

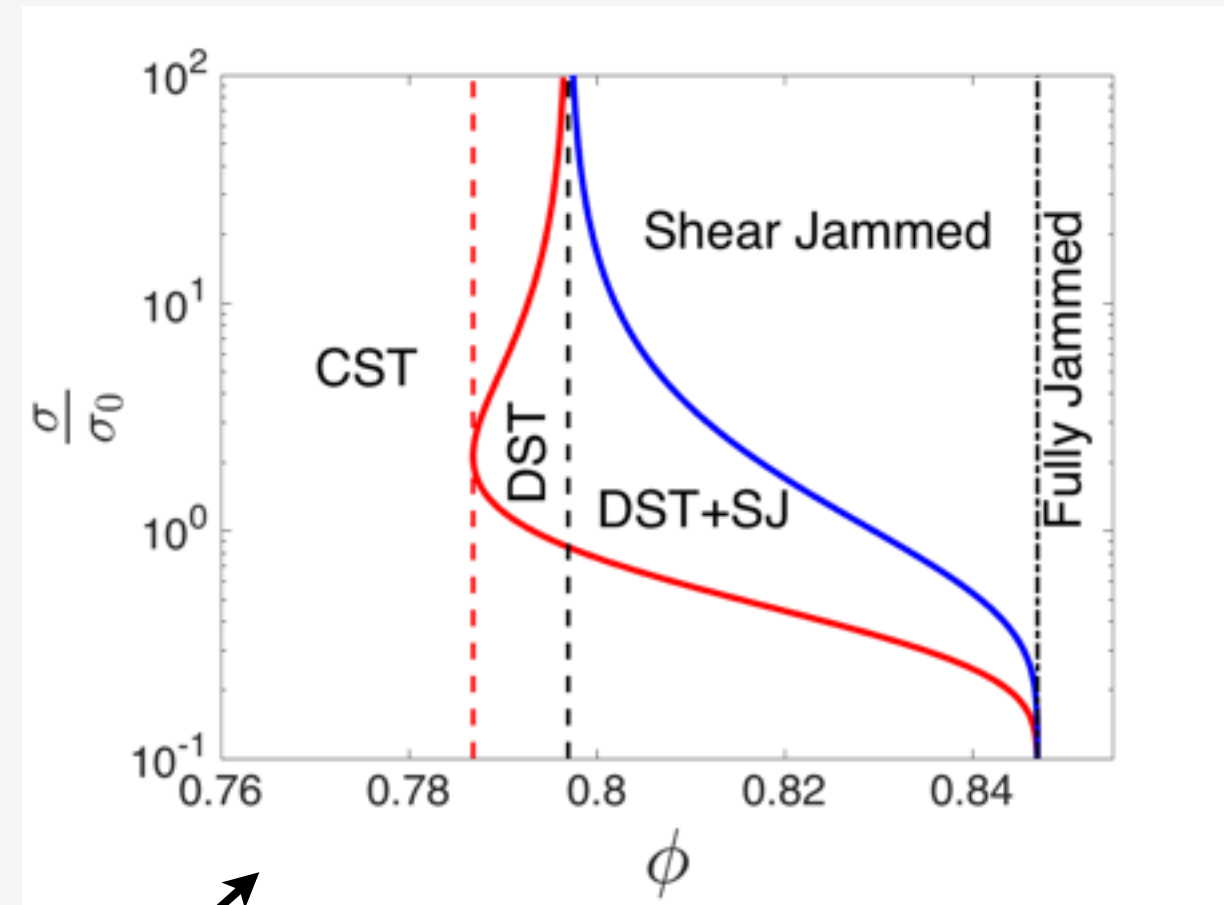
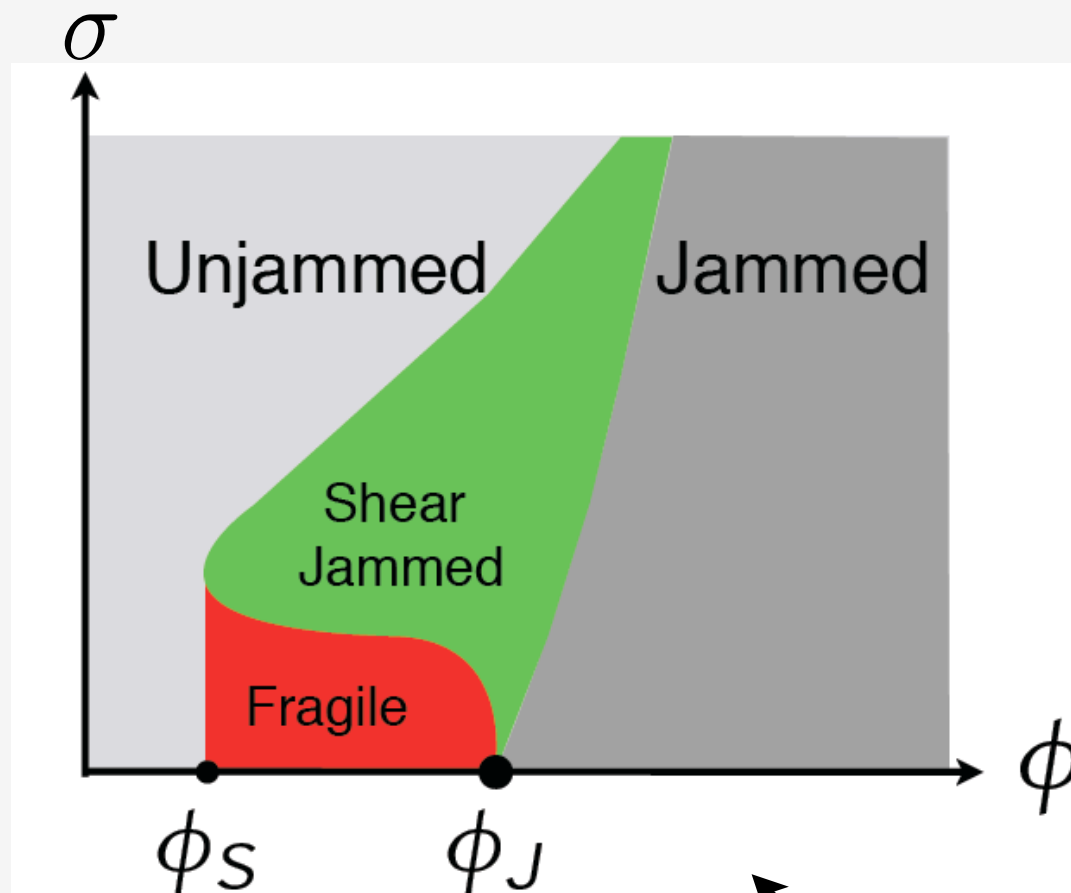
Shear-induced Rigidity in Granular Materials

Statistical Mechanics with Friction

Dapeng Bi, Sumantra Sarkar, Kabir Ramola, Jetin Thomas, Jishnu Nampoothiri

The Behringer Group

Romain Mari, Abhi Singh, Jeff Morris



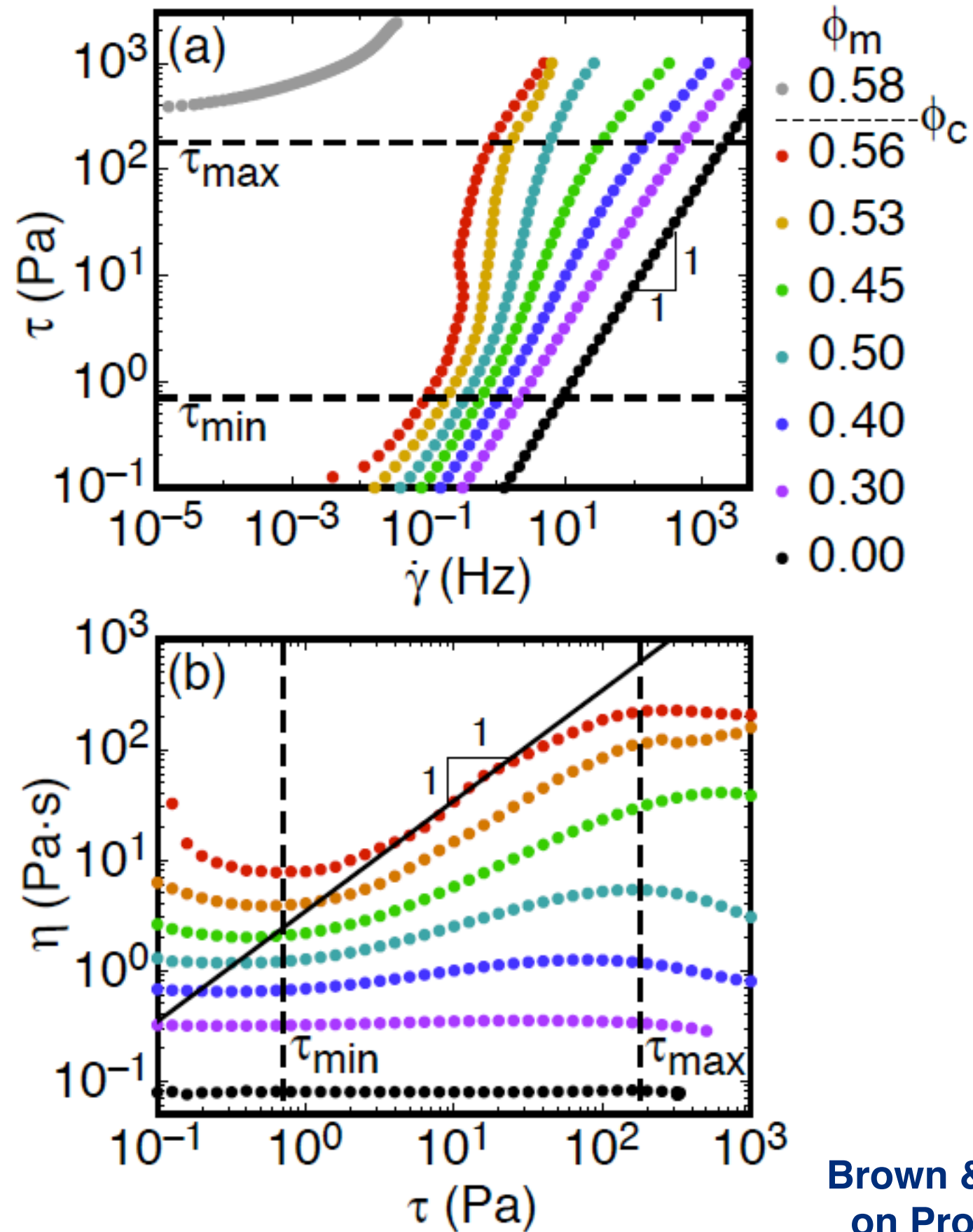
Dry Grains

Suspensions

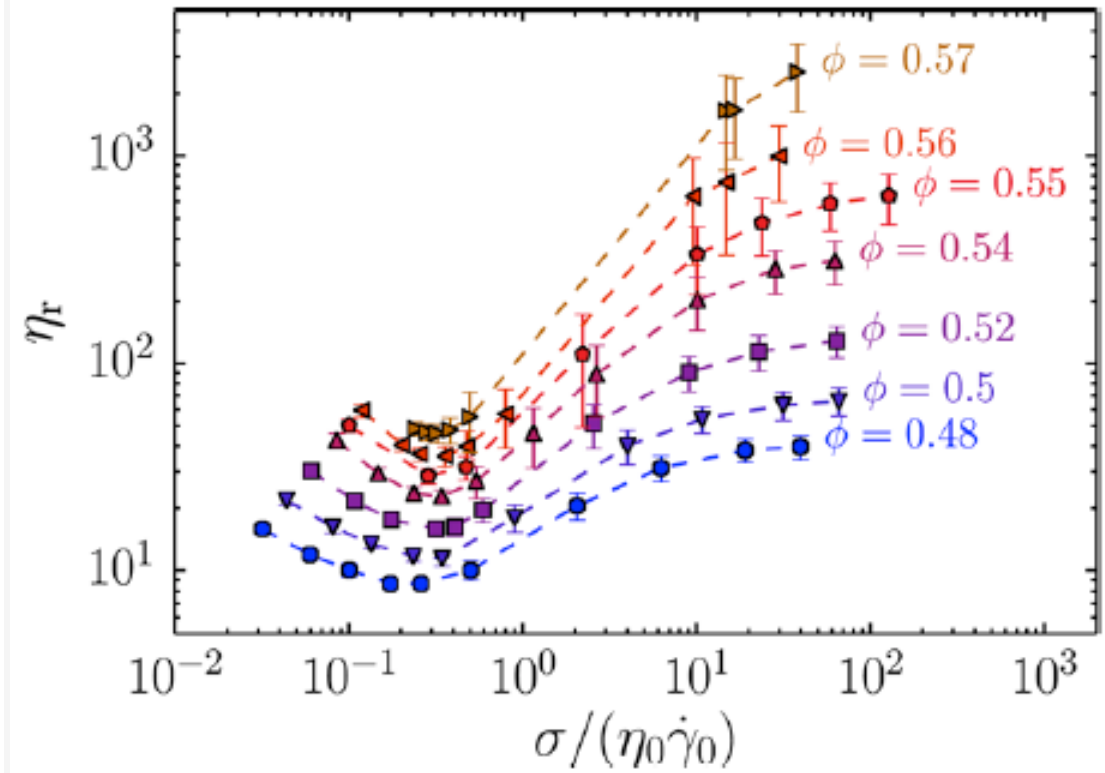
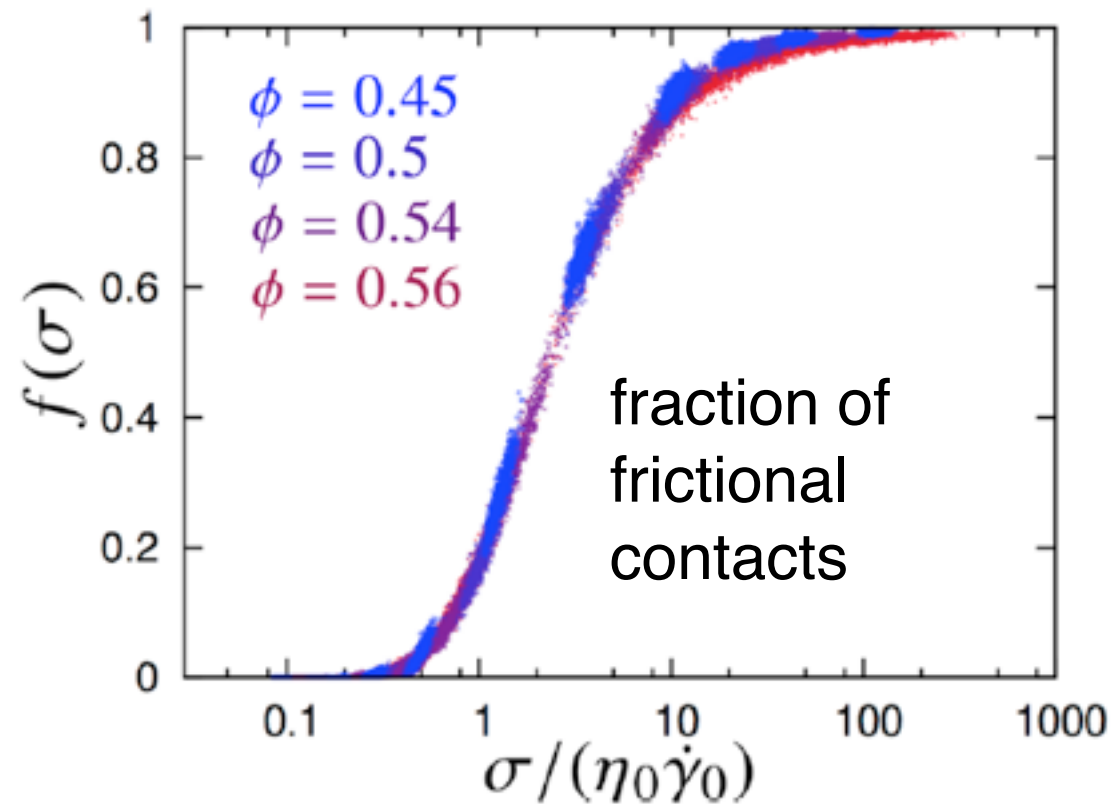
All states are "jammed"
these are static states

Flowing States (Non-
equilibrium steady states)

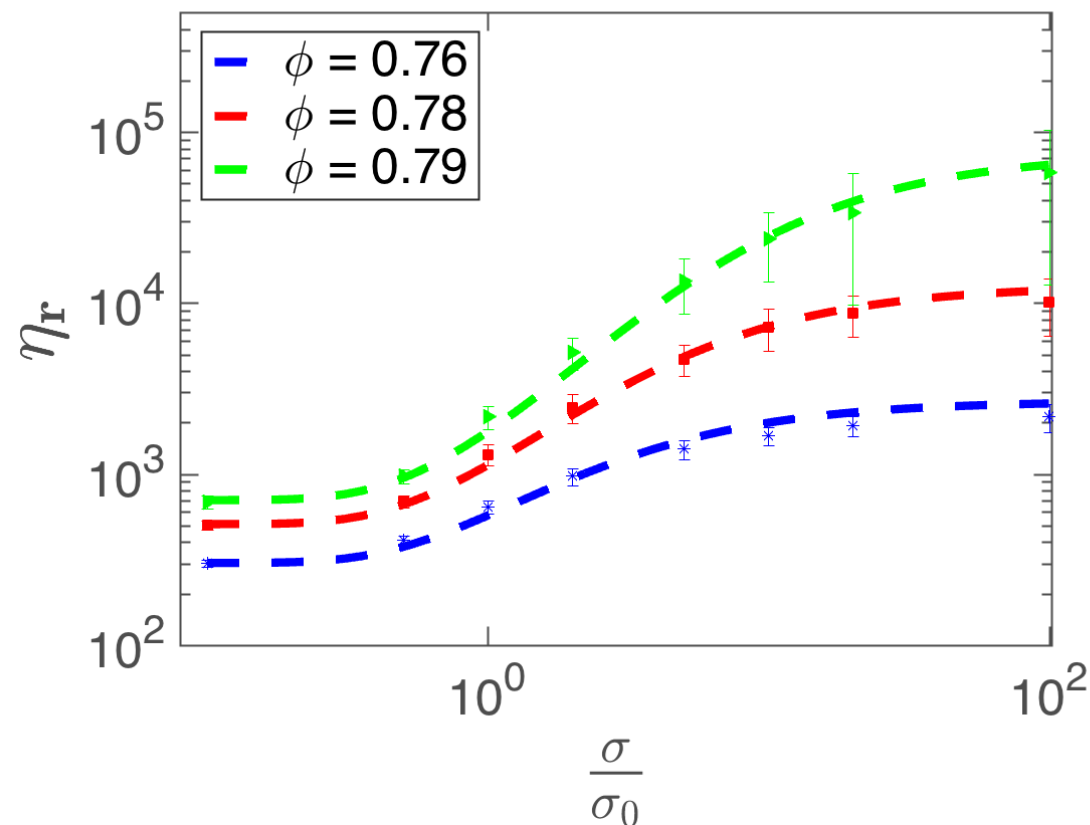
Discontinuous Shear Thickening (DST)



DST Phenomenology (Simulations)

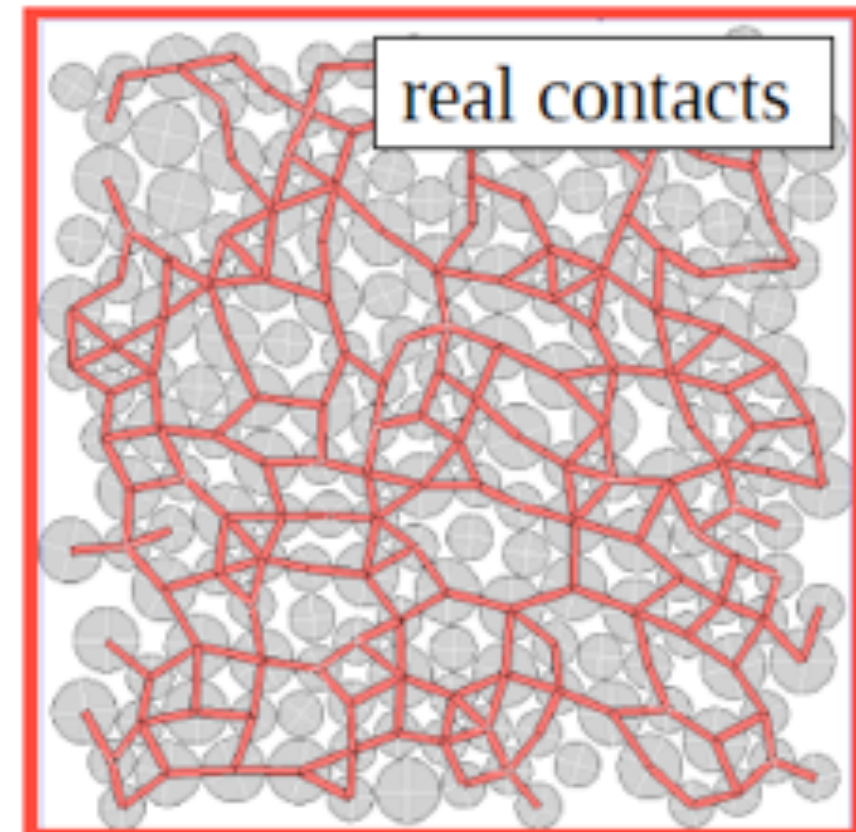
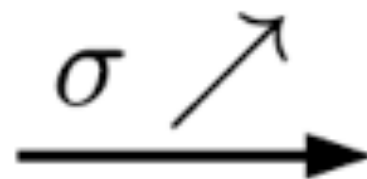
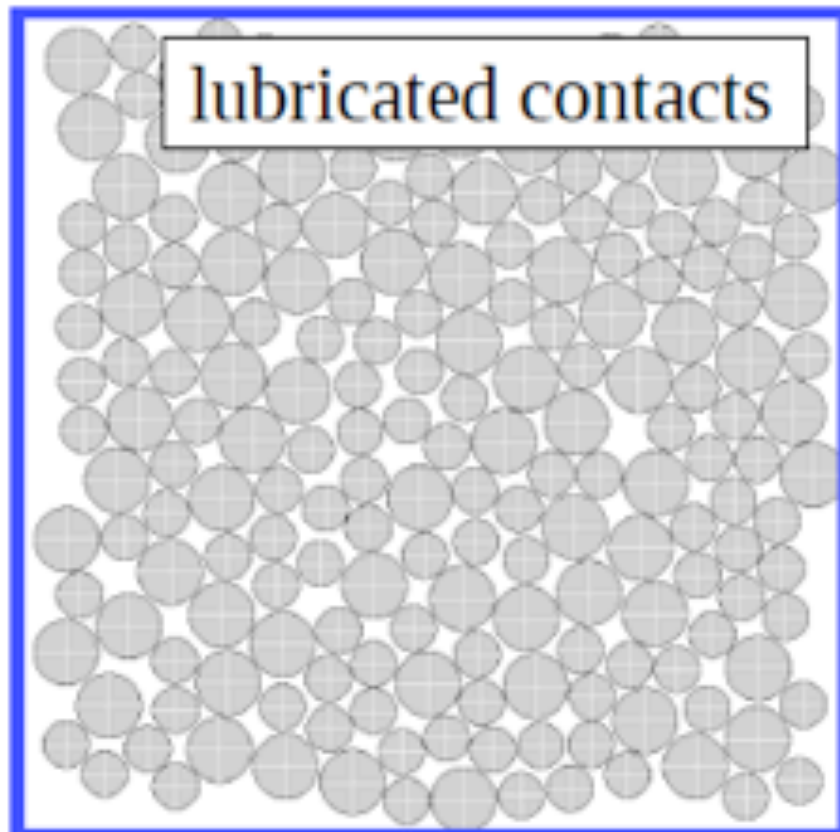
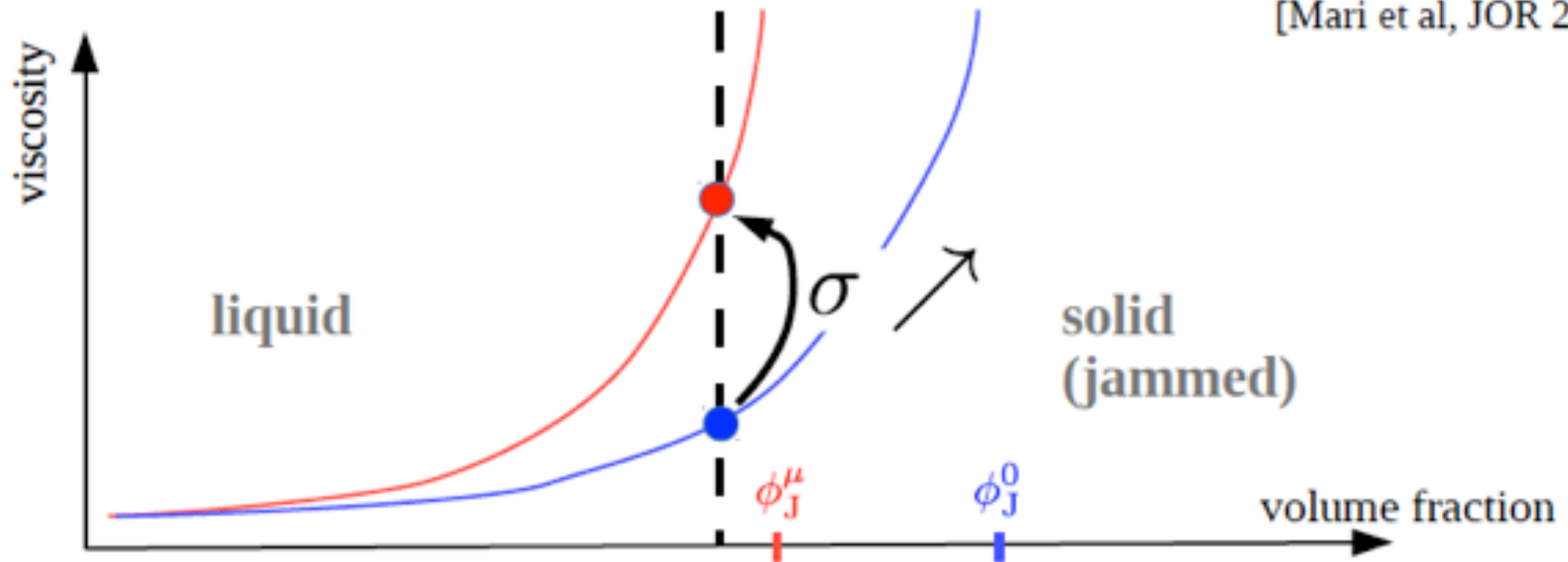


2D



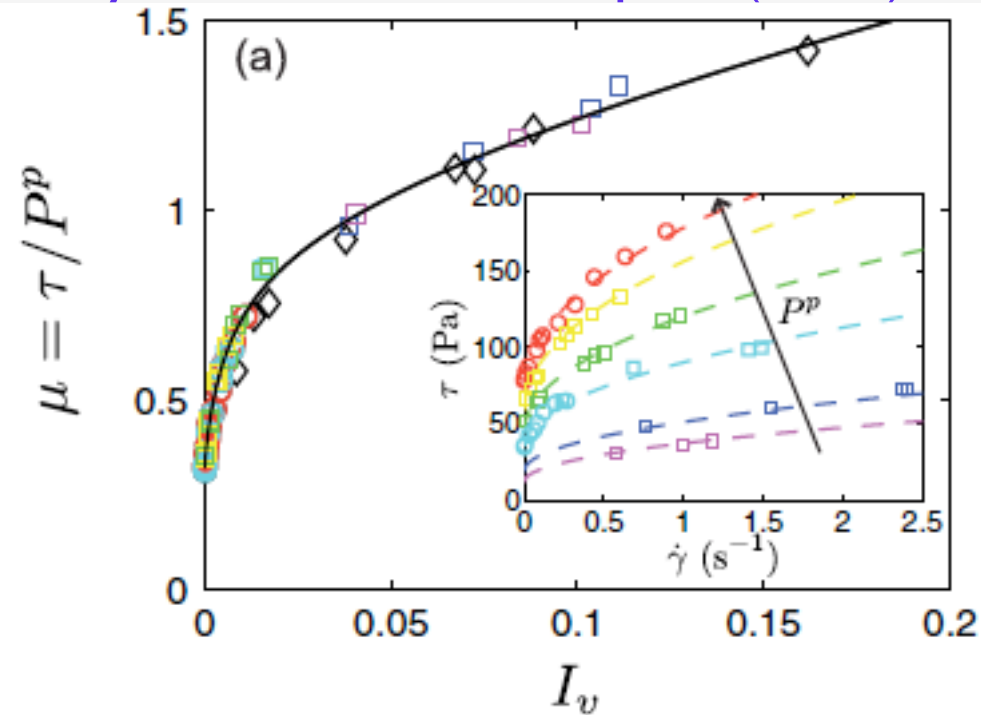
Mean-field theory based on contacts (DST)

[Fernandez et al, PRL 2013]
[Seto et al, PRL 2013]
[Heussinger, PRE 2013]
[Wyart and Cates PRL 2013]
[Mari et al, JOR 2014]



Viscosity: Suspension Rheology

Boyer, Guazzelli, Pouliquen (2011)



- A “universal” relationship between the macroscopic friction coefficient and the viscous number at constant pressure.
- When a suspension is sheared at constant volume, the shear and normal viscosities can be expressed in terms of the friction coefficient and the viscous number.

$\sigma = \eta_s \dot{\gamma}$ rate-independent but viscosity depends on packing fraction

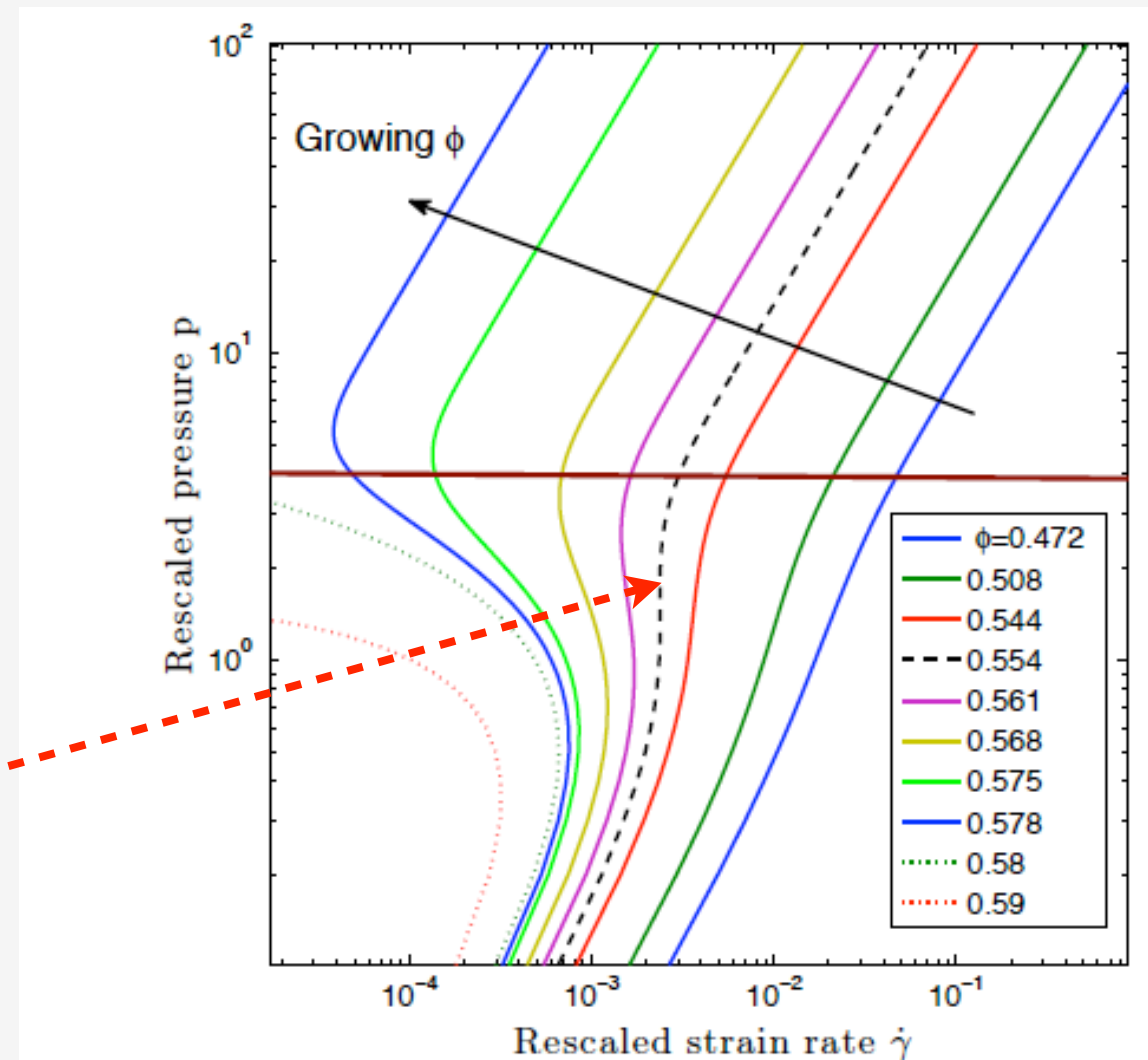
$$\phi_J(\sigma) = f(\sigma/\sigma^*)\phi_m + (1 - f(\sigma/\sigma^*))\phi_J$$

$$\eta_s(\phi) \propto \frac{1}{(\phi_J(\sigma) - \phi)^2}$$

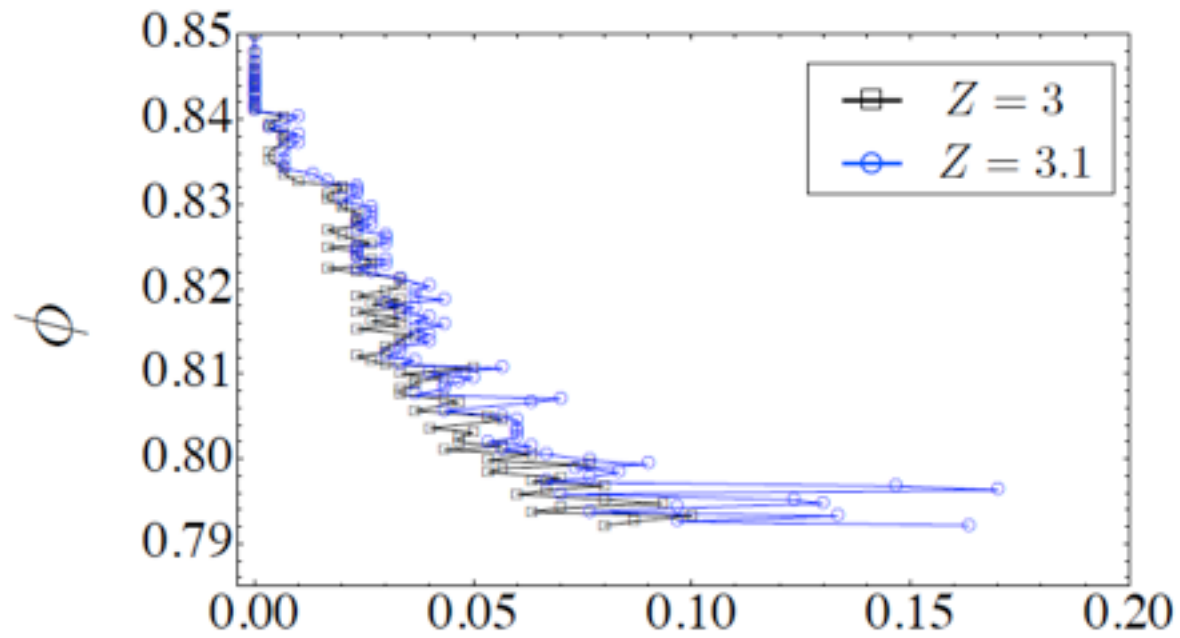
DST is regime in which the viscosity scales linearly with stress

$$\eta \propto \sigma$$

DST phase boundary: $\frac{d\dot{\gamma}}{d\sigma} = 0$

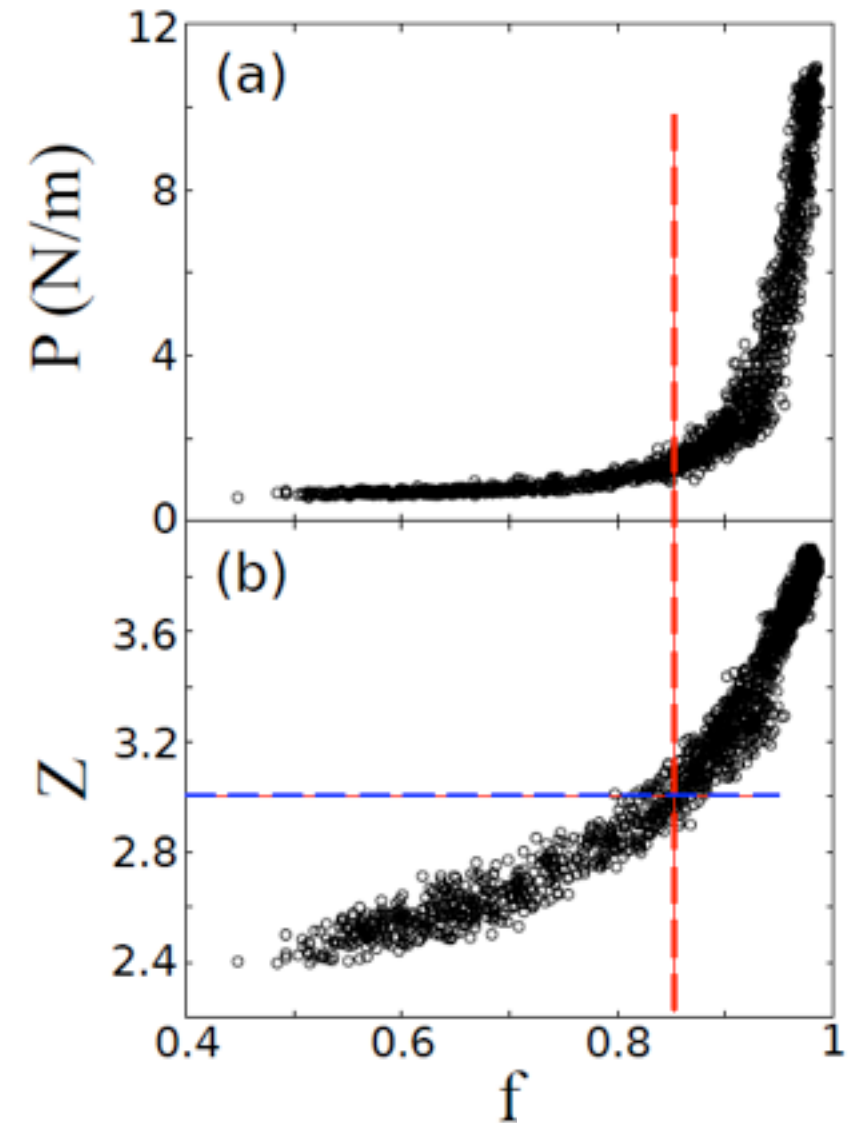
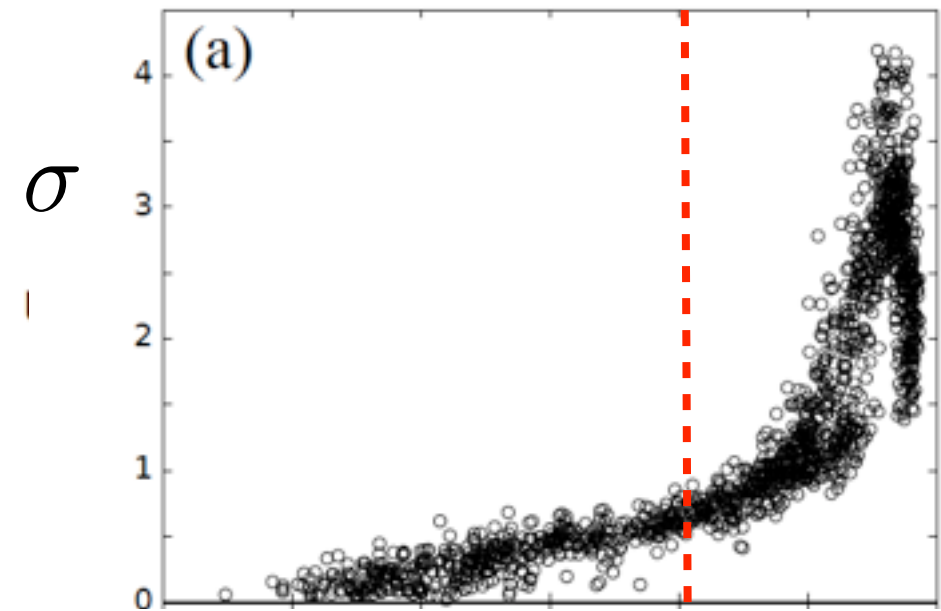
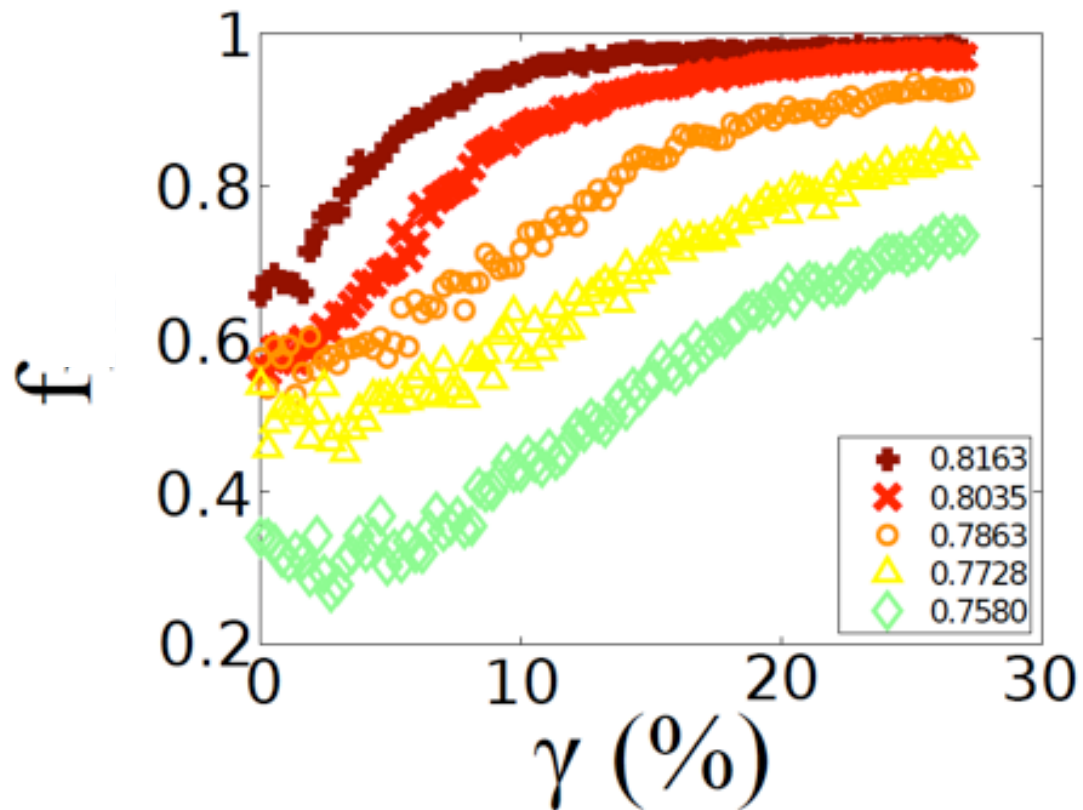


Shear Jamming Phenomenology (Experiments)



γ_{min}

fraction of grains with at least two contacts

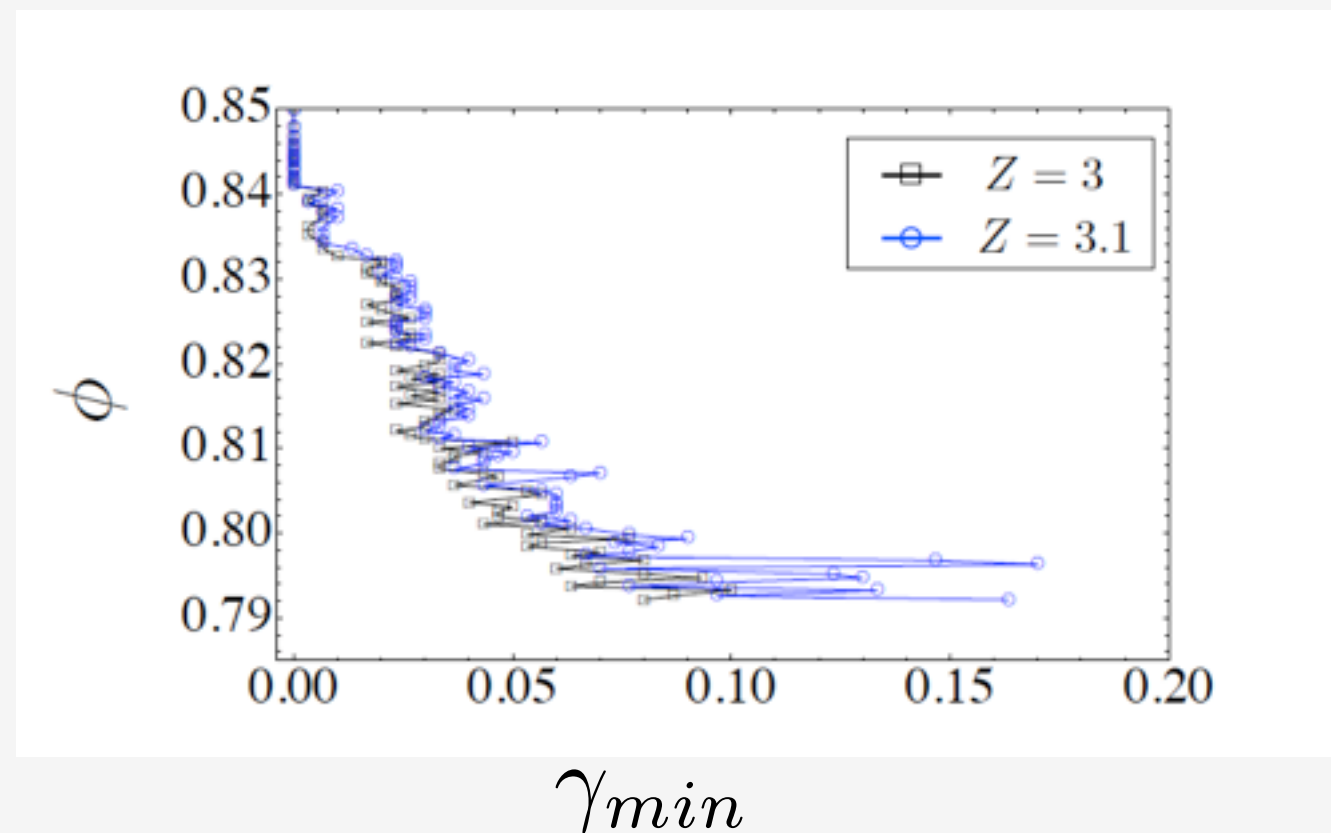
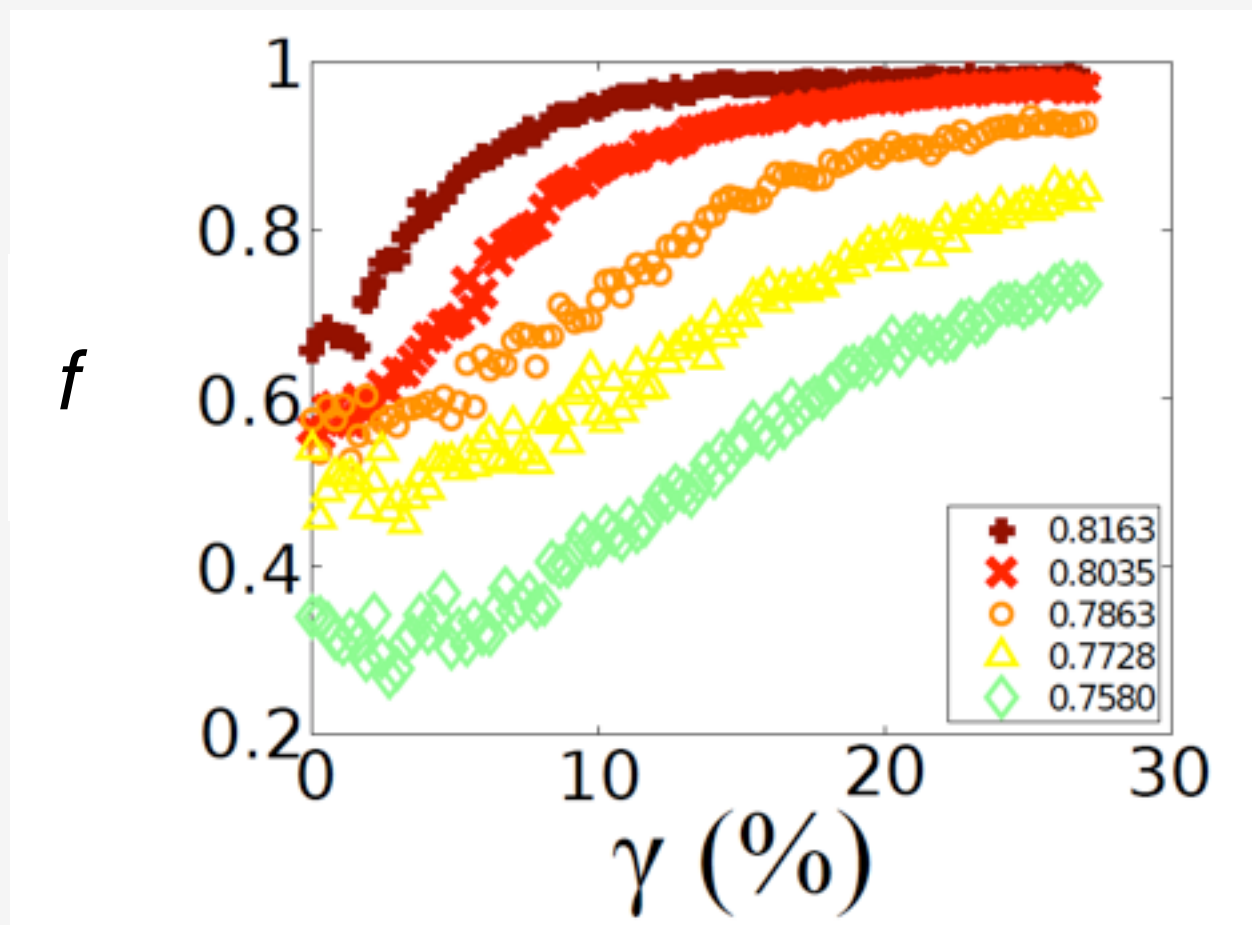


Mean-field theory based on contacts: SJ

A similar argument for SJ: f is the fraction grains with 2 or more contacts

$$\phi_J(\gamma, \phi) = f(\gamma, \phi)\phi_J(\mu) + (1 - f(\gamma, \phi))\phi_J$$

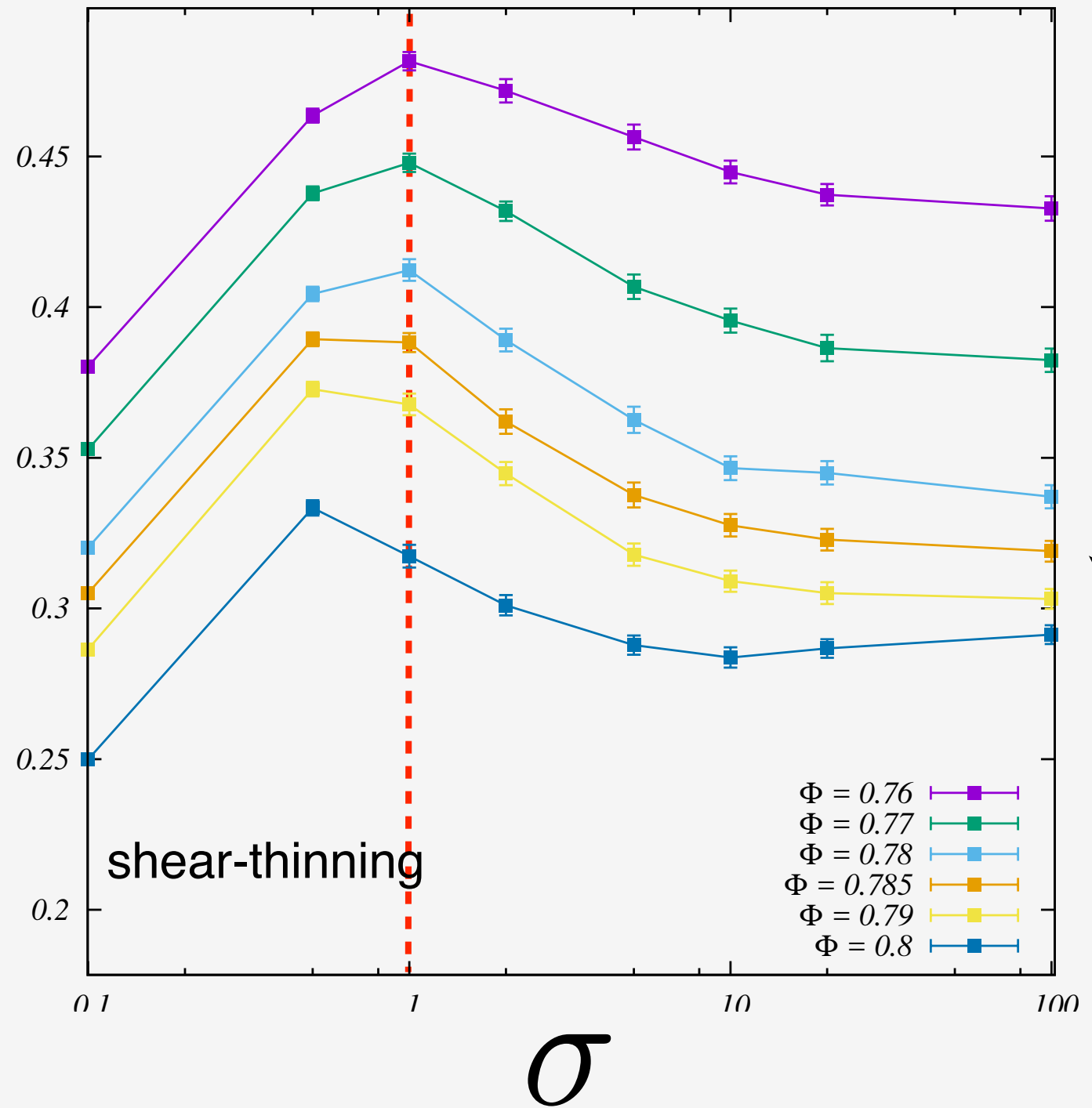
$$\phi = \phi_J(\gamma_{min}, \phi)$$



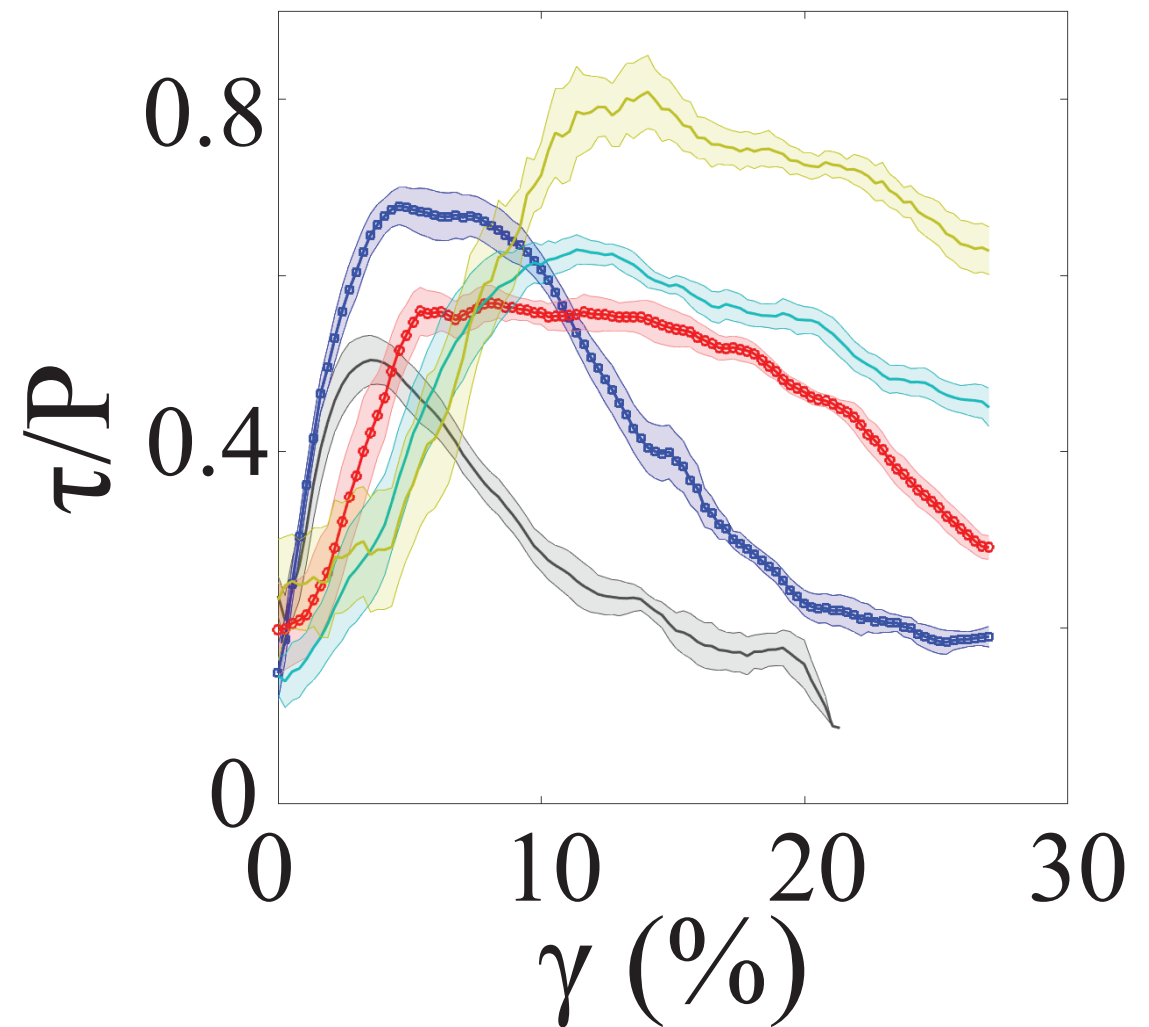
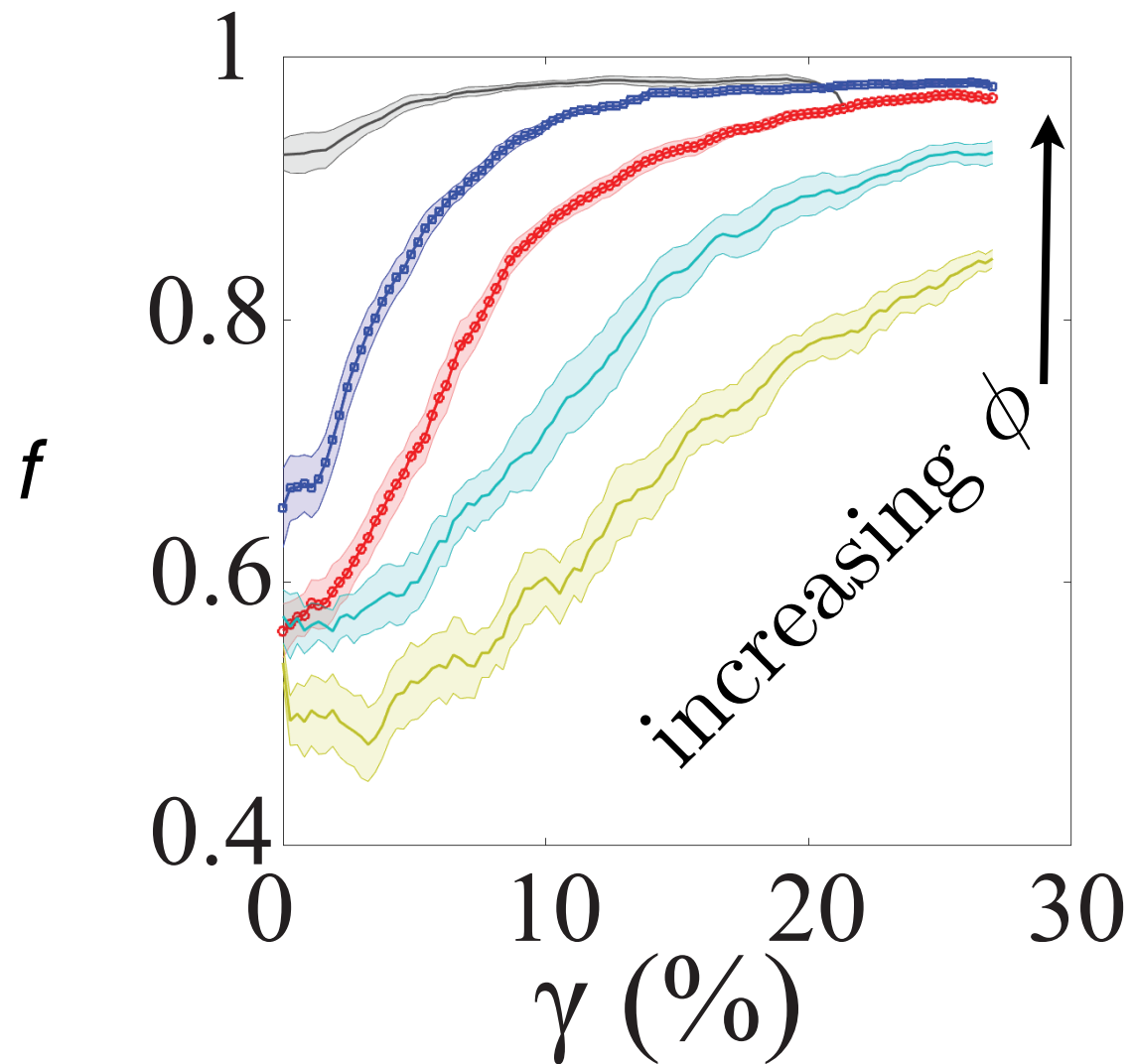
Frictional Contacts & Stress Anisotropy (DST)



$$\mu \equiv \tau / Pp$$

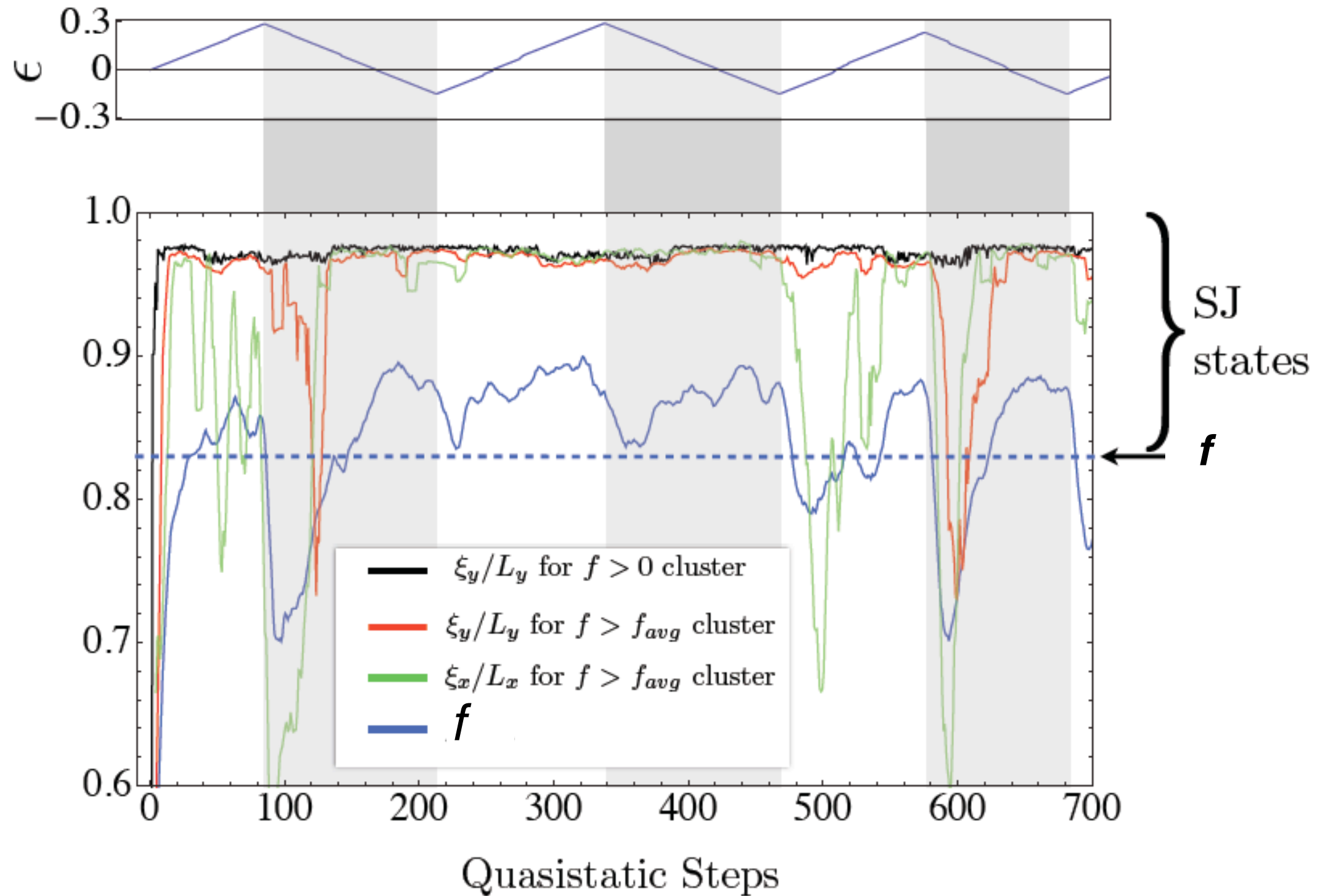


Frictional Contacts & Stress Anisotropy (SJ)

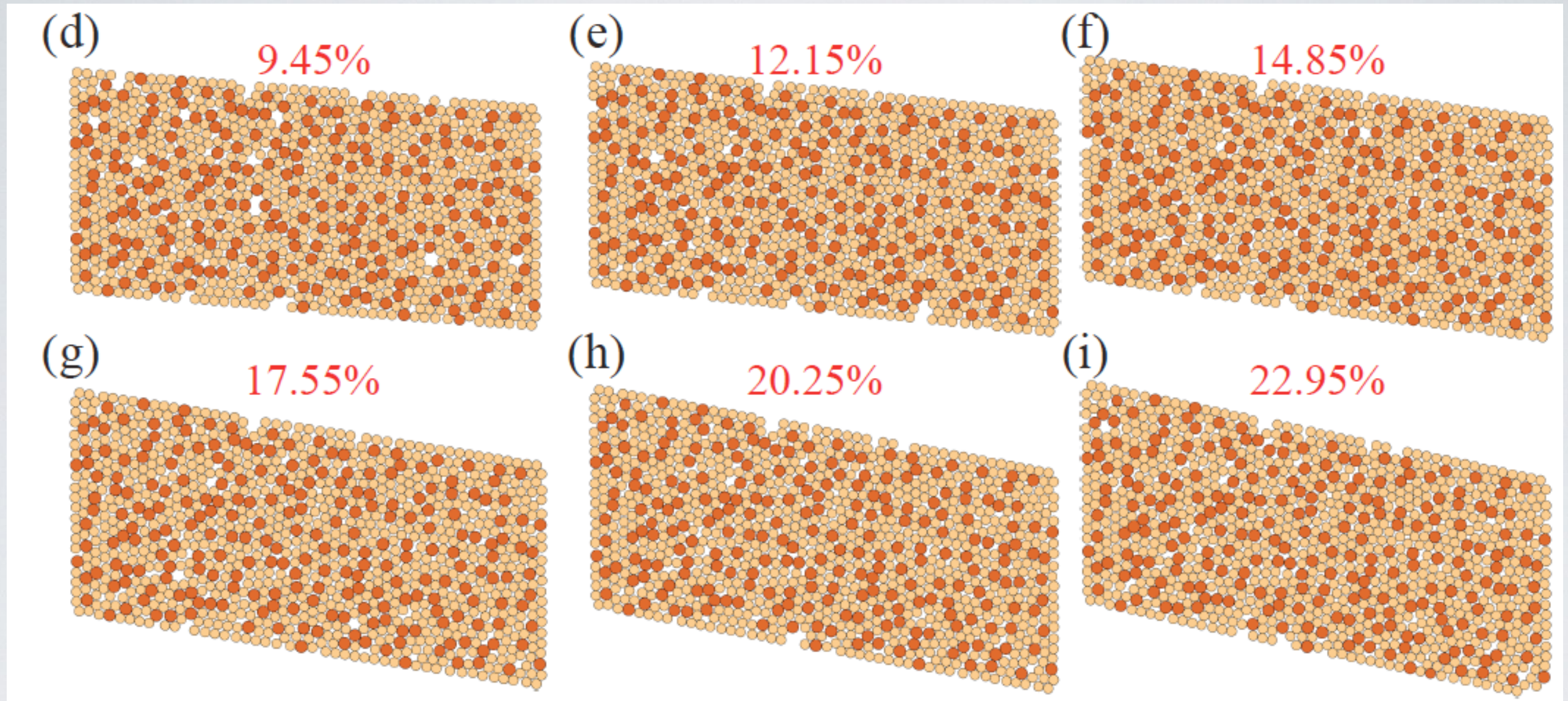


maximum stress anisotropy at transition from fragile to shear-jammed states

Response to cyclic shear

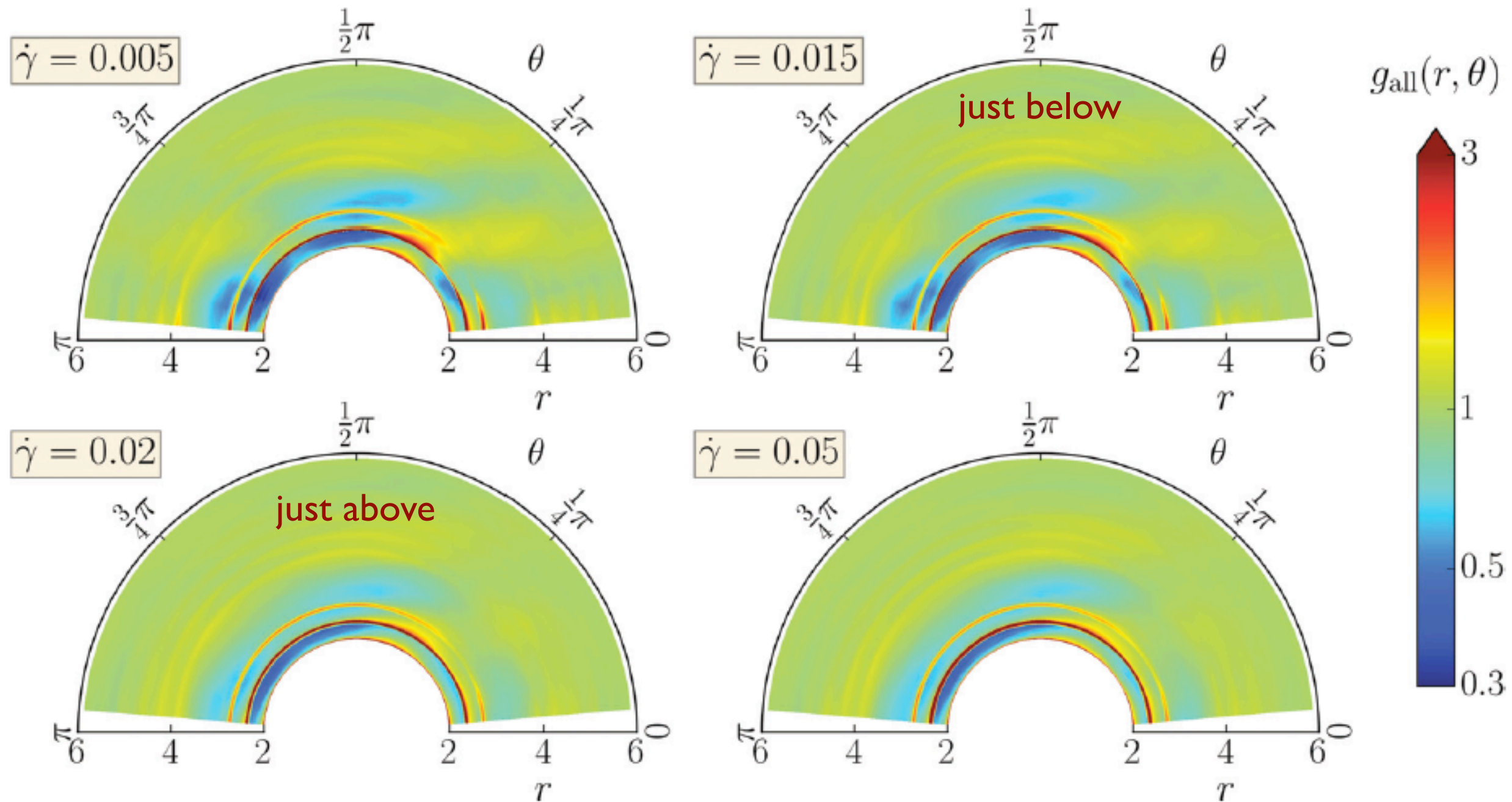


Sj: Positional patterns



Shows large and small particles: gaps are due to imaging

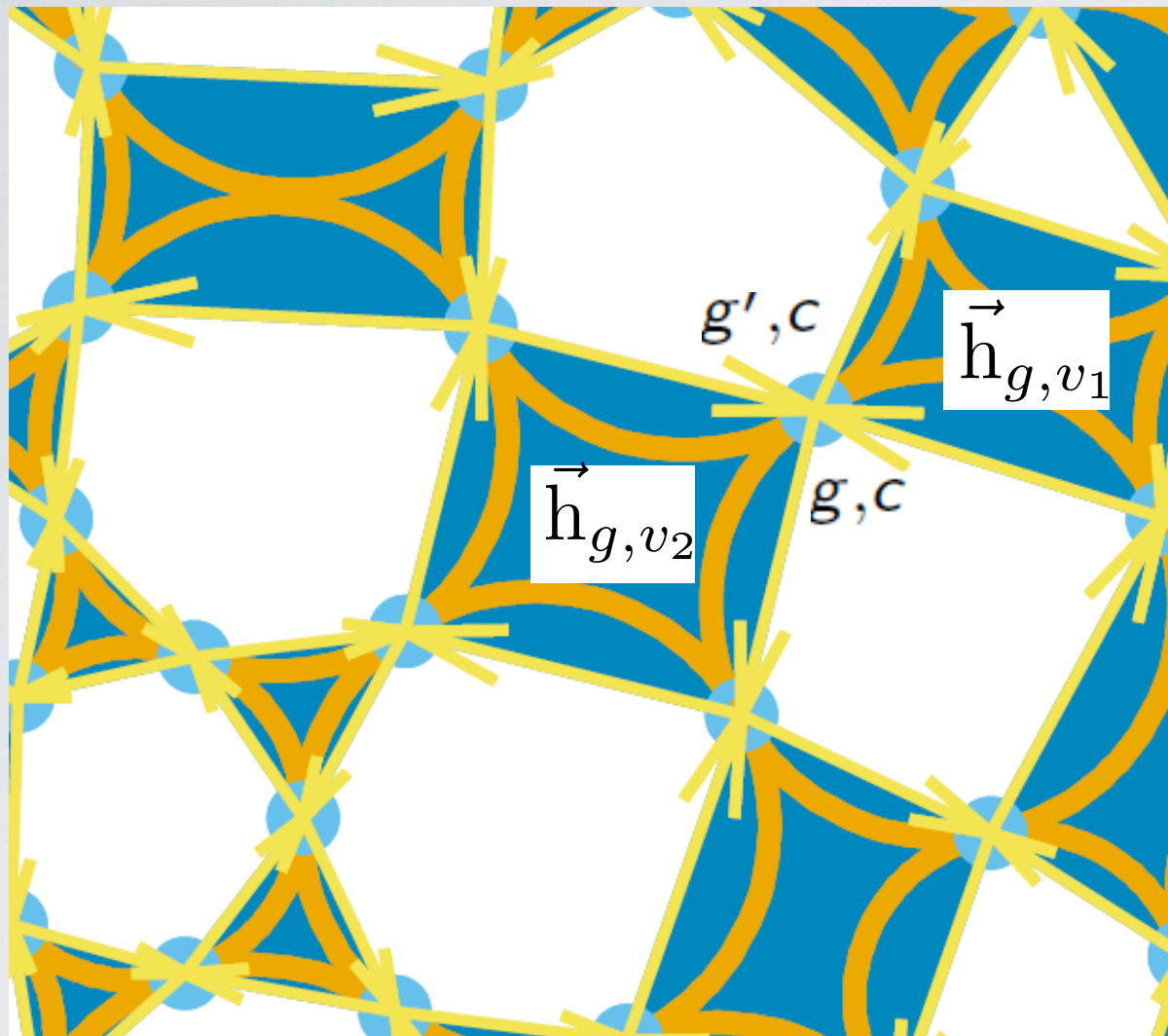
DST Microstructure: Pair Correlation Functions



Mari, Seto, Morris, Denn (JOR, 2014)

Height Representation (2D)

Ball & Blumenfeld, 2003



$$\begin{aligned}\vec{f}_{g, c_1} &= \vec{h}_{g, v_1} - \vec{h}_{g, v_2}, \\ \vec{f}_{g, c_2} &= \vec{h}_{g, v_2} - \vec{h}_{g, v_3}, \\ \vec{f}_{g, c_3} &= \vec{h}_{g, v_3} - \vec{h}_{g, v_4}, \\ \vec{f}_{g, c_4} &= \vec{h}_{g, v_4} - \vec{h}_{g, v_1}.\end{aligned}$$

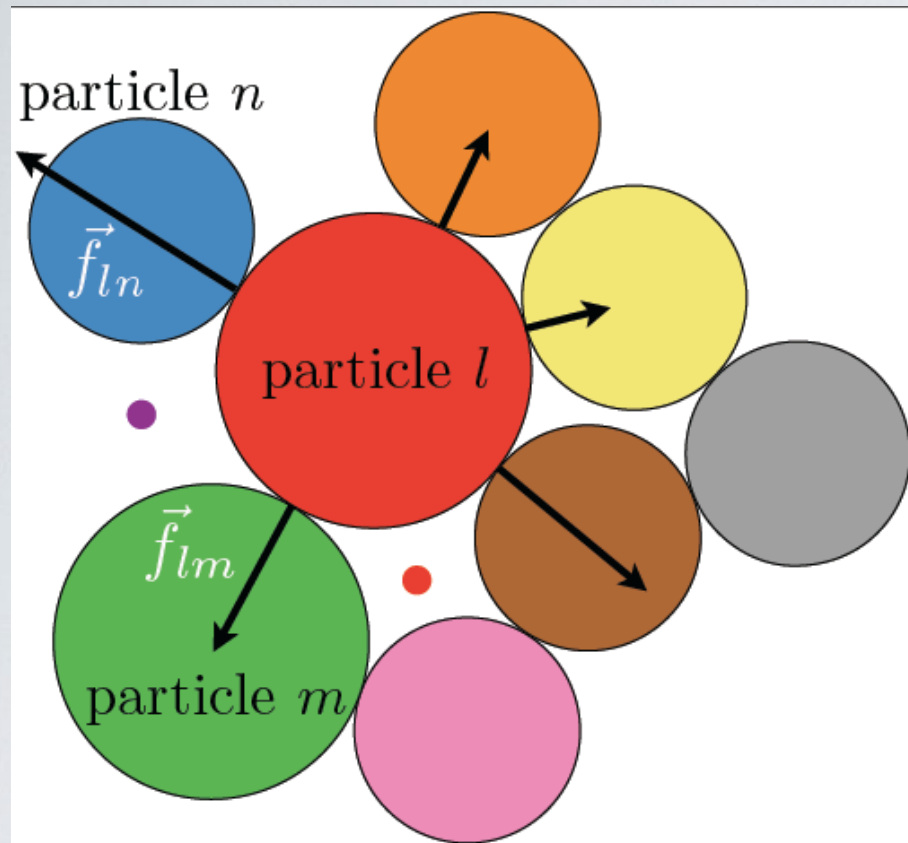
$\underbrace{\hspace{10em}}_0 \qquad \underbrace{\hspace{10em}}_0$

External stresses determine difference in heights across the system

The conditions of mechanical equilibrium ensure the uniqueness of the height representation

$$\nabla \cdot \hat{\sigma} = 0 \rightarrow \text{Vector potential}$$

2D Systems: Force Tilings



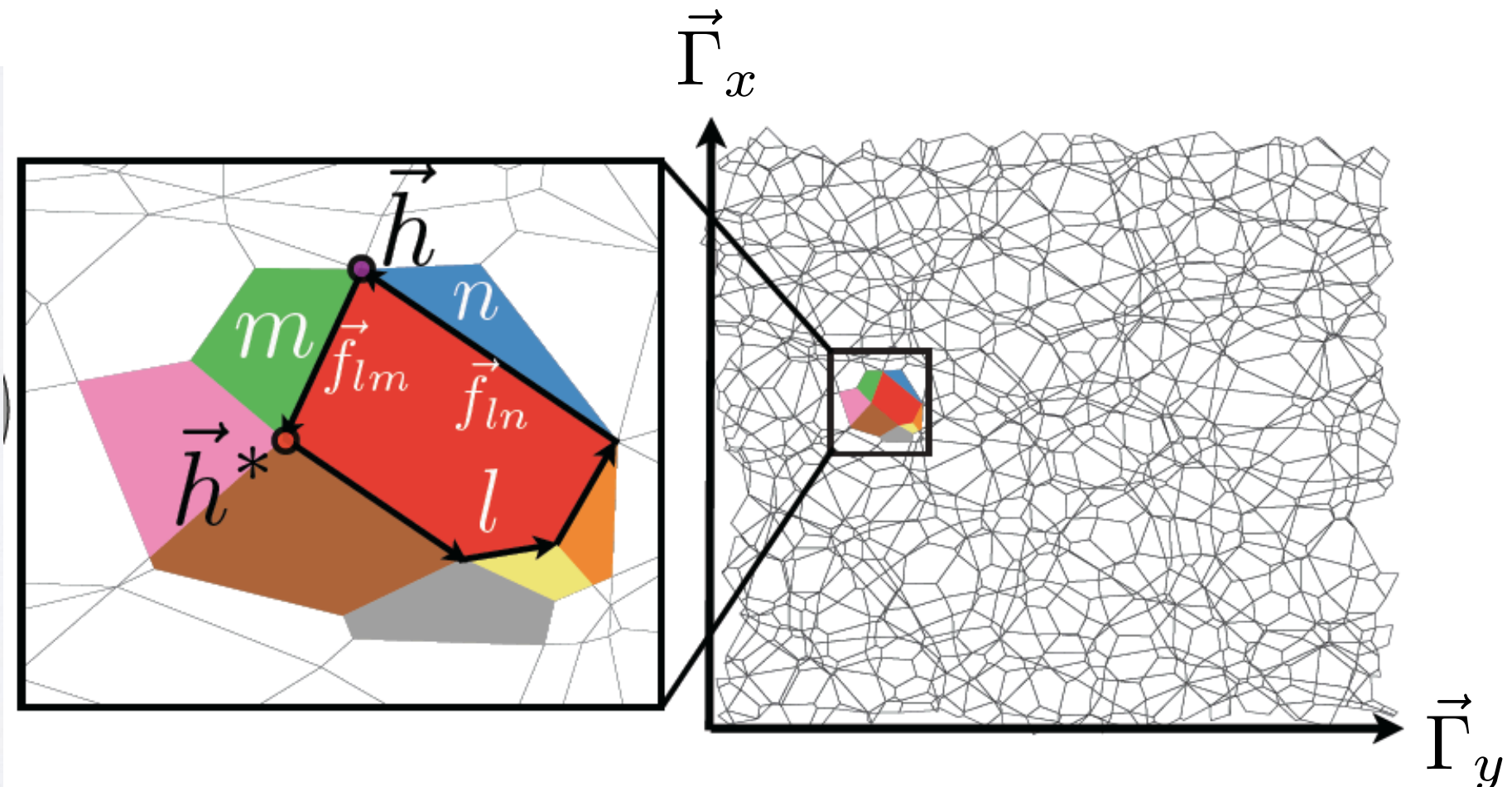
Forces at contacts can have normal and tangential components. Impose force balance on every grain, and use Newton's third law

Applied to dry grains and theory of shear jamming

Force Moment Tensor

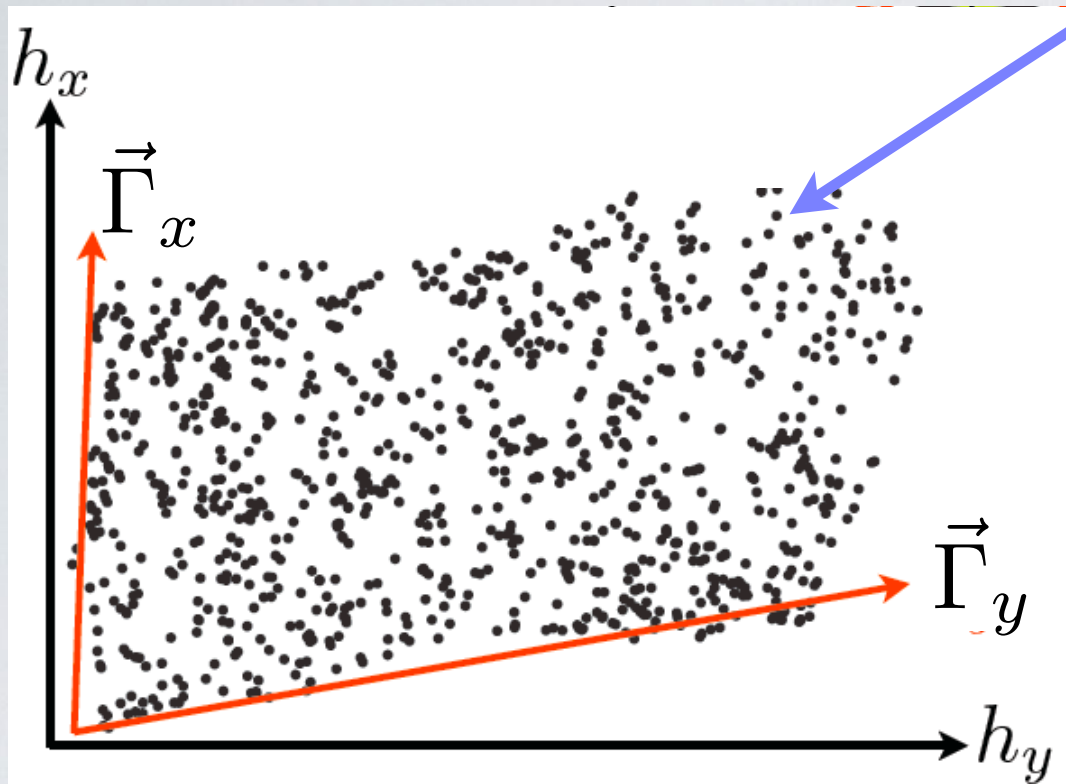
$$\hat{\Sigma} = \sum_{ij} \vec{r}_{ij} \otimes \vec{f}_{ij}$$

$$\hat{\Sigma} = \begin{pmatrix} L_y \Gamma_{yx} & L_y \Gamma_{yy} \\ -L_x \Gamma_{xx} & -L_x \Gamma_{xy} \end{pmatrix}$$



Point Patterns in force space:

Position of vertices: height vectors starting from some arbitrary origin



Macroscopic Stress Tensor

$$\mu = \frac{\tau}{P} = \frac{\sqrt{(N_1)^2 + 4\sigma^2}}{2P}$$

$$P = \frac{F_{xy} + F_{yx}}{2}$$

$$N_1 = \frac{F_{xy} - F_{yx}}{2}$$

Force space: height vectors are the “position vectors” of voids in force space

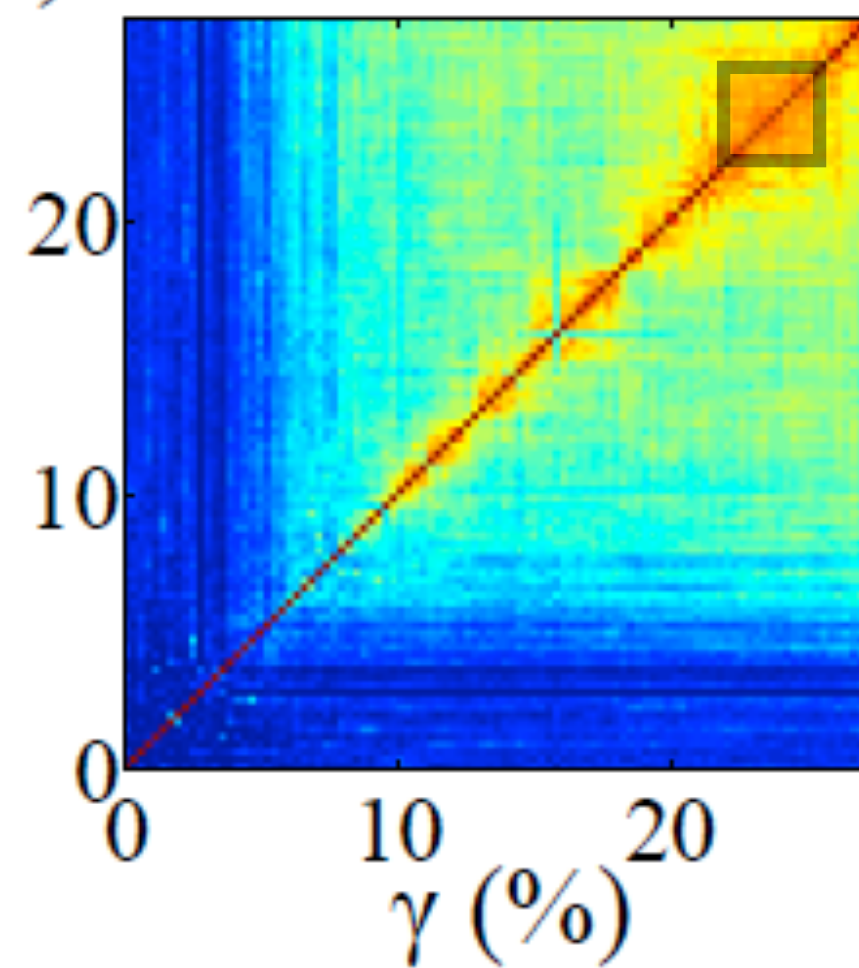
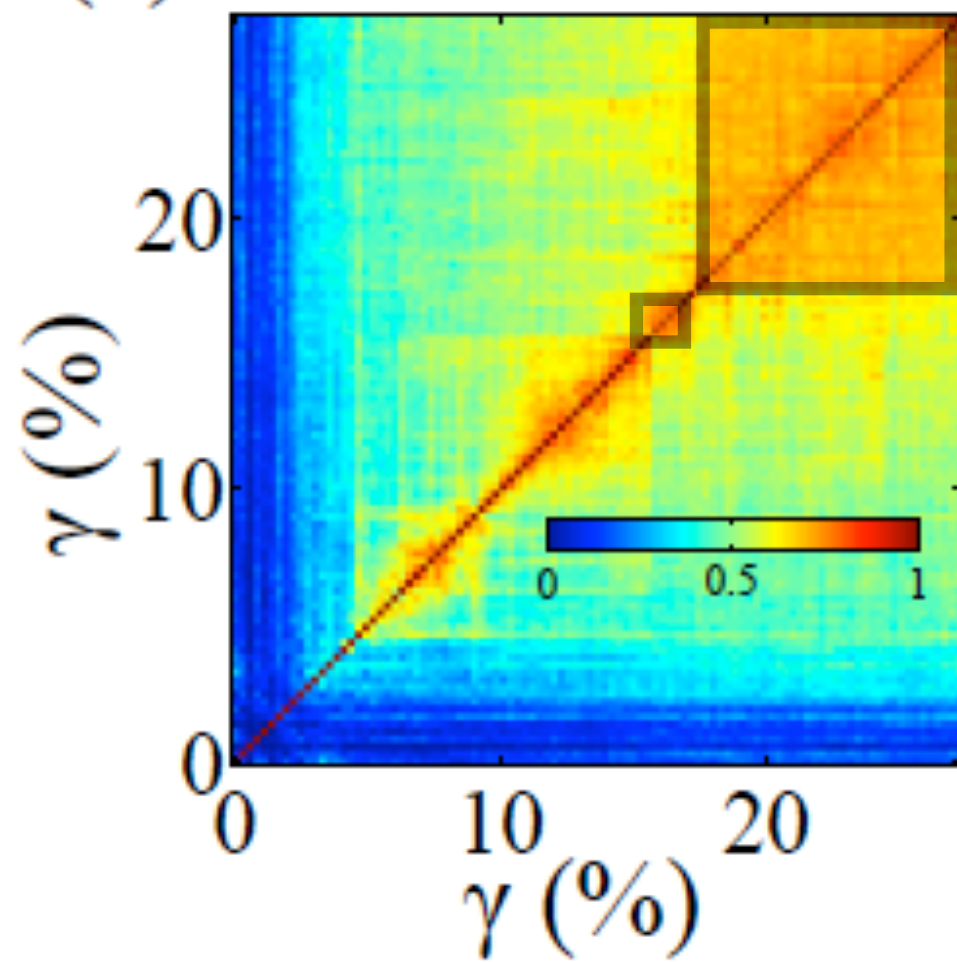
Changing shape of boundary by changing external stresses is the analog of straining: Elastic solids should resist straining: respond affinely.

Do the point patterns in force space distort affinely in the SJ state?

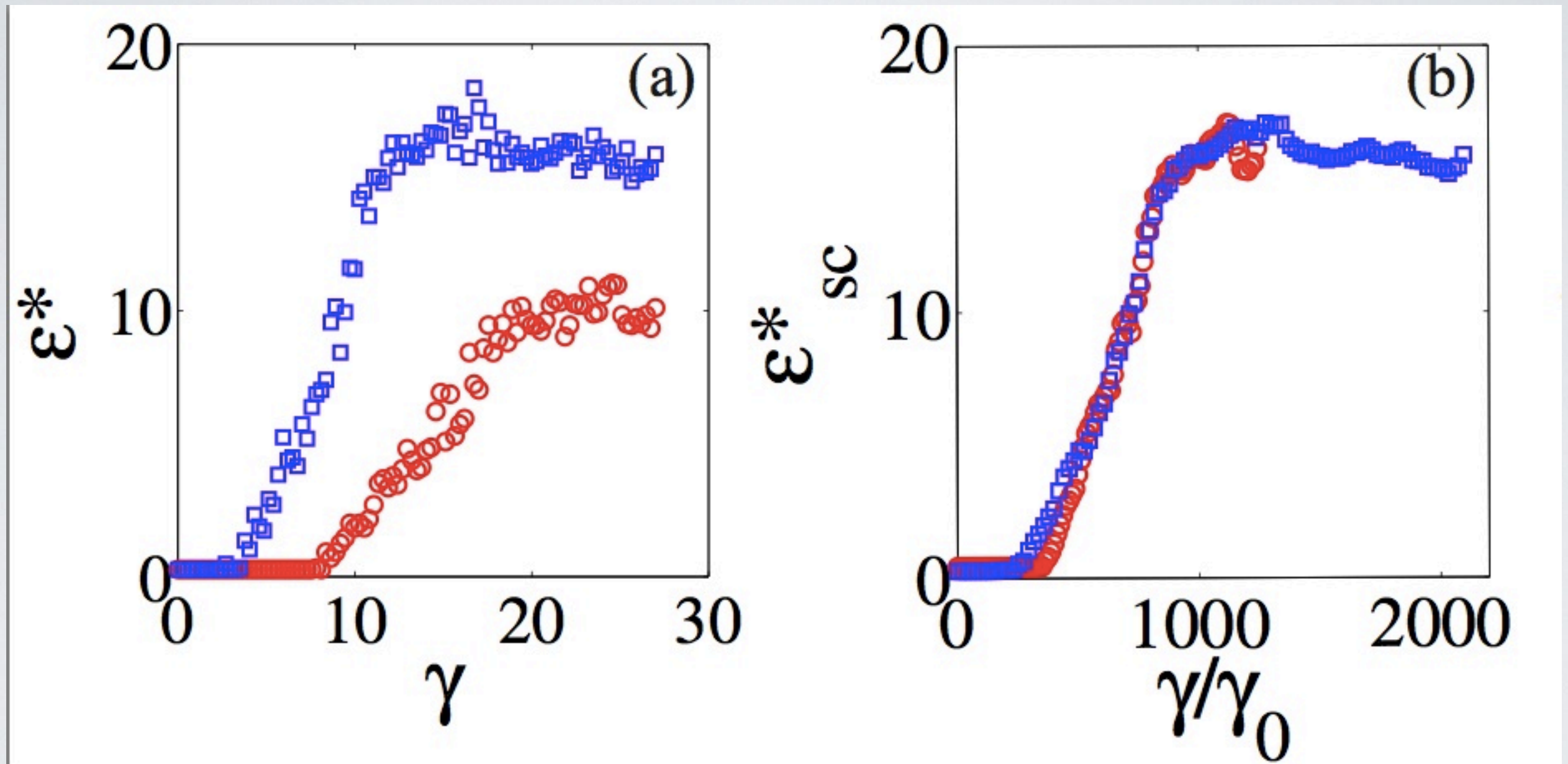
Overlap Order Parameter

Higher packing fraction

Lower packing fraction



Scalar order parameter: threshold the overlap > 0.5



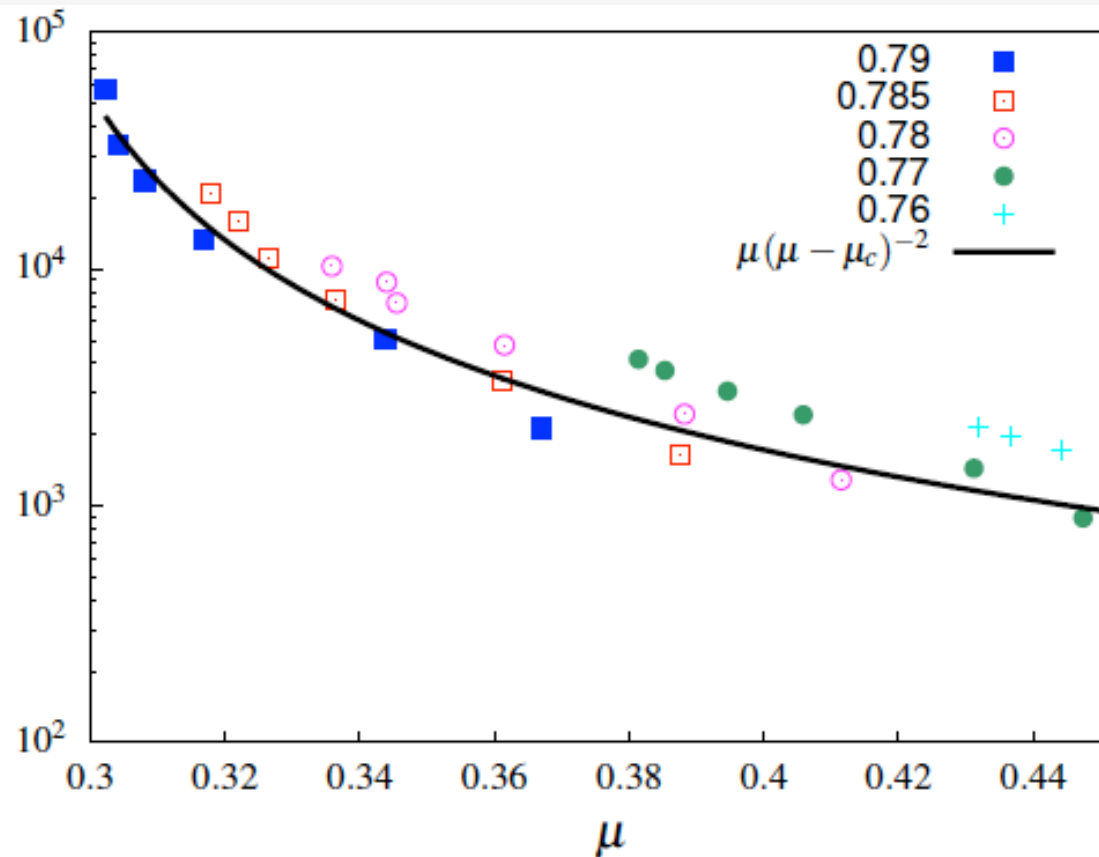
DST: theory based on stress anisotropy

Characteristic decrease in anisotropy

Boyer, Guazzelli, Pouliquen (2011)

$$\eta = \frac{\mu(I)}{I} \longrightarrow \eta = \frac{\mu}{I(\mu)}$$

$$\eta \propto \frac{\mu}{(\mu - \mu_c)^2} \quad \text{BUT} \quad \mu(\sigma, \phi)$$



The DST transition is identified by:

$$\frac{d\dot{\gamma}}{d\sigma} = 0$$

Using the “new” constitutive relation, we can write this condition as

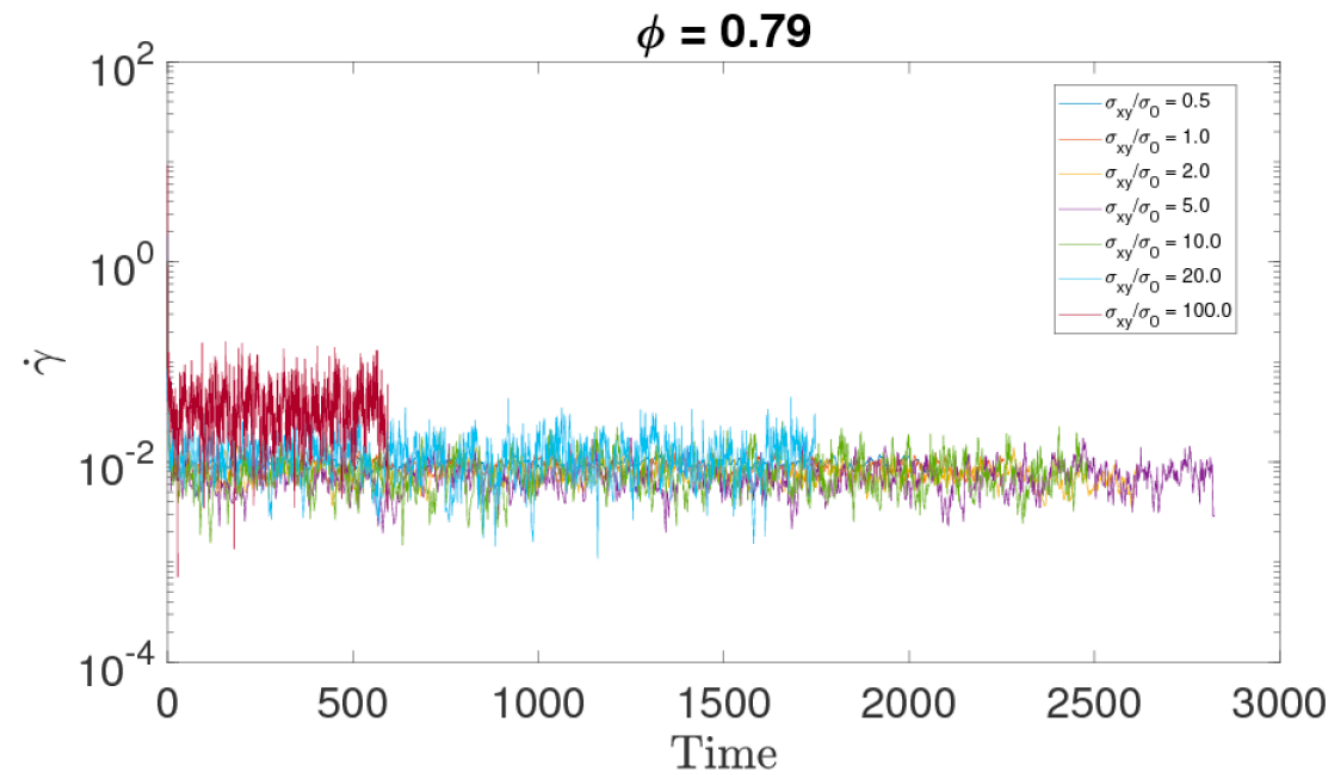
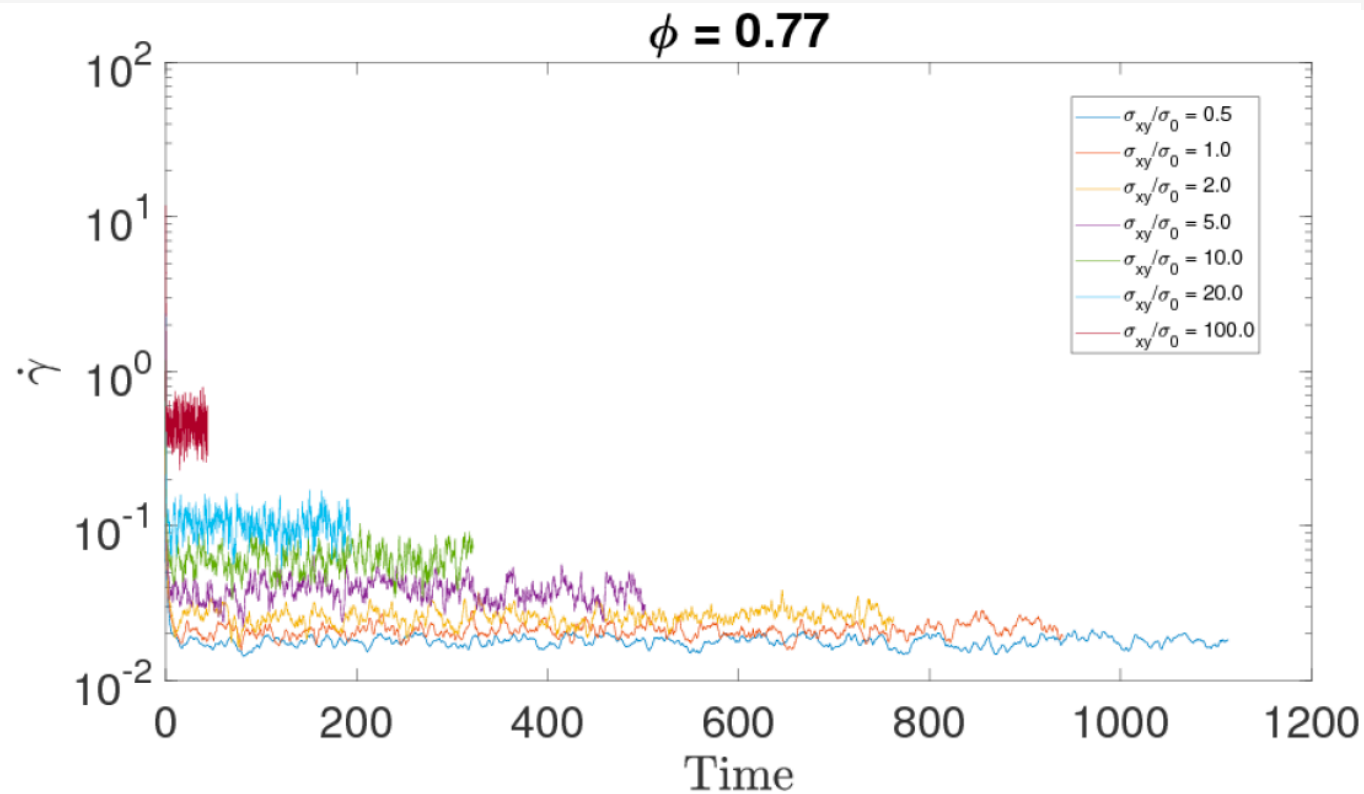
$$\frac{\sigma}{\mu} \frac{d\mu}{d\sigma} = \frac{\mu - \mu_c}{\mu + \mu_c}$$

A theory for the macroscopic friction coefficient

$\mu(\sigma, \phi)$

**from microscopic correlations
(arXiv: 1804.03155, to appear in PRL)**

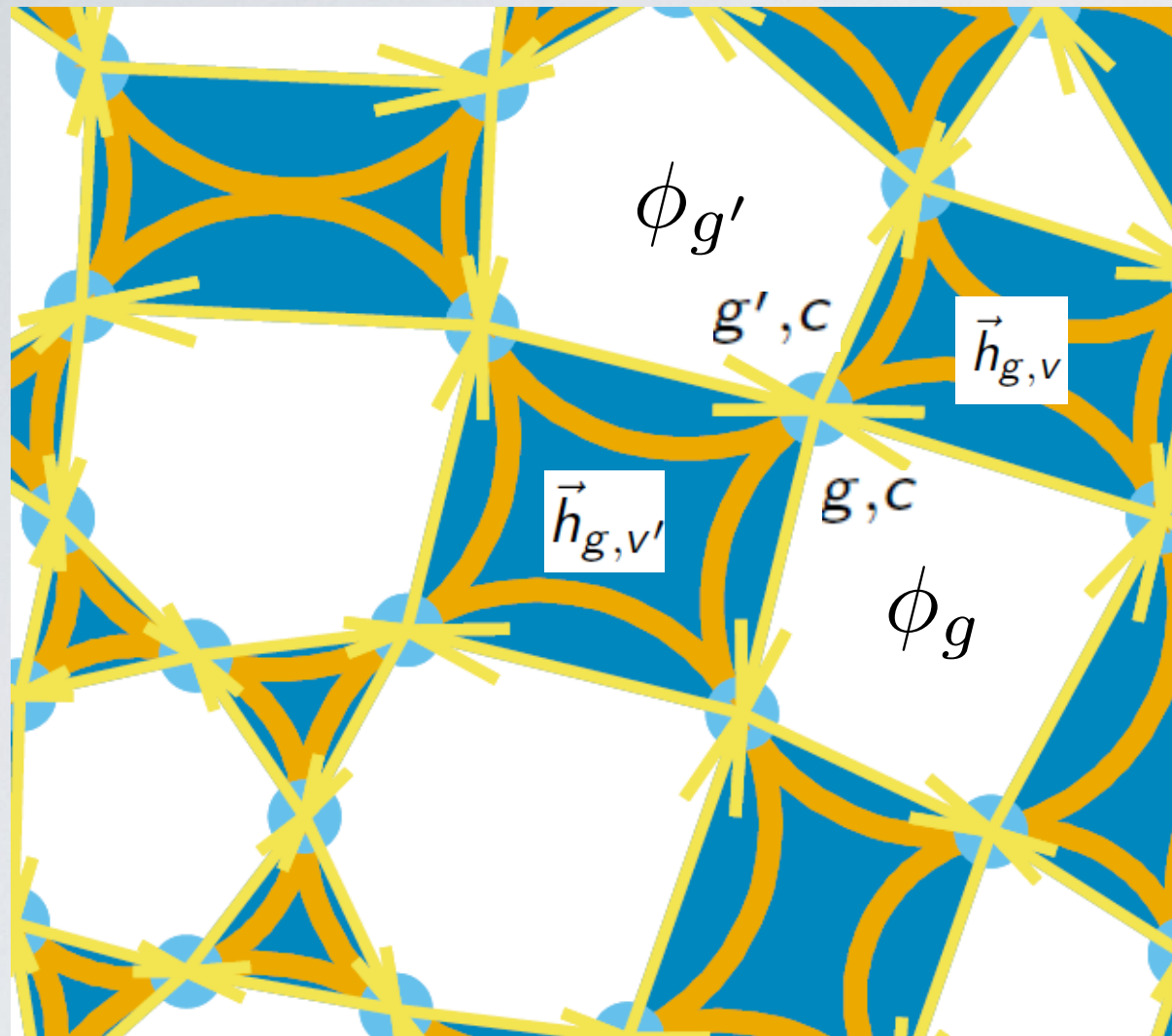
Non-equilibrium steady states sampled in DST simulations: Instantaneously in mechanical equilibrium



- Unlike dry granular materials, these are flowing states: particles have velocities
- “Contact forces”: lubricated and solid-on-solid frictional
- “Body forces”: Stokes drag
- Generalized force tilings using graph Laplacian of contact network
- (Kabir Ramola & BC, Journal of Statistical Physics, 2017)

Body Forces:

Force Response of a network to a perturbation



$$\begin{aligned}
 \vec{f}_{g, c_1} &\neq \vec{h}_{g, v_1} - \vec{h}_{g, v_2}, \\
 \vec{f}_{g, c_2} &\neq \vec{h}_{g, v_2} - \vec{h}_{g, v_3}, \\
 \vec{f}_{g, c_3} &\neq \vec{h}_{g, v_3} - \vec{h}_{g, v_4}, \\
 \vec{f}_{g, c_4} &\neq \vec{h}_{g, v_4} - \vec{h}_{g, v_1}.
 \end{aligned}$$

$$\begin{aligned}
 \vec{f}_{g, c_1} &= \vec{h}_{g, v_1} - \vec{h}_{g, v_2} + \vec{\phi}_{g_1} - \vec{\phi}_{g_0}, \\
 \vec{f}_{g, c_2} &= \vec{h}_{g, v_2} - \vec{h}_{g, v_3} + \vec{\phi}_{g_2} - \vec{\phi}_{g_0}, \\
 \vec{f}_{g, c_3} &= \vec{h}_{g, v_3} - \vec{h}_{g, v_4} + \vec{\phi}_{g_3} - \vec{\phi}_{g_0}, \\
 \vec{f}_{g, c_4} &= \vec{h}_{g, v_4} - \vec{h}_{g, v_1} + \vec{\phi}_{g_4} - \vec{\phi}_{g_0}.
 \end{aligned}$$

Geometry of contact network
represented by the network Laplacian

Matrix whose diagonal elements contain
the number of contacts, otherwise the
adjacency matrix

- This is **valid for every grain**.
- We can represent this in vectorial notation as the **basic equation**

$$\square^2 |\vec{\phi}\rangle = -|\vec{f}^{\text{body}}\rangle.$$

Localization: Diffusion on a disordered network

- We can **invert this equation** to obtain the auxiliary fields $\{\vec{\phi}_g\}$.
- Given a set of body forces $\{\vec{f}_g^{\text{body}}\}$ and the contact network, the solution $\{\vec{\phi}_g\}$ is **unique**.

Properties of the Network Laplacian

- The network Laplacian is a $N_G \times N_G$ **real symmetric matrix**.
- \square^2 has the eigenfunction expansion

$$\square^2 = \sum_{i=1}^{N_G} \lambda_i |\lambda_i\rangle \langle \lambda_i|.$$

- \square^2 has **one** zero eigenvalue, with eigenvector

$$\lambda_1 = 0, \quad |\lambda_1\rangle = (111\dots 1).$$

- The rest of the eigenvalues are **all negative**.

Framework

$$\square^2 |\vec{\phi}\rangle = -|\vec{f}_{body}\rangle \quad \text{Equation defining the auxiliary fields}$$

Given a contact network and a set of body forces, solution is unique

If the solution violates torque balance/static friction condition, network will rearrange

Disorder of contact network represented by network Laplacian

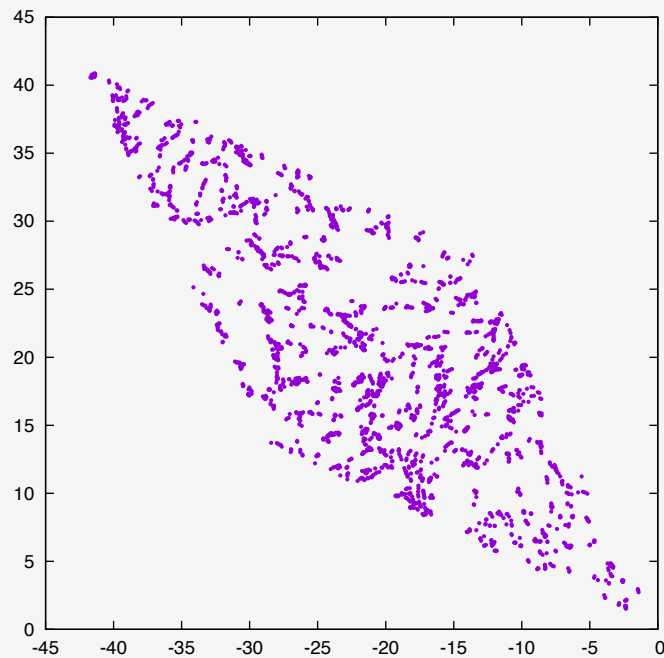
Eigenfunction expansion $\square^2 = \sum_{i=1}^N \lambda_i |\lambda_i\rangle \langle \lambda_i|$

One zero mode: $\lambda_1 = 0$, $|\lambda_1\rangle = (1 \ 1 \ 1 \dots 1)$

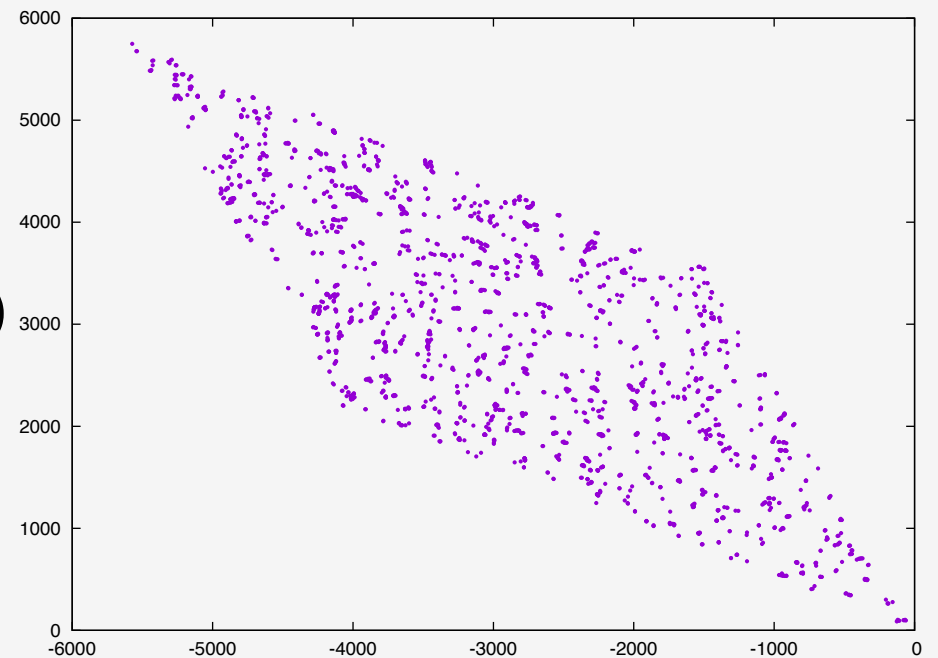
$$|\vec{\phi}\rangle = \sum_{i=1}^N \frac{1}{\lambda_i} \langle \lambda_i | \vec{f}_{body} \rangle |\lambda_i\rangle$$

Point Patterns: Vertices of Force tilings

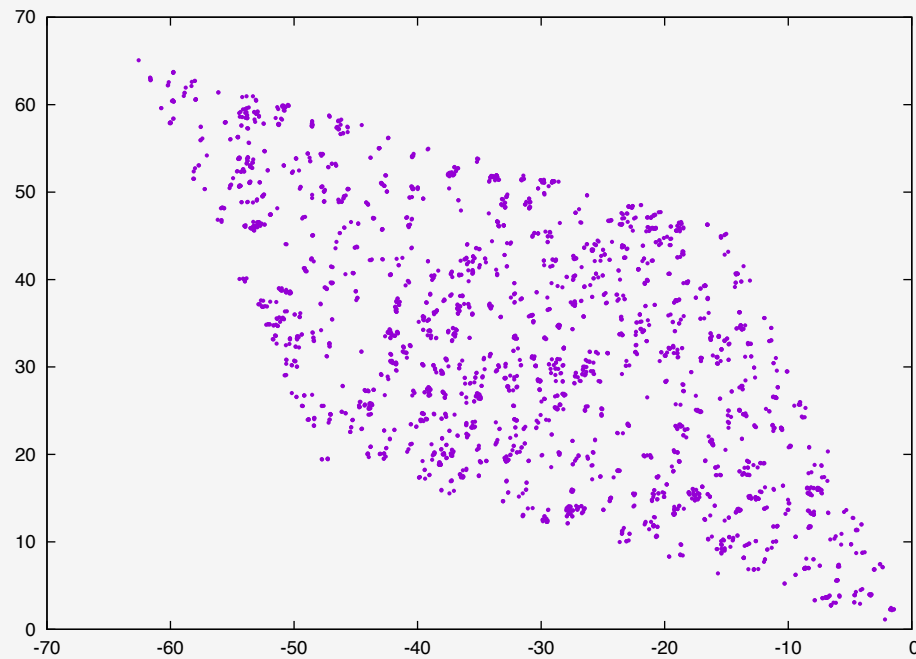
(0.76, 1)



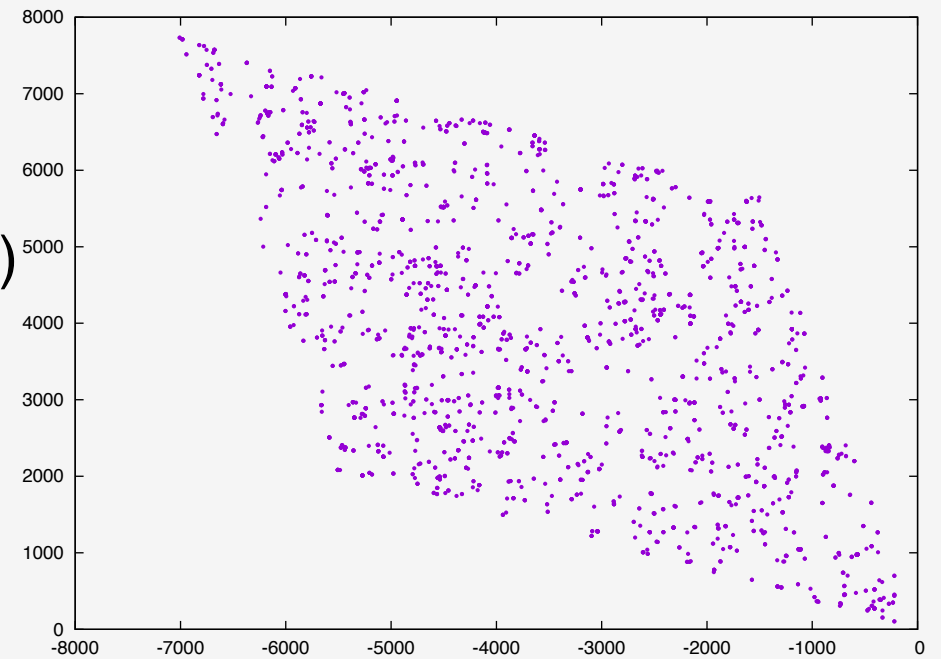
(0.76, 100)



(0.8, 1)



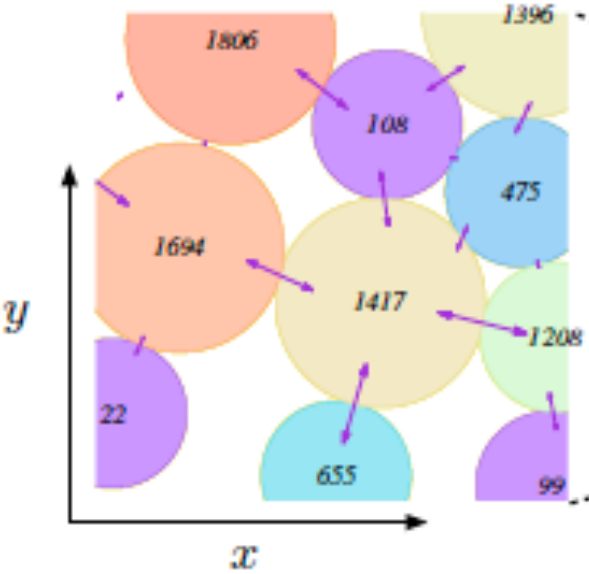
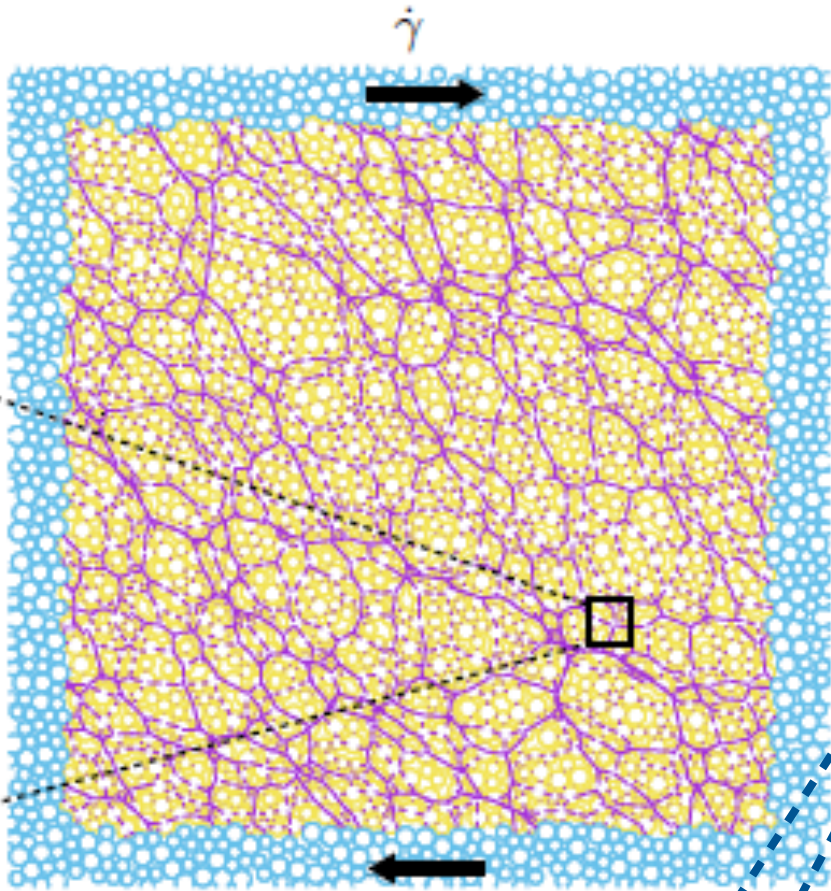
(0.8, 100)



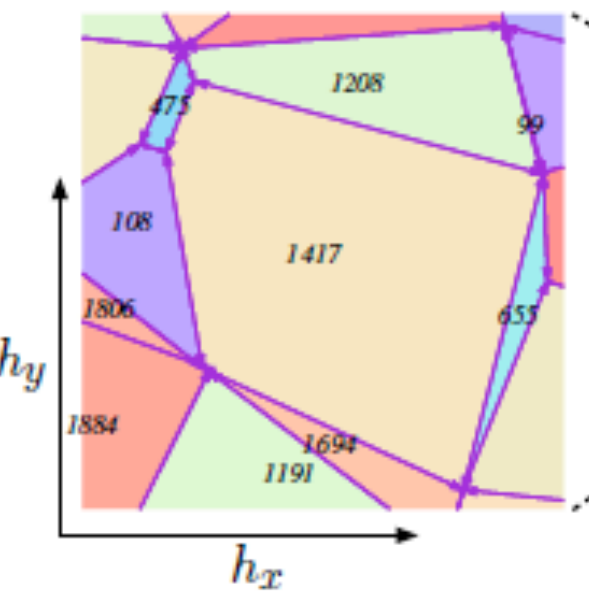
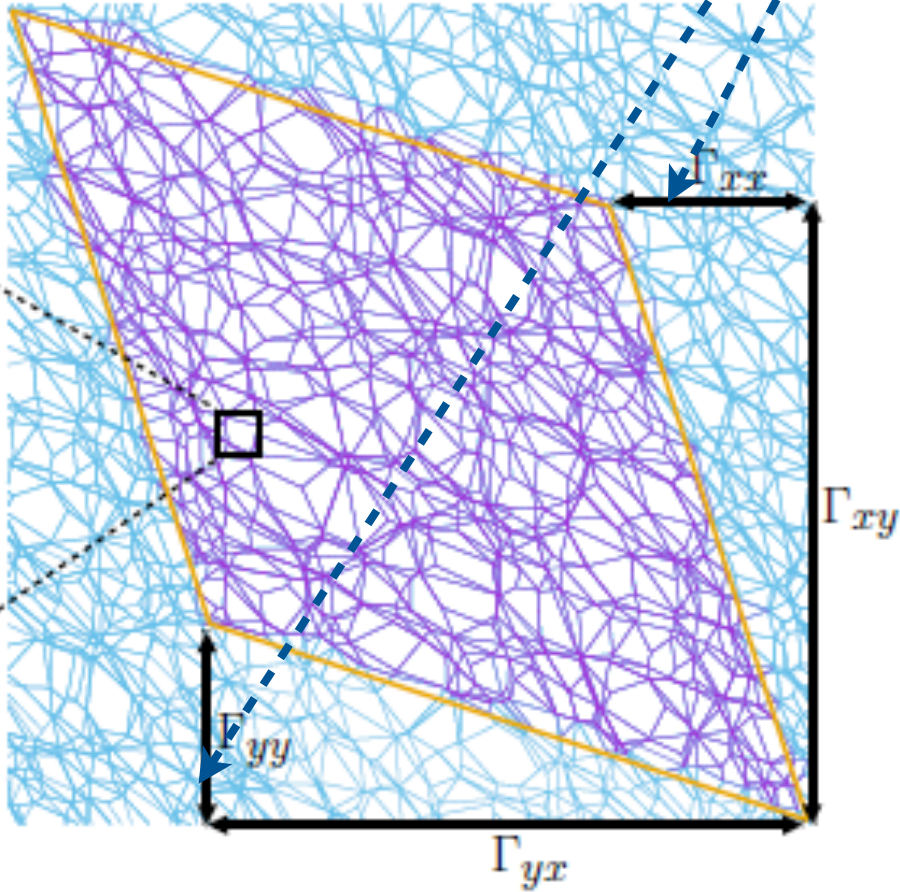
The set of points is represented by “height vectors” : $\{\vec{h}_i\}$

DST

a)



b)



Shape can Fluctuate

Fixed in stress-controlled simulations

$$\mu = \frac{\tau}{P} = \frac{\sqrt{(N_1)^2 + 4\sigma^2}}{2P}$$

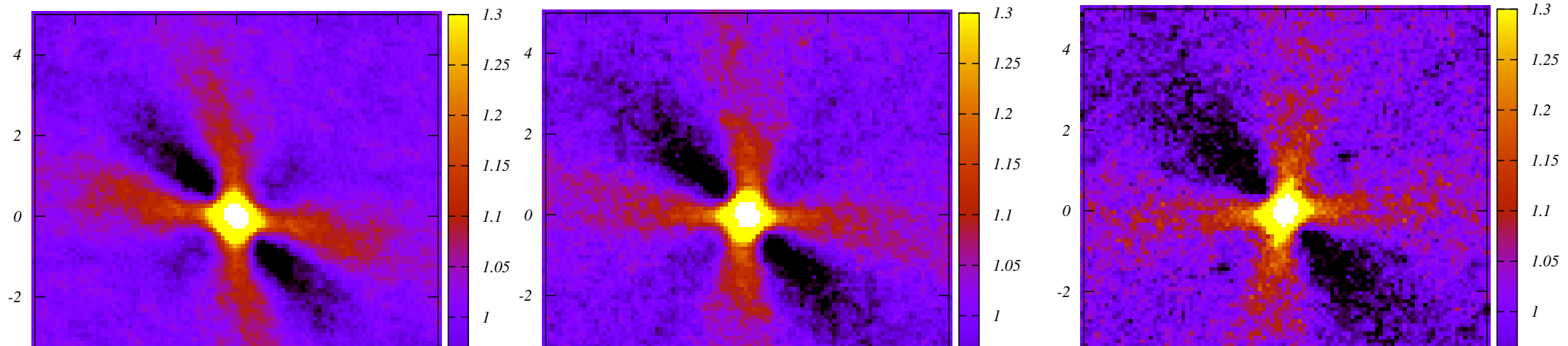
$$P = \frac{\Gamma_{yx} - \Gamma_{xy}}{2}$$

$$N_1 = \Gamma_{yx} + \Gamma_{xy}$$

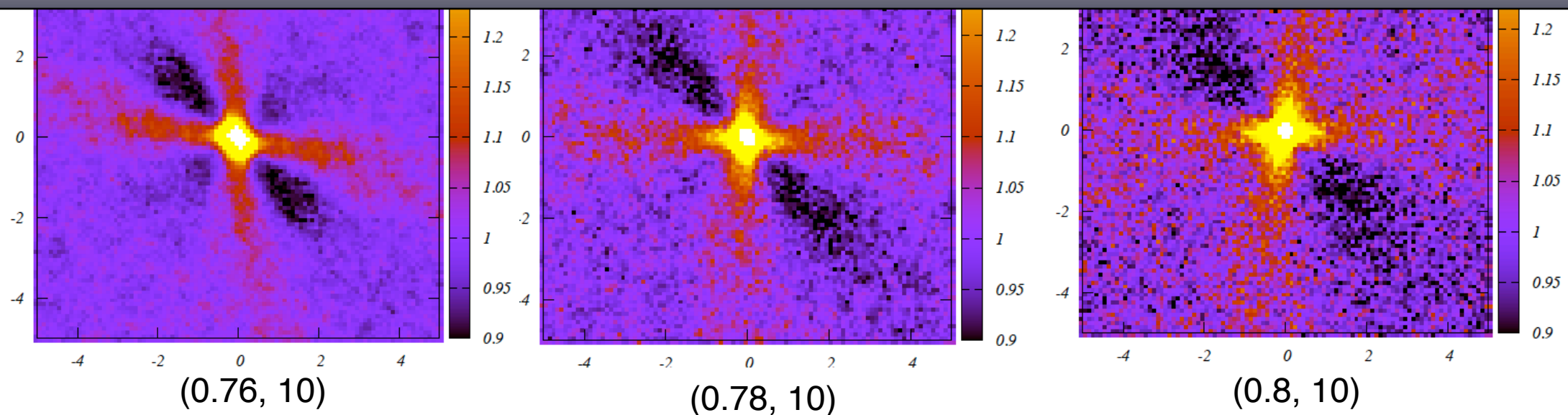
For simplicity, let's set normal stress difference to zero, then area of the box, A , is the single shape parameter.

$$A = \sigma^2 \left(\frac{1}{\mu^2} - 1 \right)$$

DST: Pair Correlation Functions



Can these changes in microscopic correlations in force-space lead to changes in $\mu(\sigma, \phi)$?

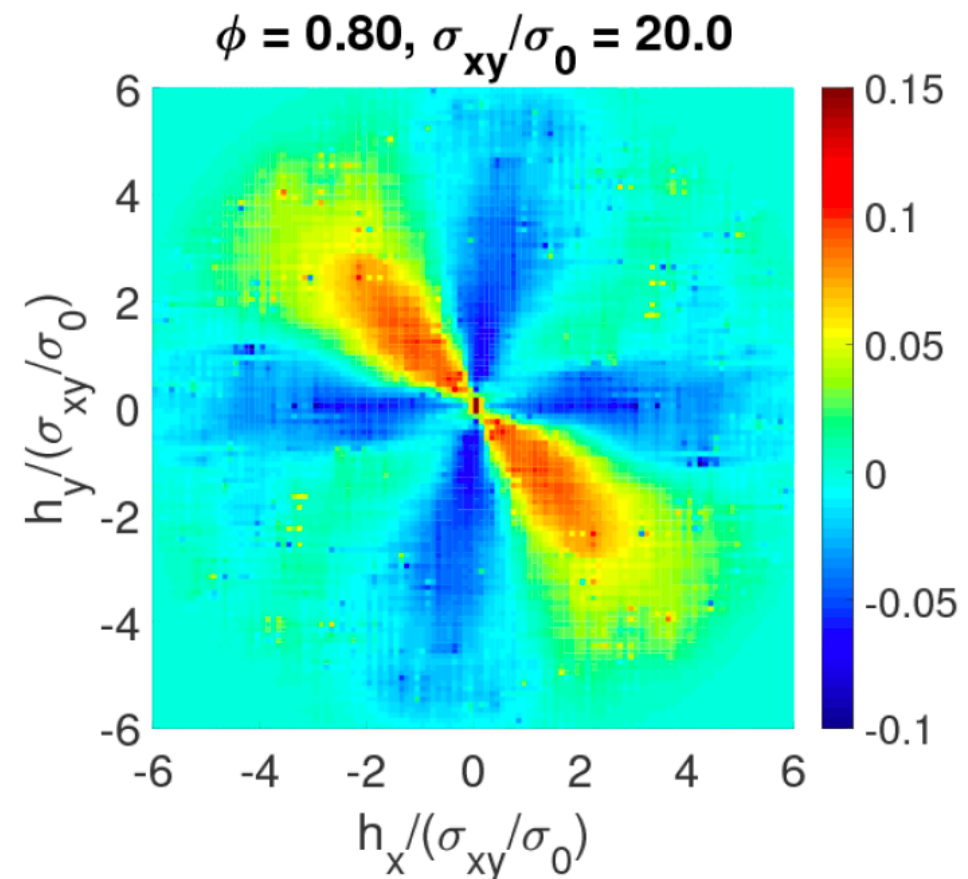
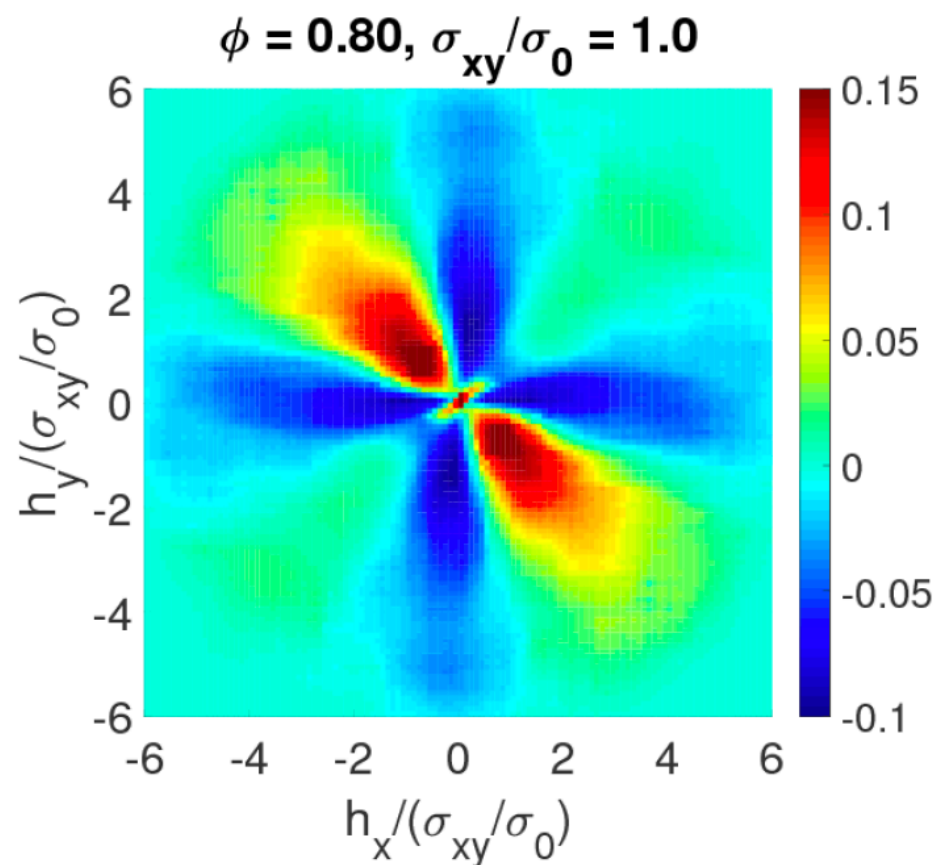
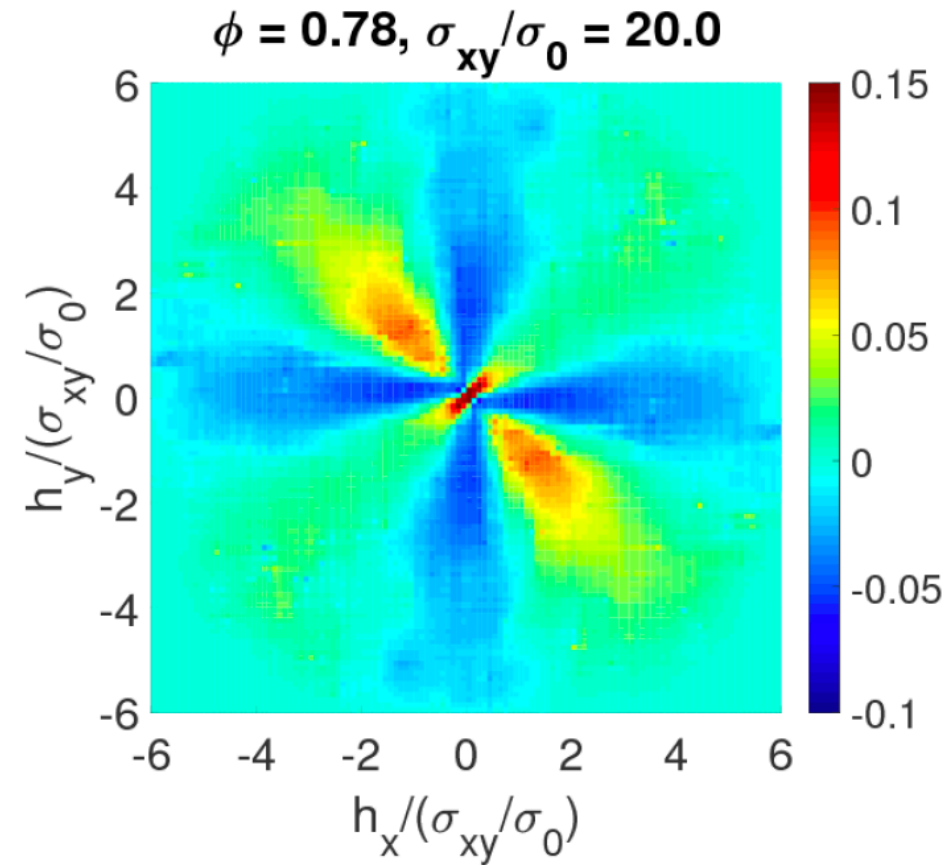
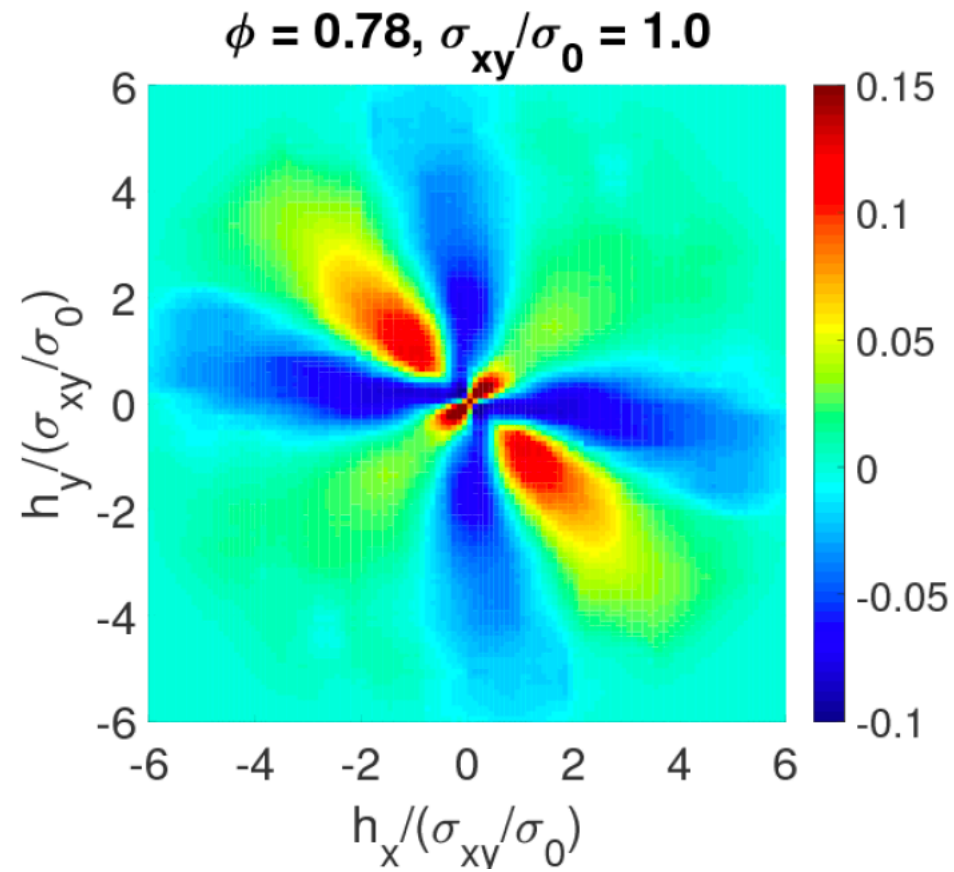


blue-black regions: statistically larger forces, primarily along the compressive direction

yellow-red regions: statistically smaller forces, rotates with increasing packing fraction

with increasing stress: contrast decreases

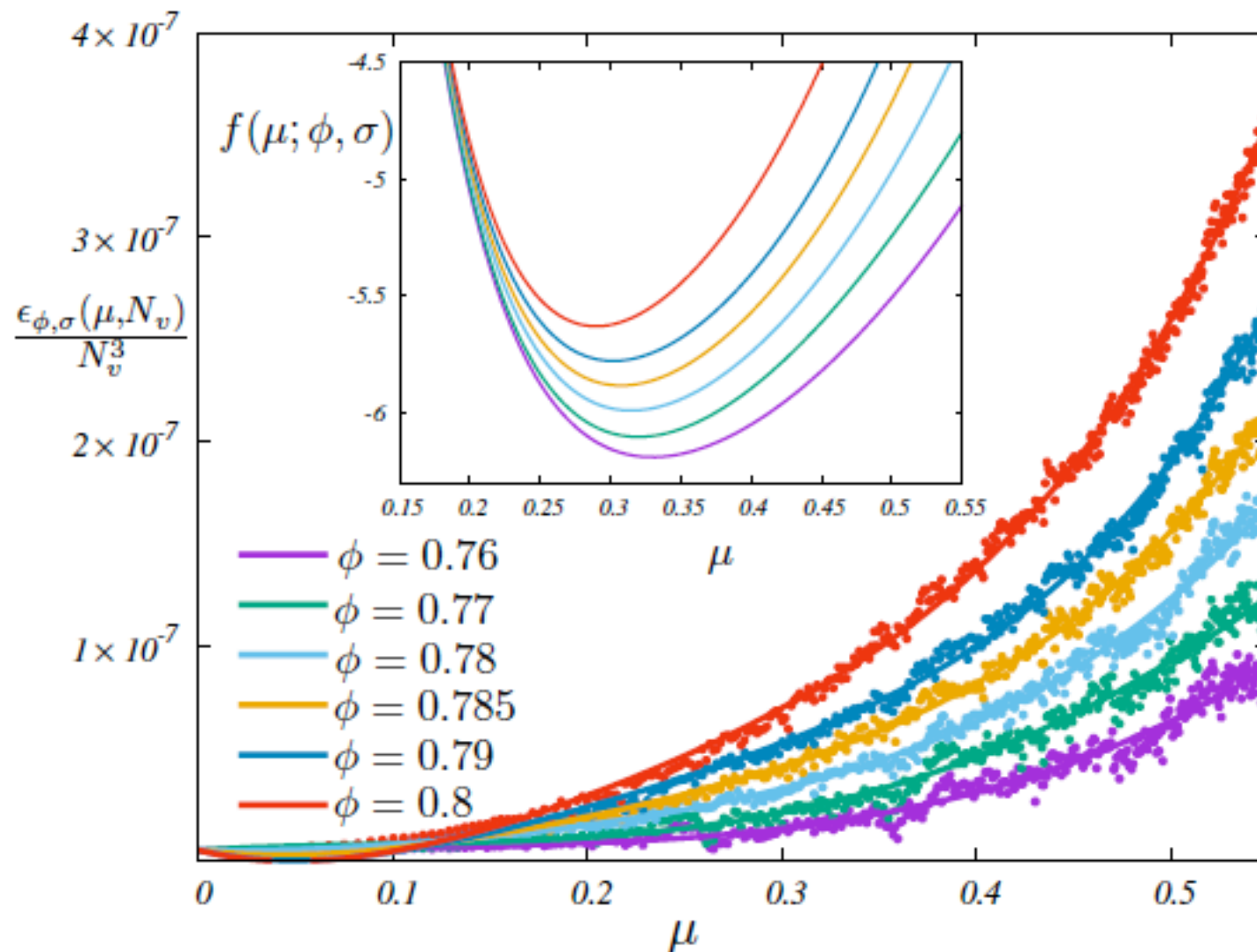
DST: Pair Potentials



DST: Statistical Mechanics based on Edwards ensemble

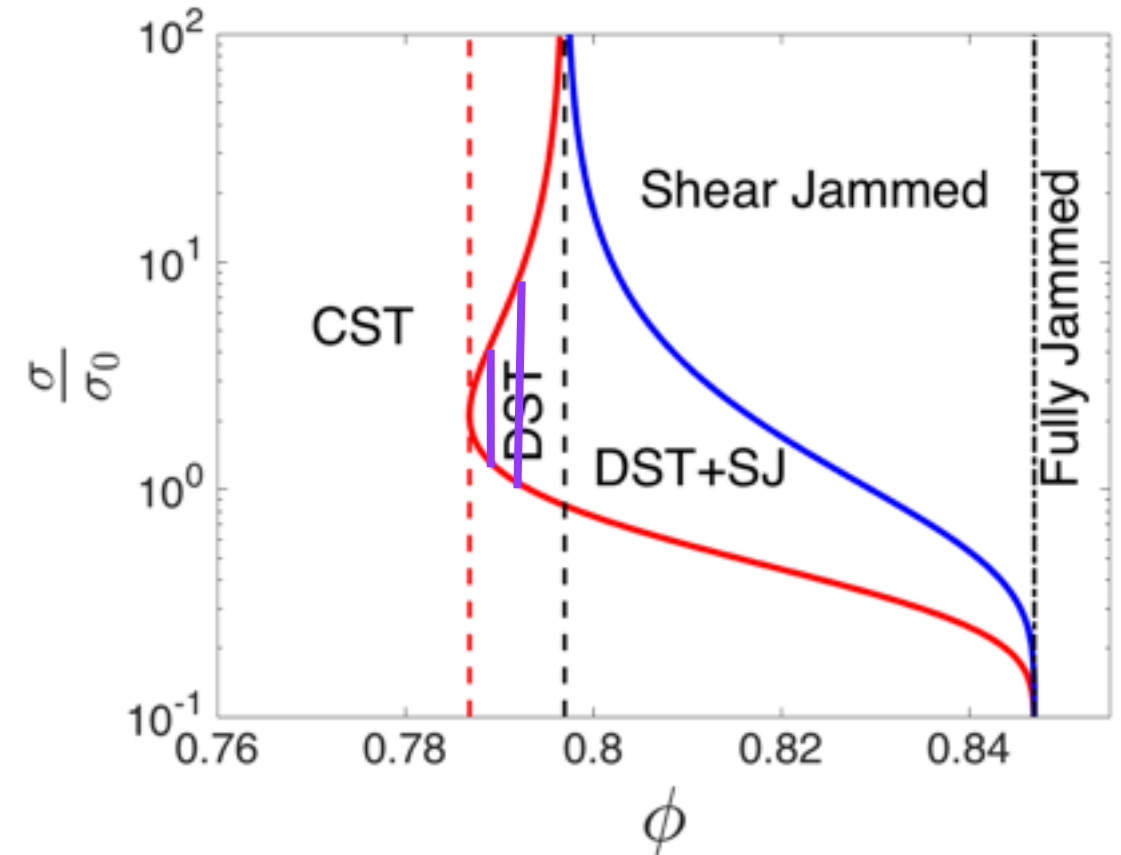
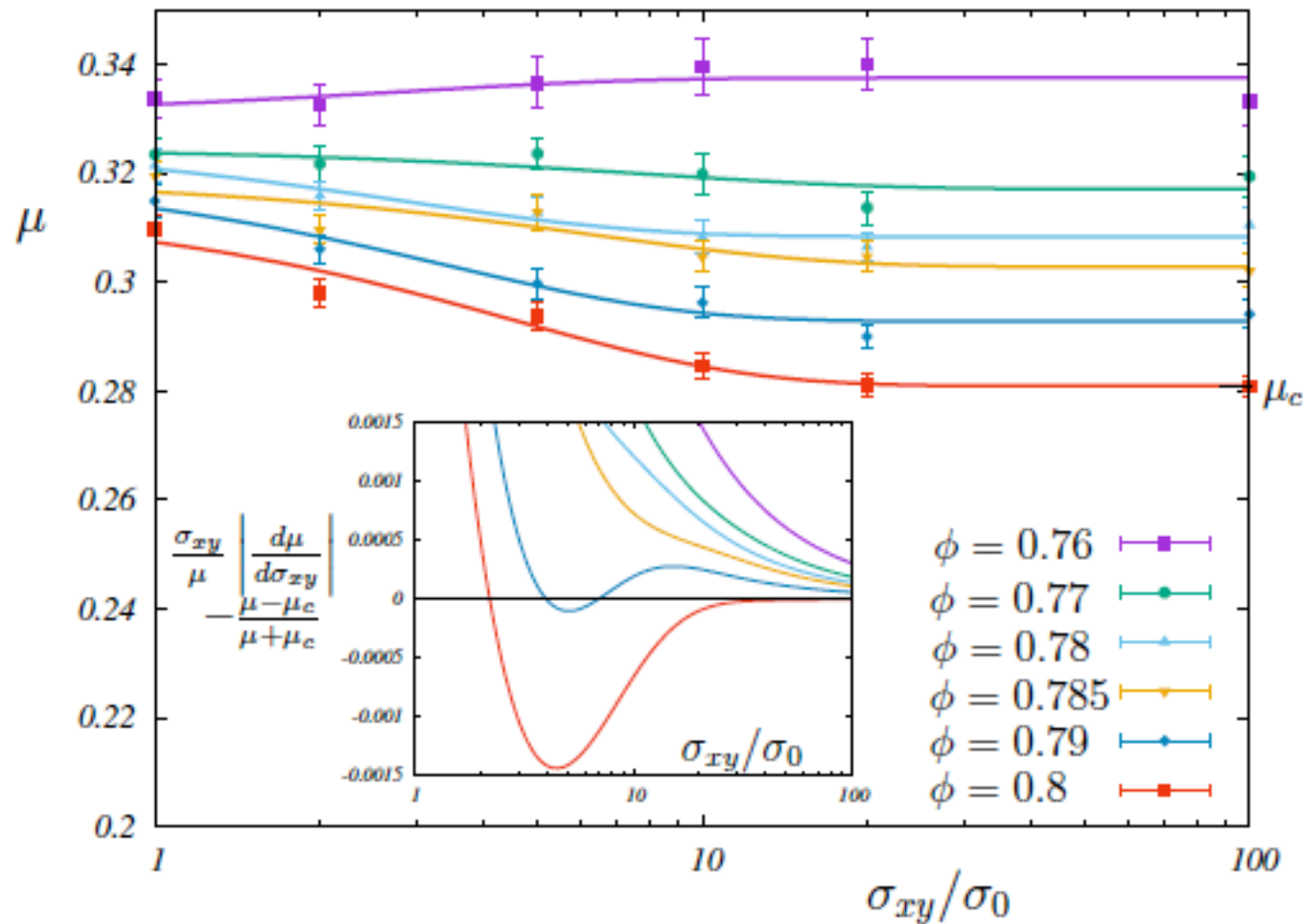
No assumption about equiprobability: measure obtained from pair potential

$$Z_{\phi,\sigma} = \frac{1}{N_v!} \int_0^\infty dA \exp(-N_v f_p^* A) \times \underbrace{\int_A \prod_{i=1}^{N_v} d\vec{h}_i \exp\left(-\sum_{i,j} V_{\phi,\sigma}(\vec{h}_i - \vec{h}_j)\right)}_{A^{N_v} \exp(-\epsilon_{\phi,\sigma}(A, N_v))} = \int_0^\infty dA \exp(-\mathcal{F}_{A;\phi,\sigma}).$$



$$A = \sigma^2 \left(\frac{1}{\mu^2} - 1 \right)$$

Results for stress anisotropy: Based on a theory of probability distributions from an effective pair potential in force space



Get DST \sim 0.785-0.79 packing fraction: at 0.785 (0.5-2) & at 0.79 (1.5 - 6)

More importantly: we show that there is a definitive change in “microstructure” between the low and high viscosity states ***in the pattern of heights***