Micro-Macro transition –
(from particles to continuum theory)

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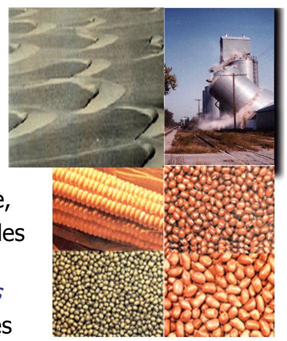
Granular Materials

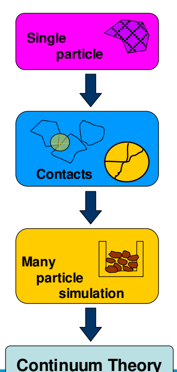


Real:
- sand, soil, rock,
- grain, rice, lentils,
- powder, pills, granulate,
- micro- and nano-particles

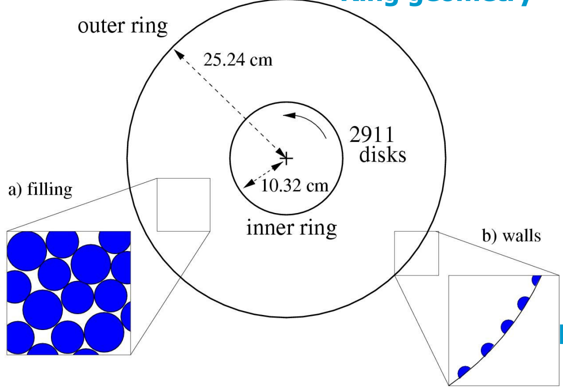
Model Granular Materials
- steel/aluminum spheres
- spheres with dissipation/friction/adhesion

Approach philosophy

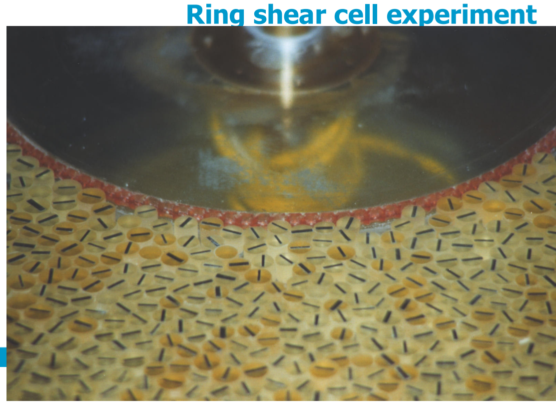
- Introduction
- Single Particles
- Particle Contacts/Interactions
- Many particle cooperative behavior
- Applications/Examples
- Conclusion

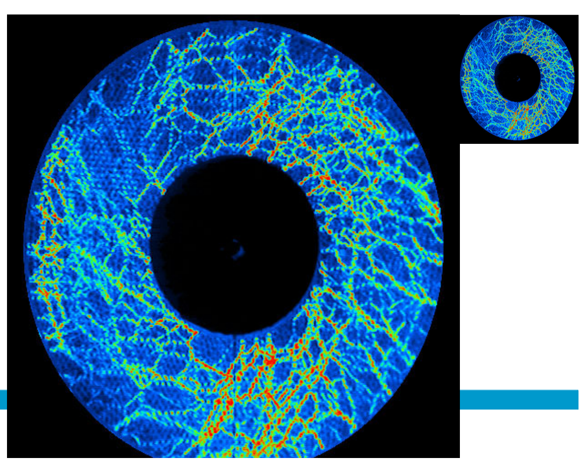


Ring geometry

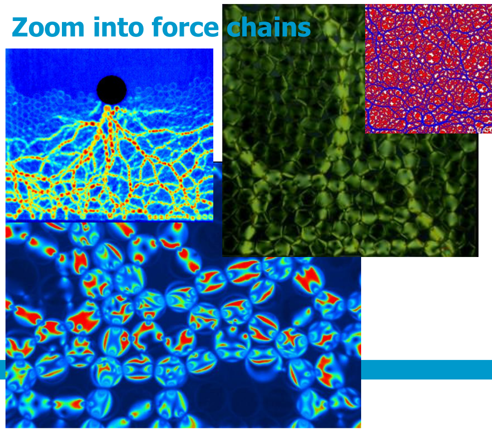


Ring shear cell experiment

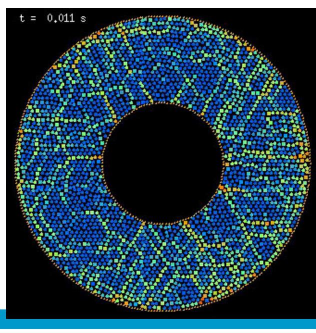




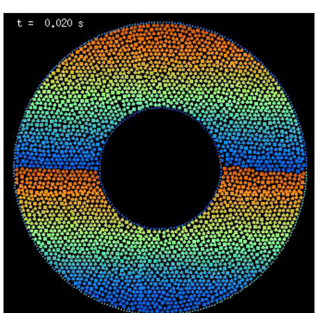
Zoom into force chains



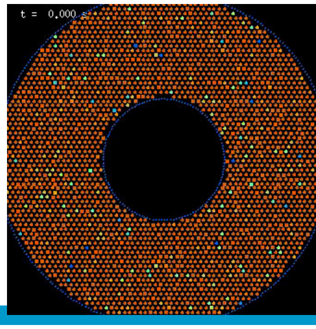
2D shear cell – force chains



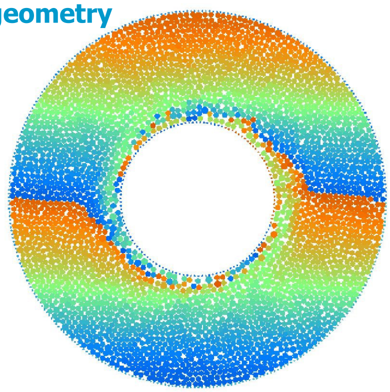
2D shear cell – shear band



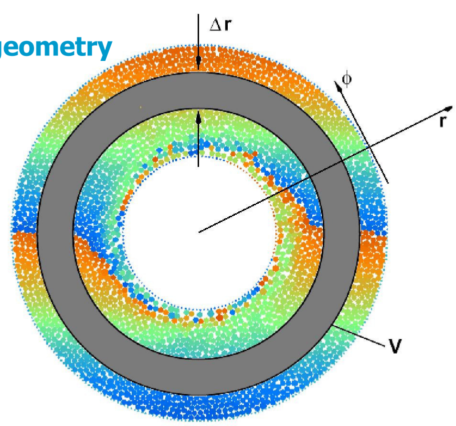
2D shear cell – energy



Ring geometry



Ring geometry



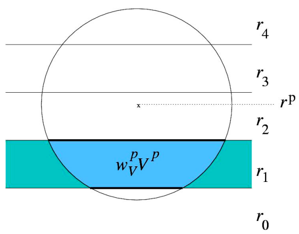
Averaging Formalism

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

Any quantity:

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

- Scalar
- Vector
- Tensor



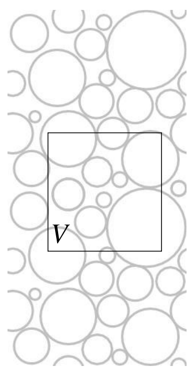
Averaging Formalism

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

Any quantity:

$$Q^p$$

In averaging volume: V



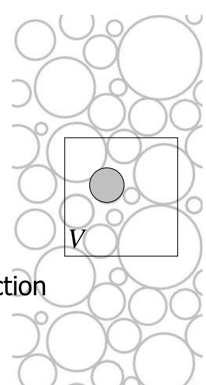
Averaging Density

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

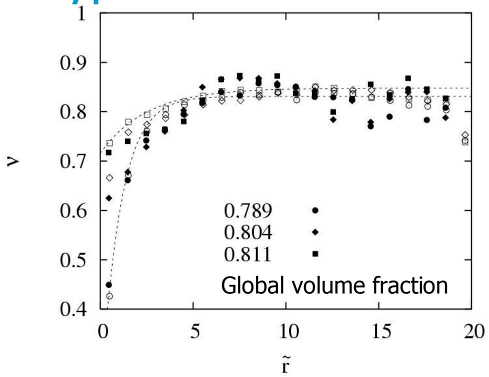
Any quantity:

$$Q^p = 1$$

- Scalar: Density/volume fraction



Density profile



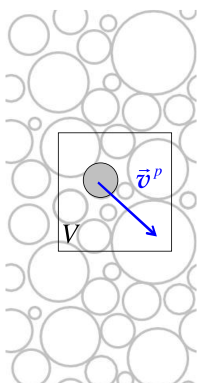
Averaging Velocity

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

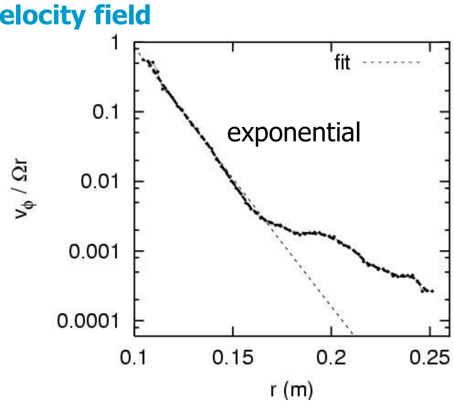
Any quantity:

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

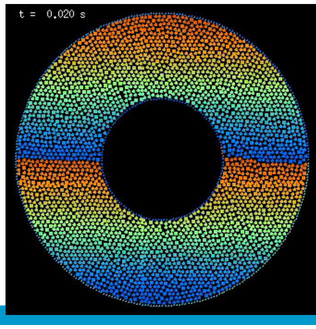
- Scalar
- Vector – velocity density



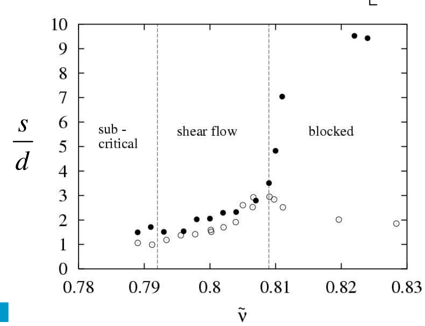
Velocity field



2D shear cell – shear band

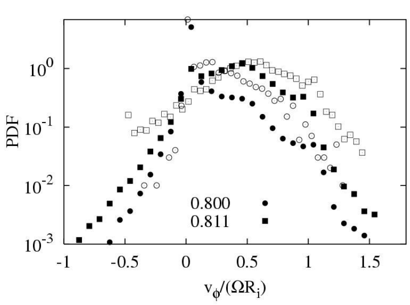


Velocity gradient $\nabla \mathbf{v} \rightarrow D_{r\phi} = \frac{1}{2}\left[\frac{\partial v_\phi}{\partial r} - \frac{v_\phi}{r}\right]$



exponential: $v_\phi(r) = v_0 \exp(-(r - R_i)/s)$

Velocity distribution



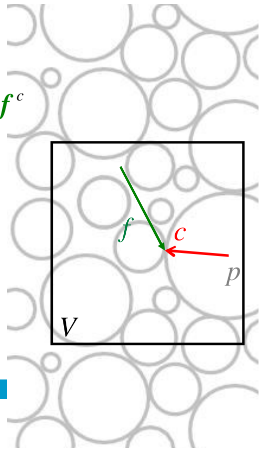
Averaging Stress

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

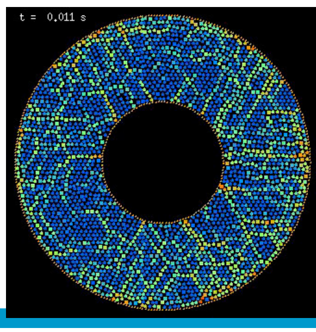
Any quantity:

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

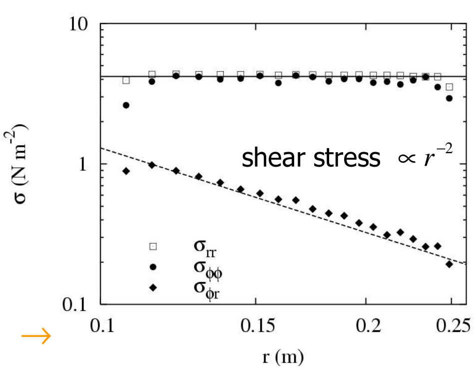
- Scalar
- Vector
- Tensor: Stress



2D shear cell – force chains

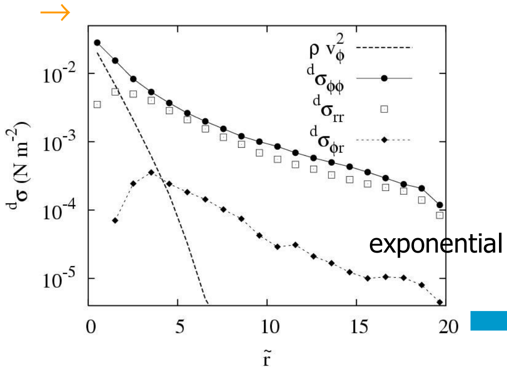


Stress tensor (static)

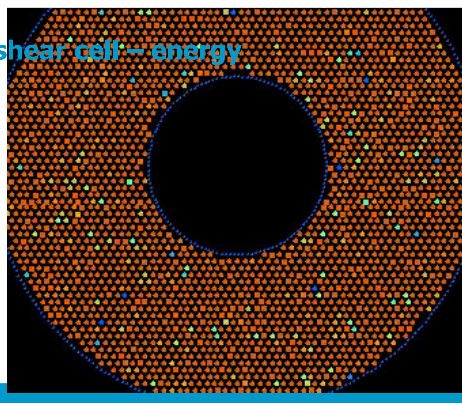


Stress tensor (dynamic)

$\rightarrow$



2D shear cell – energy



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

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

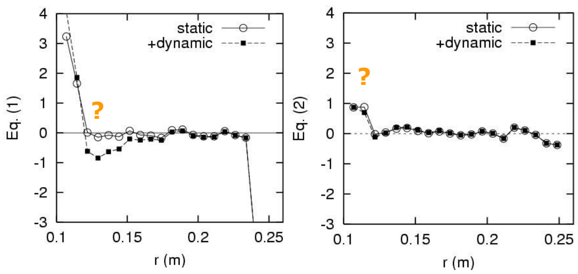
$$0 = r\frac{\partial \sigma_{r\phi}}{\partial r} + (\sigma_{r\phi}+\sigma_{\phi r}),$$

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

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

Stress equilibrium (2)

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



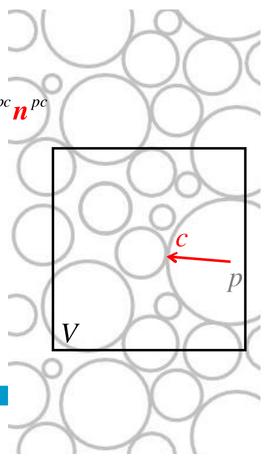
Averaging Fabric

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

Any quantity:

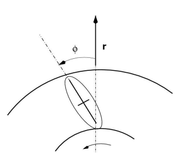
$$Q^p = \underline{\underline{\mathbf{F}}}^p = \sum_c \boldsymbol{n}^{pc}\boldsymbol{n}^{pc}$$

- Scalar: contacts
- Vector: normal
- Contact distribution



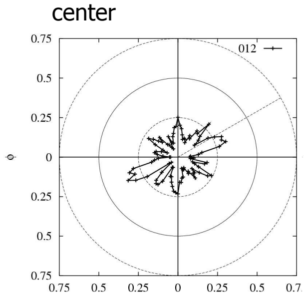
Fabric tensor

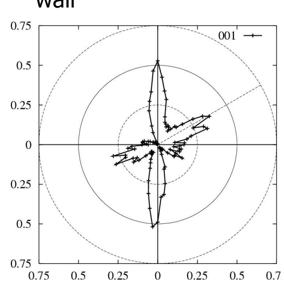
contact probability ...



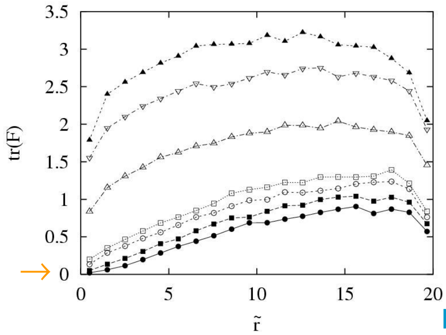
center

wall



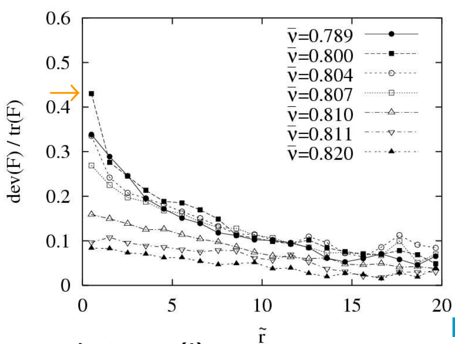


Fabric tensor (trace)



contact number density

Fabric tensor (deviator)



an-isotropy (!)

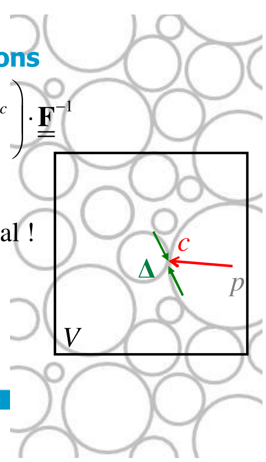
Averaging Deformations

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

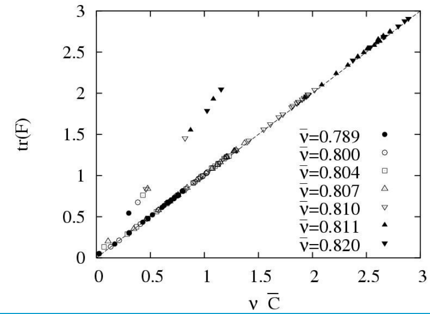
Deformation:

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

- Scalar
- Vector
- Tensor: Deformation

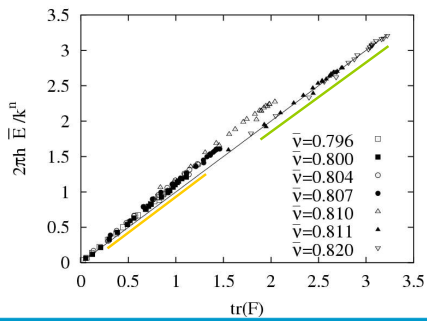


Macro (contact density)



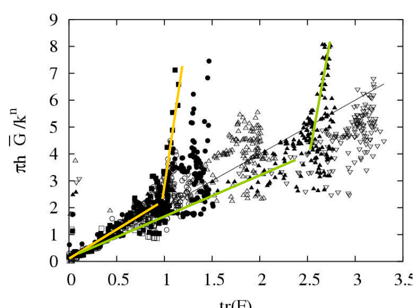
Macro (bulk modulus)

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



Macro (shear modulus)

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



Local micro-macro transition

From virtual work …
For each single contact …
⇒ Stress tensor **σ**
⇒ Stiffness matrix ***C*** (elastic)
- Normal contacts
- Tangential springs

Deformations (2D):
- Isotropic compression ε_V
- Deviatoric strain (=shear) ε_D, ϕ_ε

⇒ **Stress changes**
- Isotropic $\delta\sigma_V$
- Deviatoric $\delta\sigma_D$, ϕ_σ

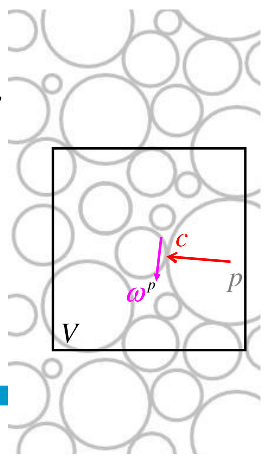
Averaging Rotations

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

Deformation:

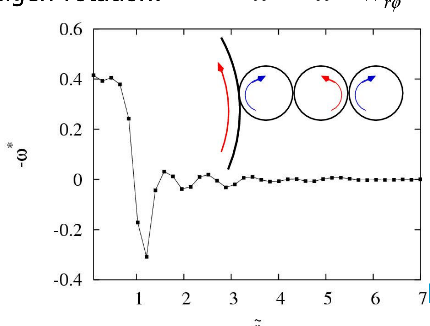
$$Q^p = \omega^p$$

- Scalar
- Vector: Spin density
- Tensor

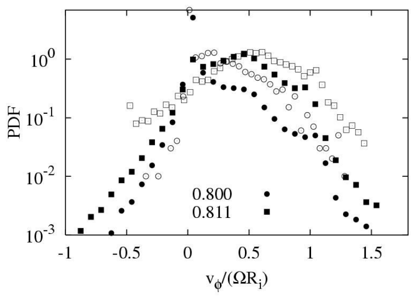


Rotations – spin density

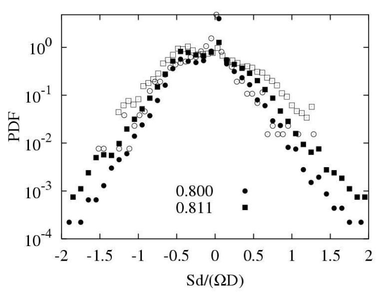
eigen-rotation: $\omega^* = \omega - W_{r\phi}$

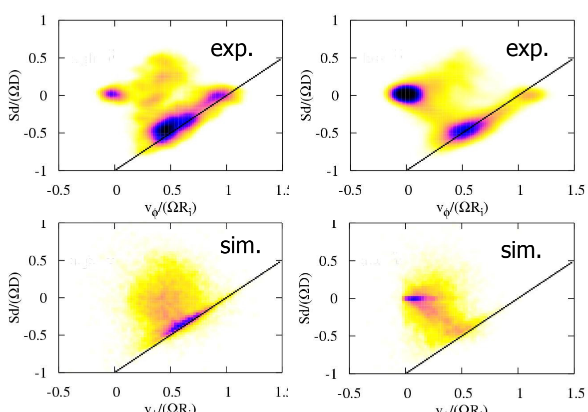


Velocity distribution



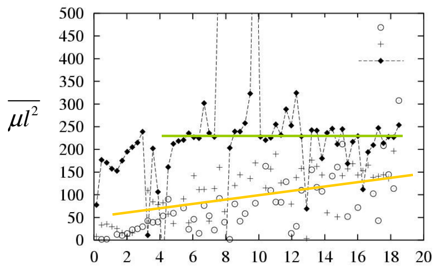
Spin distribution





Macro (torque stiffness)

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



Summary

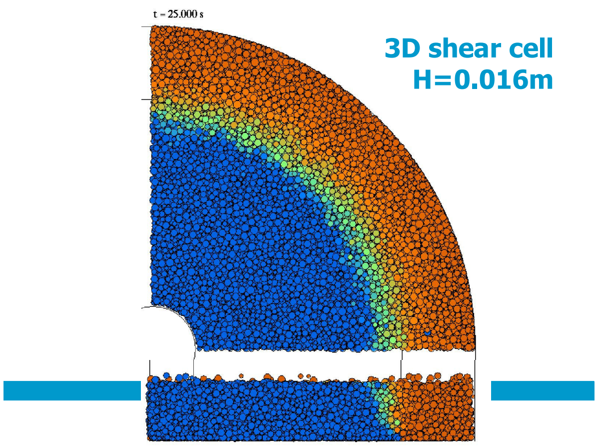
Quantitative comparison between
Experiments (2D Couette) &
MD simulations (soft disks)

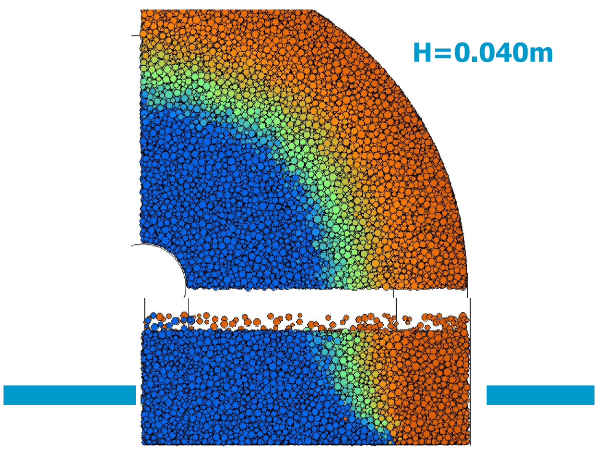
Observations:
- shear band & dilation
- inhomogeneous (force-chains)
- (almost always) an-isotropic
- micro-polar (rotations)

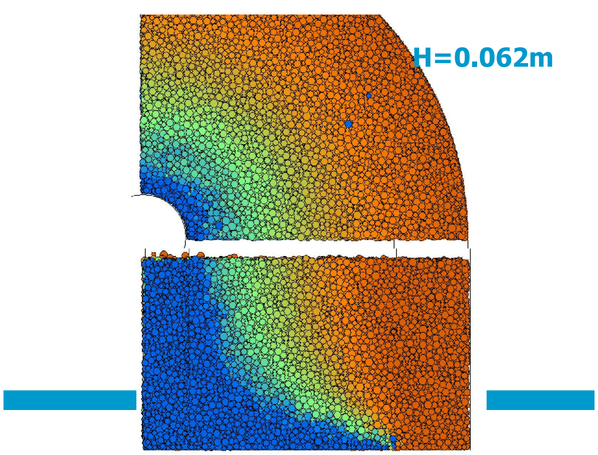
Conclusion

Qualitative agreement 100%
Subjective quant. agreement 50%-80%

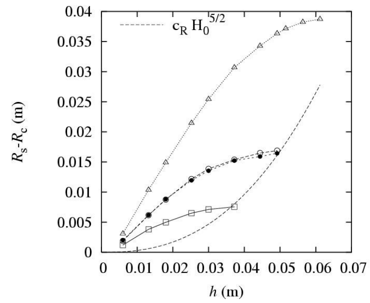
Reasons for discrepancy:
- idealized 2D disks vs. real disks
- idealized 2D motion vs. out-of-plane
- background friction (powder on base)
- small differences in geometry
- ...


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


H=0.040m

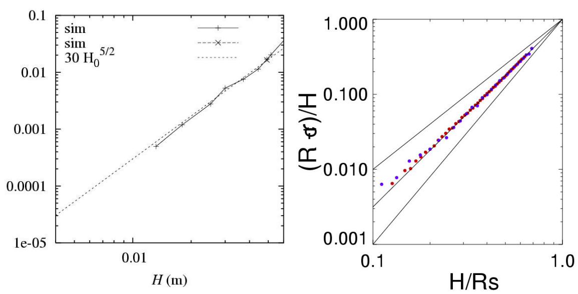

H=0.062m

3D shear band center position



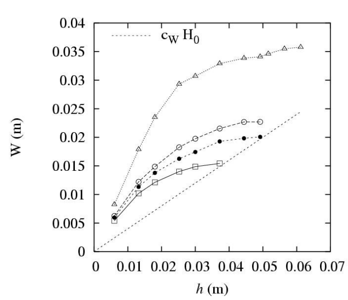
80% agreement … up to now

3D shear band center position



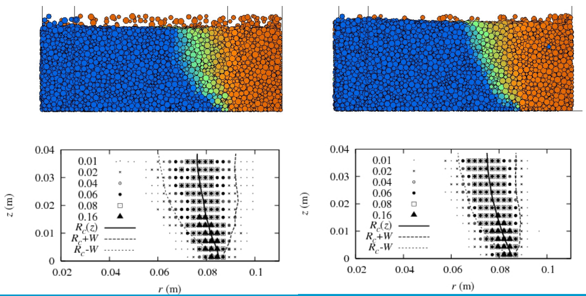
80% agreement … up to now

3D shear band width



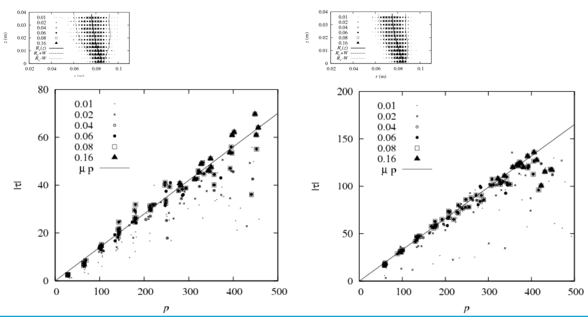
80% agreement … up to now

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



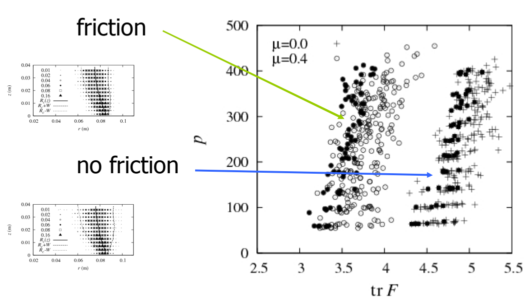
no friction | friction

Constitutive relations: Mohr-Coulomb



no friction | friction

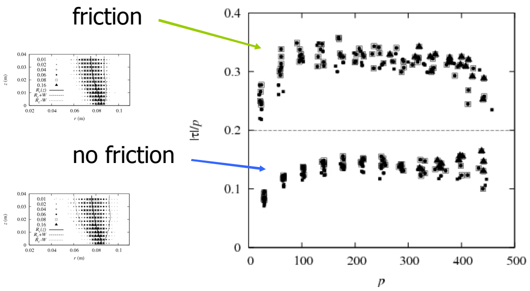
Constitutive relations: stress-structure



Constitutive relations: anisotropy

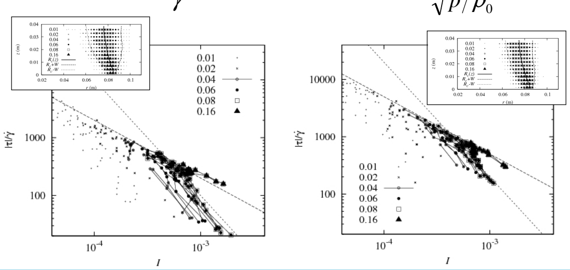
friction

no friction



Constitutive relations: shear softening

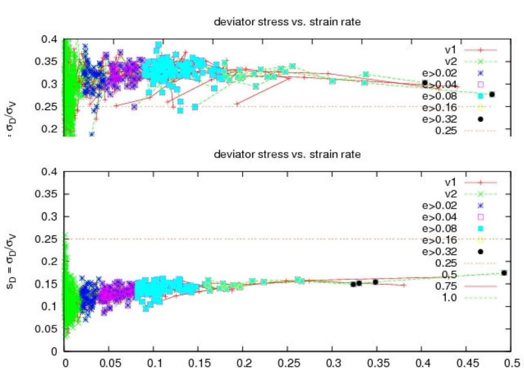
viscosity $\frac{|\tau|}{\dot{\gamma}}$ vs. shear rate $I = \frac{\dot{\gamma} d_0}{\sqrt{p/\rho_0}}$



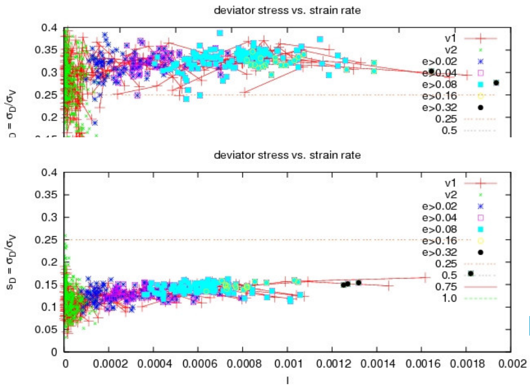
no friction

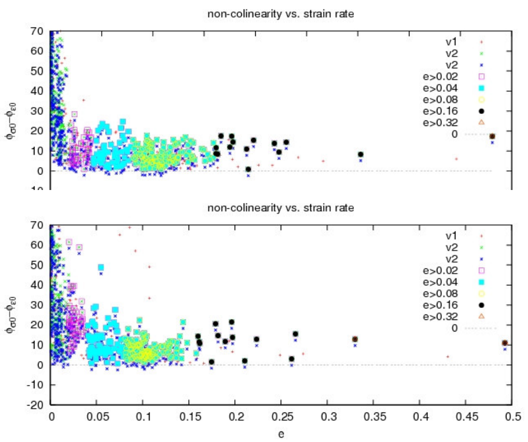
friction

stress ratio vs. shear rate



stress ratio vs. I

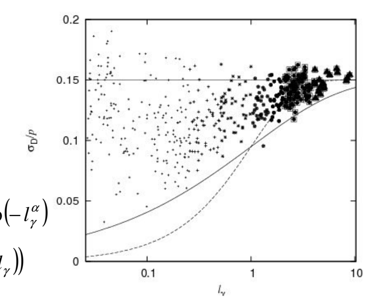




anisotropy vs. shear path

$$l_\gamma = \Delta t\,\dot{\gamma}$$

$$\mu \geq s_D(l_\gamma) \geq s_D^{\min}$$



$$s_D(l_\gamma) = \mu - (\mu - s_D^0)\exp(-l_\gamma^\alpha)$$

$$\frac{ds_D(l_\gamma)}{dl_\gamma} = \alpha l_\gamma^{\alpha-1}(\mu - s_D(l_\gamma))$$

3D Flow behavior – steady state shear

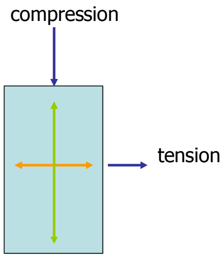
Obtain constitutive relations from one SINGLE simulation:

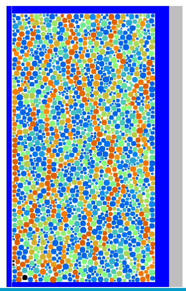
- **Mohr Coulomb yield stress**
- **shear softening viscosity**
- **compression/dilatancy …**
- **inhomogeneity (force-chains)**
- **(almost always) an-isotropy**
- **micro-polar effects (rotations) …**

The End

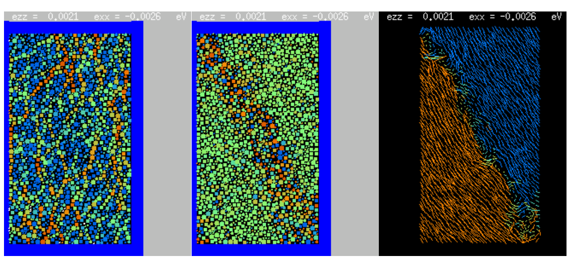
Anisotropy

Micro-macro for anisotropy – rheology





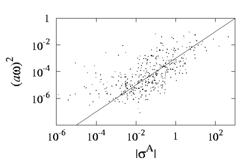
Micro informations: shear bands

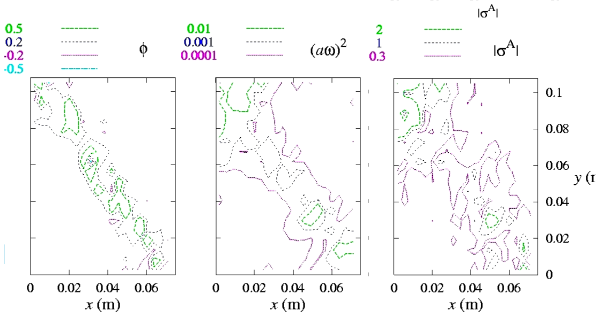


potential energy rotations displacements

Rotations (local)

Direction, amplitude,
anti-symmetric (!) stress

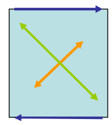




Anisotropy ↔ Shear ?

- Simple shear

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

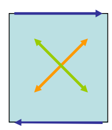


Rotation + symmetric shear

Anisotropy ↔ Shear ?

- Simple shear

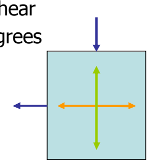
$$\varepsilon = \begin{pmatrix} 0 & 2\varepsilon_s \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & \varepsilon_s \\ -\varepsilon_s & 0 \end{pmatrix} + \begin{pmatrix} 0 & \varepsilon_s \\ \varepsilon_s & 0 \end{pmatrix}$$



Rotation + symmetric shear

- Rotate symmetric shear tensor by 45 degrees

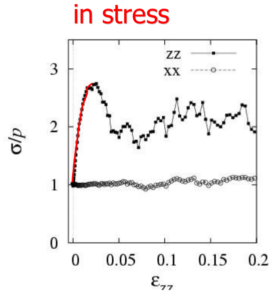
$$R_{45} \cdot \begin{pmatrix} 0 & \varepsilon_s \\ \varepsilon_s & 0 \end{pmatrix} \cdot R_{45}^T = \begin{pmatrix} \varepsilon_s & 0 \\ 0 & -\varepsilon_s \end{pmatrix}$$



- Biaxial “shear”: compression+extension

An-isotropy

in stress



An-isotropy (Stress)

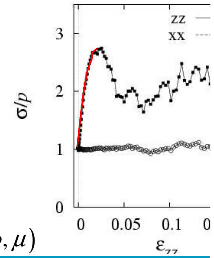
- Stress: Isotropic: $\mathrm{tr}\,\boldsymbol{\sigma}$, and deviatoric: $\mathrm{dev}\,\boldsymbol{\sigma} = \boldsymbol{\sigma}_{zz}-\boldsymbol{\sigma}_{xx}$
  - Minimal eigenvalue: $\boldsymbol{\sigma}_{xx}$
  - Maximal eigenvalue: $\boldsymbol{\sigma}_{zz}$
- Dev. Stress fraction $s_D = \mathrm{dev}\,\boldsymbol{\sigma}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

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

- Exponential approach to peak

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

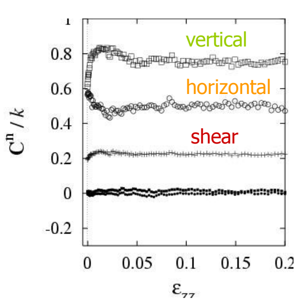
$$\beta_s\left(\rho, p, \mu\right)$$

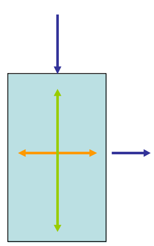


An-isotropy (Stress)

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

Stiffness tensor





Different moduli:

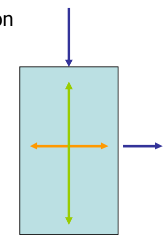
- against shear C_2
- perpendicular C_1
- *one* shear modulus

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)

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

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

Mechanical waves in sand, 3D simulations

O. Mouraille, S. Luding

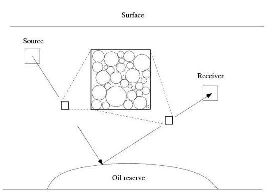
Particle Technology, NSMm TUDelft, NL

Thanks for discussions : E. Grekova, G. Herman, W. Mulder, A. Suiker, …

Content

- Motivation
- The numerical method
- Some 3D-simulation results
- Conclusions and Perspectives

Why ?



Soil investigations

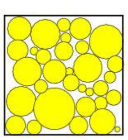
- Generally only 30% to 35% of the oil contained in a reservoir is extracted.

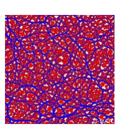
- How to take into account the complexity of granular material in the wave propagation theory ?

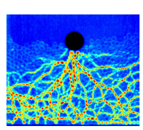
- What about rotations ?

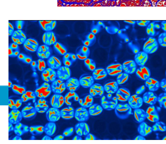
Framework

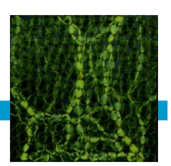
- Assembly of grains (**dense**, frictional and non-cohesive)
- Compressional (P)-wave, shear (S)-wave, (**R-wave** ?)
- Forces transmission, friction, **rotations**
- **3D** simulations (DEM)
- **Micro-Macro** theory



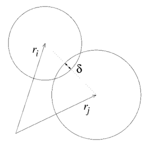








Discrete element method



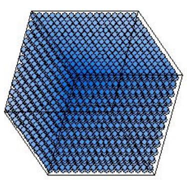
The equation of motion is solved for each particle according to the contact forces and torques.

Linear contact model

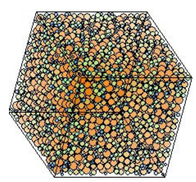
- *Normal part :* $f = k_N \delta$ ***repulsive*** and *attractive* forces (**dissipation**)
- *Tangential part :* ***Sliding*** **-(*k_T*)**, *Rolling-* and *Torsion-* resistance
  μ: friction coefficient

Model systems

Crystal structured packing

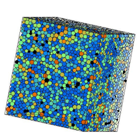


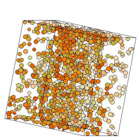
Poly-disperse packing

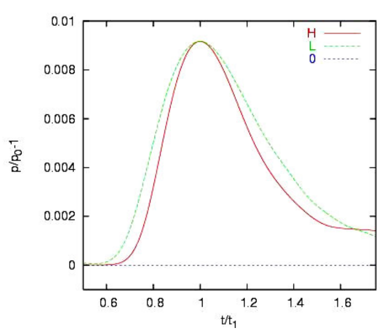


Different boundary conditions: with walls / periodic

Sound



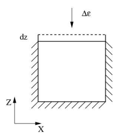




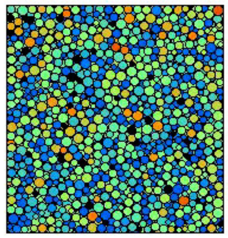
P-wave shape and speed

Stefan Luding, s.luding@tnw.tudelft.nl
Particle Technology, DelftChemTech, Julianalaan 136, 2628 BL Delft

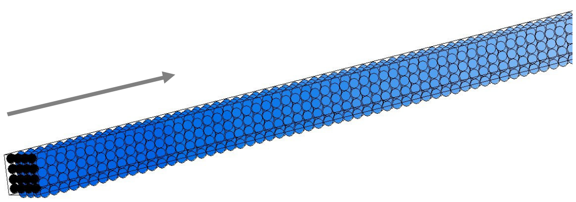
P-wave animation



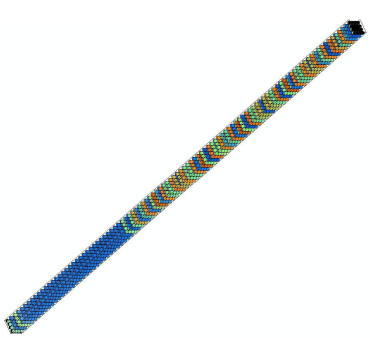
- Smooth wall motion
- Fixed side walls



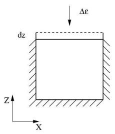
System 0: regular lattice $\Delta a=0$



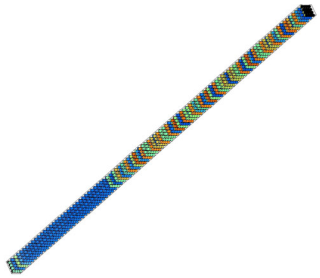
P-wave animation



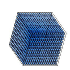
P-wave animation – regular packing

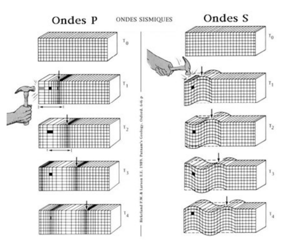


- one layer is shifted
- periodic boundaries
- black particles are fixed

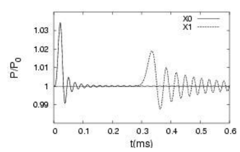


P- and S-wave

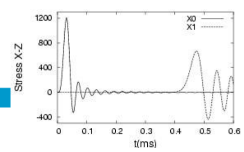




Compressive (P)-wave



Shear (S)-wave



Stiffness tensor

From the micro-macro transition theory we can derive "a" stiffness tensor:

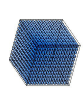
$$C_{\alpha\beta\gamma\varphi} = \frac{1}{V}\sum_{p\in V} a^2 \left(k \sum_{c=1}^{C} n_\alpha^c n_\beta^c n_\gamma^c n_\varphi^c + k^t \sum_{c=1}^{C} n_\alpha^c t_\beta^c n_\gamma^c t_\varphi^c \right)$$

Stiffness tensor of the regular packing

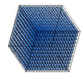
Dimensionless tensor (only structure dependent)

$$\tilde{C} = C\frac{V}{ka^2}$$

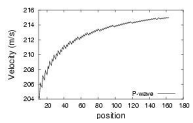
$$\tilde{C}_{1111} = \tilde{C}_{2222} = 2.5$$
$$\tilde{C}_{3333} = 2$$
$$\tilde{C}_{1133} = \tilde{C}_{2233} = \tilde{C}_{1313} = \tilde{C}_{2323} = 1$$
$$\tilde{C}_{1122} = \tilde{C}_{1212} = 0.5$$

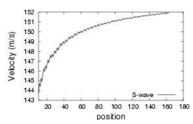


Waves and stiffnesses



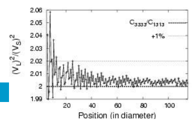
- Components of the stiffness tensor corresponding to the direction of particle-motion for both P- and S-wave
- In this case : C_{3333} for the P-wave and C_{1313} for the S-wave.
- *V_p and V_s denote the "Peak velocity".*





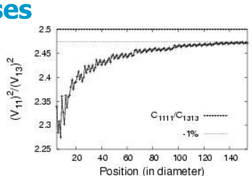
Theory : $\rho V_p^2 \propto C_{3333}$ $\rho V_s^2 \propto C_{1313}$

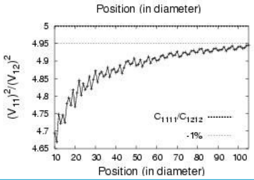
$$\frac{V_p^2}{V_s^2} \rightarrow \frac{C_{3333}}{C_{1313}}$$



Waves and stiffnesses

Ratios of C entries		Ratios of velocities	
$\frac{C_{1111}}{C_{1313}}$	2.5	$\left(\frac{V_{11}}{V_{13}}\right)^2$	≅ 2.475
$\frac{C_{3333}}{C_{1313}}$	2	$\left(\frac{V_{33}}{V_{13}}\right)^2$	≅ 2.005
$\frac{C_{1111}}{C_{1212}}$	5	$\left(\frac{V_{11}}{V_{12}}\right)^2$	≅ 4.95

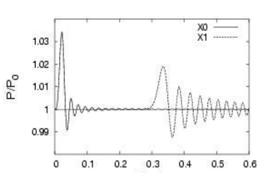




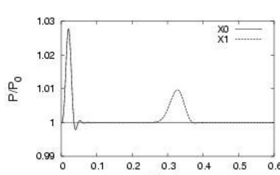
Compressive (P)-wave

Influence of "micro" properties

Elastic

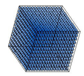


Visco-Elastic

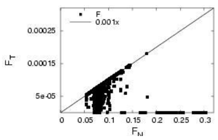


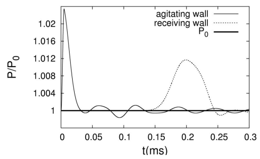
How relevant is the damping coefficient in our model ?

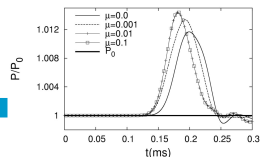
P-wave in a regular packing



- Simulations varying the friction coefficient μ
- Stick and slip contacts in the packing

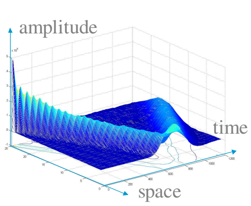


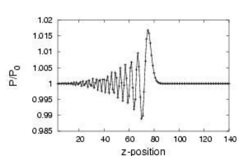


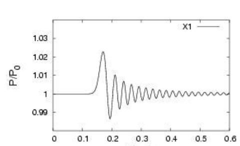


Space-Time analysis

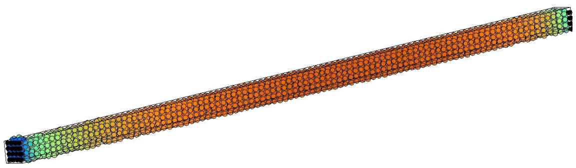
Space-Time analysis



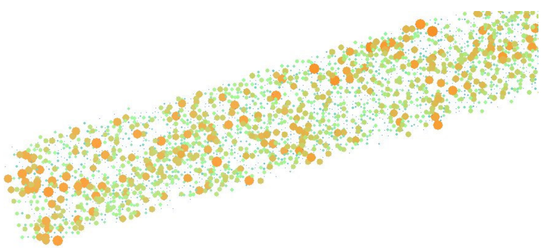




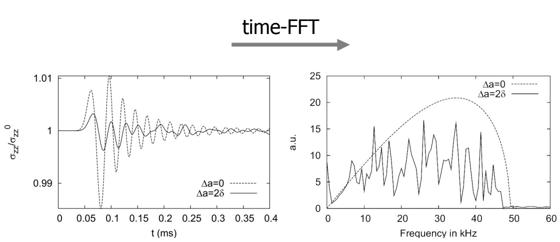
+polydispersity $\Delta a>0$



Contacts (force intensity)

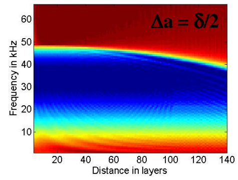


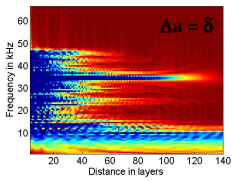
Signal Analysis

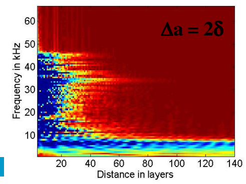


Stress-time signal Power-spectrum

Frequency-space Diagrams

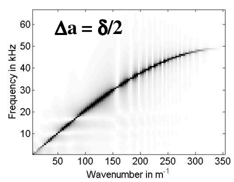


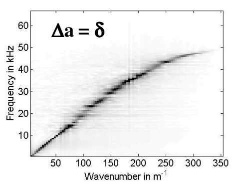


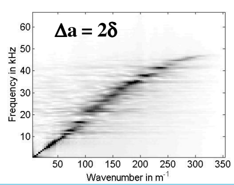


Dispersion relations

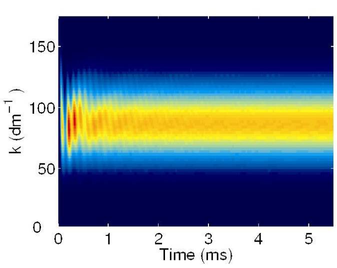
space-time-FFT



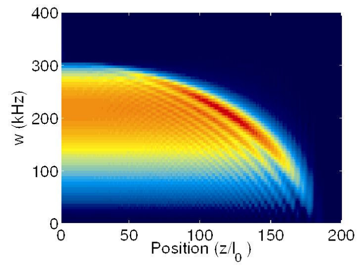




Space-Time analysis – space Fourier transform

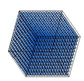


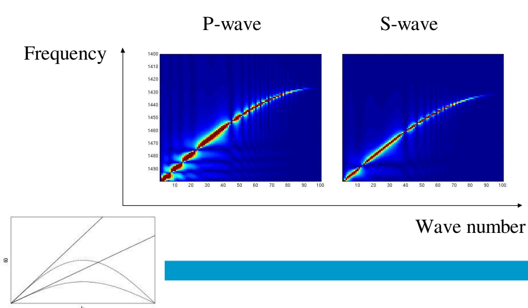
Space-Time analysis
– time Fourier transform



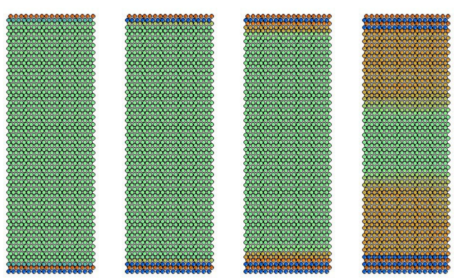
Dispersion relation

-Compressive and shear wave
- Small amplitude
- Regular packing





Rotation waves ?



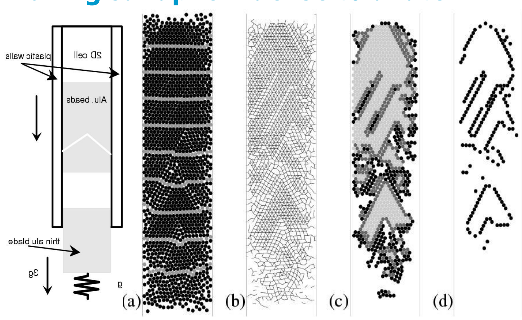
Conclusions

- The signal reveals structure- and state-changes in the packing
- Larger friction increases the velocity
- The wave gets broader and accelerates while propagating
- The wave velocity is directly related to the corresponding stiffness
- Rotational waves ?
- **The model captures the particle systems interesting features**

Perspectives

- Local (point) perturbation (Greens function): spherical waves
- Further study of rotations, and their possible propagation

Falling sandpile – dense to dilute



Rotational order