Molecular Dynamics for Experts

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Granular Materials

Real:

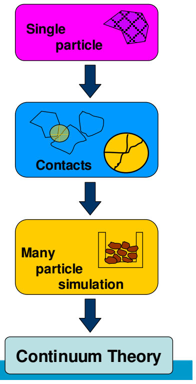
- sand, soil, rock,
- grain, rice, lentils,
- powder, pills, granulate,
- micro- and nano-particles

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



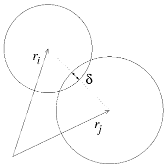
Single particle

Contacts

Many particle simulation

Continuum Theory

Discrete particle model

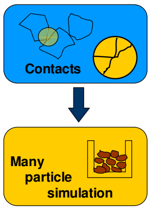


Equations of motion

$$m_i \frac{d^2\vec{r}_i}{dt^2} = \vec{f}_i$$

Forces and torques:

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



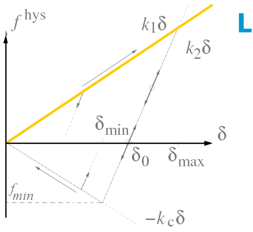
Contacts

Many particle simulation

Contact if Overlap > 0

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

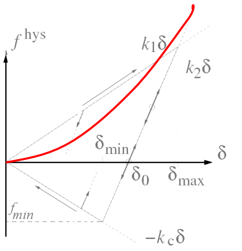
Normal $\hat{n} = \vec{n}_{ij} = \frac{\left(\vec{r}_i - \vec{r}_j\right)}{\left|\vec{r}_i - \vec{r}_j\right|}$



Linear Contact model

- (really too) simple ☺
- linear
- very easy to implement

$$f_i^{hys} = \begin{cases} k_1\delta & \text{for un-/re-loading} \\ & \\ & \end{cases}$$

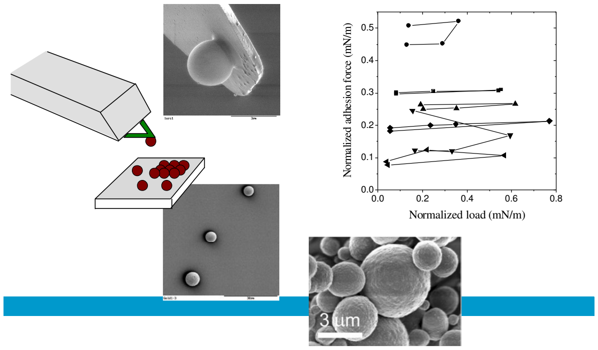


Hertz Contact model

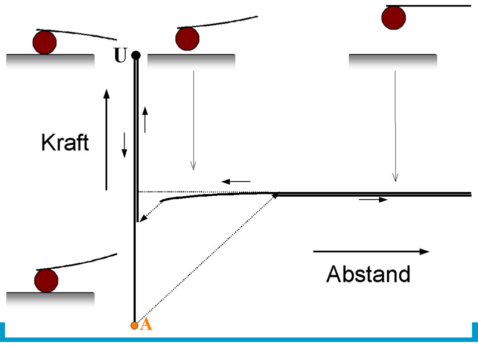
- simple ☺
- non-linear
- easy to implement

$$f_i^{hys} = \begin{cases} k_1\delta^{3/2} & \text{for un-/re-loading} \\ & \\ & \end{cases}$$

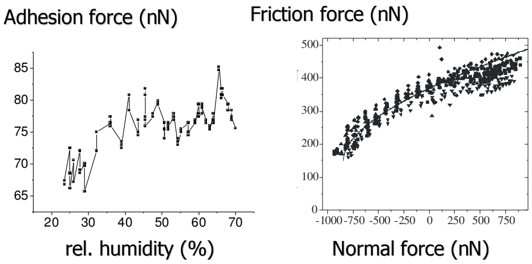
Contact force measurement (PIA)



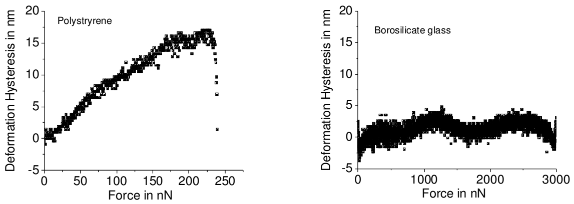
Contact Force Measurement



Adhesion and Friction



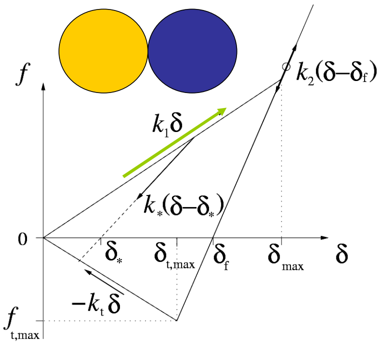
Hysteresis (plastic deformation)



Collaborations:
MPI-Polymer Science (Butt et al.)
Contact properties via AFM

Contacts

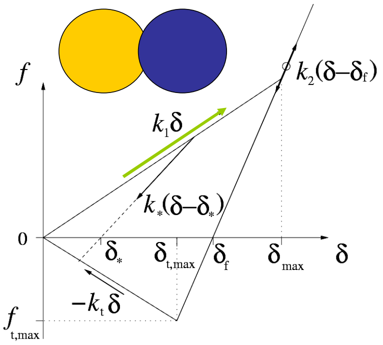
1. loading



Contacts

1. loading

plastic loading stiffness: k_1



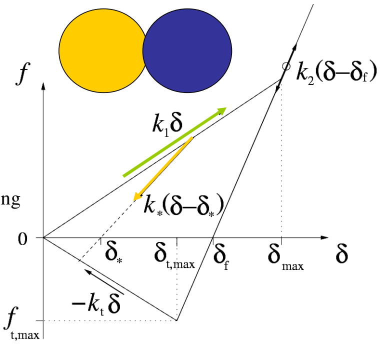
Contacts

1. loading

plastic loading stiffness: k_1

2. unloading

elastic un/re-loading stiffness: k_*



Contacts

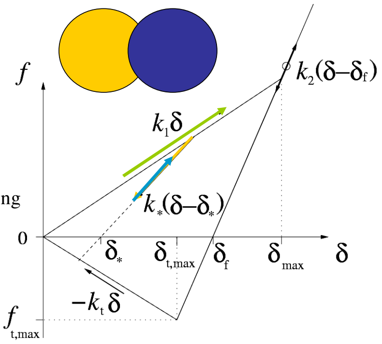
1. loading

plastic loading stiffness: k_1

2. unloading

3. re-loading

elastic un/re-loading stiffness: k_*



Contacts

1. loading

plastic loading stiffness: k_1

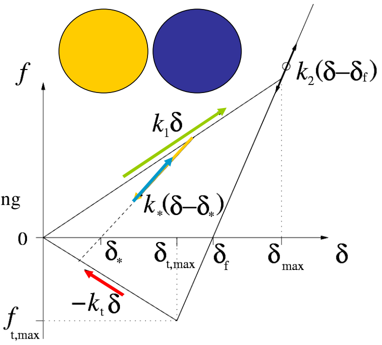
2. unloading

3. re-loading

elastic un/re-loading stiffness: k_*

4. tensile failure

tensile force



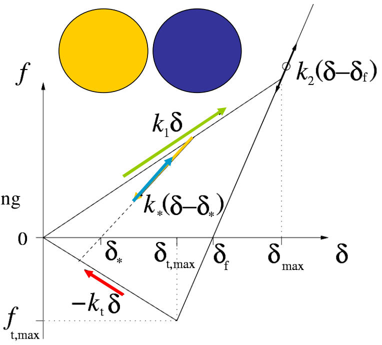
Contacts

1. loading
plastic loading stiffness: k_1

2. unloading

3. re-loading
elastic un/re-loading stiffness: k_*

4. tensile failure
tensile force



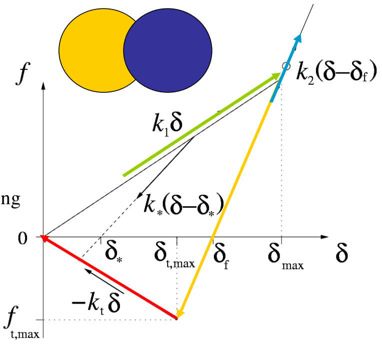
Contacts

1. loading
transition to stiffness: k_2

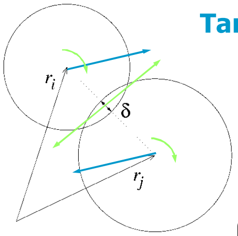
2. unloading

3. re-loading
elastic un/re-loading stiffness: k_2

4. tensile failure
max. tensile force



Tangential contact model



***Sliding* contact points:**
- Static Coulomb friction
- Dynamic Coulomb friction

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

Tangential contact model

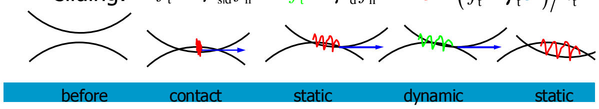
- Static friction	- spring
- Dynamic friction	- dashpot

project into tangential plane $\vartheta' = \vartheta - \hat{n}(\hat{n} \cdot \vartheta)$

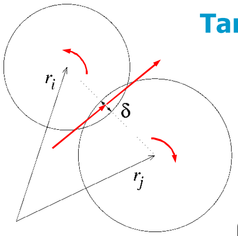
compute test force $f_\mathrm{t}^0 = -k_\mathrm{t}\vartheta' - \gamma_\mathrm{t}\dot{\vartheta}'$ and $\hat{t} = f_\mathrm{t}^0 / |f_\mathrm{t}^0|$

sticking: $f_\mathrm{t}^0 \le \mu_\mathrm{s} f_\mathrm{n}$ $\quad f_\mathrm{t} = f_\mathrm{t}^0$ $\quad \vartheta = \vartheta' + \dot{\vartheta}' \,\mathrm{d}t$

sliding: $f_\mathrm{t}^0 > \mu_\mathrm{s|d} f_\mathrm{n}$ $\quad f_\mathrm{t} = \mu_\mathrm{d} f_\mathrm{n} \hat{t}$ $\quad \vartheta = (f_\mathrm{t} + \gamma_\mathrm{t}\dot{\vartheta}') / k_\mathrm{t}$



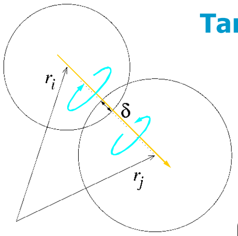
Tangential contact model



Rolling **(mimic roughness or steady contact necks)**
- **Static rolling resistance**
- **Dynamic resistance**

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

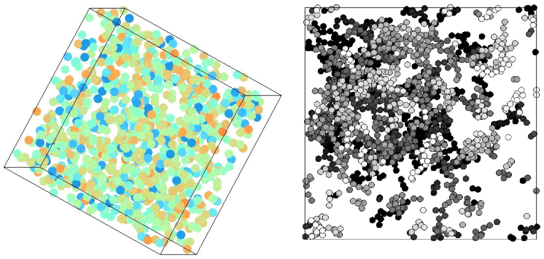
Tangential contact model



Torsion **(large contact area)**
- **Static torsion resistance**
- **Dynamic resistance**

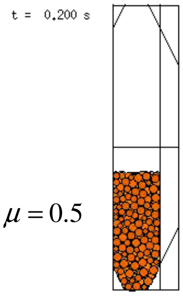
$$v_\mathrm{t} = \begin{cases} (v_i - v_j)^\mathrm{t} + \hat{n} \times (a_i\omega_i + a_j\omega_j) & \text{sliding} \\ a_{ij}\hat{n} \times (\omega_i - \omega_j) & \text{rolling} \\ a_{ij}\hat{n}\hat{n} \cdot (\omega_i - \omega_j) & \text{torsion} \end{cases}$$

… Details of interaction

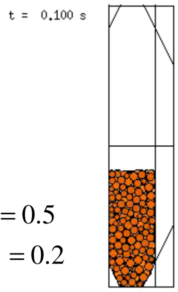


Attraction + Dissipation = Agglomeration

Silo Flow with friction

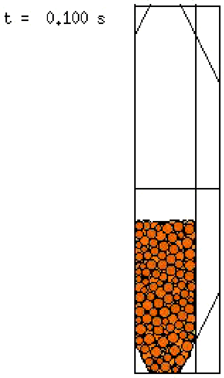


$\mu = 0.5$



$\mu = 0.5$

$\mu_r = 0.2$



$\mu = 0.5$

$\mu_r = 0.2$

Biaxial box set-up

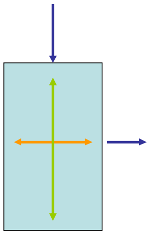
- Top wall: strain controlled

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

- Right wall: stress controlled

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

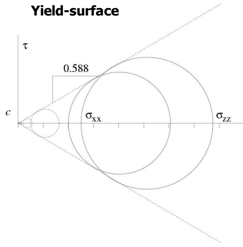
- Evolution with time … ?

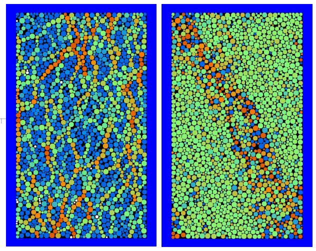


Material behavior of granular media

Non-Newtonian Flow behavior under slow shear

Yield-surface





inhomogeneity **rotations**

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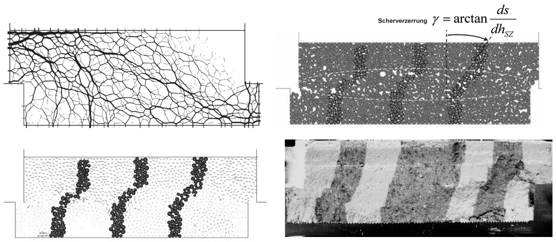
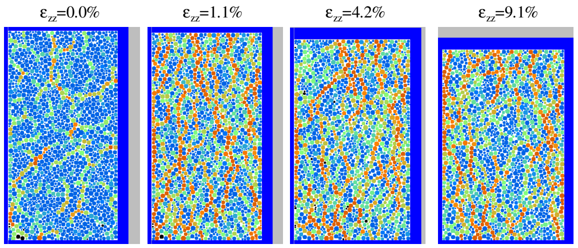
Jenike cell PFC2D



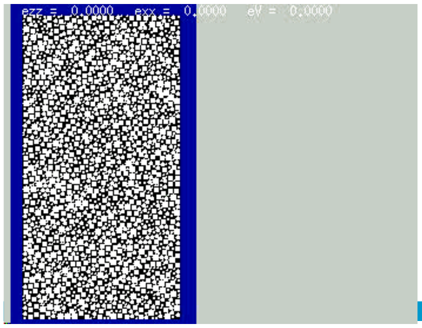
Scherverzerrung $\gamma = \arctan \frac{ds}{dh_{SZ}}$

Collaborations:
Cohesive very fine powders, MVT (Tomas)
…

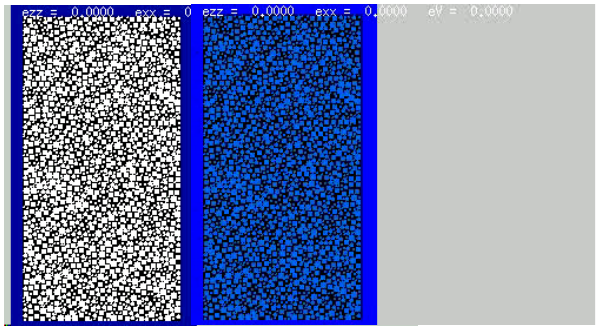
Simulation results (closer look)



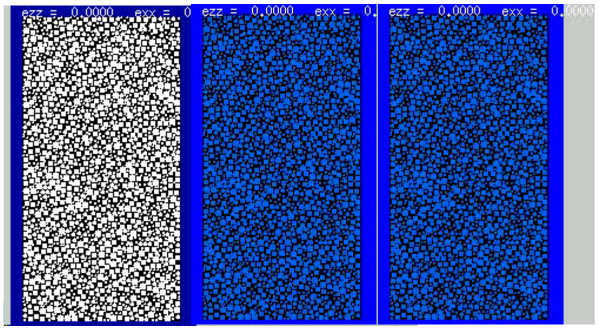
Bi-axial box (stress chains)



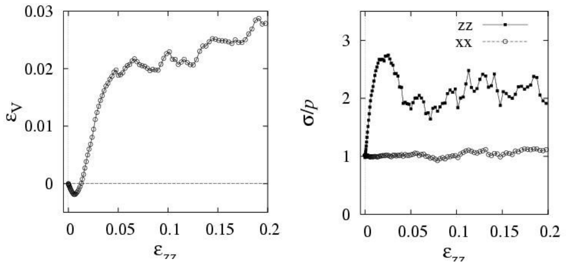
Bi-axial box (kinetic energy)



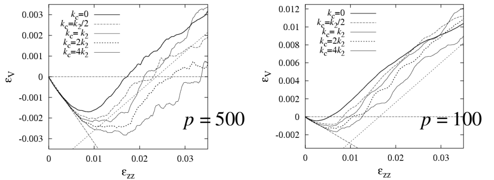
Bi-axial box (rotations)



Bi-axial compression with p_x=const.



Material parameters



Initial Compression:

$$\frac{\varepsilon_v}{\varepsilon_{zz}} = \tan^{-1}(1-2\nu)$$

Poisson-ratio: $\nu \approx 0.66$

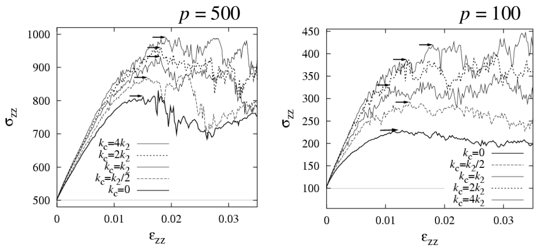
Dilatancy: $d' = \tan^{-1}\left(\frac{2\sin\psi}{1-\sin\psi}\right)$

Dilatancy Angle:

$\psi \approx 0.088$ **for** $p = 500$

$\psi \approx 0.190$ **for** $p = 100$

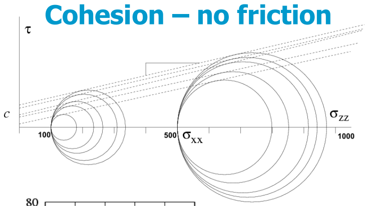
Young modulus and yield stress



Young's Modulus
(initial slope)

Yield Stress ....
(peak value)

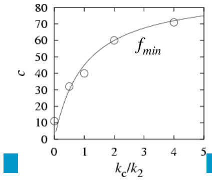
Cohesion – no friction



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

geometrical friction angle

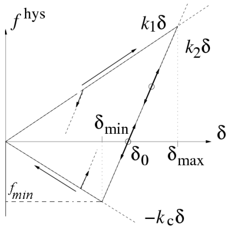
$\phi \approx 13^\circ$



macro cohesion

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

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



Contact model

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

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

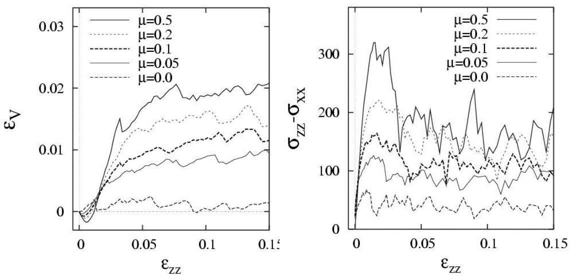
Maximum overlap $\delta_{\max}$

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

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

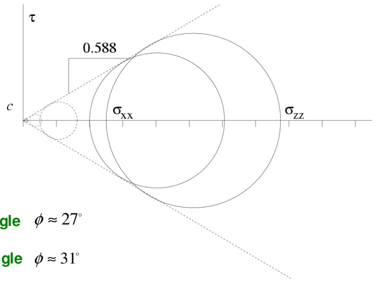
the max. attractive force: $f_{\min} = -k_c\delta_{\min}$

Bi-axial: p_x=200 – varying friction



Friction – no cohesion

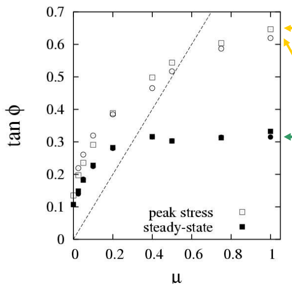
k_c = 0 and μ = 0.5



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

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

Bi-axial: p_x=200 – varying friction



prepared μ=0

prepared μ=0.5

steady-state shear

Open questions

- Quantitative experimental verification
  - Micro-/Nano Flows for polymers, nano-materials, …
- Main challenges
  - micro-macro transition & constitutive modeling

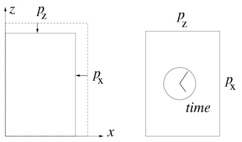
Open questions

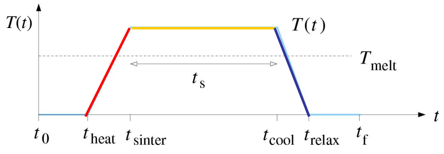
- Collective flow behavior (Rheology)
  - Size distributions (nano-micro-macro)
  - Friction/Cohesion/Shape effects
  - Size dependent properties (heat, conductivity)
  - Micro-polar (rotations) continuum theory

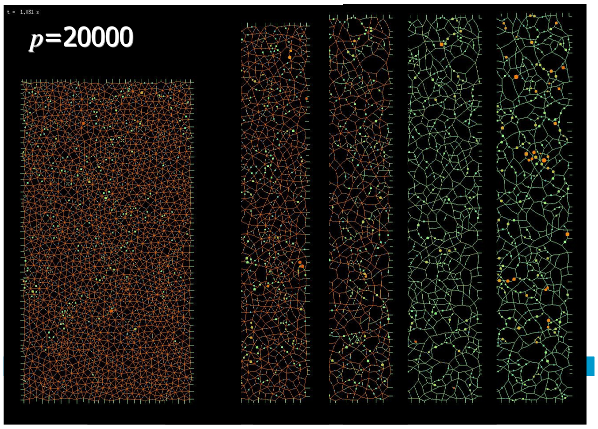
Collaborations:
ICP (Herrmann), DIGA, MVT
…

Sintering (pressure and temperature)

1. **Preparation**
2. **Heating**
3. **Sintering**
4. **Cooling**
5. **Relaxation**
6. **Testing**



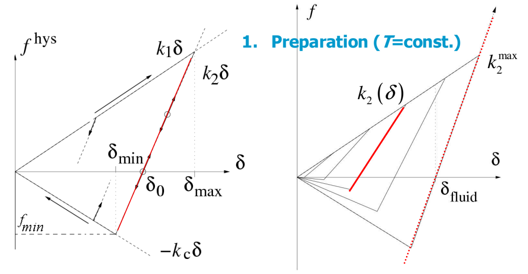




Open questions

- Understanding the collective behavior
  - Size distributions (nano-micro-macro)
  - Composite Material properties
  - Size dependent properties (heat, conductivity)
  - Self-Healing properties via nano-particles (ν-bots)

Sintering – cold contacts



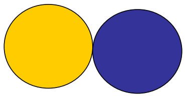
1. **Preparation (*T*=const.)**

loading stiffness: $k_1 = k_1(T)$

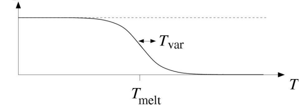
contact stiffness: $k_2 = k_2(\delta)$

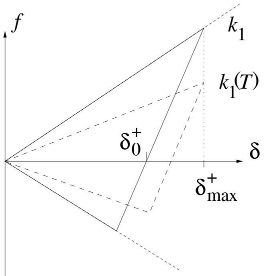
Sintering 2

2. Heating



loading stiffness: $k_1 = k_1(T)$



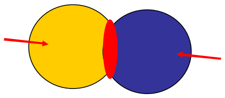


maximum overlap fixed: $\delta_{\max}^+$

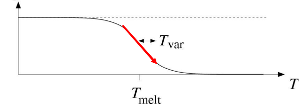
neutral overlap increasing: δ_0^+

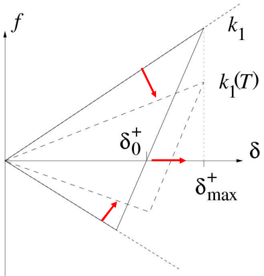
Sintering 2

2. Heating



loading stiffness: $k_1 = k_1(T)$



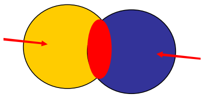


maximum overlap fixed: $\delta_{\max}^+$

neutral overlap increasing: δ_0^+

Sintering 3

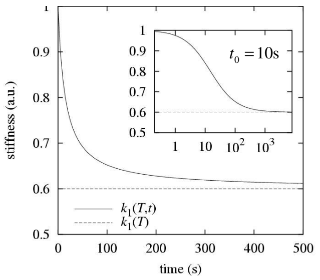
3. Sintering



Sintering 3

3. Sintering

- slow dynamics (t_0)
- diffusion, …
- trick: increase t_0

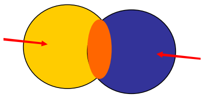


time delay:

$$\frac{\partial}{\partial t} k_1(T,t) = \pm \frac{\left[k_1(T) - k_1(T,t)\right]^2}{k_1(T)\, t_0} \qquad k_1(T,t) = k_1(T)\left\{1 - \left(\frac{1}{1 - k_1(T_0)/k_1(T)} - \frac{t}{t_0}\right)^{-1}\right\}$$

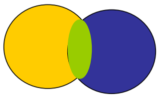
Sintering 4

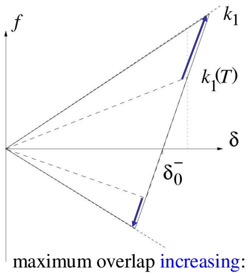
4. Cooling



Sintering 4

4. Cooling



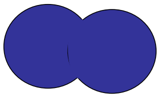


maximum overlap increasing: $\delta_{\max}^-$

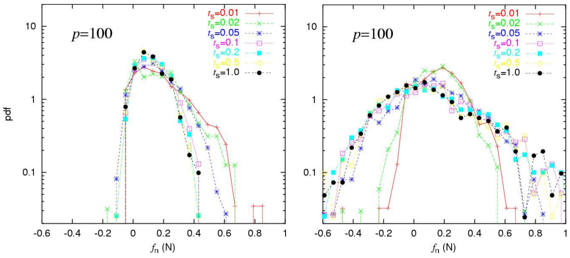
neutral overlap fixed: δ_0^-

Sintering 5

5. **Relaxation**



Contact forces

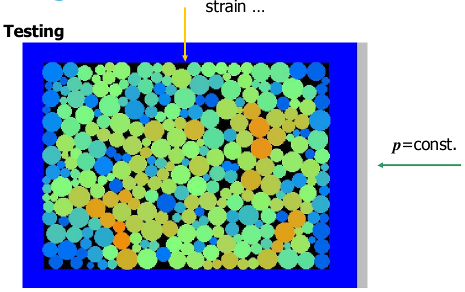


after Sintering

after Relaxation

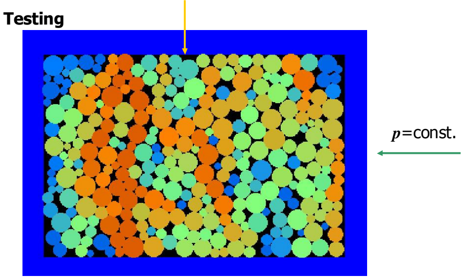
Sintering 6

6. **Testing**



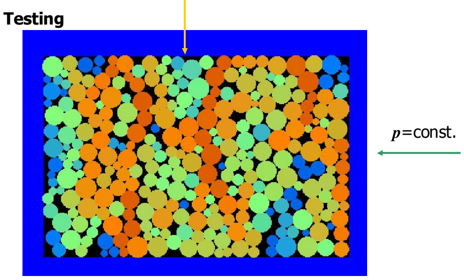
Sintering 6

6. **Testing**



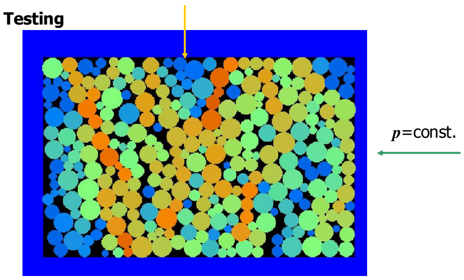
Sintering 6

6. **Testing**



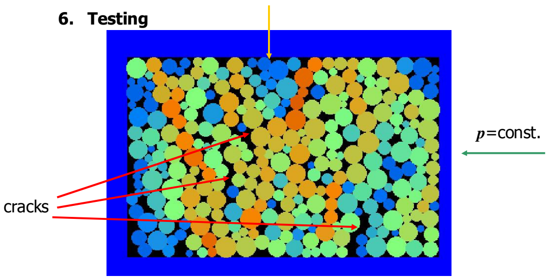
Sintering 6

6. **Testing**



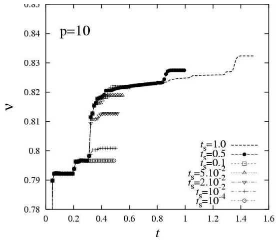
Sintering 6

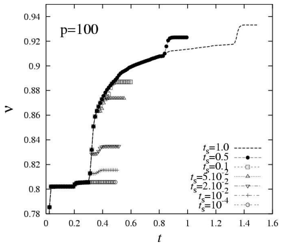
6. Testing



Sintering 6

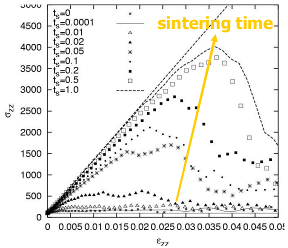
Density – Shrinkage!



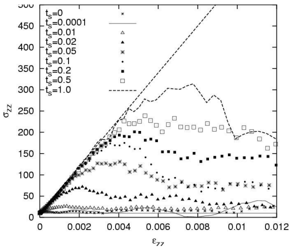


Sintering 6

Stiffness …



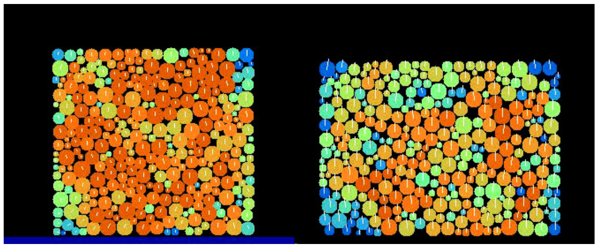
p=100



p=10

Sintering 7

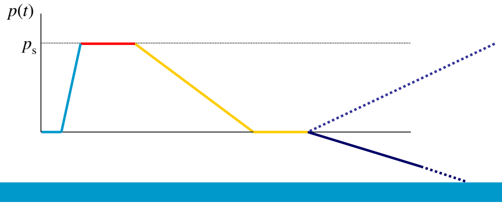
7. **Vibration test**



p=100 p=10

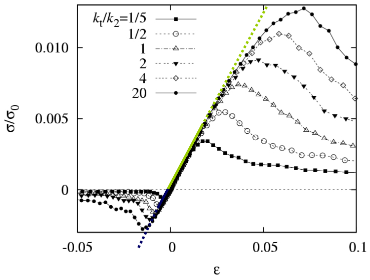
PCT (pressure-compression-tension)

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



uni-axial compression-tension

- **Compression**
- **Tension**



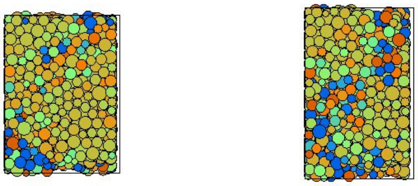
compression - uni-axial

$k_t / k_2 = 1/2$

compression - uni-axial

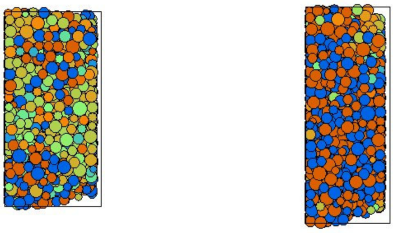
$k_t / k_2 = 1/2$

compression - uni-axial



$k_t / k_2 = 1/2$

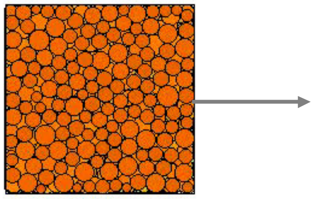
compression - uni-axial



$k_t / k_2 = 1/2$

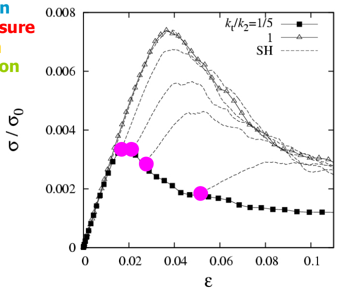
tension - uni-axial

$k_t / k_2 = 1/2$



healing (compression)

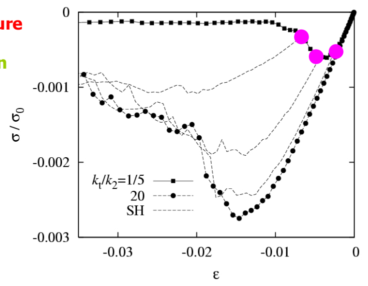
1. **Preparation**
2. **HIGH pressure**
3. **Relaxation**
4. **Compression**
5. **Tension**
6. **Healing**



Olaf Herbst, PostDoc

healing (tension)

1. Preparation
2. HIGH pressure
3. Relaxation
4. Compression
5. Tension
6. Healing



Olaf Herbst, PostDoc

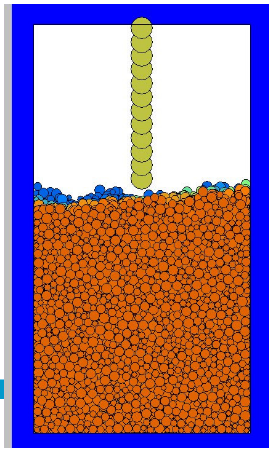
Summary

Make the material …
Break the material …
Self Healing (increase contact adhesion)
- **pre-emptive healing = max. effect**
- **later healing leads to minor effect**

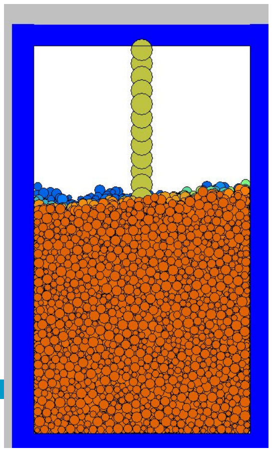
… master curve is reached … always?

Selective healing …
Active healing mechanisms …
where? when? how?

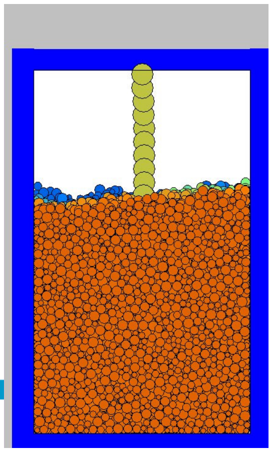
Pile penetration 8



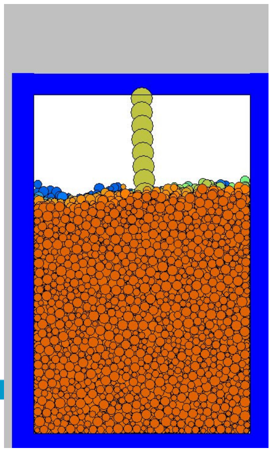
Pile penetration 10



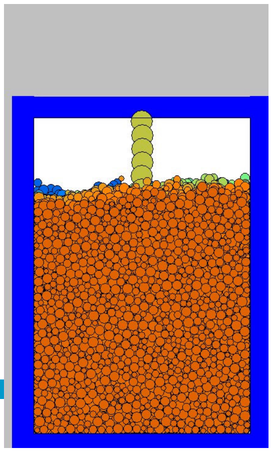
Pile penetration 12



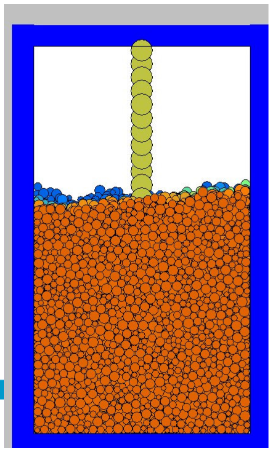
Pile penetration 14



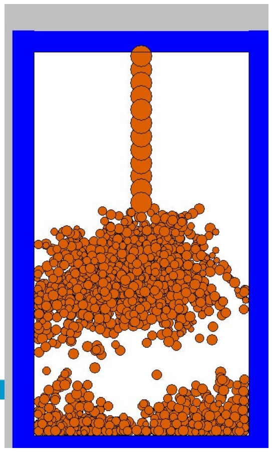
Pile penetration 16



Pile penetration 10



Pile penetration



The End

Summary

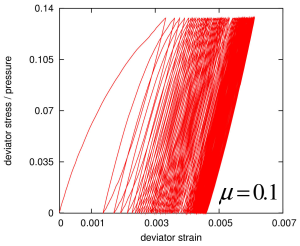
Contact properties:
- **adhesion/cohesion/friction, …**
- **pressure-dependence**
- **temperature-dependence**
- **time-dependence**

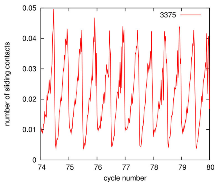
…

… Sintered Solids

Cyclic loading

3D
3375 spheres

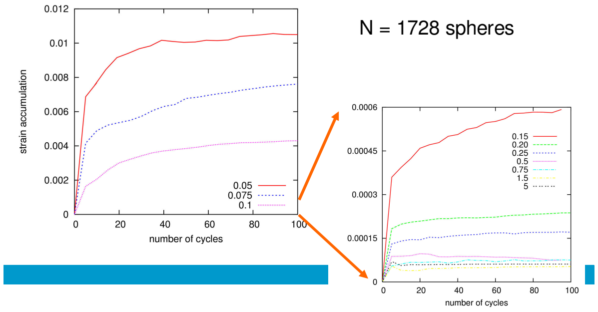




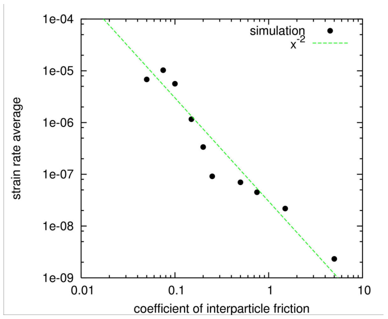
ratcheting …

Strain accumulation with decreasing friction

N = 1728 spheres

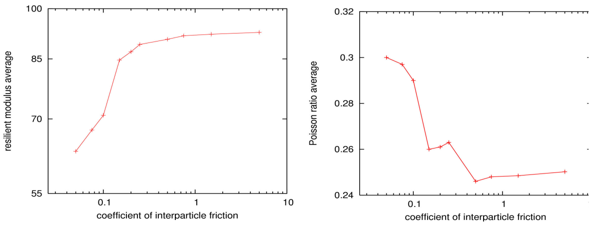


Strain rate



Modulus and Poisson ratio

N = 1728 spheres



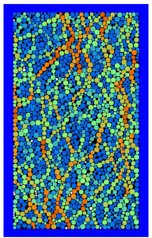
Summary

Cyclic loading …
… system size
… friction dependence
… stiffness kn and kt – in progress

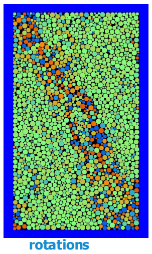
The End

4 Lectures on:
Micro-macro methods for particulate materials

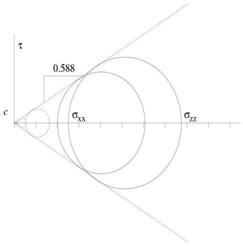
16:00 – 18:30 – 13, 20, 27 Jan. & 03 Feb. 2005 – PSE zaal, Julianalaan 136 (DCT)



inhomogeneity



rotations



Lecturers: Dr. Stefan Luding, s.luding@tnw.tudelft.nl
Dr. Akke Suiker, a.suiker@lr.tudelft.nl

For attending these lectures, please register by e-mail before 10.01.2005 !!!