From particle simulations to continuum theory for GM

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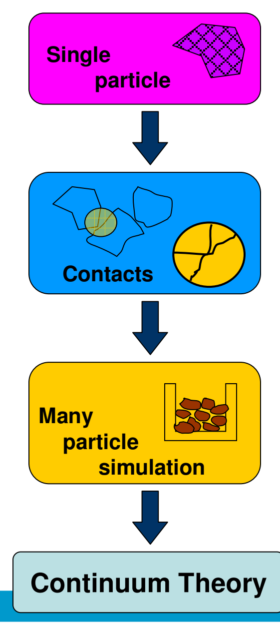
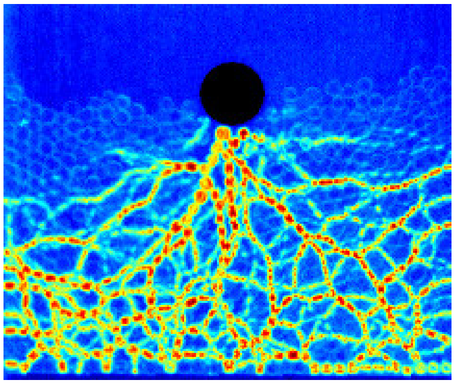
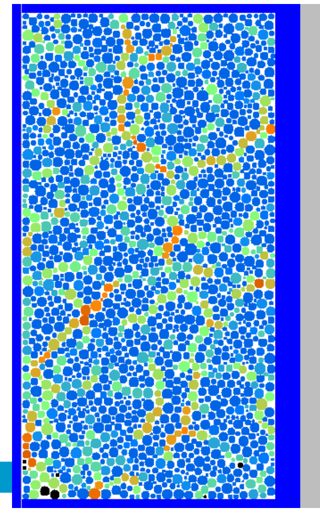


Force-chains

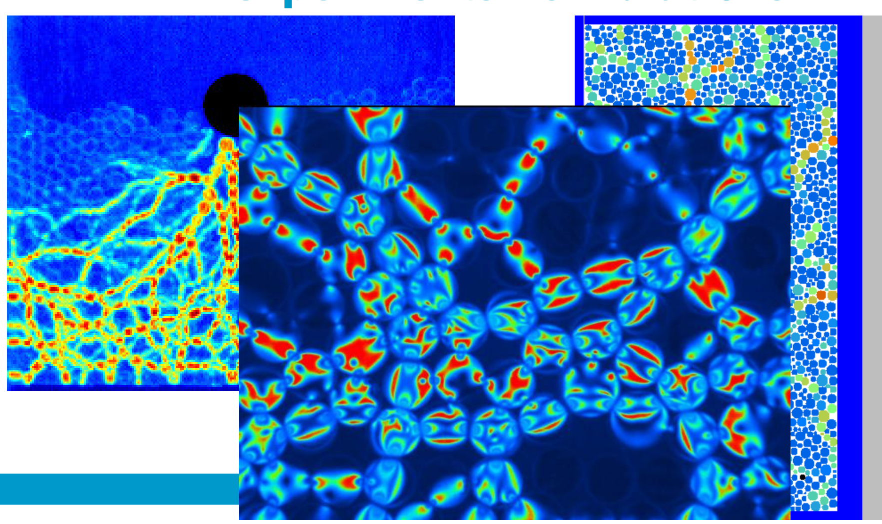
experiments - simulations





Force-chains

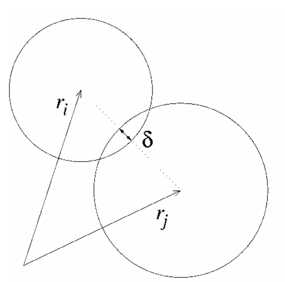
experiments - simulations



What? Why? How?

- DEM = MD simulations
  … based on contact models
- simulation of granular materials
- account for disorder/inhomogeneity
- applications:
  sand, clay, concrete, …
  powders, ceramics, tabletting, …

Discrete particle model



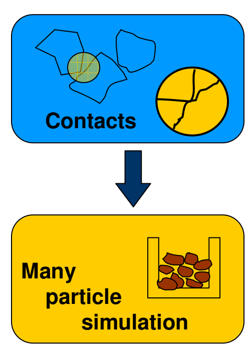
Equations of motion

$$m_i \frac{d^2 \vec{r}_i}{dt^2} = \vec{f}_i \qquad I_i \frac{d\vec{\omega}_i}{dt} = \vec{t}_i$$

Forces and torques:

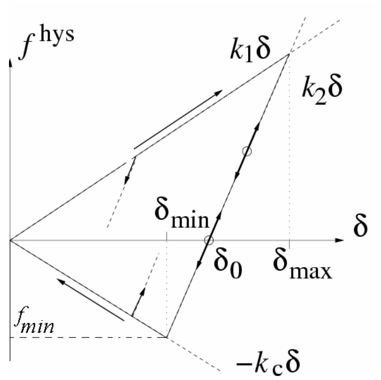
$$\vec{f}_i = \sum_c \vec{f}_i^{\,c} + \sum_w \vec{f}_i^{\,w} + m_i g$$

$$\vec{t}_i = \sum_c \vec{r}_i^{\,c} \times \vec{f}_i^{\,c}$$



Overlap $\delta = \frac{1}{2}(d_i + d_j) - (\vec{r}_i - \vec{r}_j) \cdot \vec{n}$

Normal $\hat{n} = \vec{n}_{ij} = \frac{(\vec{r}_i - \vec{r}_j)}{|\vec{r}_i - \vec{r}_j|}$



Contact model

- (too) simple ☺
- piecewise linear
- easy to implement

$$f_i^{hys} = \begin{cases} k_1\delta & \text{for loading} \\ k_2(\delta - \delta_0) & \text{for un-/reloading} \\ -k_c\delta & \text{for unloading} \end{cases}$$

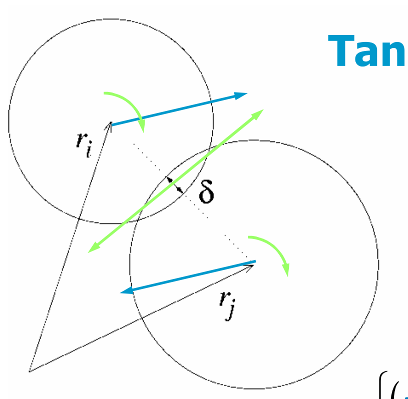
Maximum overlap $\delta_{\max}$

stress-free overlap $\delta_0 = (1 - k_1/k_2)\delta_{\max}$

strongest attraction at: $\delta_{\min} = \dfrac{k_2 - k_1}{k_2 + k_c}\delta_{\max}$

the max. attractive force: $f_{\min} = -k_c\delta_{\min}$

stiffness
plastic deform.
adhesion



Tangential contact model

***Sliding* contact points:**
- static Coulomb friction
- dynamic Coulomb friction
- objectivity

Sliding/Rolling/Torsion

$$v_t = \begin{cases} (v_i - v_j)^t + \hat{n}\times(a_i\omega_i + a_j\omega_j) & \text{sliding} \\ a_{ij}\hat{n}\times(\omega_i - \omega_j) & \text{rolling} \\ a_{ij}\hat{n}\hat{n}\cdot(\omega_i - \omega_j) & \text{torsion} \end{cases}$$

Biaxial box set-up

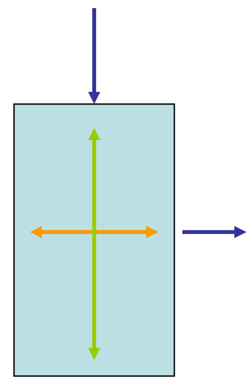
- Top wall: strain controlled

$$z(t) = z_f + \frac{z_0 - z_f}{2}\left(1 + \cos \omega t\right)$$

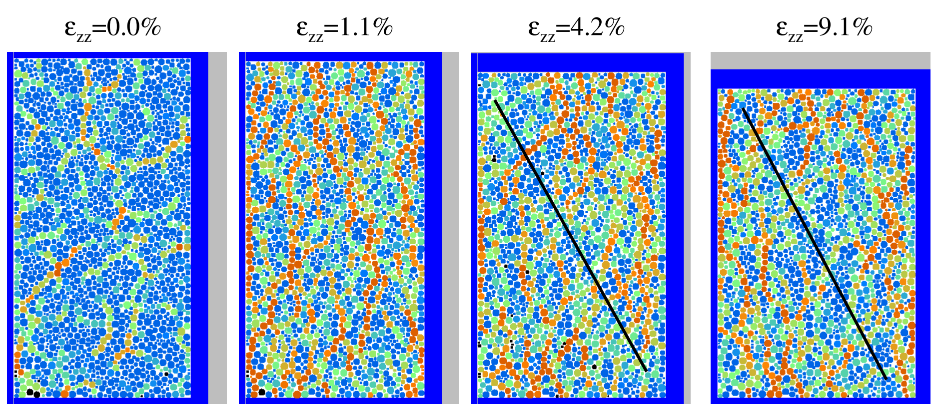
- Right wall: stress controlled

$$p = \text{const.}$$

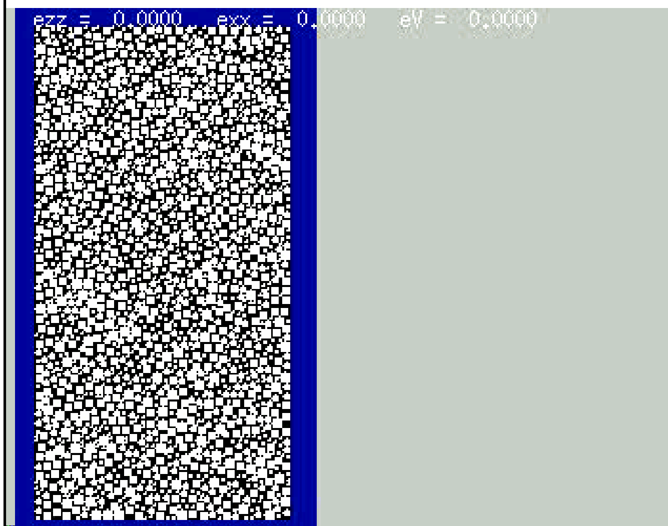
- Evolution with time … ?



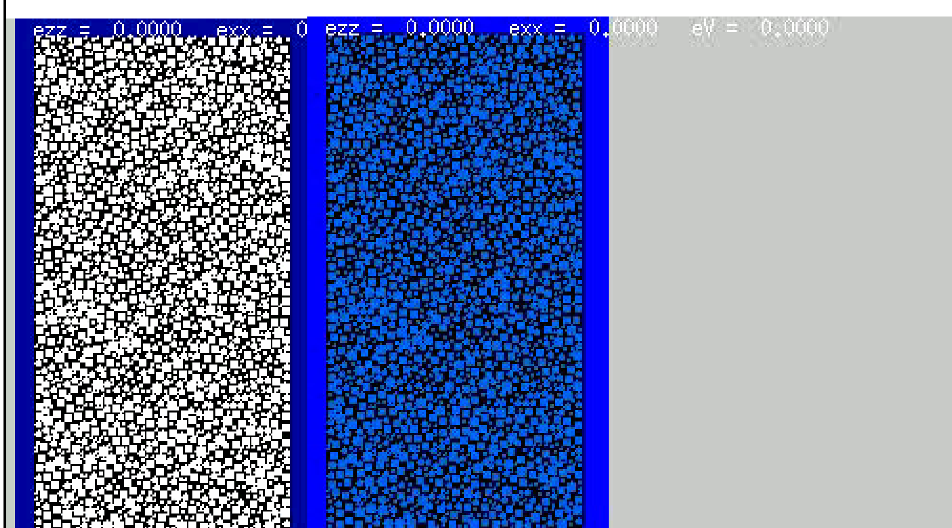
Simulation results (closer look)



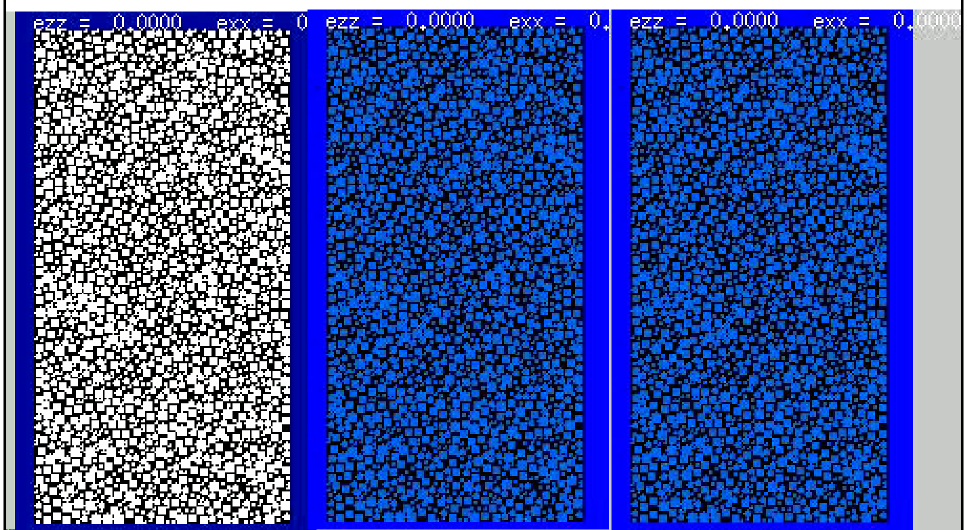
Bi-axial box (stress chains)



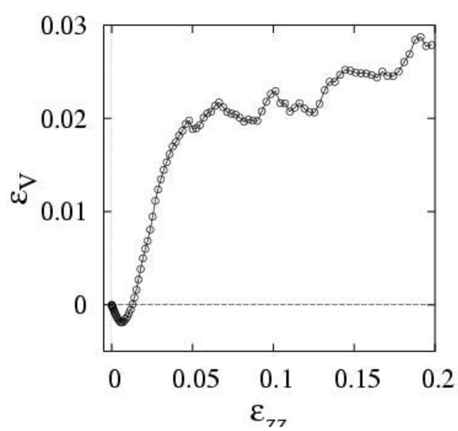
Bi-axial box (kinetic energy)

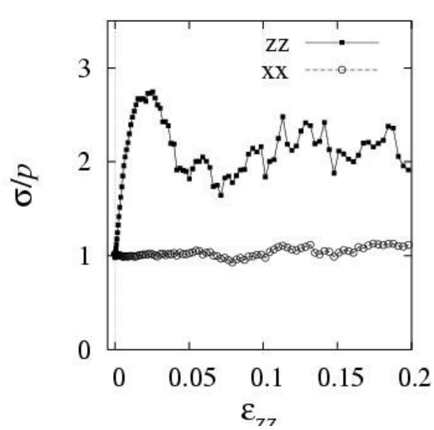


Bi-axial box (rotations)

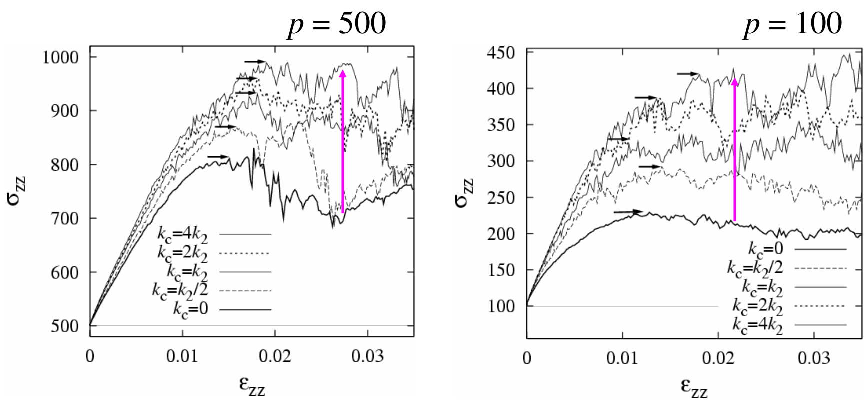


Bi-axial compression with p_x=const.





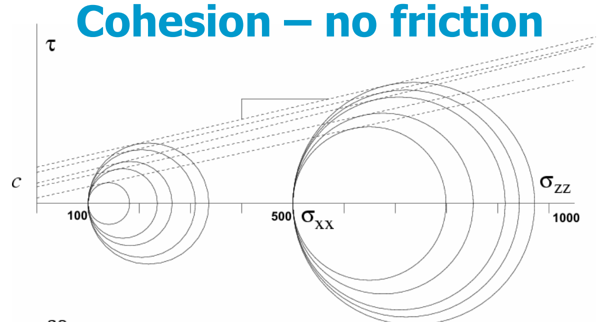
Modulus and yield stress cohesion



Modulus **(initial slope)**

Yield Stress .... **(peak value)**

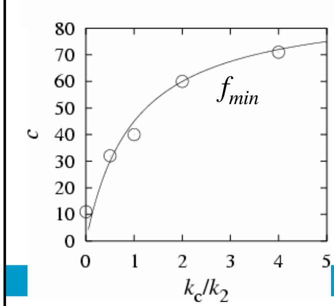
Cohesion – no friction



$k_c / k_2 = 0, 1/2, 1, 2, \text{and } 4$

geometrical friction angle

$\phi \approx 13^\circ$

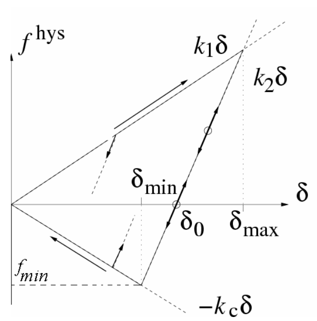


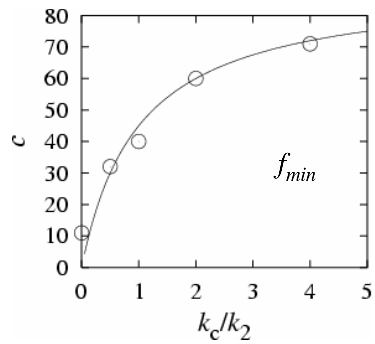
macro cohesion

$c = 1.8 \times 10^{-3} \frac{1 - k_1/k_2}{1 + k_2/k_c}$

k_c/k_2	p_x	σ_{zz}	p_x	σ_{zz}	c
0	100	183	500	798	11
½	100	234	500	853	32
1	100	264	500	915	40
2	100	310	500	941	60
4	100	336	500	972	71

Micro-macro for cohesion

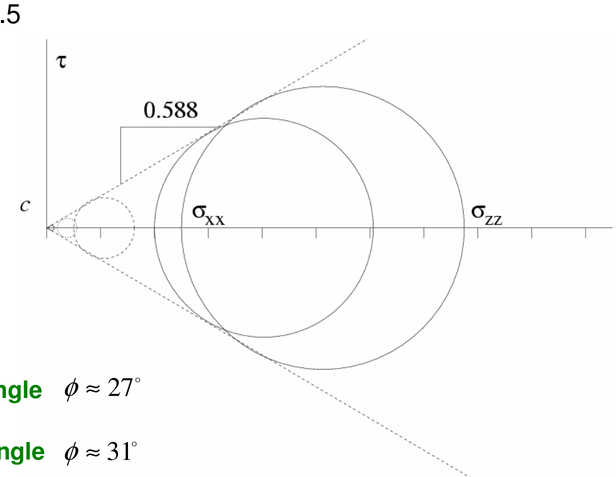




micro adhesion: f_{min} macro cohesion $c = c_0 \frac{1 - k_1/k_2}{1 + k_2/k_c}$

Friction – no cohesion

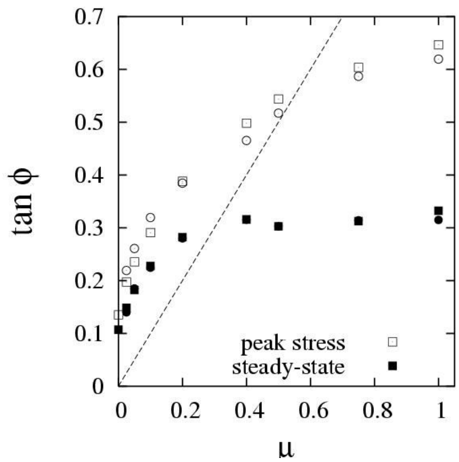
$k_c = 0$ and $\mu = 0.5$



Internal friction angle $\phi \approx 27^\circ$

Total friction angle $\phi \approx 31^\circ$

Micro-macro for friction



prepared μ=0

prepared μ=0.5

steady-state shear

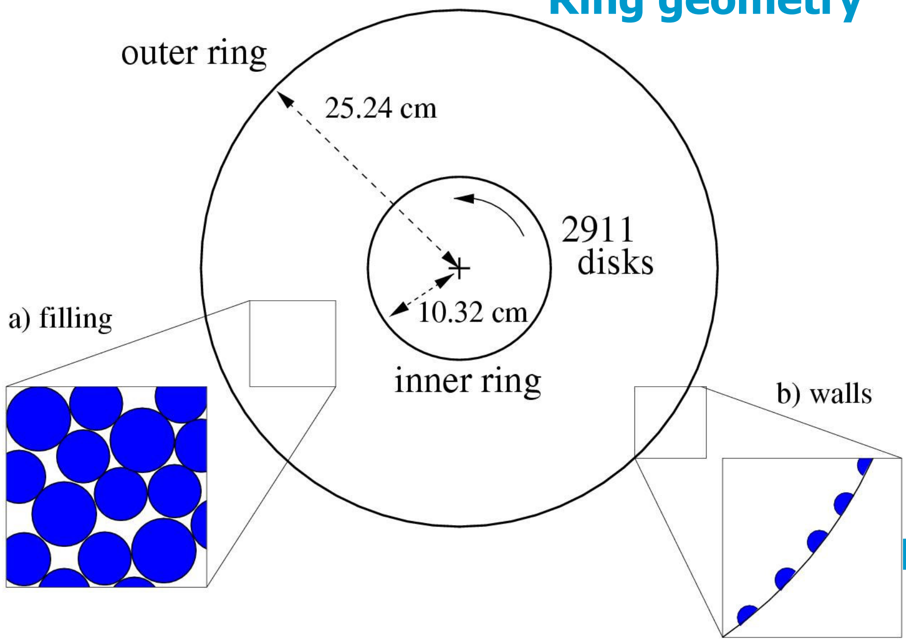
micro contact-friction μ macro friction-angle ϕ

Summary micro-macro GLOBAL

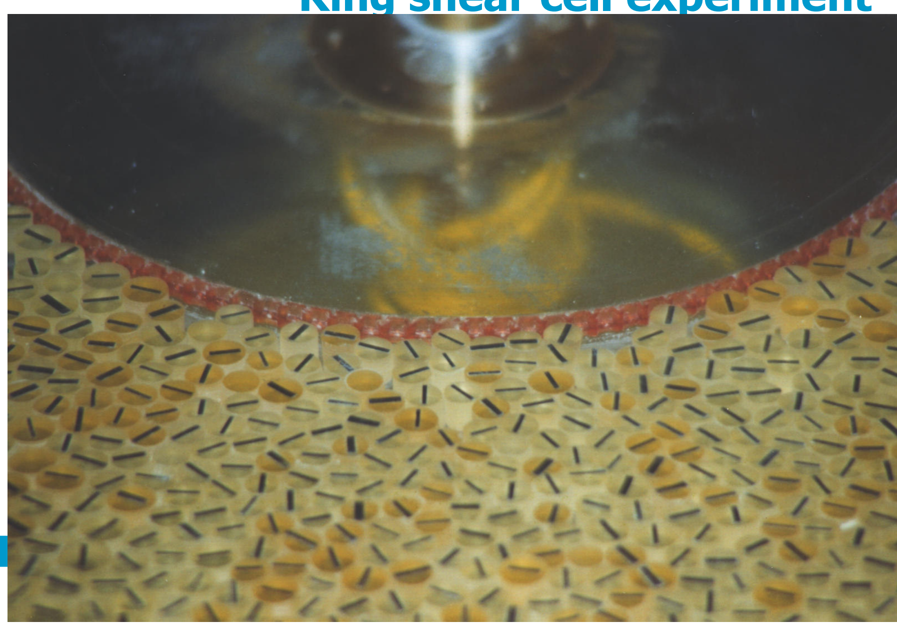
- Micro-/Macro-Flow Rheology
  - micro-adhesion … macro-cohesion
  - micro-contact-friction … macro-friction-angle
- Non-Newtonian Rheology (Anisotropy?, Micro-polar?)

- **Does global averaging make sense anyway?**

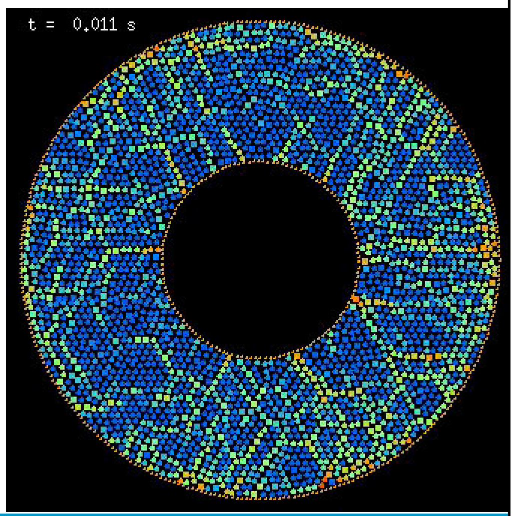
Ring geometry



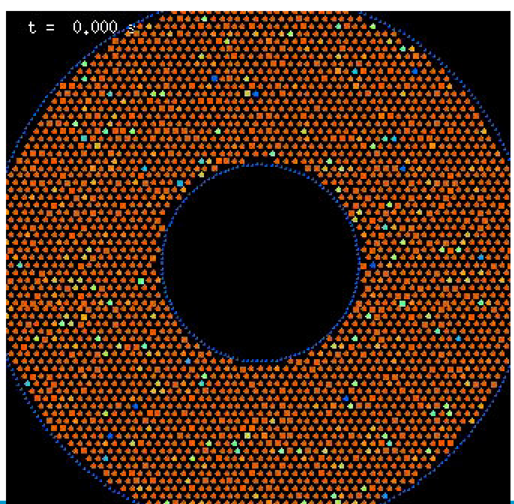
Ring shear cell experiment



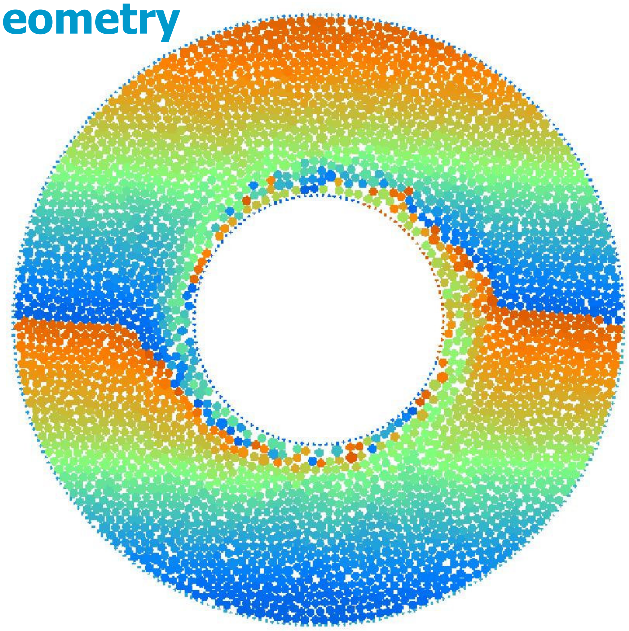
2D shear cell – force chains
= inhomogeneity
+ anisotropy



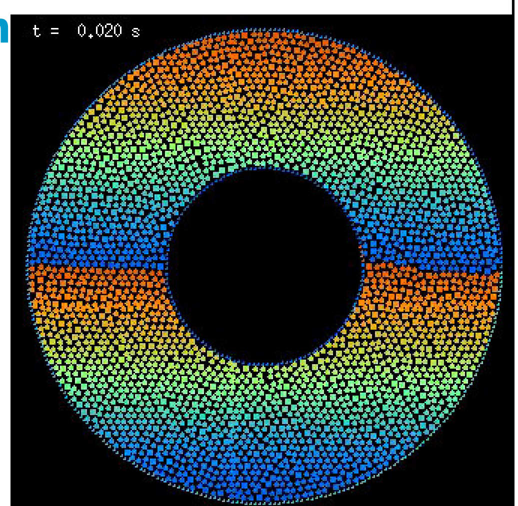
2D shear cell – energy



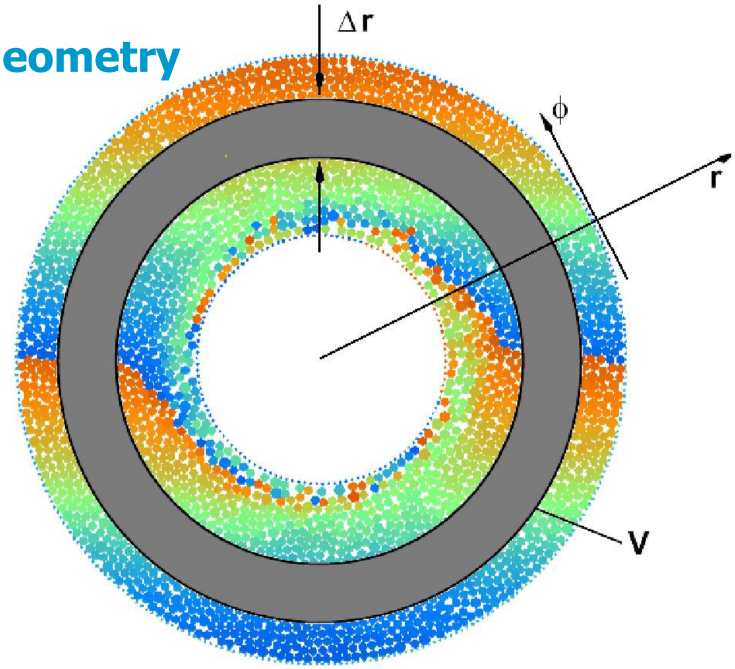
Ring geometry



2D shear cell
shear localization
non-Newtonian



Ring geometry



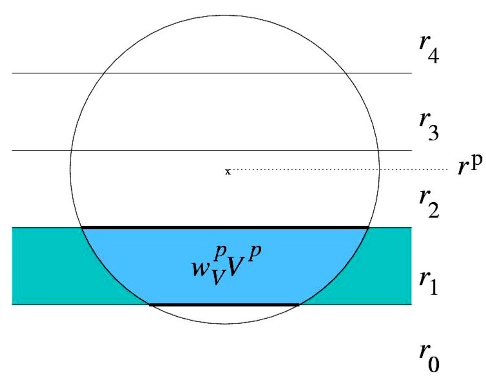
Averaging Formalism

$$Q = \left\langle Q^p \right\rangle = \frac{1}{V} \sum_{p \in V} w_V^p V^p Q^p$$

Any quantity:

$$Q^p = \sum_c Q^c$$

- Scalar
- Vector
- Tensor



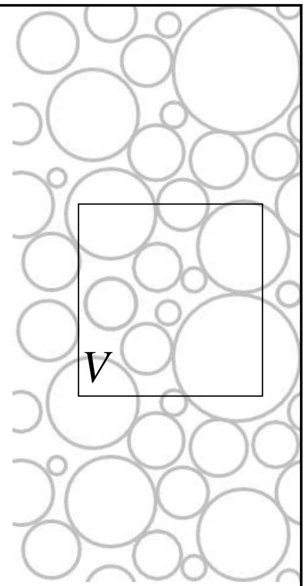
Averaging Formalism

$$Q = \left\langle Q^p \right\rangle = \frac{1}{V} \sum_{p \in V} w_V^p V^p Q^p$$

Any quantity:

$$Q^p$$

In averaging volume: V



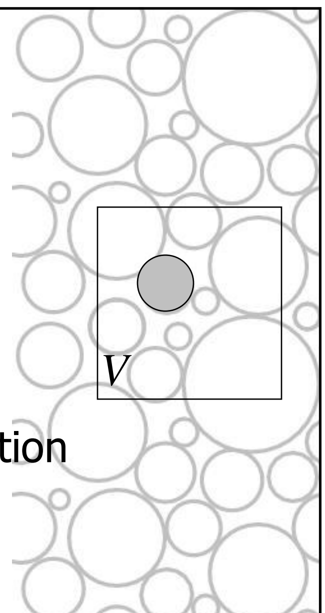
Averaging Density

$$Q = \nu = \frac{1}{V} \sum_{p \in V} w_V^p V^p$$

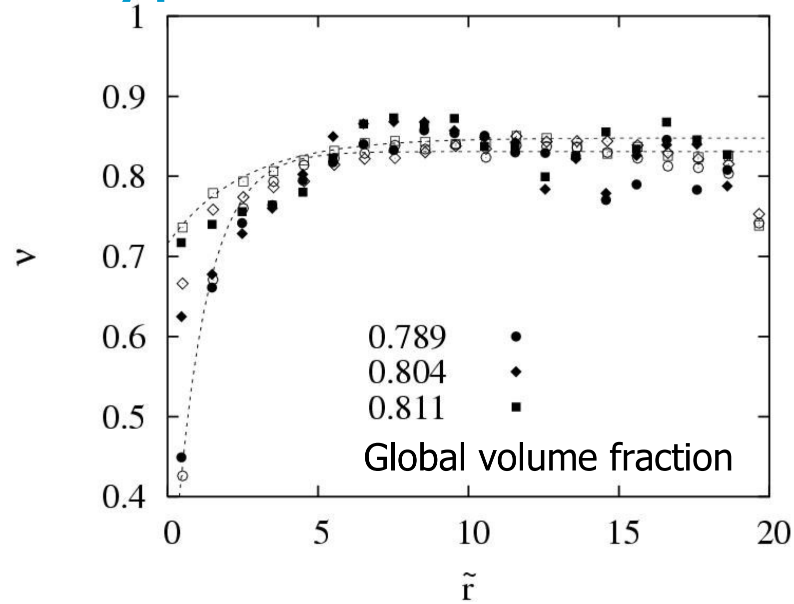
Any quantity:

$$Q^p = 1$$

- Scalar: Density/volume fraction



Density profile



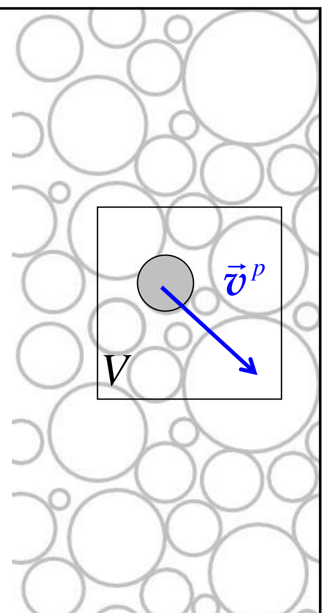
Averaging Velocity

$$Q = \nu \vec{v} = \frac{1}{V} \sum_{p \in V} w_V^p V^p \vec{v}^p$$

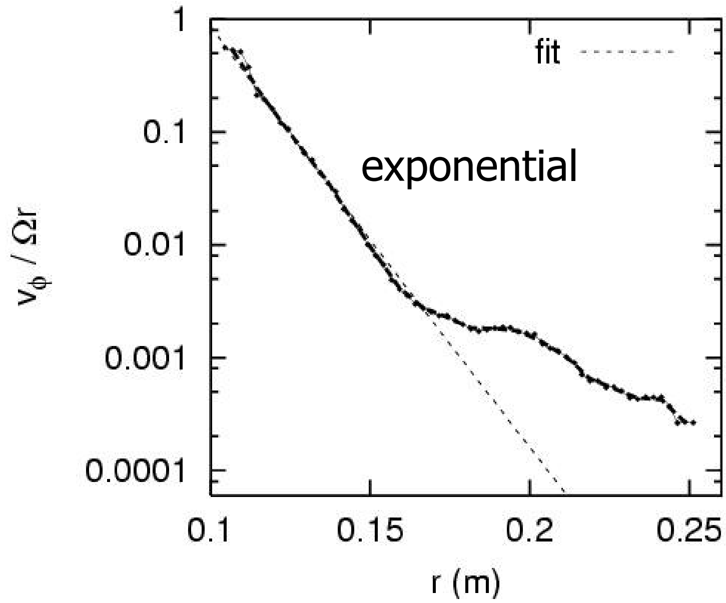
Any quantity:

$$Q^p = \vec{v}^p$$

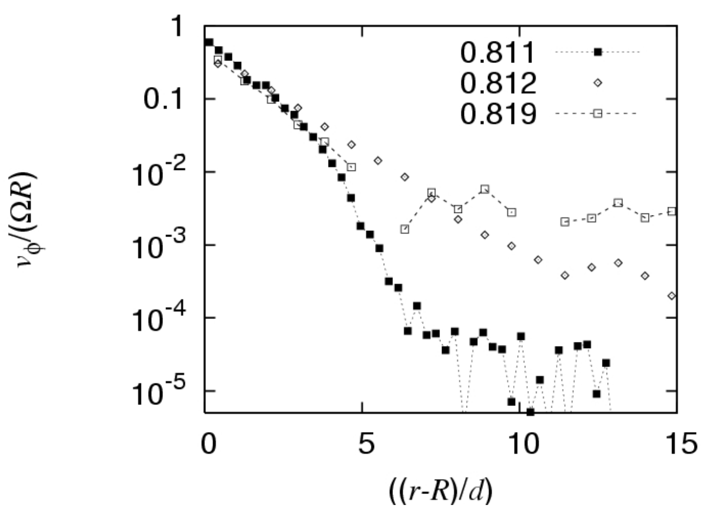
- Scalar
- Vector – velocity density



Velocity field -> velocity gradient



Velocity field -> velocity gradient



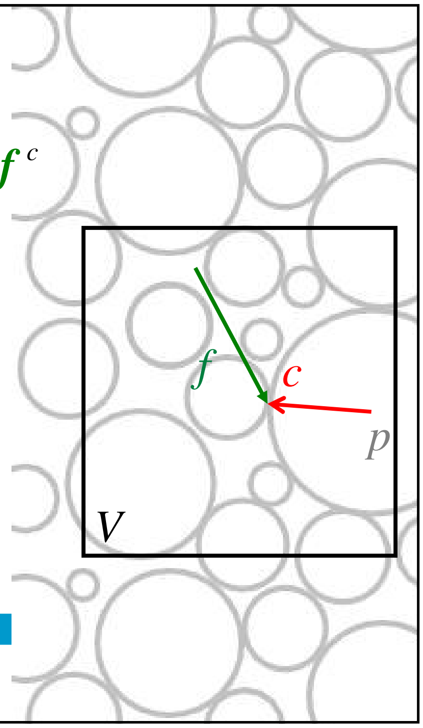
Averaging Stress

$$Q = \underline{\underline{\boldsymbol{\sigma}}} = \frac{1}{V} \sum_{p \in V} \sum_{c} w_V^p \, \boldsymbol{l}^{pc} \boldsymbol{f}^{c}$$

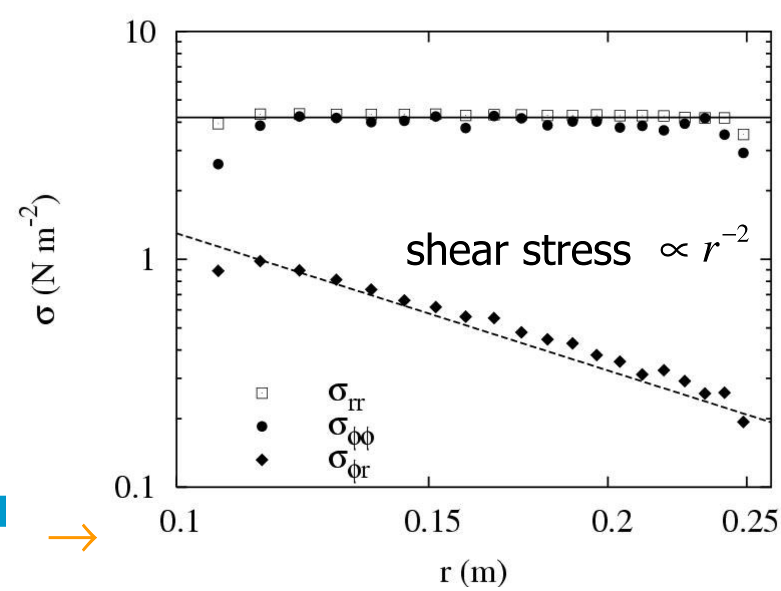
Any quantity:

$$Q^p = \underline{\underline{\boldsymbol{\sigma}}}^p = \frac{1}{V^p} \sum_{c} \boldsymbol{l}^{pc} \boldsymbol{f}^{c}$$

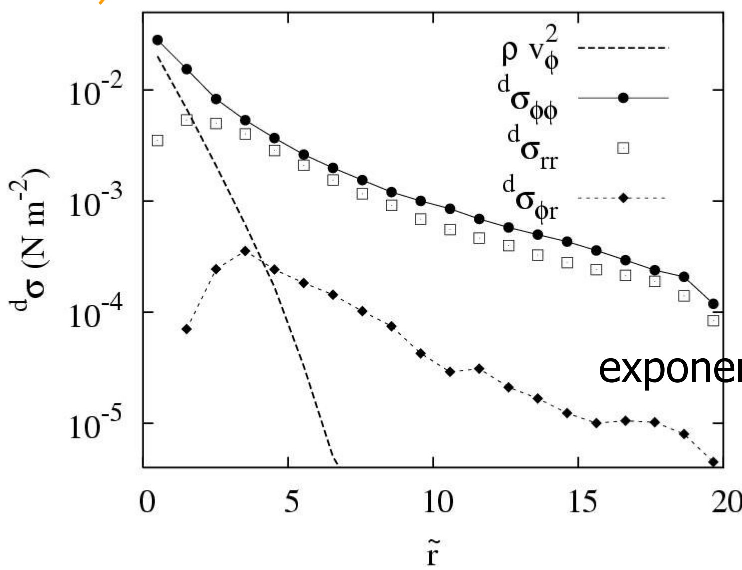
- Scalar
- Vector
- Tensor: Stress



Stress tensor (static)



Stress tensor (dynamic)



exponential

Stress equilibrium (1)

$$\Rightarrow \nabla\cdot\sigma = \frac{1}{r}\left[\frac{\partial(r\sigma_{rr})}{\partial r} - \sigma_{\phi\phi}\right]\vec{e}_r + \frac{1}{r}\left[\frac{\partial(r\sigma_{r\phi})}{\partial r} + \sigma_{\phi r}\right]\vec{e}_\phi$$

acceleration: $\vec{a} = \frac{d}{dt}\vec{v} = \frac{\partial}{\partial t}\vec{v} + (\vec{v}\cdot\vec{\nabla})\vec{v}$

$$\rho\vec{a} = \vec{\nabla}\cdot\sigma \Rightarrow \quad 0 = \rho v_\phi^2 + r\frac{\partial\sigma_{rr}}{\partial r} + (\sigma_{rr} - \sigma_{\phi\phi}),$$

$$0 = r\frac{\partial\sigma_{r\phi}}{\partial r} + (\sigma_{r\phi} + \sigma_{\phi r}),$$

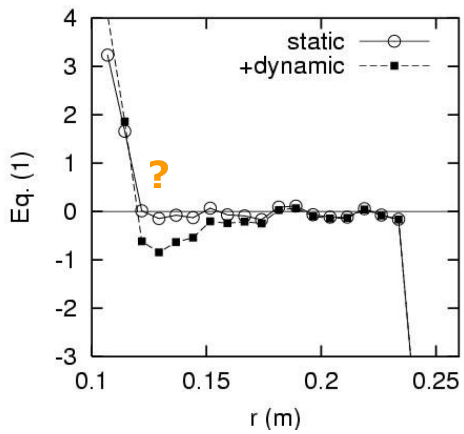
$$\Rightarrow \frac{\partial(r\sigma_{rr})}{\partial r} = \sigma_{\phi\phi} \qquad \frac{\partial(r\sigma_{r\phi})}{\partial r} = -\sigma_{\phi r}$$

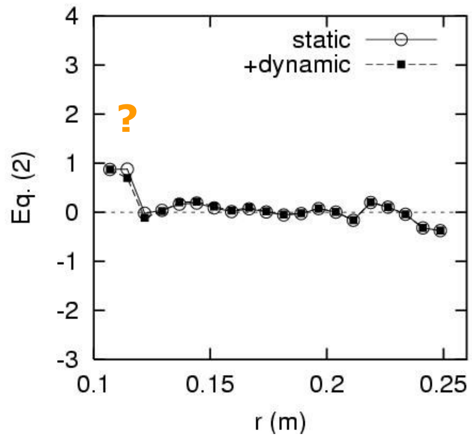
$$(\ \sigma_{rr} \propto \sigma_{\phi\phi} \propto r^0 \qquad \sigma_{r\phi} \propto \sigma_{\phi r} \propto r^{-2}\ )$$

Stress equilibrium (2)

$$0 = \rho v_\phi^2 + r\frac{\partial \sigma_{rr}}{\partial r} + (\sigma_{rr} - \sigma_{\phi\phi}),$$

$$0 = r\frac{\partial \sigma_{r\phi}}{\partial r} + (\sigma_{r\phi} + \sigma_{\phi r}),$$





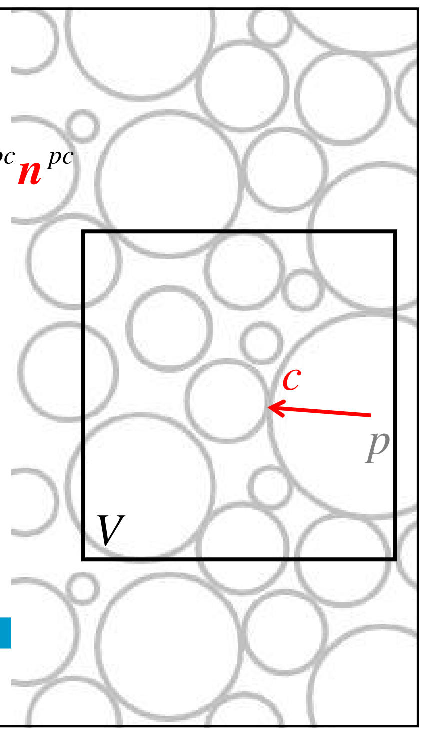
Averaging Fabric

$$Q = \underline{\underline{\mathbf{F}}} = \frac{1}{V}\sum_{p \in V} w_V^p V^p \sum_c \boldsymbol{n}^{pc}\boldsymbol{n}^{pc}$$

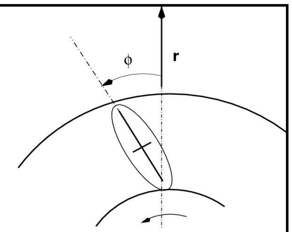
Any quantity:

$$Q^p = \underline{\underline{\mathbf{F}}}^p = \sum_c \boldsymbol{n}^{pc}\boldsymbol{n}^{pc}$$

- Scalar: contacts
- Vector: normal
- Contact distribution

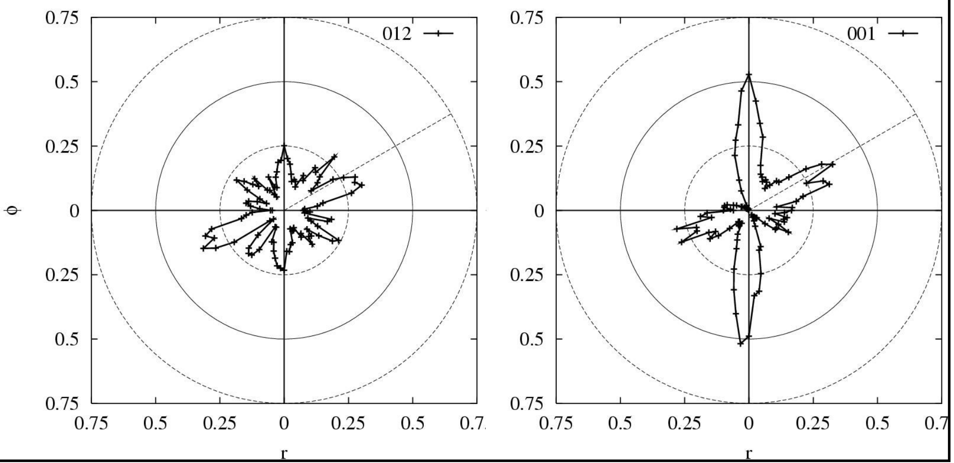


Fabric tensor

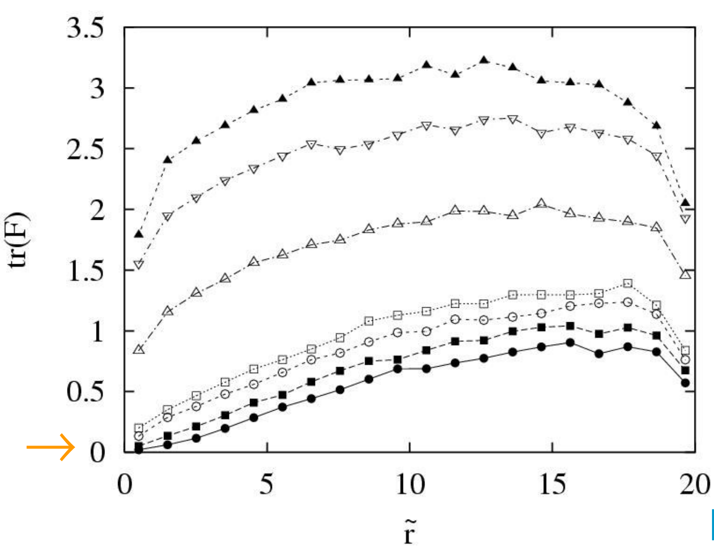


contact probability …

center   wall

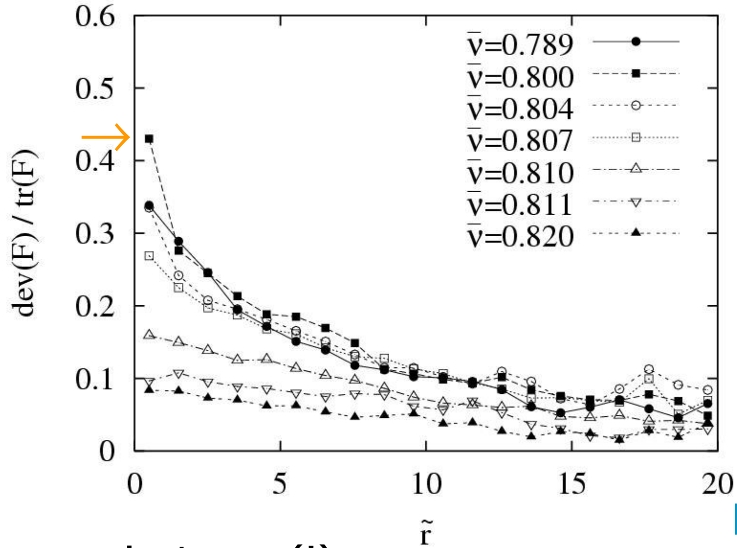


Fabric tensor (trace)



contact number density

Fabric tensor (deviator)



an-isotropy (!)

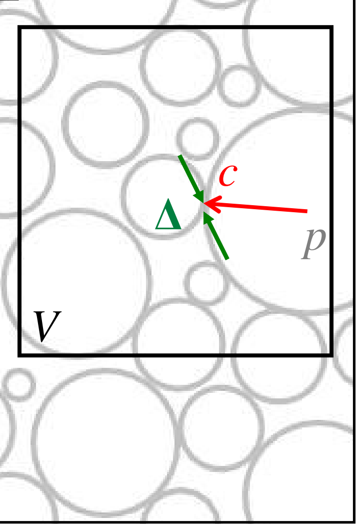
Averaging Deformations

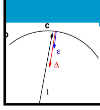
$$Q = \underline{\underline{\varepsilon}} = \frac{\pi h}{V}\left(\sum_{p\in V} w_V^p \sum_c \boldsymbol{l}^{pc} \Delta^c \right)\cdot \underline{\underline{\mathbf{F}}}^{-1}$$

Deformation:

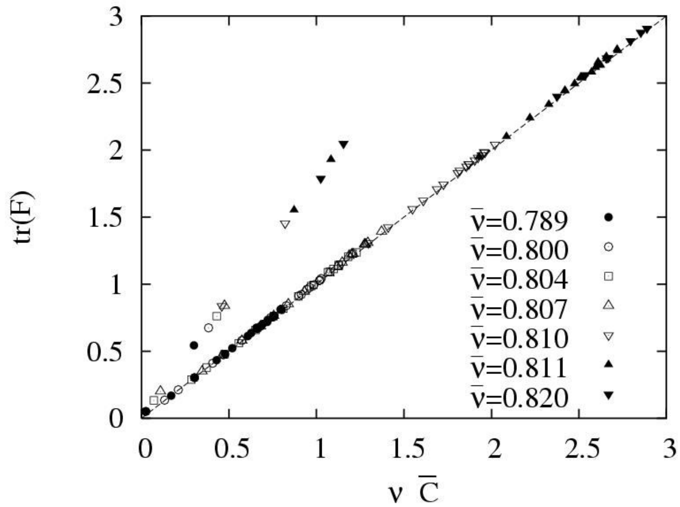
$$S = \left(\Delta^c - \underline{\underline{\varepsilon}}\cdot \boldsymbol{l}^{pc}\right)^2 \quad \text{minimal !}$$

- Scalar
- Vector
- Tensor: Deformation



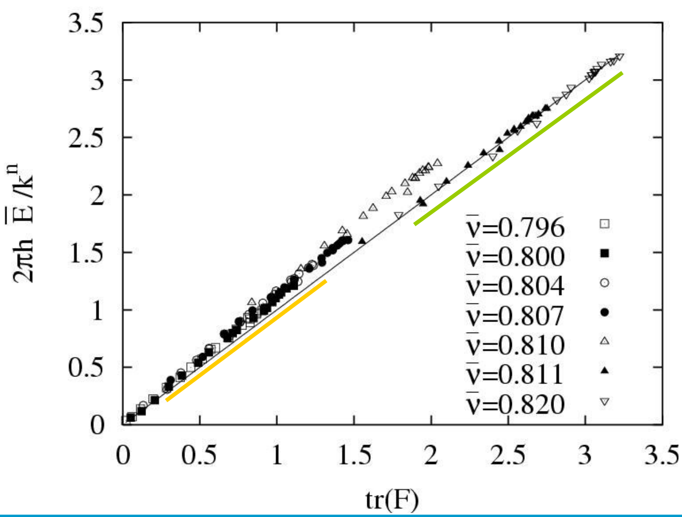


Macro (contact density)



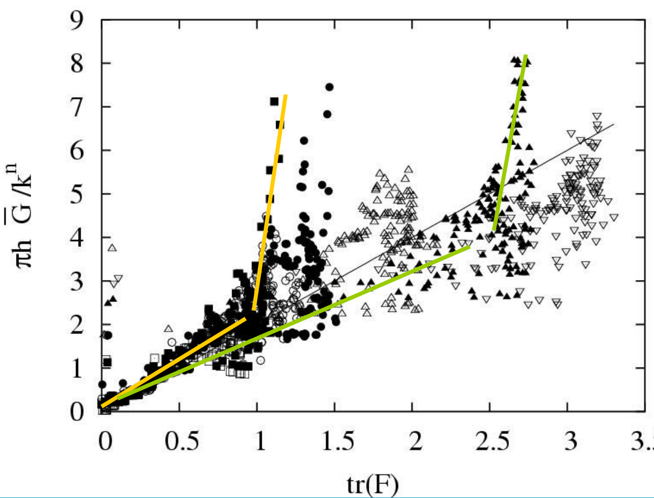
Macro (bulk modulus)

$$\overline{E} = \frac{\mathrm{tr}\underline{\underline{\sigma}}}{\mathrm{tr}\underline{\underline{\varepsilon}}}$$

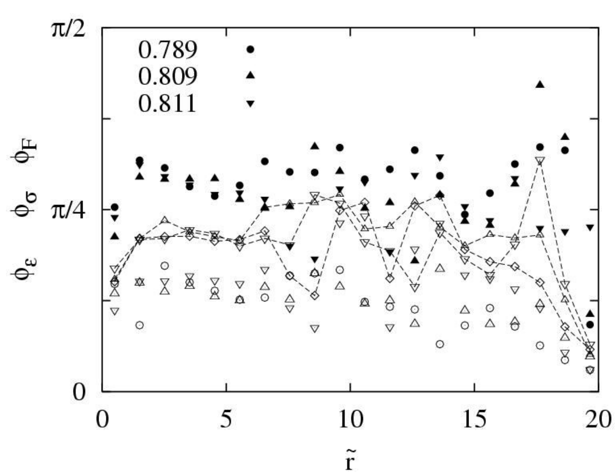


Macro (shear modulus)

$$\overline{G} = \frac{\mathrm{dev}\underline{\underline{\sigma}}}{\mathrm{dev}\underline{\underline{\varepsilon}}}$$



Anisotropy – non-colinearity



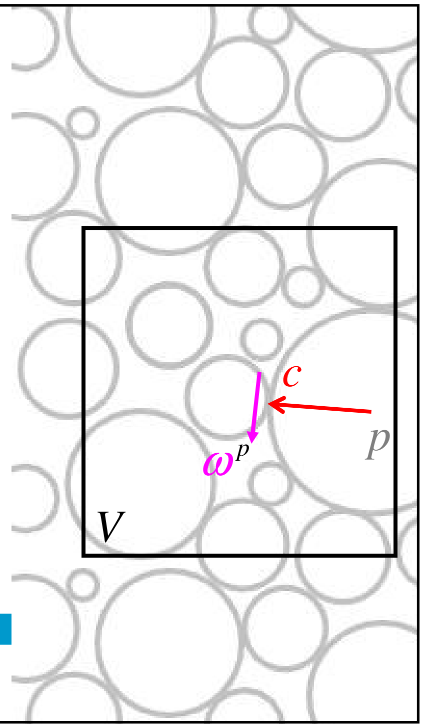
Averaging Rotations

$$Q = \nu\omega = \frac{1}{V}\sum_{p\in V}\sum_{c} w_V^p V^p \omega^p$$

Deformation:

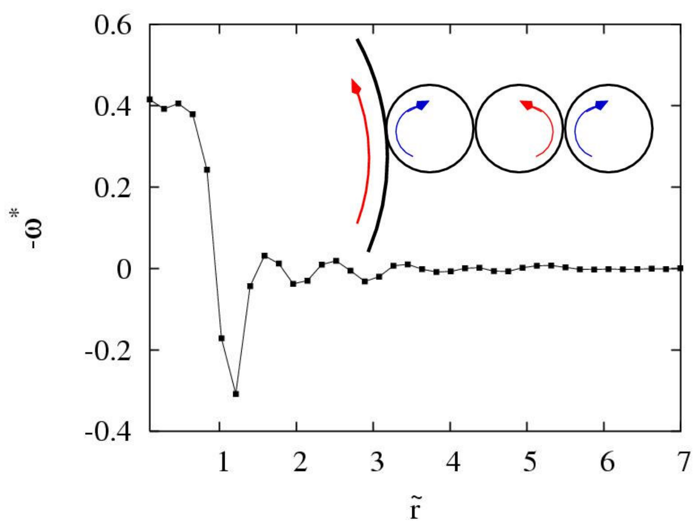
$$Q^p = \omega^p$$

- Scalar
- Vector: Spin density
- Tensor



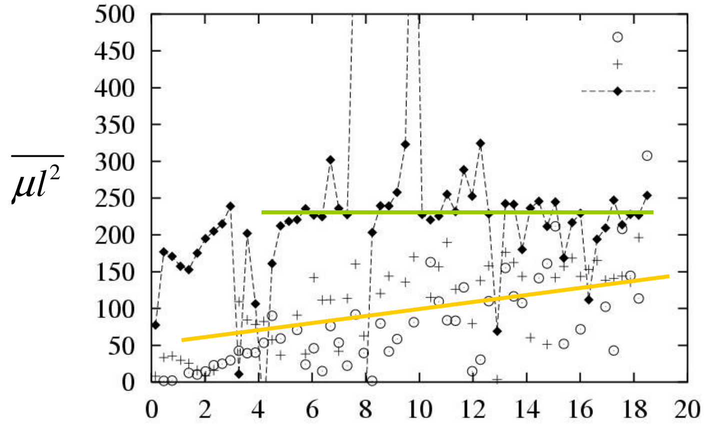
Rotations – spin density

eigen-rotation: $\omega^* = \omega - W_{r\phi}$



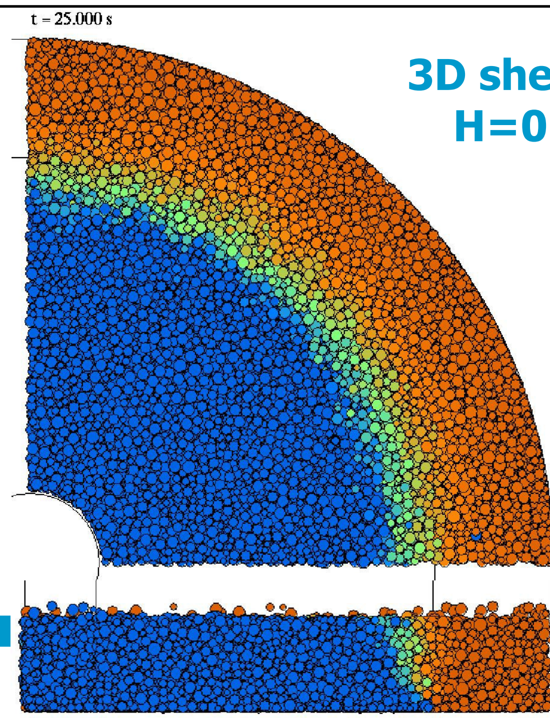
Macro (torque stiffness)

$$\overline{\mu l^2} = \frac{\underline{\underline{M}}}{\underline{\underline{\kappa}}}$$

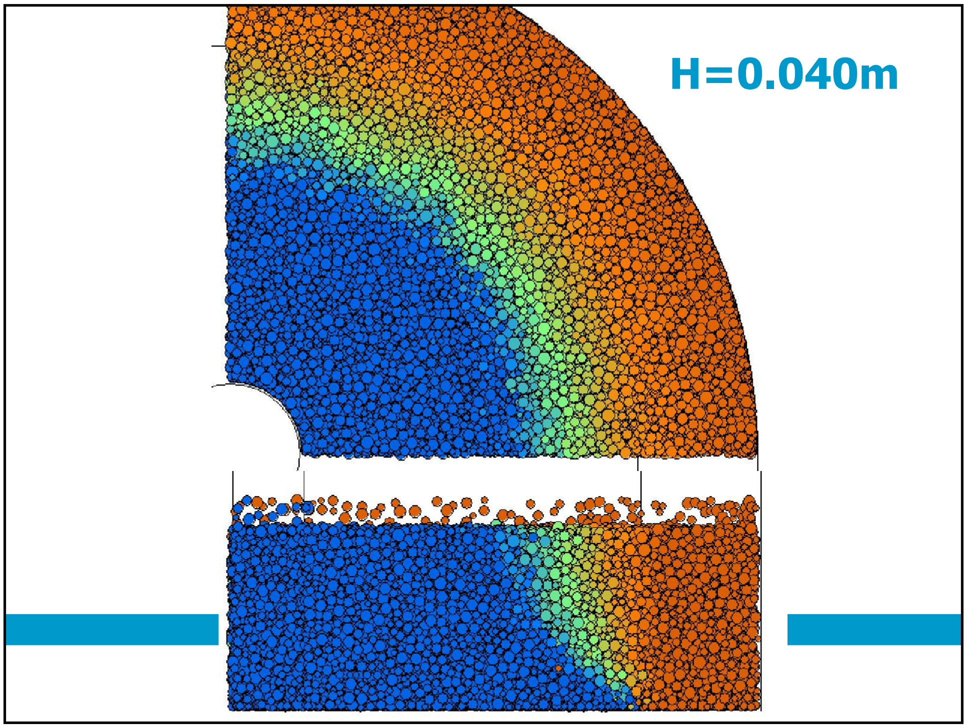


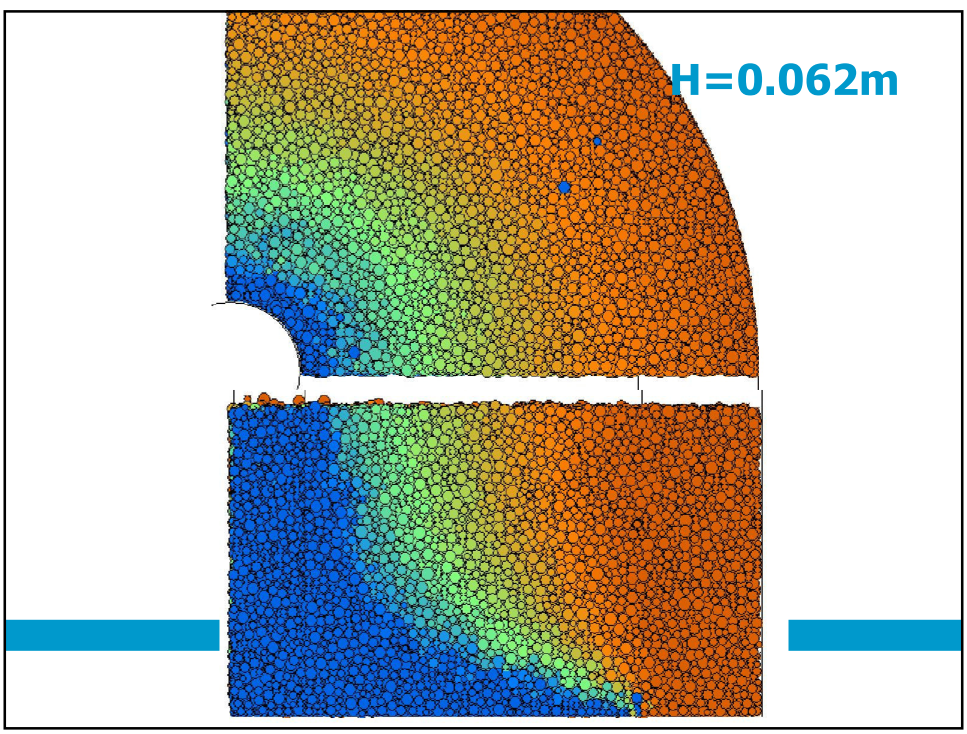
The End ?

3D ring shear cell
micro-macro for shear viscosity

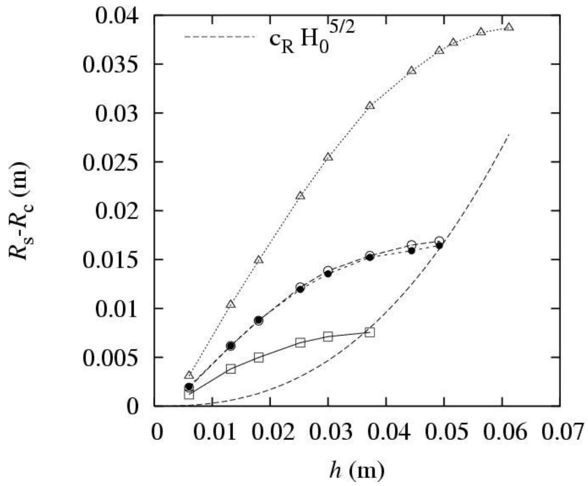


3D shear cell
H=0.016m


H=0.040m

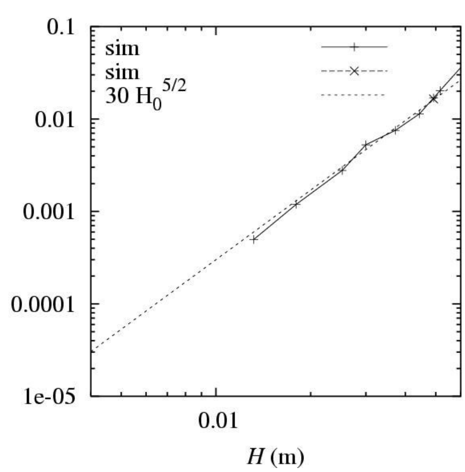

H=0.062m

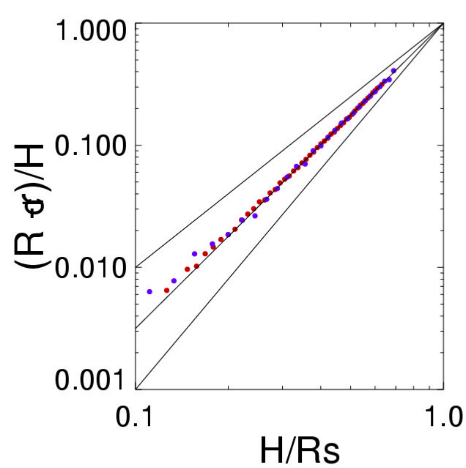
3D shear band center position



80% agreement … up to now

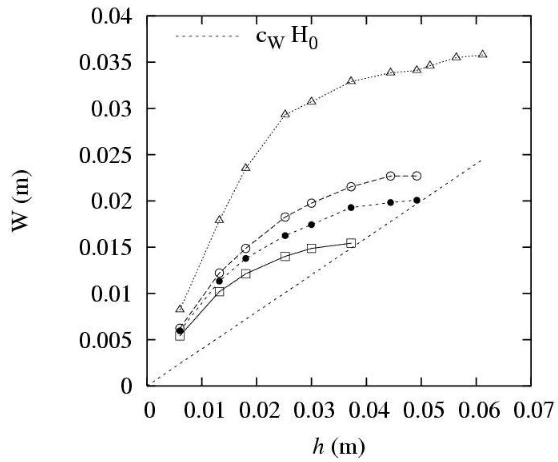
3D shear band center position





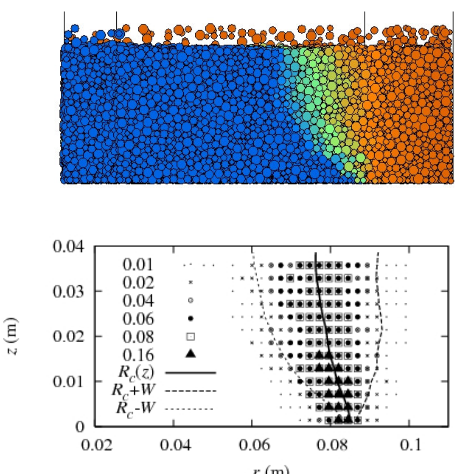
80% agreement … up to now

3D shear band width

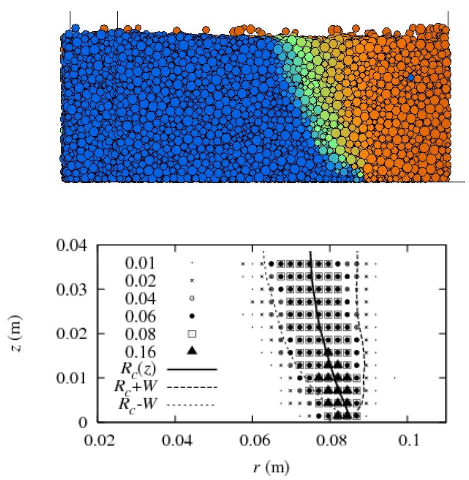


80% agreement … up to now

Constitutive relations – shear rate $\dot{\gamma}$

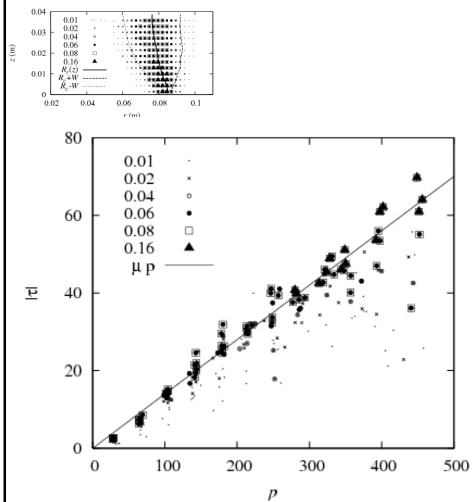


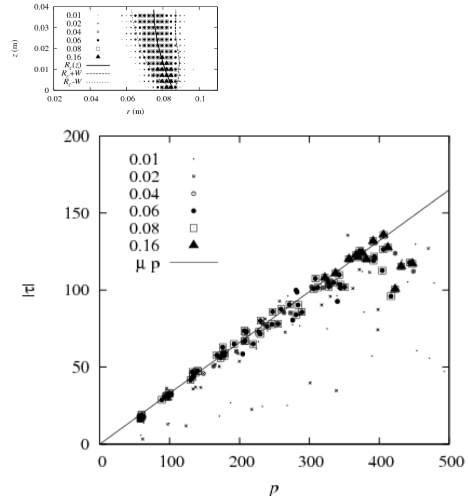
no friction



friction

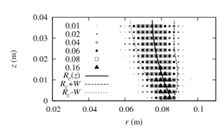
Constitutive relations: Mohr-Coulomb

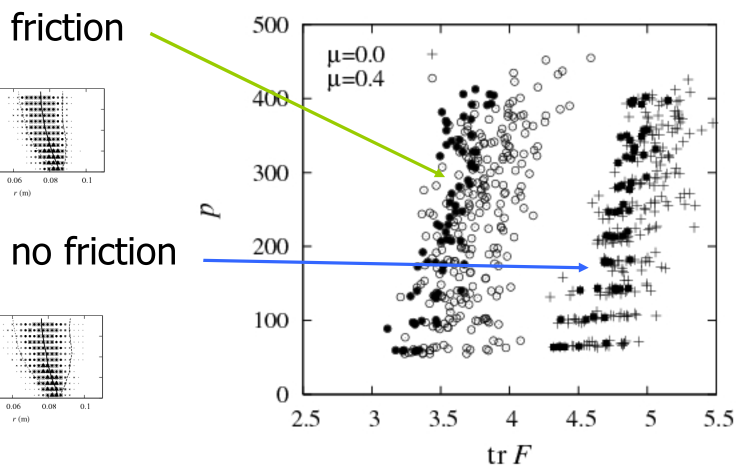


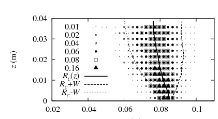


no friction friction

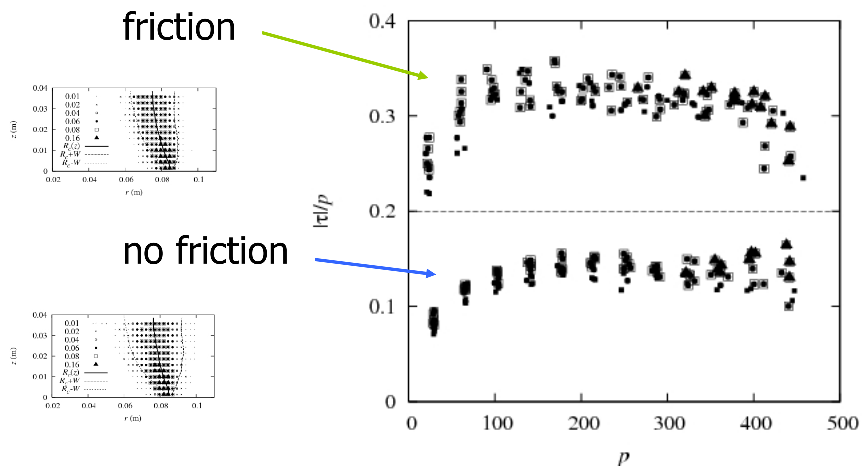
Constitutive relations: stress-structure





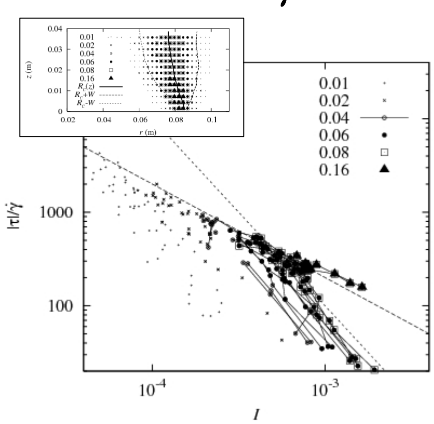


Constitutive relations: anisotropy

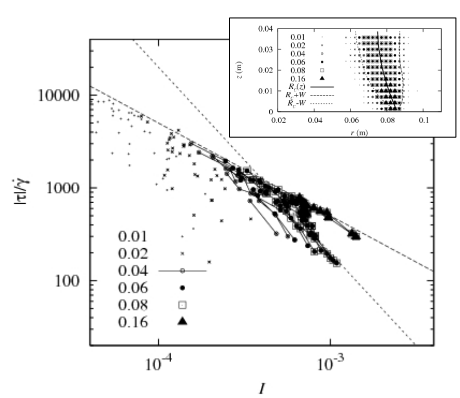


Constitutive relations: shear softening

viscosity $\frac{|\tau|}{\dot{\gamma}}$ vs. shear rate $I = \frac{\dot{\gamma} d_0}{\sqrt{p/\rho_0}}$

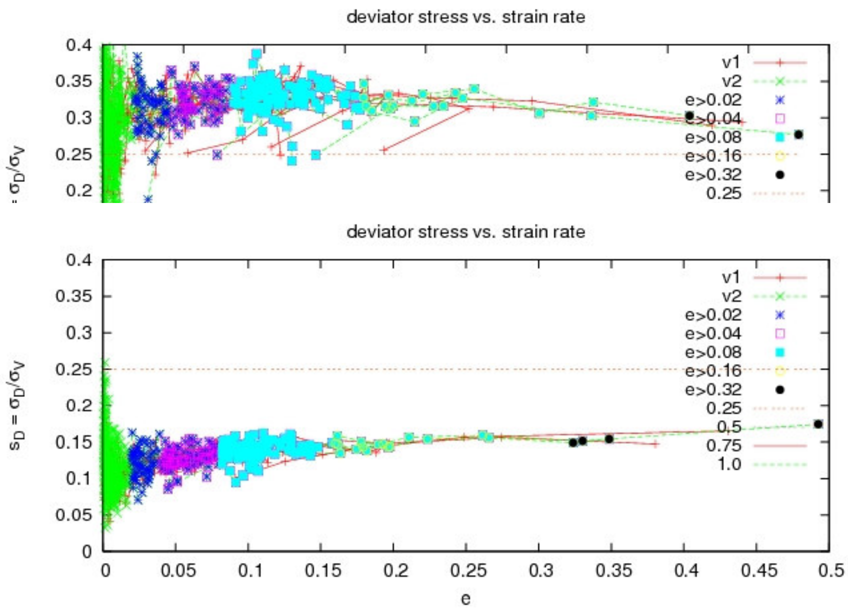


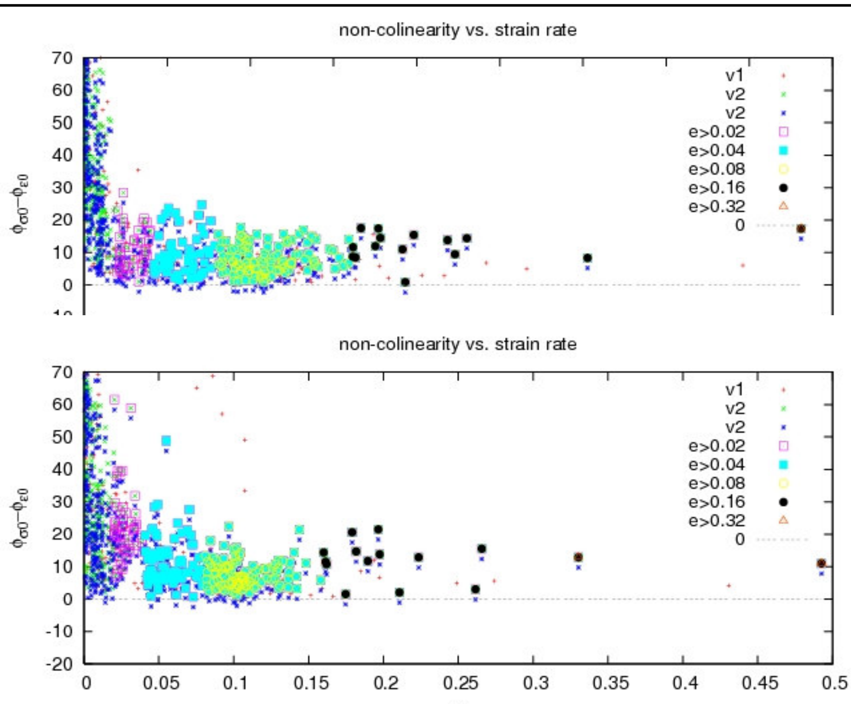
no friction



friction

stress ratio vs. shear rate





3D Flow behavior – steady state shear

Obtain constitutive relations from one SINGLE simulation:

- **Mohr Coulomb yield stress**
- **shear softening viscosity**
- **compression/dilatancy …**
- **inhomogeneity (force-chains)**
- **(almost always) an-isotropy**
- **micro-polar effects (rotations) …**