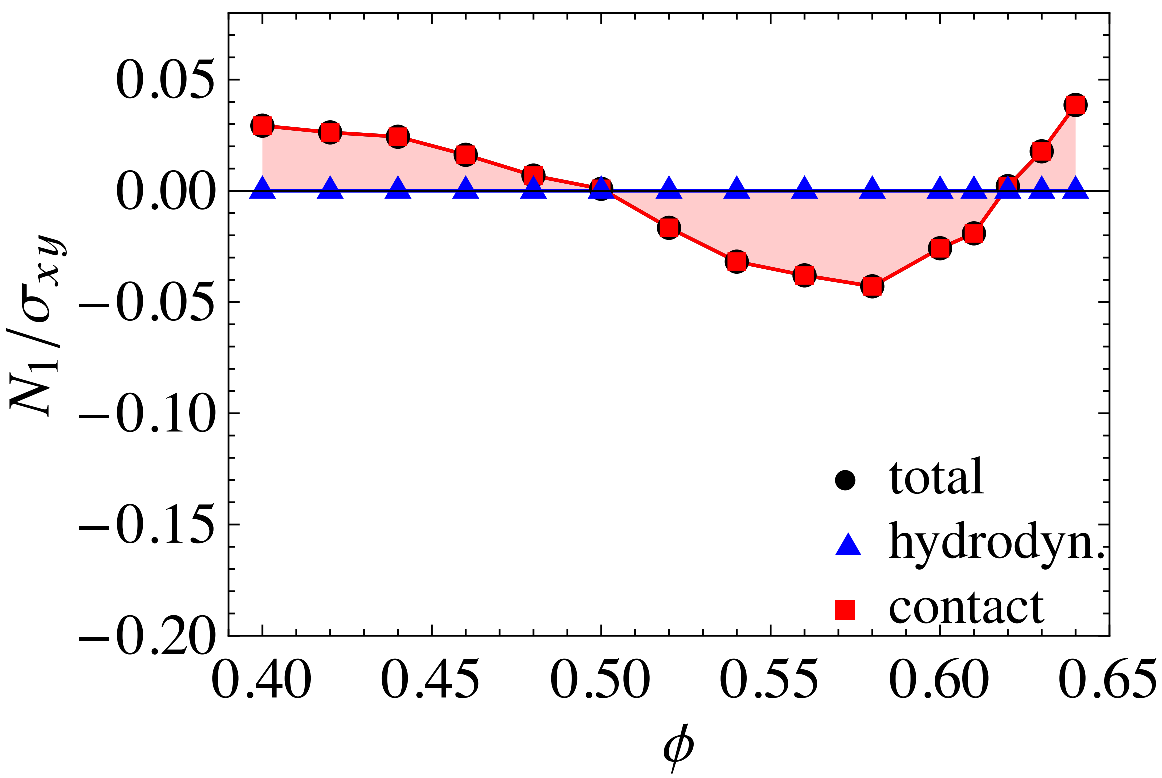




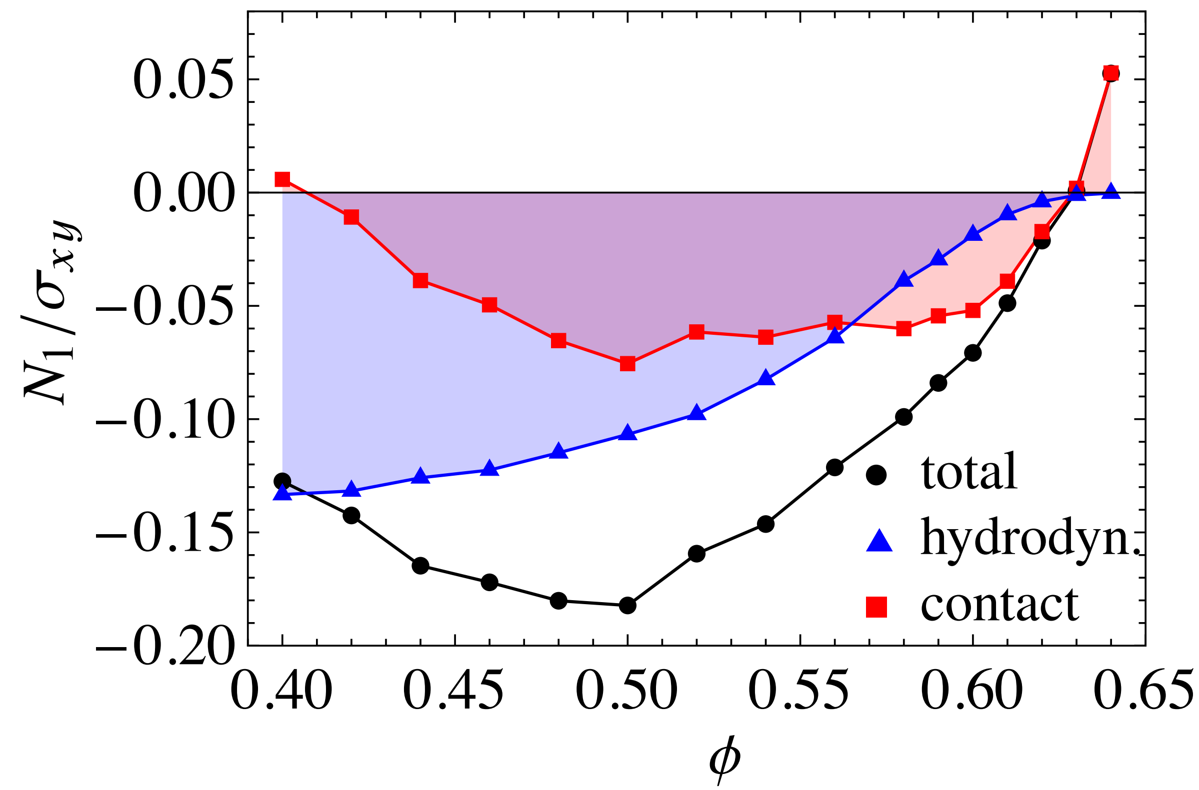
Hydrodynamic interaction vs. Contact force



Without
hydrodynamics interaction
(frictionless)

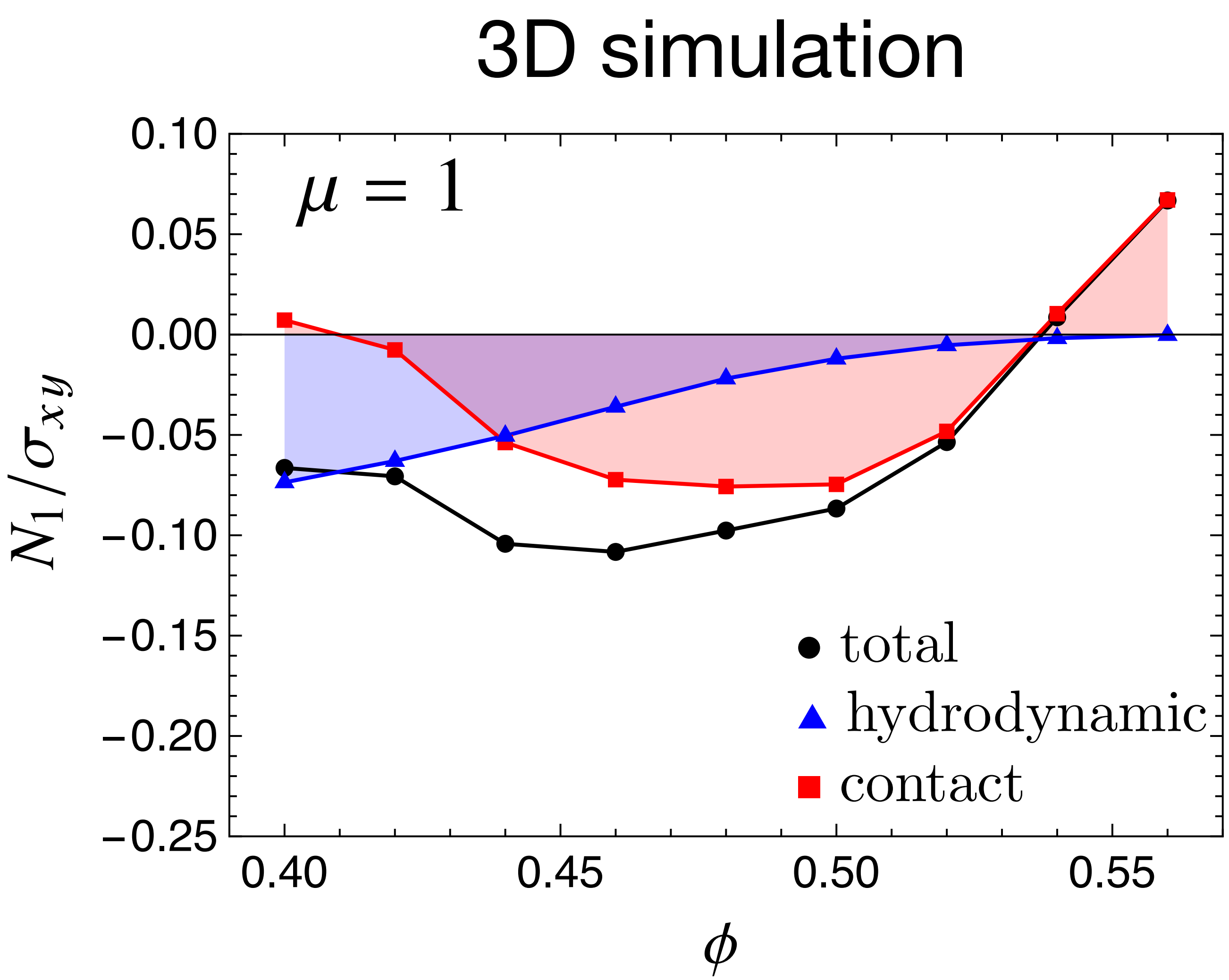


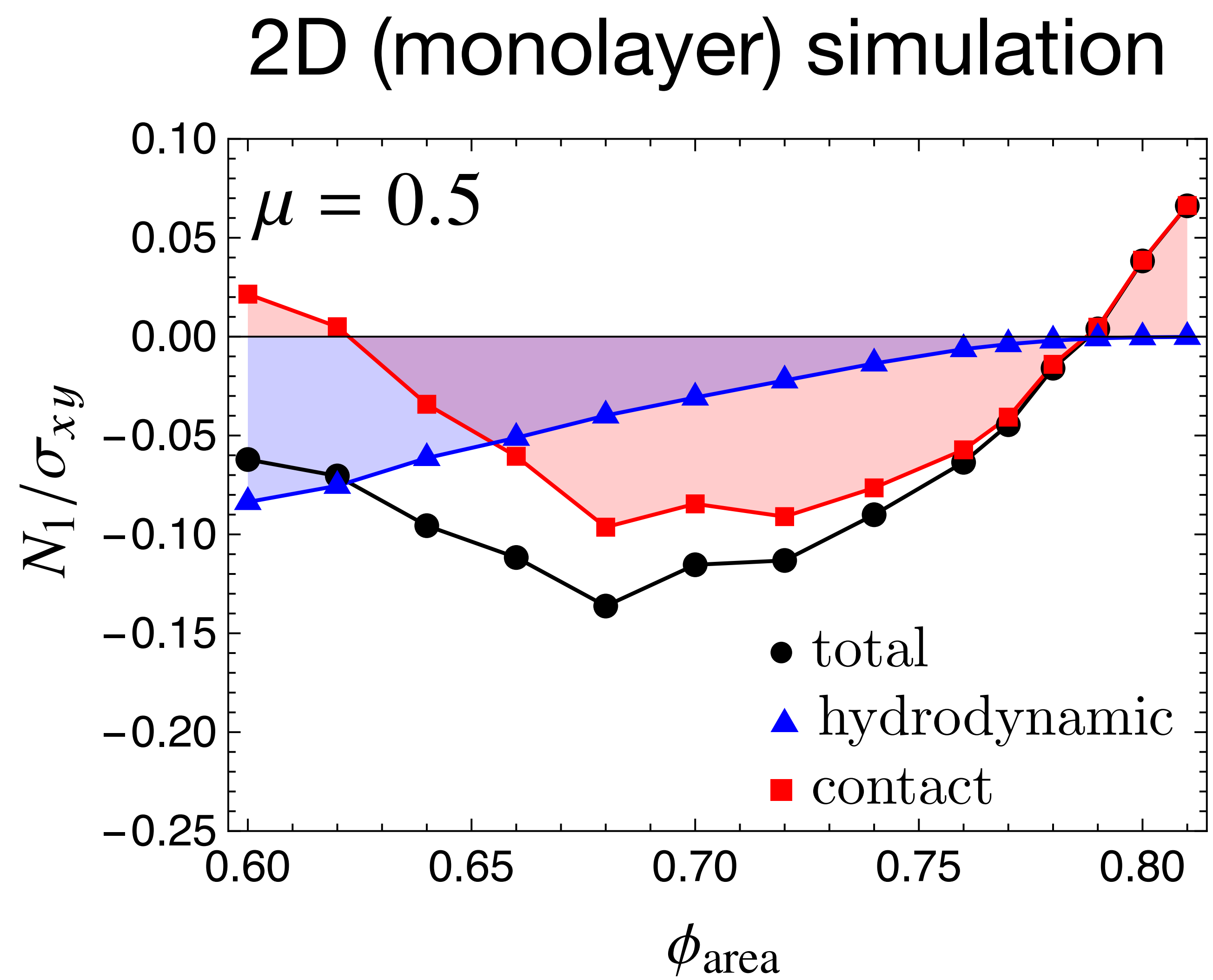
With
hydrodynamics interaction
(frictionless)



→ Hydrodynamic interaction may be essential for the microstructure giving the negative N_1.

Monolayer simulation gives similar results





2D (monolayer) simulations
are easier for visualization and data analysis.

Approximation of N_1 using only normal forces

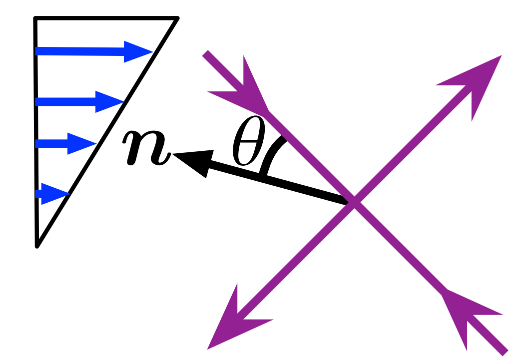
$$\bar{F}_{ij} \equiv -\boldsymbol{F}^{(ij)} \cdot \boldsymbol{n}^{(ij)}$$
$$\bar{\boldsymbol{F}}^{(ij)} = \bar{F}_{ij}\boldsymbol{n}^{(ij)}$$

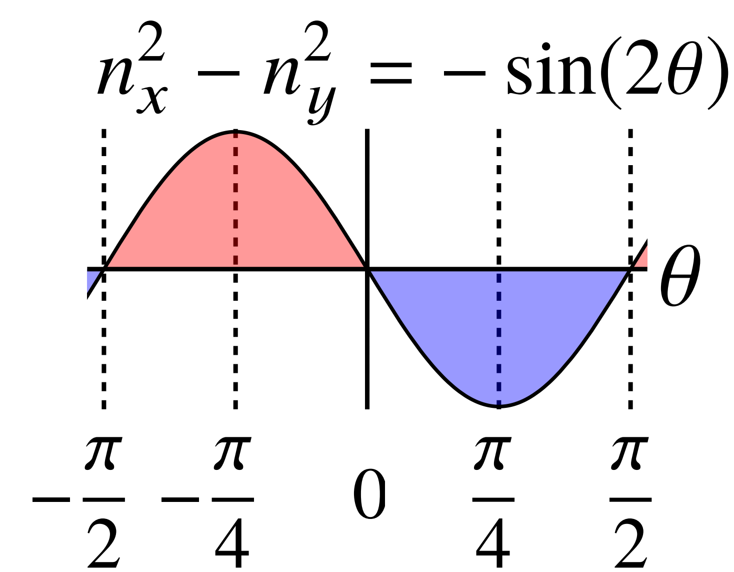
Stress tensor using only normal forces

$$\tilde{\boldsymbol{\sigma}} \equiv -p\mathsf{I} + 2\eta_0\mathsf{D} + V^{-1}\sum_{i>j}(\boldsymbol{r}^j - \boldsymbol{r}^i)\bar{\boldsymbol{F}}^{(ij)}$$

First normal stress difference using only normal forces

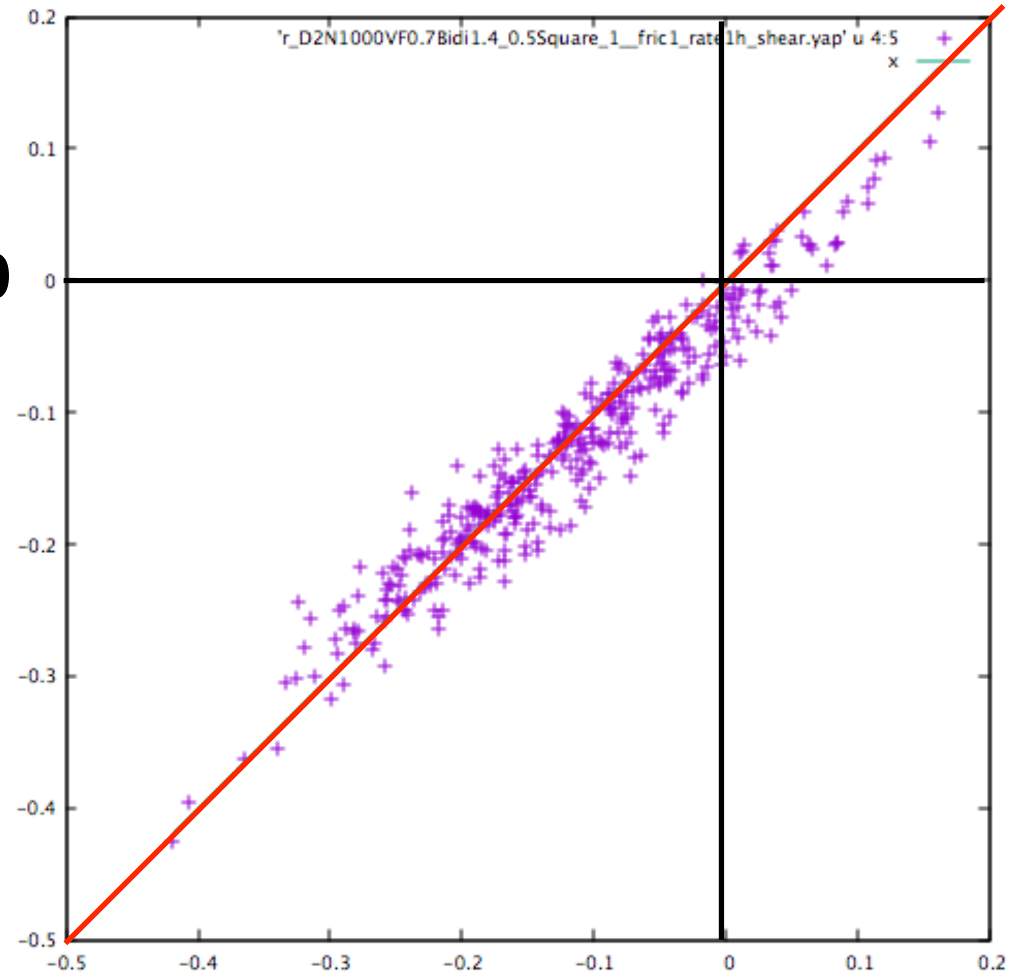
$$\begin{aligned}\tilde{N}_1 &\equiv \tilde{\sigma}_{xx} - \tilde{\sigma}_{yy} \\ &= V^{-1}\sum_{i>j} r_{ij}\bar{F}_{ij}\left[\left(n_x^{(ij)}\right)^2 - \left(n_y^{(ij)}\right)^2\right] \\ &= V^{-1}\sum_{i>j}\left(-r_{ij}\bar{F}_{ij}\sin 2\theta_{ij}\right) \\ &= \sum_{i>j}\tilde{N}_1^{ij}\end{aligned}$$



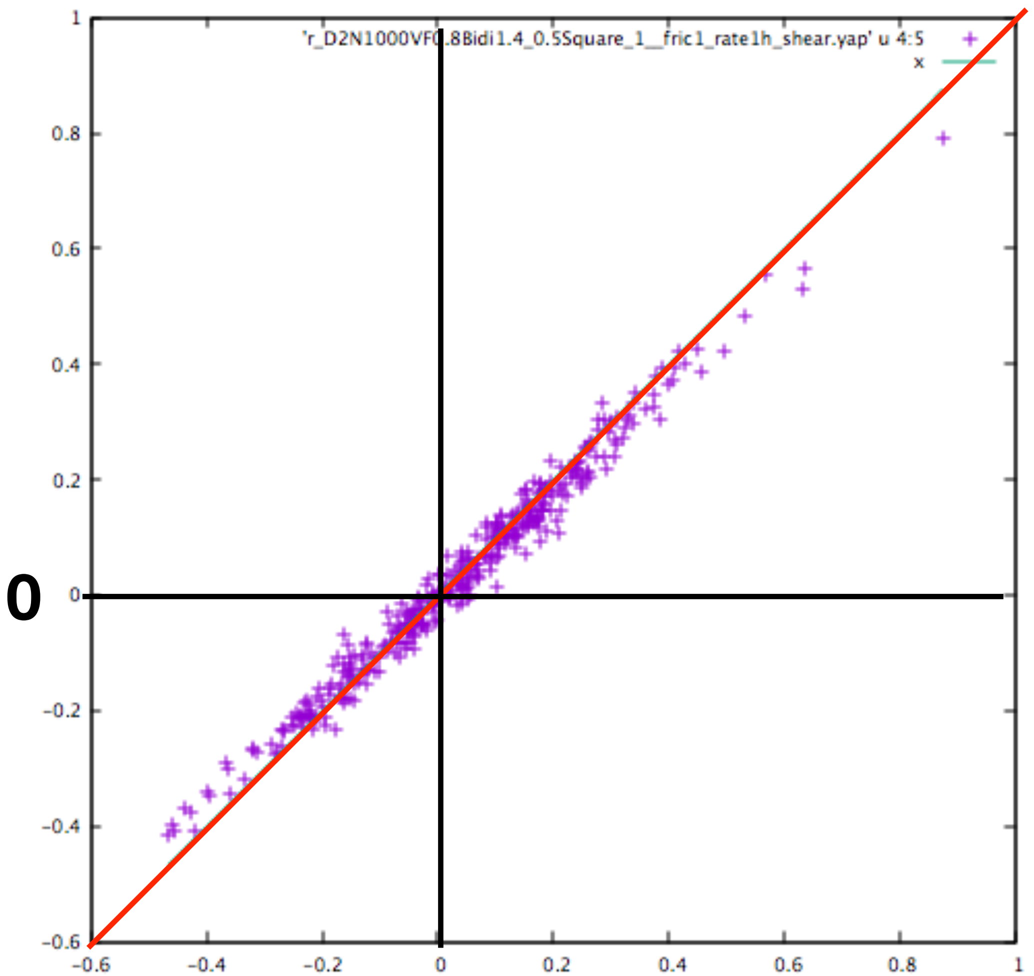


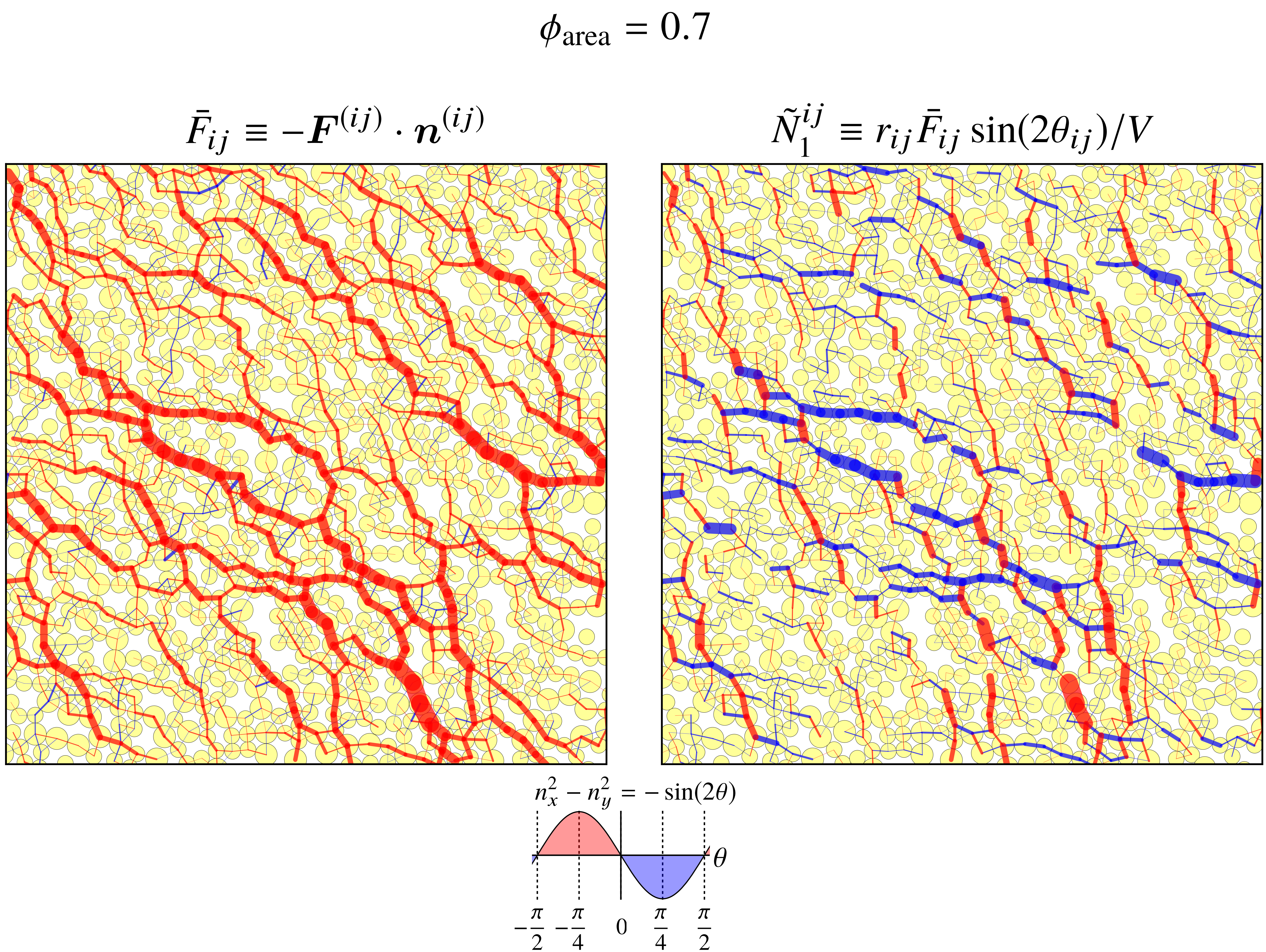
The approximated N_1 works

$\phi_{\text{area}} = 0.7$

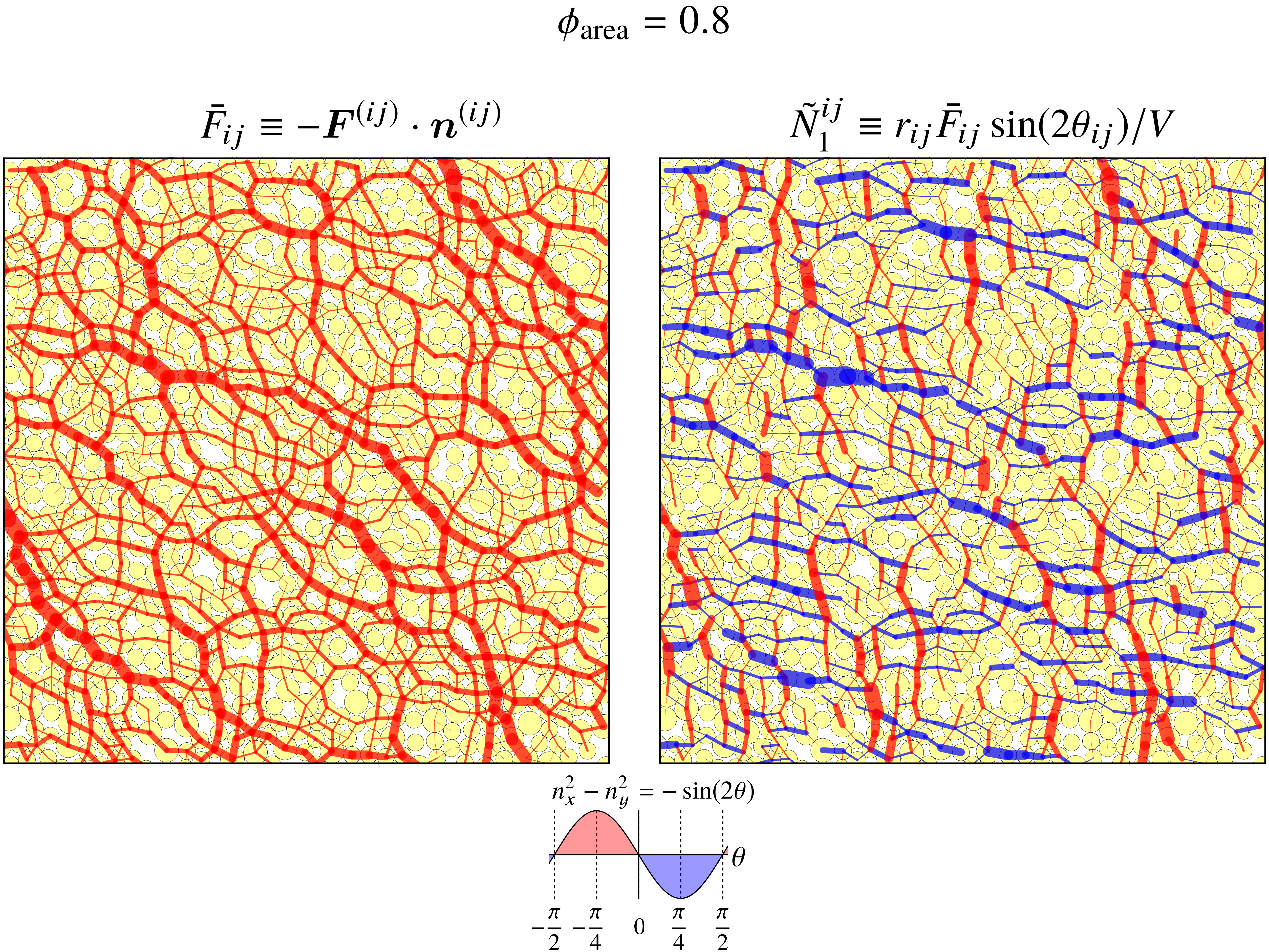


$\phi_{\text{area}} = 0.8$





$\phi_{\mathrm{area}} = 0.7$
$\bar{F}_{ij} \equiv -\boldsymbol{F}^{(ij)} \cdot \boldsymbol{n}^{(ij)}$
$\tilde{N}_1^{ij} \equiv r_{ij} \bar{F}_{ij} \sin(2\theta_{ij})/V$
$n_x^2 - n_y^2 = -\sin(2\theta)$
θ
$-\frac{\pi}{2}$
$-\frac{\pi}{4}$
0
$\frac{\pi}{4}$
$\frac{\pi}{2}$

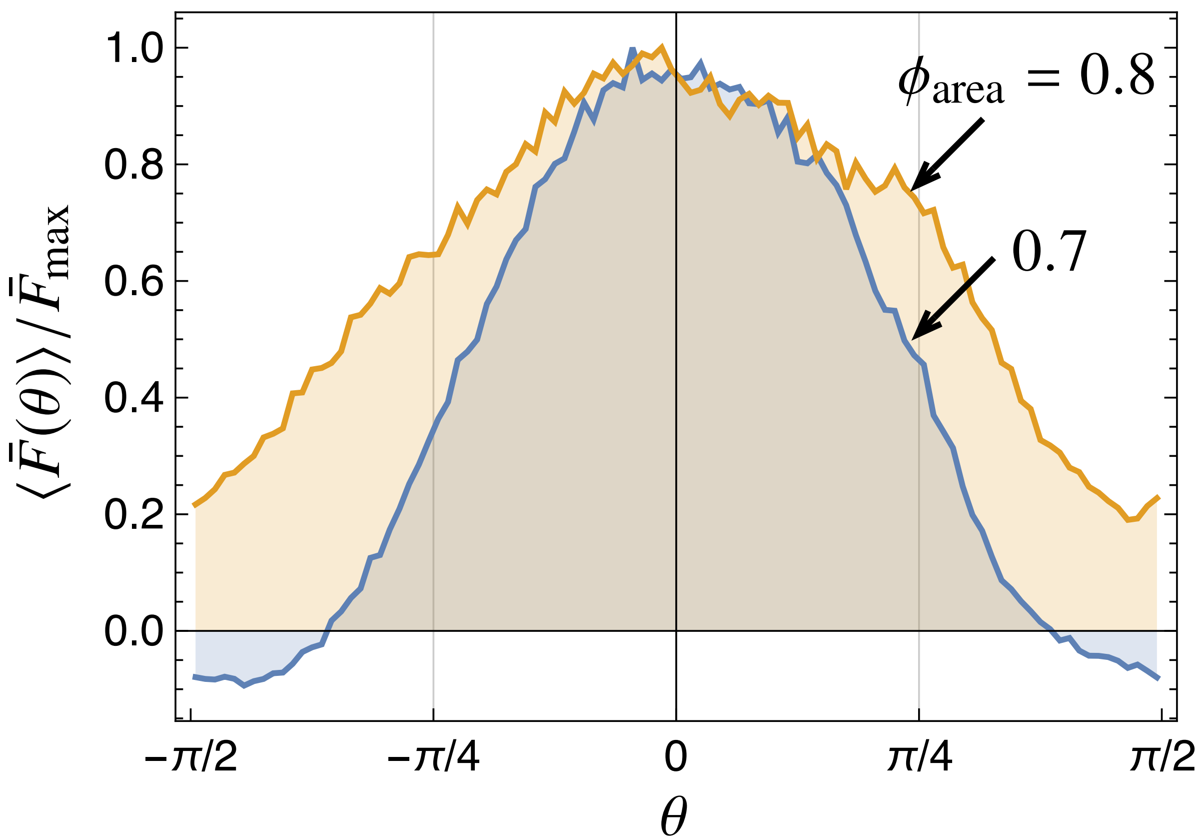


$\phi_{\text{area}} = 0.8$
$\bar{F}_{ij} \equiv -\boldsymbol{F}^{(ij)} \cdot \boldsymbol{n}^{(ij)}$
$\tilde{N}_1^{ij} \equiv r_{ij} \bar{F}_{ij} \sin(2\theta_{ij})/V$
$n_x^2 - n_y^2 = -\sin(2\theta)$
θ
$-\frac{\pi}{2}$
$-\frac{\pi}{4}$
0
$\frac{\pi}{4}$
$\frac{\pi}{2}$

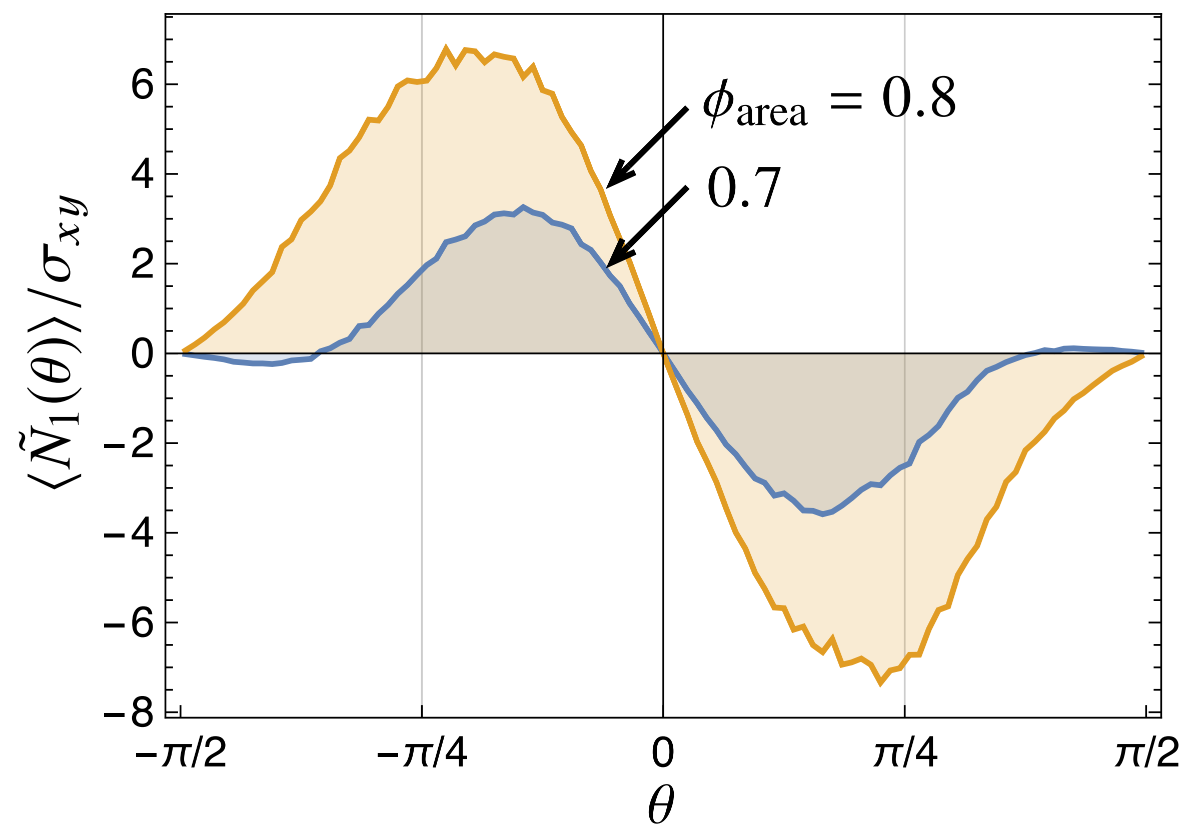
Angular distribution

normal force

$$\bar{F}_{ij} \equiv -\boldsymbol{F}^{(ij)} \cdot \boldsymbol{n}^{(ij)}$$

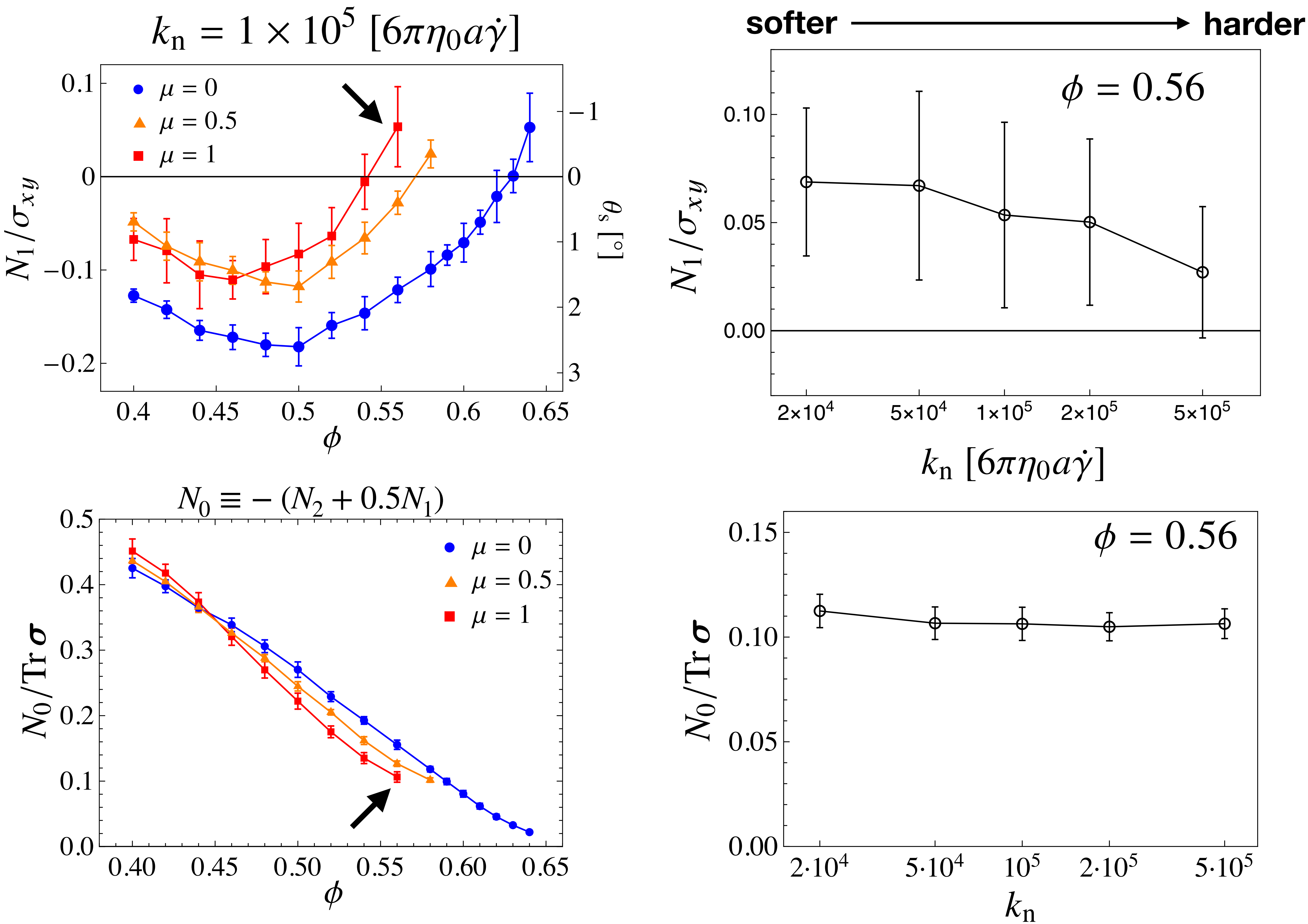


$$\tilde{N}_1^{ij} / \sigma_{xy}$$

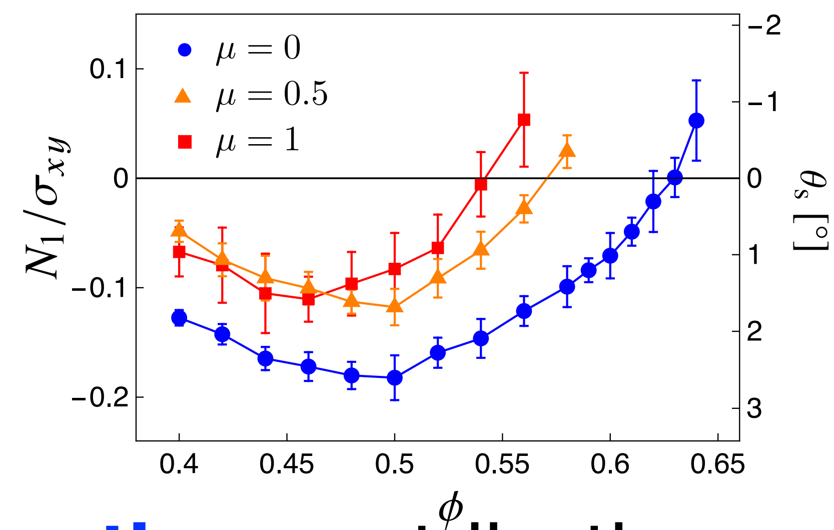


$$N_1 \approx \frac{1}{\pi} \int_{-\pi/2}^{\pi/2} \langle \tilde{N}_1(\theta) \rangle \mathrm{d}\theta$$

Anisotropies exist at jamming points of hard spheres?



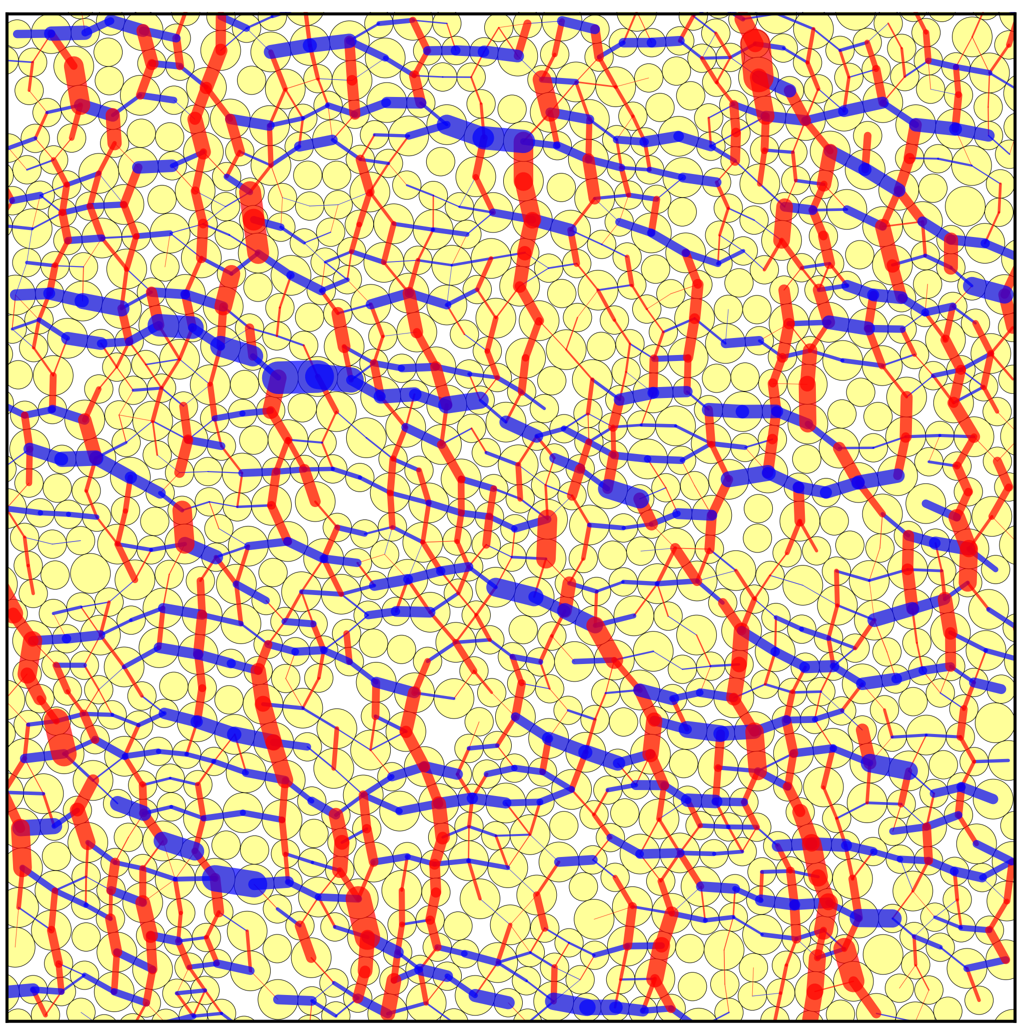
Summary

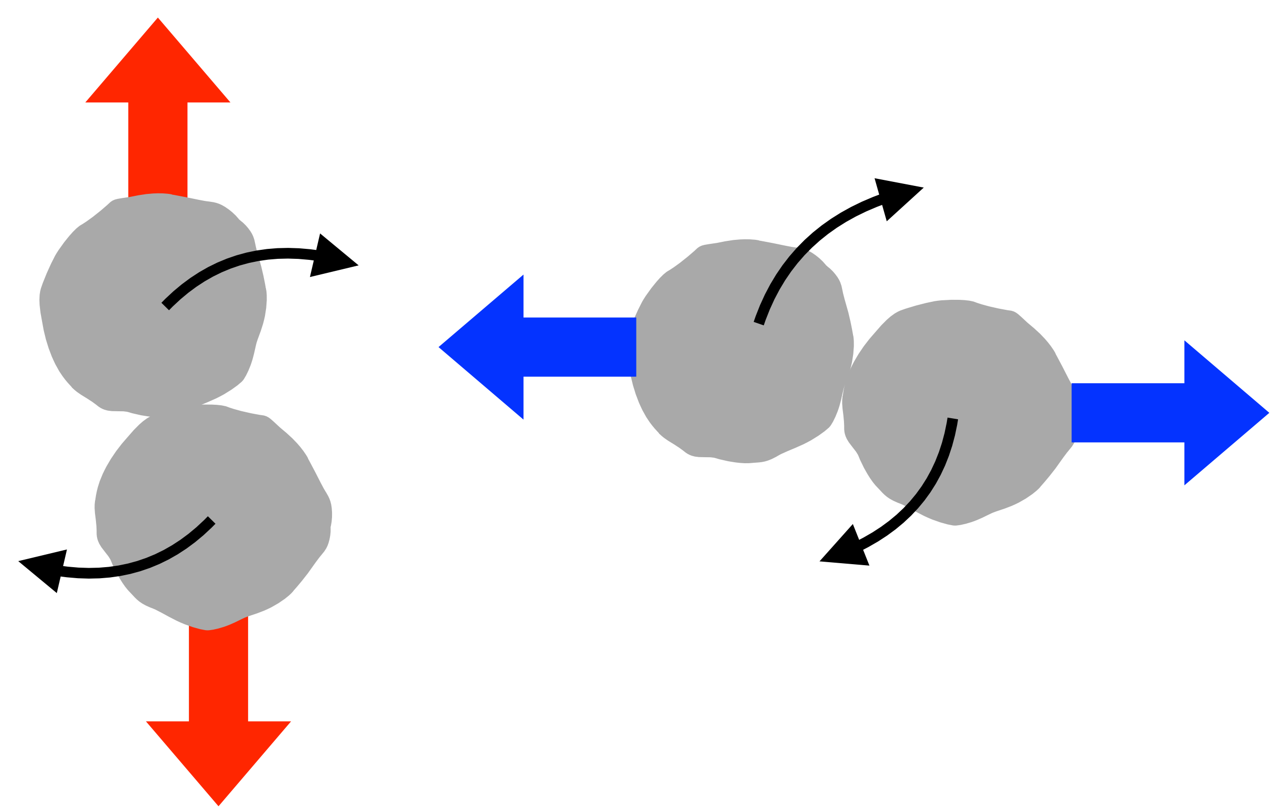


Smallness of the reorientation angle.
(Observed finite N_1 due to high shear stress)

Large N_1 fluctuation around zero
due to competition between **positive** and **negative** contributions

Positive N_1 in simulation is due to softness of particles.





Seto and Giusteri, arXiv:1806.09423