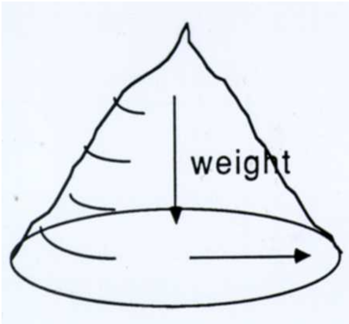
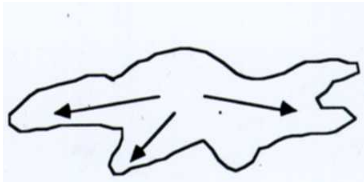
Powder and Liquid Flow (differences)

Inherent Yield Stress



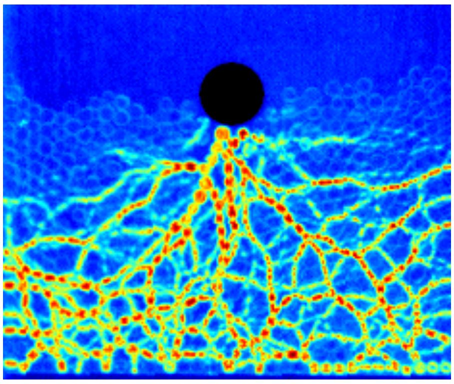


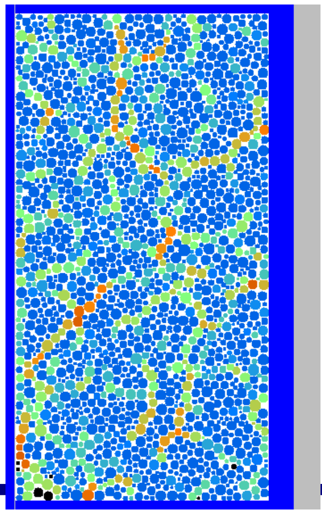
Powders heap

Liquid spreads

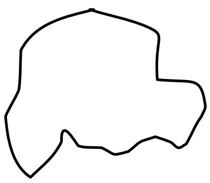
Yield stress = resistance against flow

Dense particle systems: experiments - simulations

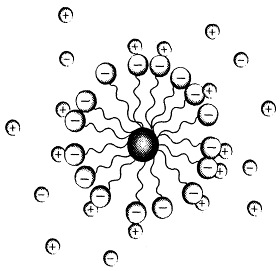




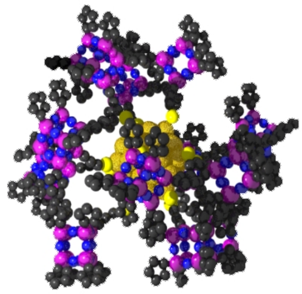
Particle Interactions



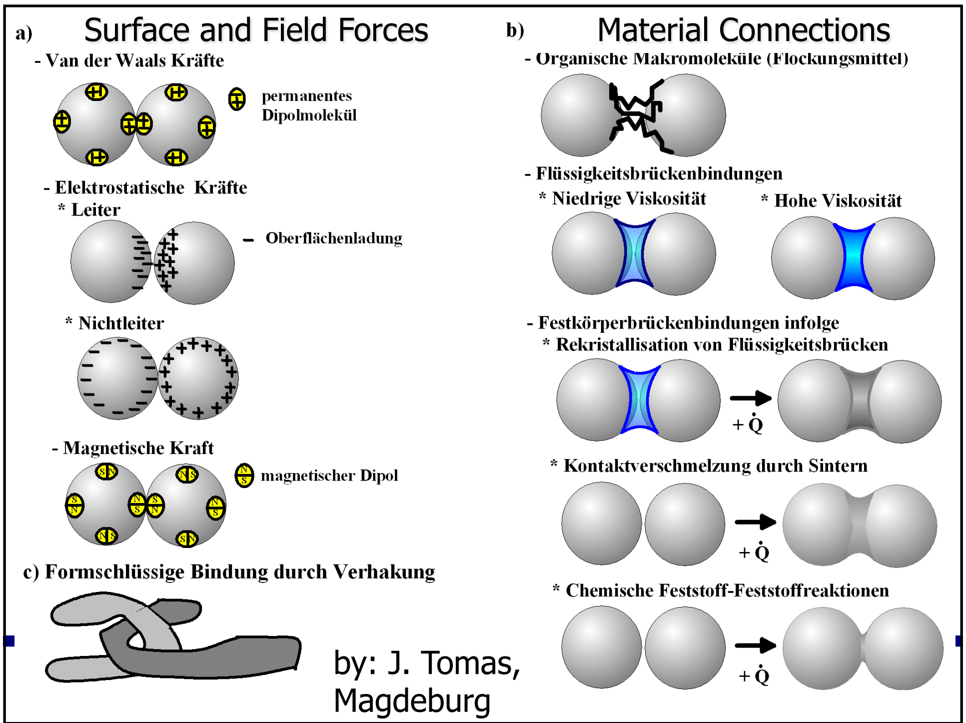
Mechanical (d_p>10µm)



Chemical (10nm<d_p<10µm)



Atomic Cluster (d_p<10nm)



by: J. Tomas, Magdeburg

How to model Contacts?

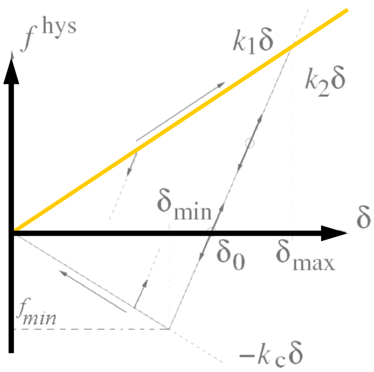
Atomistic/Molecular …

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. $\eta = \frac{\gamma}{2m_{ij}}$

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

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

contact duration $t_c = \pi/\omega$

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

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** $t_c^{large} > t_c^{small}$

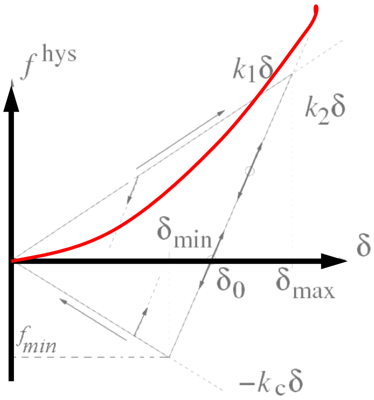
time between contacts

$t_n > t_c$

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

experiment T

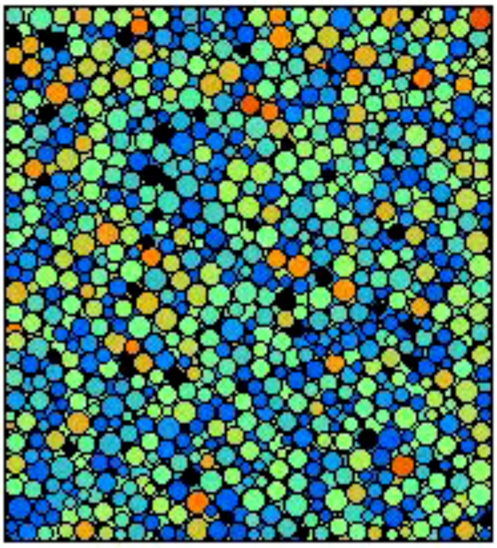
http://www2.msm.ctw.utwente.nl/sluding/PAPERS/coll2p.pdf



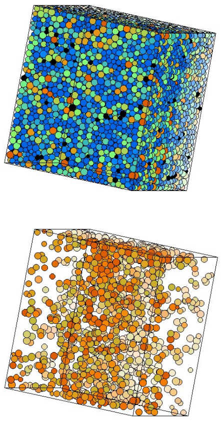
Hertz Contact model

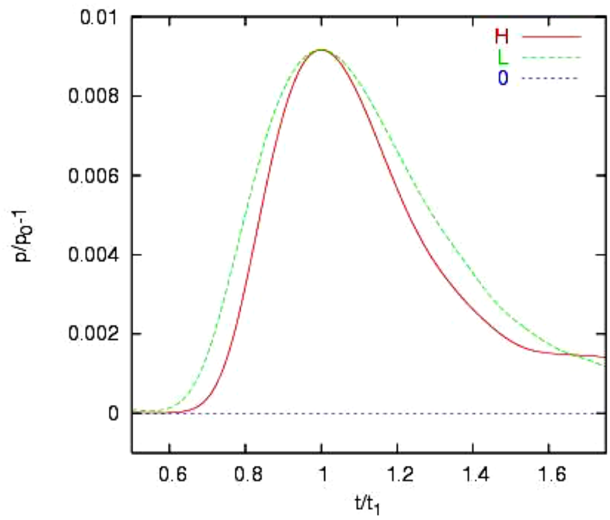
- simple ☺
- non-linear
- easy to implement

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



Sound





P-wave shape and speed

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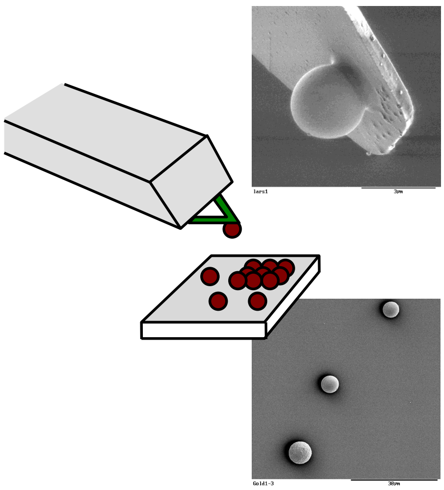
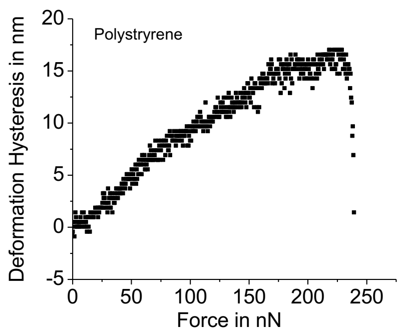
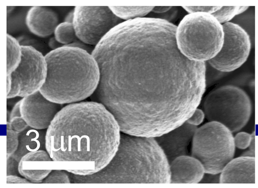
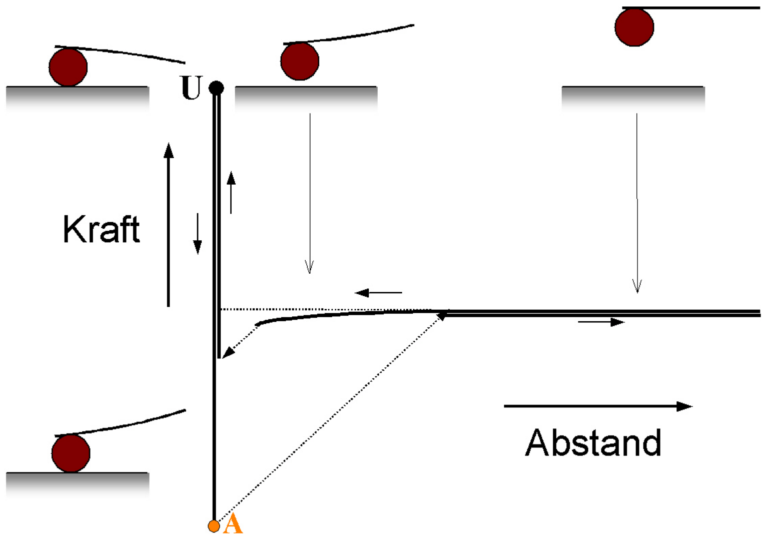
Contact force measurement (AFM)



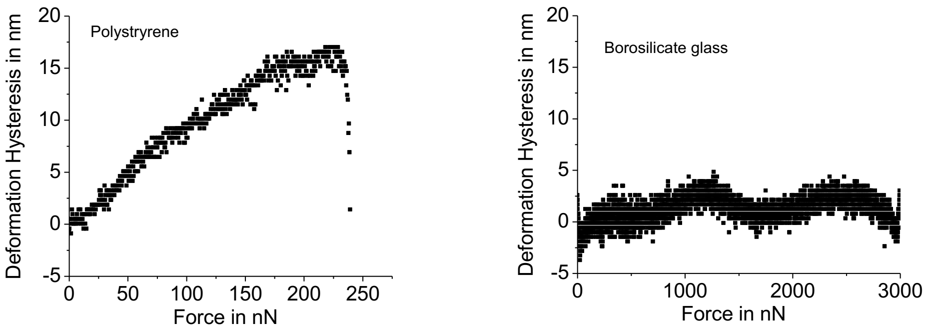




Contact Force Measurement



Hysteresis (plastic deformation)

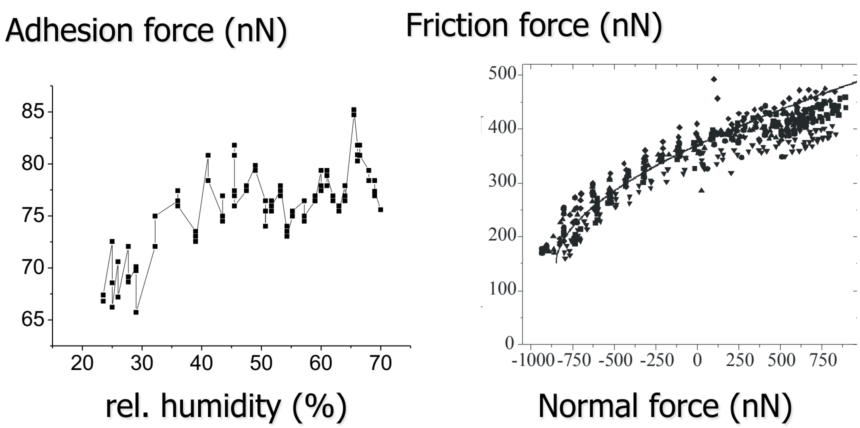


Collaborations:

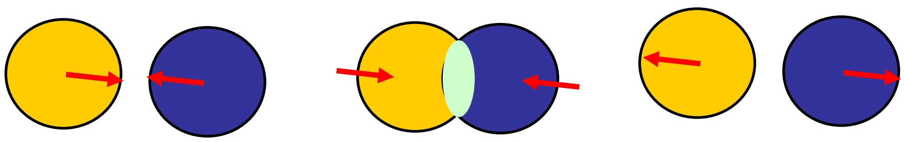
MPI-Polymer Science (Kappl, Butt)

Contact properties via AFM

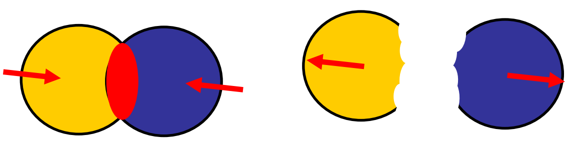
Adhesion and Friction



Elastic spheres



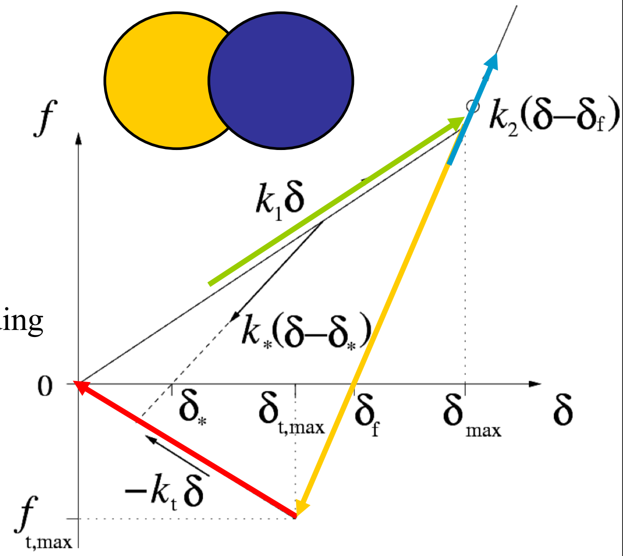
Elasto-plastic spheres



Before
During
After

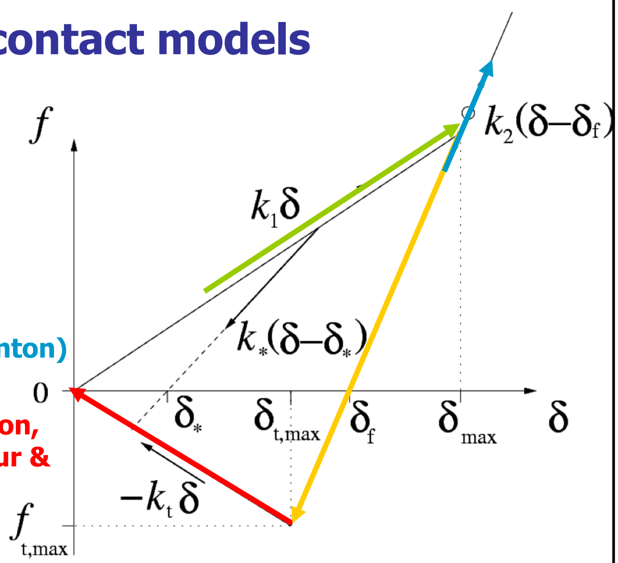
Contacts

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

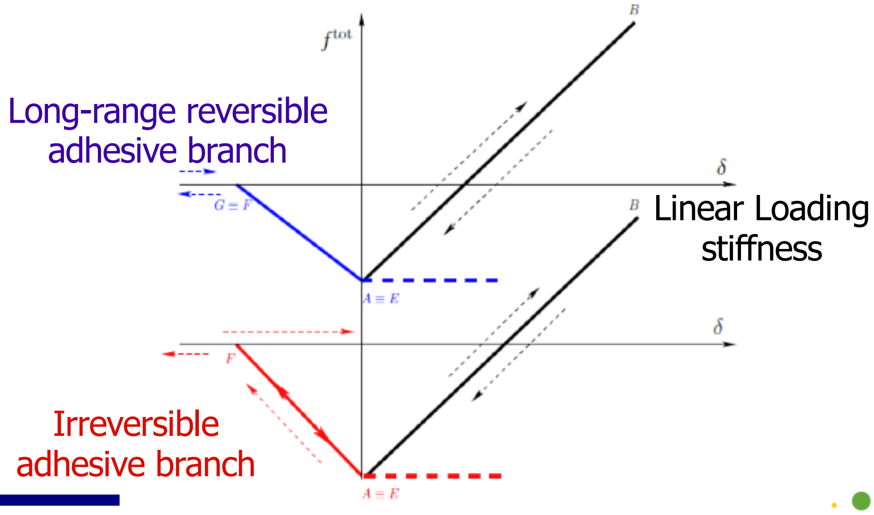


Alternative contact models

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)



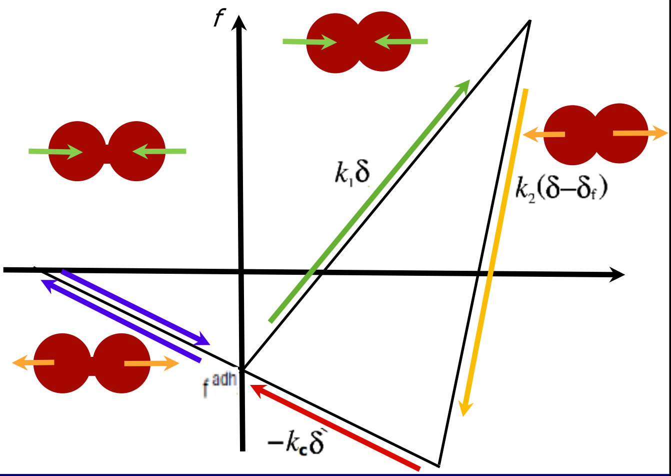
Elastic adhesive contacts



UNIVERSITEIT TWENTE.

Reversible elasto-plastic adhesive contacts

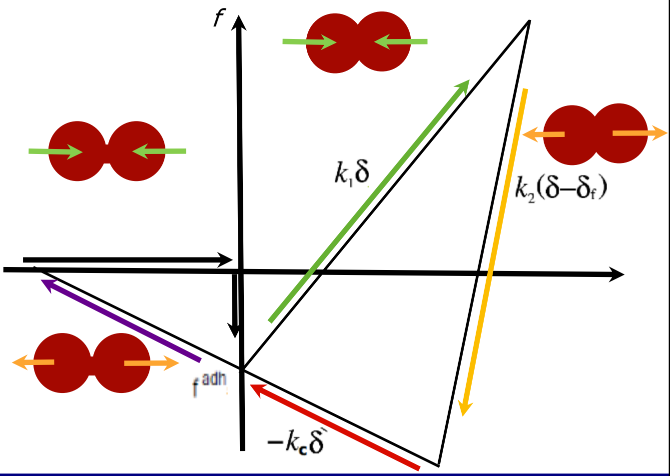
- Long range force.
- Loading
  Plastic def.
- Unloading
  "elasto-plastic"
- Re-loading
  "elastic"
- Cohesion



Van-der Waals type interaction.

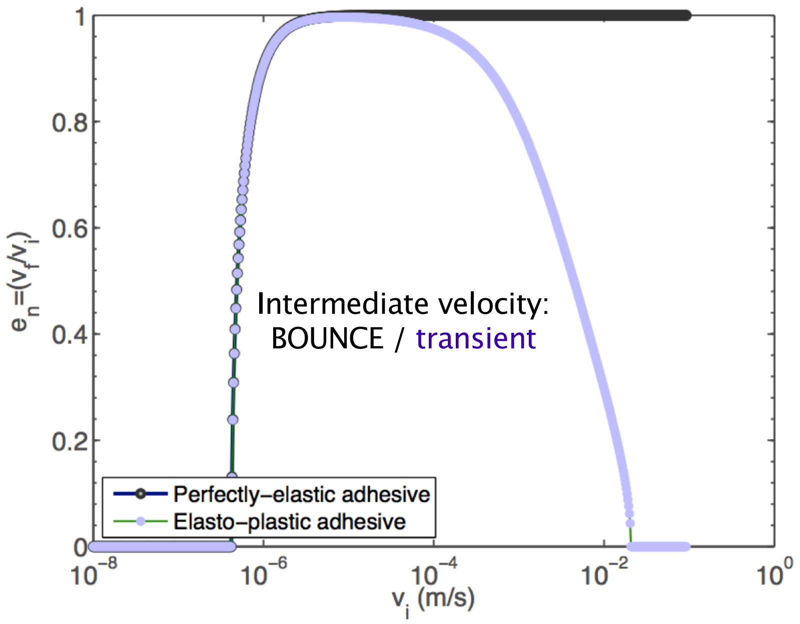
Irreversible elasto-plastic adhesive contacts

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



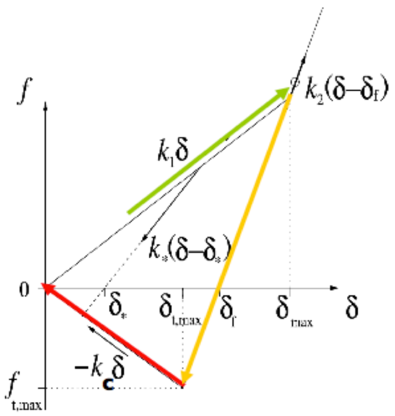
Low velocity: STICKING
Behavior is similar

High velocity: STICKING
Behavior is different



Energy Calculations

msm FOM



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

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

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

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

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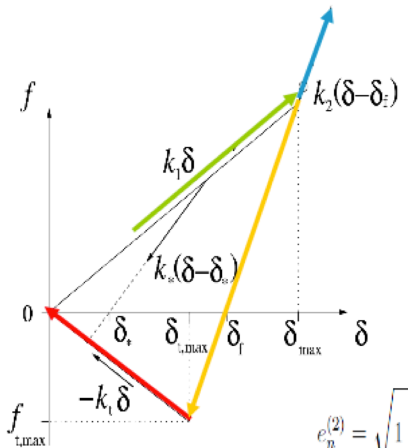
msm FOM



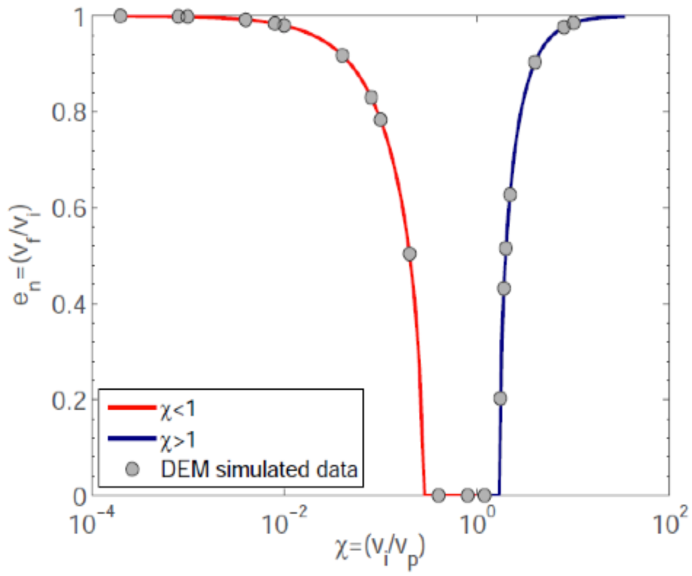
$$\frac{1}{2}m_r v_i^2 - \frac{1}{2}m_r v_1^2 = \frac{1}{2}k_1\delta^{*2}_{\max}$$

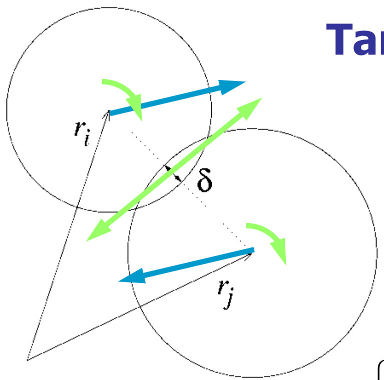
$$\frac{1}{2}m_r v_1^2 - \frac{1}{2}m_r v_0^2 = \frac{1}{2}k_1\delta^*_{\max}(\delta^*_{\max}-\delta_0)$$

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

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

Coefficient of Restitution





Tangential contact model

Sliding **contact points:**

- static Coulomb friction

- dynamic Coulomb friction

- objectivity

Sliding/Rolling/Torsion

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

Tangential contact model

- Static friction
- Dynamic friction

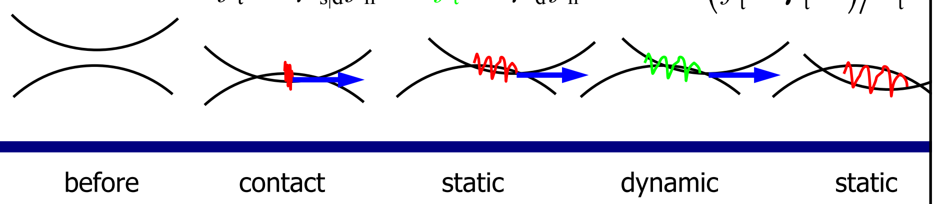
- spring
- dashpot

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

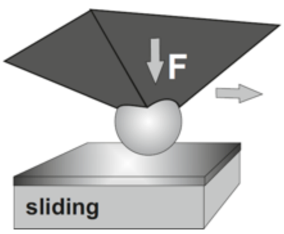
compute test force $f_t^0 = -k_t\vartheta' - \gamma_t\dot{\vartheta}'$ and $\hat{t} = f_t^0 / |f_t^0|$

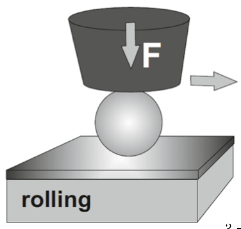
sticking: $f_t^0 \le \mu_s f_n$ $\quad f_t = f_t^0$ $\quad \vartheta = \vartheta' + \dot{\vartheta}'\,dt$

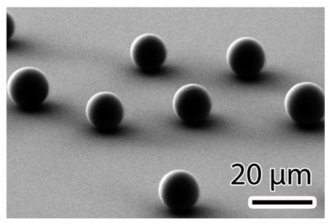
sliding: $f_t^0 > \mu_{s|d} f_n$ $\quad f_t = \mu_d f_n \hat{t}$ $\quad \vartheta = (f_t + \gamma_t\dot{\vartheta}')/k_t$

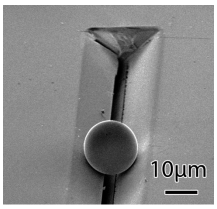


Nano-indenter -> contacts

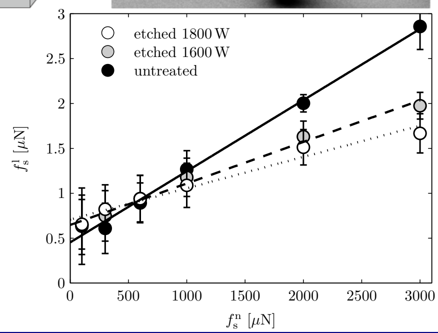






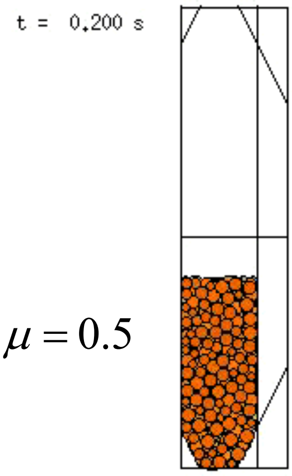


torsion
+rolling

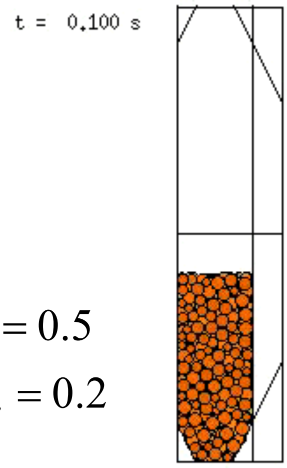


R. Fuchs et al. Granular Matter, 2014

Flow with friction & rolling resistance



$\mu = 0.5$



$\mu = 0.5$

$\mu_r = 0.2$

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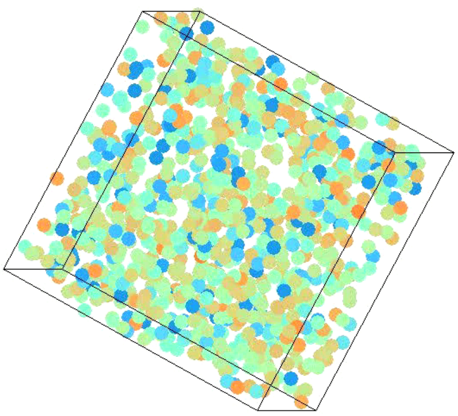
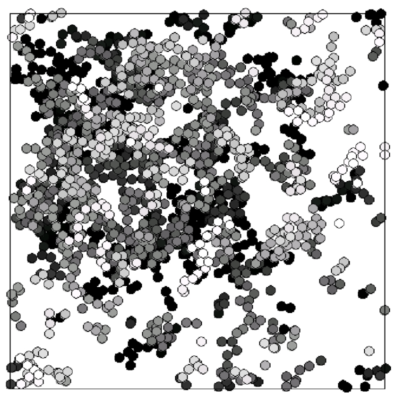
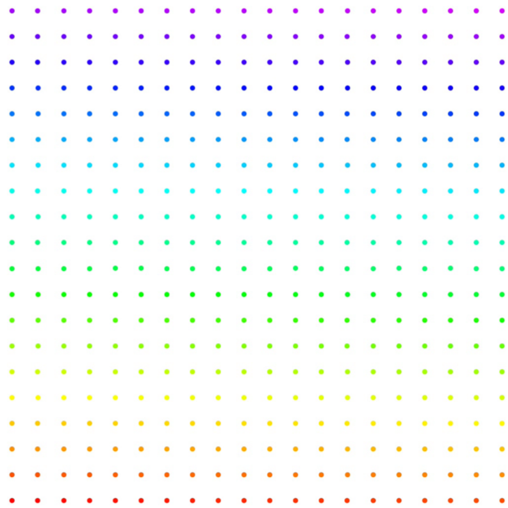
… details of interaction





Attraction + Dissipation = Agglomeration

Example: Agglomeration



S. Gonzalez-Briones, MSM, 2010

Asphalt modeling

T. Ormel, V. Magnanimo, H. ter Huerne, S. Luding

Tire&Road Consortium, CTW, University of Twente

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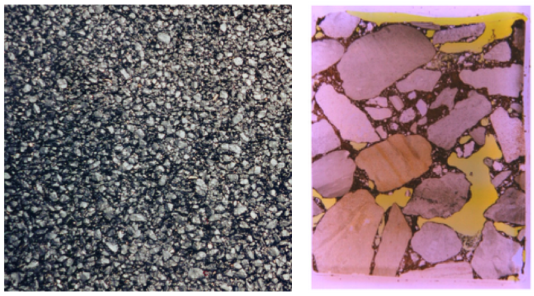
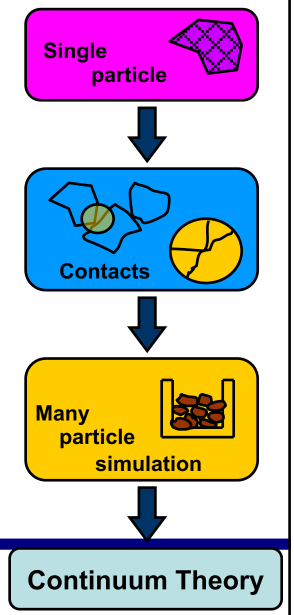
Materials with Microstructure

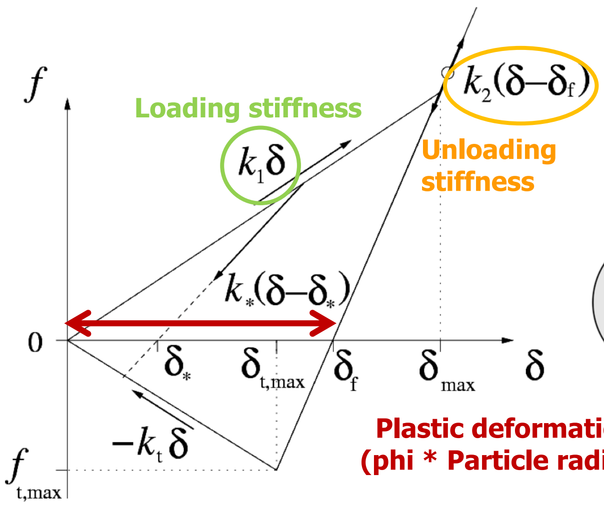


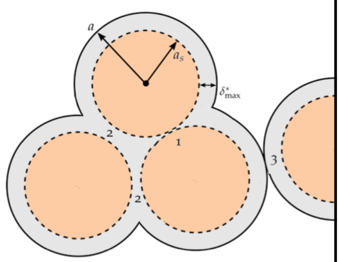
Asphalt samples

Can we model its internal structure and macroscopic response ?



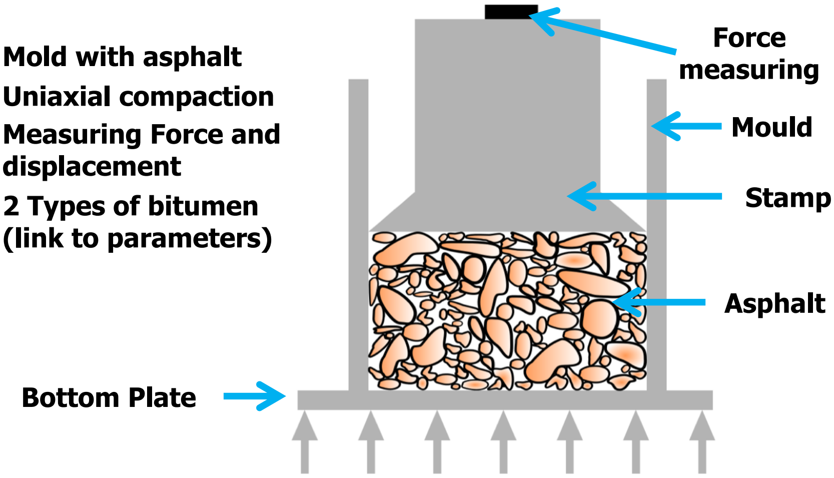
Loading/ Unloading stiffness



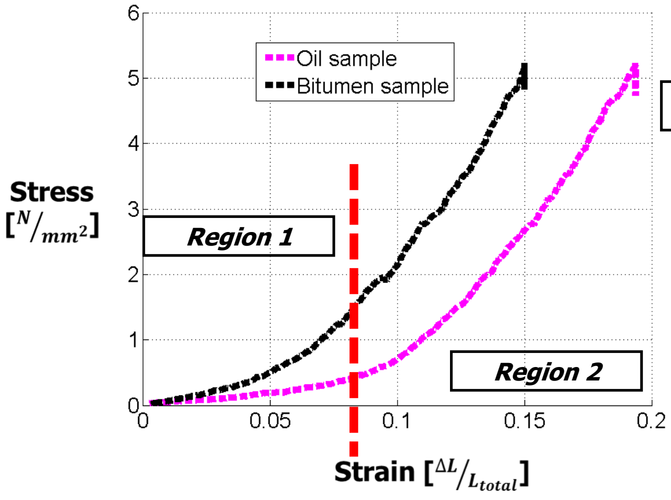


Experimental Compaction

- Mold with asphalt
- Uniaxial compaction
- Measuring Force and displacement
- 2 Types of bitumen (link to parameters)

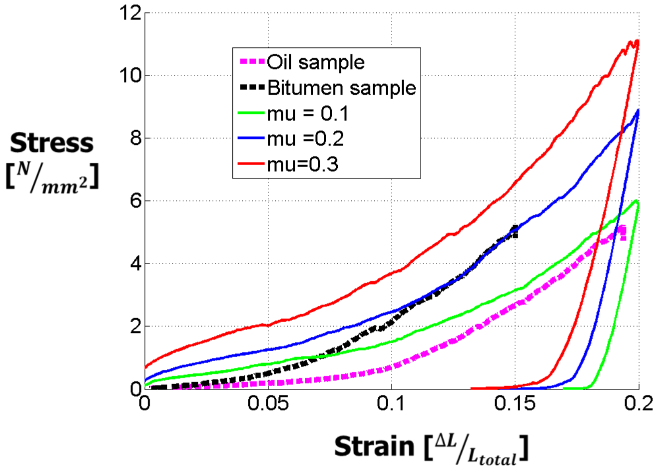


Results (Experimental)



Porous asphalt

Results (Experimental+DEM)



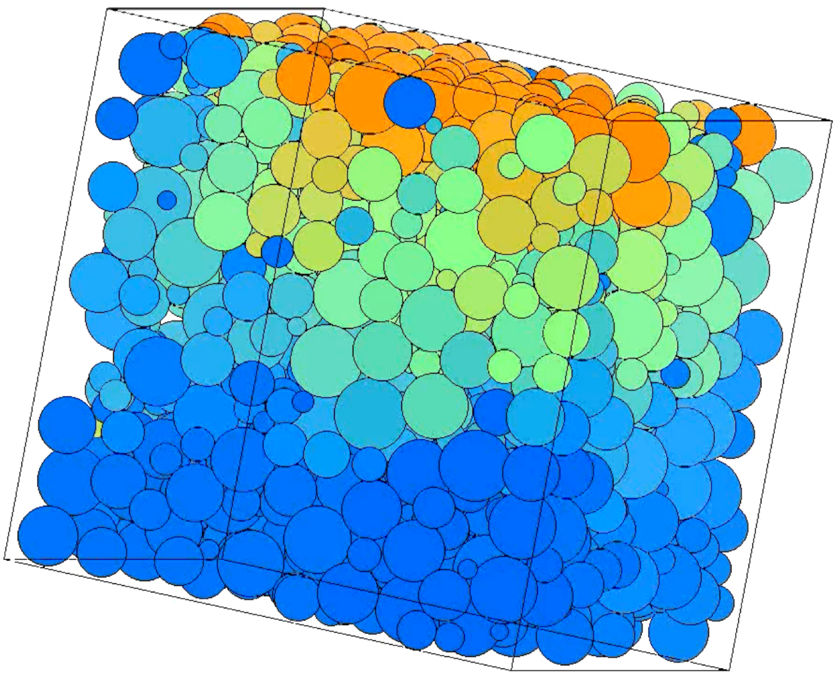
Phi=0.1
K1/K2 = 0.1

Conclusions & further research

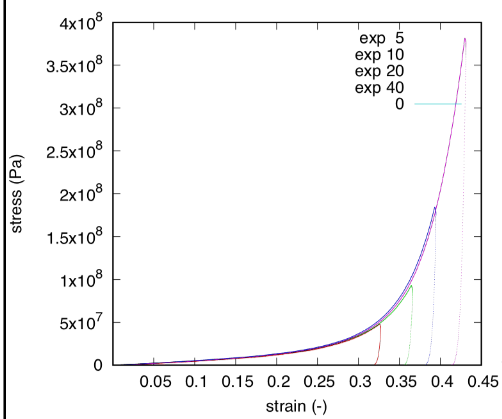
- **Simple DEM Model fits the experiments**
- **Parameters influencing the fit:**

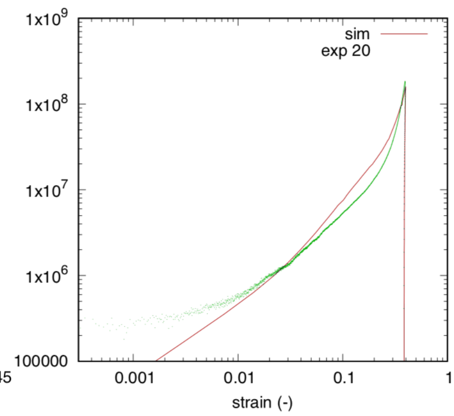
-	**Friction**	**(Scaling the curves)**
-	**K1**	**(Stress slope in region 1)**
-	**Phi**	**(Thickness of bitumen layer)**

- **Further research:**
  - **Link model to other asphalt mixes**
  - **Link discrete model to continuum material models**

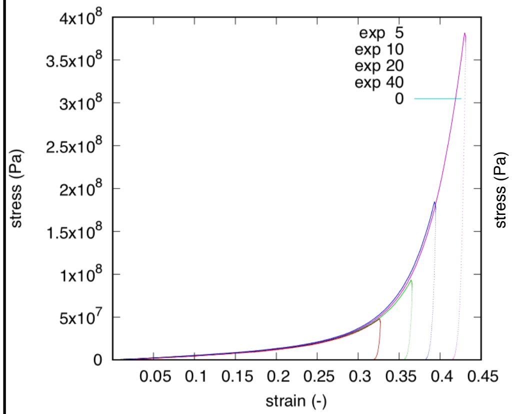


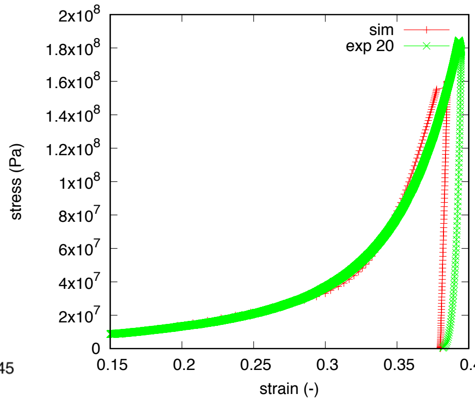
Tabletting (cohesive, fine limestone powder)
Experiments: R. Cabiscol TUBS
DEM: S. Luding



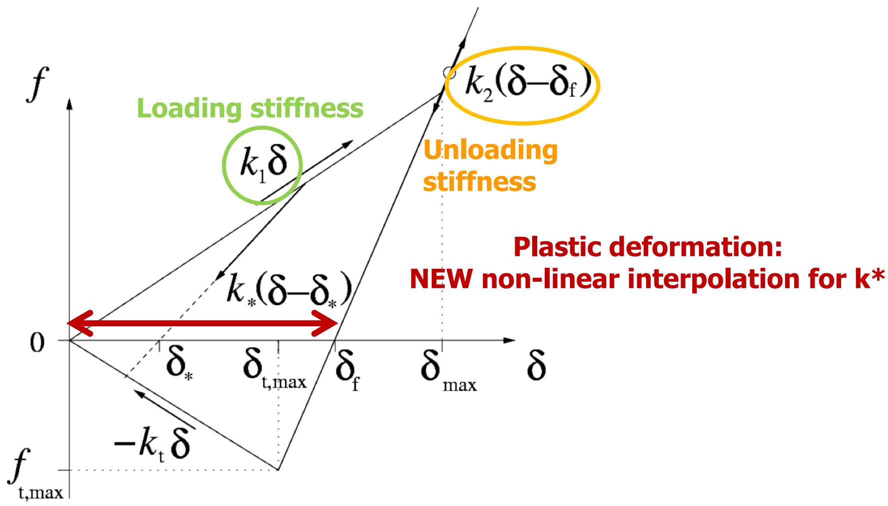


Tableting (cohesive, fine limestone powder)
Experiments: R. Cabiscol TUBS
calibration of DEM: S. Luding vs. H. Cheng



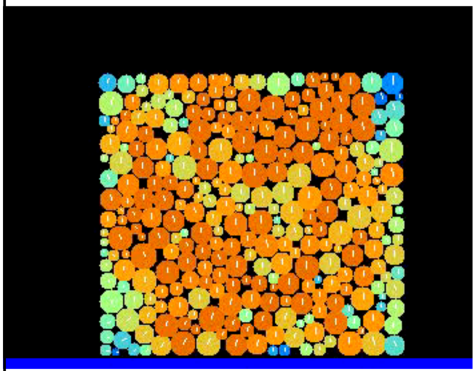


High stress tableting => NEW ingredient



Tabletting

Vibration test



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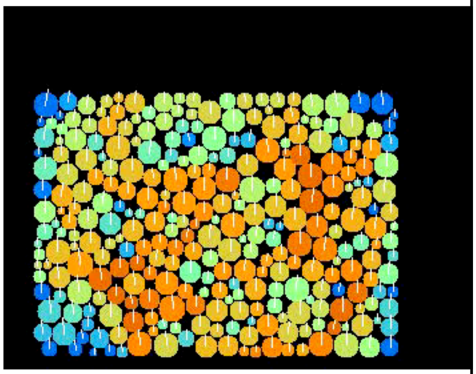

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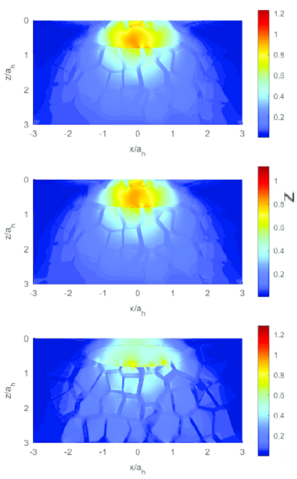
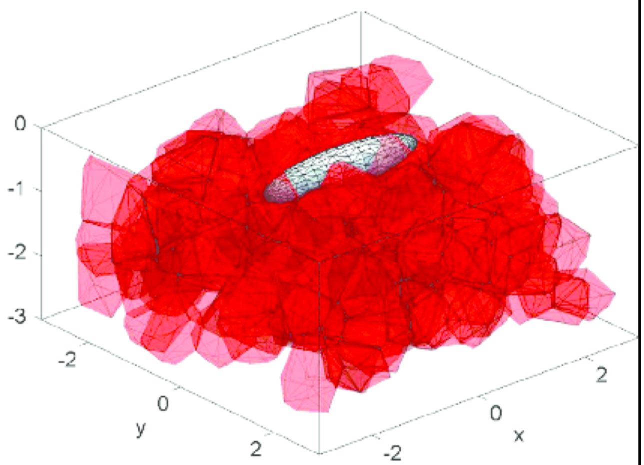
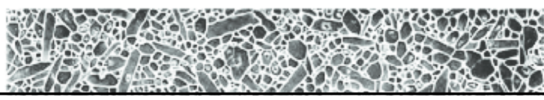
Results (3D Multigrid FEM)

H. Boffy and K. Venner, 2014







We can simulate:

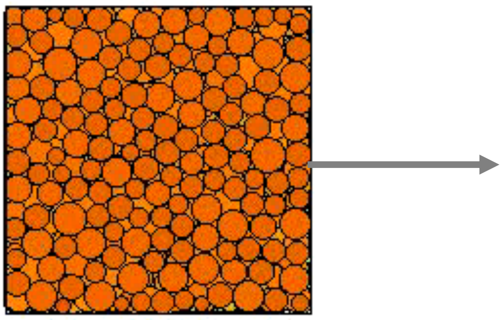
+ element tests (REV)
+ small processes & equipment

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

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

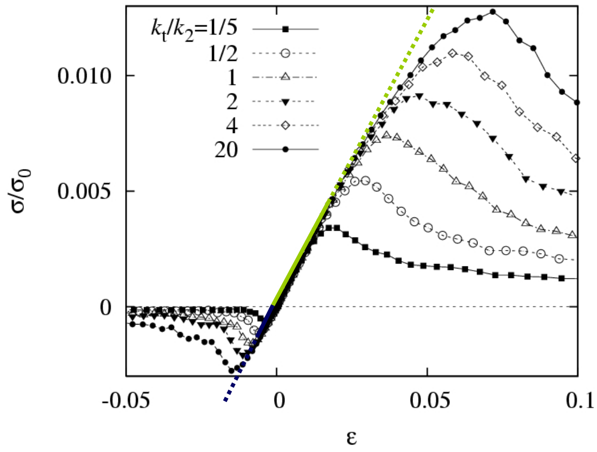
tension - uni-axial

$k_t / k_2 = 1/2$



uni-axial compression-tension

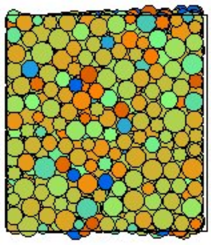
- Compression
- Tension

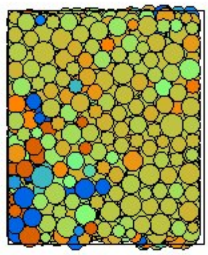


compression - uni-axial

$k_t / k_2 = 1/2$

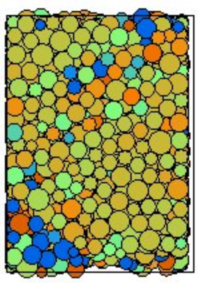
compression - uni-axial

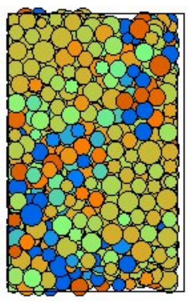




$k_t/k_2 = 1/2$

compression - uni-axial





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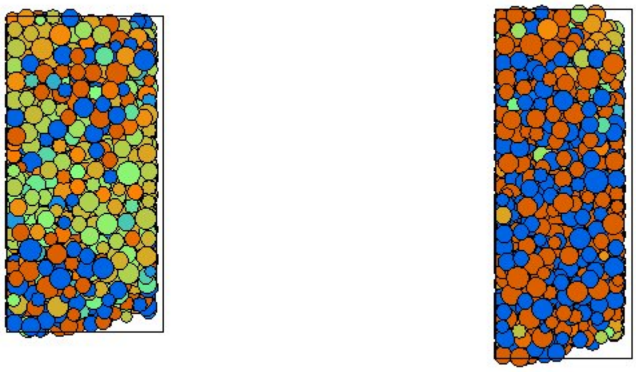
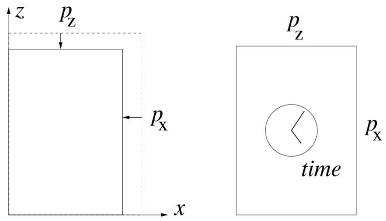
compression - uni-axial

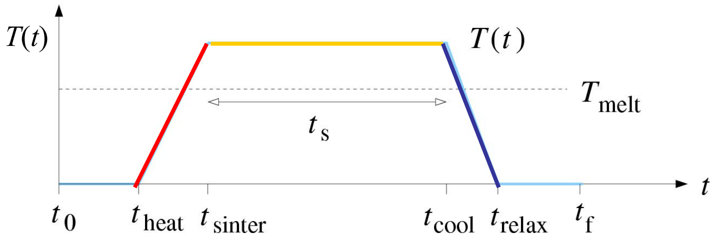


$k_t / k_2 = 1/2$

Sintering / Cementation (back to 2D)

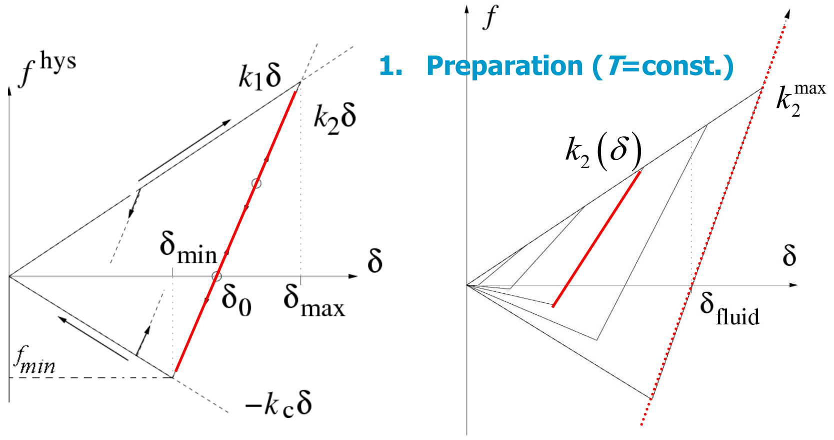
1. Preparation
2. Heating
3. Sintering / Cementation
4. Cooling
5. Relaxation
6. Testing





cold contacts – loose grains

1. Preparation (T=const.)

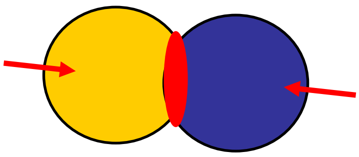


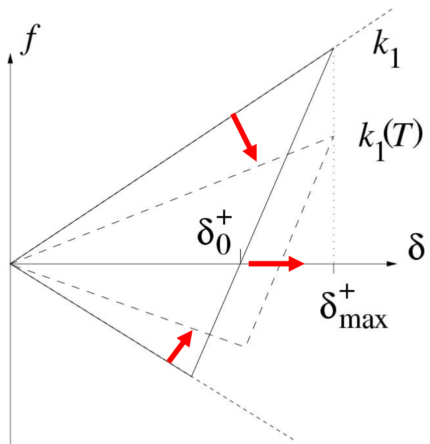
loading stiffness: $k_1 = k_1(T)$

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

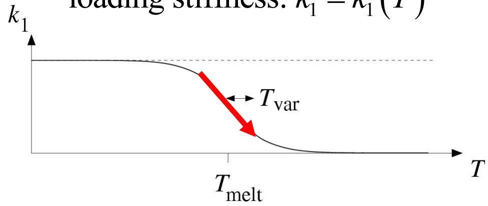
Sintering / Cem.

2. Heating





loading stiffness: $k_1 = k_1(T)$

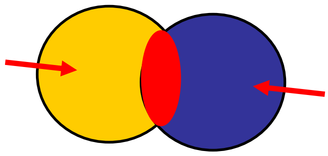


maximum overlap fixed: δ_{max}^+

neutral overlap increasing: δ_0^+

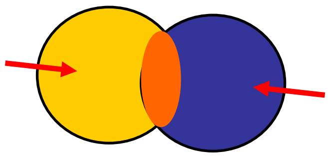
Sintering / Cem. 3

3. Sintering / Cementation - Reaction



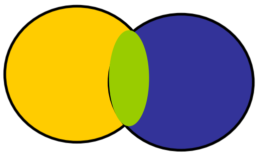
Sintering 4

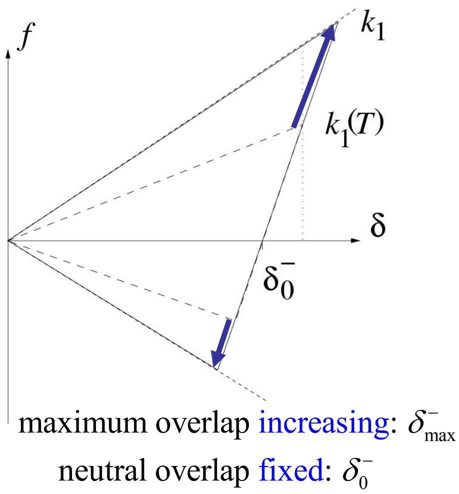
4. Cooling



Sintering 4

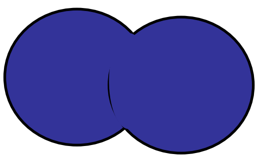
4. **Cooling**





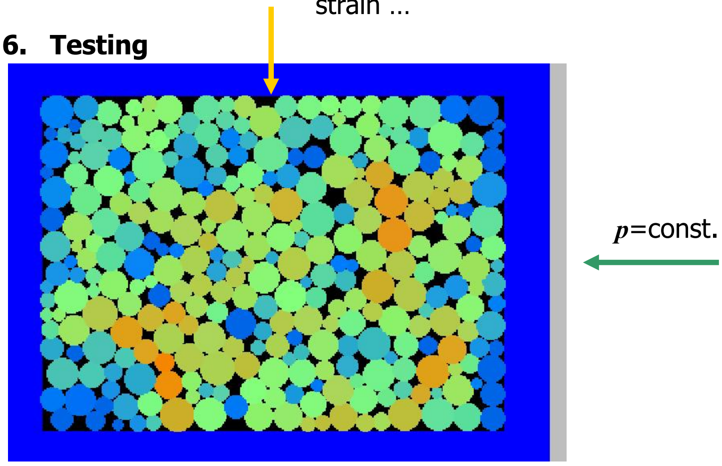
Sintering 5

5. **Relaxation**



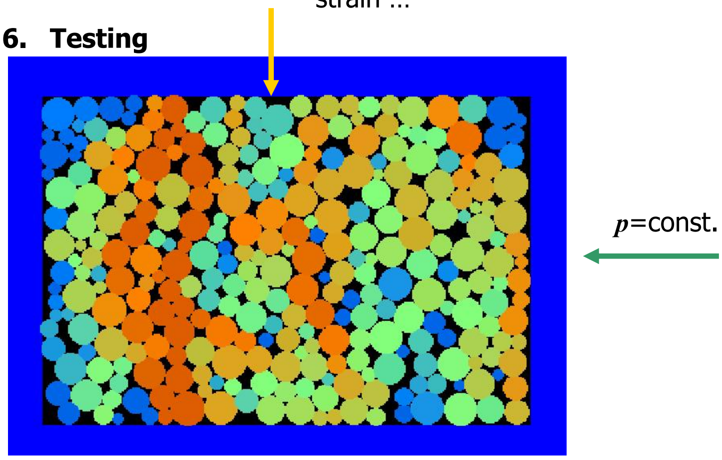
Sintering 6

6. **Testing**



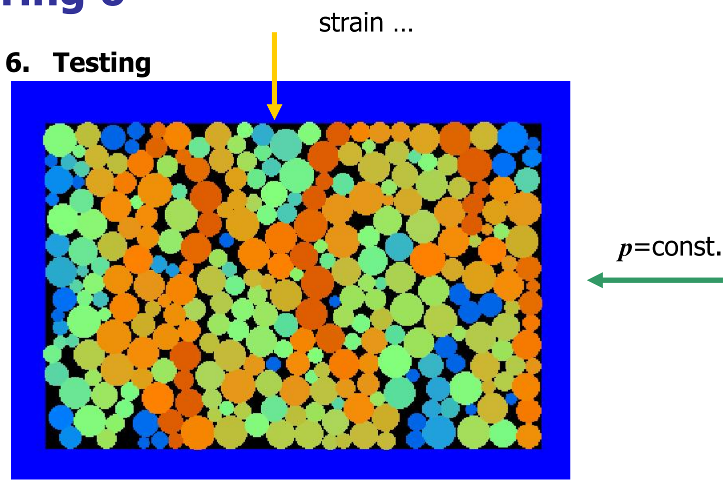
Sintering 6

6. **Testing**



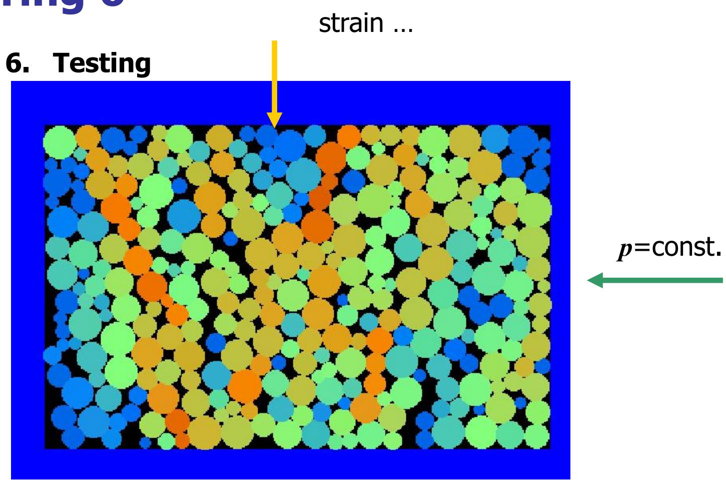
Sintering 6

6. Testing



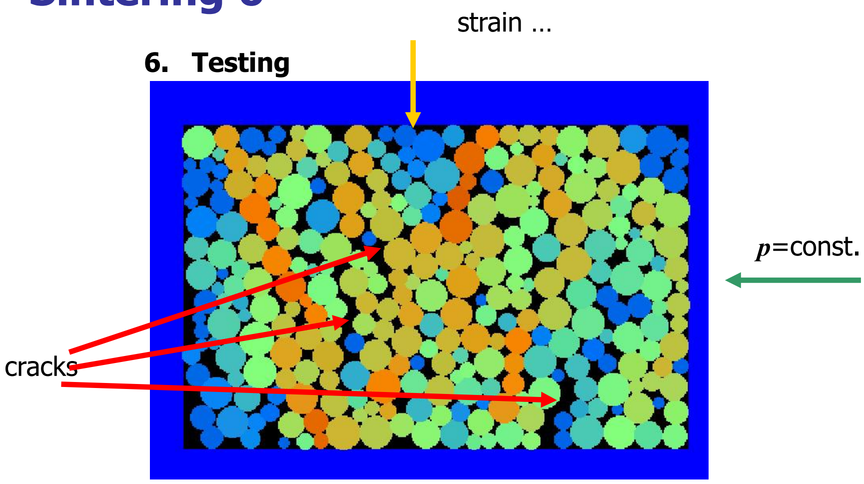
Sintering 6

6. Testing



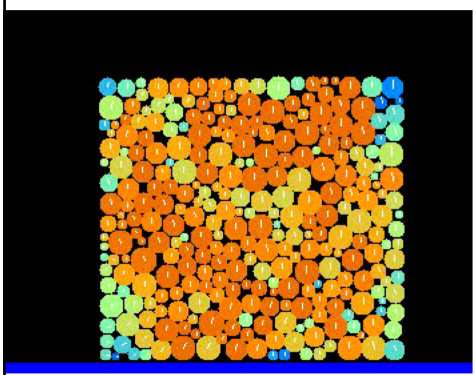
Sintering 6

6. Testing



Sintering (Temperature+Pressure)

Vibration test



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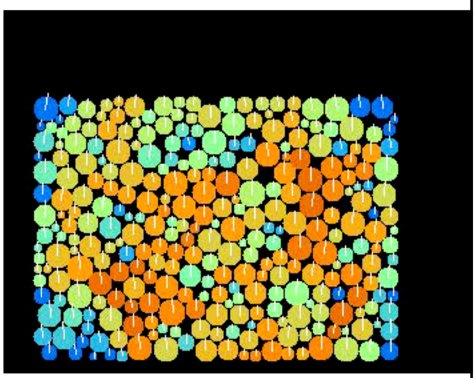

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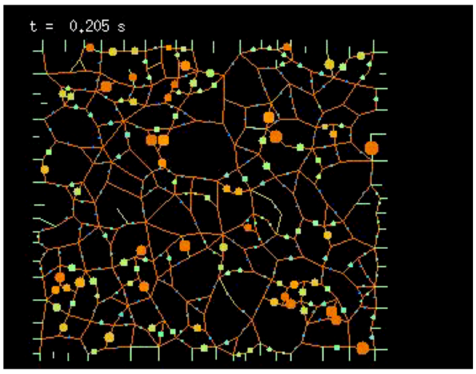
Sintering

Vibration test



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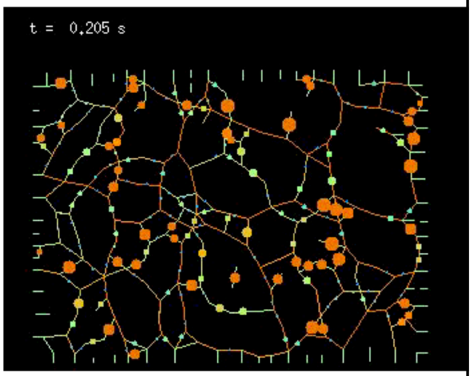

p=10

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– especially of fine, cohesive powders

Instead:
+ provide constitutive relations
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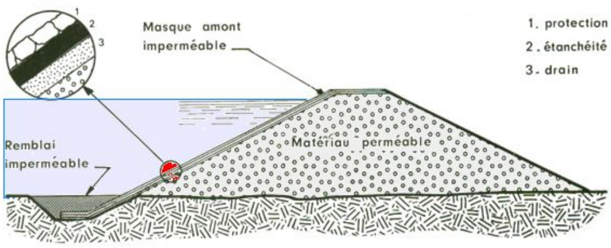
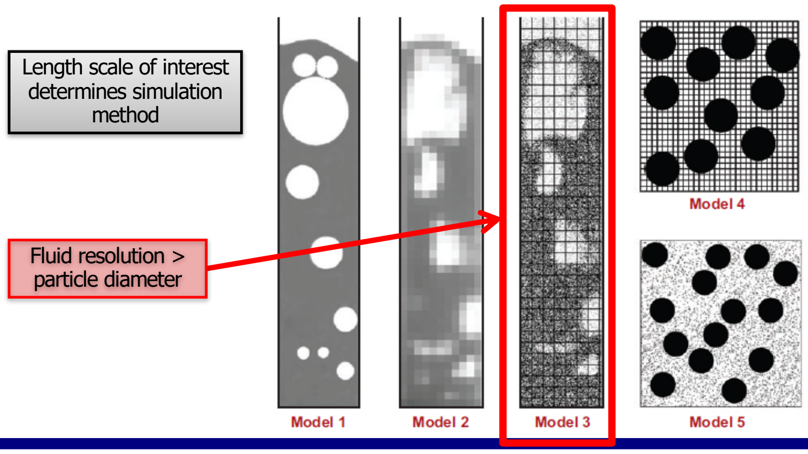
Literature (http://www2.msm.ctw.utwente.nl/sluding/publications.html)
[1] S. Luding *Collisions & Contacts between two particles,*
in: Physics of dry granular Media, eds. H. J. Herrmann, J.-P. Hovi, and S. Luding, Kluwer Academic Publishers, Dordrecht, 1998
[http://www2.msm.ctw.utwente.nl/sluding/PAPERS/coll2p.pdf]
[2] S. Luding, I*ntroduction 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]
[3] S. Luding, C*ohesive frictional powders: Contact models for tension*
Granular Matter 10(4), 235-246, 2008
[http://www2.msm.ctw.utwente.nl/sluding/PAPERS/LudingC5.pdf]
[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]



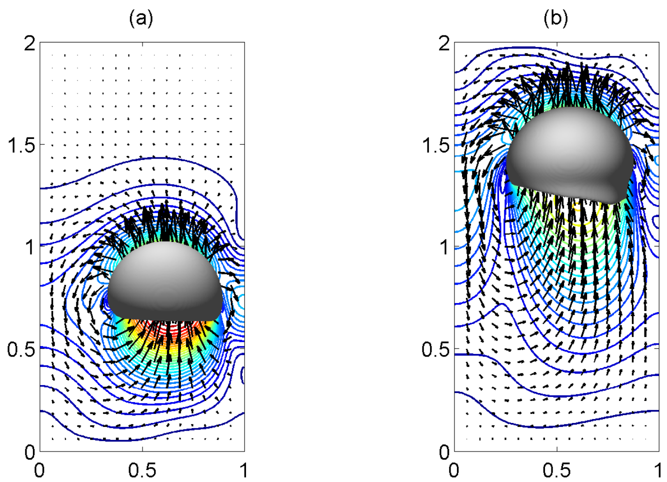
N. Limmen and J. F. van den hoogen

Fluid-particle simulation – multiscale …
but which length scale?



Van der Hoef, M. A., van Sint Annaland, Deen, N. G., & Kuipers, J. A. M. (2008).
Numerical simulation of dense gas-solid uidized beds: A multiscale modeling strategy.
Annual Review of Fluid Mechanics, 40 (1), 47-70.

Recent research: 1. bubble 2-phase flow
PhD thesis: *P. Cifani* (H. Kuerten, B. Geurts) UT



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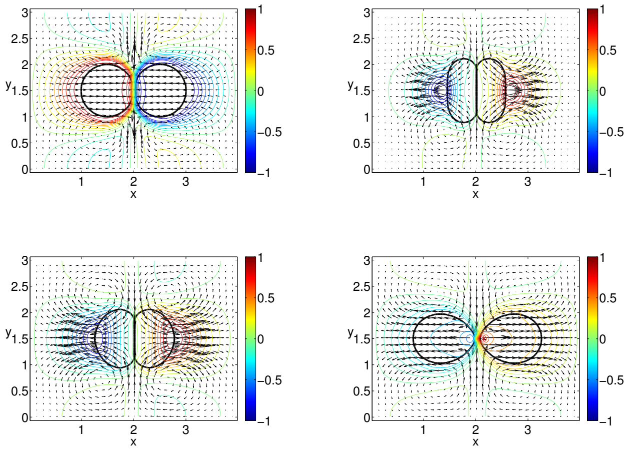

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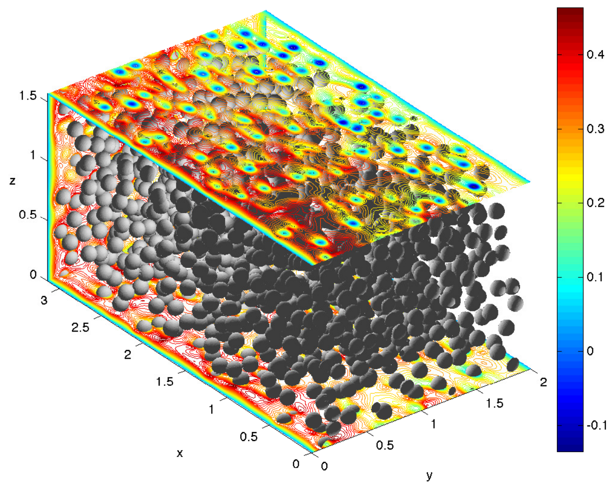
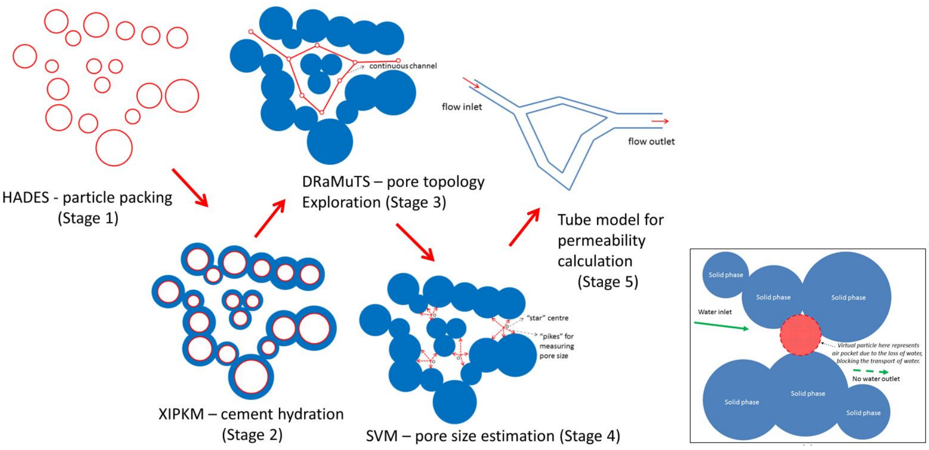


Recent research: 2. porous/cement 3-phase flow PhD thesis: K. Li (M. Stroeven, L. J. Sluys) TUD



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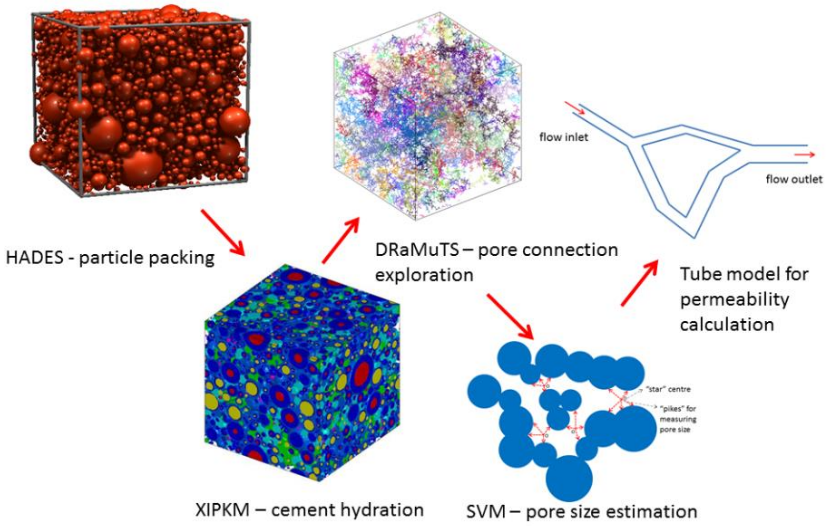
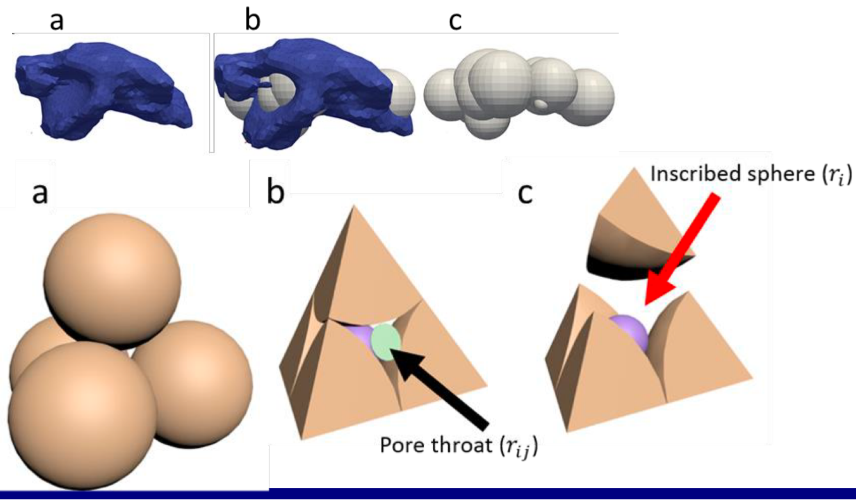


Recent research: 3. swelling particles (YADE, UU)
PhD thesis: T. Sweijen (B. Chareyre, M. Hasanizadeh)



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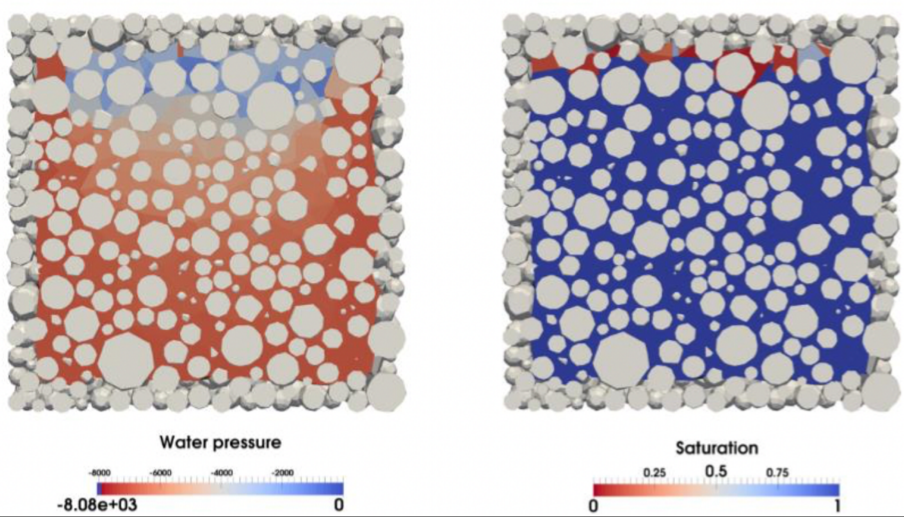
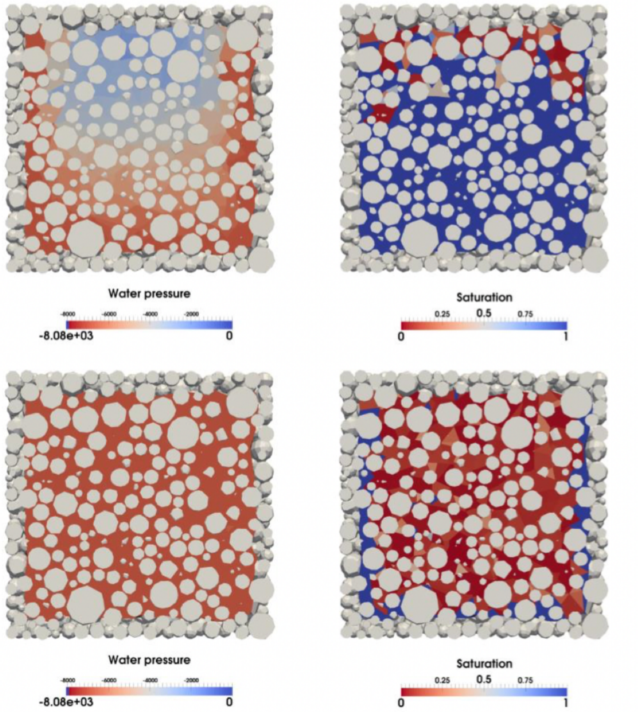
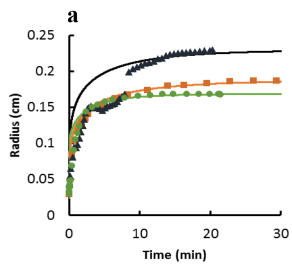
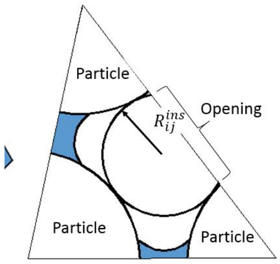
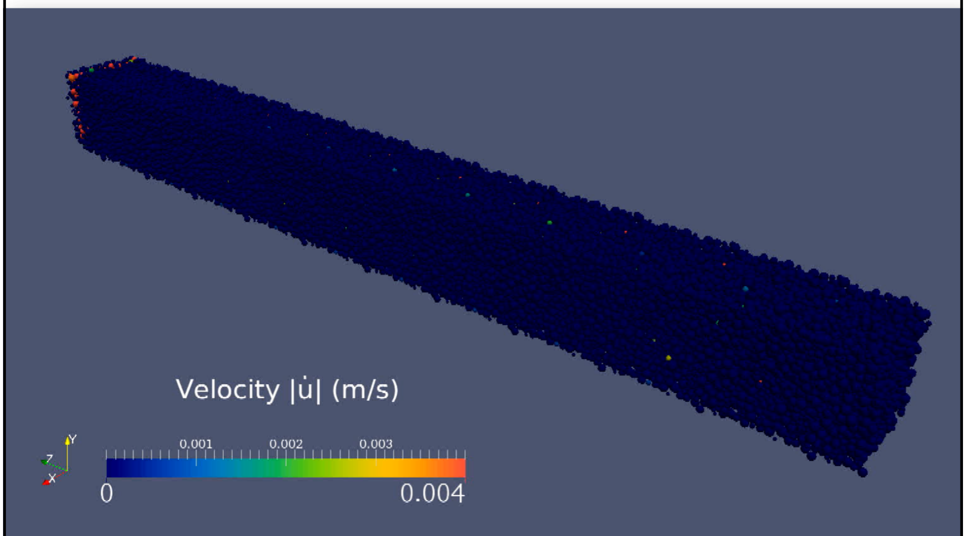




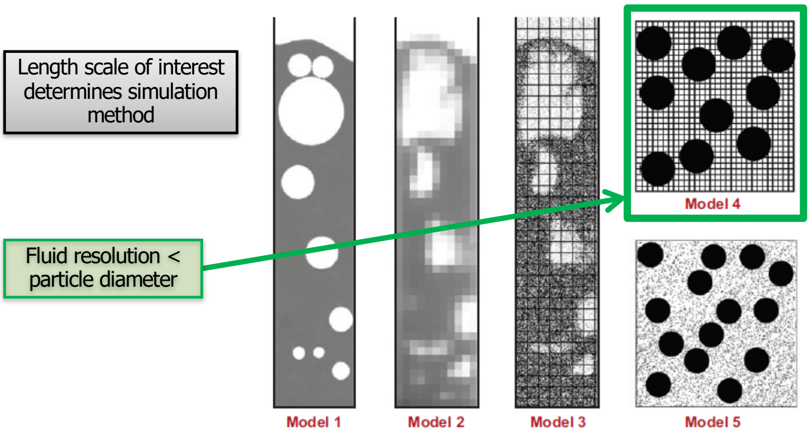




Example: Mechanical Wave Propagation in Solids



Fluid-particle simulation – multiscale …
but which length scale?



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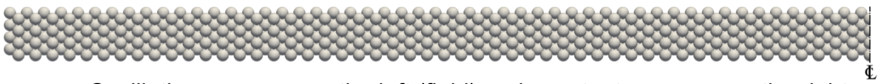
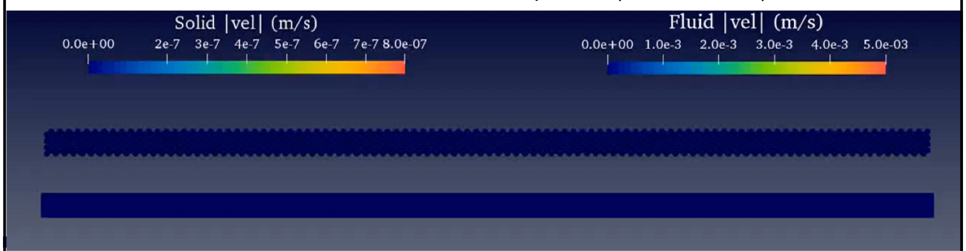
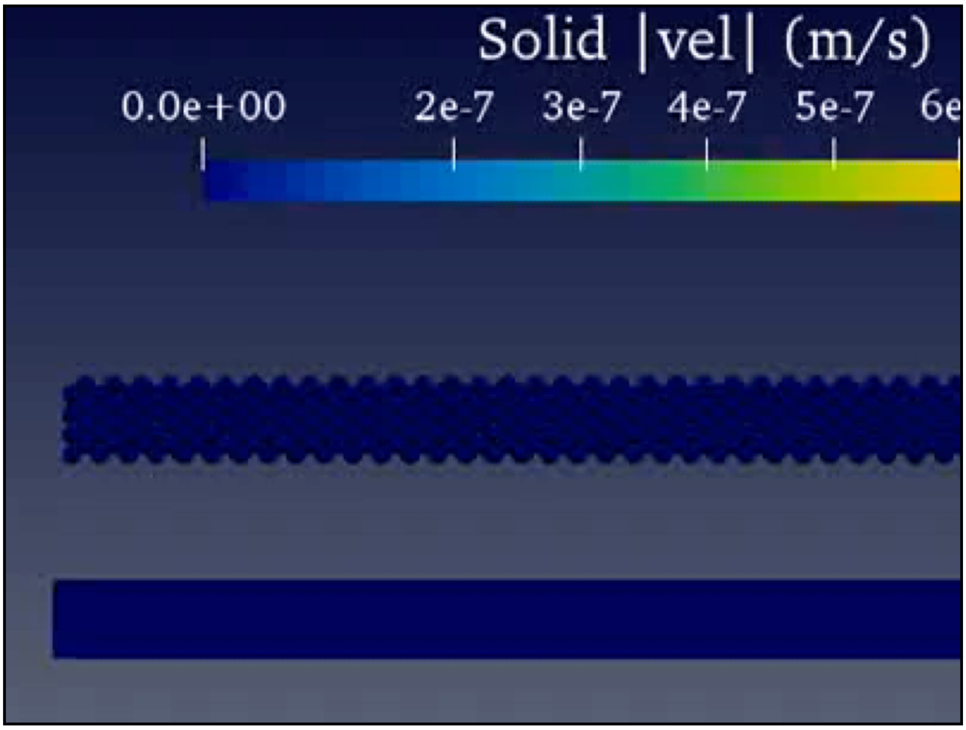
System setup

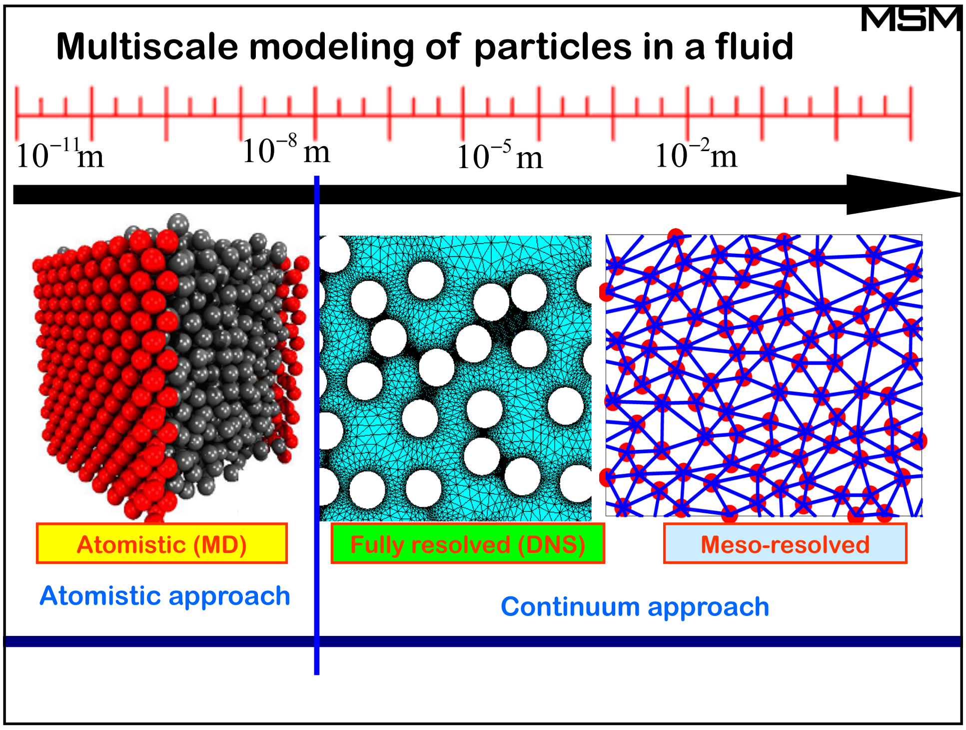
- A fully saturated granular system (FCC + fluid):



  - Oscillating pressure on the left (fluid) and constant pressure on the right (fluid) and periodic boundary condition
  - First and last layer fixed to have effective pressure on the solid, ranging from 0.1 Mpa to 30 MPa
  - Young's modulus and Poisson's ratio: 70 GPa and 0.2
  - Contact law: Hertzian for frictionless spheres (R = 0.02 mm)

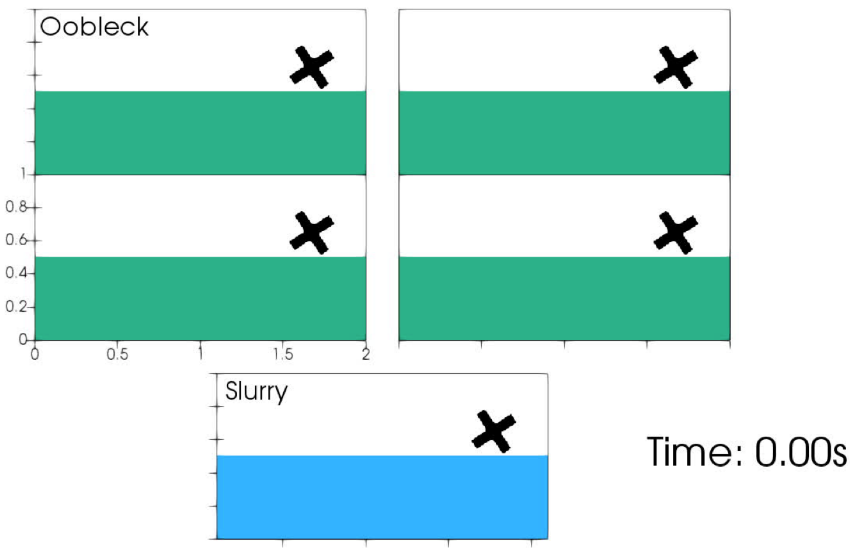



Solid |vel| (m/s)
0.0e+00
2e-7
3e-7
4e-7
5e-7
6e


MSM
Multiscale modeling of particles in a fluid
10^-11 m
10^-8 m
10^-5 m
10^-2 m
Atomistic (MD)
Fully resolved (DNS)
Meso-resolved
Atomistic approach
Continuum approach

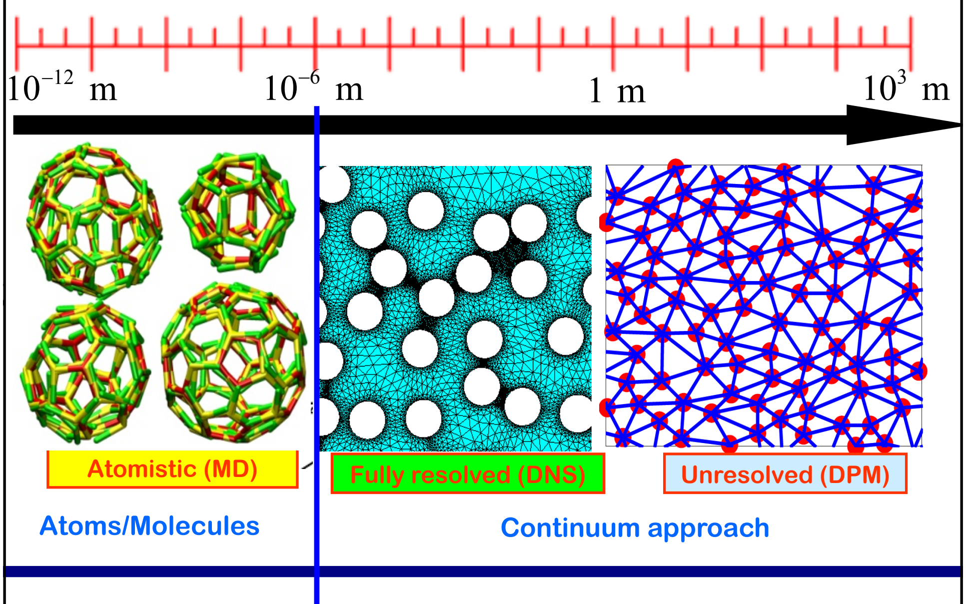
Upscaling challenge (movie by: Ken Kamrin)

Constitutive relations => continuum solver



MSM

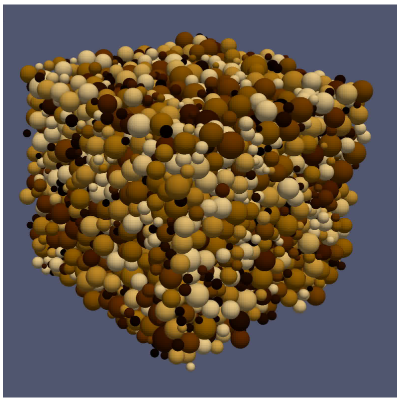
Multiscale modeling



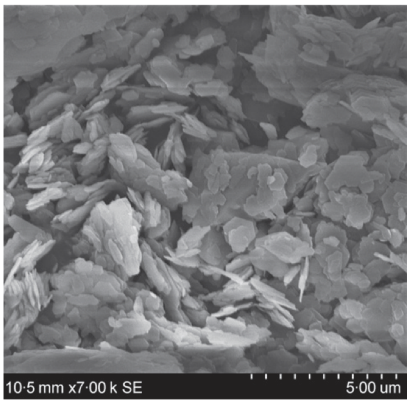
W.denOtter & R.Hartkamp K. Yazdchi, I. Gueven M. Robinson, S. Srivastava

Modelling non-spherical (clay) particles

Numerical sample

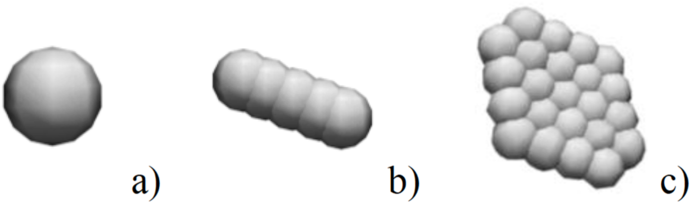


SEM of kaolin clay in water

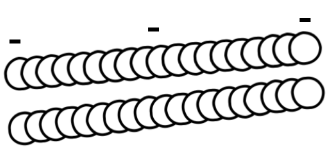


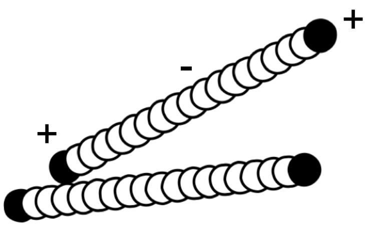
[Pedrotti & Tarantino, Strathclyde]

Clay particles



Sphere | Flexible Rod/Fiber | Platelet

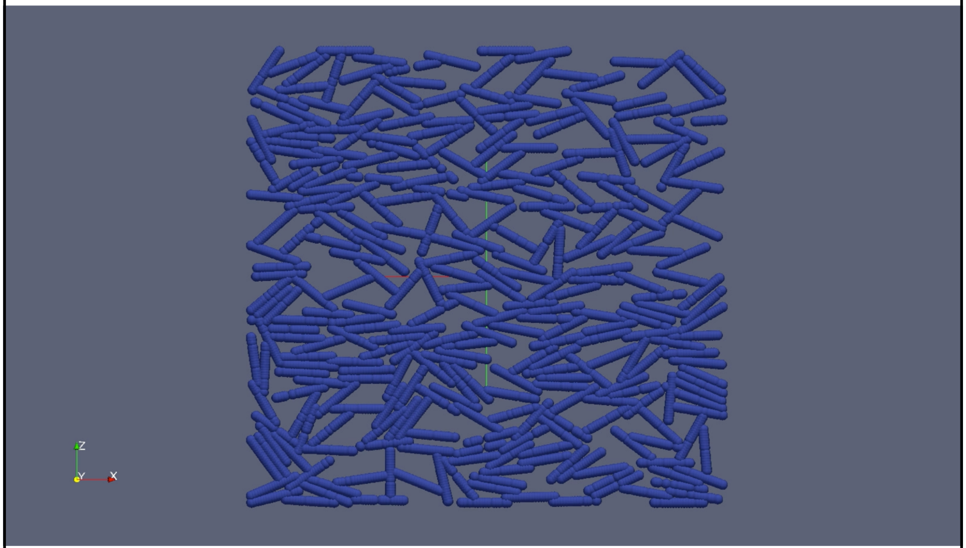




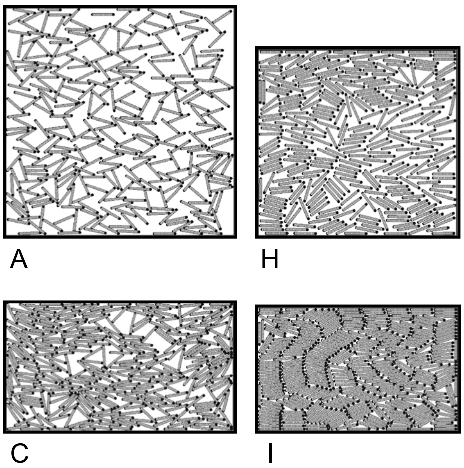
Face-to-Face
negative charges

Edge-to-Face
negative/positive charges

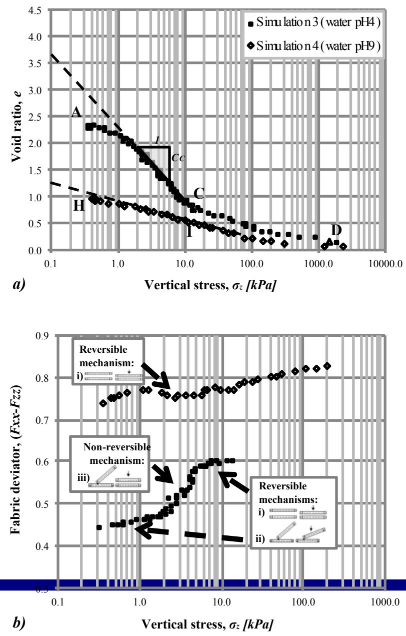
Clay particles



Clay particles

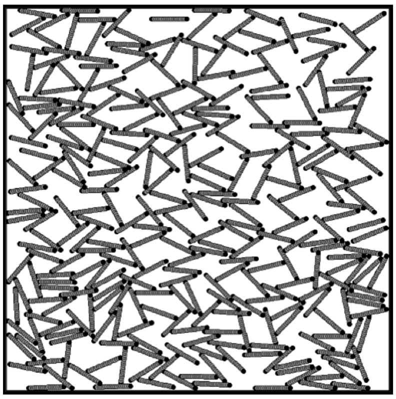


Water pH4 Water pH9

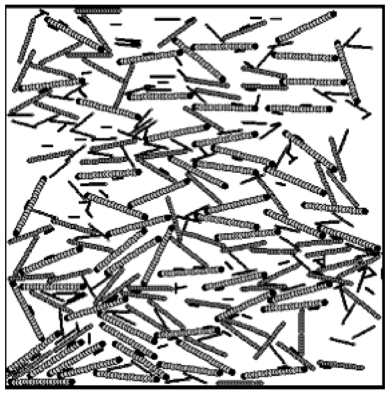


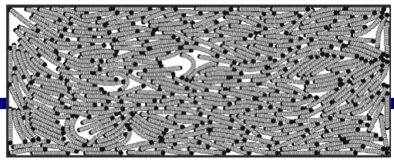
[Pagano, Magnanimo, et al., under review, Géotechnique, 2018]

Additional features of rods/fibers



A





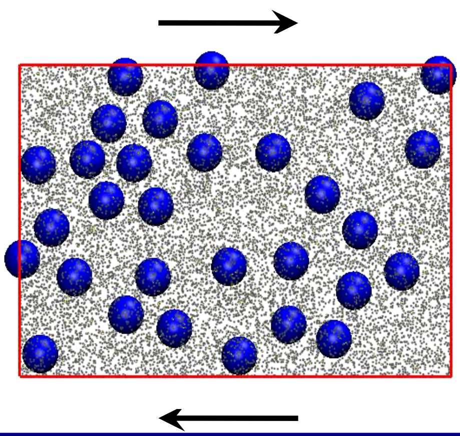
D

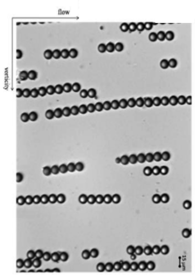
Polydispersity

Bending = soft fibers

What if? nanoscopic particles in visco-elastic fluids

paint, toothpaste, mayonaise, etc



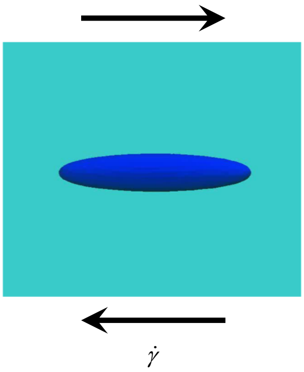


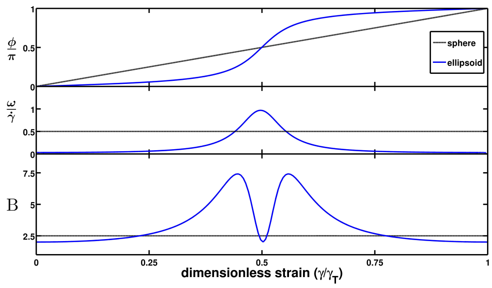
continued in project with
CBP and Apollo-Vredestein

5

Simulation of ellipsoid under shear

(using analytical mobility matrix, non-Brownian)





simulations agree with Jeffery

S. Kim and S.J. Karrila, *Microhydrodynamics Principles and selected applications (1991)*
G.B. Jeffery, *Proc. Royal Soc. London A* **102** 161 (1922)

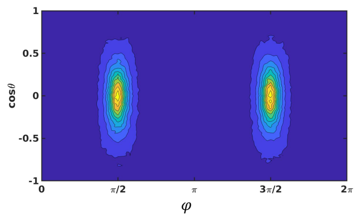
6

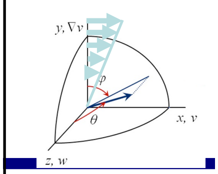
Orientation of ellipsoid under shear

(with-Brownian)

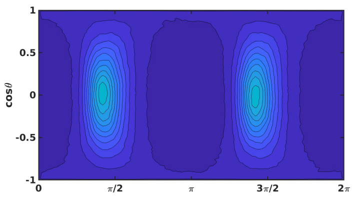
$$Pe = \frac{\dot{\gamma}}{D_{rot}}$$

$Pe = 100$

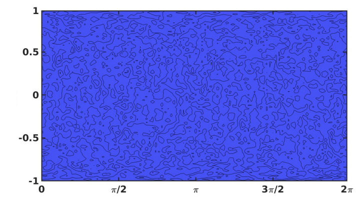


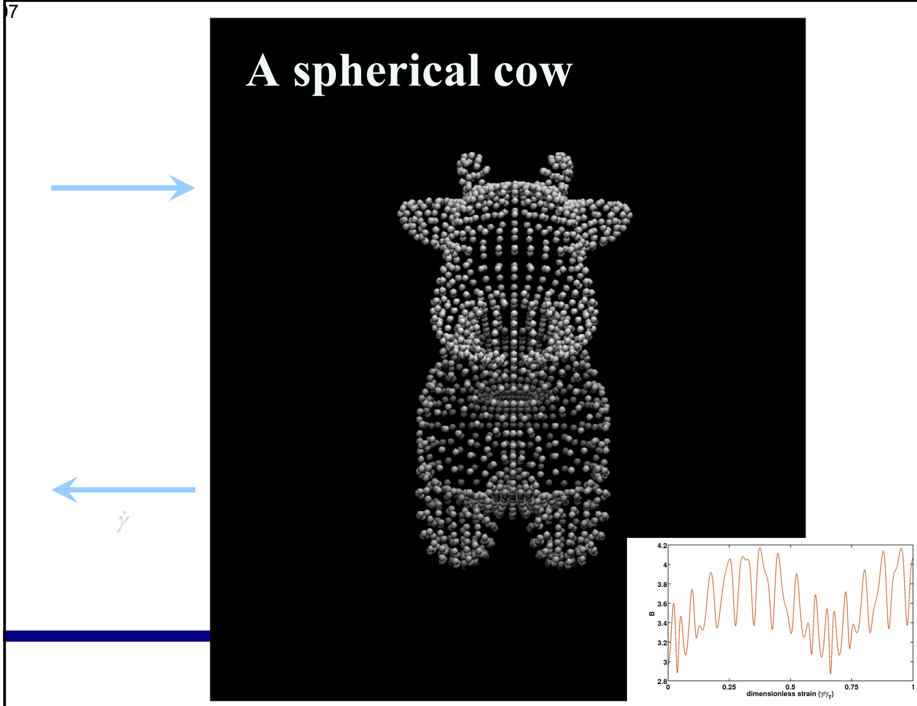


$Pe = 1$



$Pe = 0$





Biaxial box element test

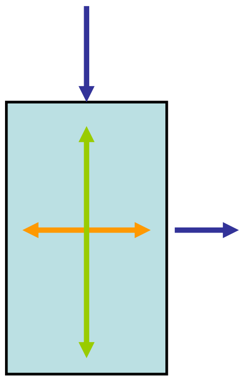
- Top wall: strain controlled

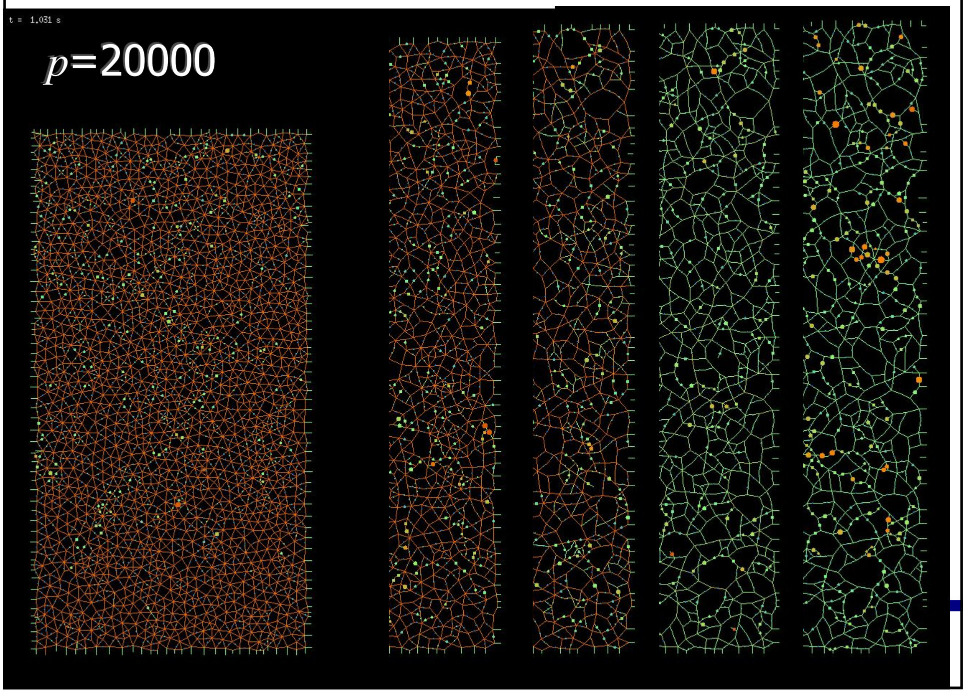
$$z(t) = z_f + \frac{z_0 - z_f}{2}\left(1 + \cos \omega t\right)$$

- Right wall: stress controlled

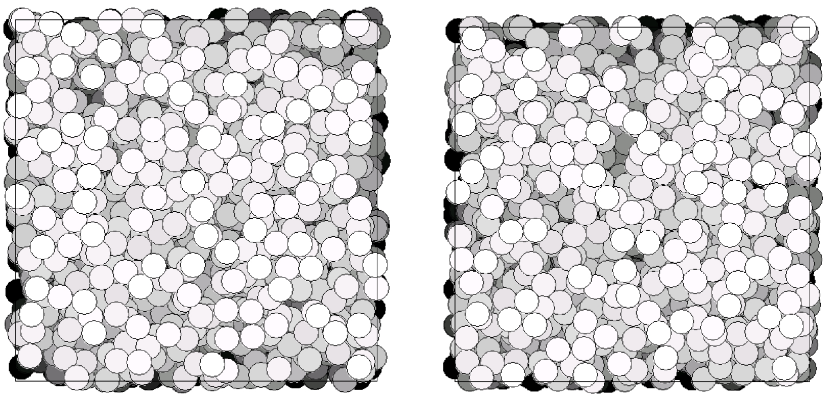
$$p = \text{const.}$$

- Evolution with time … ?



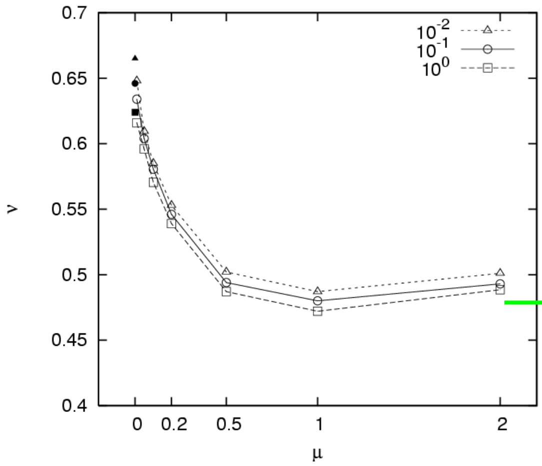


3D - Initial Condition Density ?
… van der Waals adhesion



- clusters/agglomerates form …

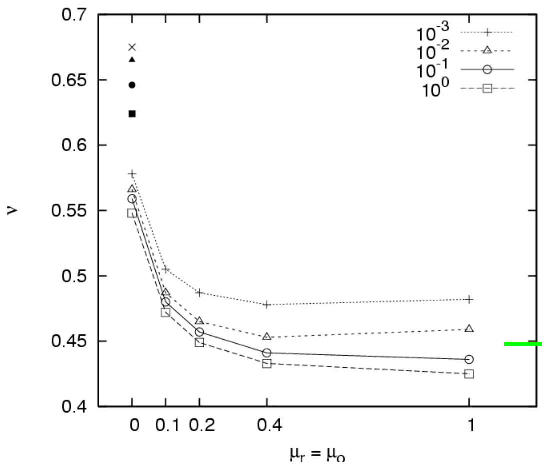
3D – Density vs. friciton …



ν=0.48

- Sättigung bei hoher Reibung

3D – Density vs. rolling-resistance



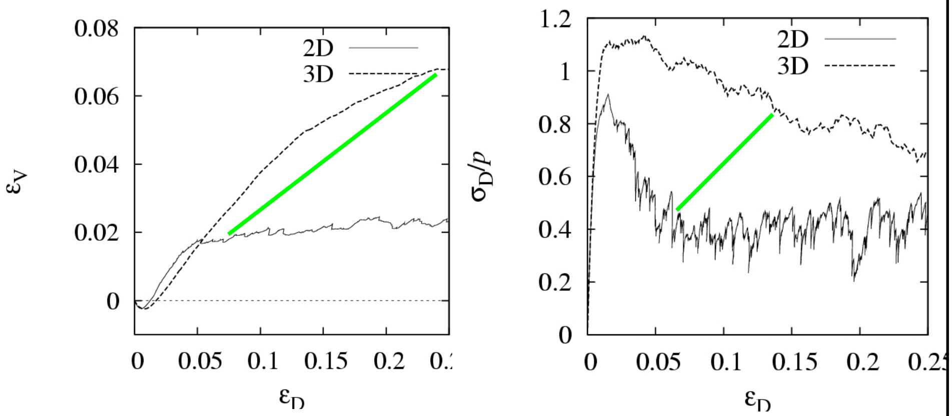
ν=0.45

- Sättigung bei hohem Rollwiderstand

2 dimensions or 3 dimensions?

2D	3D
• disks	spheres
• polygons, …	polyedra, …
• density/porosity	
Area-fraction	Volume-fraction
• Visualization	
SIMPLE ☺	less simple
• learn …	
	practical use

2D-3D – comparison?



• Saturation at large friction coefficients

Constitutive model
various deformation modes

Mode 0: Isotropic $d\gamma = 0$

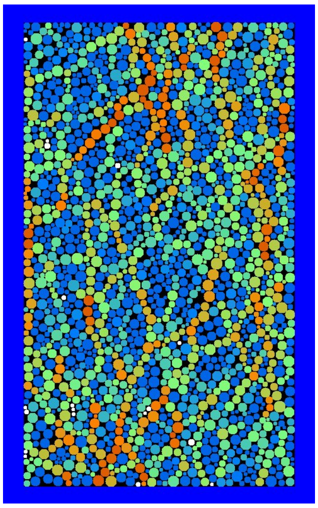
Mode 1: Uni-axial

Mode 2: Deviatoric $\varepsilon_V = 0$

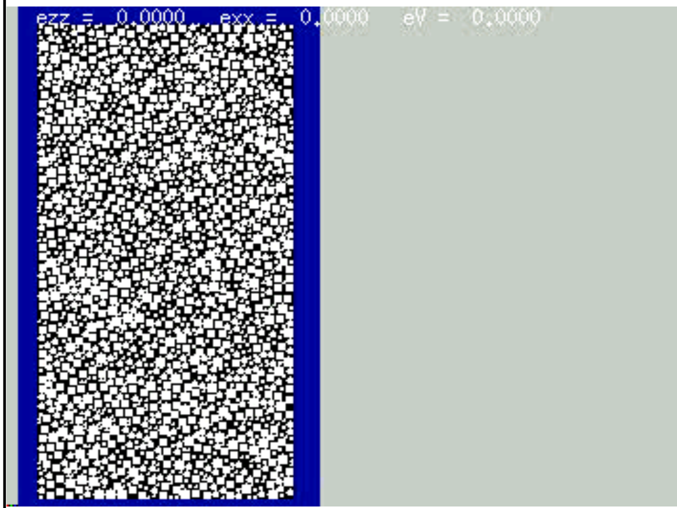
Mode 3: Bi-axial (side-stress controlled)

Mode 4: Bi-axial (isobaric, p-contolled)

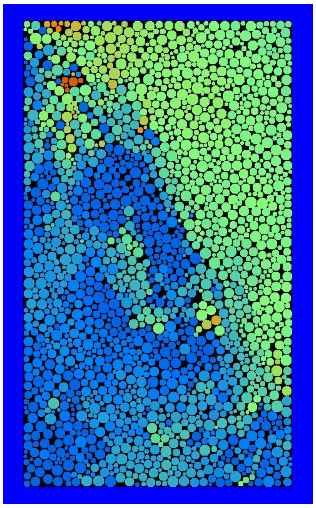
Bi-axial box (stress chains)



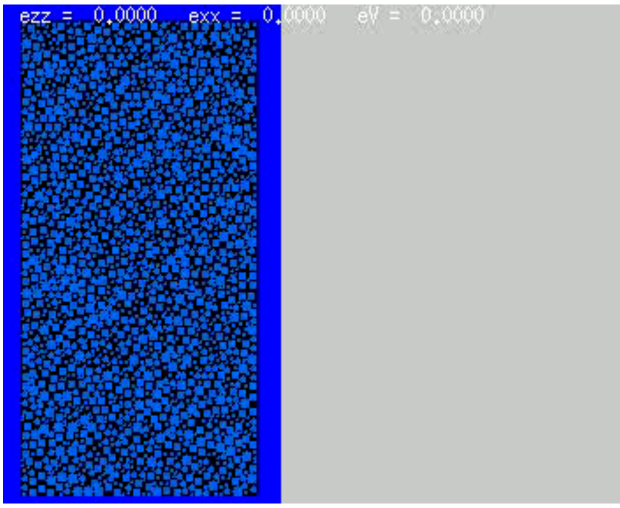
Bi-axial box (stress chains)



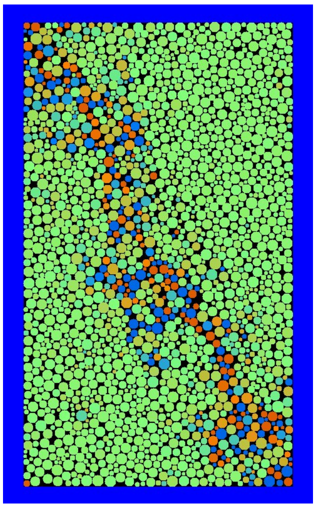
Bi-axial box (kinetic energy)



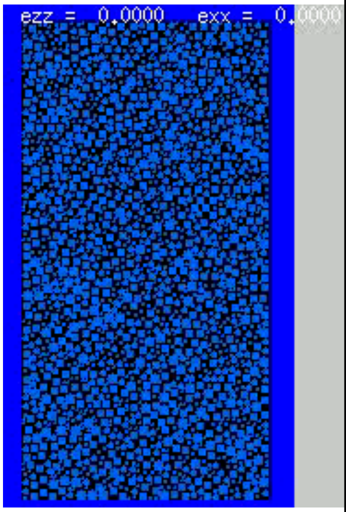
Bi-axial box (kinetic energy)



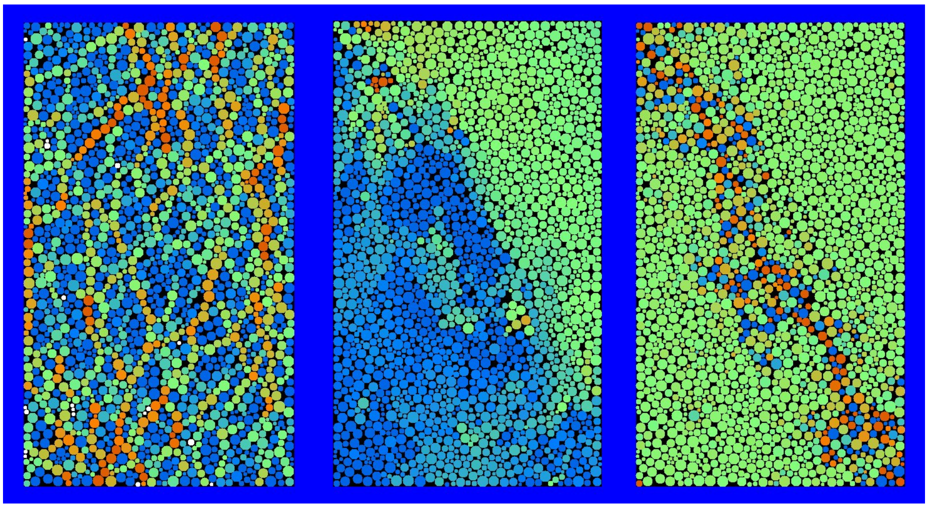
Bi-axial box (rotations)



Bi-axial box (rotations)

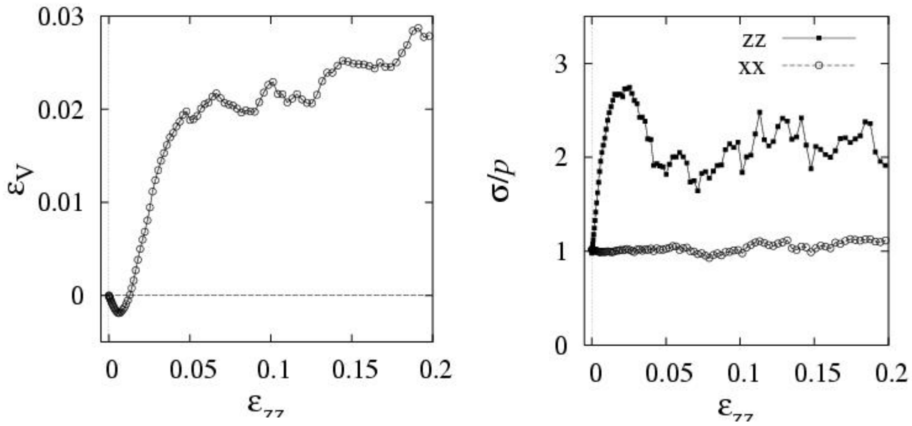


Multiple micro-mechanisms - challenge

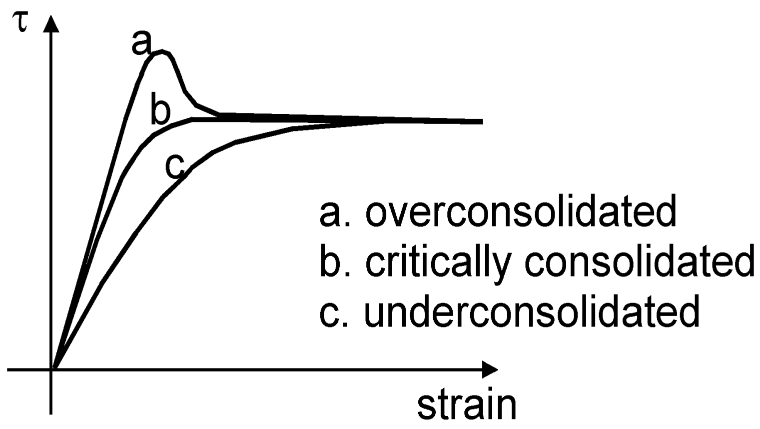


inhomogeneity & anisotropy, instabilities & structures, rotations

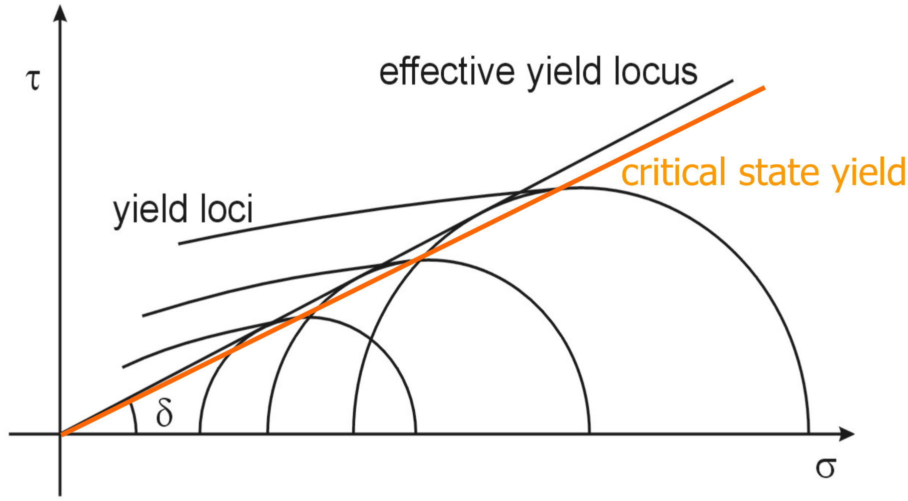
Bi-axial compression with p_x=const.



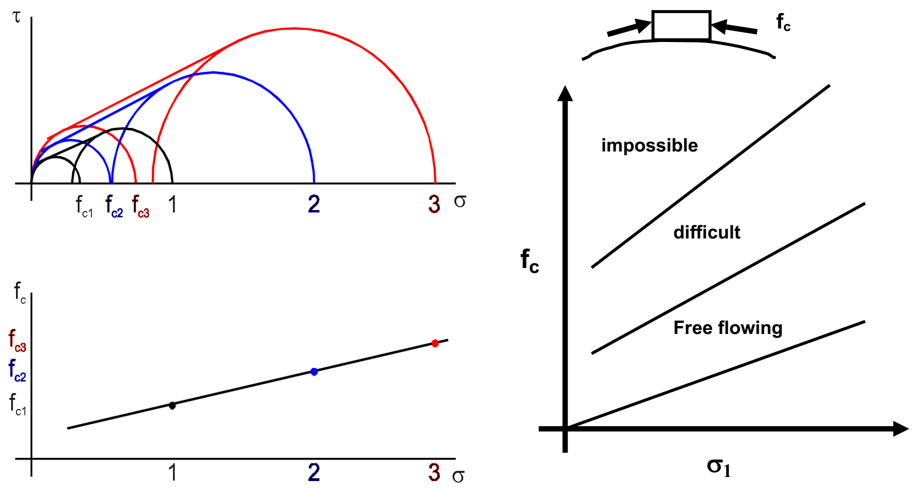
Microscopic interpretation: memory?



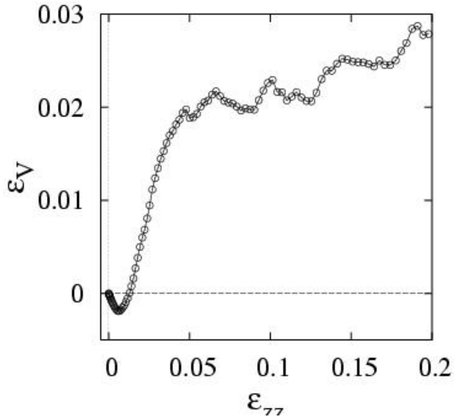
Yield loci

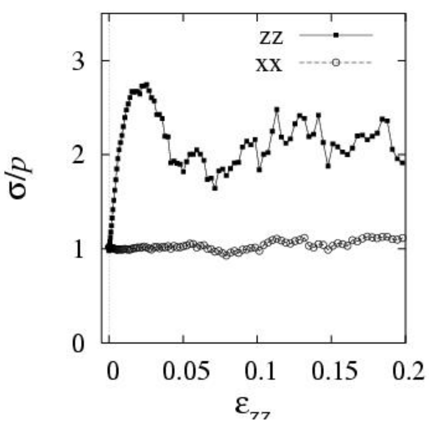


Flow behavior

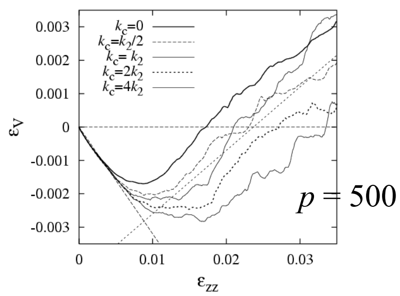


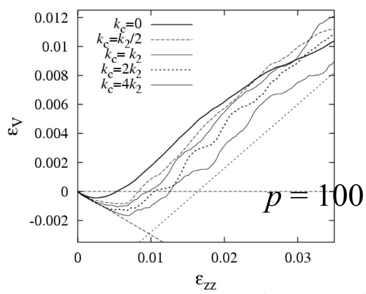
Bi-axial compression with p_x=const.





Material parameters





Initial Compression:

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

Poisson-ratio: $\nu \approx 0.66$

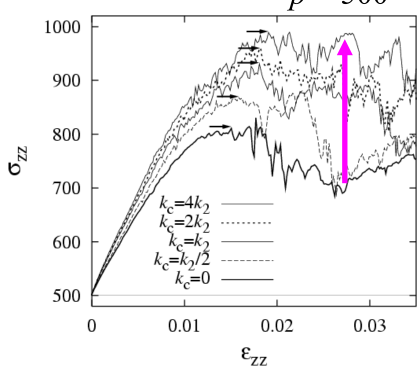
Dilatancy: $d' = \tan^{-1}\left(\frac{2\sin\psi}{1-\sin\psi}\right)$

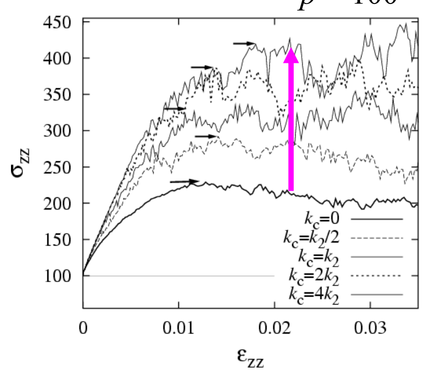
Dilatancy Angle:

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

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

Modulus and yield stress cohesion

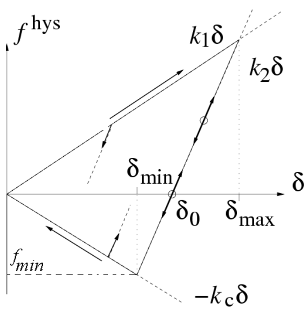


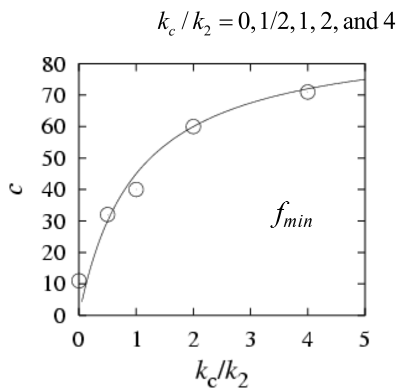


Modulus (initial slope)

Yield Stress …. (peak value)

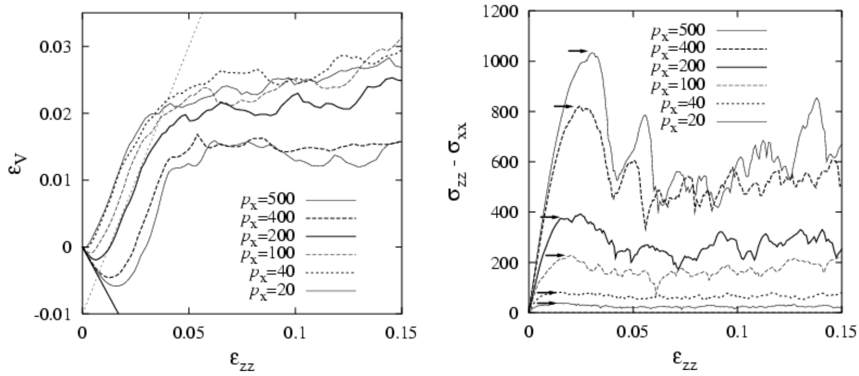
Micro-macro for cohesion





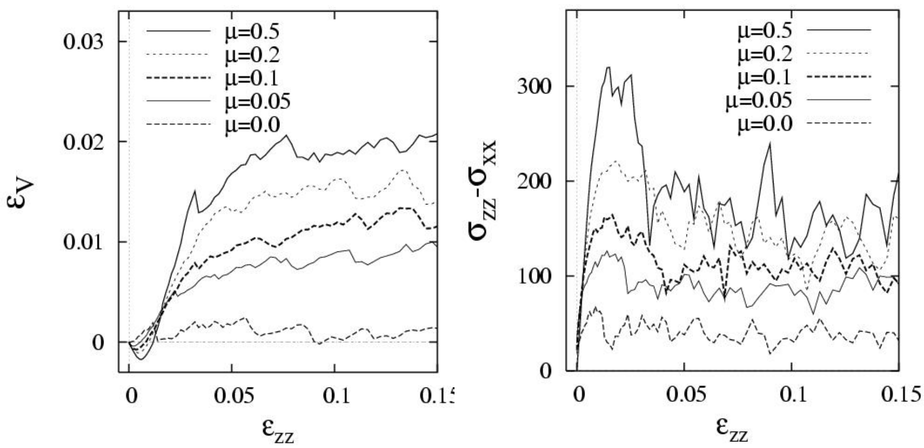
micro adhesion: f_{min} macro cohesion $c = c_0 \dfrac{1 - k_1/k_2}{1 + k_2/k_c}$

Pressure dependence



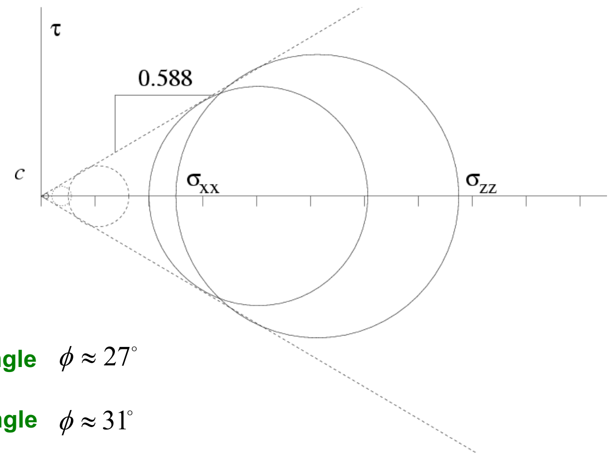
Results for friction μ=0.5 and different p_x *and* k_c*=0*

Bi-axial: p_x=200 – varying friction



Friction – no cohesion

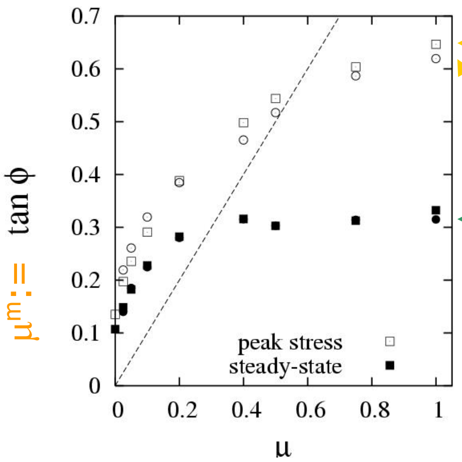
$k_c = 0$ and $\mu = 0.5$



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

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

Micro-macro for friction



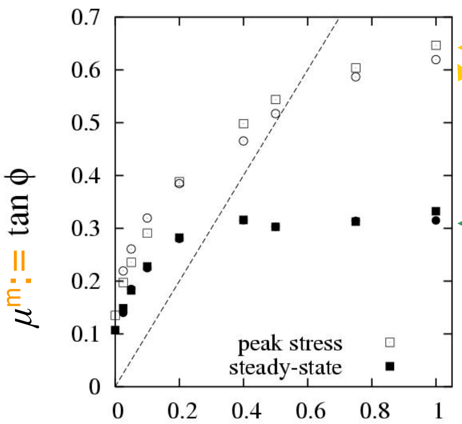
prepared μ=0

prepared μ=0.5

steady-state shear

micro contact-friction μ macro friction-angle ϕ

Micro-macro for friction



prepared μ=0

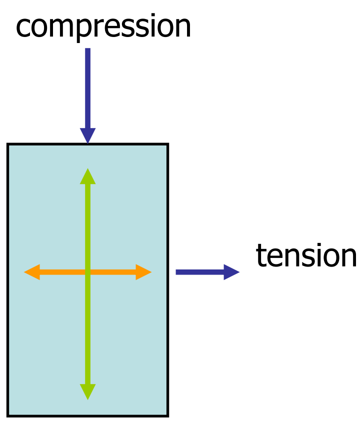
prepared μ=0.5

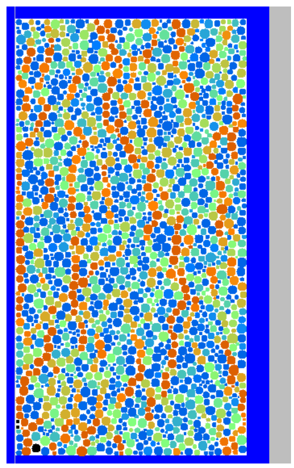
steady-state shear

micro contact-friction μ macro friction-angle μ^m

NOTE: each point = 5-10 simulations

Micro-macro for anisotropy – rheology



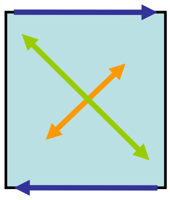


Anisotropy <-> Shear ?

- 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

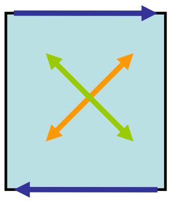


Anisotropy <-> Shear ?

- Simple shear

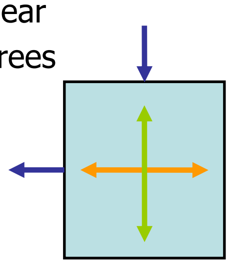
$$\varepsilon = \begin{pmatrix} 0 & 2\varepsilon_s \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & \varepsilon_s \\ -\varepsilon_s & 0 \end{pmatrix} + \begin{pmatrix} 0 & \varepsilon_s \\ \varepsilon_s & 0 \end{pmatrix}$$

Rotation + symmetric shear



- Rotate symmetric shear tensor by 45 degrees

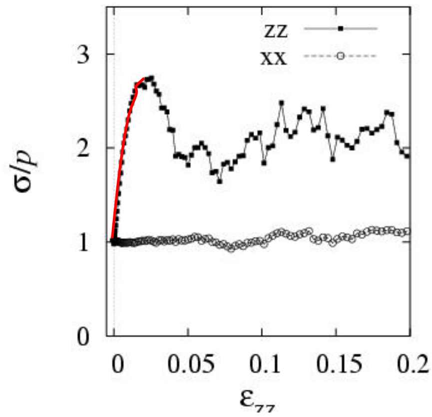
$$R_{45} \cdot \begin{pmatrix} 0 & \varepsilon_s \\ \varepsilon_s & 0 \end{pmatrix} \cdot R_{45}^T = \begin{pmatrix} \varepsilon_s & 0 \\ 0 & -\varepsilon_s \end{pmatrix}$$



- Biaxial "shear": compression+extension

An-isotropy

in stress



An-isotropy (Stress)

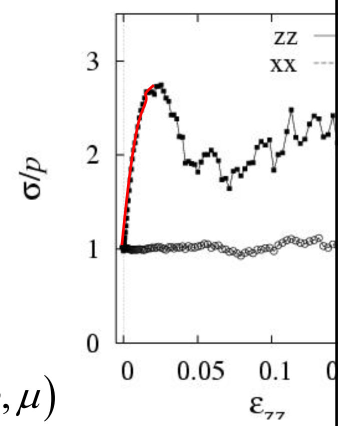
- Stress: Isotropic: $\mathrm{tr}\,\boldsymbol{\sigma}$, and deviatoric: $\mathrm{dev}\,\boldsymbol{\sigma} = \sigma_{zz}-\sigma_{xx}$
  - Minimal eigenvalue: σ_{xx}
  - Maximal eigenvalue: σ_{zz}
- Dev. Stress fraction $s_D = \mathrm{dev}\,\boldsymbol{\sigma} / \mathrm{tr}\,\boldsymbol{\sigma}$

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

- Exponential approach to peak

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

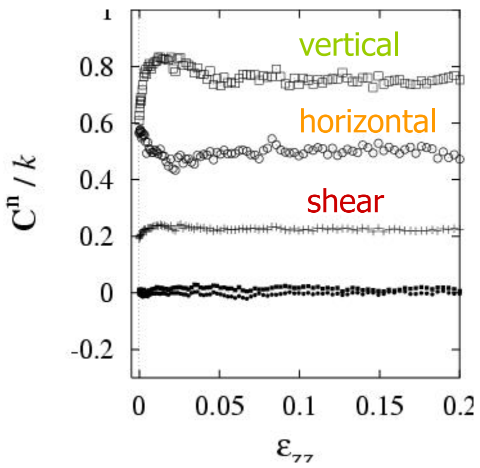
$$\beta_s\left(\rho, p, \mu\right)$$

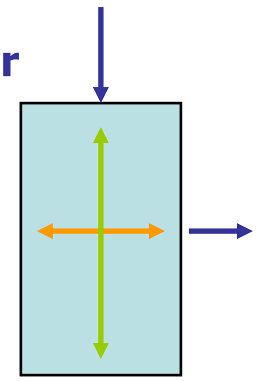


An-isotropy (Stress)

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

Stiffness/structure tensor





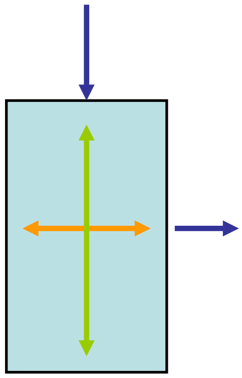
Different moduli:

- 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

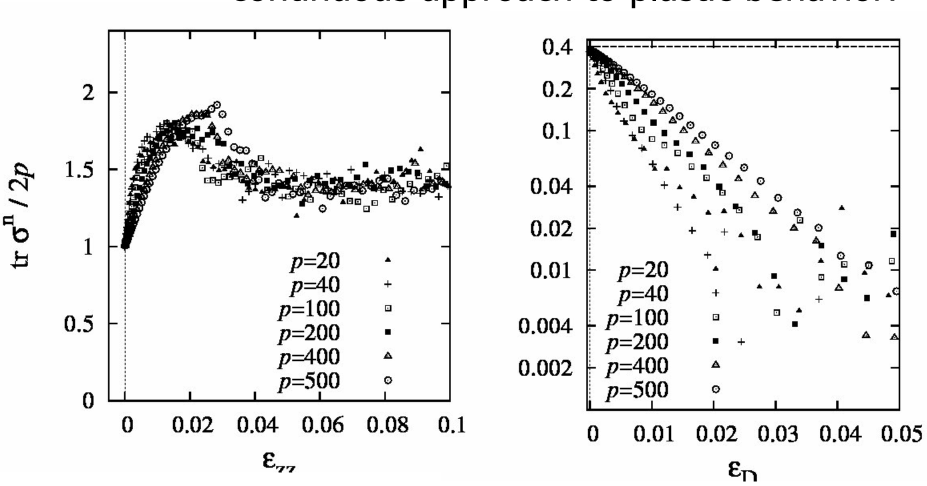
(in the biaxial box eigen-system)

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

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

Stress

continuous approach to plastic behavior!

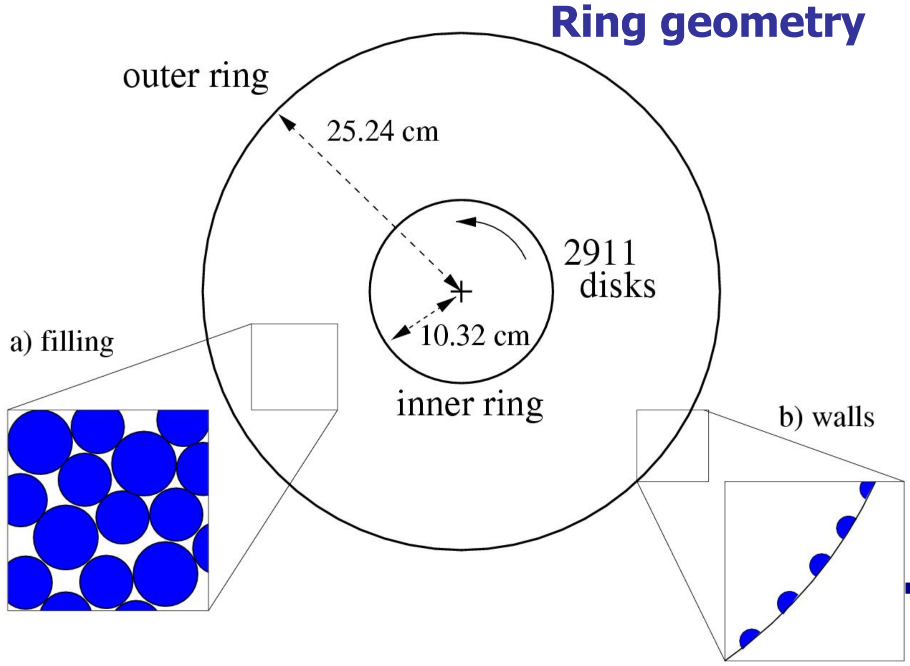


Summary micro-macro GLOBAL

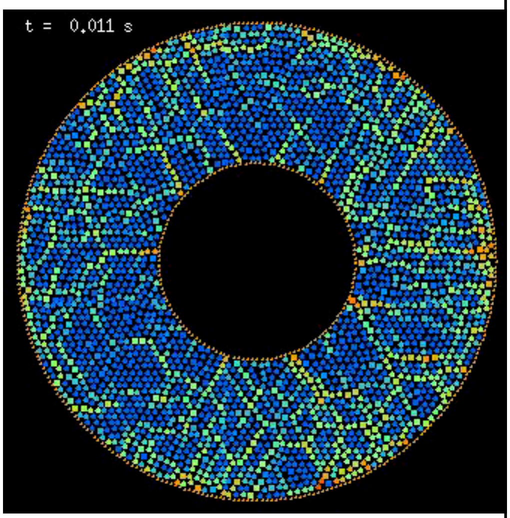
- Micro-/Macro-Flow Rheology
  - micro-adhesion … macro-cohesion
  - micro-contact-friction … macro-friction-angle
- Non-Newtonian Rheology (Anisotropy?, Micro-polar?)

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

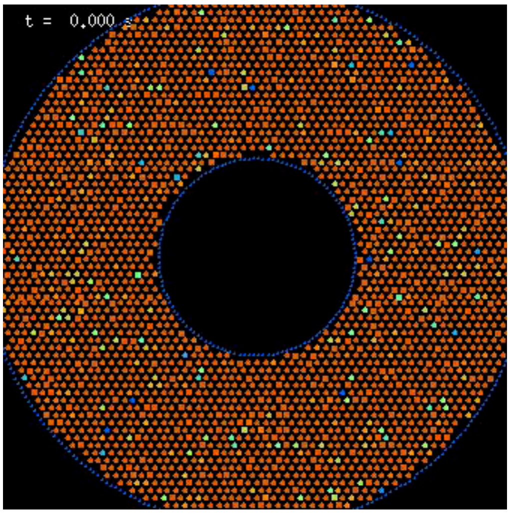
Ring geometry



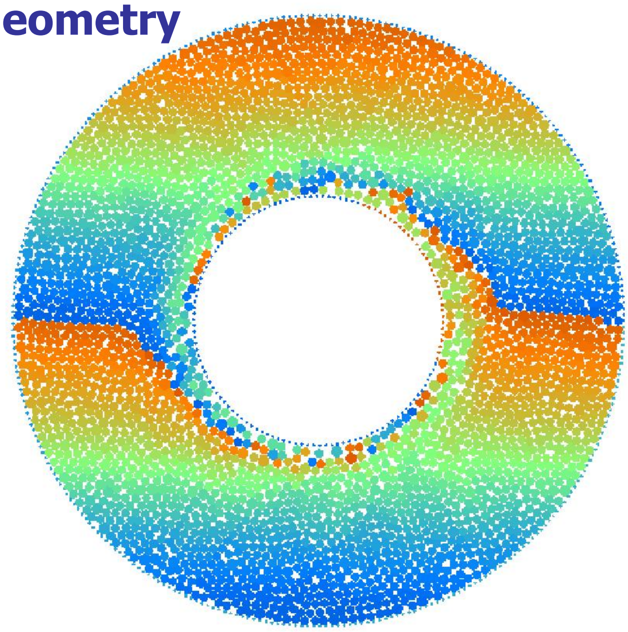
2D shear cell – force chains
= inhomogeneity
+ anisotropy



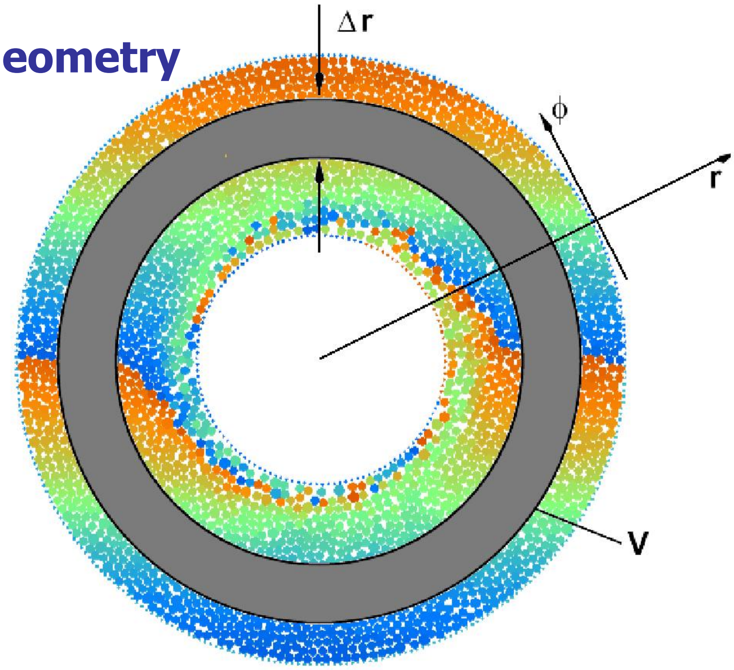
2D shear cell – energy



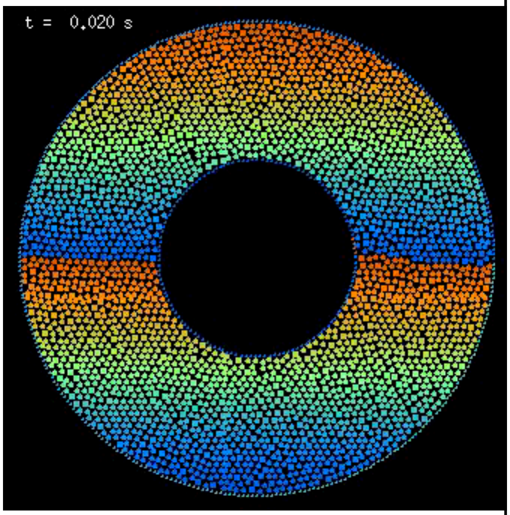
Ring geometry



Ring geometry



2D shear cell:
- shear localization
- non-Newtonian



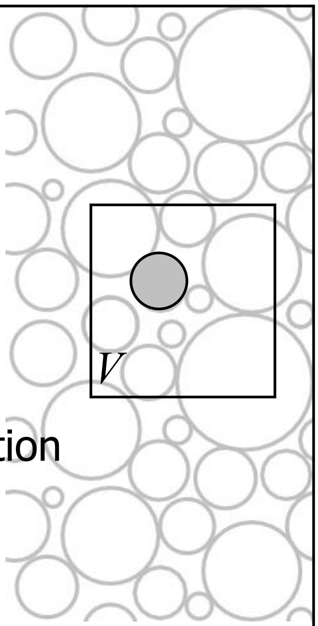
Averaging Density

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

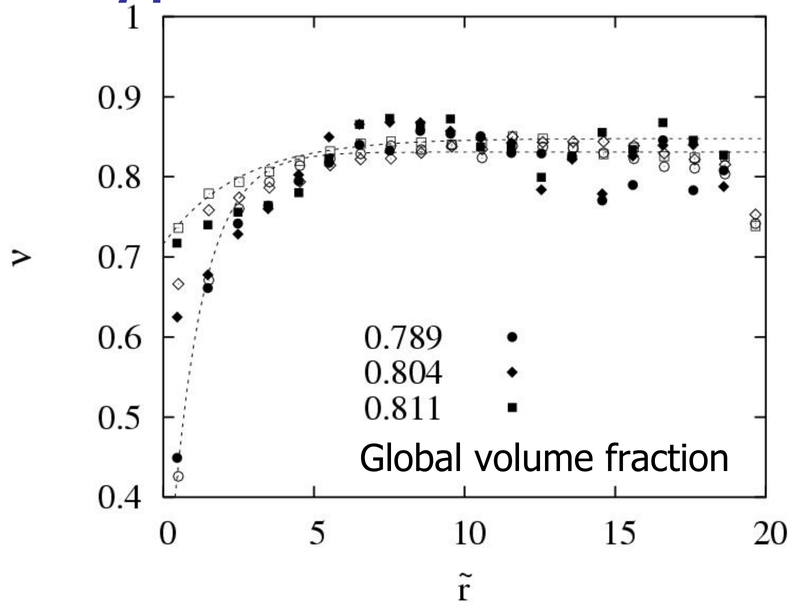
Any quantity:

$$Q^p = 1$$

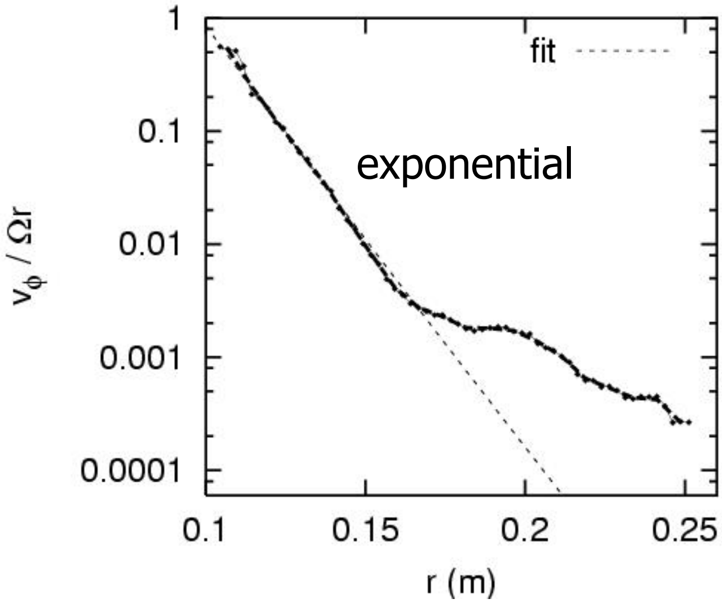
- Scalar: Density/volume fraction



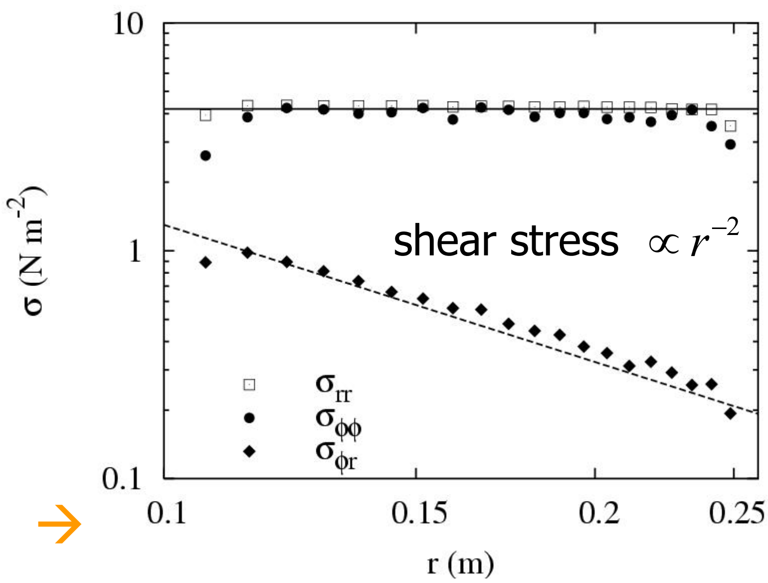
Density profile



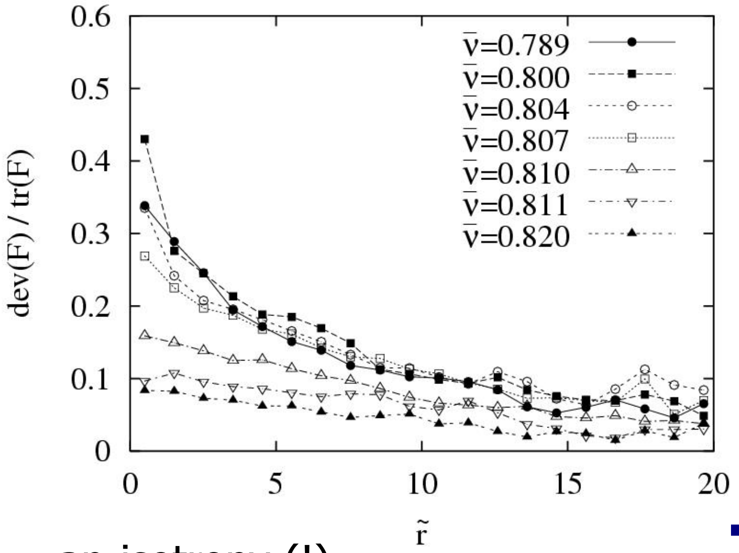
Velocity field -> velocity gradient



Stress tensor (static)



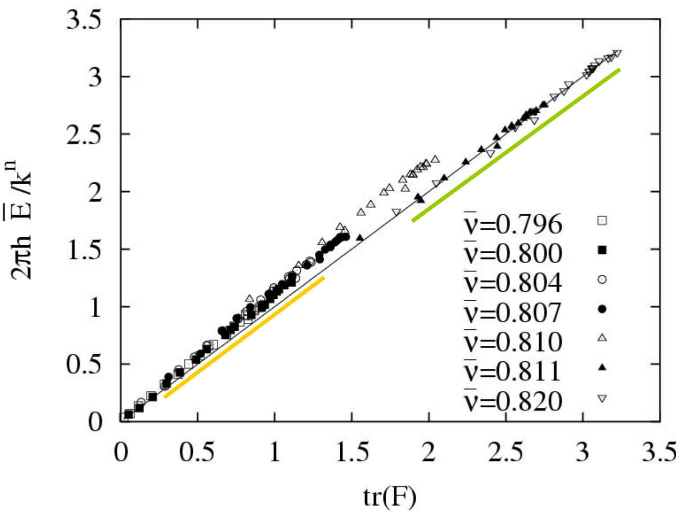
Fabric tensor (deviator)



an-isotropy (!)

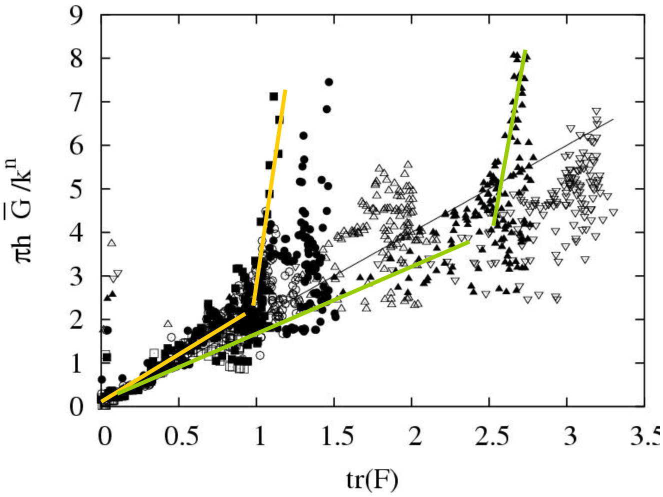
Macro (bulk modulus)

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



Macro (shear modulus)

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



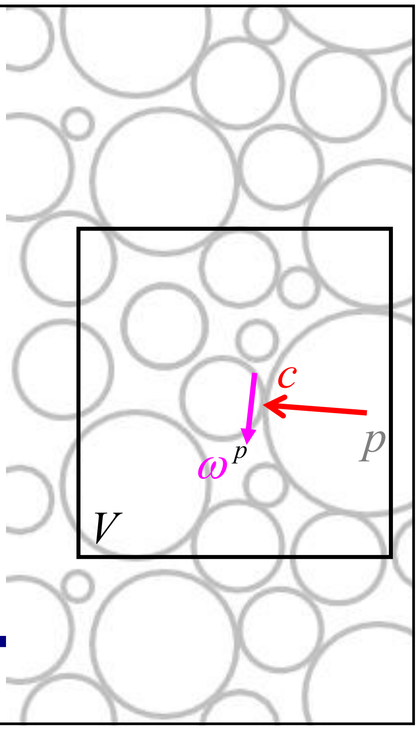
Averaging Rotations

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

Deformation:

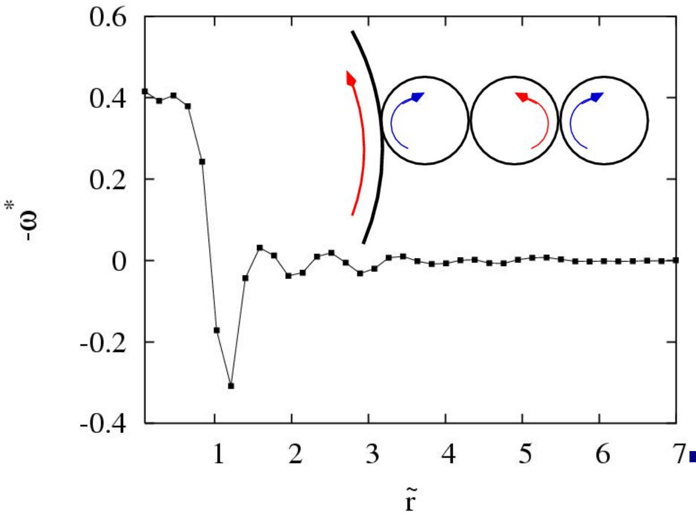
$$Q^p = \omega^p$$

- Scalar
- Vector: Spin density
- Tensor

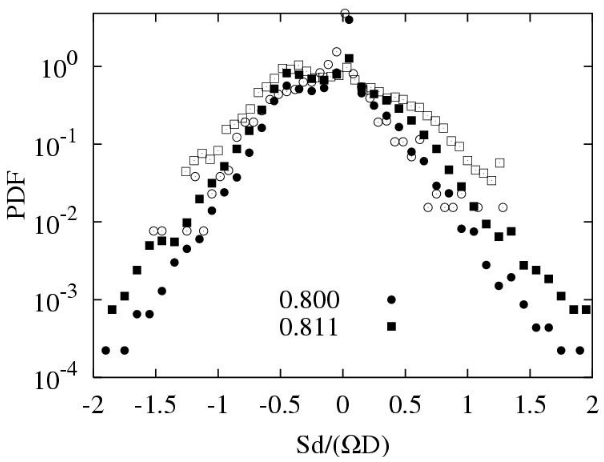


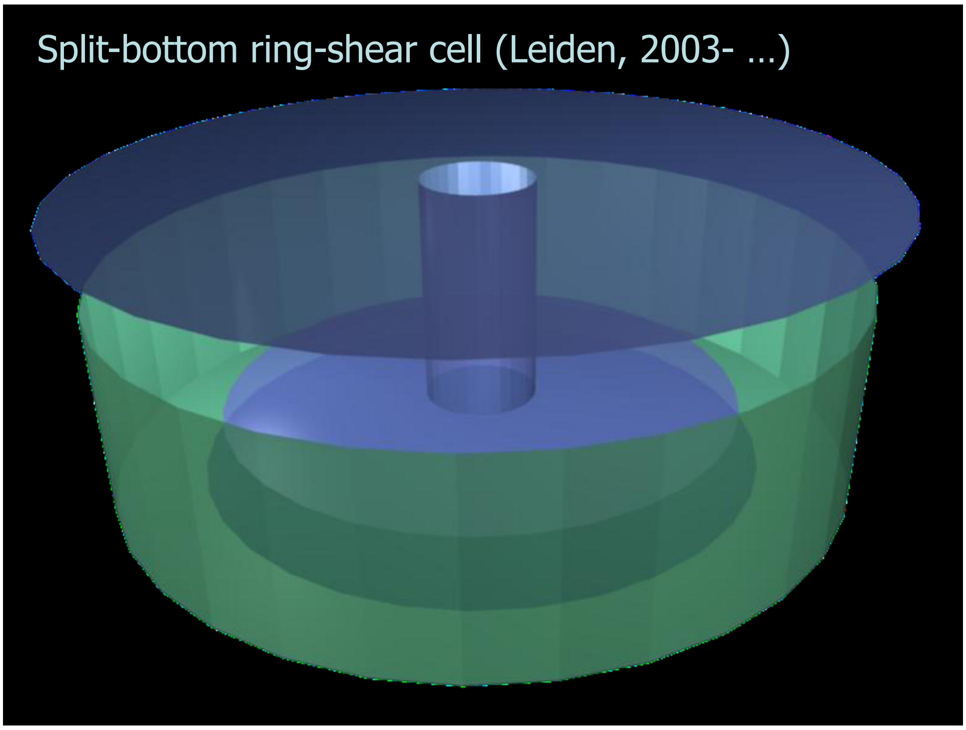
Rotations – spin density

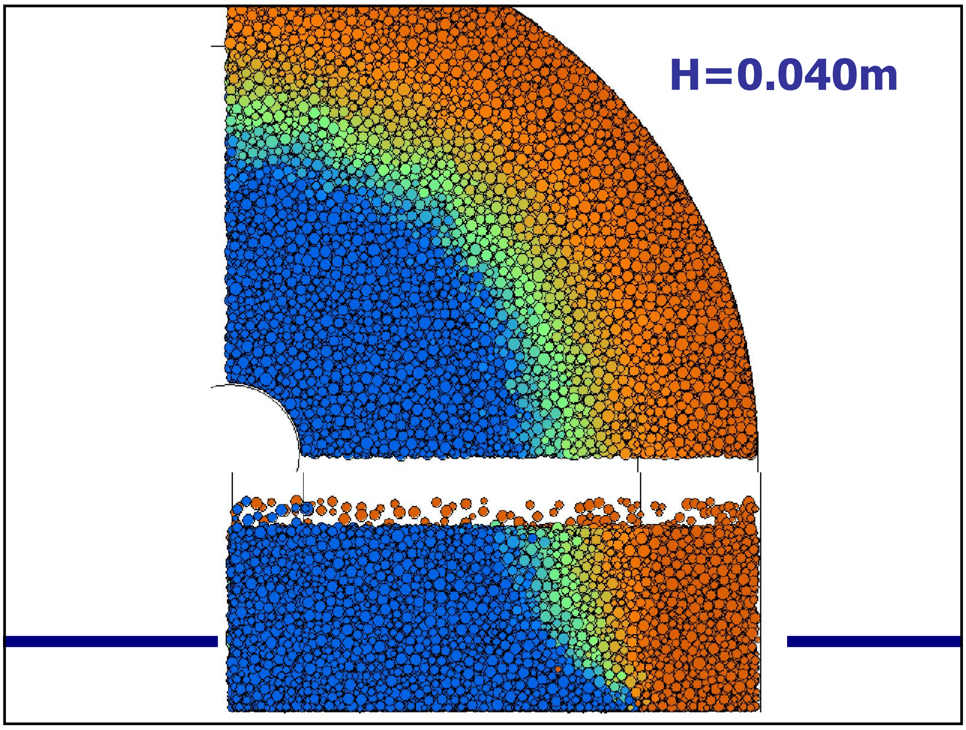
eigen-rotation: $\omega^* = \omega - W_{r\phi}$



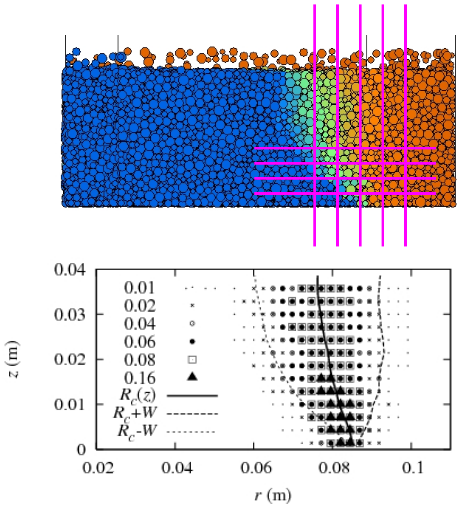
Spin distribution




Split-bottom ring-shear cell (Leiden, 2003- …)

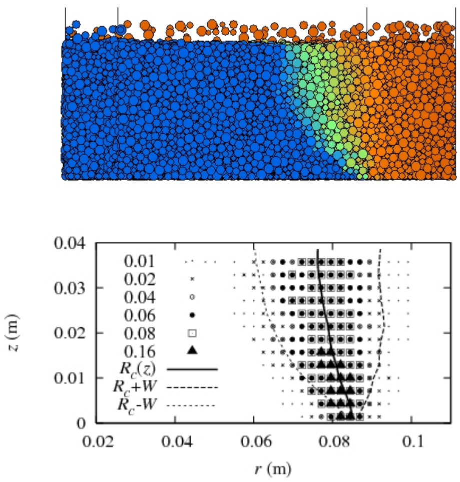

H=0.040m

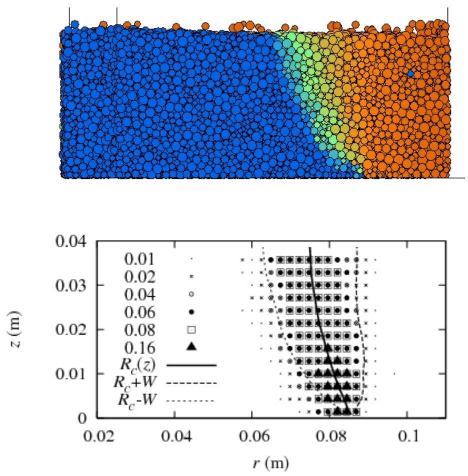
Constitutive relations – shear rate $\dot{\gamma}$



no friction

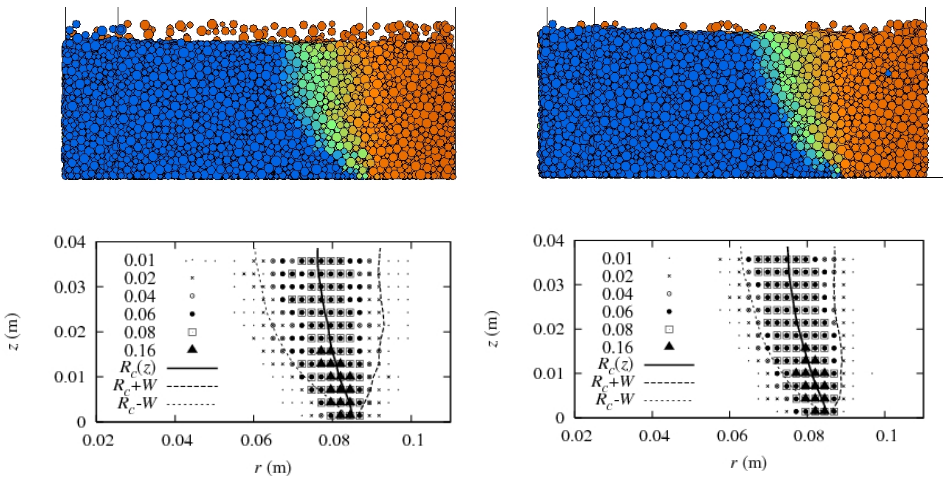
Constitutive relations – shear rate $\dot{\gamma}$





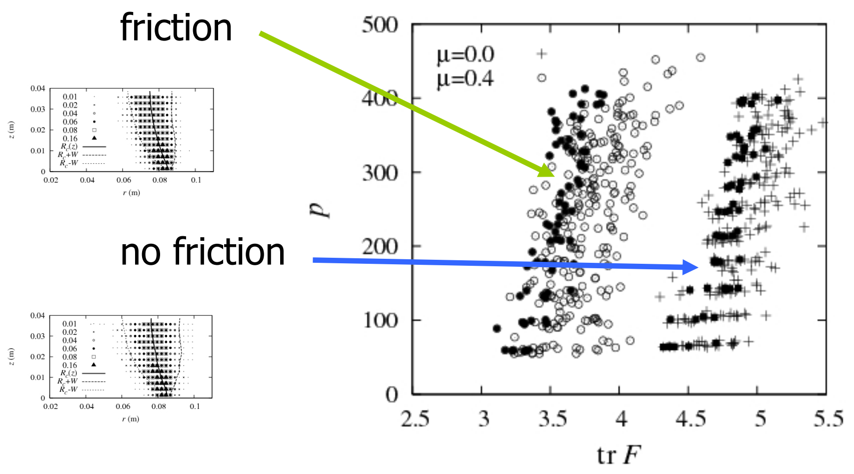
no friction friction

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

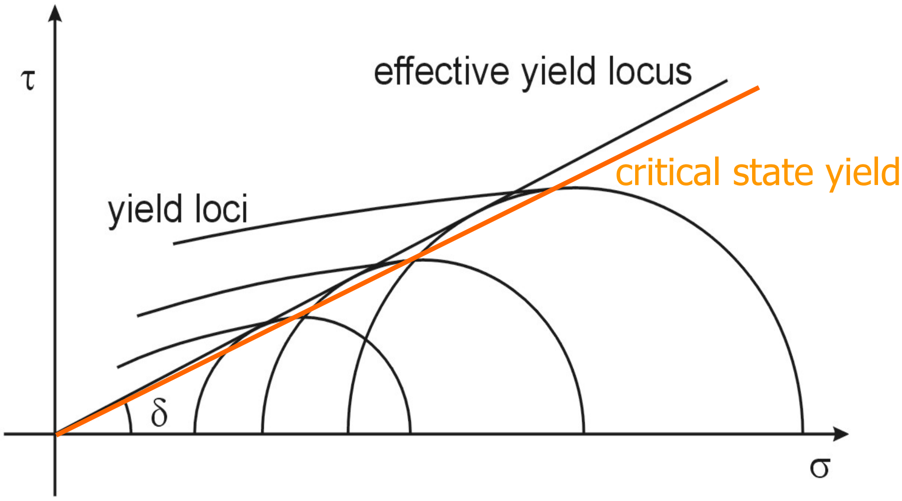


90% quantitative agreement with experiments …

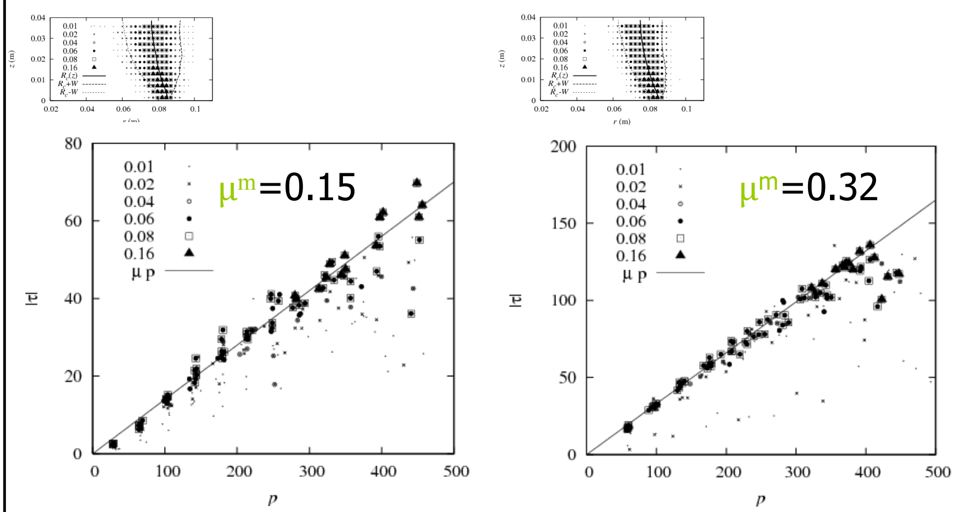
Constitutive relations: stress-structure



Yield loci

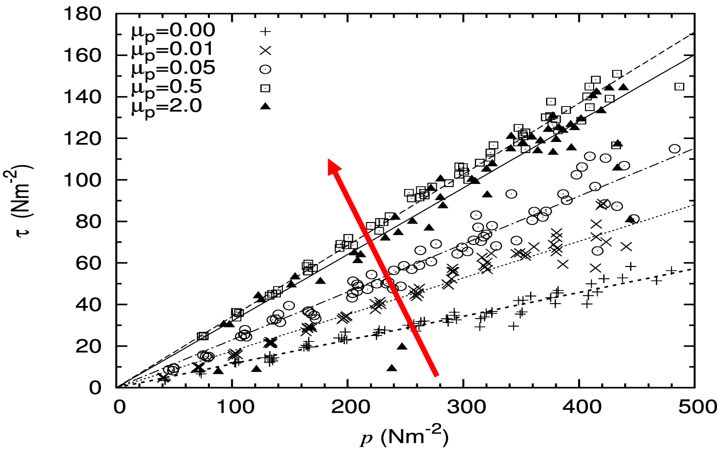


Constitutive relations: Mohr-Coulomb



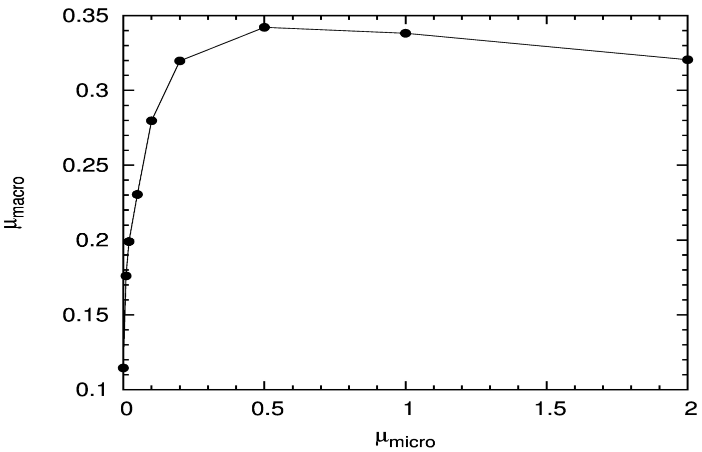
no friction μ=0 friction μ=0.4

Friction at contact



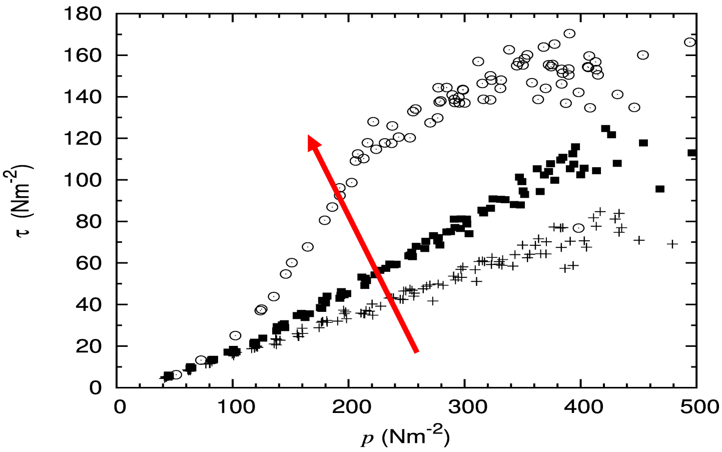
The slope of termination locus increases with friction.

Friction at contact



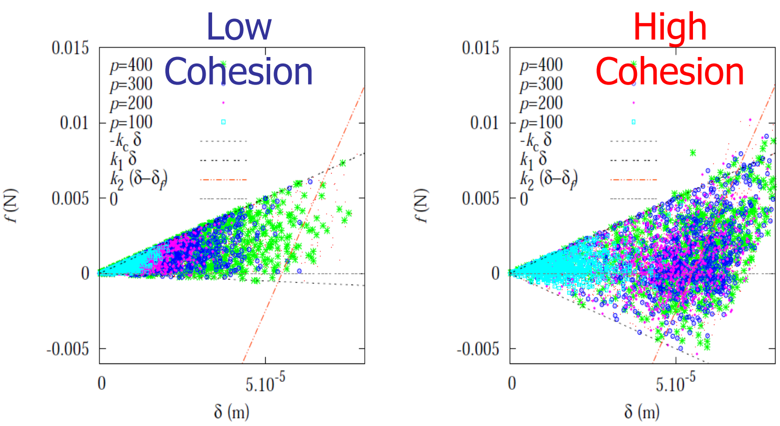
- Low friction: Increase with particle friction.
- High friction: Asymptotic saturation.

Cohesion at contact



The termination locus becomes non-linear with cohesion.

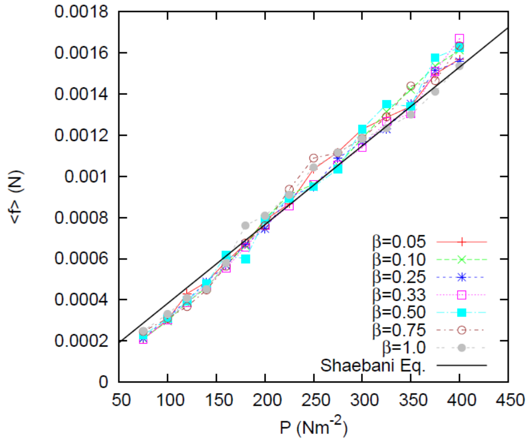
Force statistics



Increasing cohesion, particles tend to drift to limit branch.

705

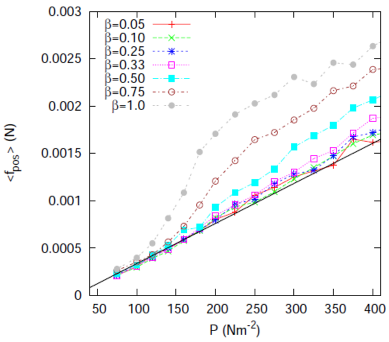
Mean force

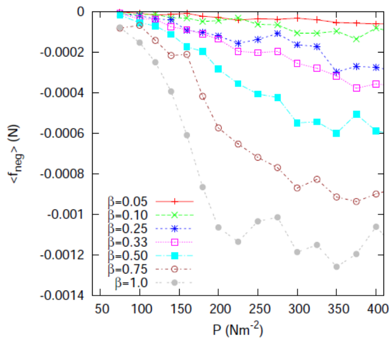


- Mean force is linear against pressure.
- Cohesion does not affect mean force.

706

Mean attractive and repulsive forces

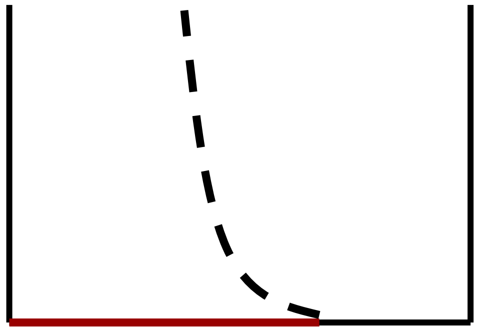




- Low cohesion: Mean forces are linear → cohesion can be ignored.
- High cohesion: Mean forces are non-linear → cohesion cannot be ignored

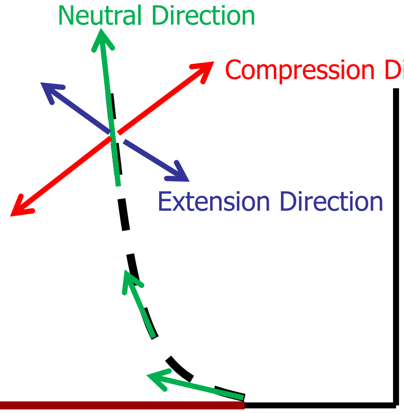
708

Split-bottom setup

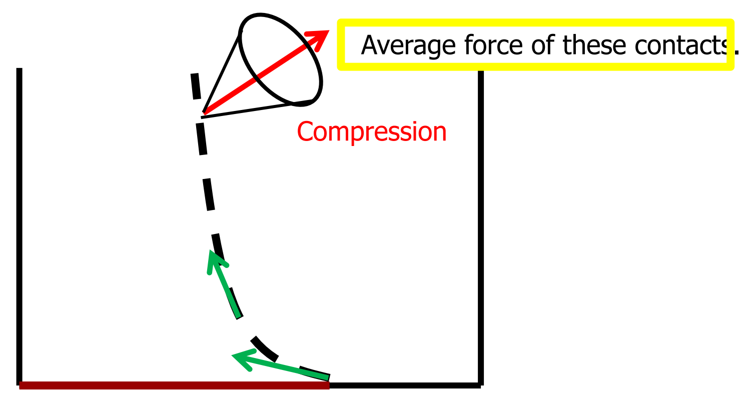


Let us look closely!

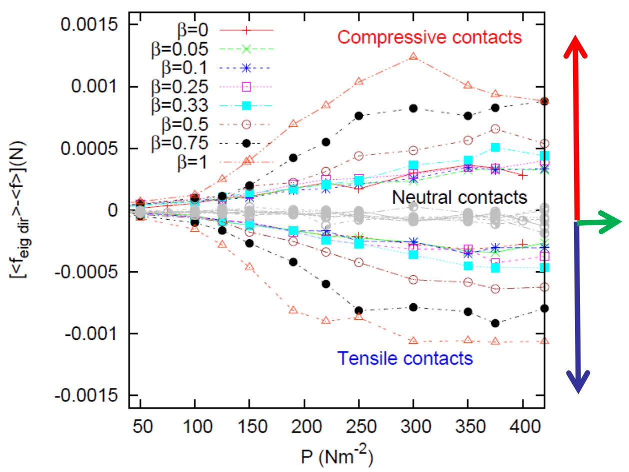
Principal directions in split-bottom



Principal directions in split-bottom

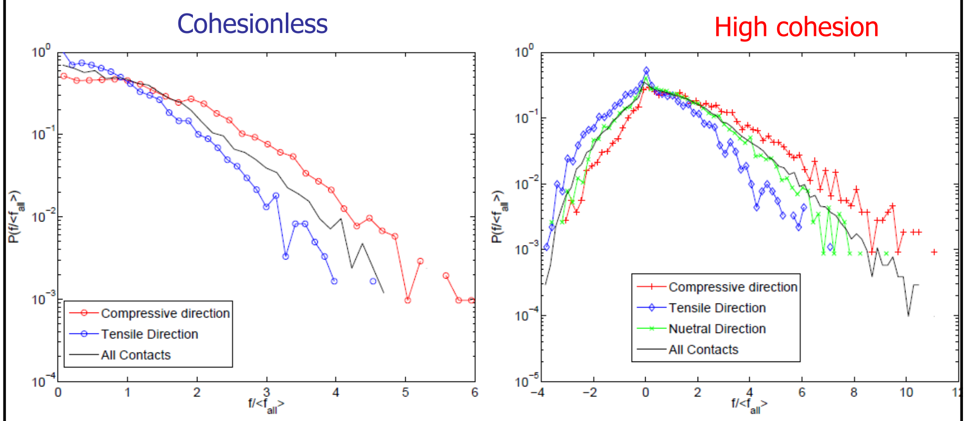


Mean forces in principal directions.



Cohesion by tension is activated in one major direction only!

Probability distribution of forces.



The probability distribution in two major directions switches for attractive and repulsive forces!

Summary

realistic DEM meso particle simulations
+ interaction forces (contact physics)
+ hierarchical grid (wide size-distributions)

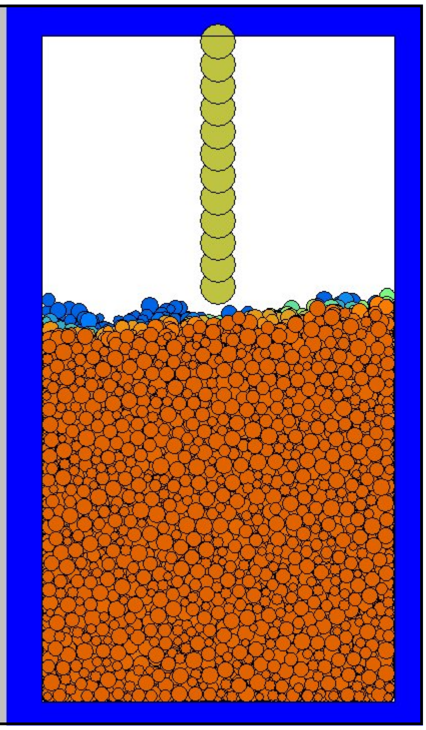
+ micro-macro transition to continuum
=> macro flow behavior …

+ understand interplay micro-macro
=> in *shear*: ~1/3 of contacts are cohesive
~1/3 are under compressive stress

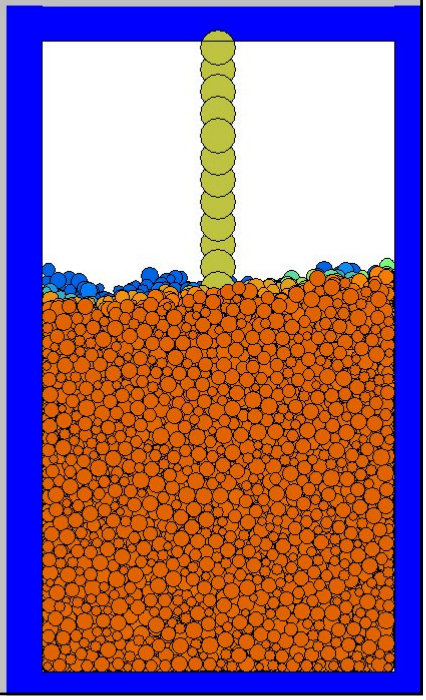
Thanks for your attention

Questions ?

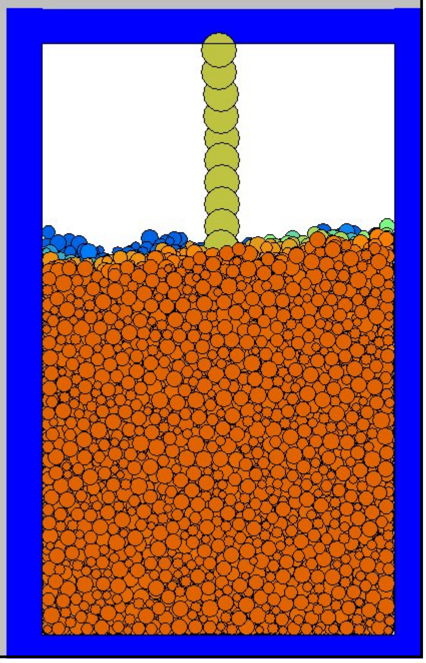
Pile penetration 8



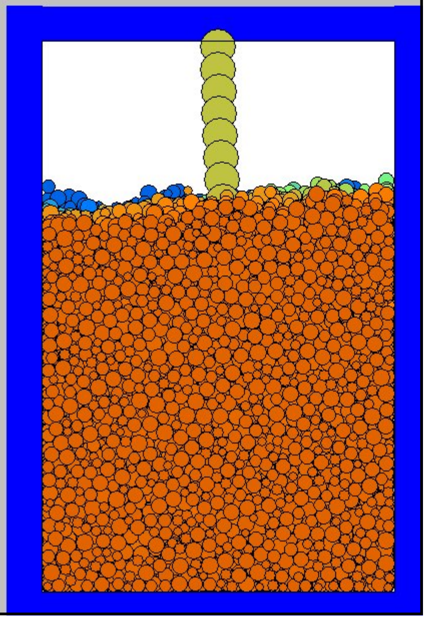
Pile penetration 10



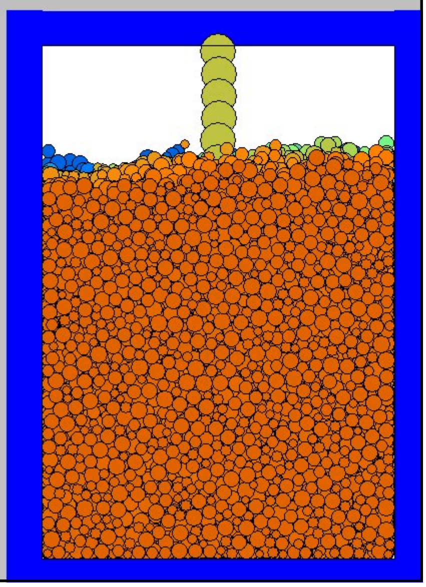
Pile penetration 12



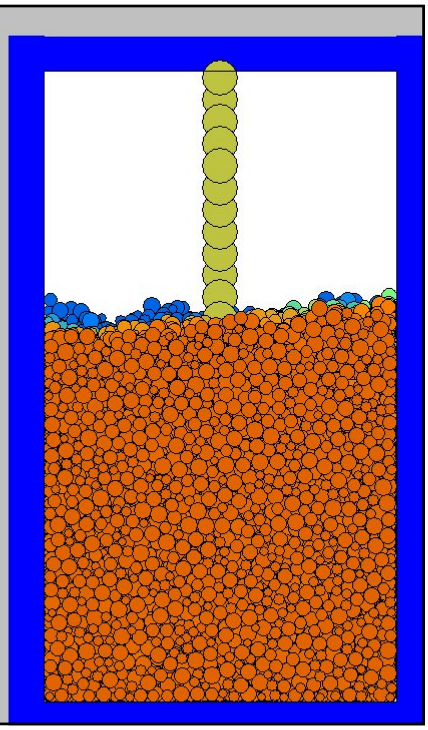
Pile penetration 14



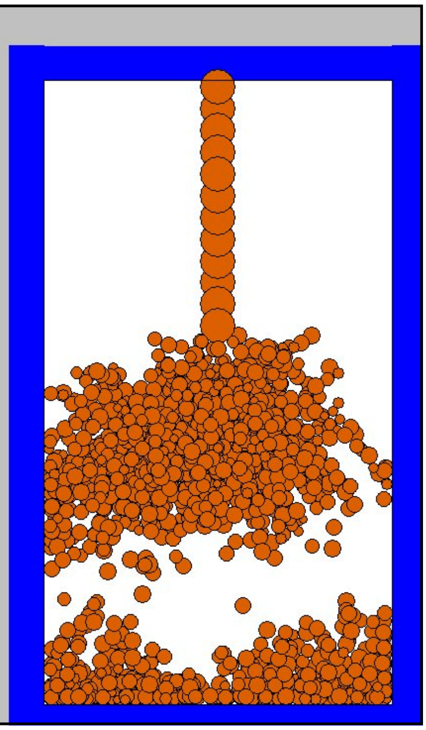
Pile penetration 16



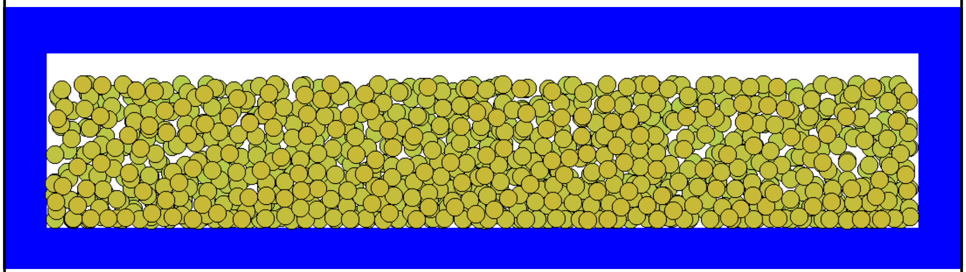
Pile penetration 10

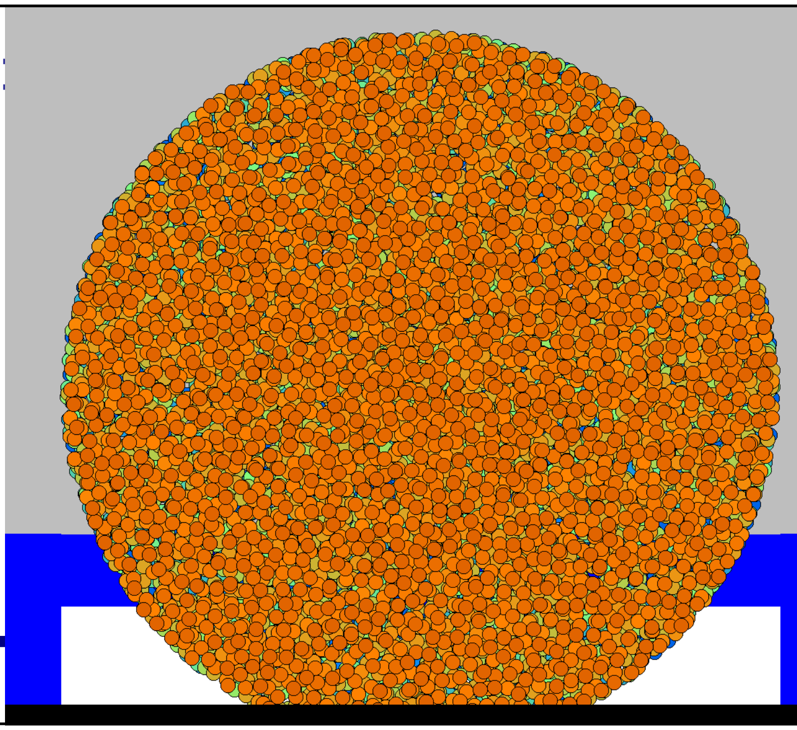


Pile penetration

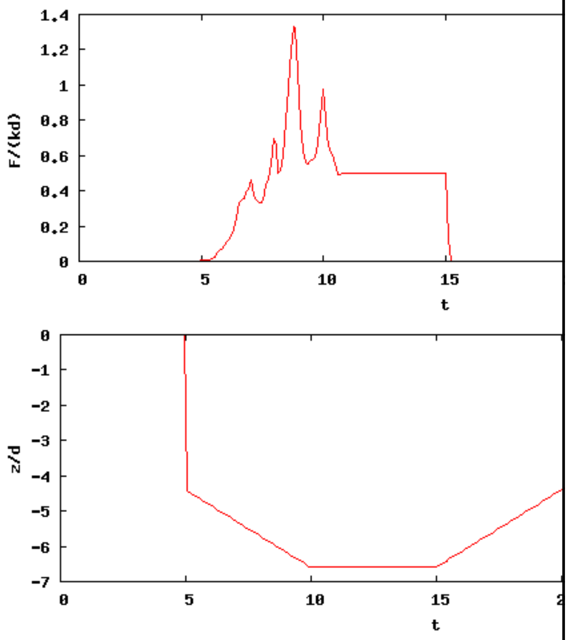


Indenter test (DEM)

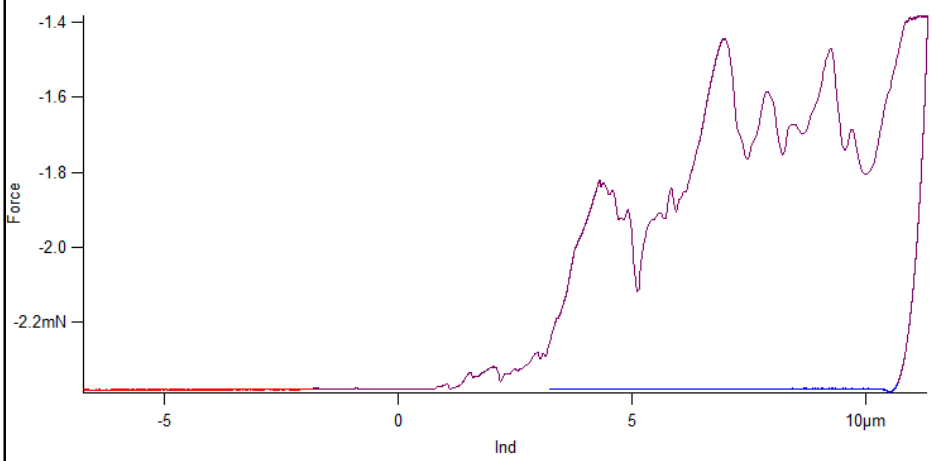




Indenter test



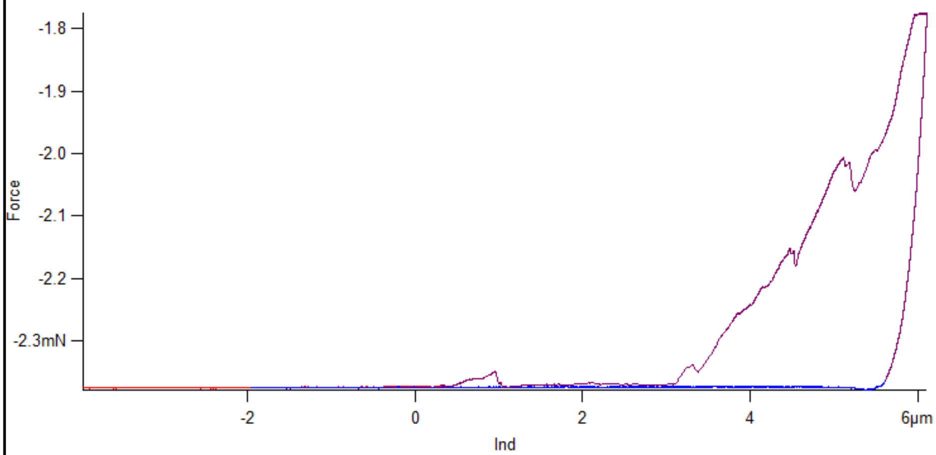
Indenter test (Exp. MPIP Ming&Kappl)



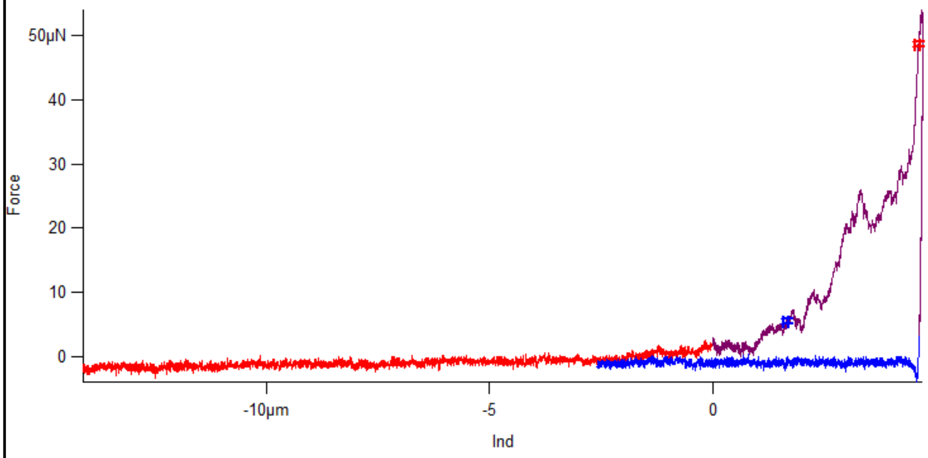
Indenter test (Exp. Sphere sample.avi)

MPIP Ming&Kappl

Indenter test (Exp. MPIP Ming&Kappl)



Indenter test (Exp. MPIP Ming&Kappl)



Application: Oil exploration (SHELL)

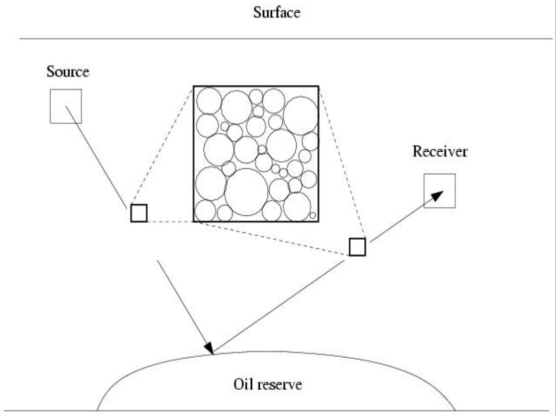
Fast

Small amplitude

Single pulse

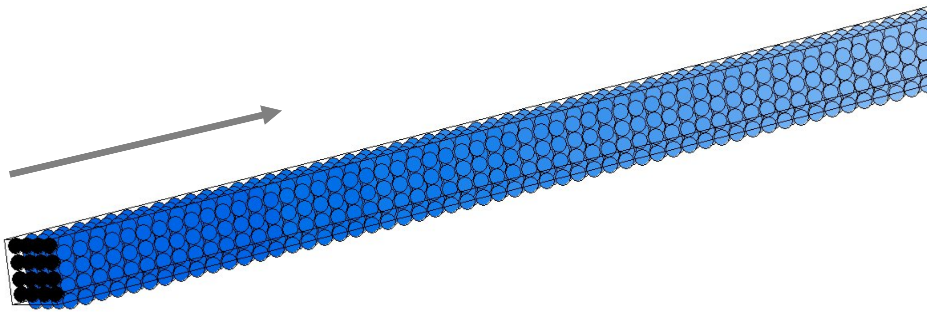
⇩

Sound propagation

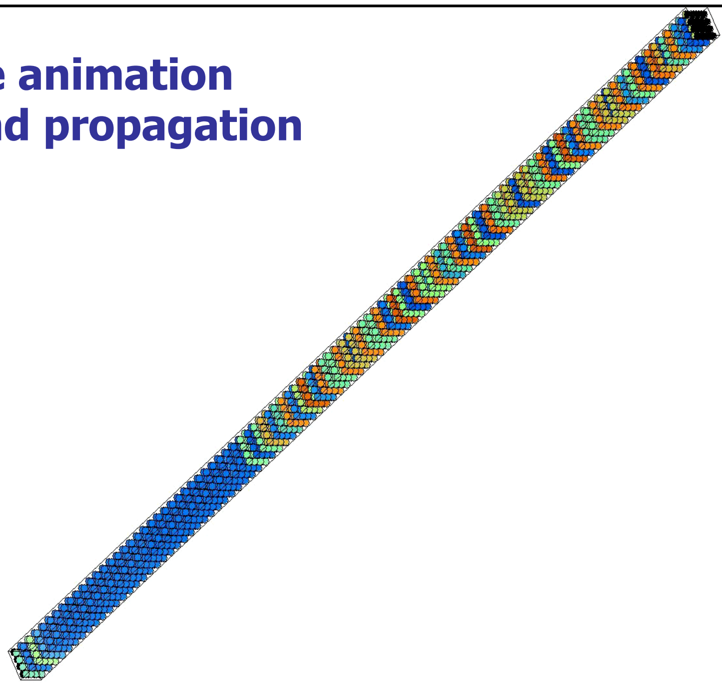


Orion Mouraille, PhD thesis, 27.02.2009

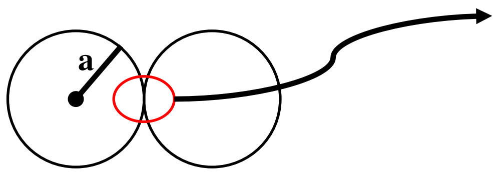
System 0: regular lattice Δa=0



P-wave animation
… sound propagation



Weak polydispersity



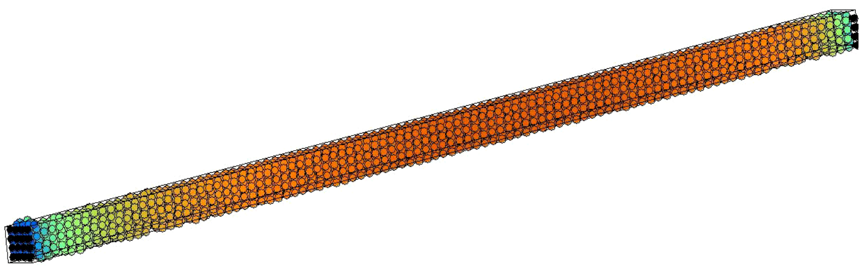
$\delta = a/1000$

$\Delta a = \delta/2, \delta$ and 2δ

-The system is practically unchanged at the grain level

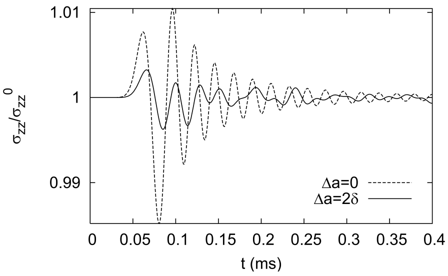
-Distribution of weak and strong contacts

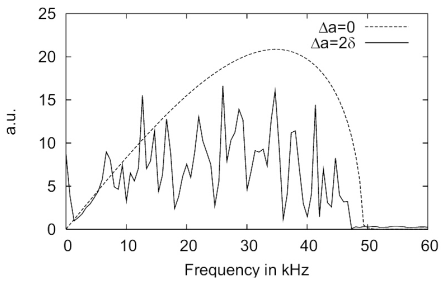
Sound propagation + polydispersity $\Delta a > 0$



Signal Analysis

time-FFT

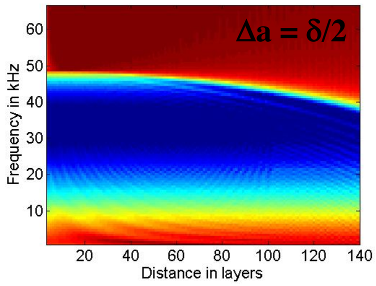


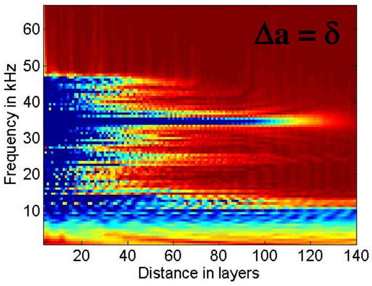


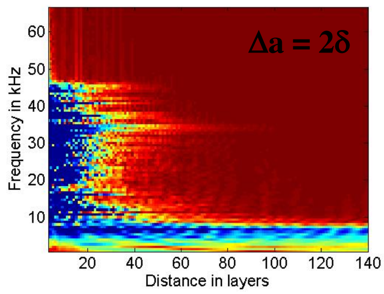
Stress-time signal

Power-spectrum

Frequency-space Diagrams







Dispersion relations

space-time-FFT