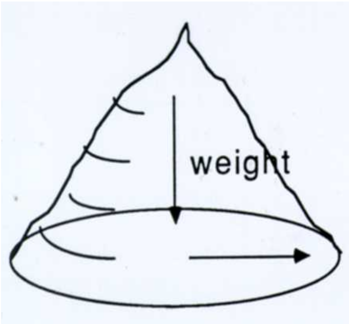
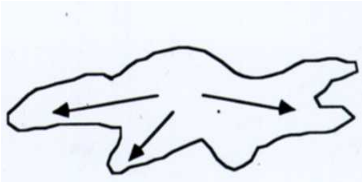
Powder and Liquid Flow (differences)

Inherent Yield Stress



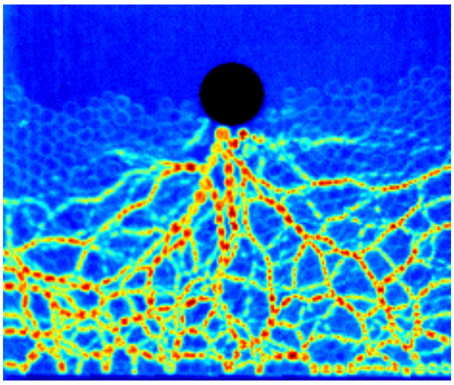


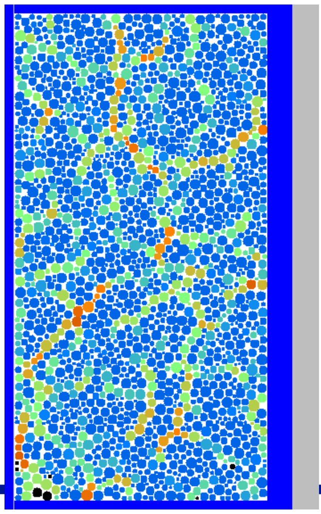
Powders heap

Liquid spreads

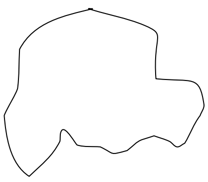
Yield stress = resistance against flow

Dense particle systems: experiments - simulations

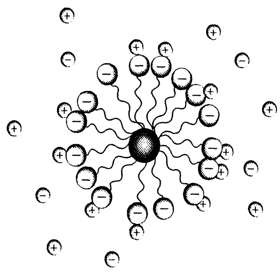




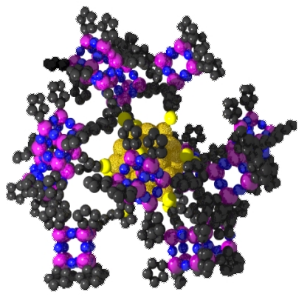
Particle Interactions



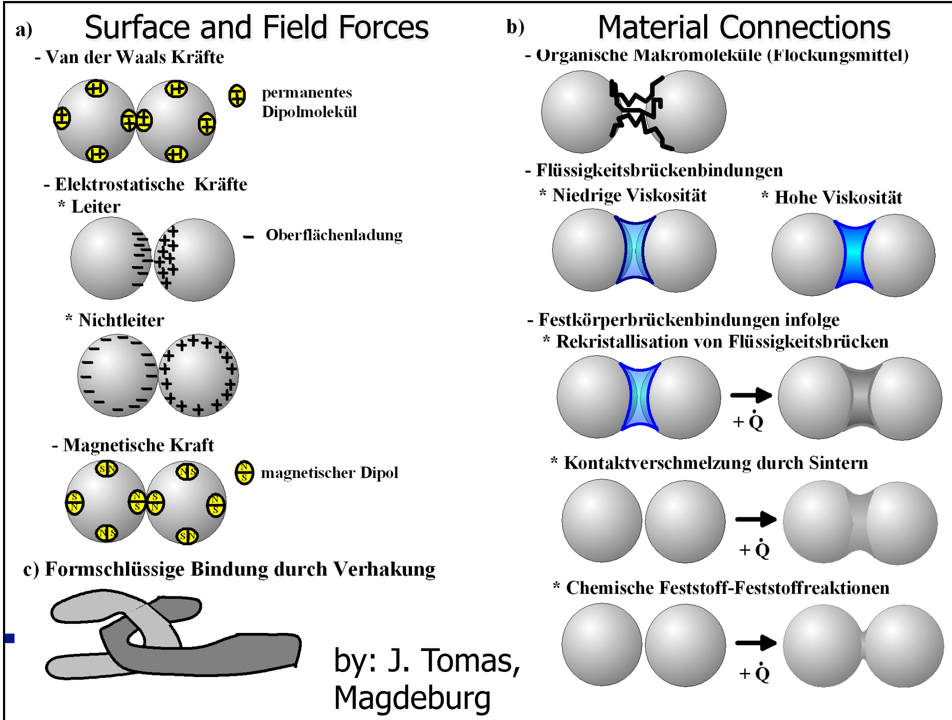
Mechanical
(d_p>10µm)



Chemical
(10nm<d_p<10µm)



Atomic Cluster
(d_p<10nm)



by: J. Tomas, Magdeburg

How to model Contacts?

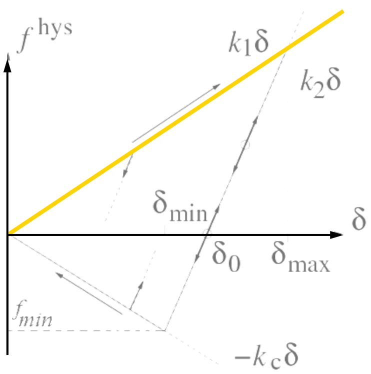
Atomistic/Molecular …

Continuum theory + Contact Mechanics

Experiments (Nano-Ind., AFM, Mech., HSMovies)

Contact Modeling

- Full/All Details … too much!
- **Mesoscopic type Models**
- (Over-)Simplified Models



Linear Contact model

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

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

Linear Contact model

- really simple ☺
- linear, analytical
- very easy to implement

$$f_i = -m_{ij}\ddot{\delta} = k\delta + \gamma\dot{\delta}$$

$$k\delta + \gamma\dot{\delta} + m_{ij}\ddot{\delta} = 0$$

$$\frac{k}{m_{ij}}\delta + 2\frac{\gamma}{2m_{ij}}\dot{\delta} + \ddot{\delta} = 0$$

$$\omega_0^2\delta + 2\eta\dot{\delta} + \ddot{\delta} = 0$$

elastic freq. $\omega_0 = \sqrt{k/m_{ij}}$

eigen-freq. $\omega = \sqrt{\omega_0^2 - \eta^2}$

visc. diss. $\eta = \dfrac{\gamma}{2m_{ij}}$

$$\delta(t) = \frac{v_0}{\omega}\exp(-\eta t)\sin(\omega t)$$

$$\dot{\delta}(t) = \frac{v_0}{\omega}\exp(-\eta t)\left[-\eta\sin(\omega t) + \omega\cos(\omega t)\right]$$

contact duration $t_c = \pi/\omega$

restitution coefficient $r = -\dfrac{v(t_c)}{v_0} = \exp(-\eta t_c)$

http://www2.msm.ctw.utwente.nl/sluding/PAPERS/coll2p.pdf

Time-scales

time-step $\Delta t <= t_c/50$

contact duration $t_c = \pi/\omega$

$t_n < t_c$ — different sized particles $t_c^{large} > t_c^{small}$

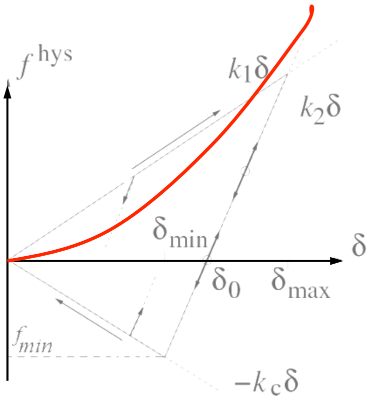
time between contacts

$t_n > t_c$

sound propagation $N_L t_c$ ... with number of layers N_L

experiment T

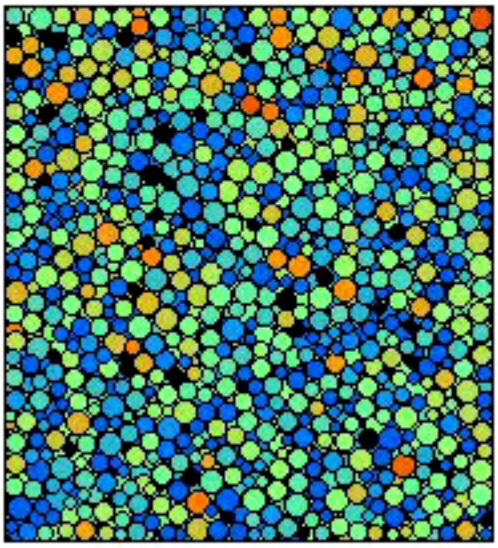
http://www2.msm.ctw.utwente.nl/sluding/PAPERS/coll2p.pdf



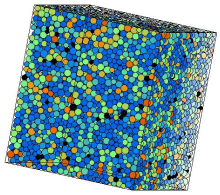
Hertz Contact model

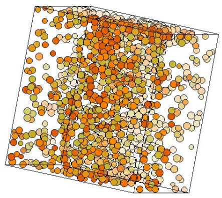
- **simple ☺**
- **non-linear**
- **easy to implement**

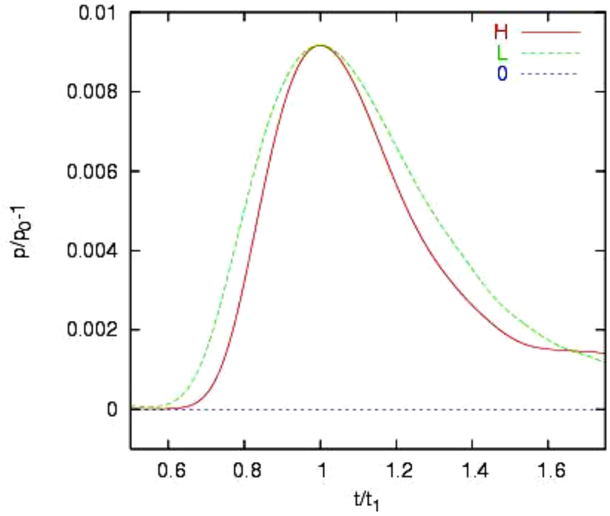
$$f_i^{hys} = \begin{cases} k_1\delta^{3/2} & \text{for un-/re-loading} \end{cases}$$



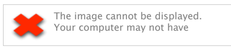
Sound



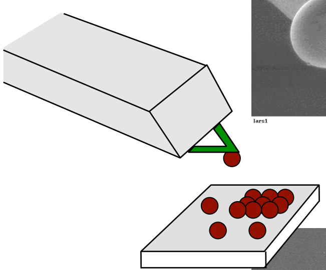


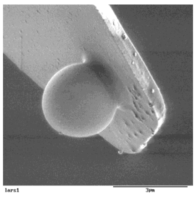


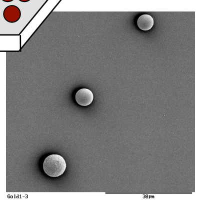
P-wave shape and speed

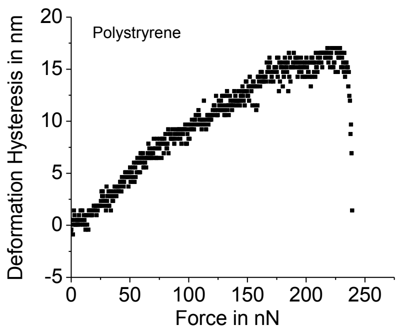


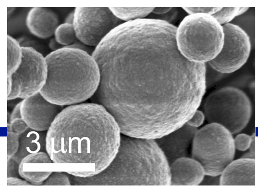
Contact force measurement (AFM)



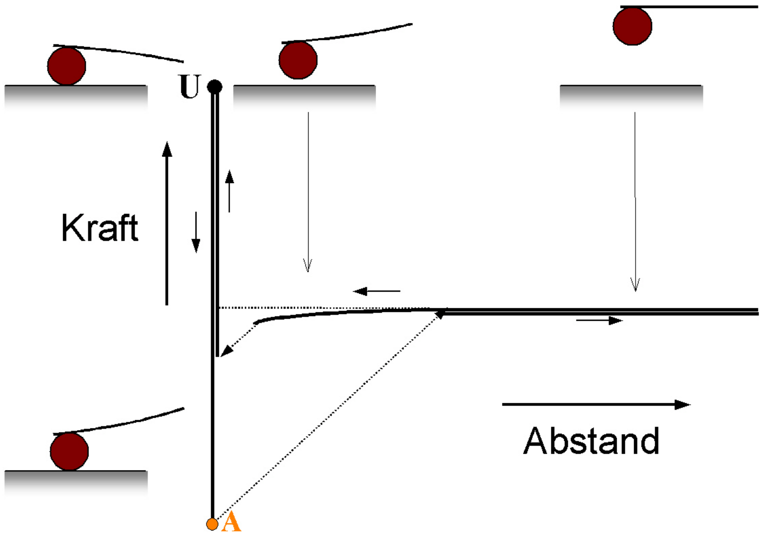




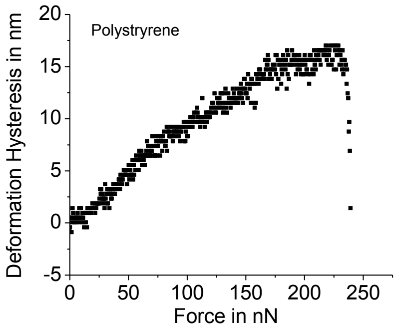


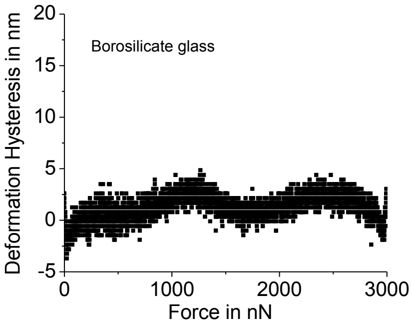


Contact Force Measurement



Hysteresis (plastic deformation)



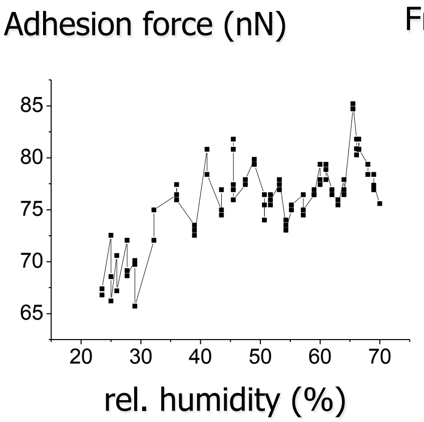


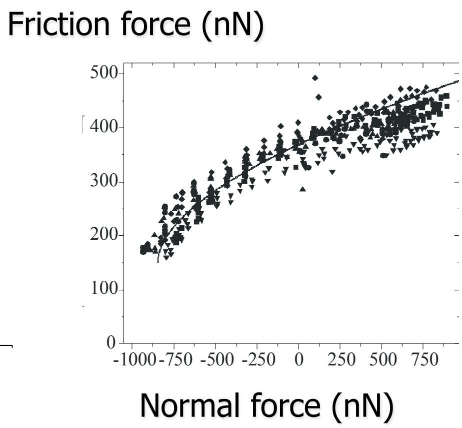
Collaborations:

MPI-Polymer Science (Kappl, Butt)

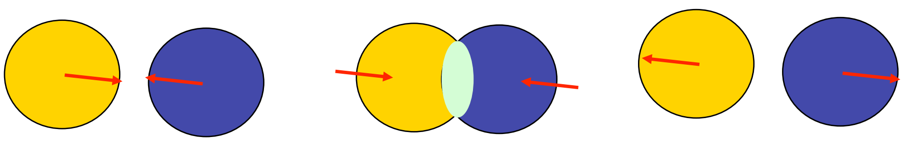
Contact properties via AFM

Adhesion and Friction

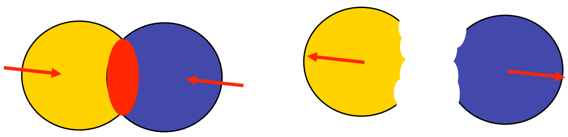




Elastic spheres



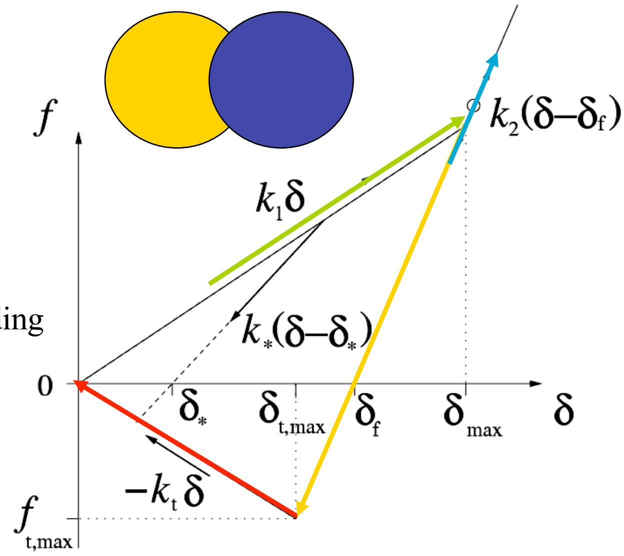
Elasto-plastic spheres



Before **During** **After**

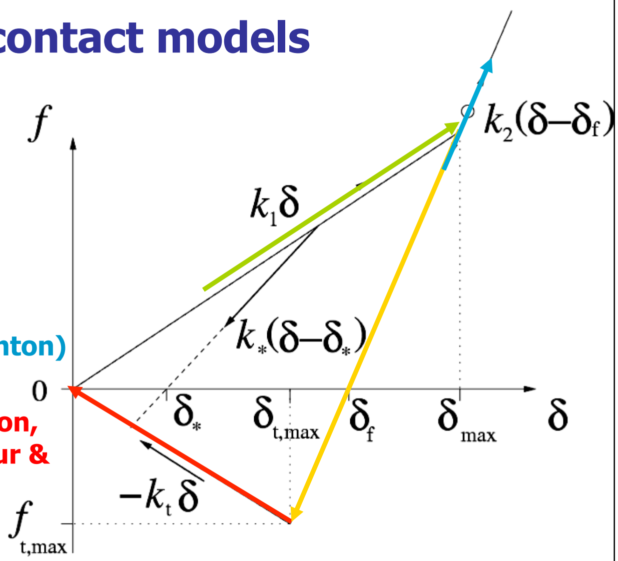
Contacts

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

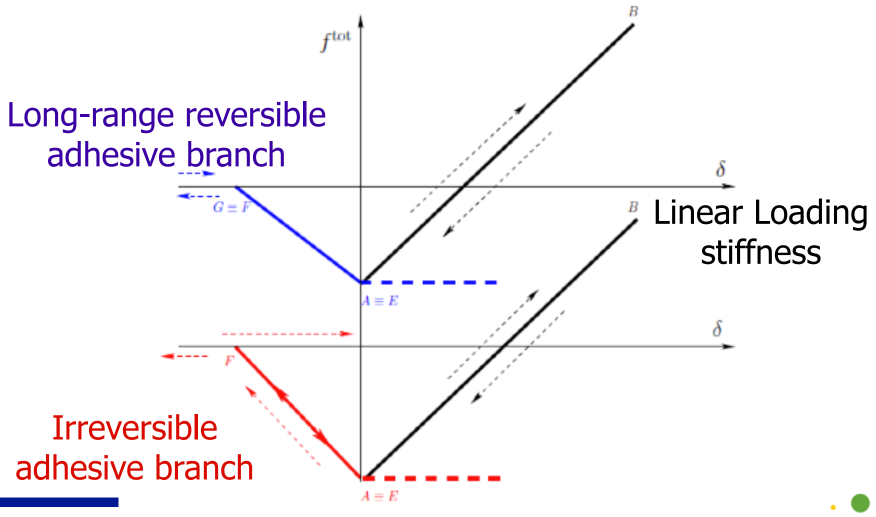


Alternative contact models

1. loading
   => early elastic phase (Tomas)
2. unloading
   => non-linear (Thornton, Tomas)
3. re-loading
   => more elastic (Thornton)
4. tensile failure
   => more abrupt (Walton, Pasha & Ghadiri, Thakur & Ooi)

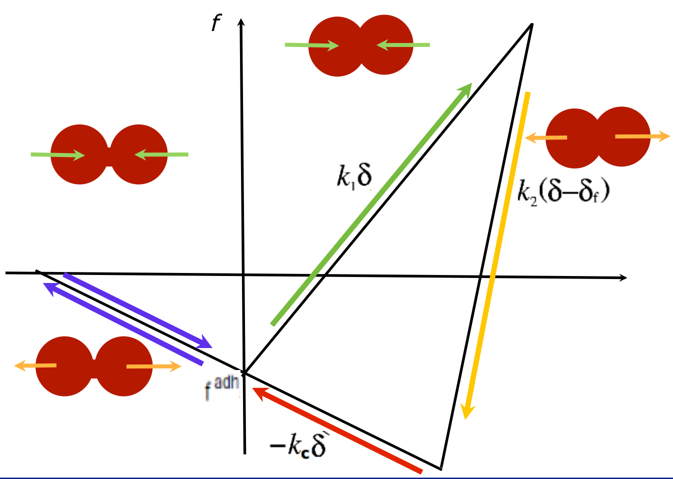


Elastic adhesive contacts



Reversible elasto-plastic adhesive contacts

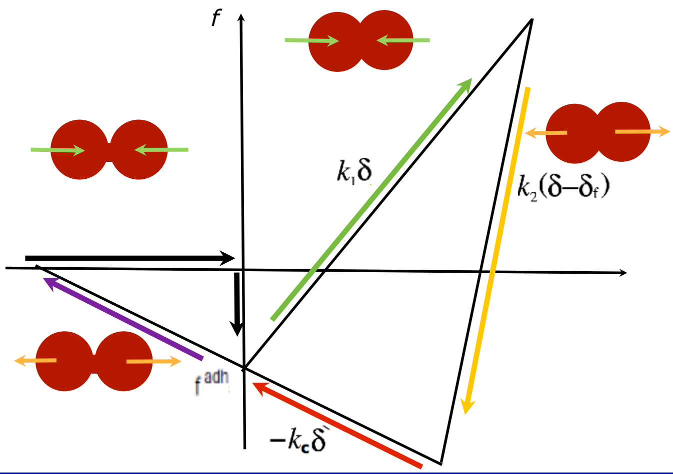
- Long range force.
- Loading
  Plastic def.
- Unloading
  "elasto-plastic"
- Re-loading
  "elastic"
- Cohesion

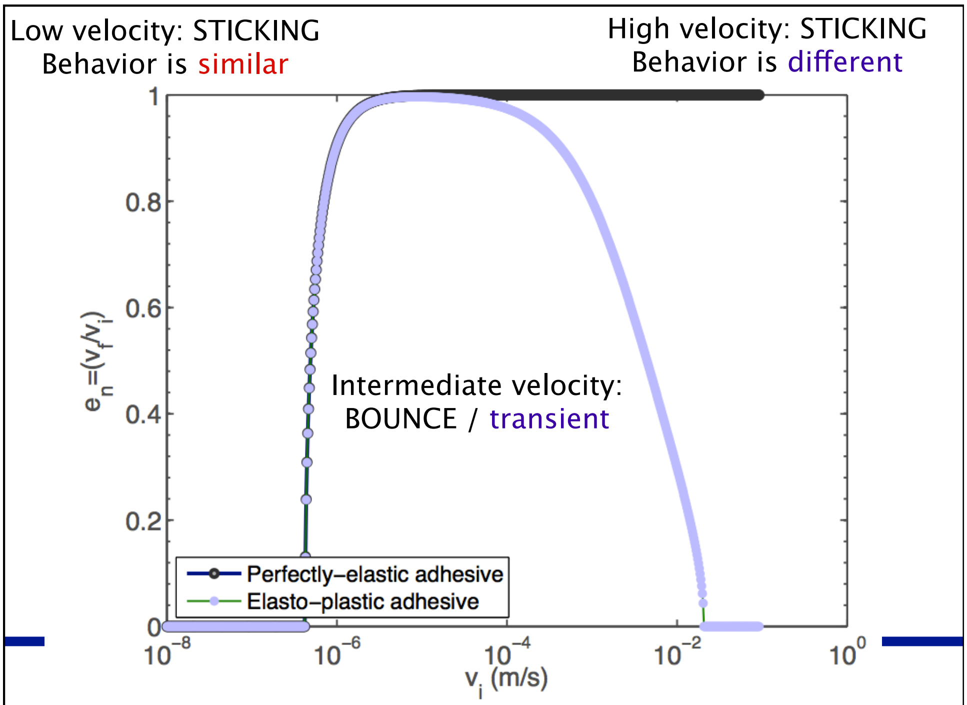


Van-der Waals type interaction.

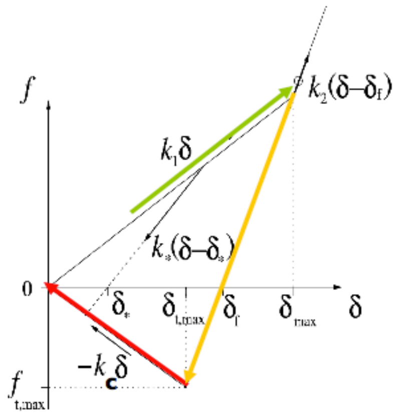
Irreversible elasto–plastic adhesive contacts

- Loading
  Plastic def.
- Unloading
  "elasto-plastic"
- Re-loading
  "elastic"
- Cohesion
- Long-range
  forces …





Energy Calculations



$$\frac{1}{2}m_r v_i^2 = \frac{1}{2}k_1\delta_{max}^2$$

$$\frac{1}{2}m_r v_0^2 = \frac{1}{2}k_1\delta_{max}(\delta_{max}-\delta_0)$$

$$\frac{1}{2}m_r v_f^2 - \frac{1}{2}m_r v_0^2 = -\frac{1}{2}k_c\delta_{min}\delta_0$$

$$e_n^{(1)} = \frac{v_f}{v_i} = \sqrt{\frac{k_1}{k_*} - \frac{k_c\,(k_*-k_1)}{k_1\,(k_*+k_c)}\frac{(k_*-k_1)}{k_*}}$$

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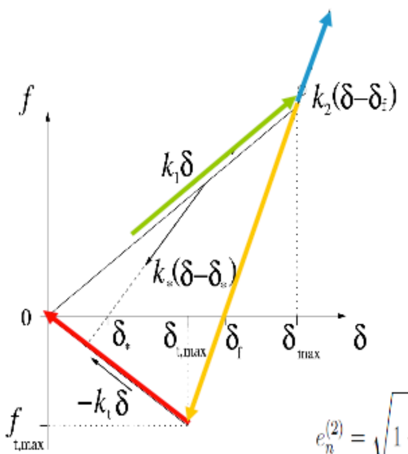


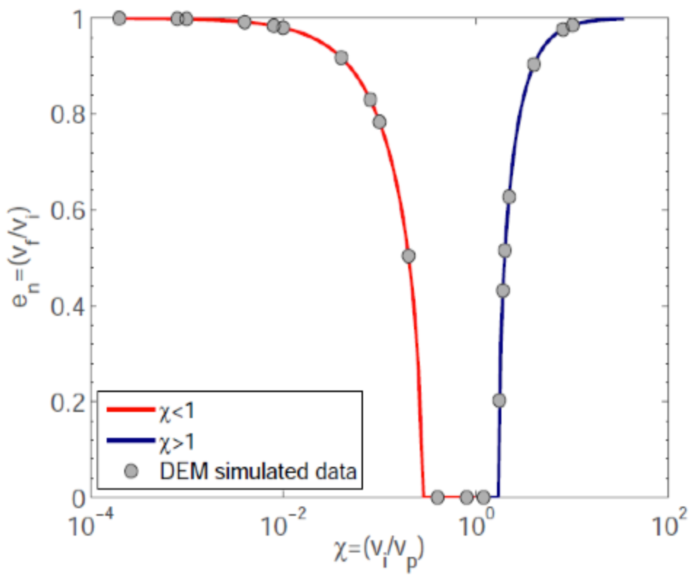
$$\frac{1}{2}m_r v_i^2 - \frac{1}{2}m_r v_1^2 = \frac{1}{2}k_1\delta^{*2}_{max}$$

$$\frac{1}{2}m_r v_1^2 - \frac{1}{2}m_r v_0^2 = \frac{1}{2}k_1\delta^*_{max}(\delta^*_{max}-\delta_0)$$

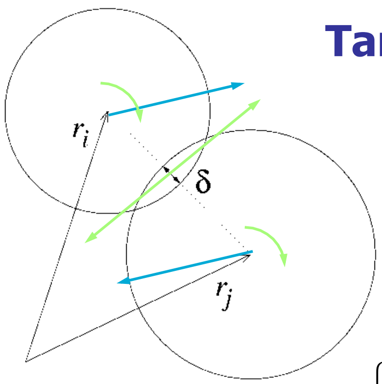
$$\frac{1}{2}m_r v_f^2 - \frac{1}{2}m_r v_0^2 = -\frac{1}{2}k_c\delta_{min}\delta_0$$

$$e_n^{(2)} = \sqrt{1-\left[k_1+\frac{k_1^2}{k_2}-k_c\frac{(k_2-k_1)}{(k_2+k_c)}\frac{(k_2-k_1)}{k_2}\right]\kappa^2} \qquad \kappa^2 = \frac{\delta^{*2}_{max}}{m_r v_i^2}$$

Coefficient of Restitution



Tangential contact model



Sliding **contact points:**

- **static Coulomb friction**
- **dynamic Coulomb friction**
- **objectivity**

Sliding/Rolling/Torsion

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

Tangential contact model

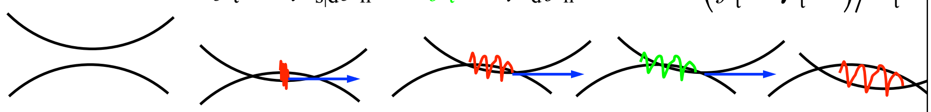
- Static friction — spring
- Dynamic friction — dashpot

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

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

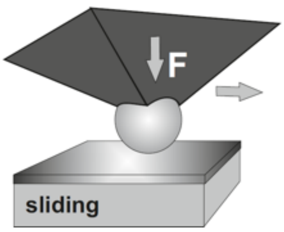
sticking: $f_{\mathrm{t}}^{0} \le \mu_{\mathrm{s}} f_{\mathrm{n}}$ $\quad f_{\mathrm{t}} = f_{\mathrm{t}}^{0}$ $\quad \vartheta = \vartheta' + \dot{\vartheta}' \mathrm{d}t$

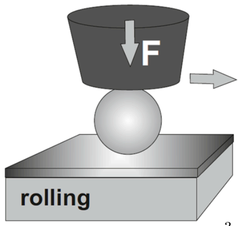
sliding: $f_{\mathrm{t}}^{0} > \mu_{\mathrm{s|d}} f_{\mathrm{n}}$ $\quad f_{\mathrm{t}} = \mu_{\mathrm{d}} f_{\mathrm{n}} \hat{t}$ $\quad \vartheta = \left(f_{\mathrm{t}} + \gamma_{\mathrm{t}} \dot{\vartheta}'\right) / k_{\mathrm{t}}$

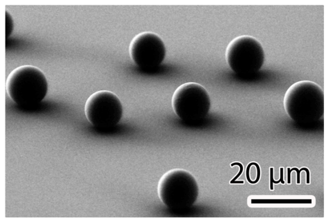


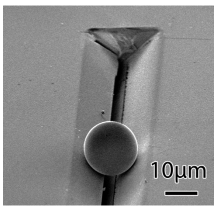
before | contact | static | dynamic | static

Nano-indenter -> contacts

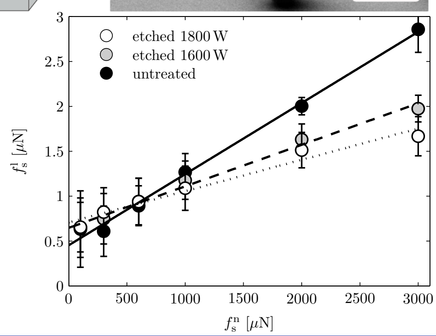






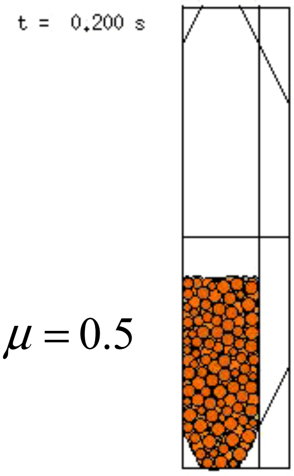


torsion
+rolling

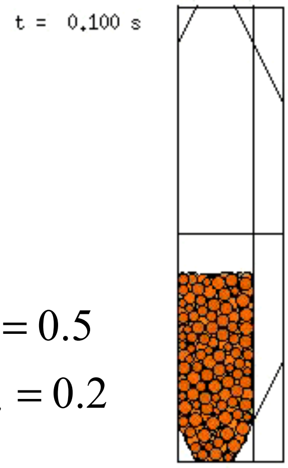


R. Fuchs et al. Granular Matter, 2014

Flow with friction & rolling resistance



$\mu = 0.5$

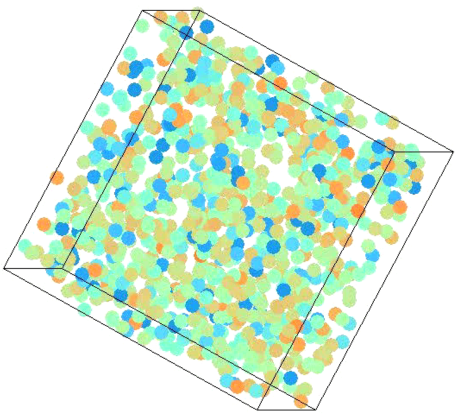


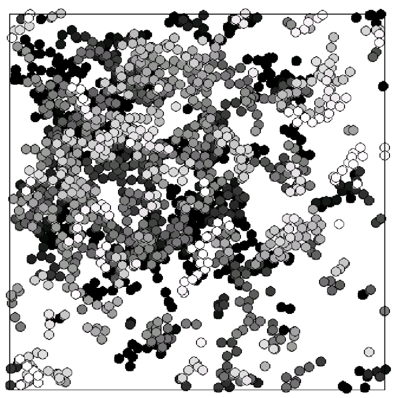
$\mu = 0.5$

$\mu_r = 0.2$

The image cannot be displayed. Your computer may not have

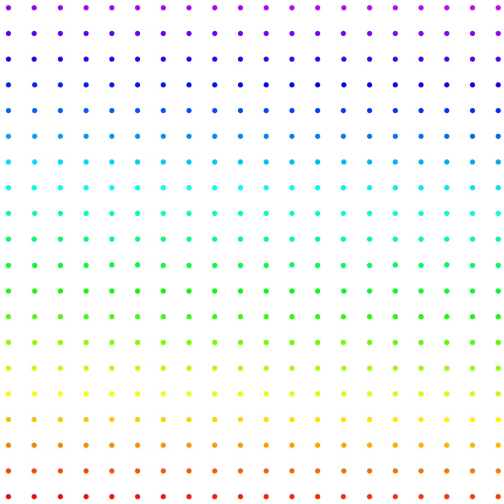
… details of interaction





Attraction + Dissipation = Agglomeration

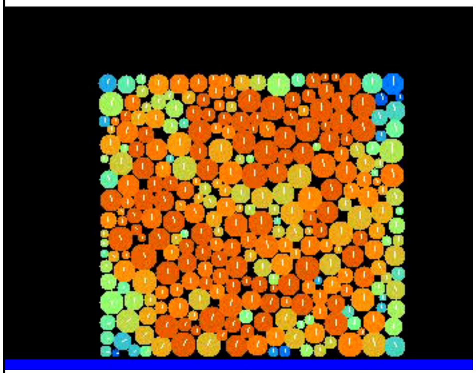
Example: Agglomeration

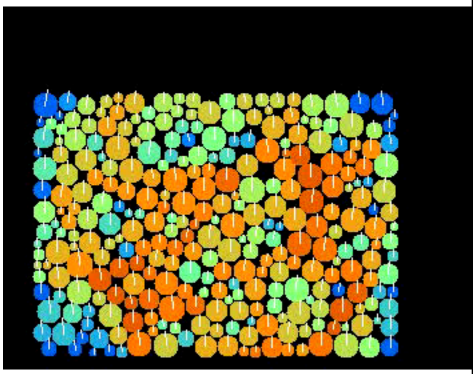


S. Gonzalez-Briones, MSM, 2010

Tabletting

Vibration test





p=100 p=10

We can simulate:

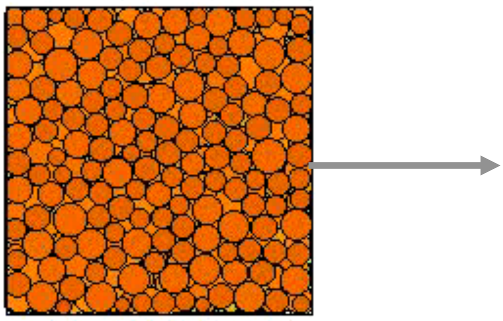
+ element tests (REV)
+ small processes & equipment

– large scales (processes/plants/geophysical scales)
– especially of fine, cohesive powders

Instead:
+ provide constitutive relations = f(contact)
+ model large scales with continuum methods

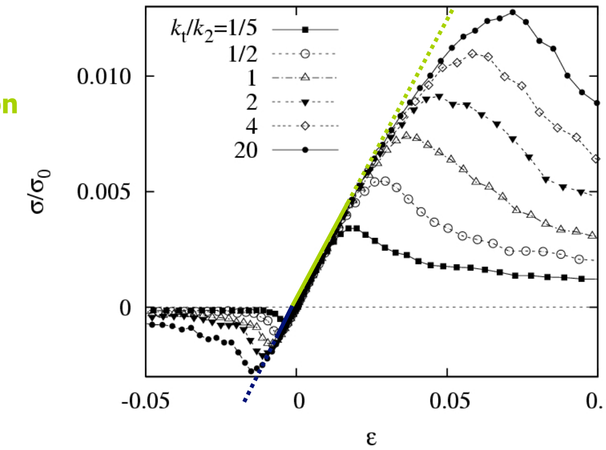
tension - uni-axial

$k_t/k_2 = 1/2$



uni-axial compression-tension

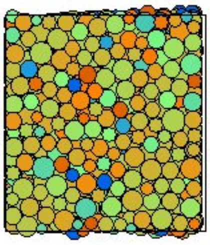
- Compression
- Tension

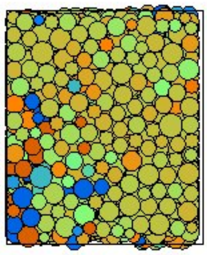


compression - uni-axial

$k_t/k_2 = 1/2$

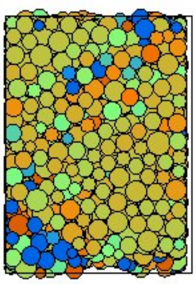
compression - uni-axial

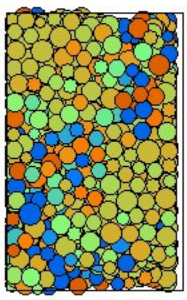




$k_t / k_2 = 1/2$

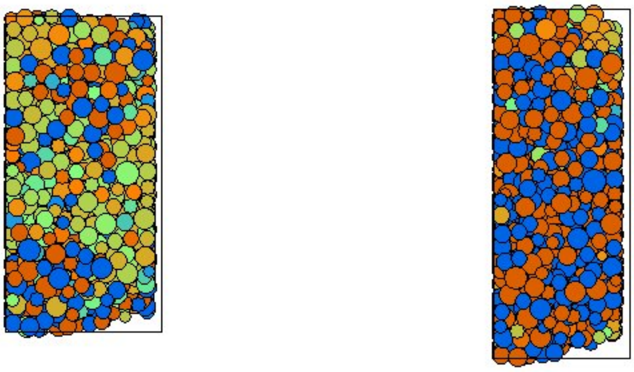
compression - uni-axial





$k_t / k_2 = 1/2$

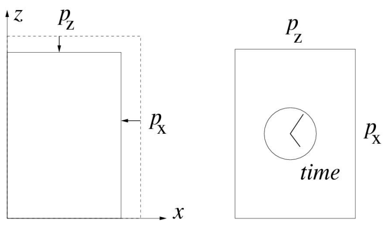
compression - uni-axial

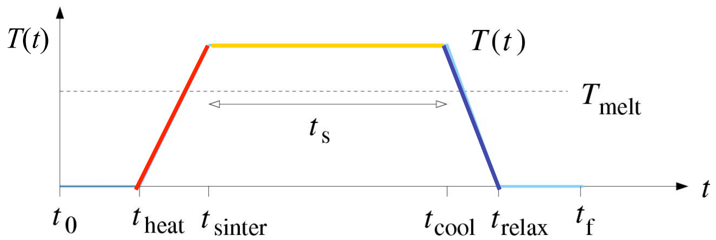


$k_t / k_2 = 1/2$

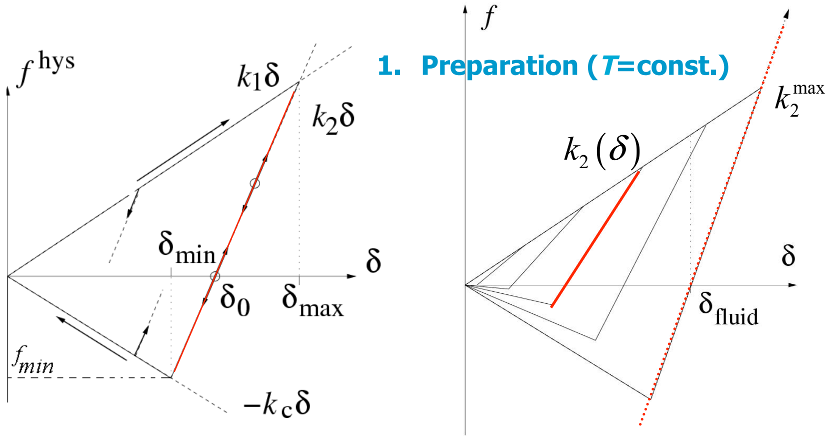
Sintering / Cementation (back to 2D)

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





cold contacts – loose grains

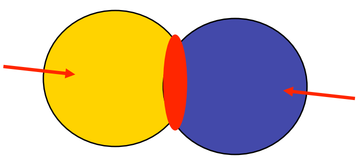


loading stiffness: $k_1 = k_1(T)$

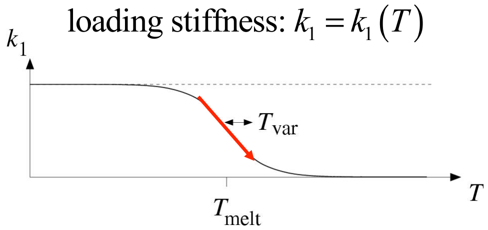
contact stiffness: $k_2 = k_2(\delta)$

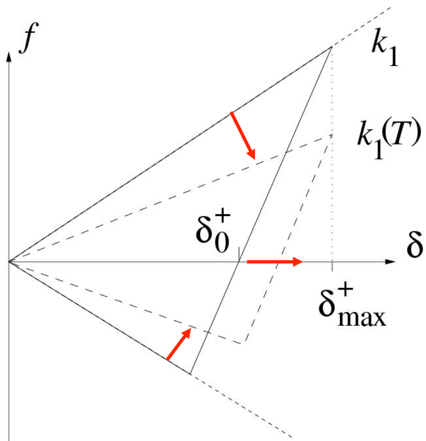
Sintering / Cem.

2. Heating



loading stiffness: $k_1 = k_1(T)$



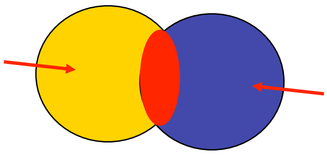


maximum overlap fixed: δ_{max}^+

neutral overlap increasing: δ_0^+

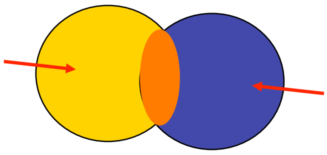
Sintering / Cem. 3

3. Sintering / Cementation - Reaction



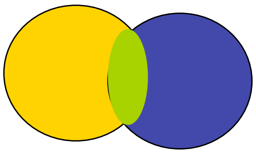
Sintering 4

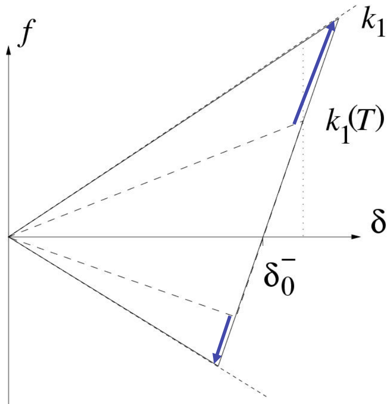
4. Cooling



Sintering 4

4. **Cooling**



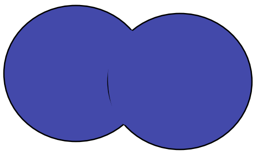


maximum overlap increasing: δ_{max}^-

neutral overlap fixed: δ_0^-

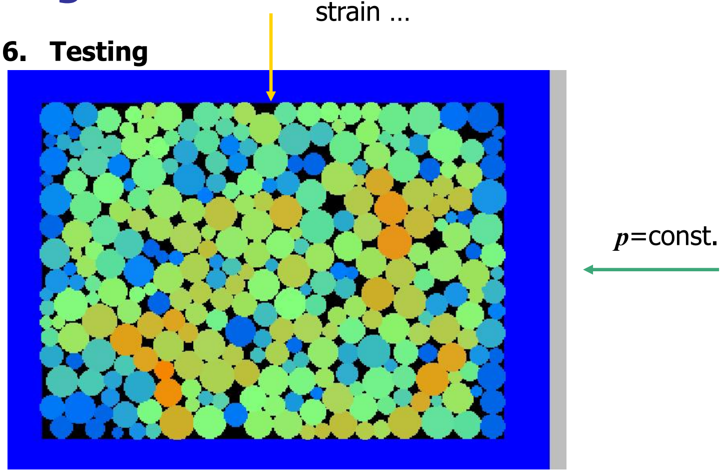
Sintering 5

5. **Relaxation**



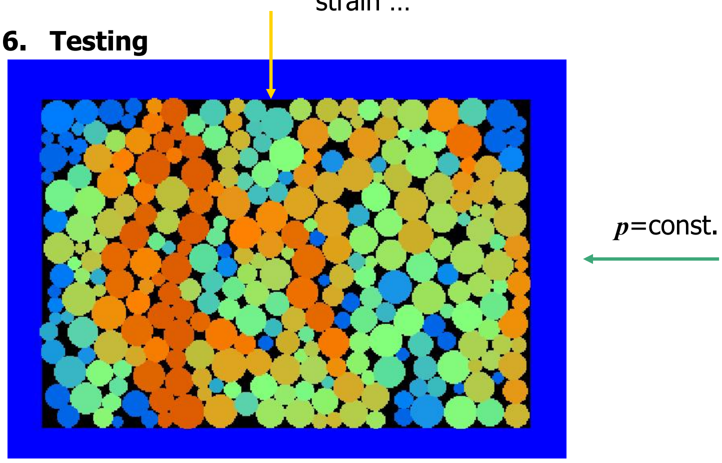
Sintering 6

6. Testing



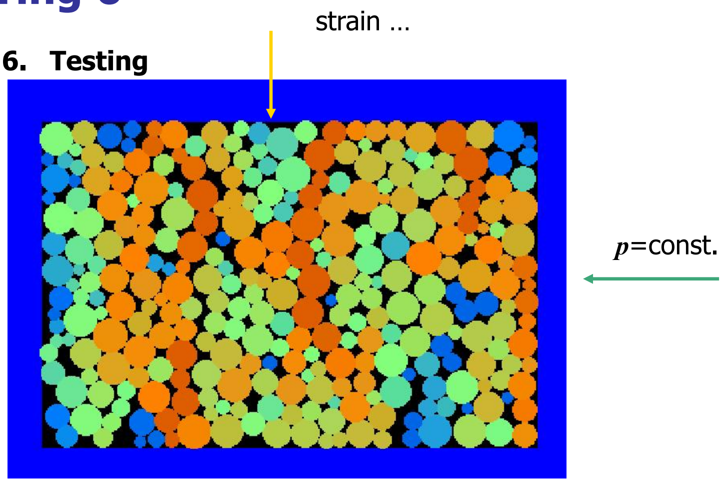
Sintering 6

6. Testing



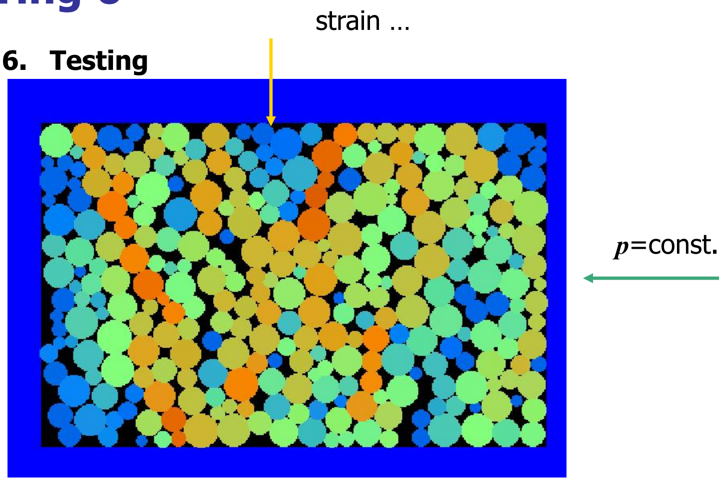
Sintering 6

6. Testing



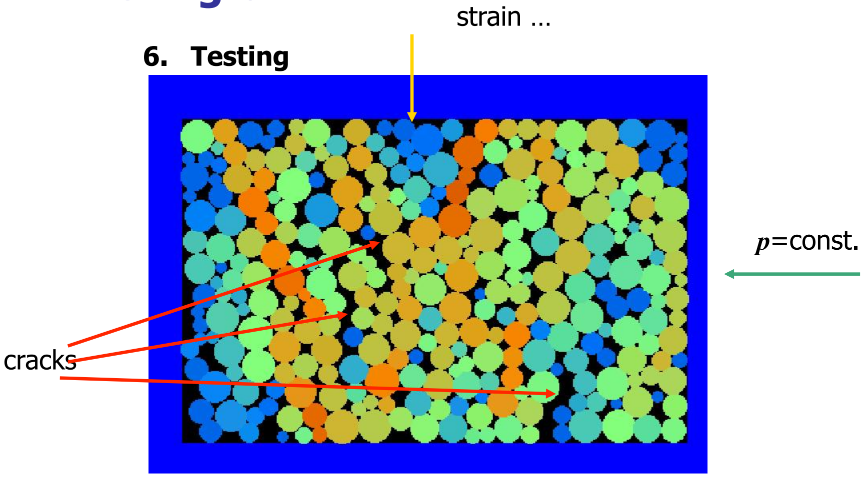
Sintering 6

6. Testing



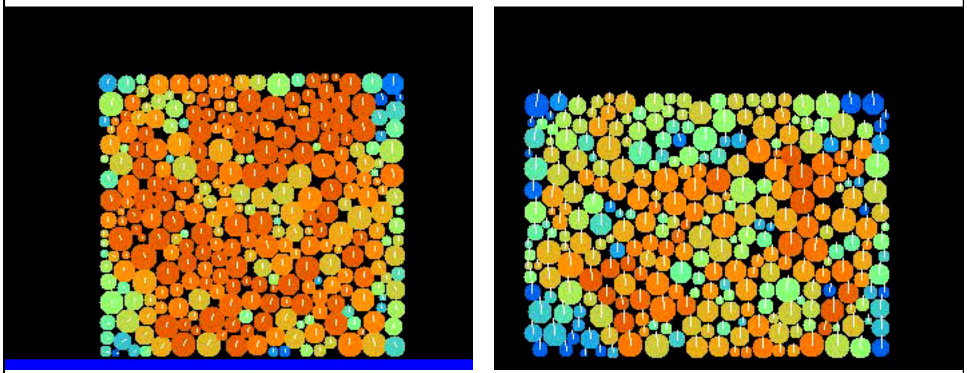
Sintering 6

6. Testing



Sintering (Temperature+Pressure)

Vibration test



p=100

p=10

We can simulate:

+ element tests (REV)
+ small processes & equipment

– large scales (processes/plants/geophysical scales)
– especially of fine, cohesive powders

Instead:
+ provide constitutive relations
+ model large scales with continuum methods

Literature (http://www2.msm.ctw.utwente.nl/sluding/publications.html)
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[2] S. Luding, *Introduction to Discrete Element Methods: Basics of Contact Force Models and how to perform the Micro-Macro Transition to Continuum Theory*, European Journal of Environmental and Civil Engineering - EJECE 12 - No. 7-8 (Special Issue: Alert Course, Aussois), 785-826 (2008), [http://www2.msm.ctw.utwente.nl/sluding/PAPERS/luding_alert2008.pdf]
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[4] M. Lätzel, S. Luding, and H. J. Herrmann,
Macroscopic material properties from quasi-static, microscopic simulations of a two-dimensional shear-cell , Granular Matter 2(3), 123-135, 2000 [http://www2.msm.ctw.utwente.nl/sluding/PAPERS/micmac.pdf]
[5] S. Luding, *Anisotropy in cohesive, frictional granular media*
J. Phys.: Condens. Matter 17, S2623-S2640, 2005 [http://www2.msm.ctw.utwente.nl/sluding/PAPERS/jpcm1.pdf]