Rheology of dense suspensions under oscillatory shear with lattice Boltzmann Method

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Physics of Jammed Matter
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Suspensions

→ **particle radius** $a \approx 1 - 100\mu m$ → **Stokes Equation**

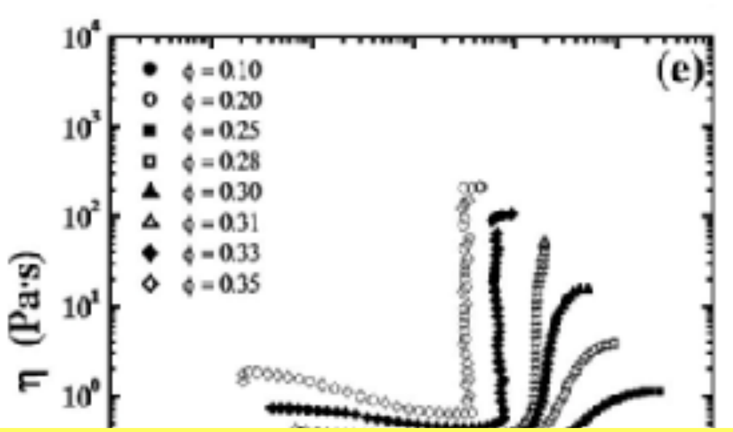
$$\eta \nabla^2 \mathbf{u} = \nabla p$$
$$\nabla \cdot \mathbf{u} = 0$$

Discontinuous shear thickening!

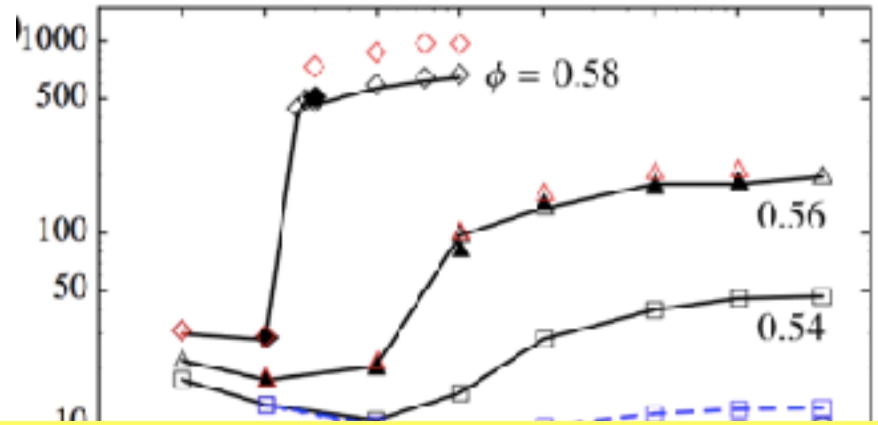
source: https://www.youtube.com/watch?v=hP88C-_LgnE&list=PLVjiIPzFTOLpxiwdwrFuPYSIBpr6jFm32

STEADY SHEAR

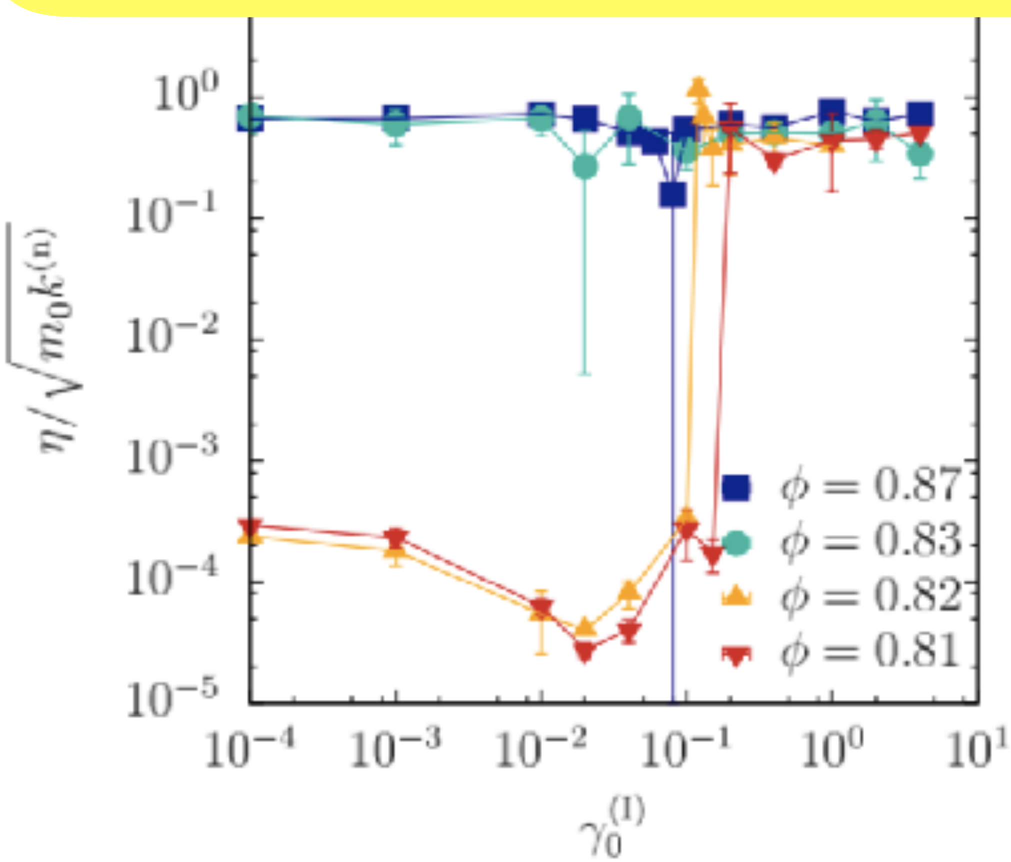
Experimental Observation:



Numerical Simulations:

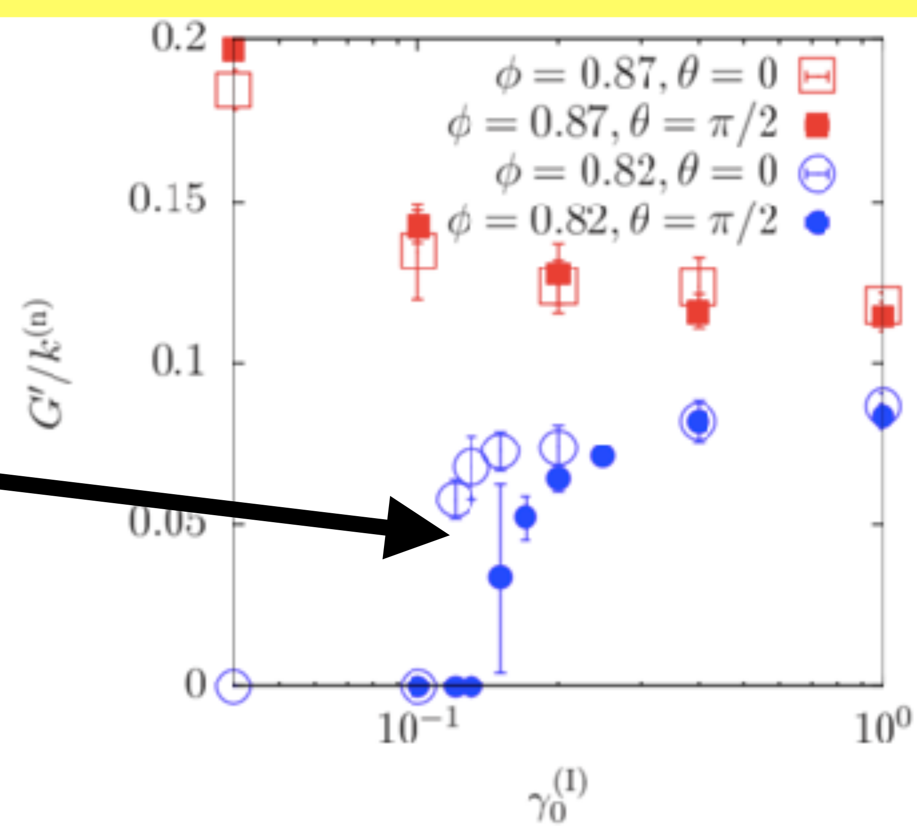


WHAT HAPPEN IF WE IMPOSE OSCILLATORY SHEAR TO SUSPENSIONS?



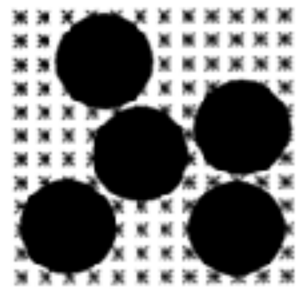
Phase dependence

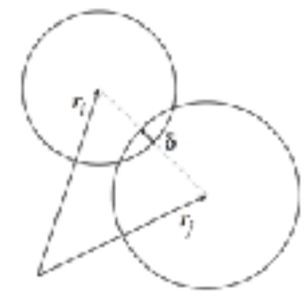
Fragile state

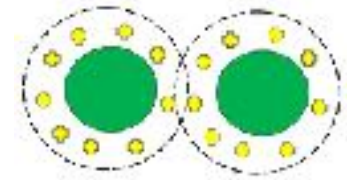


Lattice Boltzmann Method (LBM)

Hydrodynamics + **Contact** + **Electrostatic repulsive force**







Equation of motion

$$m \cdot \frac{d}{dt}\begin{pmatrix}\mathbf{U}\\ \mathbf{\Omega}\end{pmatrix} = \sum_{\alpha}\begin{pmatrix}\mathbf{F}_{\alpha}\\ \mathbf{T}_{\alpha}\end{pmatrix} \qquad \sum_{\alpha}\mathbf{F}_{\alpha} = \mathbf{F}^{h} + \mathbf{F}^{c} + \mathbf{F}^{R}$$

Ladd's LBM A.J.C Ladd, JFM, **271,**285-339 (1994)

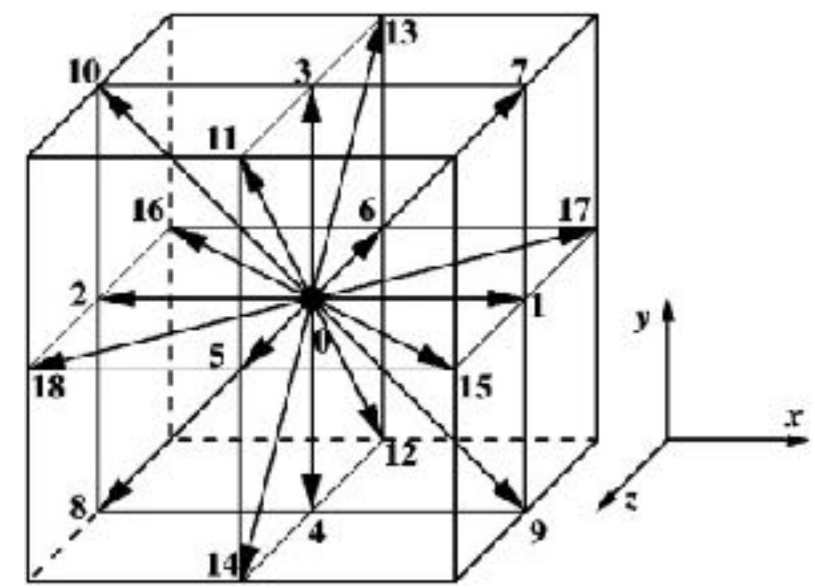
$$n_i(\mathbf{r}+\mathbf{c}_i, t+1) = n_i(\mathbf{r},t) + \Delta_i(\mathbf{r},t)$$

discrete velocity distribution function on lattice

discrete velocity

Streaming

Collision



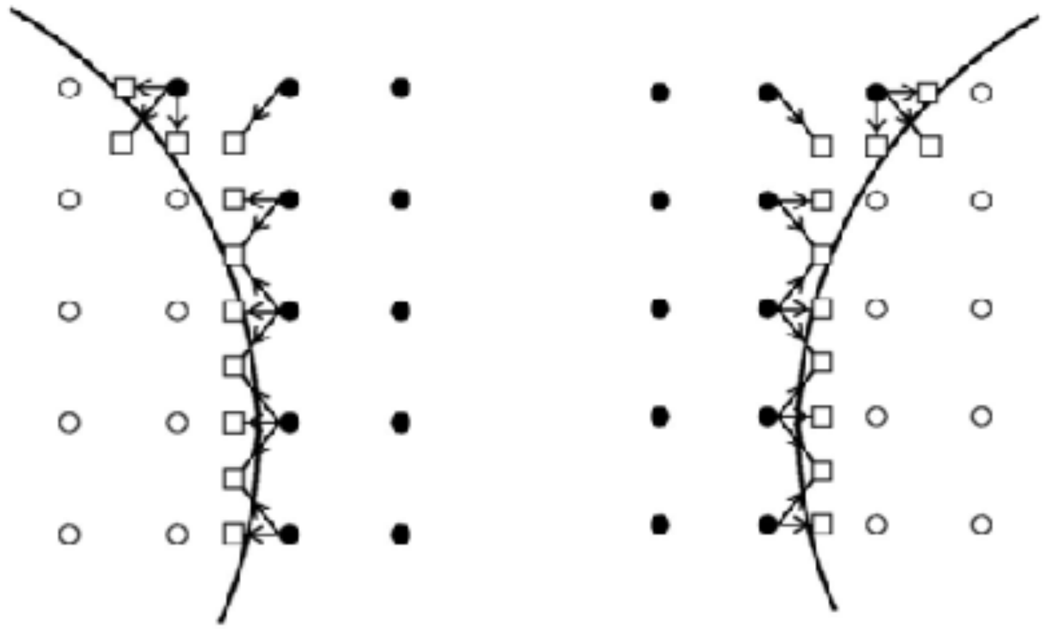
mass density $\rho = \sum_i n_i$

momentum density $\mathbf{j} = \sum_i n_i \mathbf{c}_i$

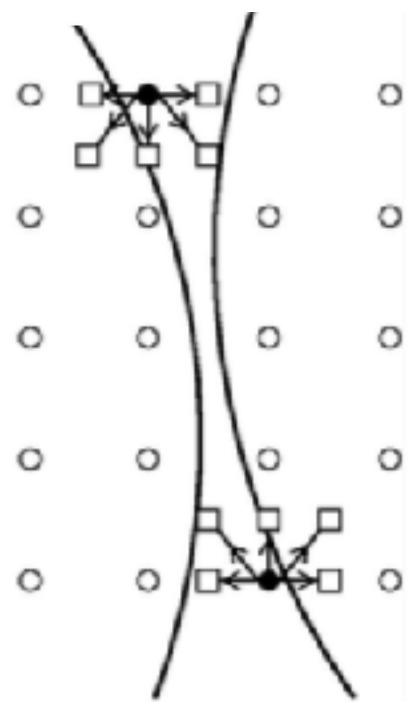
momentum flux $\Pi = \sum_i n_i \mathbf{c}_i \mathbf{c}_i$

Treatment of hydrodynamics and contact forces

Forces on boundary nodes →



shared nodes →



→ ***Use resistance matrix formulation for the lubrication forces***

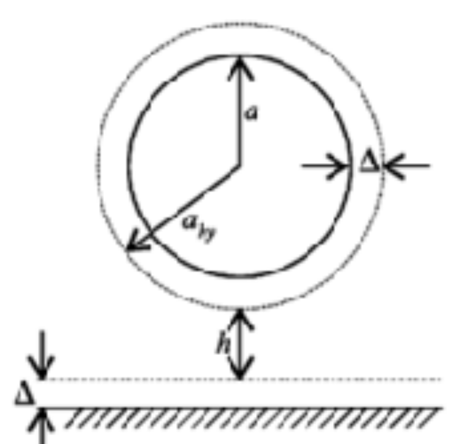
(Kim and Karilla, 1991)

Nguyen and Ladd, PRE **66**, 046708,(2002)

Contact

Linear spring model used in DEM (with friction)

Luding, Granular Matter **10**:235–246 , (2008)



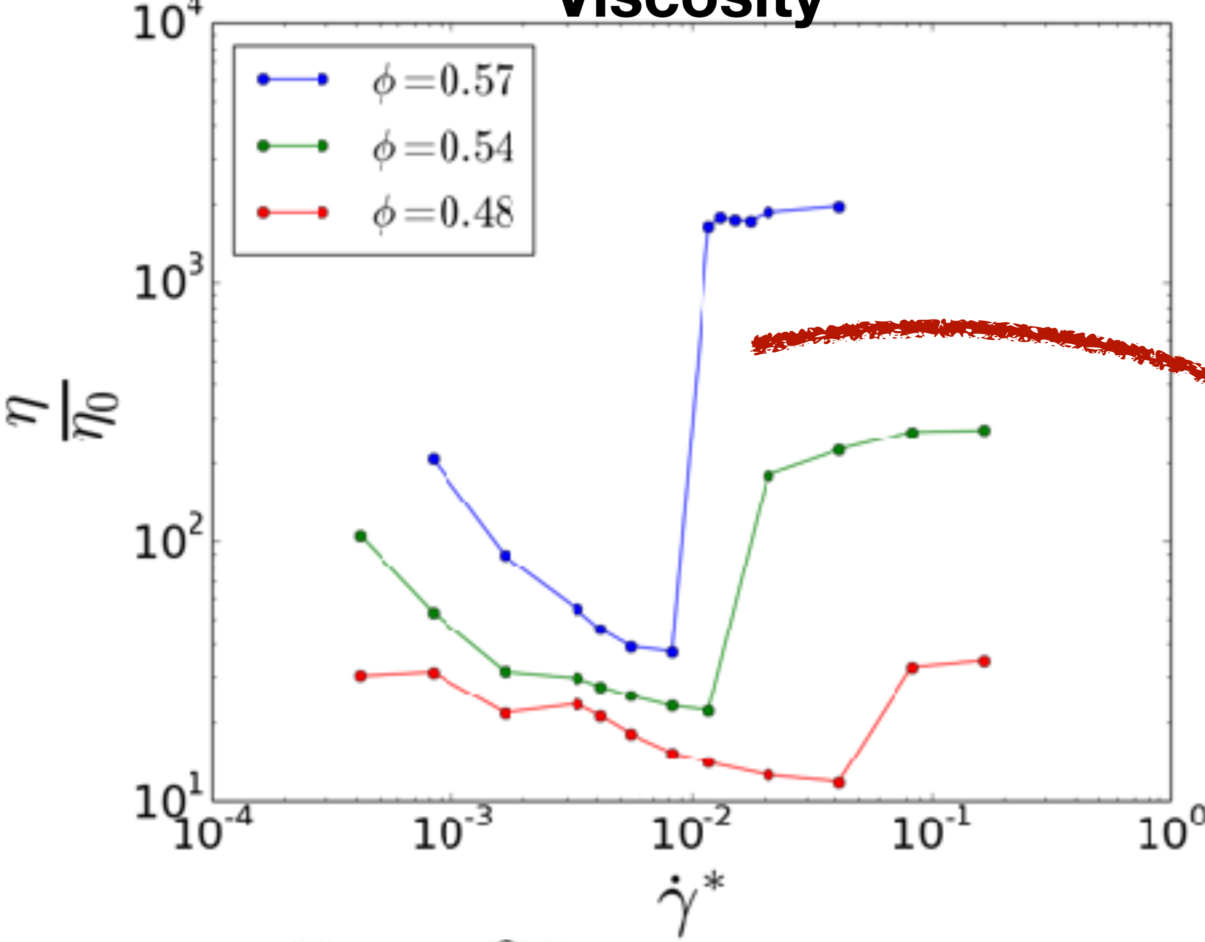
→ **Lubrication vanishes at some distances to allow contact**

$$\Delta = \frac{a_{\mathrm{contact}} - a_{\mathrm{hydro}}}{a_{\mathrm{contact}}}$$

Steady shear simulation

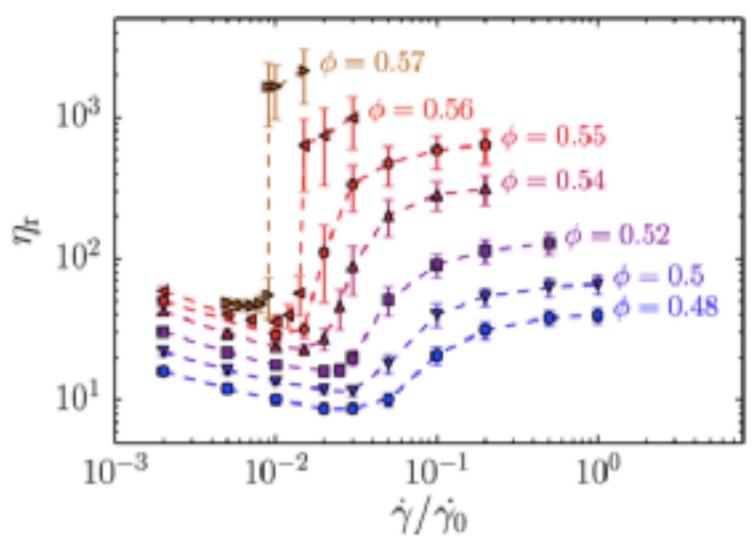
N=512 particles

Viscosity



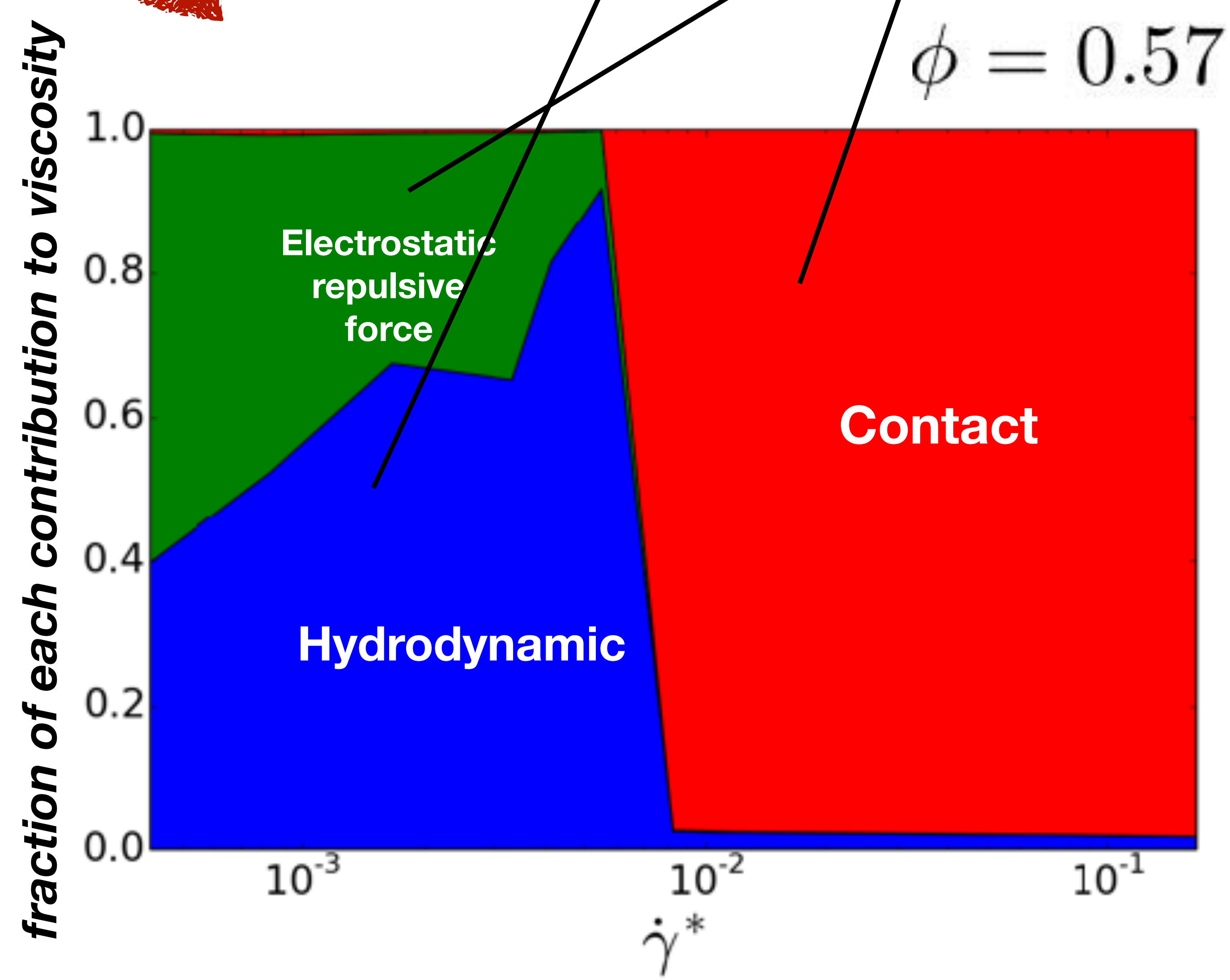
$$\dot{\gamma}^* = \frac{6\pi\eta_0 a^2 \dot{\gamma}}{F^{er}}$$

Magnitude of electrostatic repulsive forces



Mari, et al, Journal of Rheology **58 (6)** , 1693-1724(2014)

Shear stress $\sigma = \sigma^h + \sigma^c + \sigma^r$



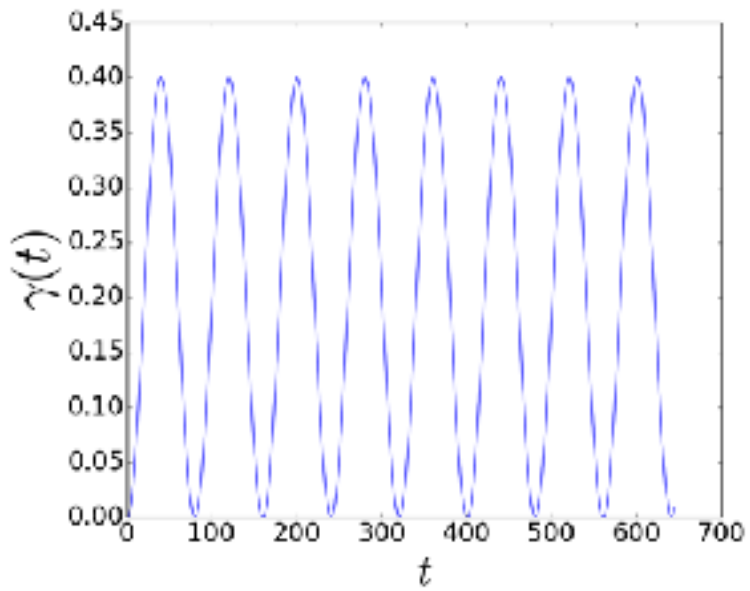
Oscillatory shear simulation

Strain

$$\gamma(t) = \gamma_0(\cos\theta - \cos(\omega t + \theta))$$

Strain rate

$$\dot{\gamma}(t) = \gamma_0 \omega \sin(\omega t + \theta)$$



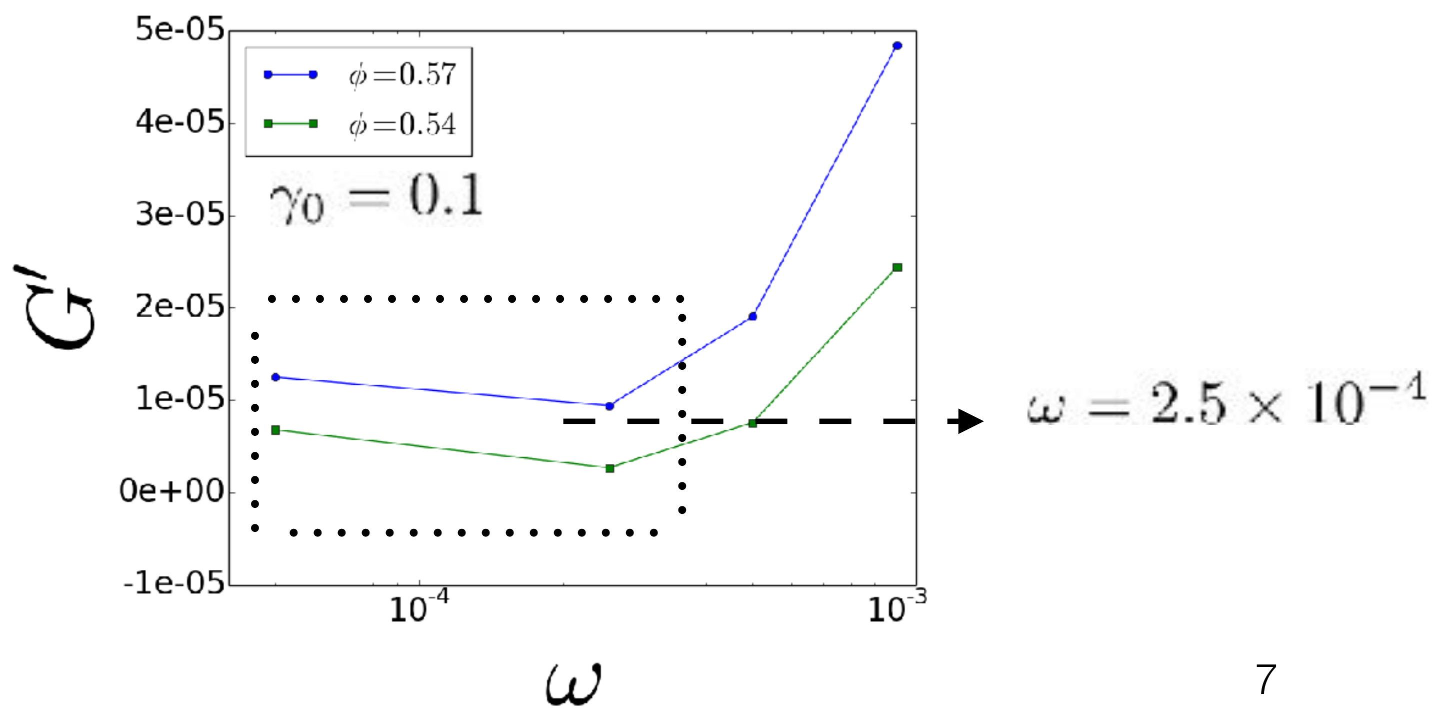
Storage modulus

$$G' = -\frac{\omega}{\pi}\int_0^{2\pi/\omega} dt \frac{\sigma(t)\cos(\omega t + \theta)}{\gamma_0}$$ **rigidity**

Loss modulus

$$G'' = \frac{\omega}{\pi}\int_0^{2\pi/\omega} dt \frac{\sigma(t)\sin(\omega t + \theta)}{\gamma_0}$$ **viscosity**

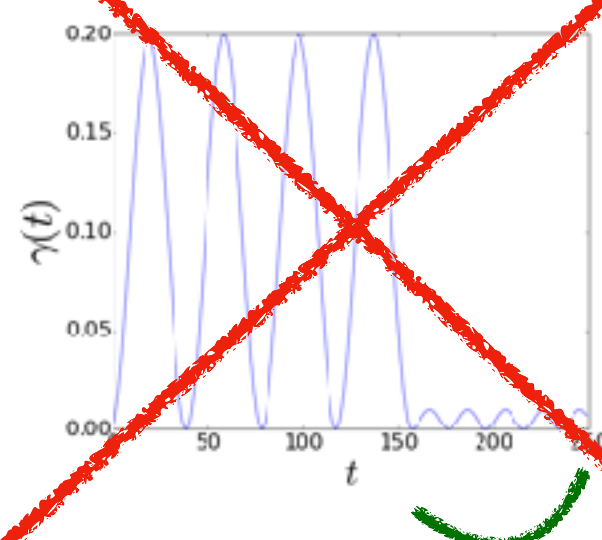
ω dependence



Michio Otsuki's protocol

using initial strain amplitude γ_0^I

$\gamma_0 = 10^{-1}$ **(very small for observation)**

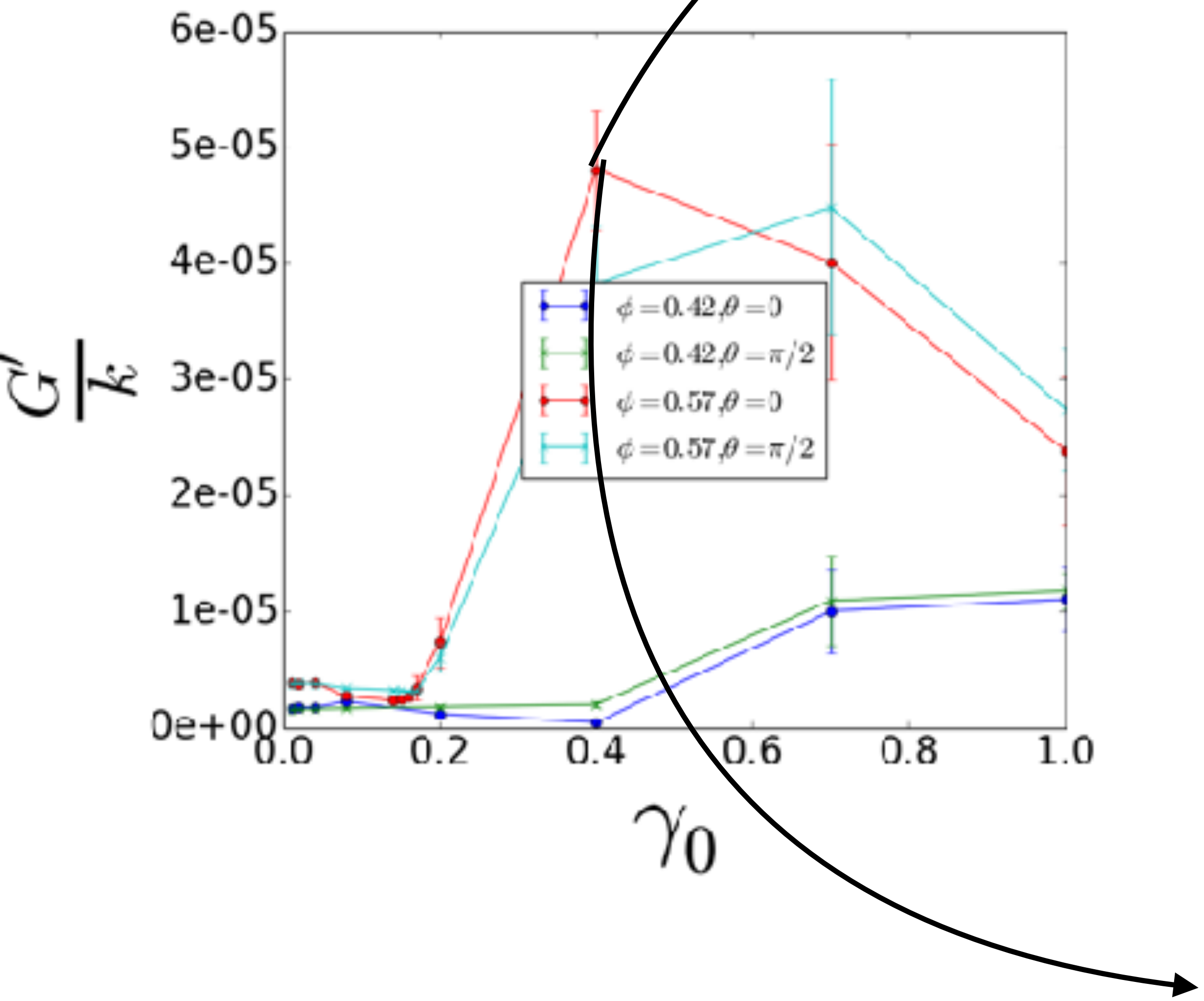


observation

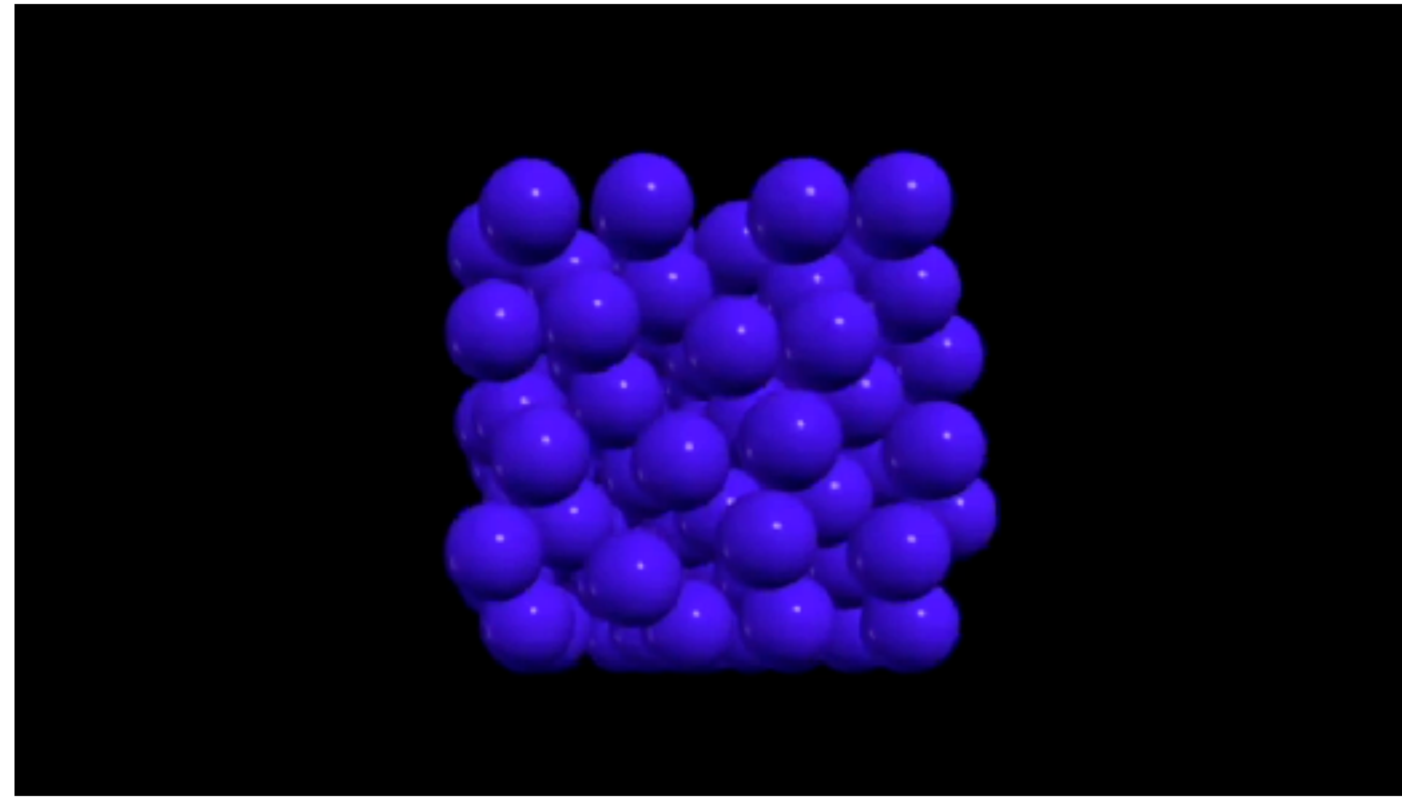
no contact observed during observation by using this protocol!

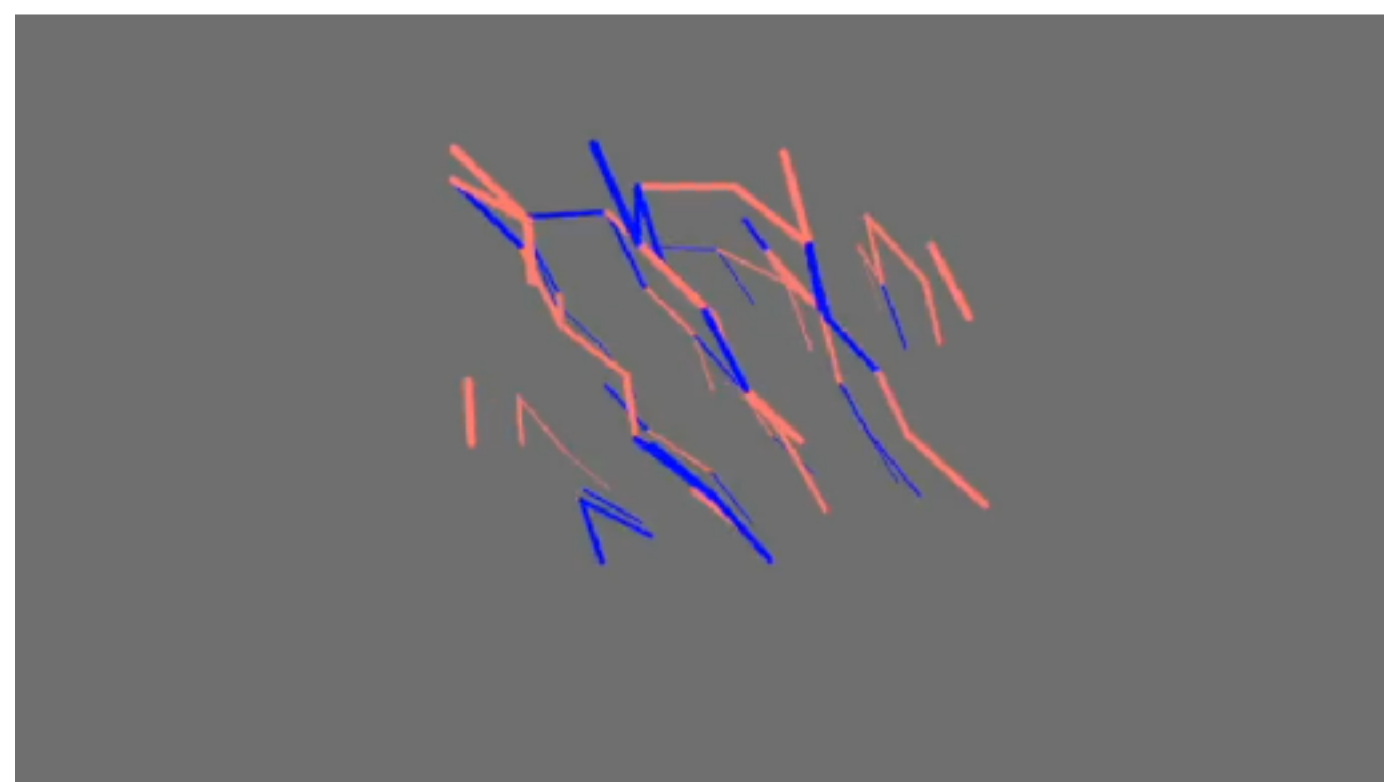
Oscillatory shear simulation

N=128 particles



Particle motion

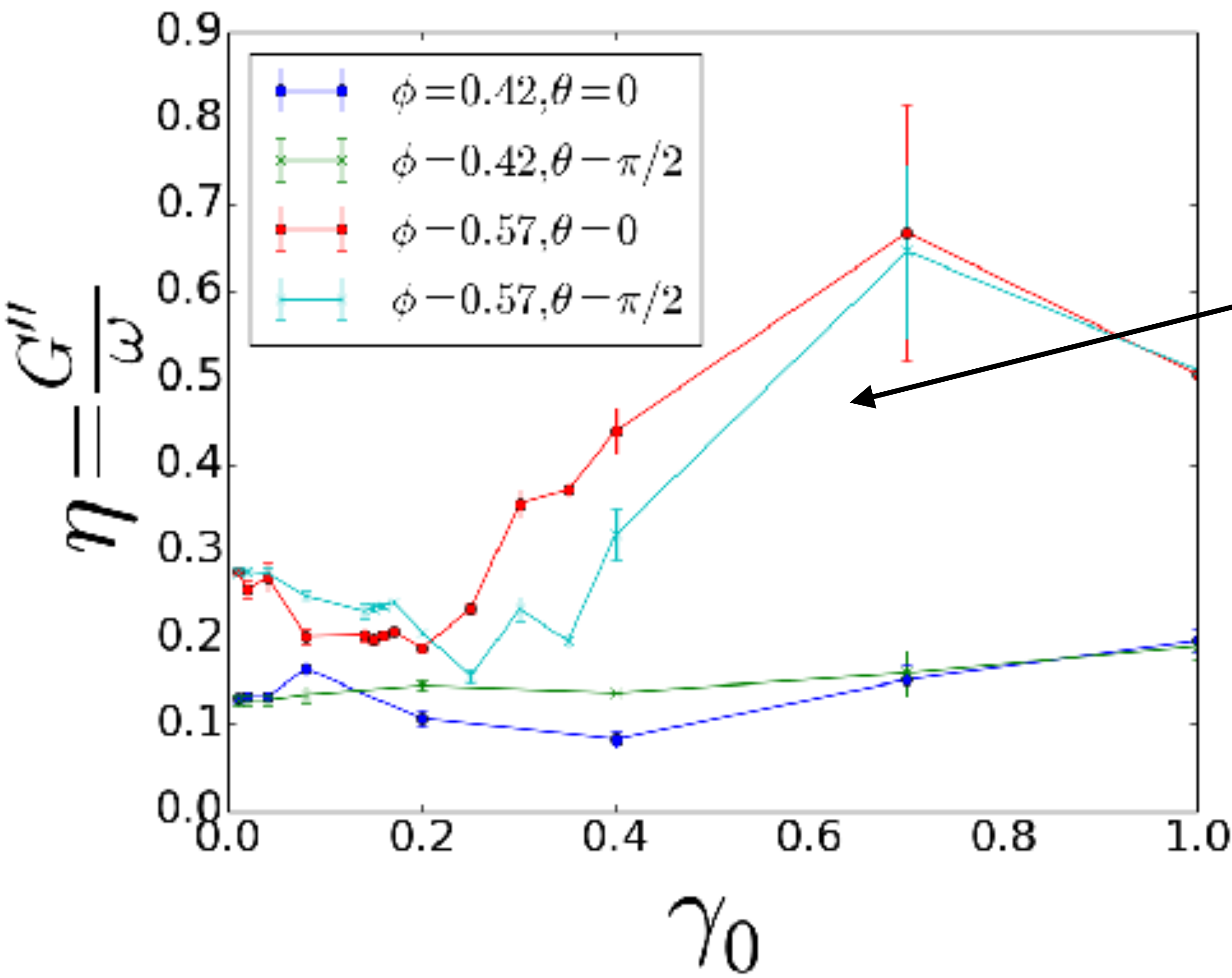




Contact network

Viscosity   N=128 particles

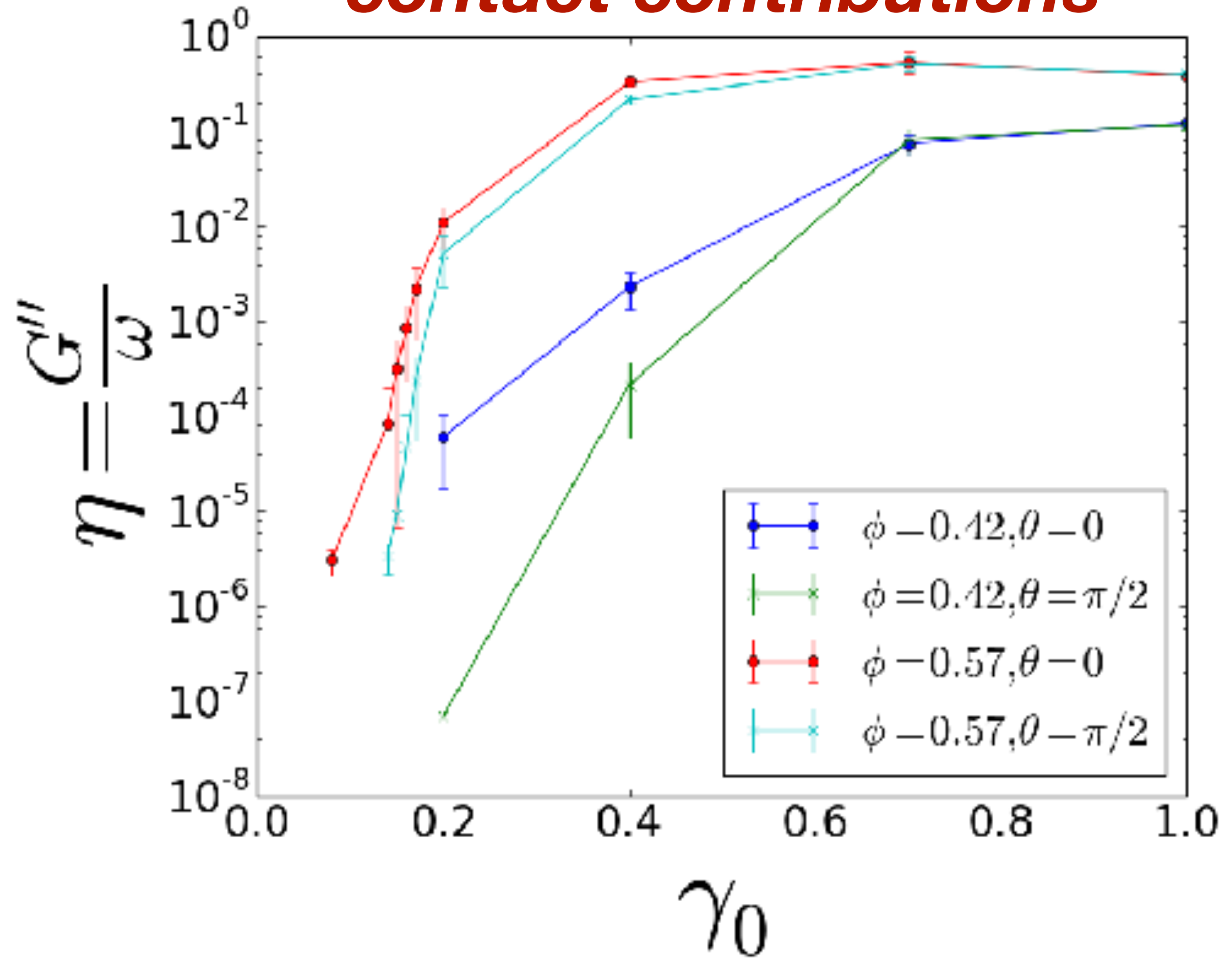
all contributions



No discontinuous jump

Hydrodynamics is still strong

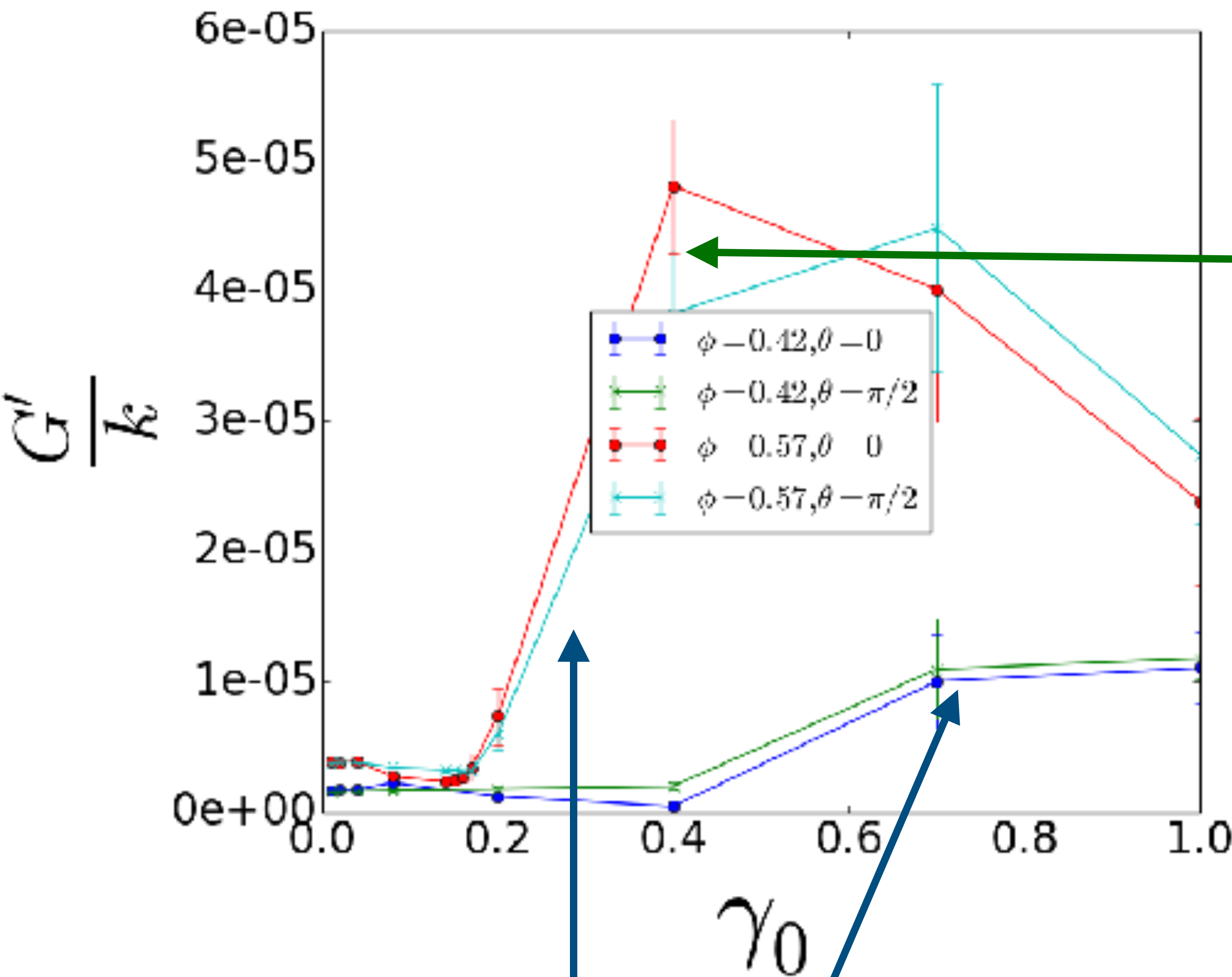
contact contributions



Thickening is caused by contact

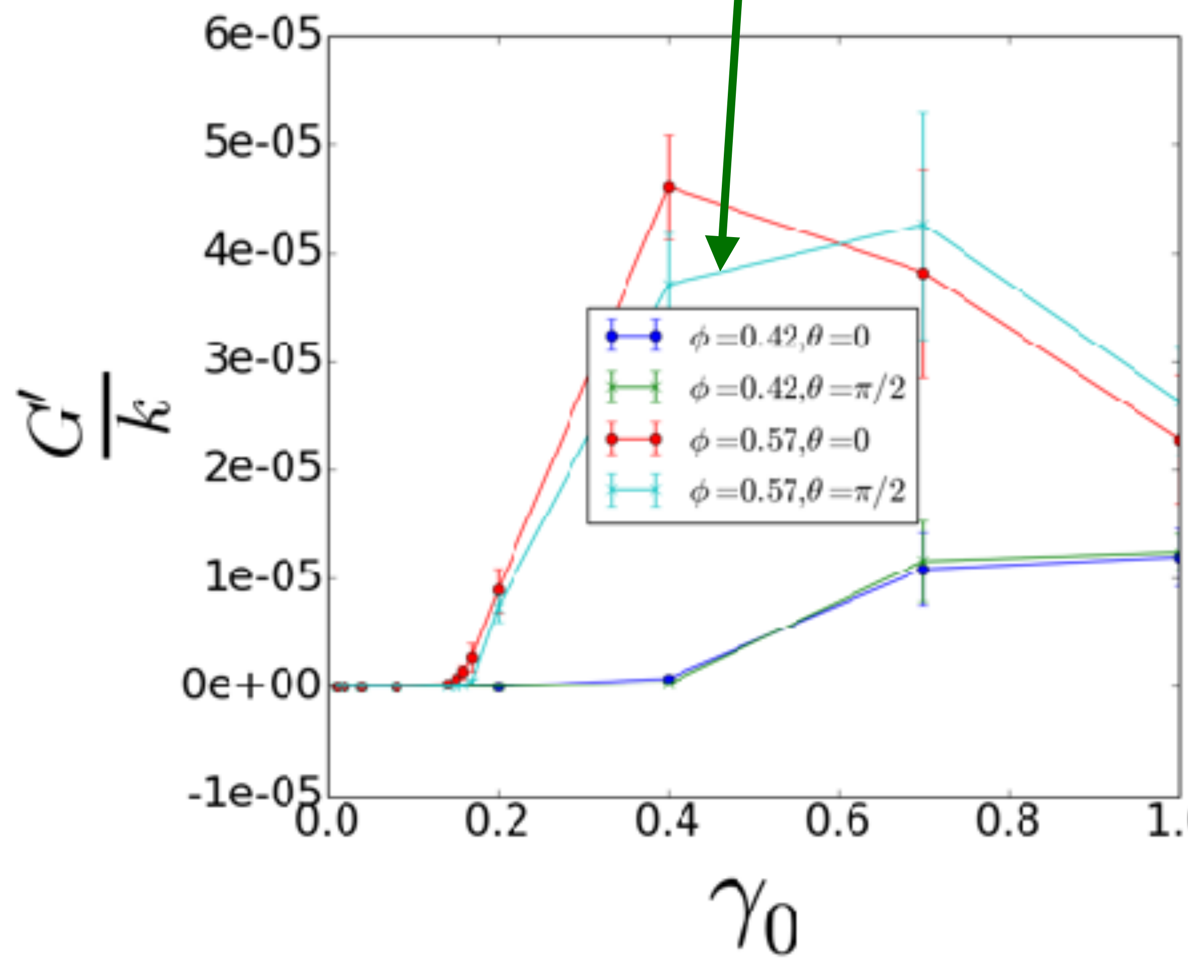
Storage modulus N=128 particles

all contributions



phase dependence ?

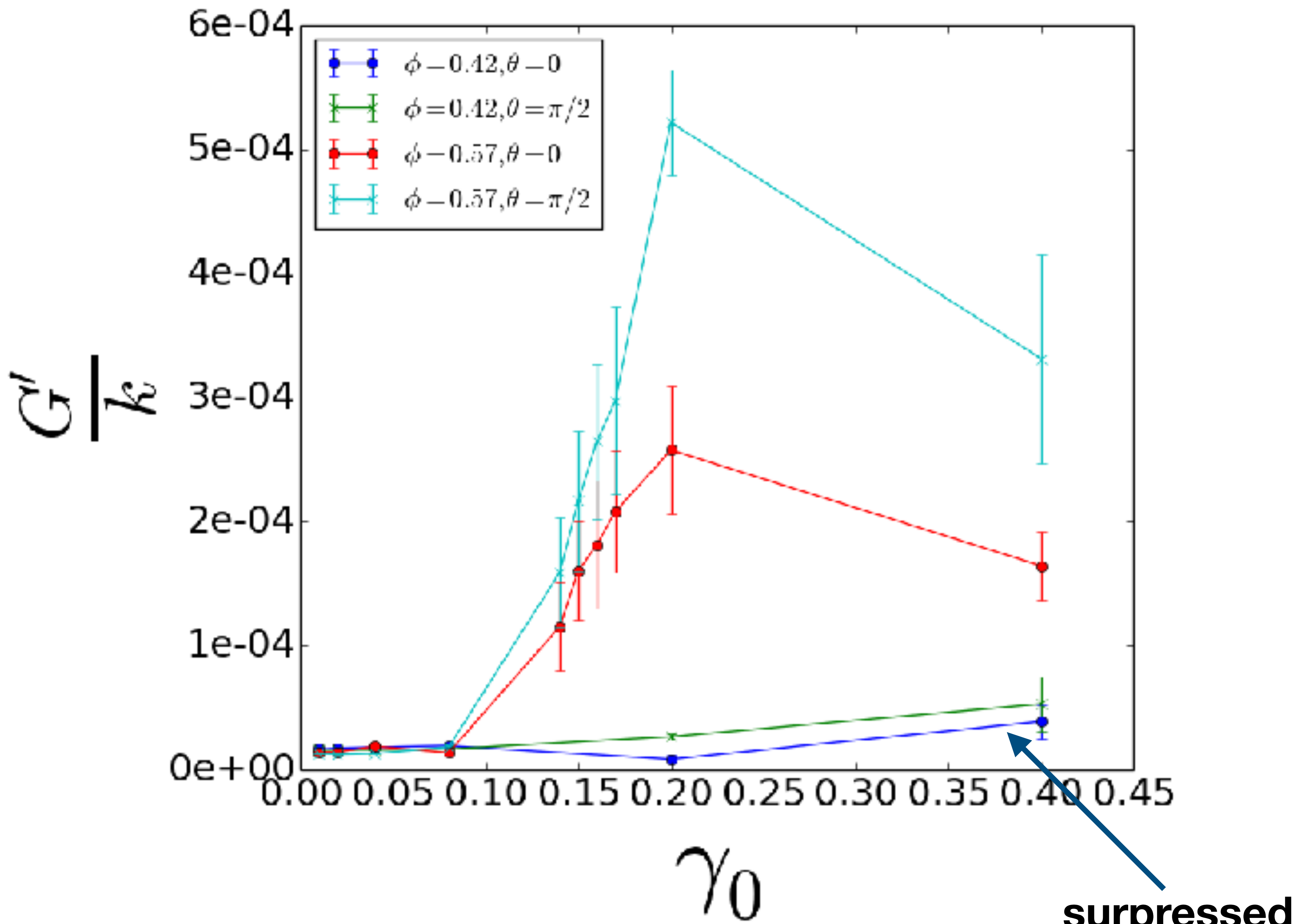
shear jamming ?



Dominated by contact

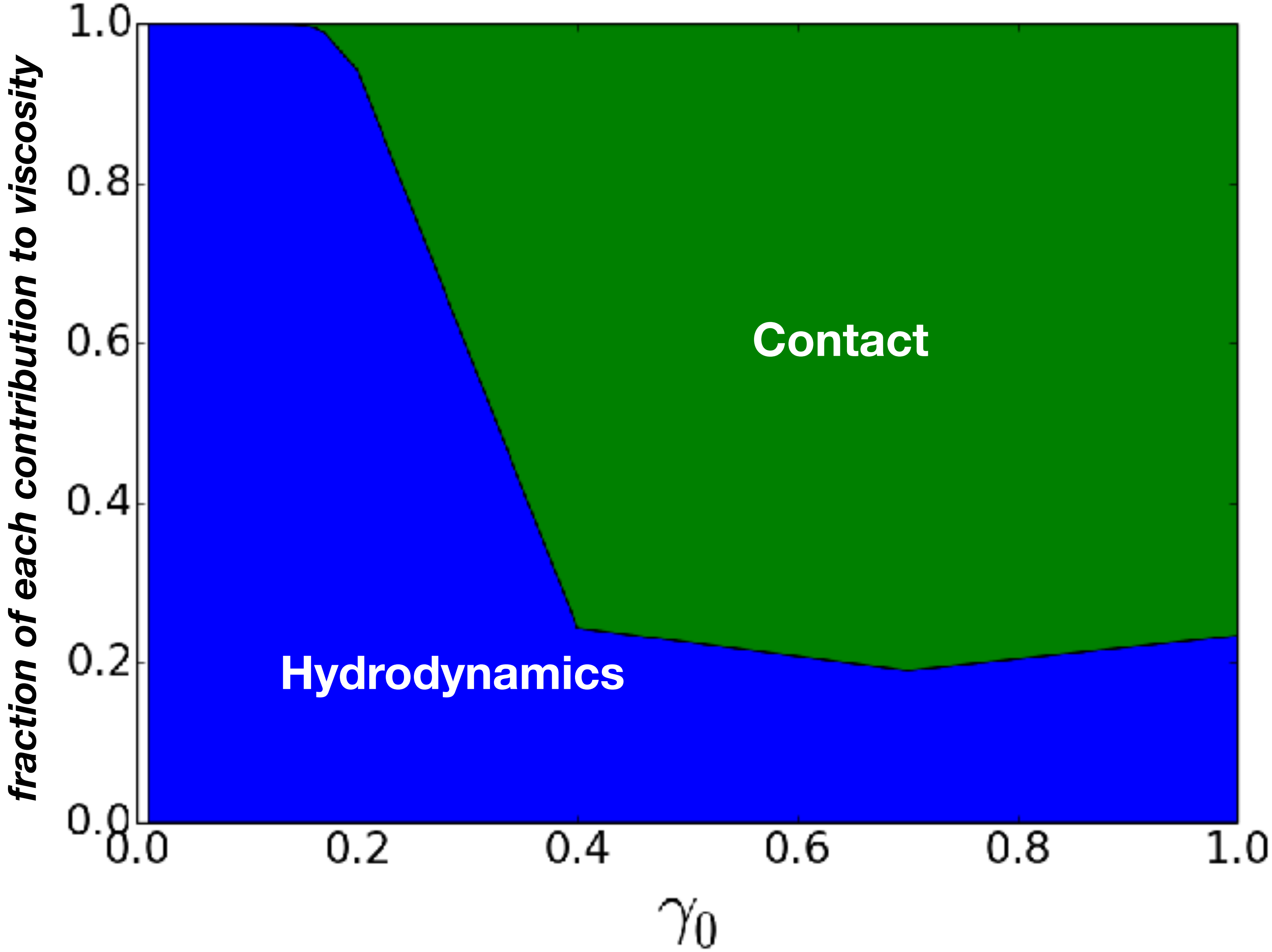
Contact contributions

Storage modulus   N=512 particles



shear jamming in low density was fake! (size dependence)

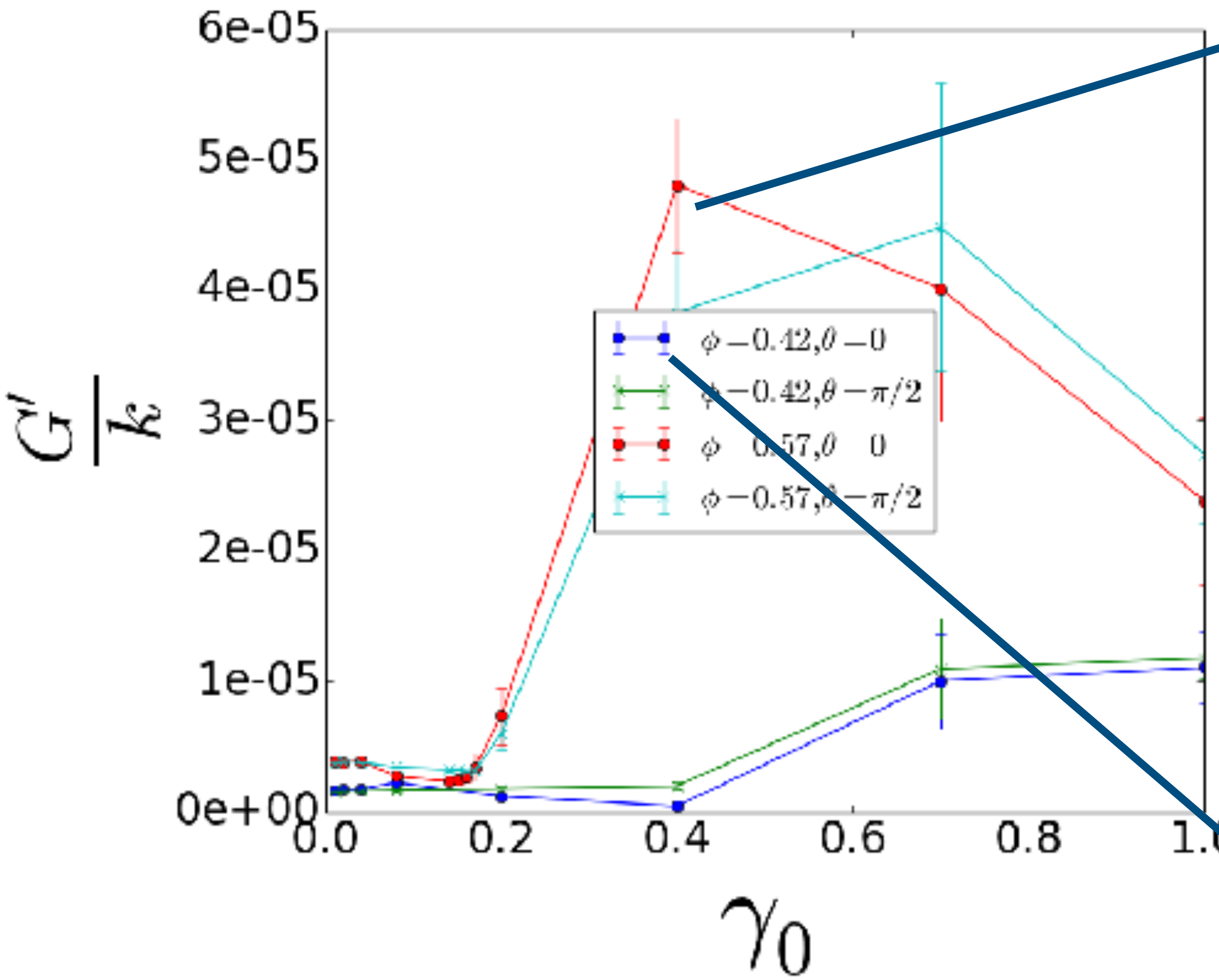
Contributions to viscosity



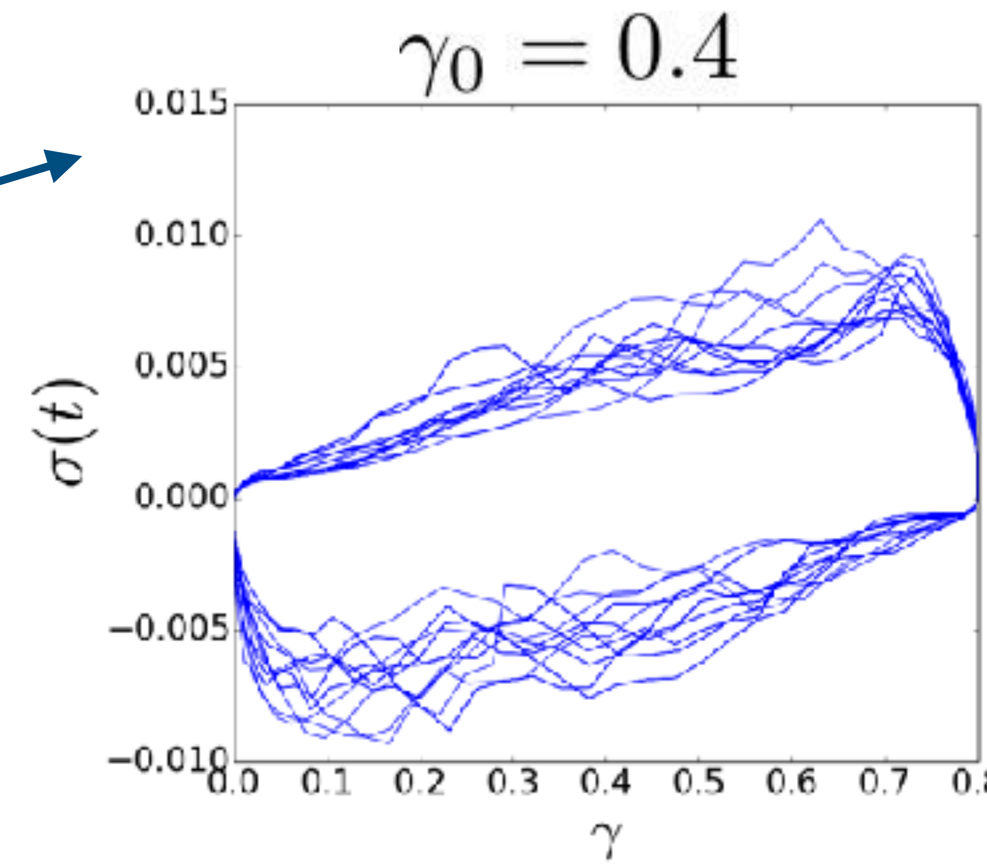
$$\theta = 0$$

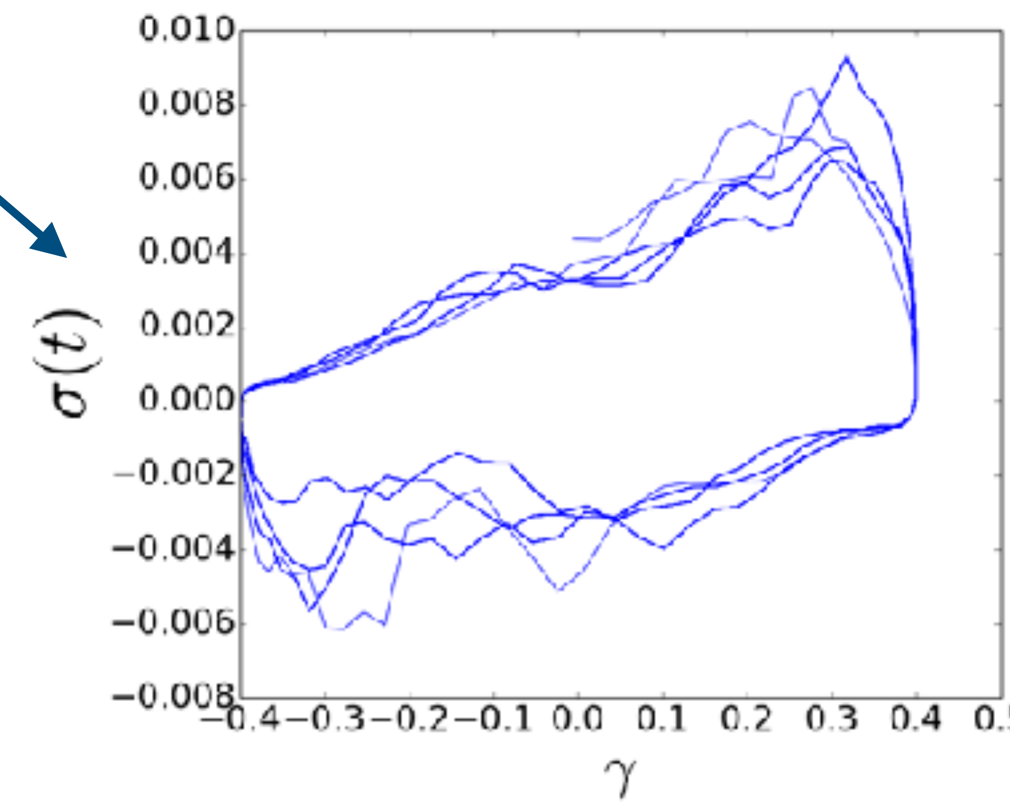
$$\phi = 0.57$$

Fragile state?

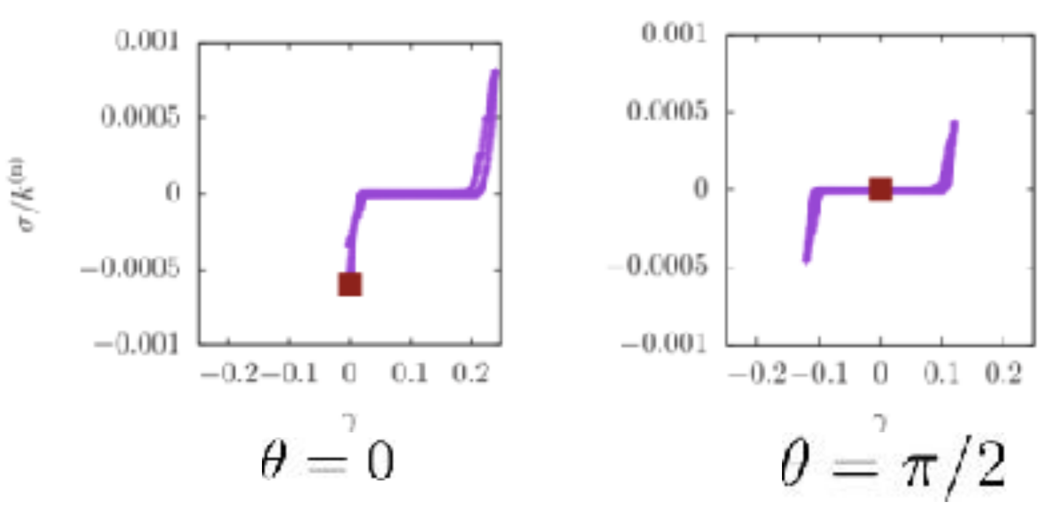


stress-strain curve



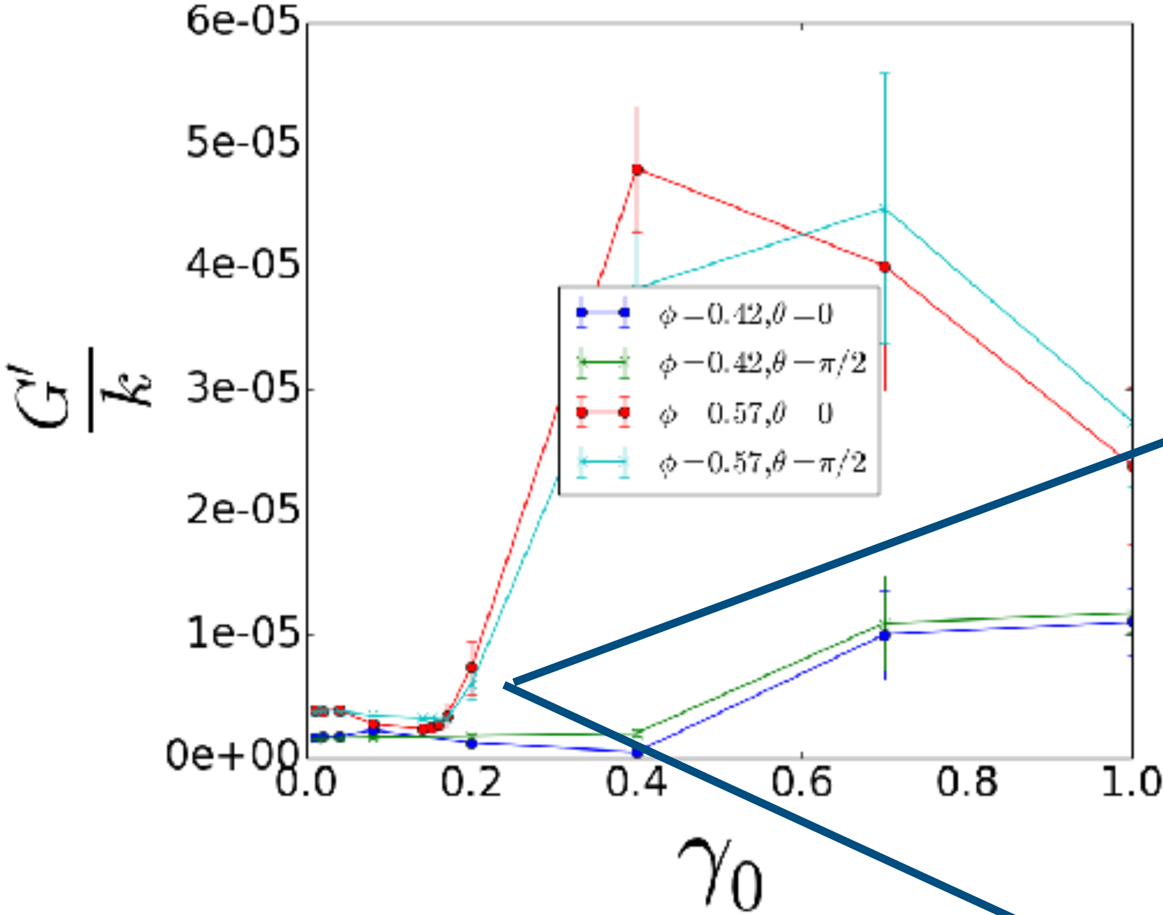


the stress strain curve of the fragile state in Otsuki san's talk



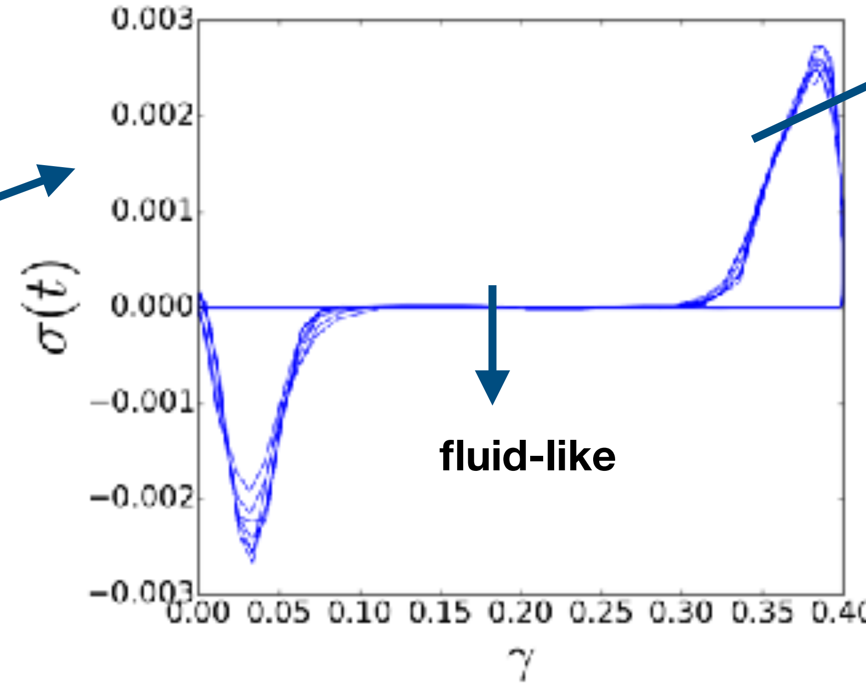
the phase dependence in this simulation might be caused by insufficient simulation time

Fragile state?



stress-strain curve

(only contact contributions)

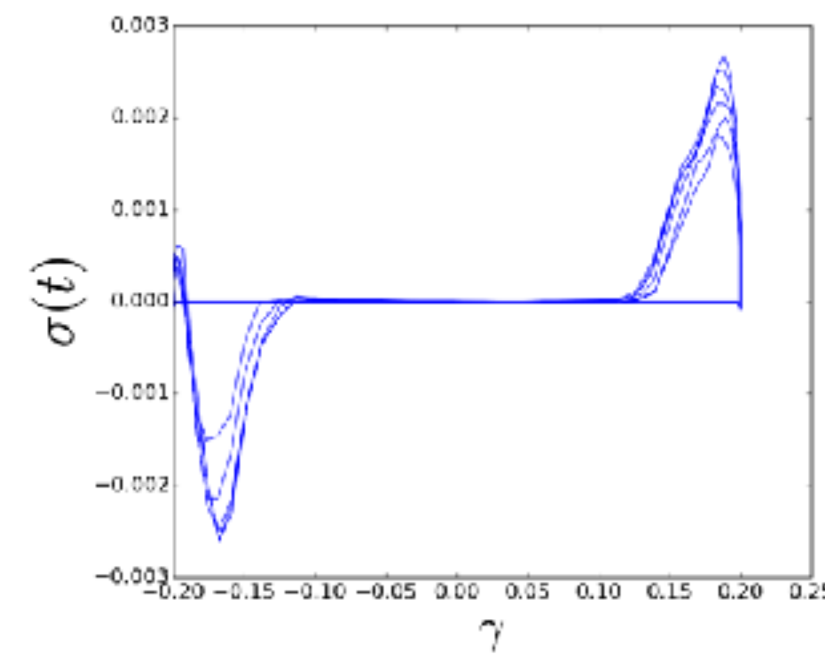


solid-like

fluid-like

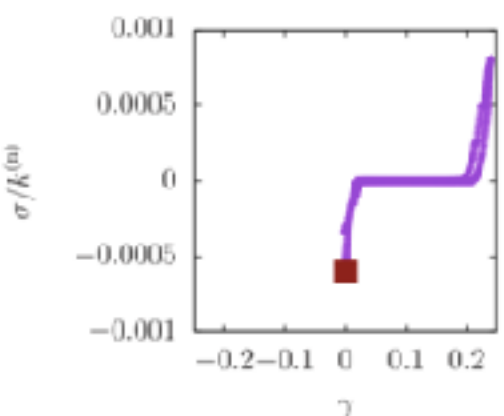
$\theta = 0$

$\gamma_0 = 0.2$

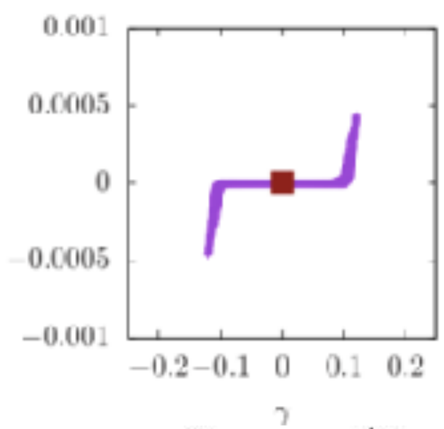


$\theta = \pi/2$

the stress strain curve of the fragile state in Otsuki san's talk



$\theta = 0$



$\theta = \pi/2$

Discussions

$$|\sigma_{ij} - \lambda\delta_{ij}| = 0$$

$$\Delta\lambda = \sigma_1 - \sigma_3$$

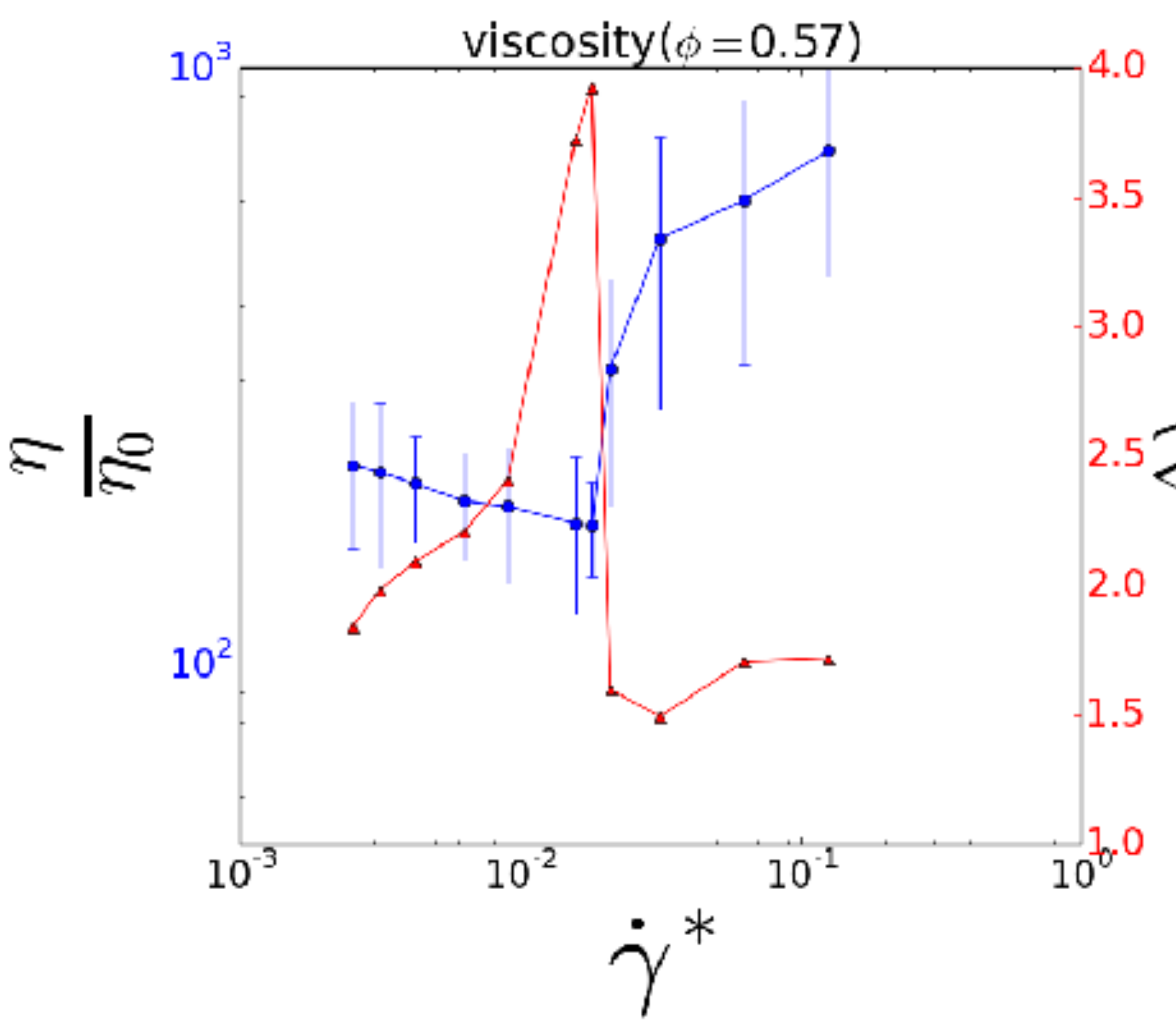
$$\sigma_1 = \max(\lambda_1, \lambda_2, \lambda_3)$$

$$\sigma_3 = \min(\lambda_1, \lambda_2, \lambda_3)$$

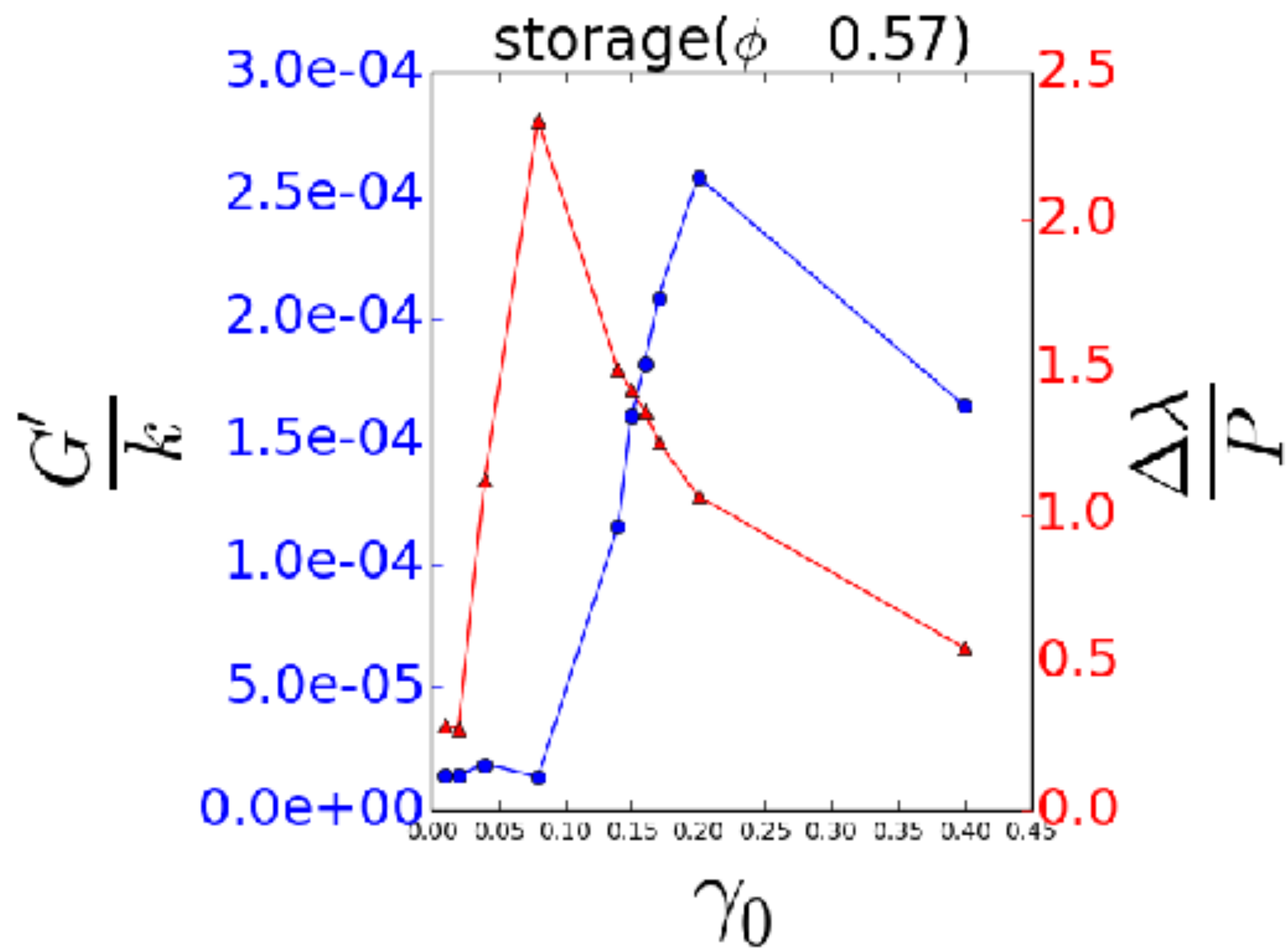
$$P = \frac{1}{3}(\sigma_1 + \sigma_2 + \sigma_3)$$

When DST takes place in steady shear, the anisotropy becomes maximum.

Anisotropy is also maximum at the onset of shear jamming.



Steady shear



Oscillatory shear

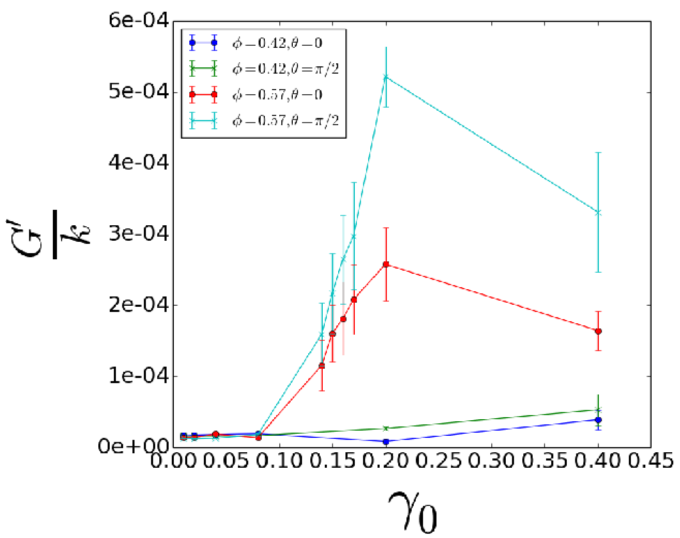
DST ⟷ Anisotropy

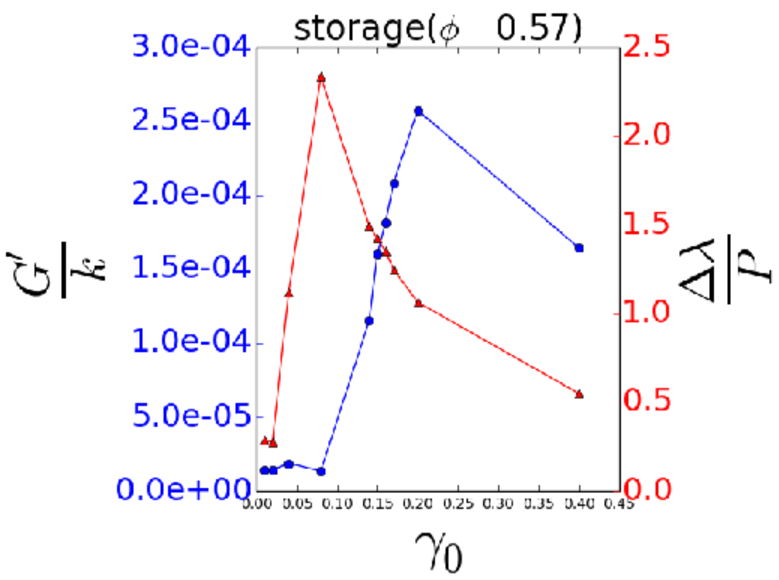
Conclusions

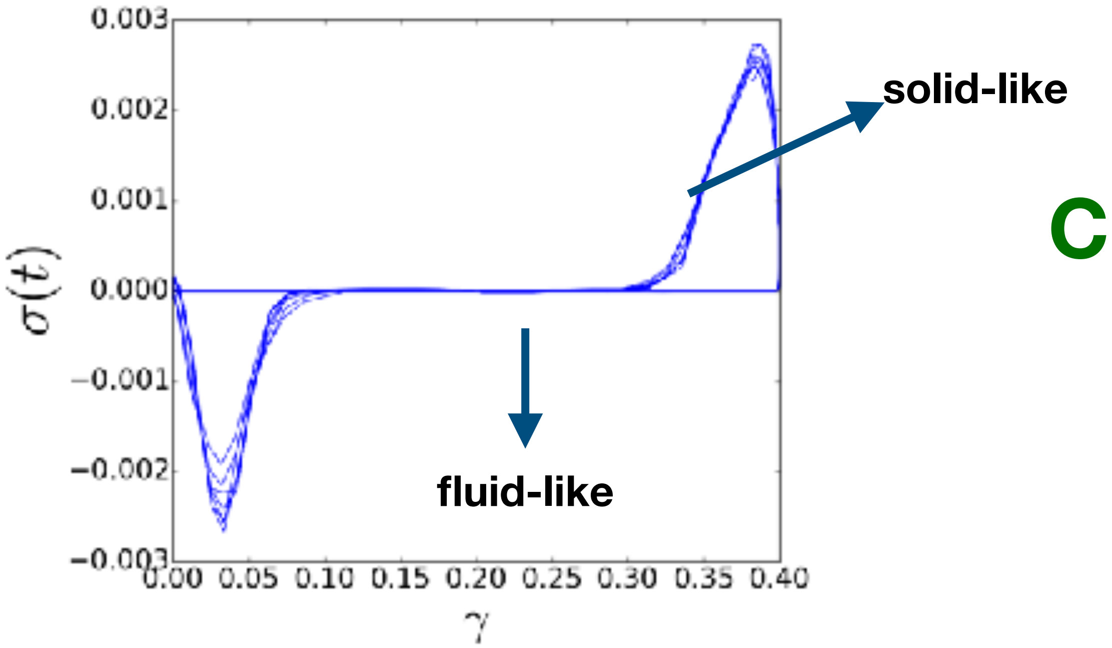
We simulate rheology of dense suspensions by using LBM.

Big increment of the viscosity and shear jamming in high strain rate has been observed.

Discontinuous change of the viscosity and the onset of shear jamming might be related to anisotropy.





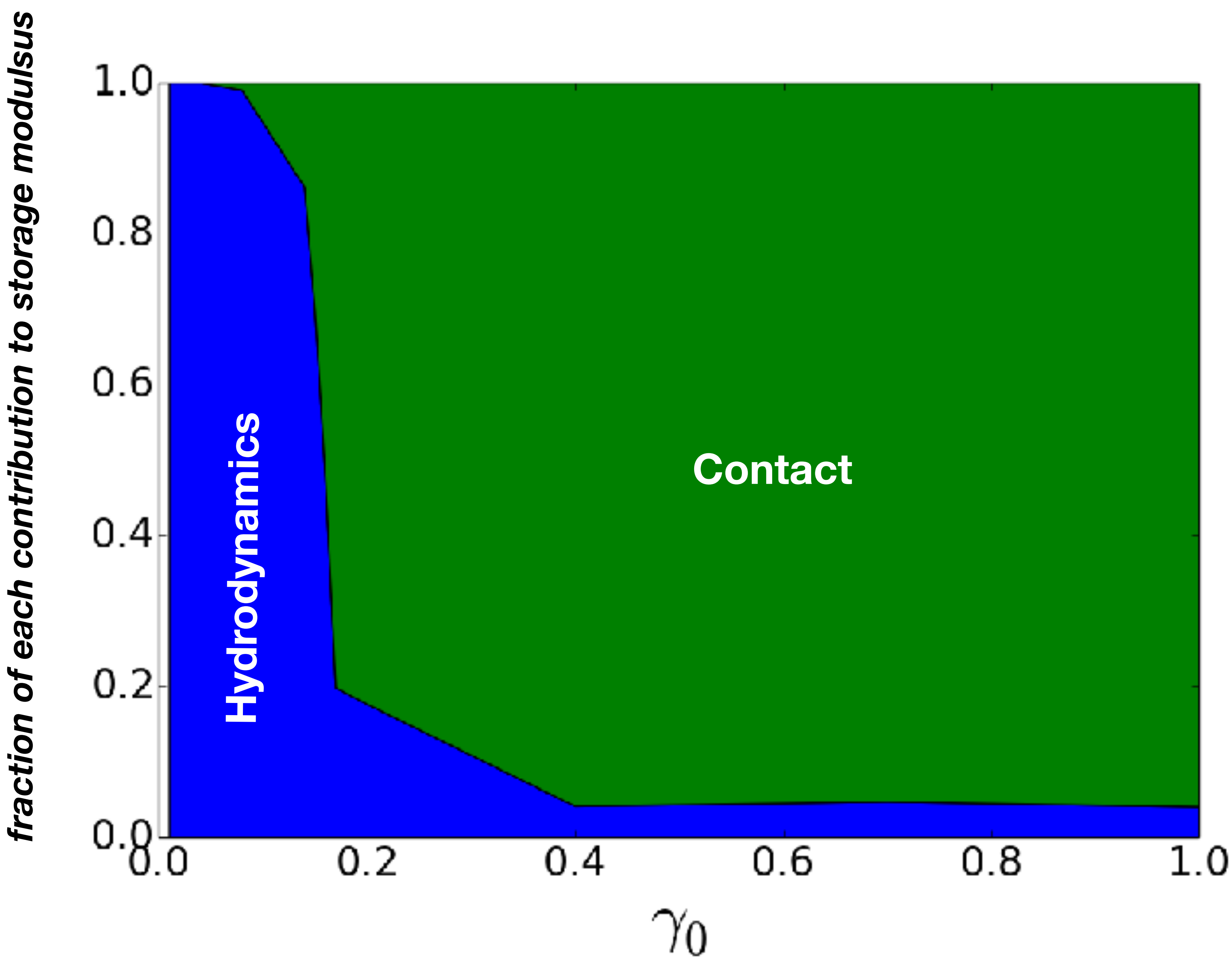


Future works

Clarify the existence of fragile state.

Analyze the percolation network (by simulating more particles in 2D).

appendix:
Contributions to storage modulus



$$\theta = 0$$

$$\phi = 0.57$$

appendix: details of the lbm (collision operator)

Discrete equilibrium d.f

$$n_i^{eq} = a^{c_i}\left(\rho + \frac{\mathbf{j}\cdot\mathbf{c}_i}{c_s^2} + \frac{(\rho\mathbf{u}\mathbf{u}) : (\mathbf{c}_i\mathbf{c}_i - c_s^2 1)}{2c_s^4}\right)$$

Post collision d.f

$$n_i^{*} = a^{c_i}\left(\rho + \frac{\mathbf{j}\cdot\mathbf{c}_i}{c_s^2} + \frac{(\rho\mathbf{u}\mathbf{u} + \mathbf{\Pi}^{neq,*}) : (\mathbf{c}_i\mathbf{c}_i - c_s^2 1)}{2c_s^4}\right)$$

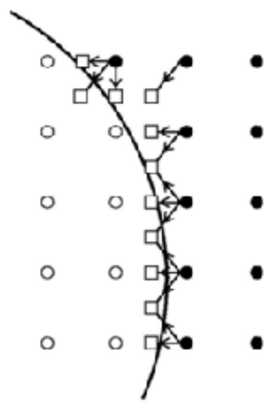
$$\mathbf{\Pi}^{neq,*} = (1+\lambda)\bar{\mathbf{\Pi}}^{neq} + \frac{1}{3}(1+\lambda_\nu)(\mathbf{\Pi}^{neq} : 1)1$$

Related to solvent viscosity

$$\eta = -\rho c_s^2 \Delta t\left(\frac{1}{\lambda} + \frac{1}{2}\right) \qquad \eta_\nu = -\rho c_s^2 \Delta t\left(\frac{2}{3\lambda_\nu} + \frac{1}{3}\right)$$

appendix: Stress Calculation

Hydrodynamics



$$\mathbf{f}(\mathbf{r}_b, t+\frac{1}{2}\Delta t) = \frac{\Delta x^3}{\Delta t}\left[2n_b^*(\mathbf{r},t) - \frac{2a^{c_b}\rho_0 \mathbf{u}_b \cdot \mathbf{c}_b}{c_s^2}\right]\mathbf{c}_b$$

$$\sigma^h = \sum_b \mathbf{r}_b \mathbf{f}(\mathbf{r}_b)$$

or

$$\begin{pmatrix} \mathbf{F}_1 \\ \mathbf{T}_1 \\ \mathbf{T}_2 \\ \mathbf{S}_1 \\ \mathbf{S}_2 \end{pmatrix} = -\begin{pmatrix} \mathbf{A}_{11} & -\mathbf{B}_{11} & \mathbf{B}_{22} \\ \mathbf{B}_{11} & \mathbf{C}_{11} & \mathbf{C}_{12} \\ -\mathbf{B}_{22} & \mathbf{C}_{12} & \mathbf{C}_{22} \\ \mathbf{G}_{11} & \mathbf{H}_{11} & \mathbf{H}_{12} \\ \mathbf{G}_{22} & -\mathbf{H}_{21} & \mathbf{H}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{U}_{12} \\ \boldsymbol{\Omega}_1 \\ \boldsymbol{\Omega}_2 \end{pmatrix}$$

lubrication grand resistance formulation

Contact

$$\sigma^c = \sigma^{\mathrm{nor}} + \sigma^{\mathrm{tan}}$$

$$\sigma^{nor} = -\frac{1}{2V}\sum_i \sum_{j\neq i}(\mathbf{r}_{ij,\alpha}\mathbf{F}^{nor}_{ij,\beta} + \mathbf{r}_{ij,\beta}\mathbf{F}^{nor}_{ij,\alpha})$$

$$\sigma^{tan} = -\frac{1}{V}\sum_i \sum_{j\neq i}\mathbf{r}_{ij,\alpha}\mathbf{F}^{tan}_{ij,\beta}$$

Electrostatic repulsive

$$\sigma^r = -\frac{1}{V}\sum_i \sum_{j\neq i}\mathbf{R}_{ij,\alpha}\mathbf{F}^{R}_{ij,\beta}$$