From particle simulations to continuum theory for GM

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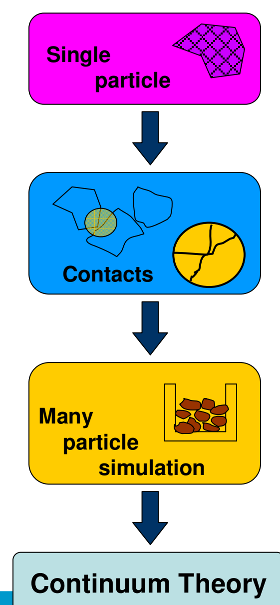
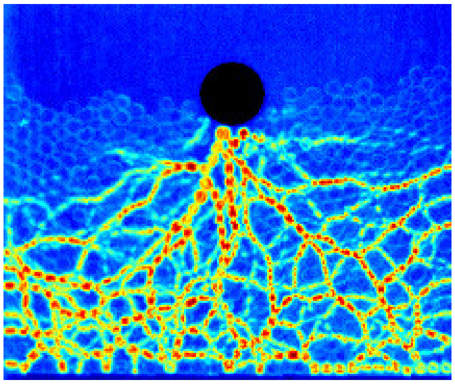
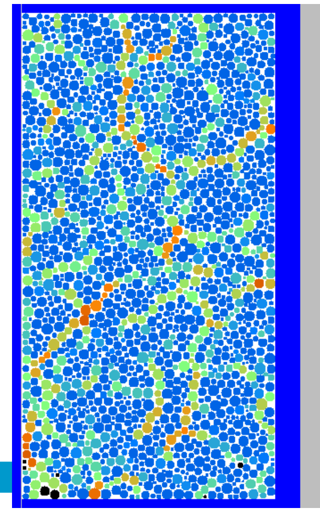


Force-chains

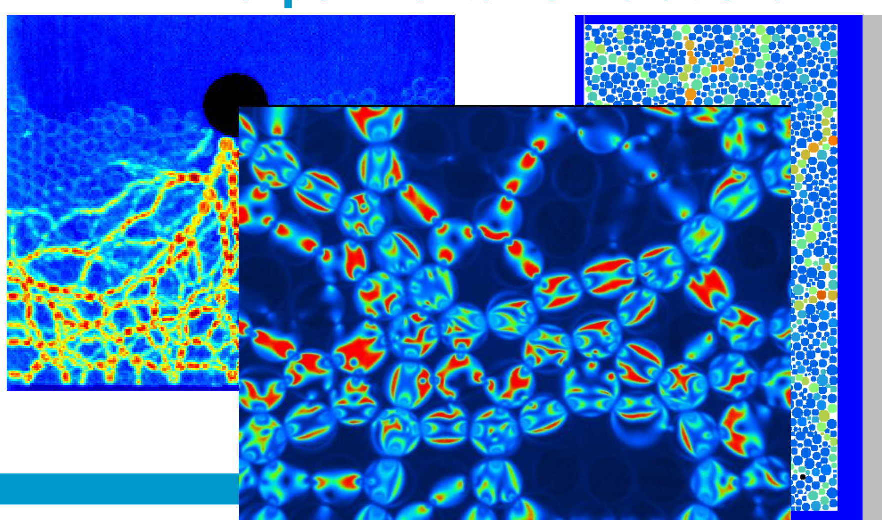
experiments - simulations





Force-chains

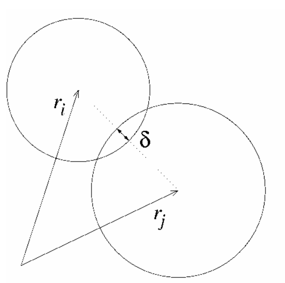
experiments - simulations



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



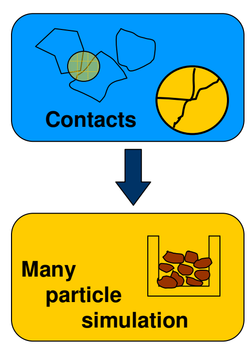
Equations of motion

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

Forces and torques:

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

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

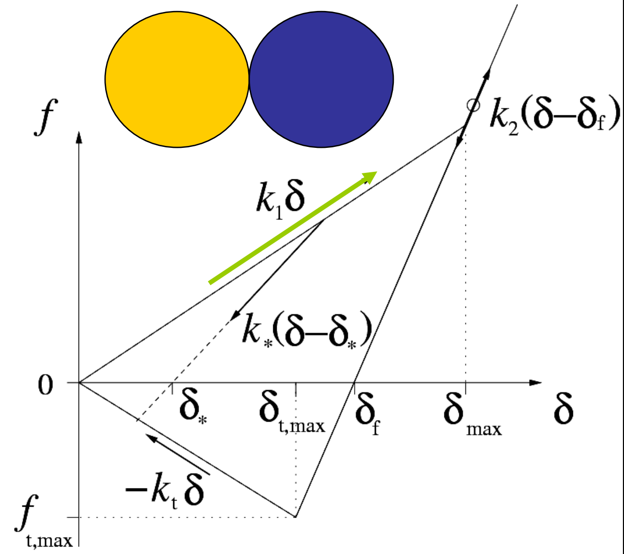


Overlap $\delta = \frac{1}{2}\left(d_i + d_j\right) - \left(\vec{r}_i - \vec{r}_j\right) \cdot \vec{n}$

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

Contacts

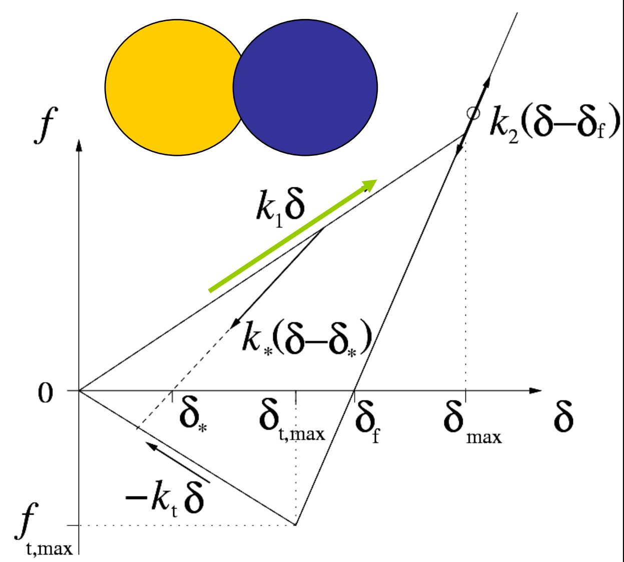
1. loading



Contacts

1. loading

plastic loading
stiffness: k_1



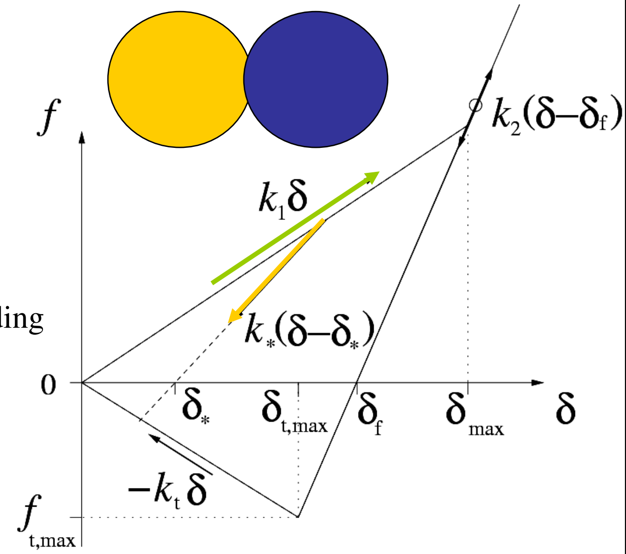
Contacts

1. loading

plastic loading
stiffness: k_1

2. unloading

elastic un/re-loading
stiffness: k_*



Contacts

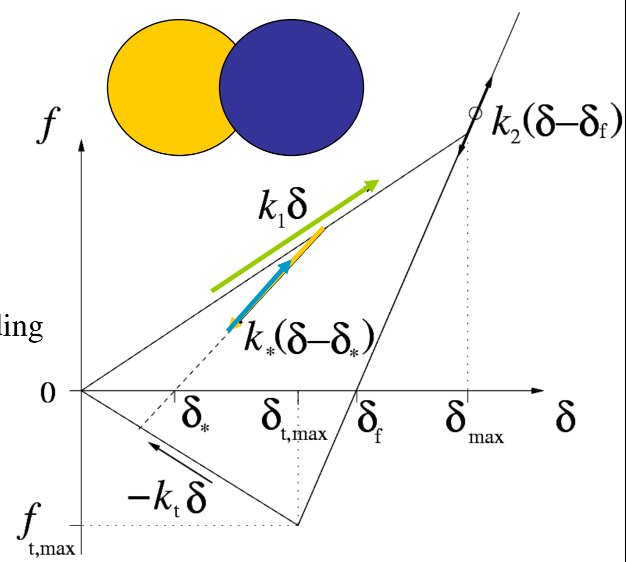
1. loading

plastic loading
stiffness: k_1

2. unloading

3. re-loading

elastic un/re-loading
stiffness: k_*



Contacts

1. loading

plastic loading
stiffness: k_1

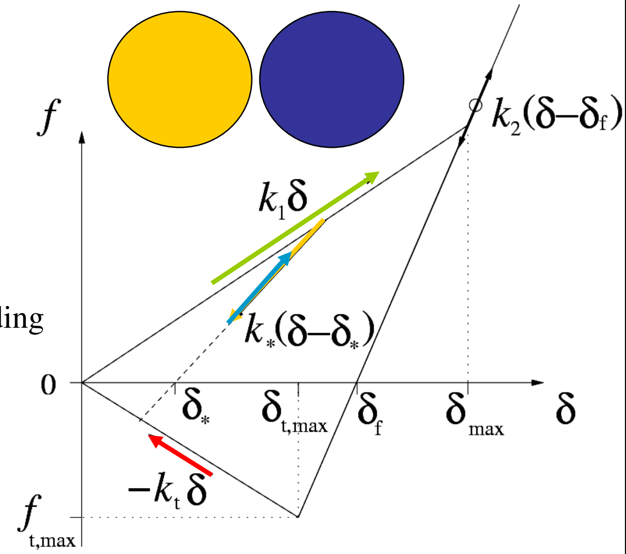
2. unloading

3. re-loading

elastic un/re-loading
stiffness: k_*

4. tensile failure

tensile force



Contacts

1. loading

plastic loading
stiffness: k_1

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elastic un/re-loading
stiffness: k_*

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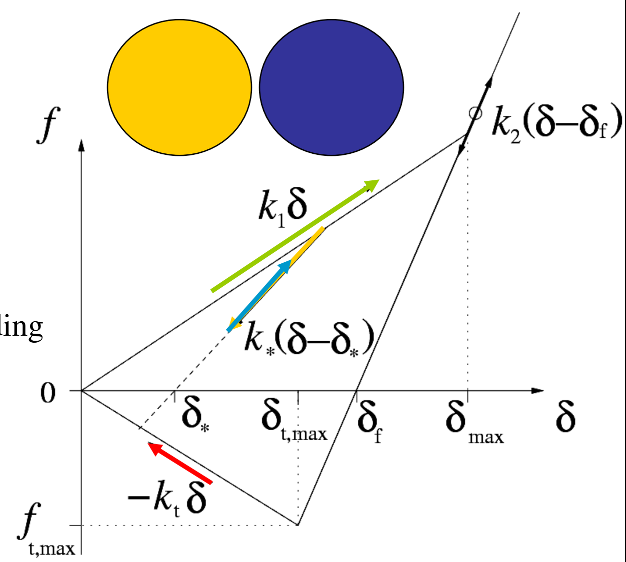
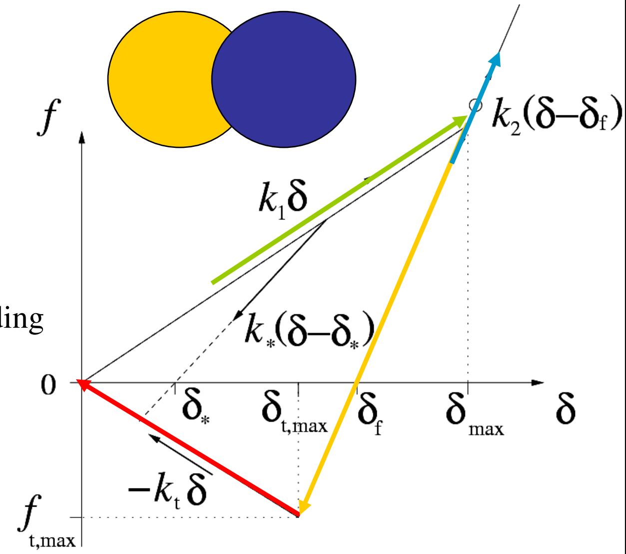
tensile force

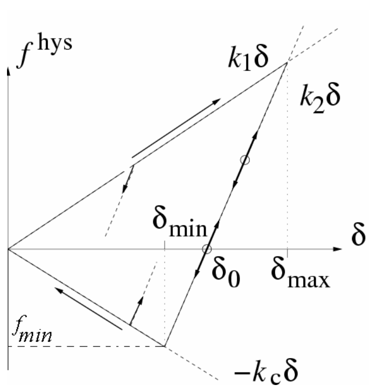


Contacts



1. **loading**
   transition to stiffness: k_2
2. **unloading**
3. **re-loading**
   elastic un/re-loading stiffness: k_2
4. **tensile failure**
   max. tensile force

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 δ_{max}

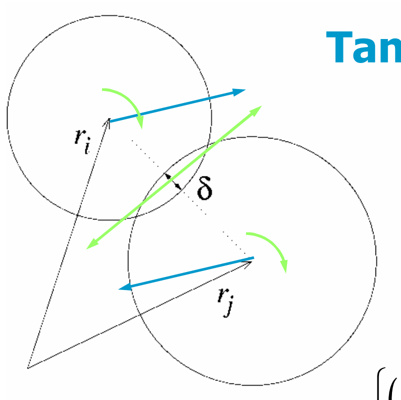
stress-free overlap $\delta_0 = (1-k_1/k_2)\,\delta_{max}$

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

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

stiffness
plastic deform.
adhesion

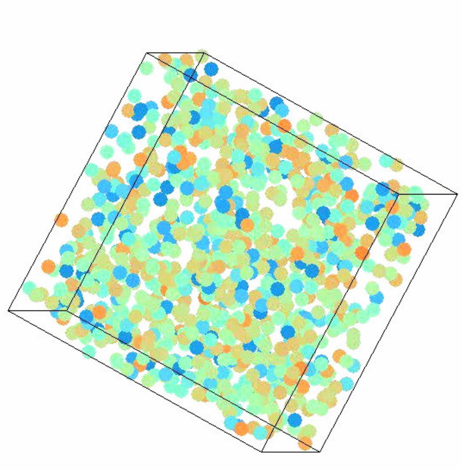
Tangential contact model

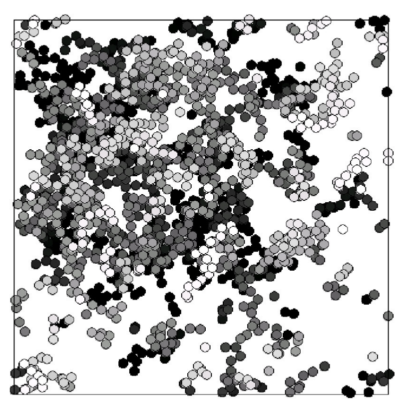


Sliding **contact points:**
- static Coulomb friction
- dynamic Coulomb friction
- objectivity
Sliding/Rolling/Torsion

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

… Details of interaction

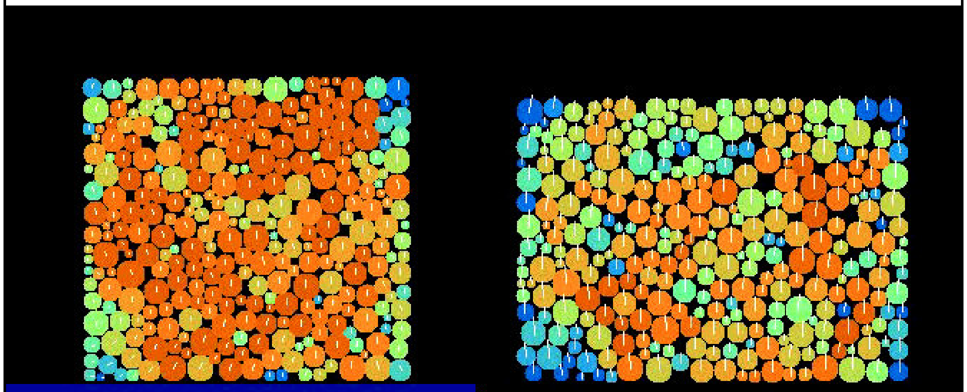




Attraction + Dissipation = Agglomeration

Sintering 7

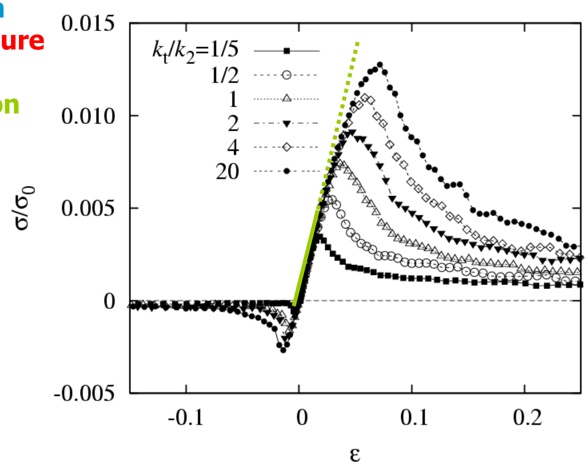
7. **Vibration test**



p=100 *p*=10

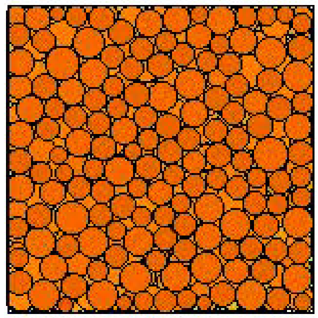
compression-tension

1. **Preparation**
2. **HIGH pressure**
3. **Relaxation**
4. **Compression**



tension

$k_t/k_2 = 1/2$



Biaxial box set-up

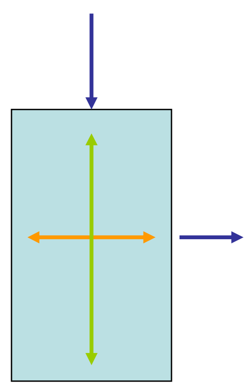
- Top wall: strain controlled

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

- Right wall: stress controlled

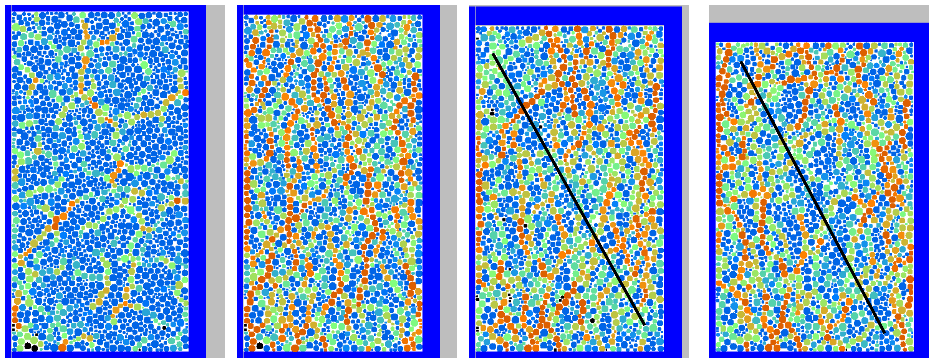
$$p = \text{const.}$$

- Evolution with time … ?

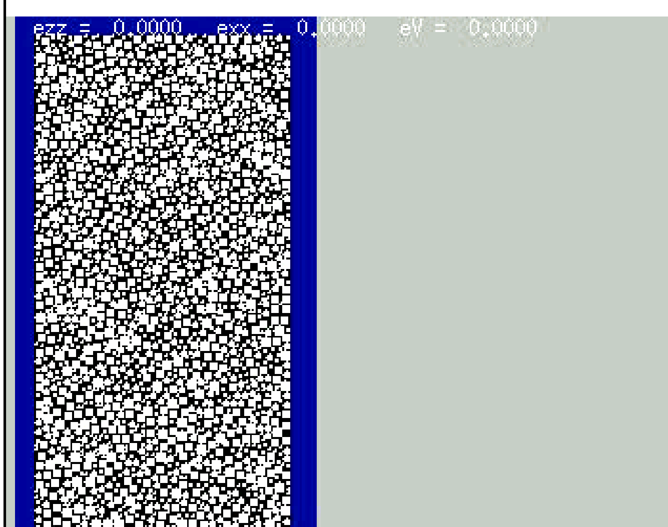


Simulation results (closer look)

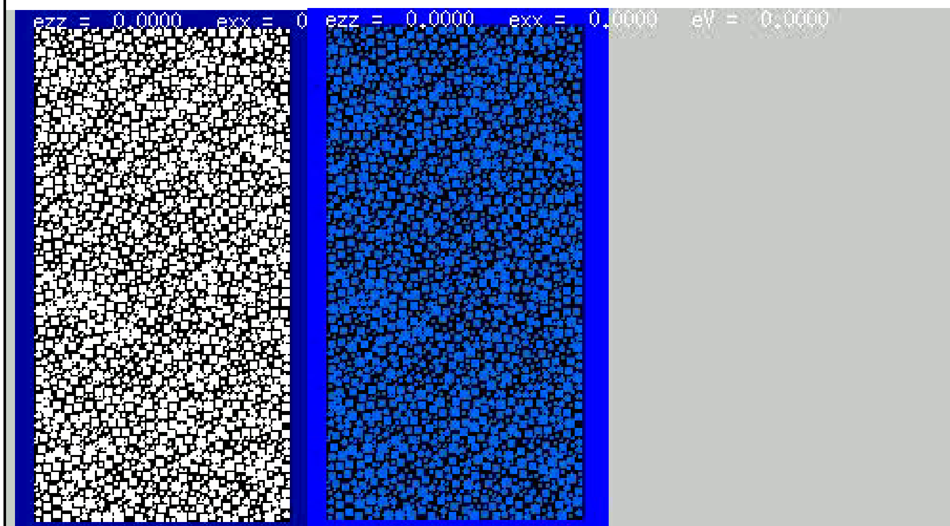
ε_{zz}=0.0% ε_{zz}=1.1% ε_{zz}=4.2% ε_{zz}=9.1%



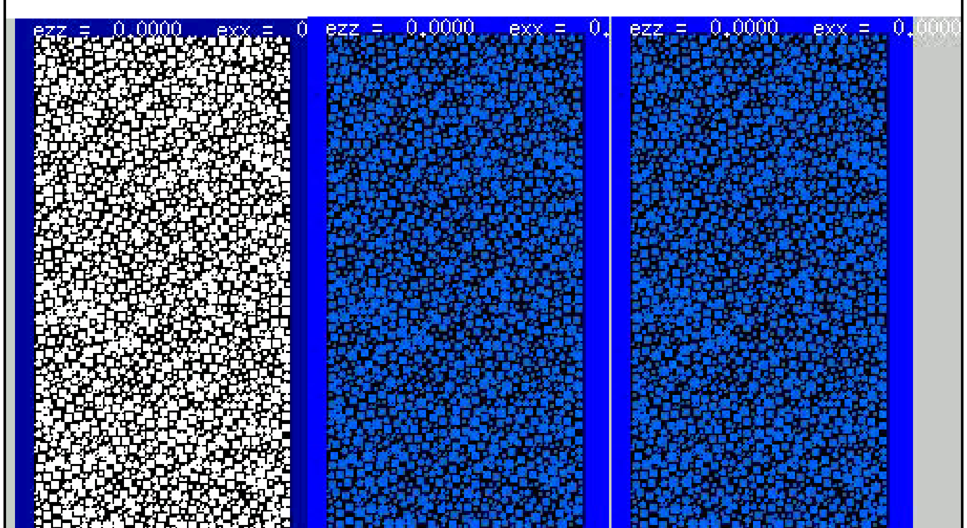
Bi-axial box (stress chains)



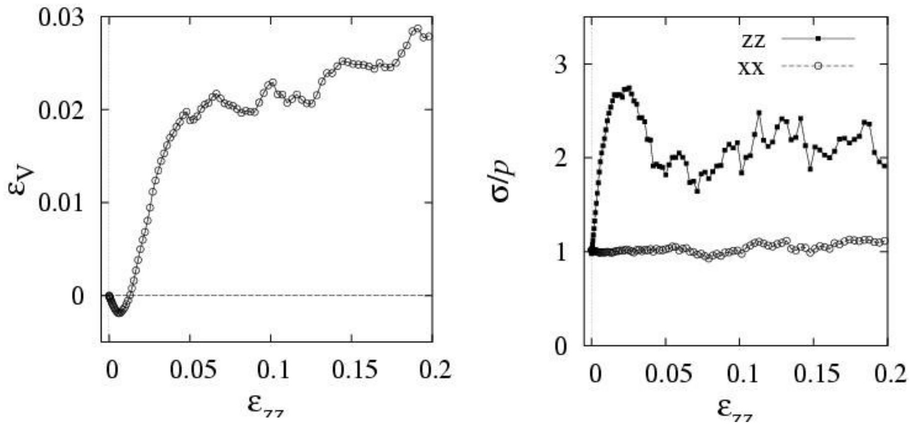
Bi-axial box (kinetic energy)



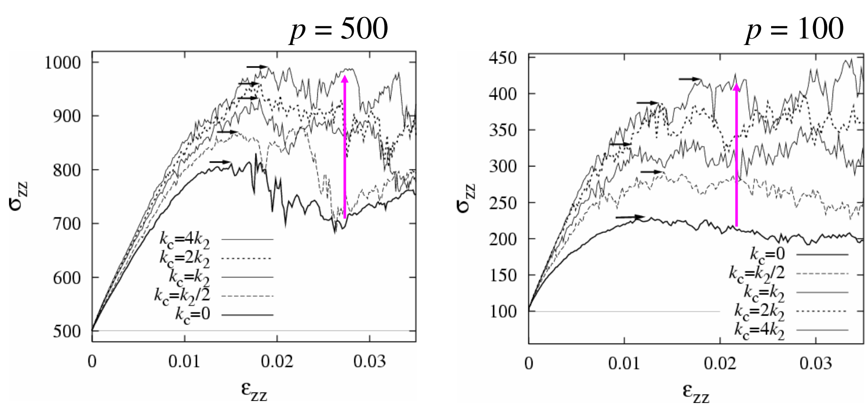
Bi-axial box (rotations)



Bi-axial compression with p_x=const.



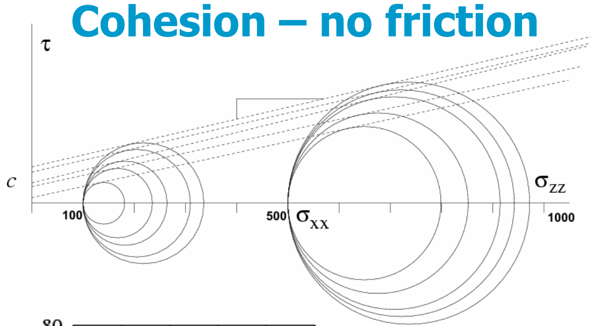
Modulus and yield stress cohesion



Modulus (initial slope)

Yield Stress .... (peak value)

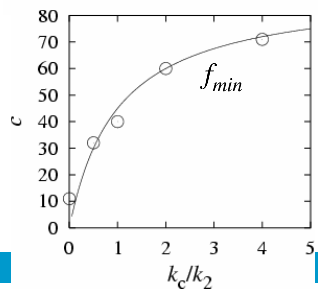
Cohesion – no friction



$k_c / k_2 = 0, 1/2, 1, 2,$ and 4

geometrical friction angle

$\phi \approx 13^\circ$



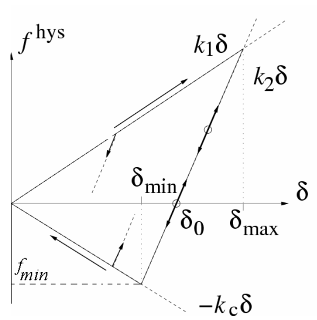
macro cohesion

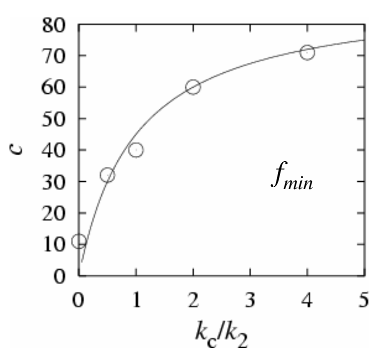
$c = 1.8\times10^{-3}\,\frac{1-k_1/k_2}{1+k_2/k_c}$

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

$k_c / k_2 = 0, 1/2, 1, 2,$ and 4



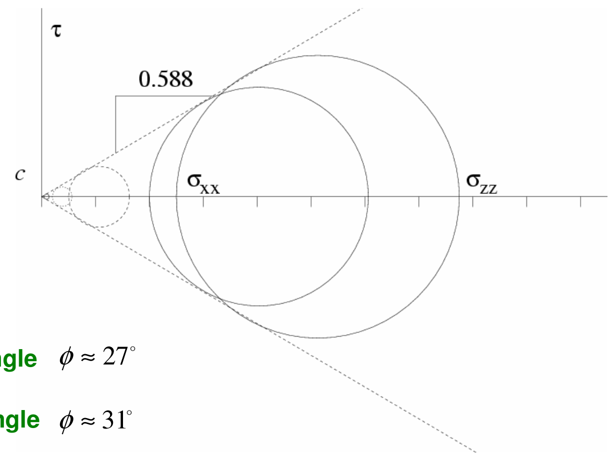


micro adhesion: f_{min}

macro cohesion $c = c_0\,\frac{1-k_1/k_2}{1+k_2/k_c}$

Friction – no cohesion

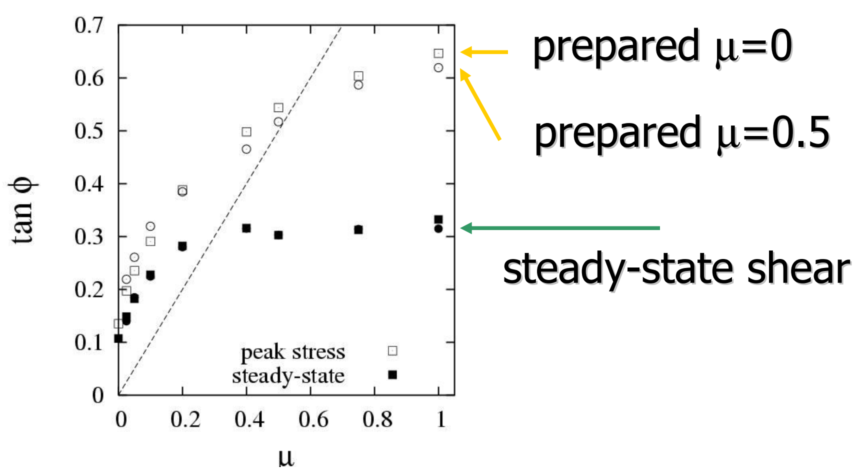
$k_c = 0$ and $\mu = 0.5$



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

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

Micro-macro for friction



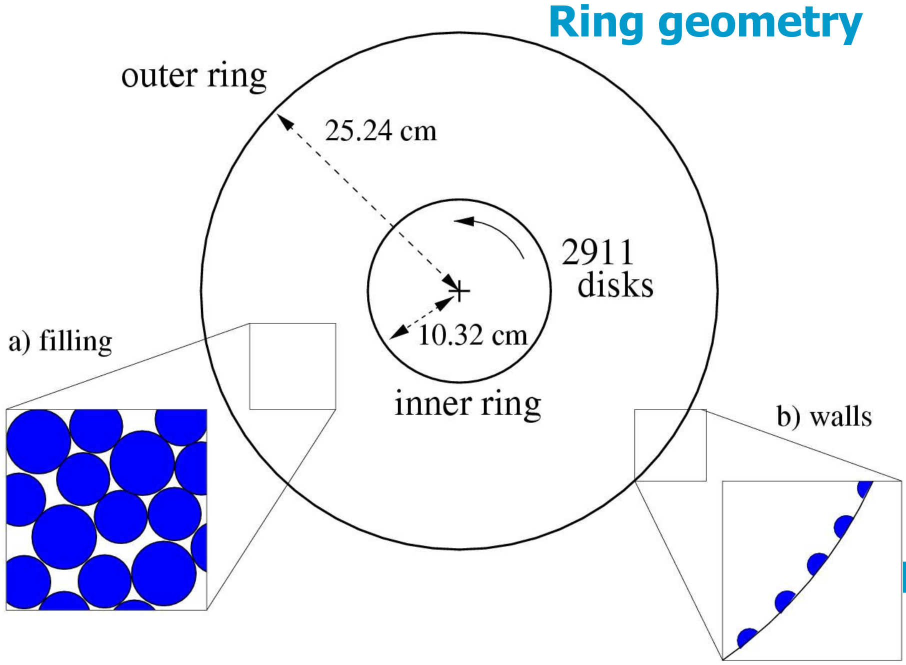
micro contact-friction μ macro friction-angle ϕ

Summary micro-macro GLOBAL

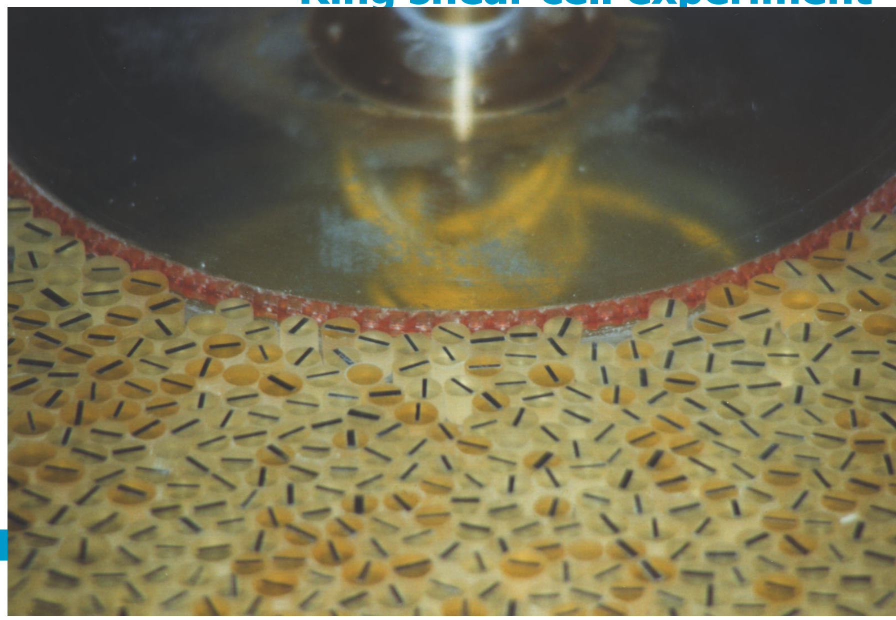
- Micro-/Macro-Flow Rheology
  - micro-adhesion … macro-cohesion
  - micro-contact-friction … macro-friction-angle
- Non-Newtonian Rheology (Anisotropy?, Micro-polar?)

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

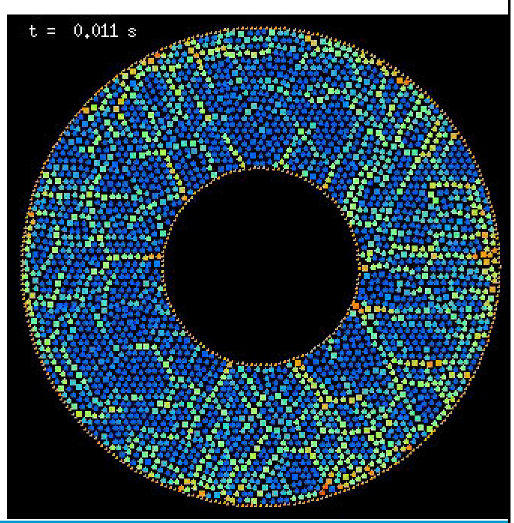
Ring geometry



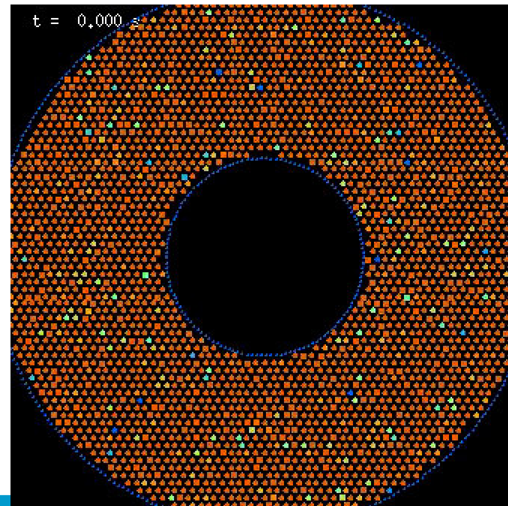
Ring shear cell experiment



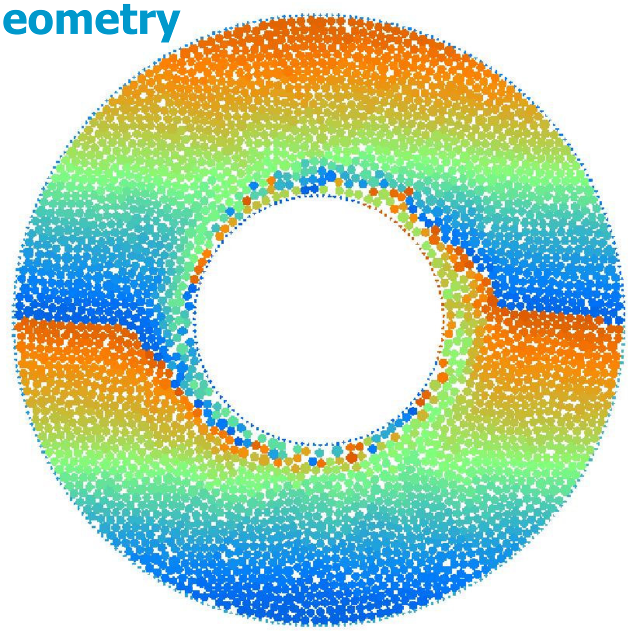
2D shear cell – force chains = inhomogeneity + anisotropy



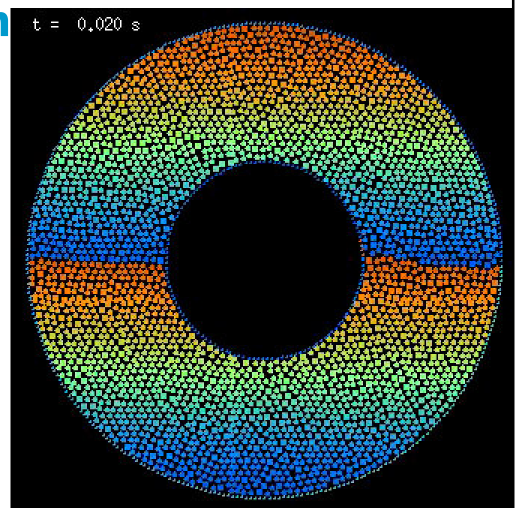
2D shear cell – energy



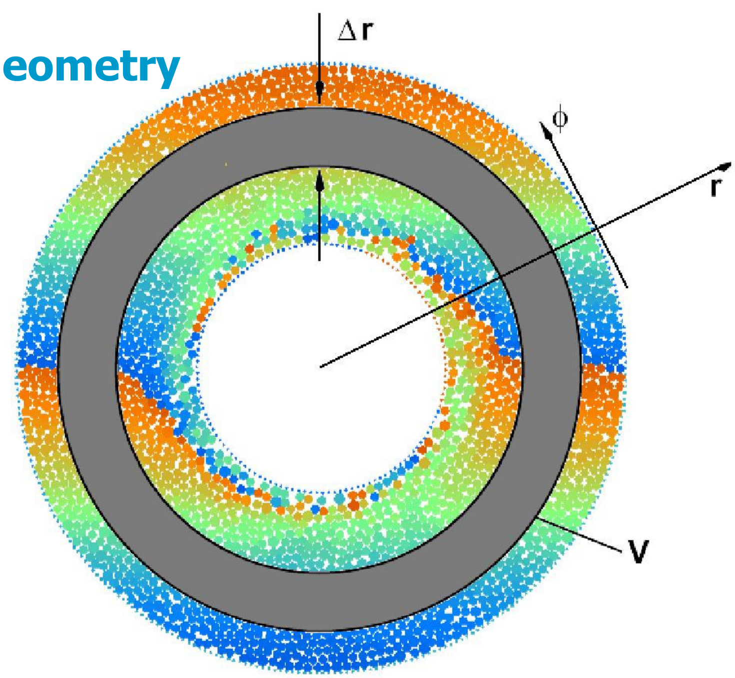
Ring geometry



2D shear cell
shear localization
non-Newtonian



Ring geometry



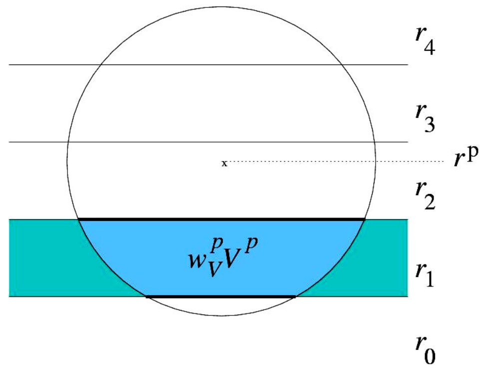
Averaging Formalism

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

Any quantity:

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

- Scalar
- Vector
- Tensor



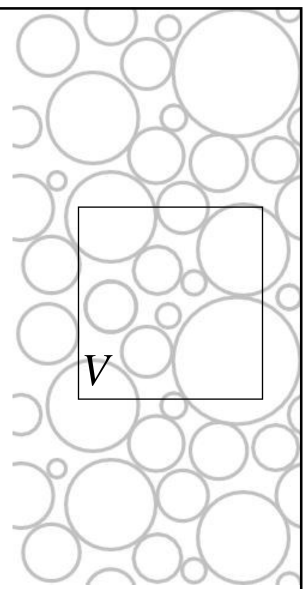
Averaging Formalism

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

Any quantity:

$$Q^p$$

In averaging volume: V



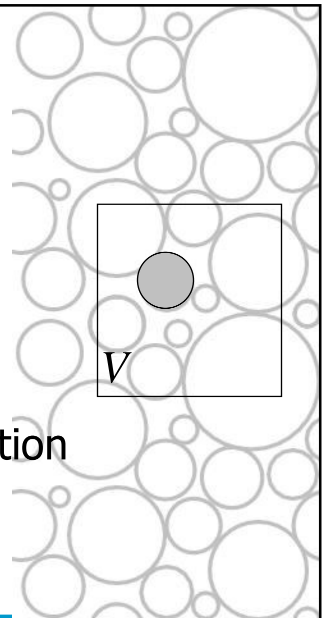
Averaging Density

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

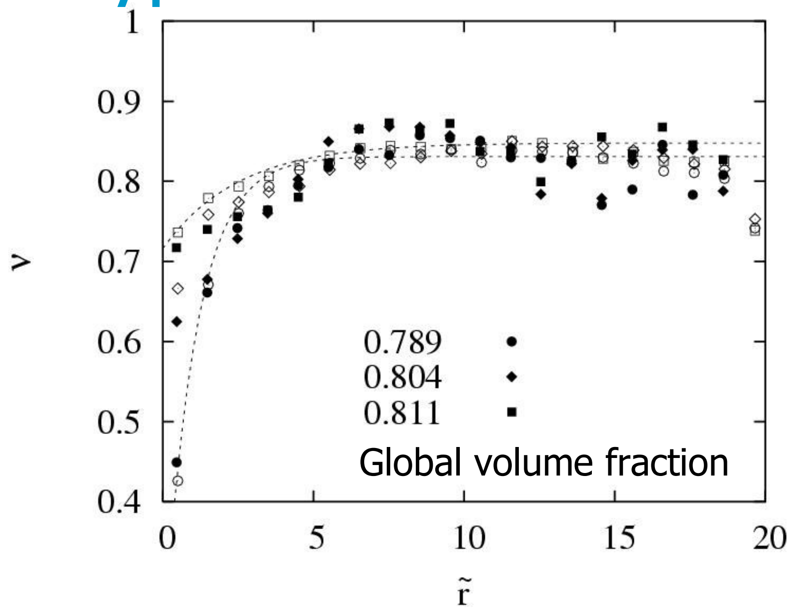
Any quantity:

$$Q^p = 1$$

- Scalar: Density/volume fraction



Density profile



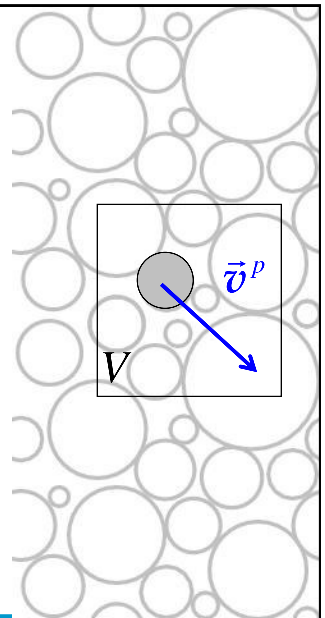
Averaging Velocity

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

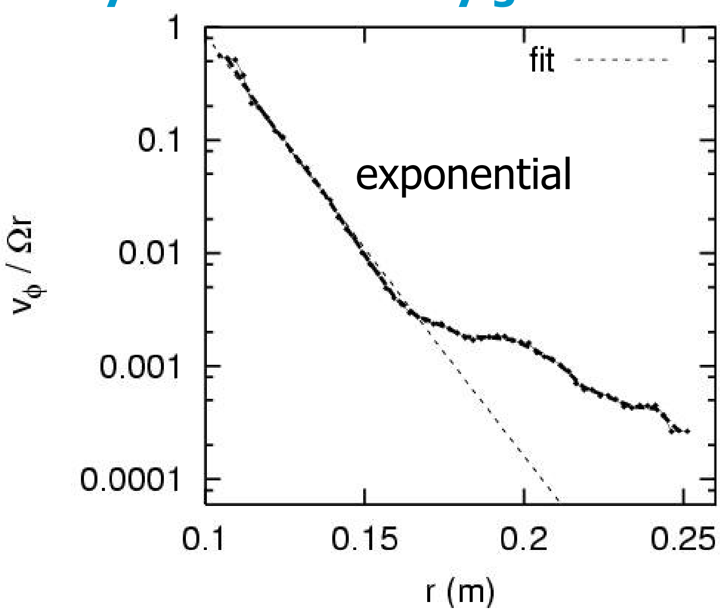
Any quantity:

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

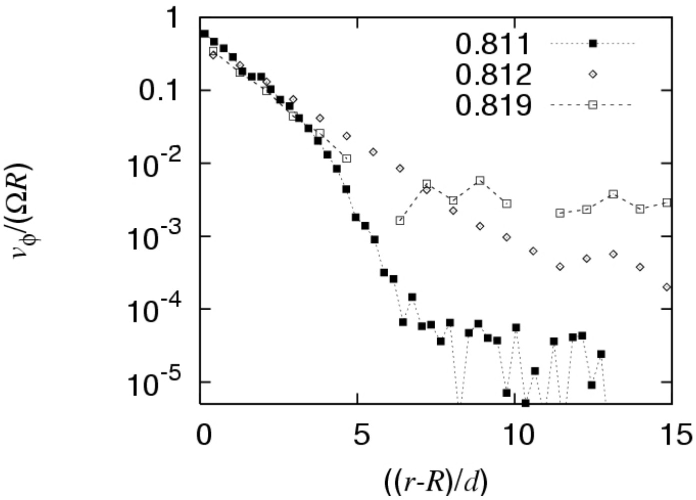
- Scalar
- Vector – velocity density



Velocity field -> velocity gradient



Velocity field -> velocity gradient



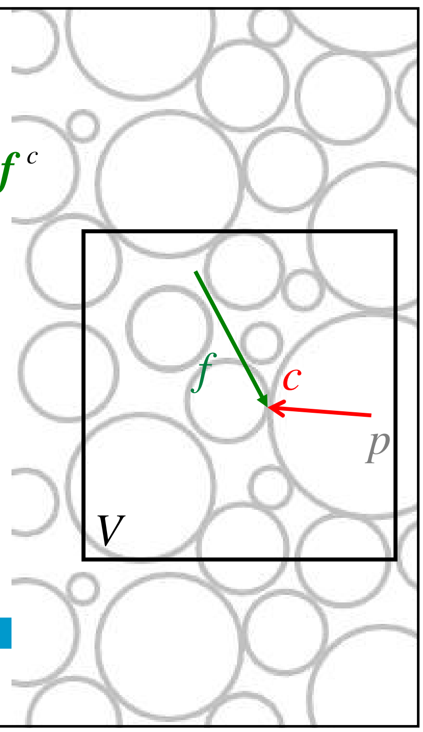
Averaging Stress

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

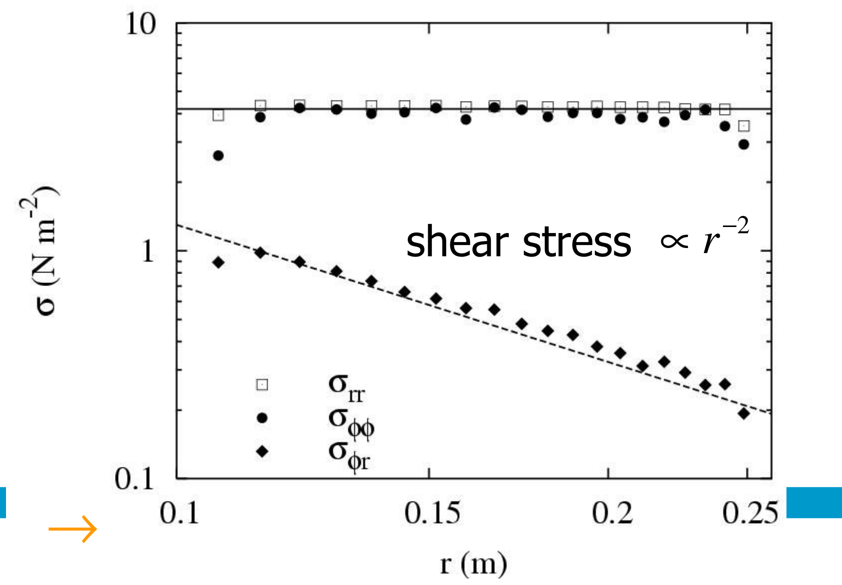
Any quantity:

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

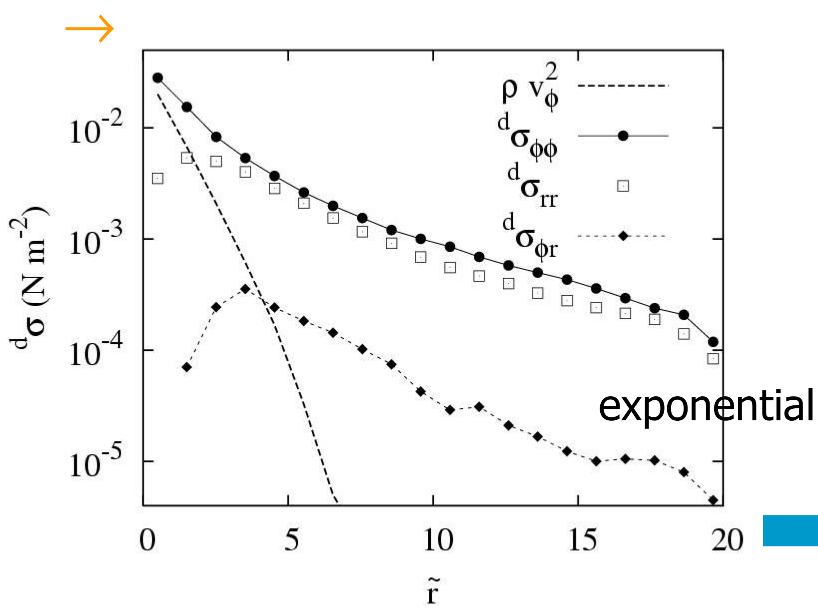
- Scalar
- Vector
- Tensor: Stress



Stress tensor (static)



Stress tensor (dynamic)



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

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

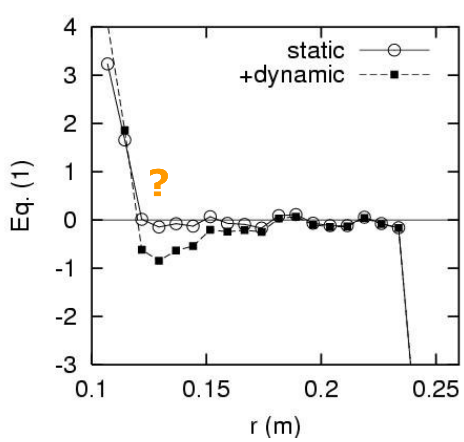
$$0 = r\frac{\partial\sigma_{r\phi}}{\partial r} + (\sigma_{r\phi} + \sigma_{\phi r})\,,$$

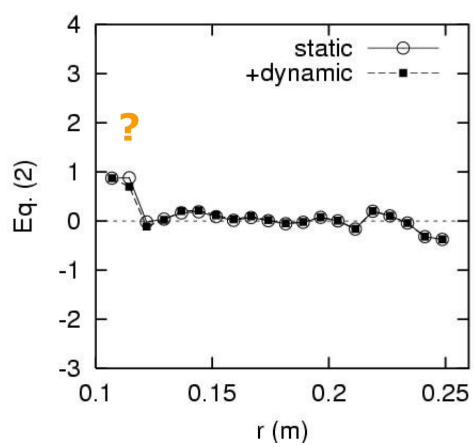
$$\Rightarrow \frac{\partial(r\sigma_{rr})}{\partial r} = \sigma_{\phi\phi} \qquad \frac{\partial(r\sigma_{r\phi})}{\partial r} = -\sigma_{\phi r}$$

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

Stress equilibrium (2)

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





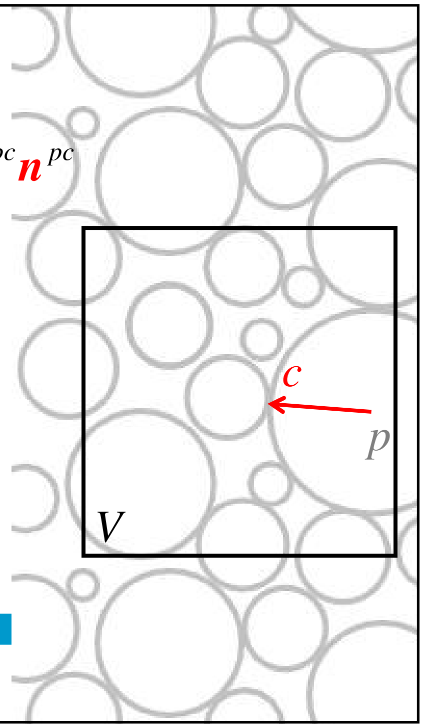
Averaging Fabric

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

Any quantity:

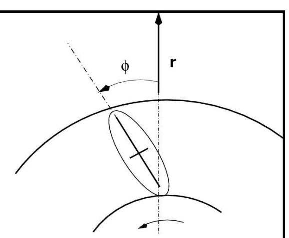
$$Q^p = \underline{\underline{\mathbf{F}}}^p = \sum_c \boldsymbol{n}^{pc}\boldsymbol{n}^{pc}$$

- Scalar: contacts
- Vector: normal
- Contact distribution

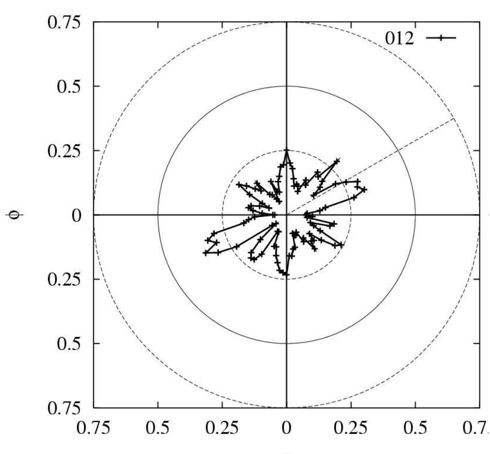


Fabric tensor

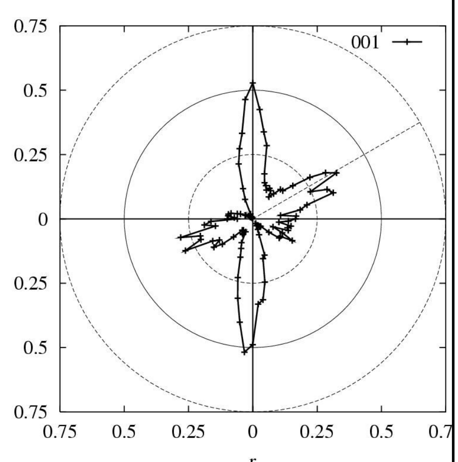
contact probability …



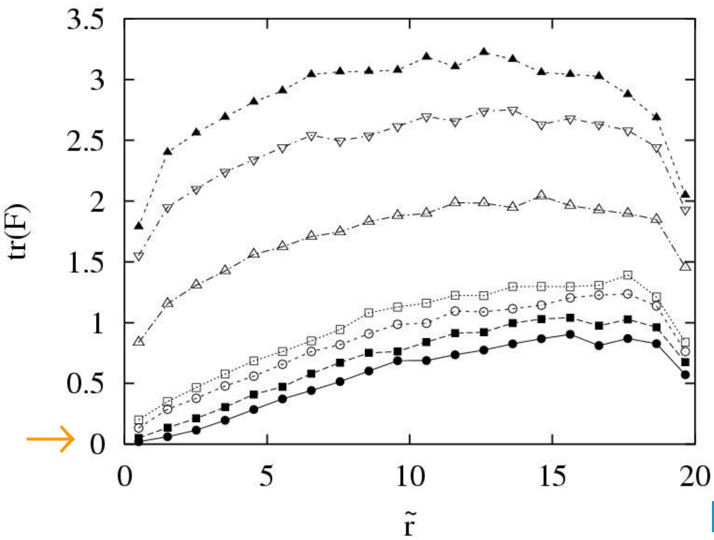
center



wall

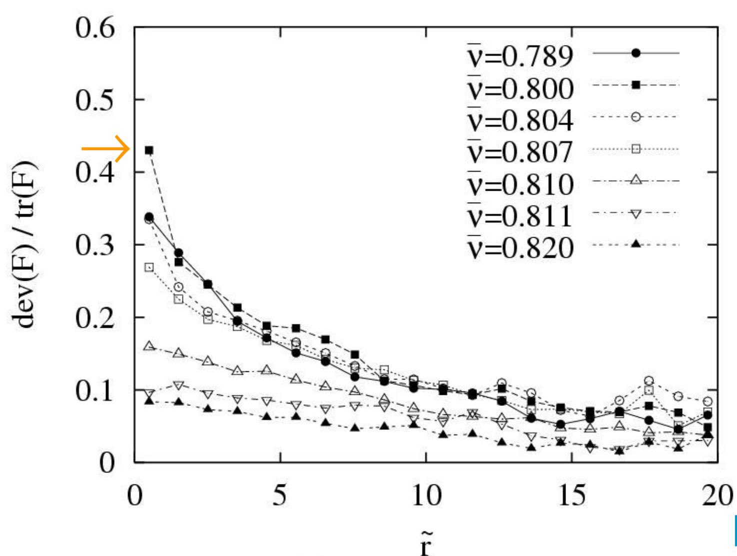


Fabric tensor (trace)



contact number density

Fabric tensor (deviator)



an-isotropy (!)

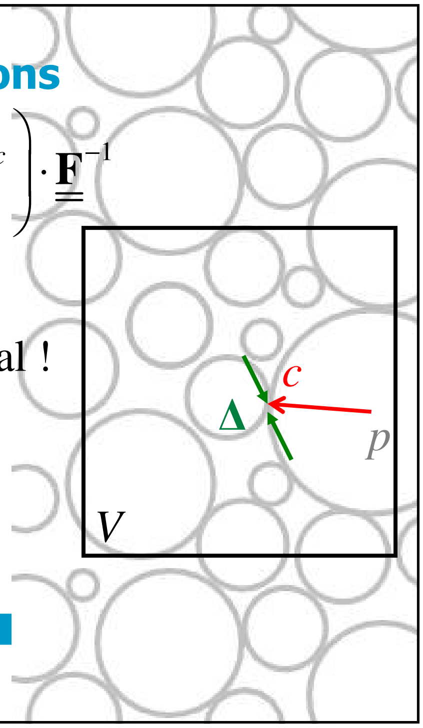
Averaging Deformations

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

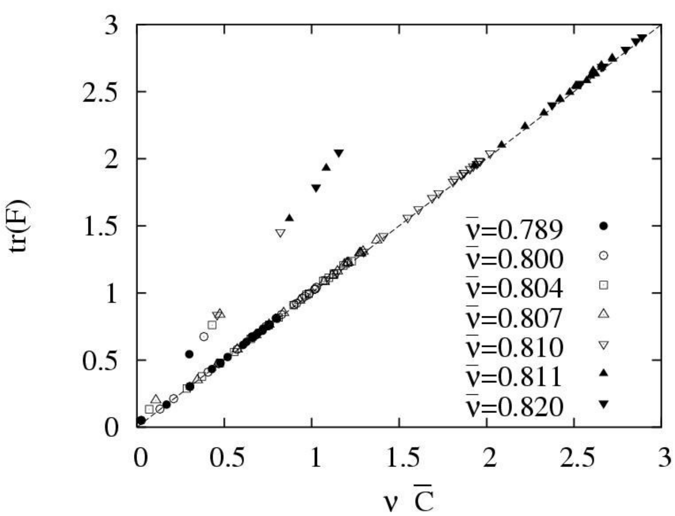
Deformation:

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

- Scalar
- Vector
- Tensor: Deformation

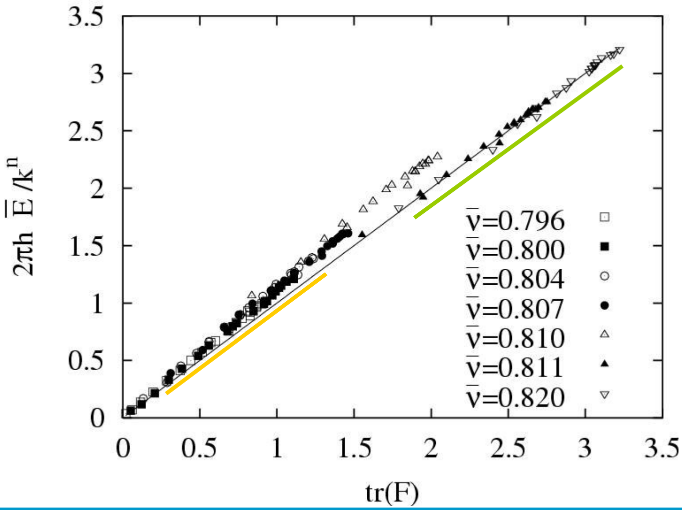


Macro (contact density)



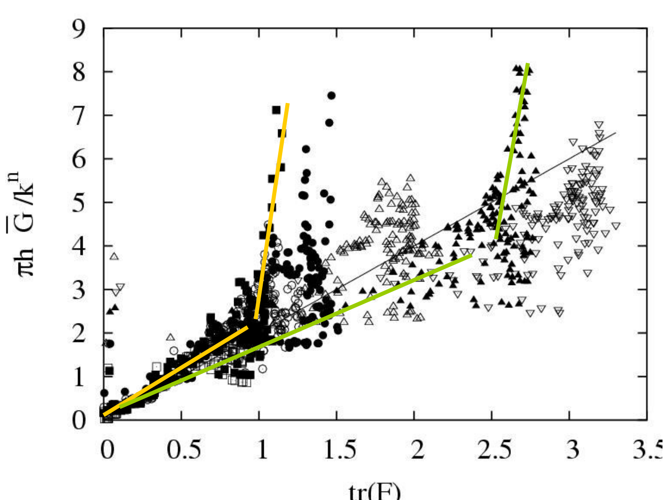
Macro (bulk modulus)

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

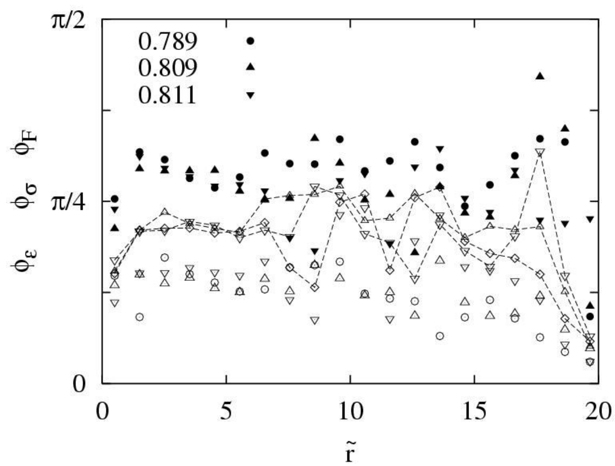


Macro (shear modulus)

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



Anisotropy – non-colinearity



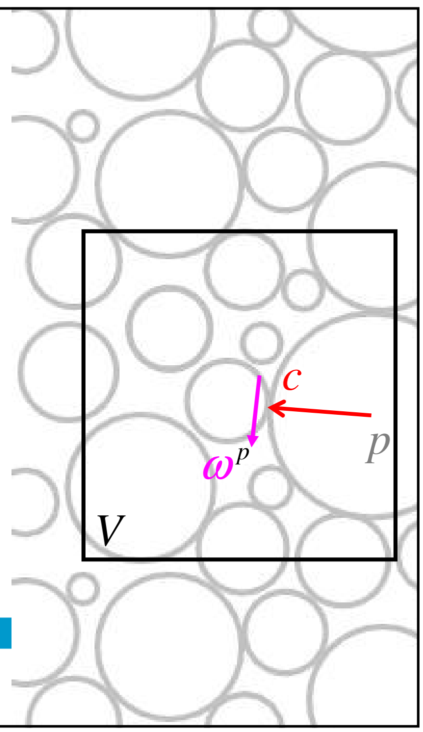
Averaging Rotations

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

Deformation:

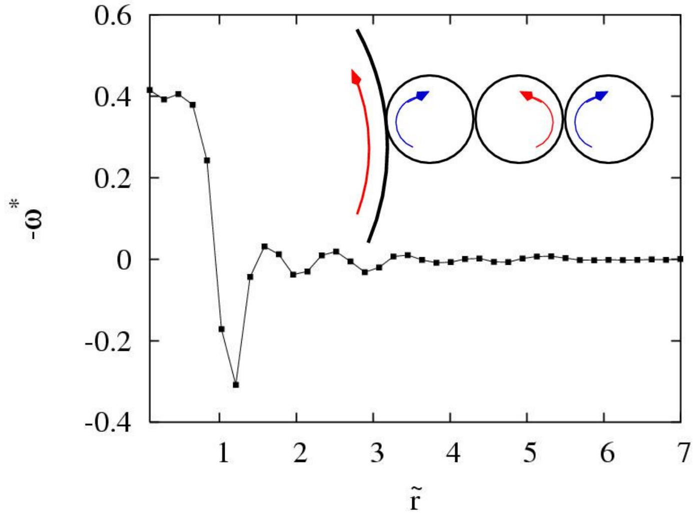
$$Q^p = \omega^p$$

- Scalar
- Vector: Spin density
- Tensor



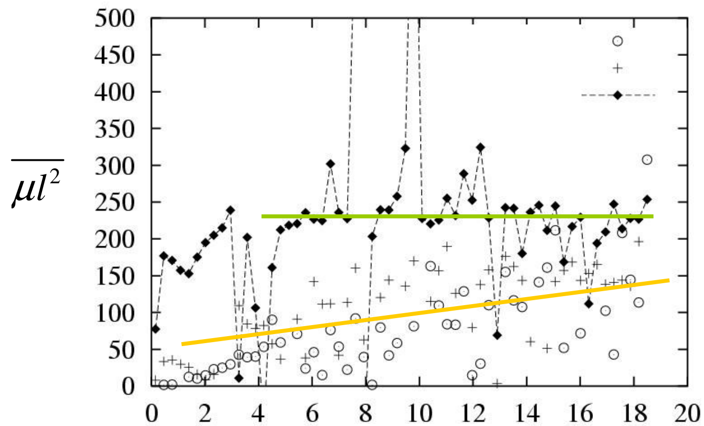
Rotations – spin density

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



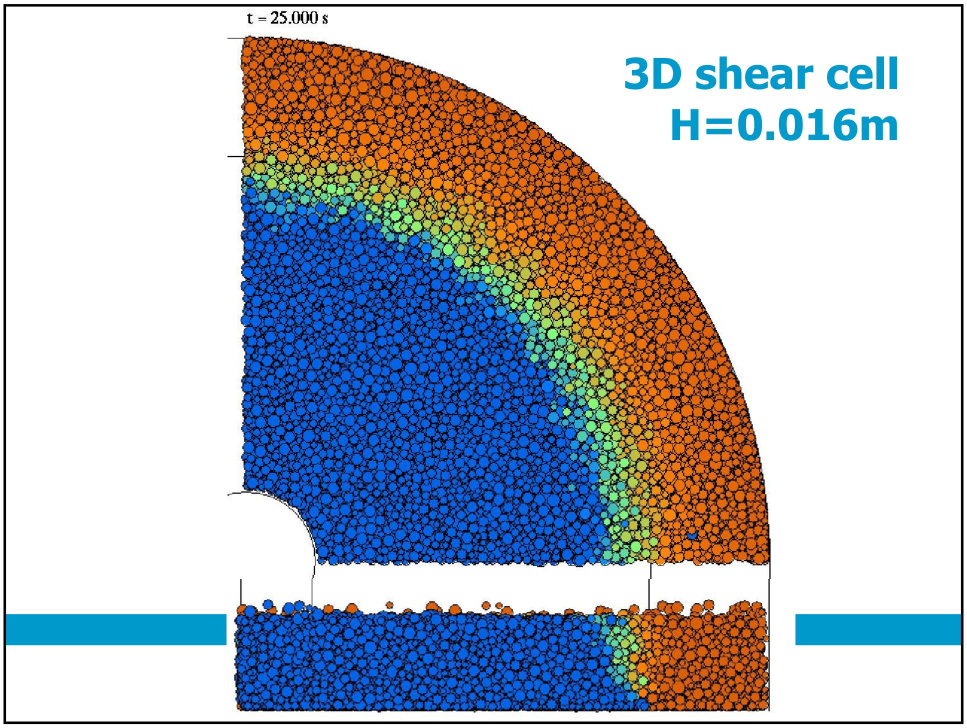
Macro (torque stiffness)

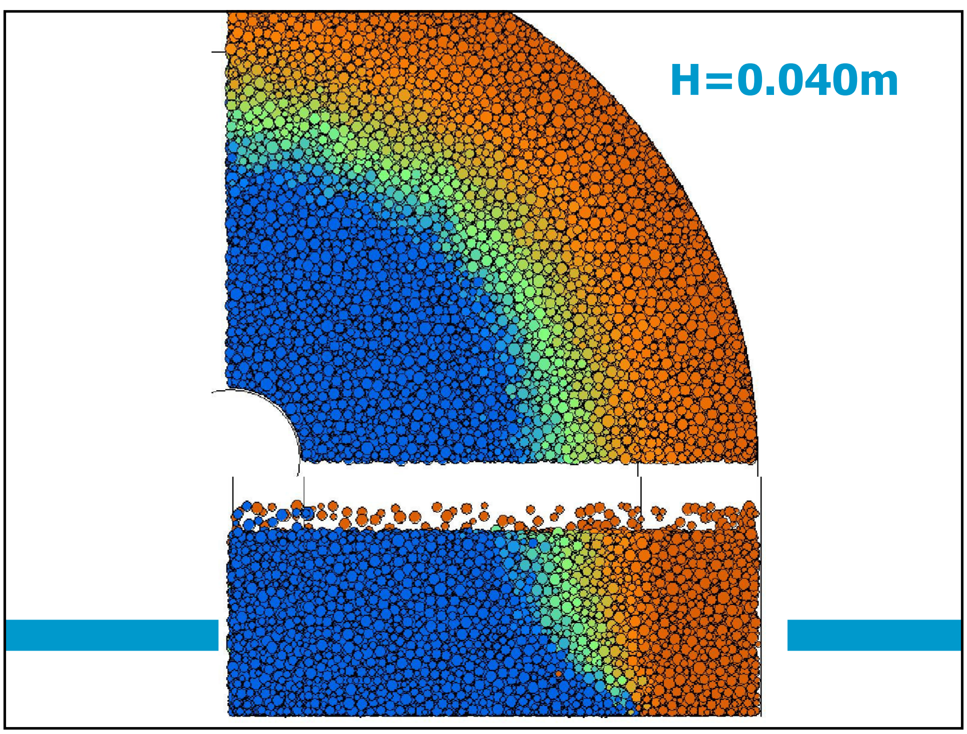
$$\overline{\mu l^2} = \frac{\underline{\underline{M}}}{\underline{\underline{\kappa}}}$$

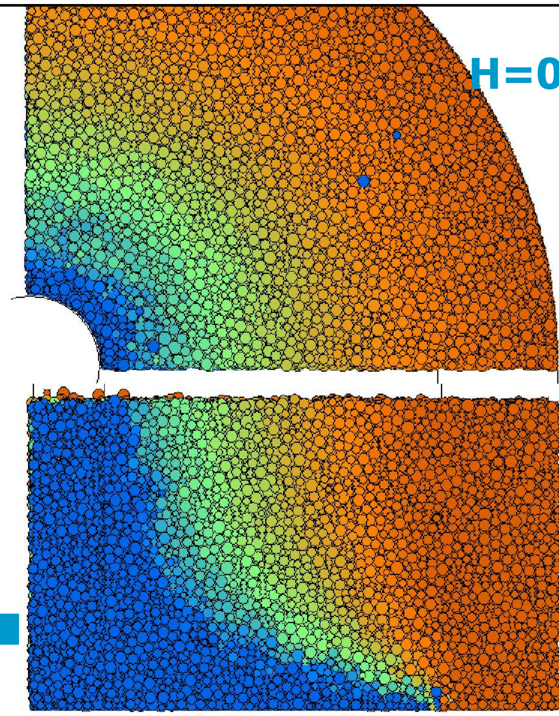


The End ?

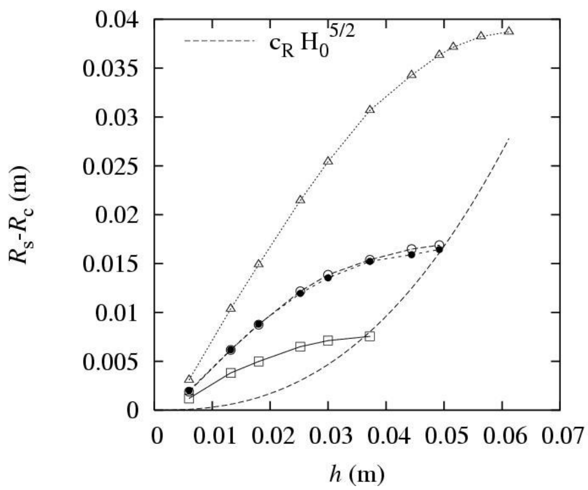
3D ring shear cell
micro-macro for shear viscosity


t = 25.000 s
3D shear cell
H=0.016m


H=0.040m

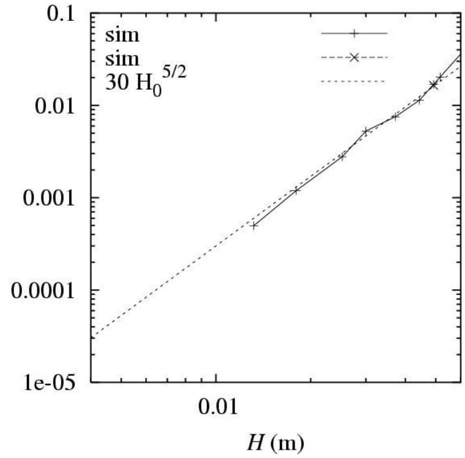


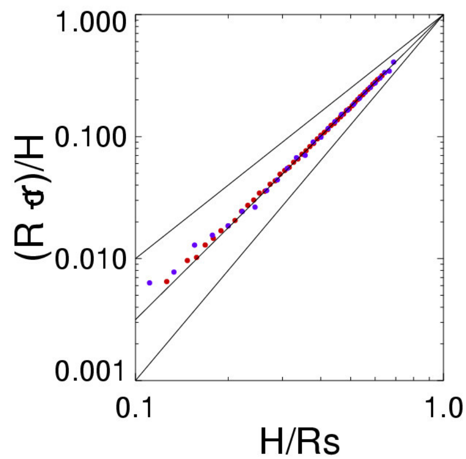
3D shear band center position



80% agreement … up to now

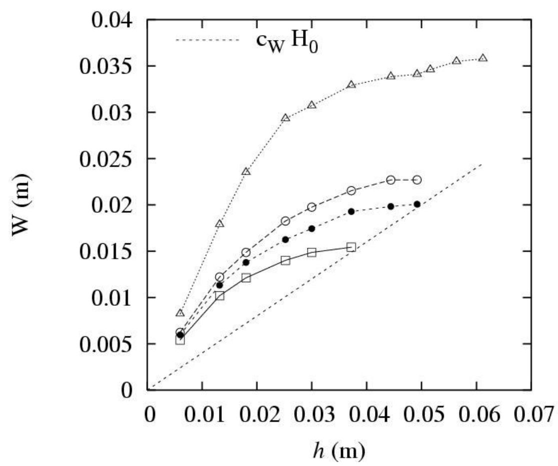
3D shear band center position





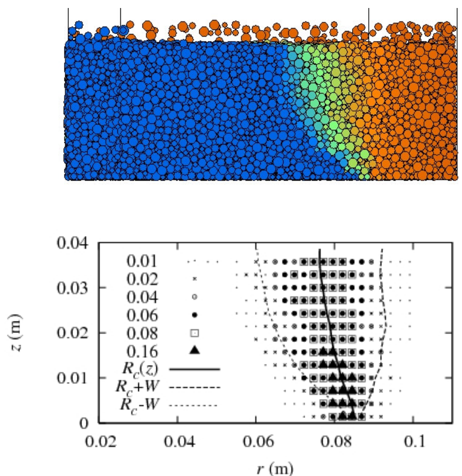
80% agreement … up to now

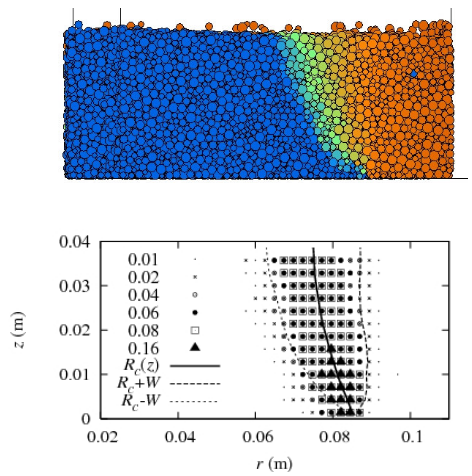
3D shear band width



80% agreement … up to now

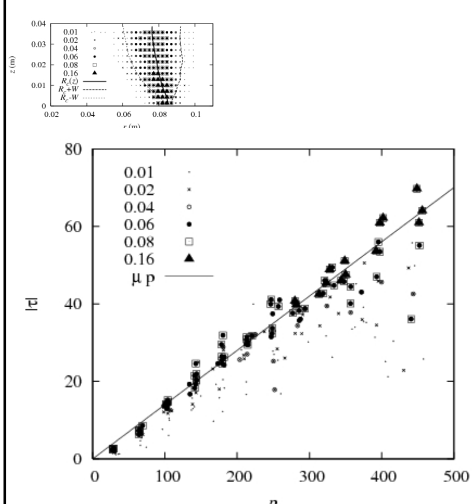
Constitutive relations – shear rate $\dot{\gamma}$

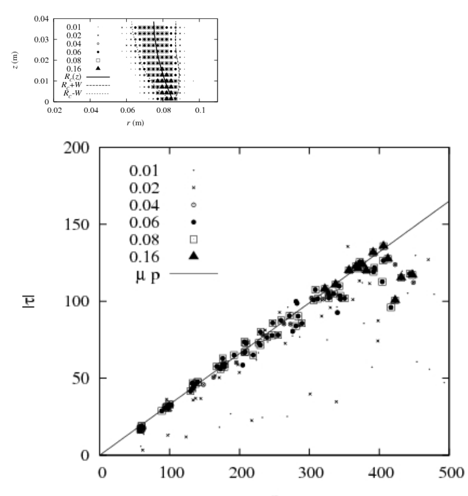




no friction   friction

Constitutive relations: Mohr-Coulomb

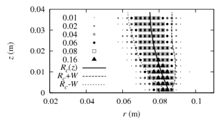




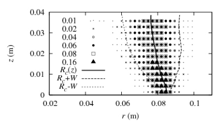
no friction   friction

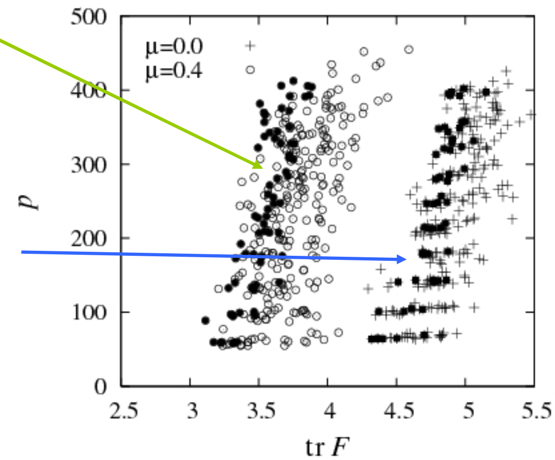
Constitutive relations: stress-structure

friction



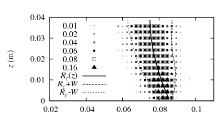
no friction



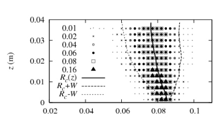


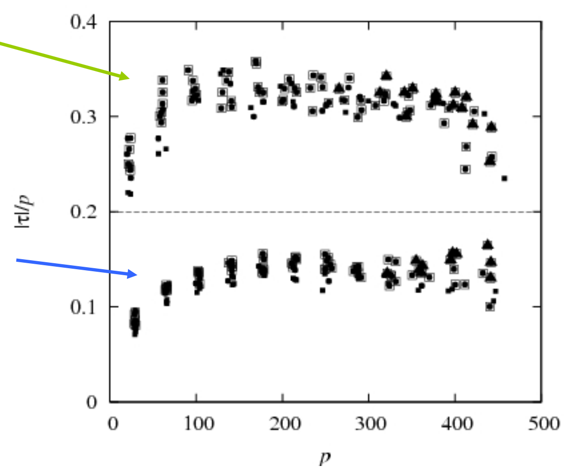
Constitutive relations: anisotropy

friction



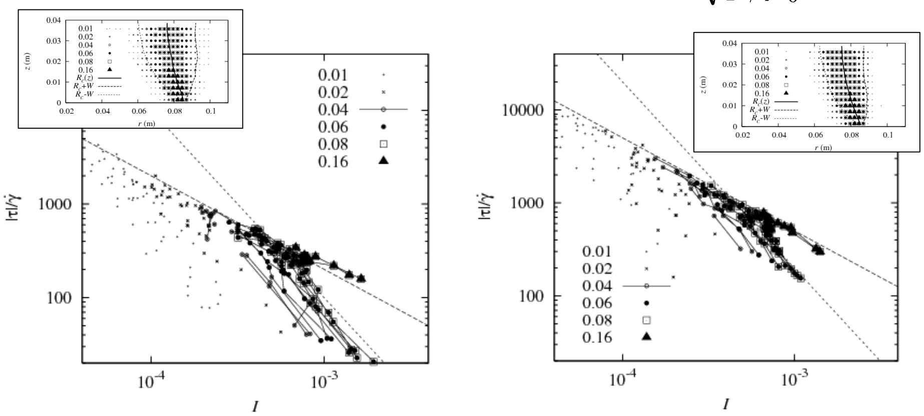
no friction





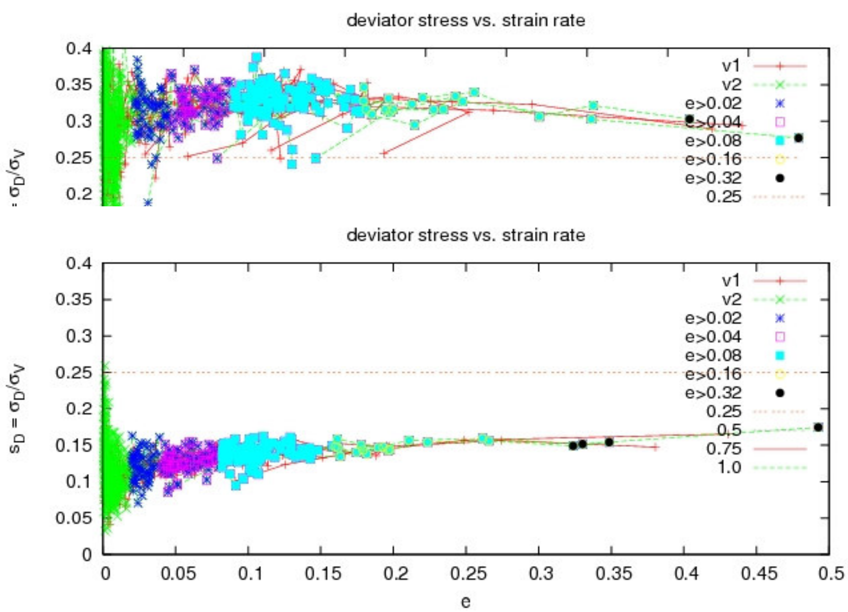
Constitutive relations: shear softening

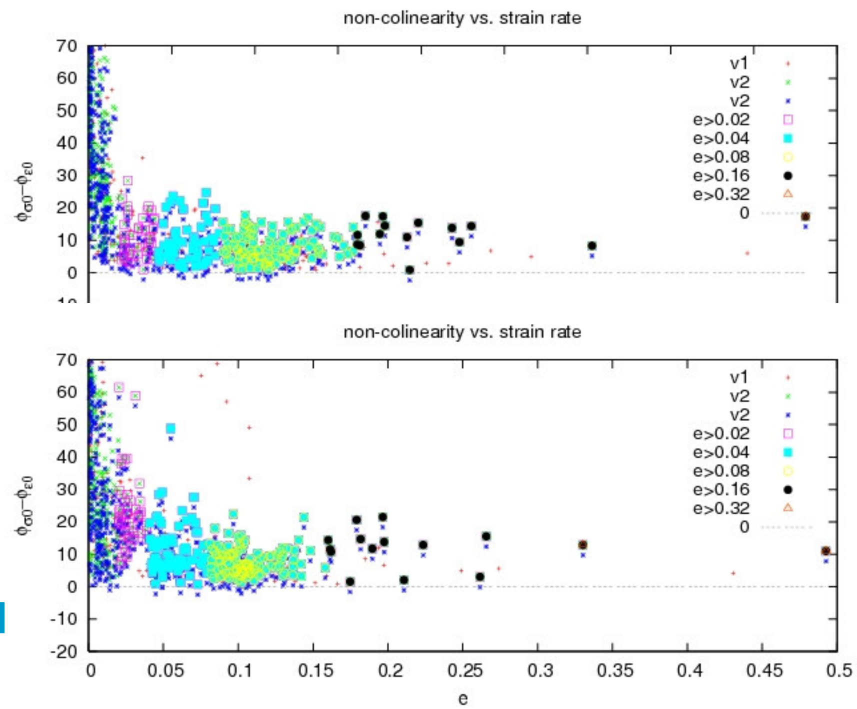
viscosity $\frac{|\tau|}{\dot{\gamma}}$ vs. shear rate $I = \frac{\dot{\gamma} d_0}{\sqrt{p/\rho_0}}$



no friction friction

stress ratio vs. shear rate





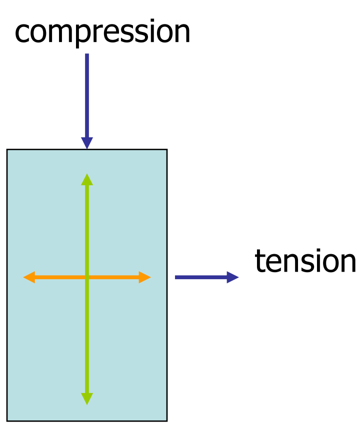
3D Flow behavior – steady state shear

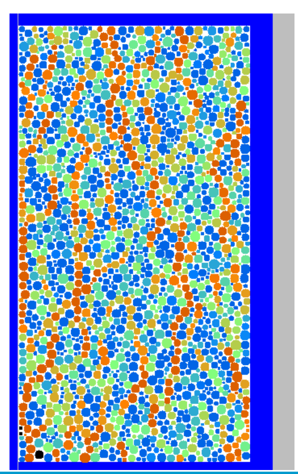
Obtain constitutive relations from one SINGLE simulation:

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

The End

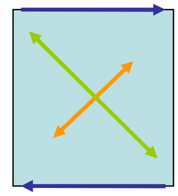
Micro-macro for anisotropy – rheology





Anisotropy ↔ Shear ?

- Simple shear

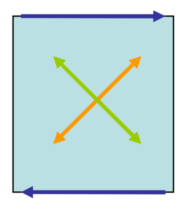


$$\varepsilon = \begin{pmatrix} 0 & 2\varepsilon_s \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & \varepsilon_s \\ -\varepsilon_s & 0 \end{pmatrix} + \begin{pmatrix} 0 & \varepsilon_s \\ \varepsilon_s & 0 \end{pmatrix}$$

Rotation + symmetric shear

Anisotropy ↔ Shear ?

- Simple shear

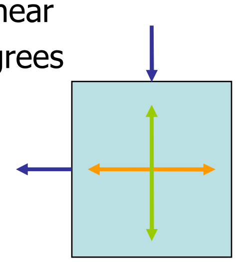


$$\varepsilon = \begin{pmatrix} 0 & 2\varepsilon_s \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & \varepsilon_s \\ -\varepsilon_s & 0 \end{pmatrix} + \begin{pmatrix} 0 & \varepsilon_s \\ \varepsilon_s & 0 \end{pmatrix}$$

Rotation + symmetric shear

- Rotate symmetric shear tensor by 45 degrees

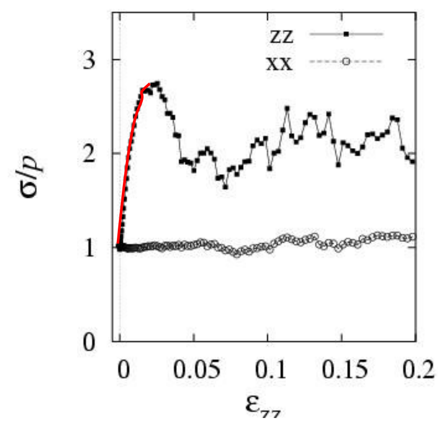
$$R_{45} \cdot \begin{pmatrix} 0 & \varepsilon_s \\ \varepsilon_s & 0 \end{pmatrix} \cdot R_{45}^T = \begin{pmatrix} \varepsilon_s & 0 \\ 0 & -\varepsilon_s \end{pmatrix}$$



- Biaxial “shear”: compression+extension

An-isotropy

in stress



An-isotropy (Stress)

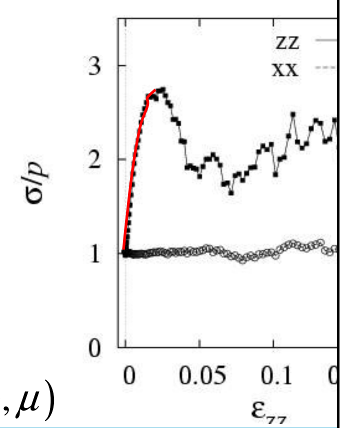
- Stress: Isotropic: $\mathrm{tr}\,\boldsymbol{\sigma}$, and deviatoric: $\mathrm{dev}\,\boldsymbol{\sigma} = \boldsymbol{\sigma}_{zz}\text{-}\boldsymbol{\sigma}_{xx}$
  - Minimal eigenvalue: $\boldsymbol{\sigma}_{xx}$
  - Maximal eigenvalue: $\boldsymbol{\sigma}_{zz}$
- Dev. Stress fraction $s_D = \mathrm{dev}\,\boldsymbol{\sigma} / \mathrm{tr}\,\boldsymbol{\sigma}$

$$\frac{\partial}{\partial \varepsilon_D} s_D = \beta_s \left(s_{\max} - s_D \right)$$

- Exponential approach to peak

$$1 - s_D / s_{\max} = \exp\left(-\beta_s \varepsilon_D \right)$$

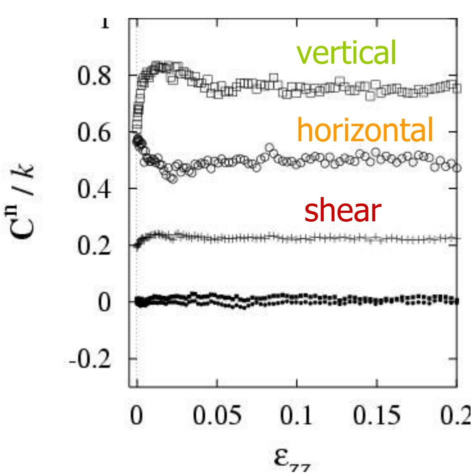
$\beta_s\left(\rho, p, \mu\right)$

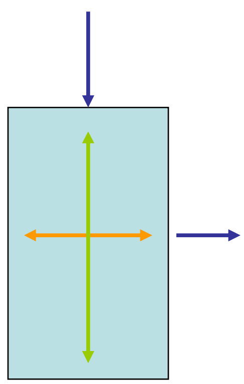


An-isotropy (Stress)

$$\frac{\partial}{\partial \varepsilon_D} s_D = \beta_s \left(s_{\max} - s_D \right)$$

Stiffness tensor





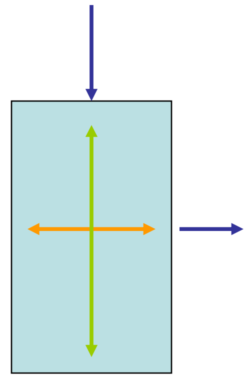
Different moduli:

- against shear C_2
- perpendicular C_1
- *one* shear modulus

An-isotropy (Structure)

- Structure changes with deformation
- Different stiffness:
  - More stiffness against shear C_2
  - Less stiffness perpendicular C_1
- One (only?) shear modulus
- Anisotropy $A = C_2 - C_1$ evolution

$$\frac{\partial}{\partial \varepsilon_D} A = \beta_F \left(A_{\max} - A \right)$$



- Exponential approach to maximal anisotropy

… see Calvetti et al. 1997

An-isotropy (Stress & Structure)

$$\frac{\partial}{\partial \varepsilon_D} s_D = \beta_s \left(s_{\max} - s_D \right)$$

$$\frac{\partial}{\partial \varepsilon_D} A = \beta_F \left(A_{\max} - A \right)$$

An-isotropy (Stress & Structure)

Modulus

Friction

$$\frac{\partial}{\partial \varepsilon_D} s_D = \beta_s \left(s_{\max} - s_D \right)$$

$$\frac{\partial}{\partial \varepsilon_D} A = \beta_F \left(A_{\max} - A \right)$$

Constitutive model – scalar

(in the biaxial box eigen-system)

$$\delta\sigma_V = E\varepsilon_V + A\varepsilon_D$$

$$\delta\sigma_D = A\varepsilon_V + B\varepsilon_D$$

Constitutive model – scalar

(in the biaxial box eigen-system)

$$\delta\sigma_V = E\varepsilon_V + A\varepsilon_D$$

$$\delta\sigma_D = A\varepsilon_V + B\varepsilon_D$$

Constitutive model – tensorial

(arbitrary eigen-system)

$$\delta\sigma_V = E\varepsilon_V + A\varepsilon_D \cos\left(2\phi_\varepsilon - 2\phi_C\right)$$

$$\delta\boldsymbol{\sigma}_D = \left[A\varepsilon_V + \left(2B - E\right)\varepsilon_D \cos\left(2\phi_\varepsilon - 2\phi_C\right)\right]\hat{\mathbf{D}}\left(\phi_C\right) + \left(E - B\right)\varepsilon_D \hat{\mathbf{D}}\left(\phi_\varepsilon\right)$$

$$\delta\boldsymbol{\sigma}_D = A\varepsilon_V \hat{\mathbf{D}}\left(\phi_C\right) + \left(2G\right)\varepsilon_D \hat{\mathbf{D}}\left(\phi_\varepsilon\right) + \tfrac{1}{2}\left(C_1 + C_2 - 6G\right)\varepsilon_D \cos\left(2\phi_\varepsilon - 2\phi_C\right)\hat{\mathbf{D}}\left(\phi_C\right)$$

Critical state flow – scalar

(in the biaxial box eigen-system)

$$0 = E\varepsilon_V + A\varepsilon_D$$

$$0 = A\varepsilon_V + B\varepsilon_D$$

Critical state flow – tensorial

(arbitrary eigen-system)

$$0 = E\varepsilon_V + A\varepsilon_D \cos\left(2\phi_\varepsilon - 2\phi_C\right)$$

$$0 = \left[A\varepsilon_V + \left(2B - E\right)\varepsilon_D \cos\left(2\phi_\varepsilon - 2\phi_C\right)\right]\hat{\mathbf{D}}\left(\phi_C\right) + \left(E - B\right)\varepsilon_D \hat{\mathbf{D}}\left(\phi_\varepsilon\right)$$

$$\delta\boldsymbol{\sigma}_D = A\varepsilon_V \hat{\mathbf{D}}\left(\phi_C\right) + \left(2G\right)\varepsilon_D \hat{\mathbf{D}}\left(\phi_\varepsilon\right) + \tfrac{1}{2}\left(C_1 + C_2 - 6G\right)\varepsilon_D \cos\left(2\phi_\varepsilon - 2\phi_C\right)\hat{\mathbf{D}}\left(\phi_C\right)$$