Landau Theory for Stresses in Dense Frictional Suspensions

Statistical Mechanics with Friction

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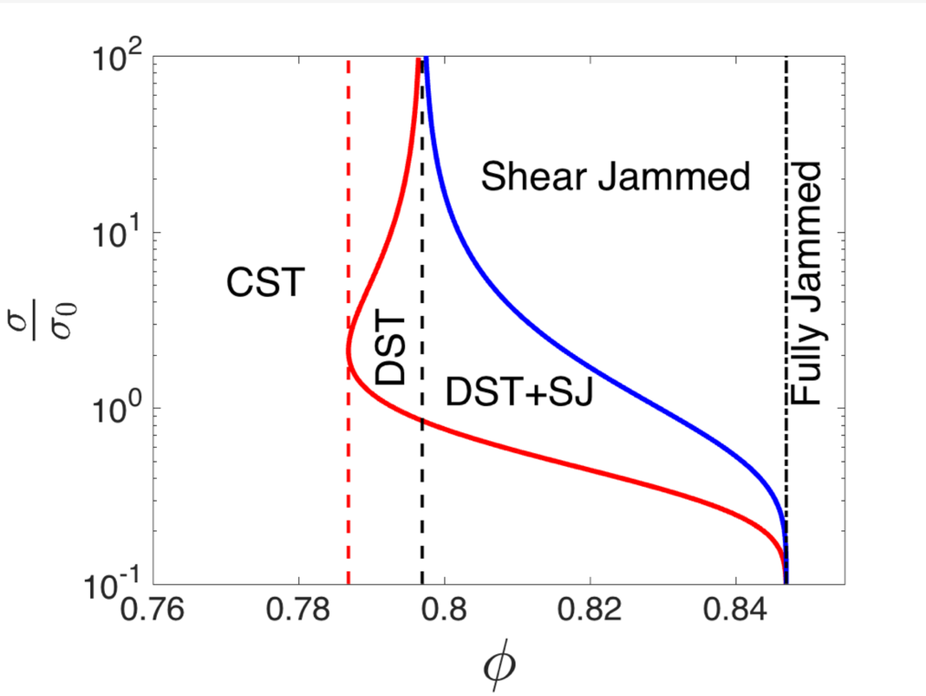
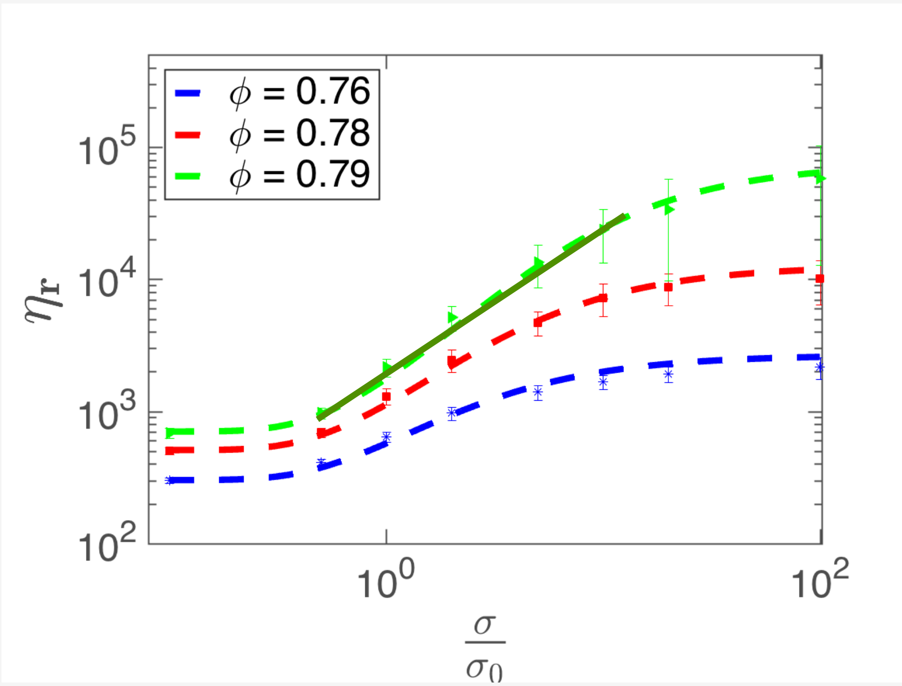
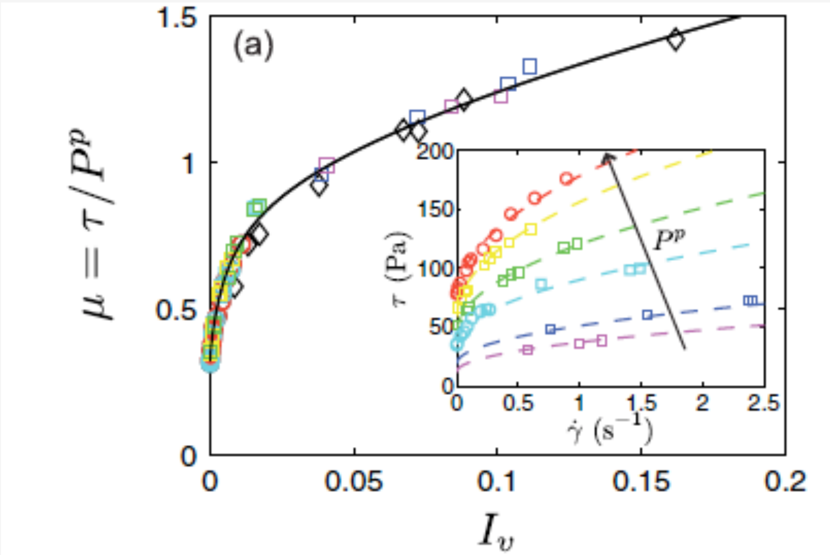




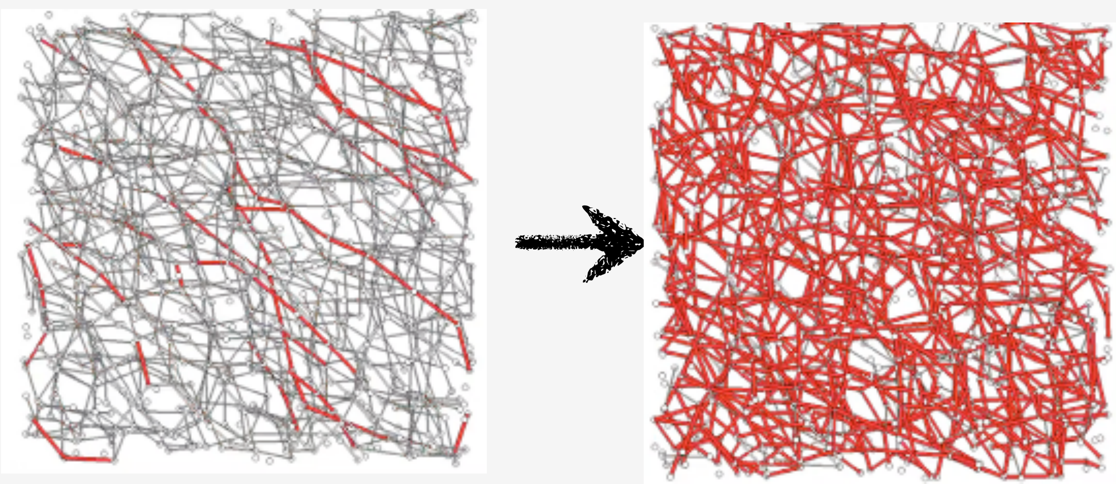
Suspension + Granular Rheology

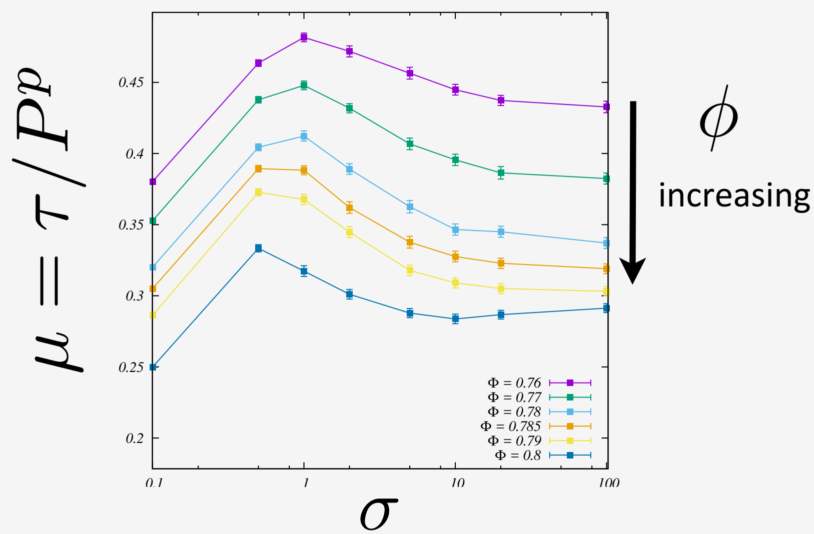
Boyer, Guazzelli, Pouliquen (2011)



- A "universal" relationship between the macroscopic friction coefficient and the viscous number
- 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:

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

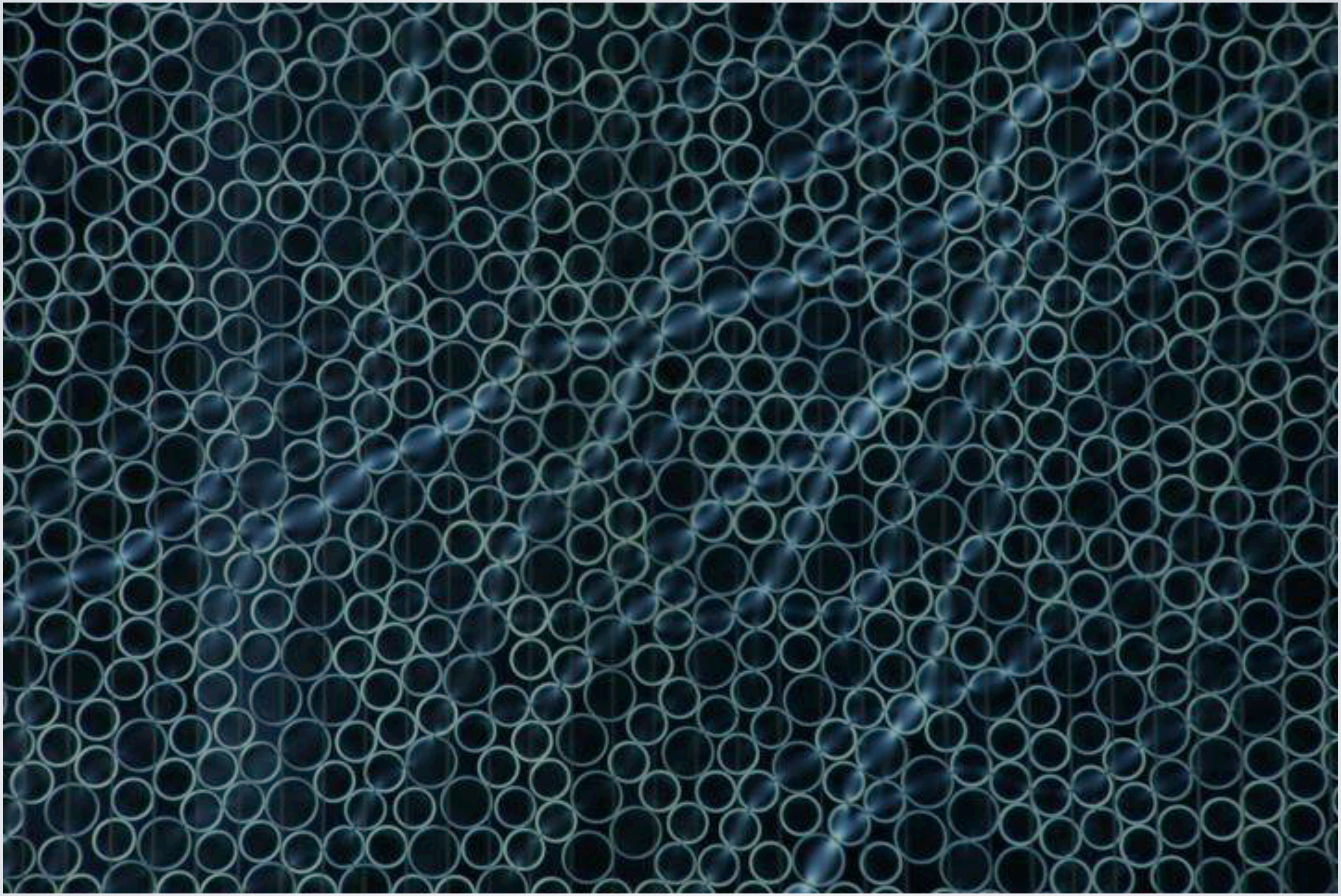




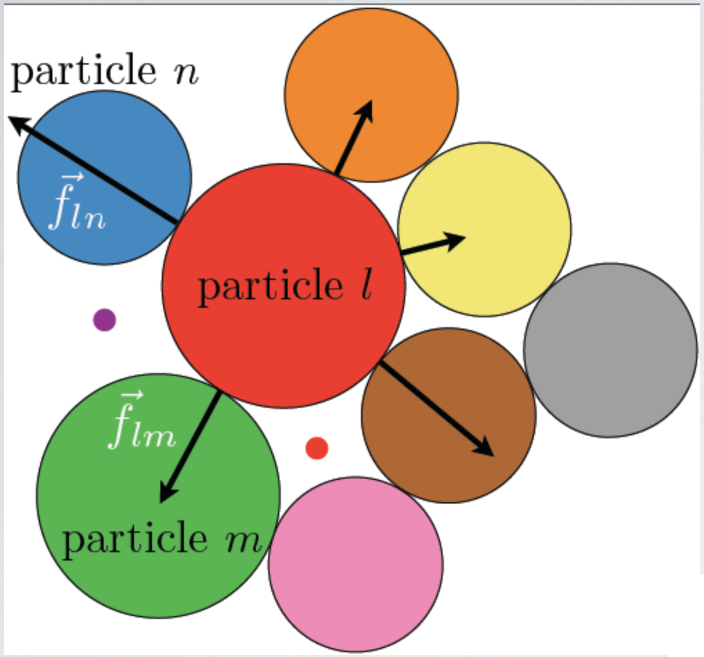
A theory for the macroscopic friction coefficient

$\mu(\sigma, \phi)$

Stress Space



2D Systems: Force Tilings

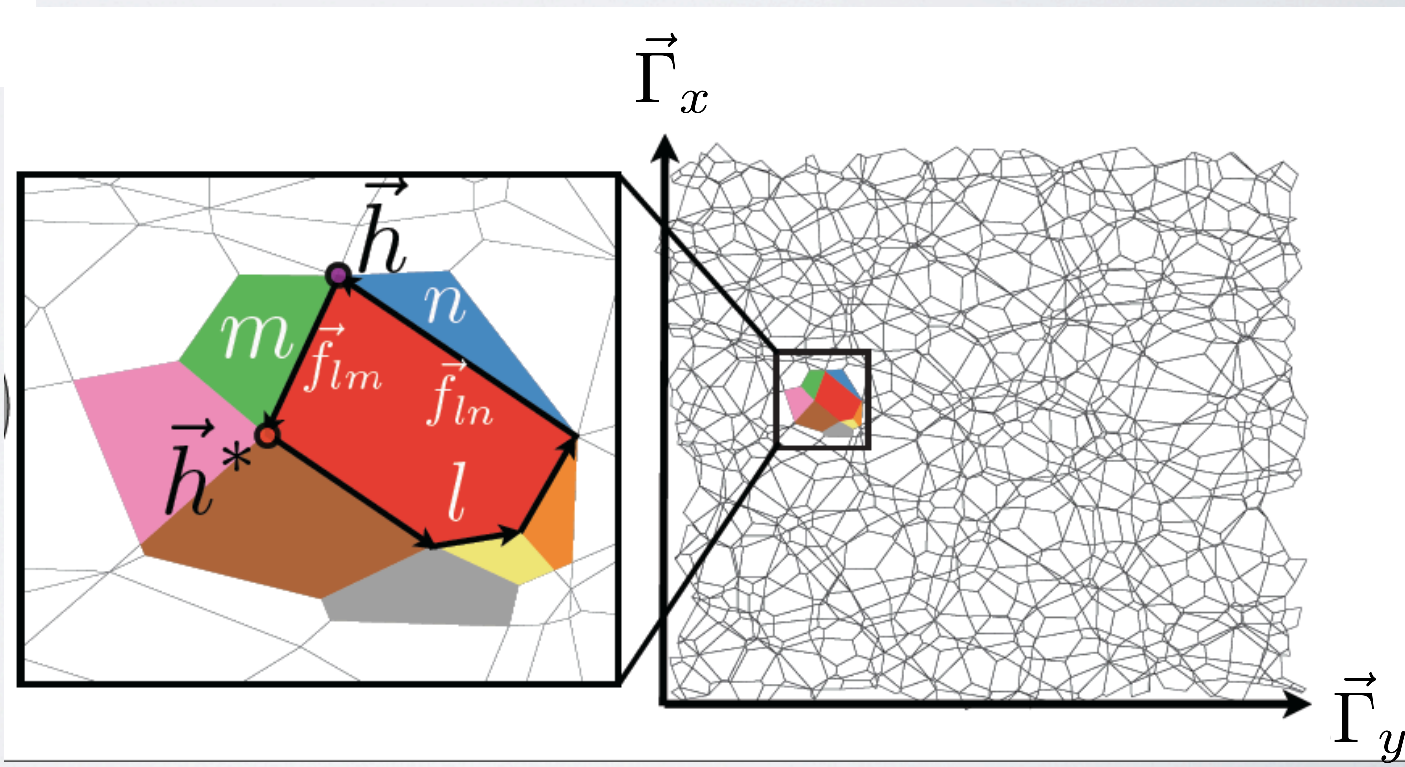


Forces at contacts can have normal and tangential components. Impose force balance on every grain, and use Newton's third law

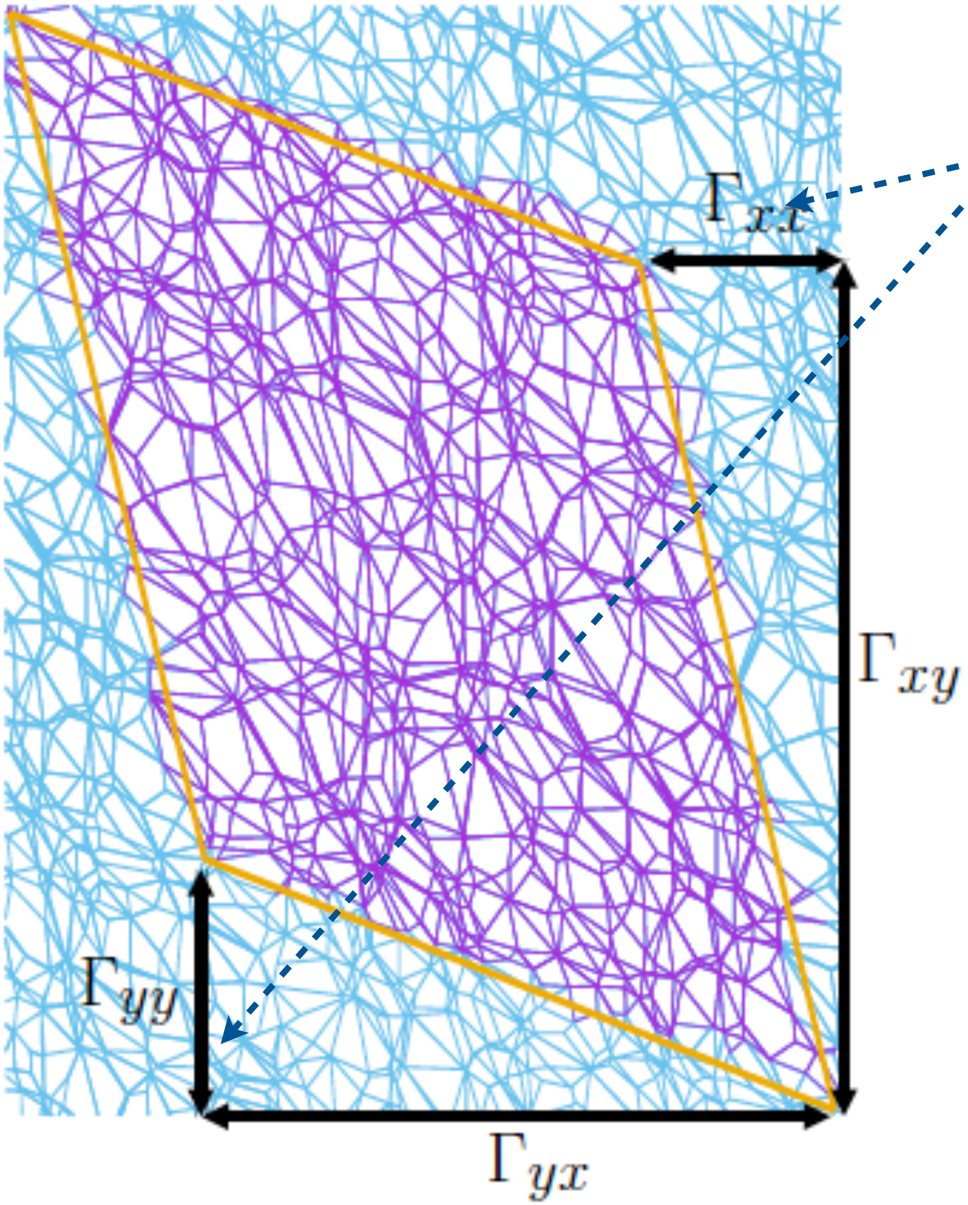
Force Moment Tensor

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

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



Force Tilings Constructed from DST Simulations



Fixed in stress-controlled simulations

Shape can Fluctuate

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

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

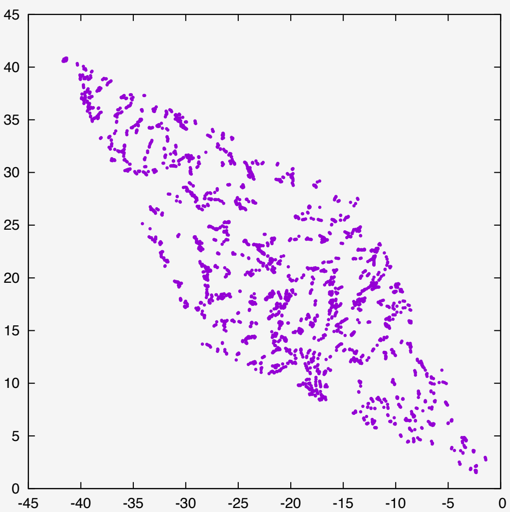
$$N_1 = \Gamma_{\mathrm{yx}} + \Gamma_{\mathrm{xy}}$$

For now, we have set normal stress difference to zero, then area of the box, A, is the single shape parameter.

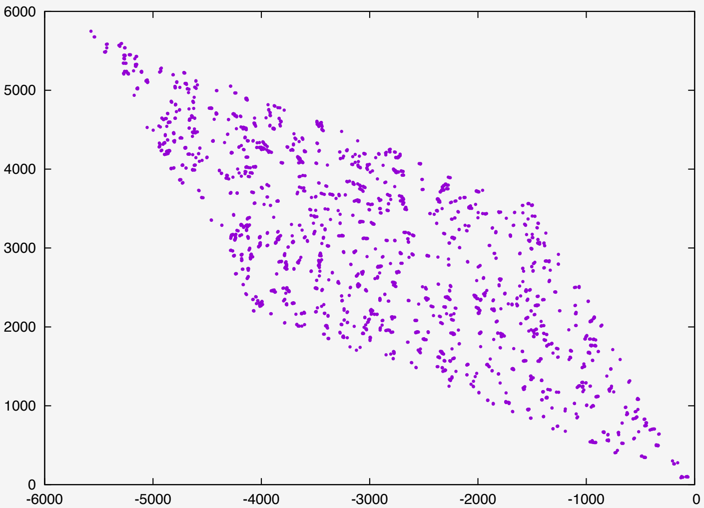
$$A = \sigma^2\left(\frac{1}{\mu^2} - 1\right)$$

Point Patterns: Vertices of Force tilings

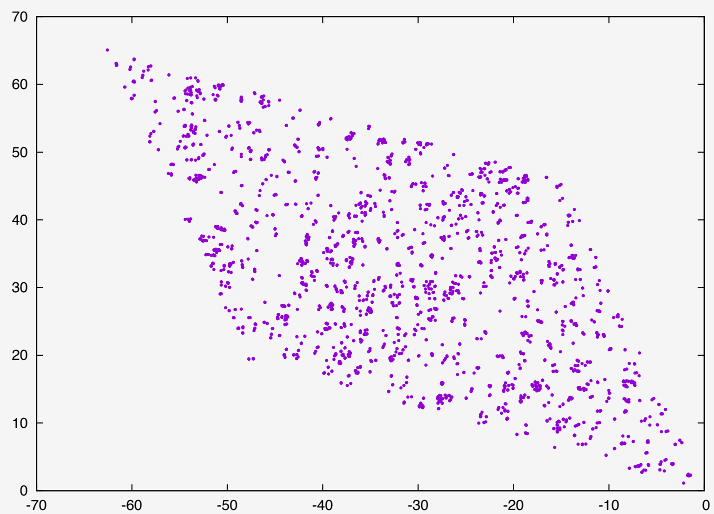
(0.76, 1)



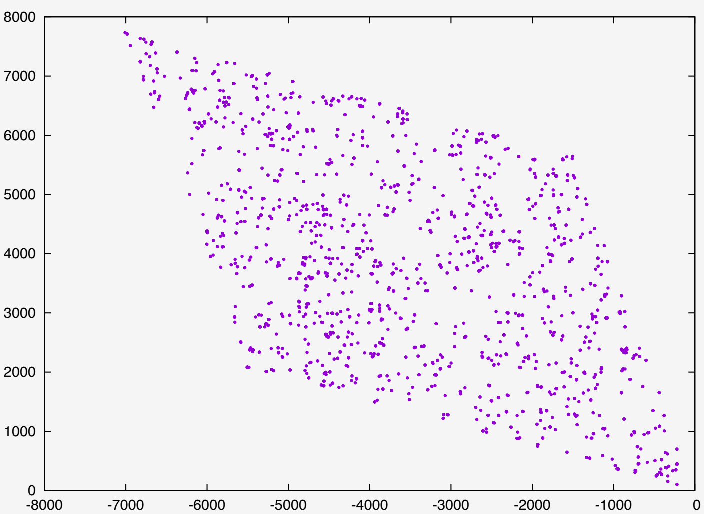
(0.76, 100)



(0.8, 1)

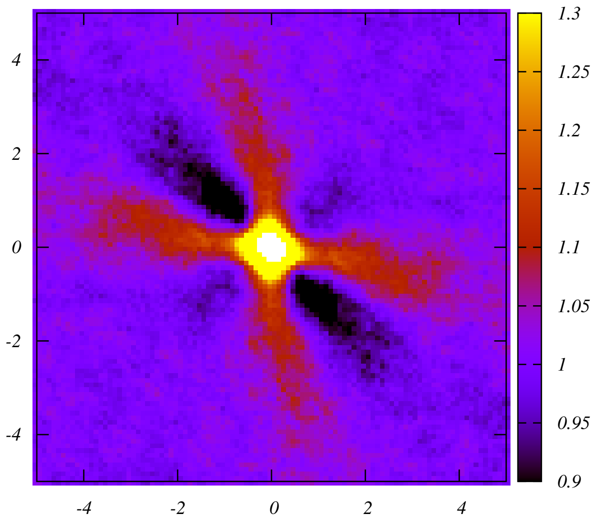


(0.8, 100)

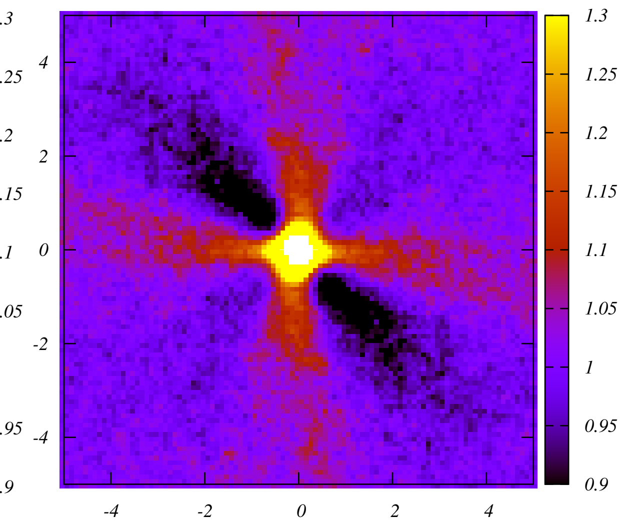


The set of points is represented by "height vectors" : $\{\vec{h}_i\}$

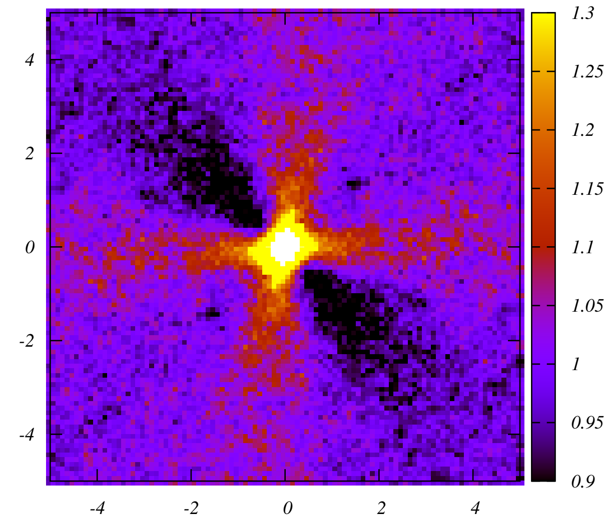
Pair Correlation Functions



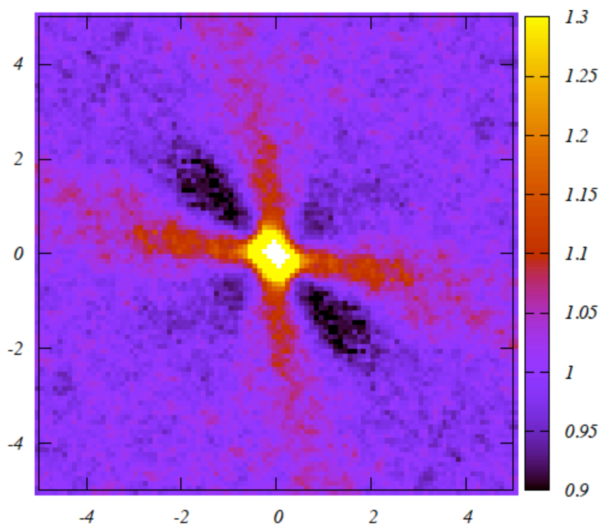
(0.76, 2)



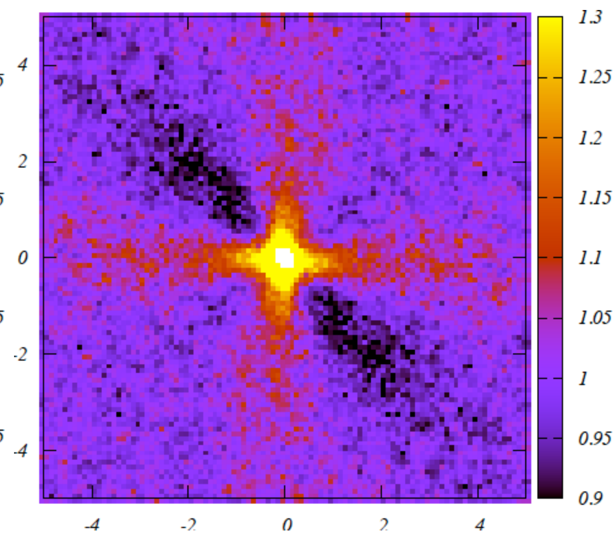
(0.78, 2)



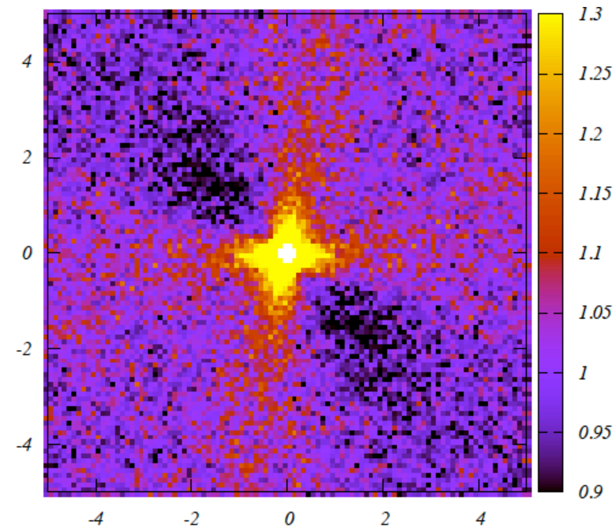
(0.8, 2)



(0.76, 10)



(0.78, 10)



(0.8, 10)

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

Stress Anisotropy from Data

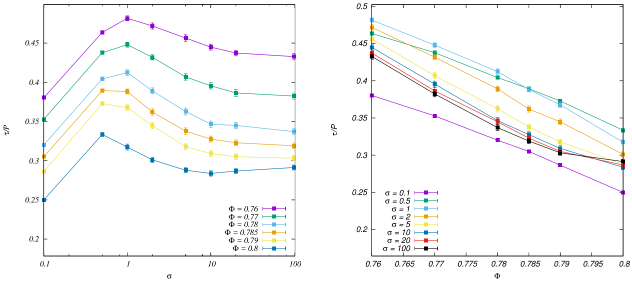


Figure: Observed $\mu = \tau/P$ from the data.

Constructing a Thermal Ensemble

- Using the pair correlations we can construct a **potential**

$$V_2^{\phi}(\vec{h}) = -\log\left(\frac{g_2(\vec{h})}{g_2(|\vec{h}|)}\right), \tag{1}$$

  that induces an **anisotropy in the interactions** based on the observed correlation functions.

- The ensemble of configurations that are sampled in the non-equilibrium dynamics are assumed to obey a **statistical mechanical description**, with each configuration $\mathcal{C}$ occurring with a **probability** $p(\mathcal{C}) \propto \exp(-V(\mathcal{C}))$.

Statistical Mechanics

- Shear stress sets the **pressure scale** (and Area): we control this by a **Lagrange multiplier** $f_p^*(\sigma)$.

- The **partition function** of the system is given by

$$Z_{\sigma,\phi} = \frac{1}{N!}\int_0^{\infty} dA \exp\left(-Nf_p^*(\sigma)A\right) \times \underbrace{\int_A \prod_{i=1}^{N} d\vec{h}_i \exp\left(-\sum_{i,j} V_2^{\phi}(\vec{h}_i - \vec{h}_j)\right)}_{\exp(-\epsilon_\phi(A))}, \qquad (2)$$

where the positions $\vec{h}_i$ are confined to be within the box defined by $A \equiv (\vec{\Gamma}_x, \vec{\Gamma}_y)$.

Testing the Potentials

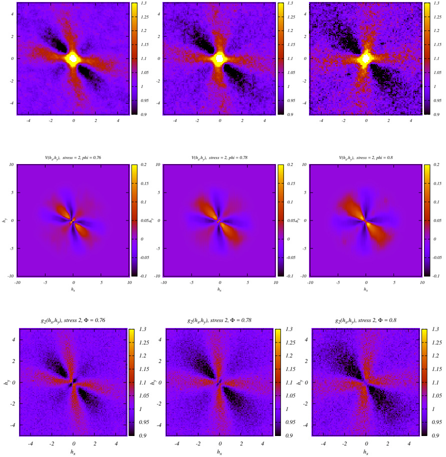


Figure: a) Observed pair correlation functions at $\sigma_{xy} = 2$, at packing fractions $\phi = 0.76, 0.785, 0.79$. b) Potentials constructed using the pair correlation functions (c) A comparision with pair correlations from Monte Carlo simulations.

Sampling the Energy Function

- We perform a **Monte Carlo sampling** of the energy function

$$\exp(-\epsilon_\phi(A)) = \int_A \prod_{i=1}^{N} d\vec{h}_i \exp\left(-\sum_{i,j} V_2^\phi(\vec{h}_i - \vec{h}_j)\right) ; \quad A = \sigma^2 \left(\frac{1}{\mu^2} - 1\right) . \quad (3)$$

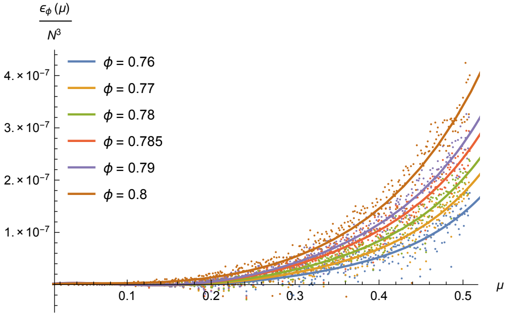


Figure: Sampled Energy Function for N = 512.

Free Energy Function

- The **free energy** of the system is then given by

$$\mathcal{F}_{\sigma,\phi} = -\log Z_{\sigma,\phi}. \quad (4)$$

- The free energy per particle is given by

$$f(\mu) = f_p^*(\sigma)\sigma^2 \left(\frac{1}{\mu^2} - 1\right) - \log\left[\sigma^2 \left(\frac{1}{\mu^2} - 1\right)\right] + \epsilon_\phi(\mu)/N. \quad (5)$$

Free Energy Function

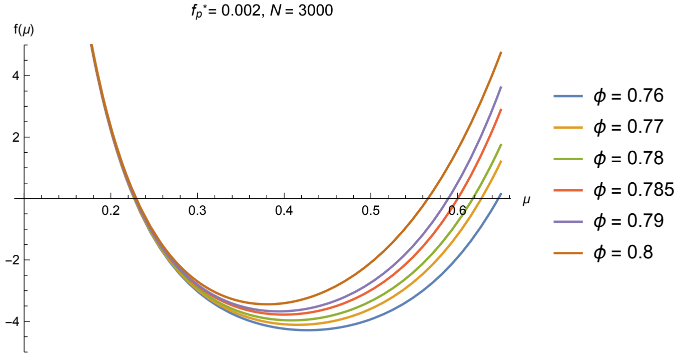


Figure: Free Energy per particle, $N = 3000$, $f_p^* = 0.002$.

Variation of μ with ϕ

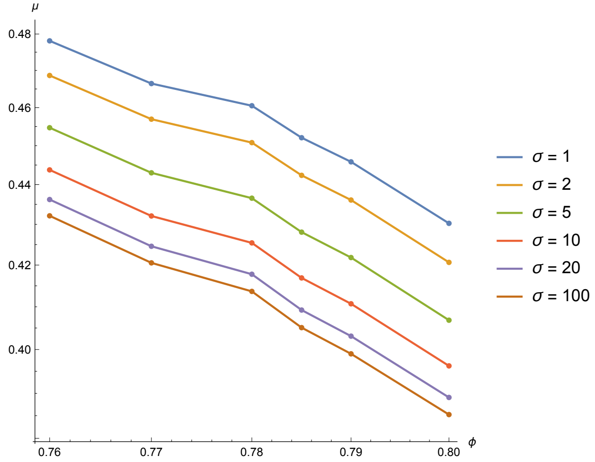


Figure: Variation of μ with ϕ at different imposed shear stresses.

Rheology from μ

- We can use μ to predict the **viscosity**

$$\eta = \frac{\mu}{(\mu - \mu_c)^2}. \quad (6)$$

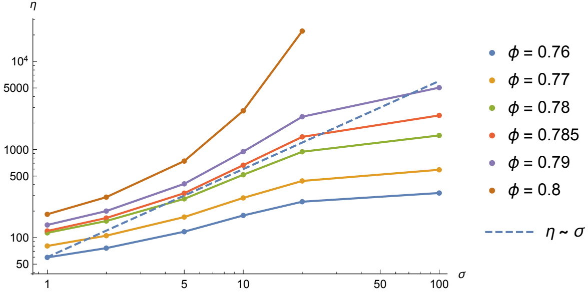
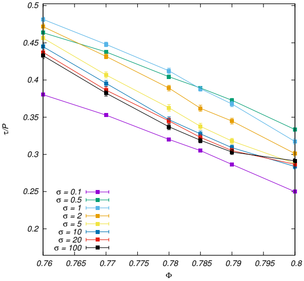
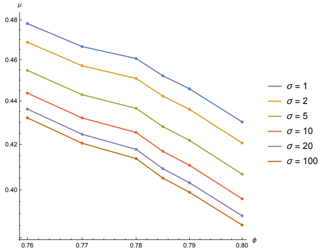


Figure: Predicted viscosity at different packing fractions ϕ. With $\mu_c \approx 0.385$.

Improving the Theory





- We can **improve the interaction** potential.
- We can include **normal stress fluctuations**.
- Finally, we can measure the **autocorrelations** in the components of the stress tensor and directly predict the **viscosity**.