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Swiss Federal Institute of Technology Zurich

Capillary interactions and particle dynamics in dense granular matter

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Computer simulations of wet granular matter

MAX-PLANCK-GESELLSCHAFT

Mixing properties

Zur Anzeige wird der QuickTime™ Dekompressor „TIFF (Unkomprimiert)“ benötigt.

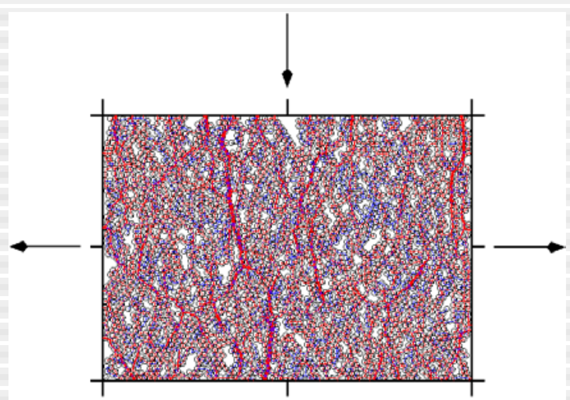
Flow properties

Goal

Couple Particle dynamics with fluid dynamics!

Stability properties

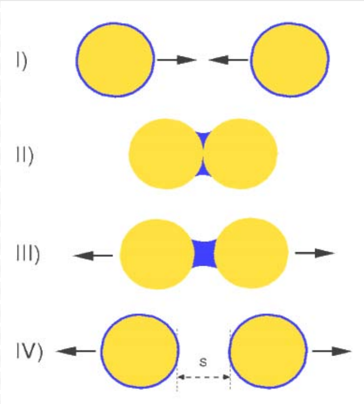
Zur Anzeige wird der QuickTime™ Dekompressor „TIFF (Unkomprimiert)“ benötigt.



Mechanical properties

Model

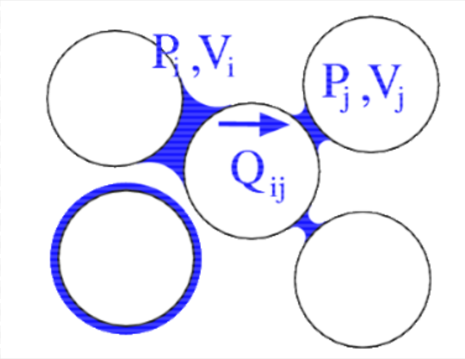
- Particle dynamics:
  - Modeled by contact dynamics (constraints)
- Fluid dynamics:



Capillary force active

Until the bridge ruptures

1) Instantaneous fluid distribution



Pressure can be measured

M Scheel et al. *Phys Condens Matter* 20: 494236 (2008)

2) Fluid transport driven by pressure difference

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Model

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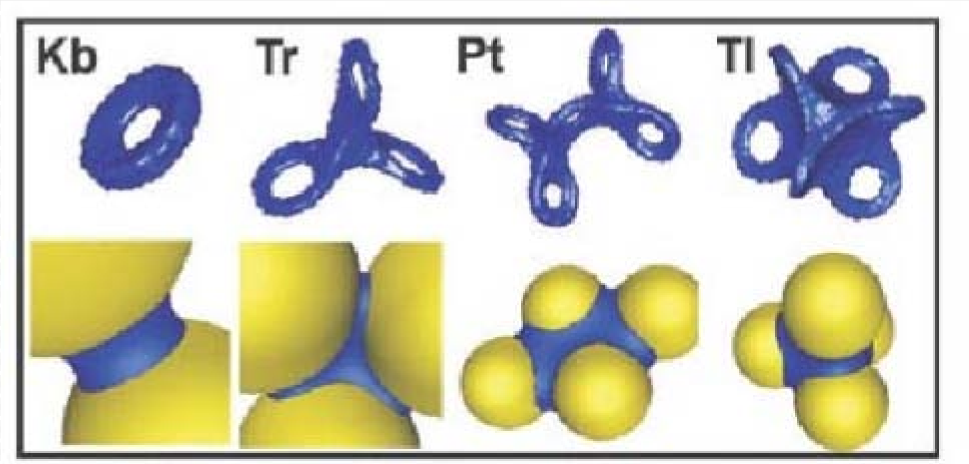
- Fluid dynamics:

  First: Only single bridges

  Later: Development of model with clusters



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Questions

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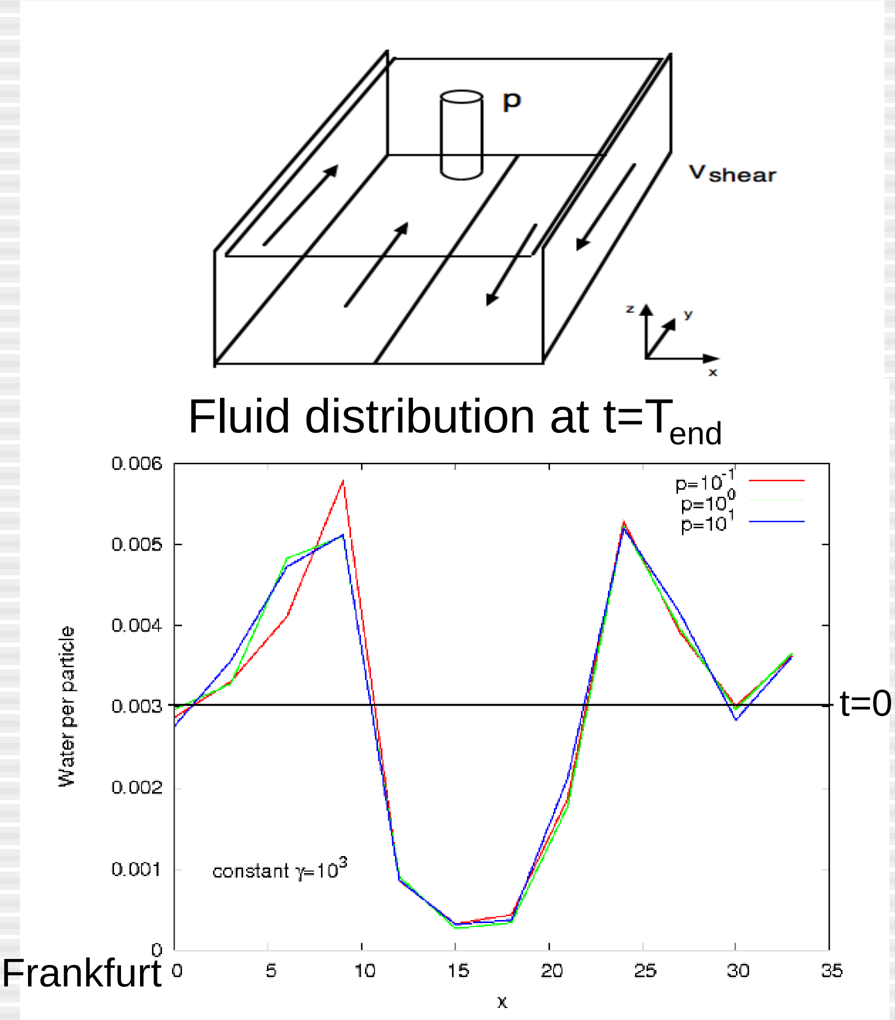
- Mixing properties of powder and fluid
- How is fluid distributed e.g. in
  - shear experiments
  - mixers/shakers

- Fluid transport
- Can fluid be mixed (unmixed) under slow deformations?

Linear split bottom cell

Transport of fluid in a shear experiment



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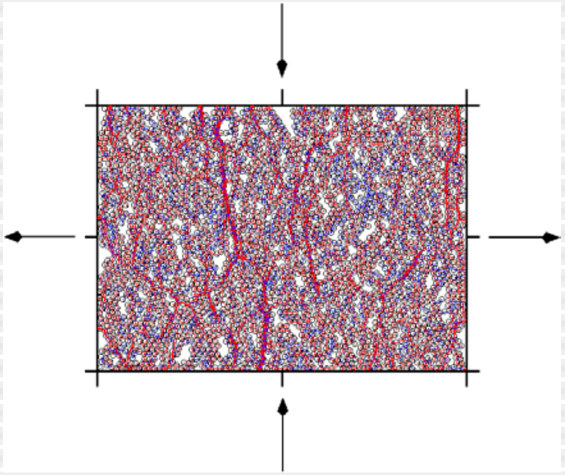
Questions

- Mechanical properties of powder
  - Shear tests
  - Compression tests
  - Tensile tests

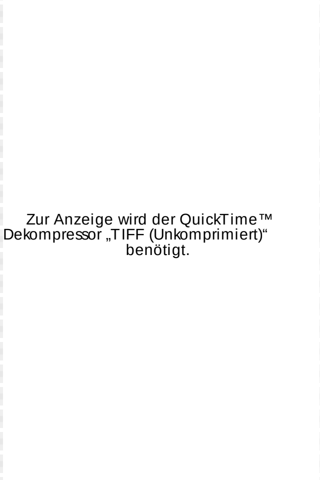


- Influence of water content
- Influence of initial fluid distribution
- etc

Questions

- Flow properties
  - Influence of fluid transport and water content

- Stability of packings
  - Drying and adding of fluid

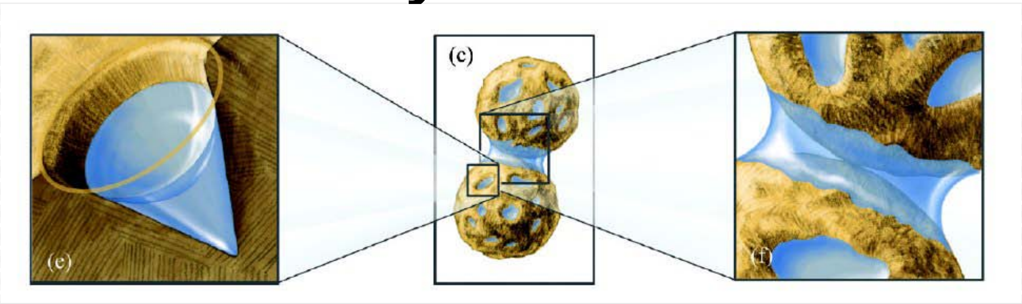


We are looking for experiments!!

How to improve the model

A more realistic model has to include:

A. Realistic dynamic of the fluid on the bead surface



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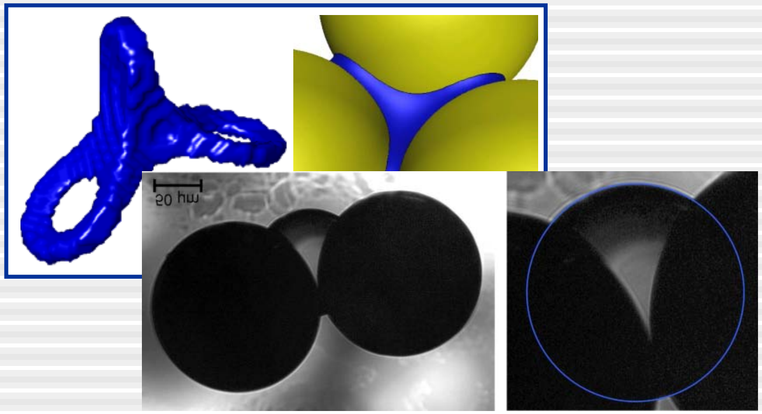

B. Multibody interactions

C. Effects of poor wettability

D. Consequences of contact angle hysteresis

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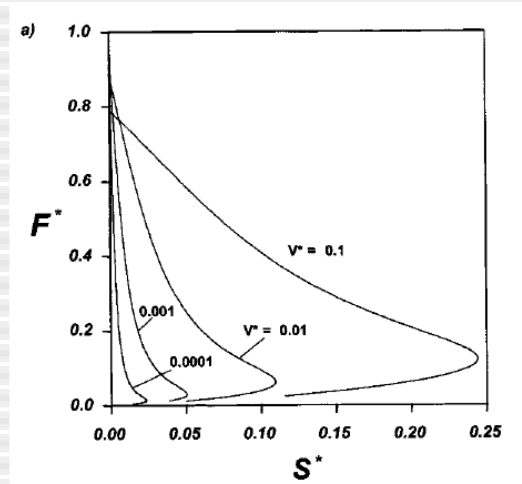
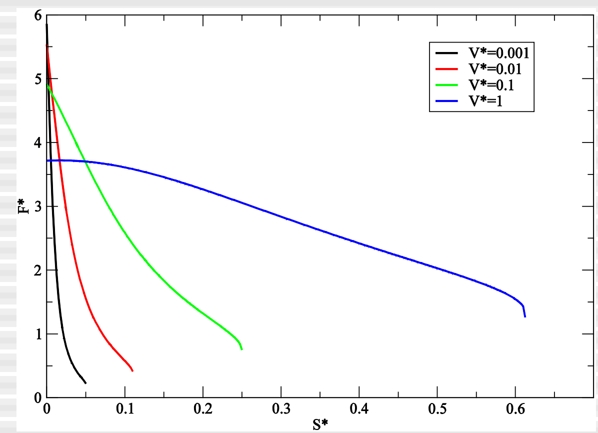
Capillary bridges

Capillary bridges (Willet):

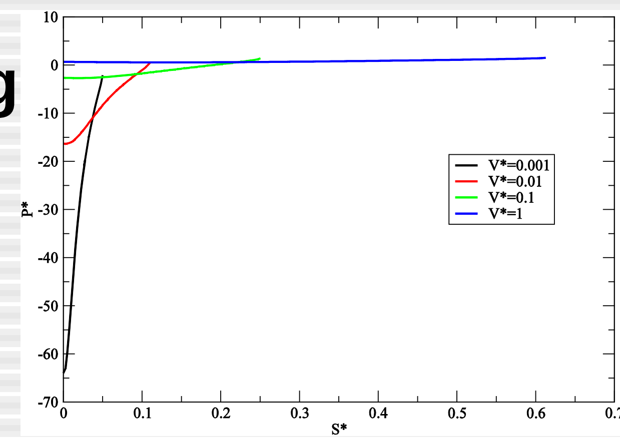
- Approximation for forces as function of separation and volume only
- Valid for small volumes
- No pressure data





Our solution: numeric look-up table including

- Case of bridges also with large volume
- Calculation of bridge pressure to account fluid transport



Calculations performed with a finite element Algorithm (Surface Evolver)

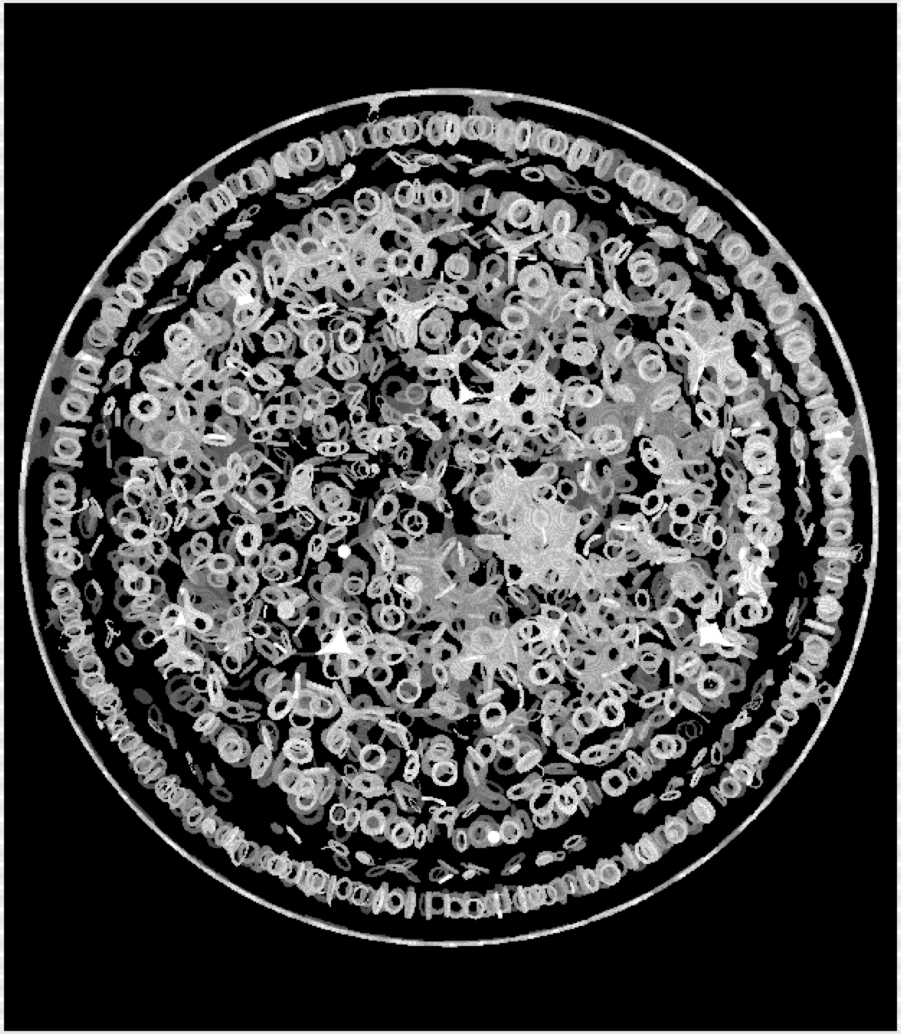
Multi body interactions

Large liquid content:
Presence of Clusters

fast X-ray
micro tomography

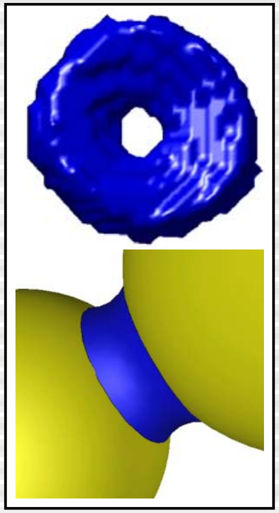
liquid content
W=0.03
bead diameter:
600 μm

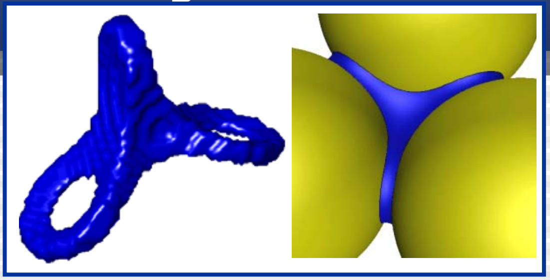
M Scheel et al. *Nature Materials* 7: 189 (2008)

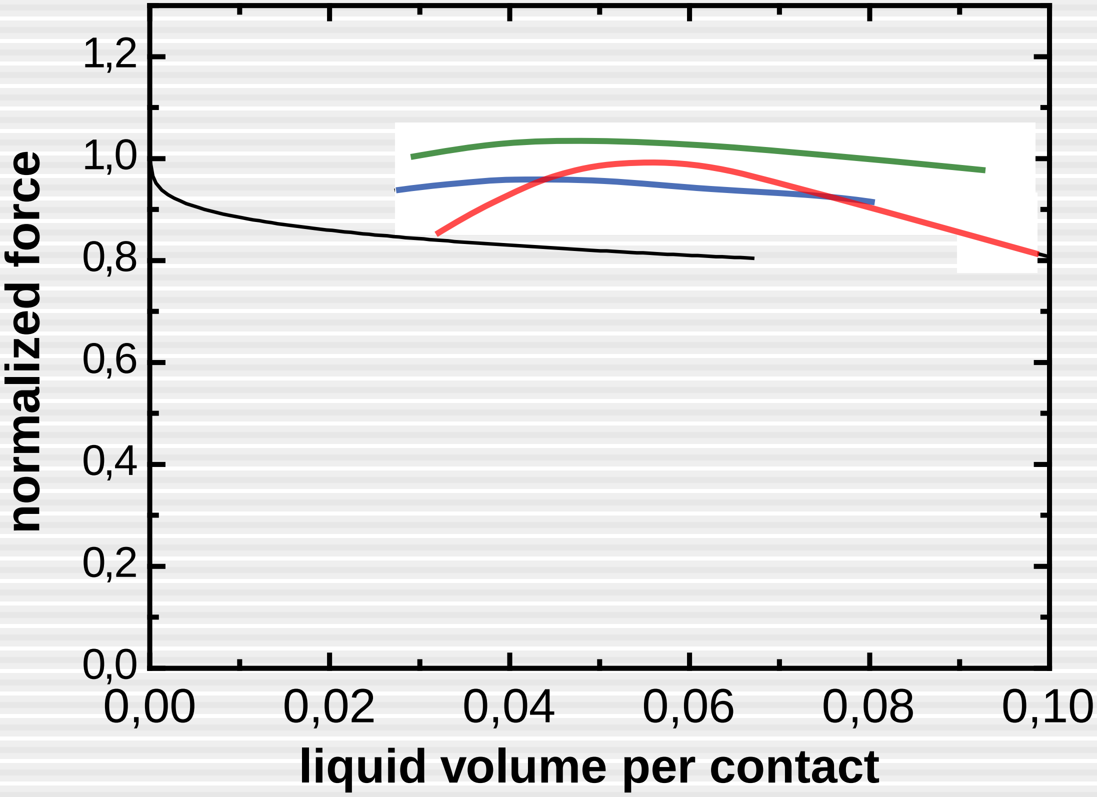


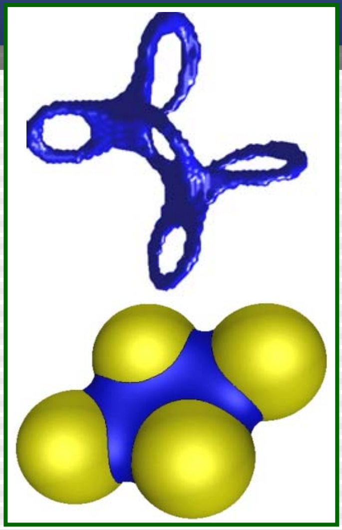
Multi body interactions

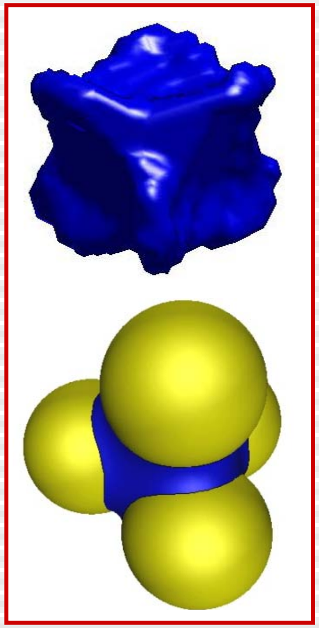
bridges





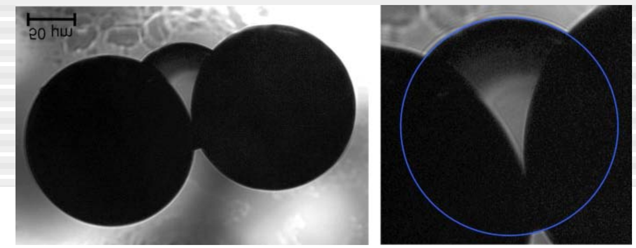






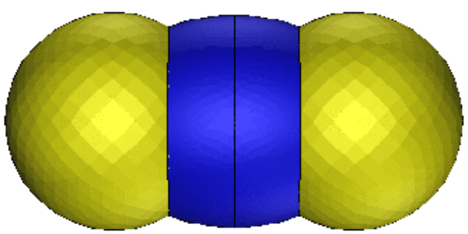
Low wettability effects

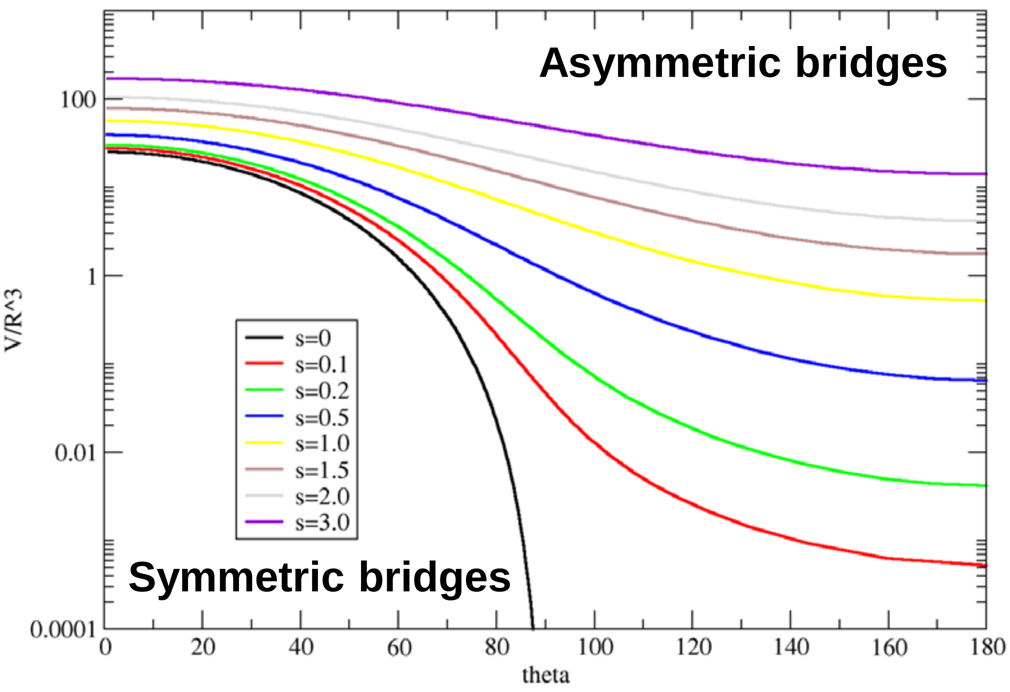
Asymmetric liquid bridge between basalt beads



Asymmetric bridges

Transition to a asymmetric bridge by increasing the contact angle





No attractive force!

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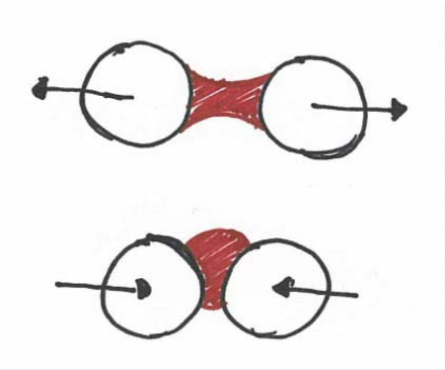
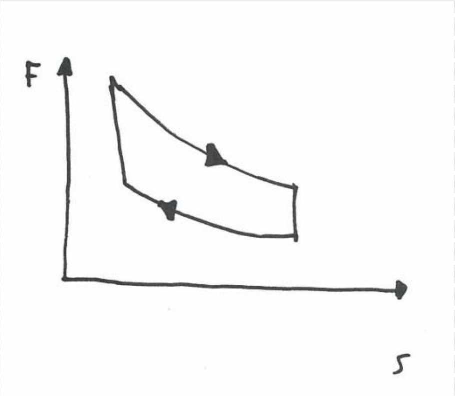
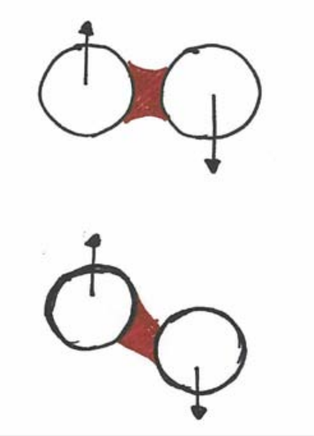
Effects of CA hysteresis

Dissipative spring

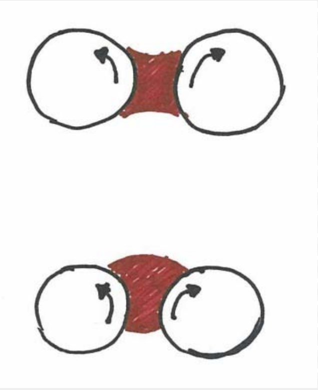




Sliding friction



Rolling friction



Summary

- Investigation of mechanical, flow, mixing and stability properties of dense wet granular matter using particle dynamics combined with fluid dynamics

- Calculation of capillary forces and Laplace pressure

- Effect of high contact angles

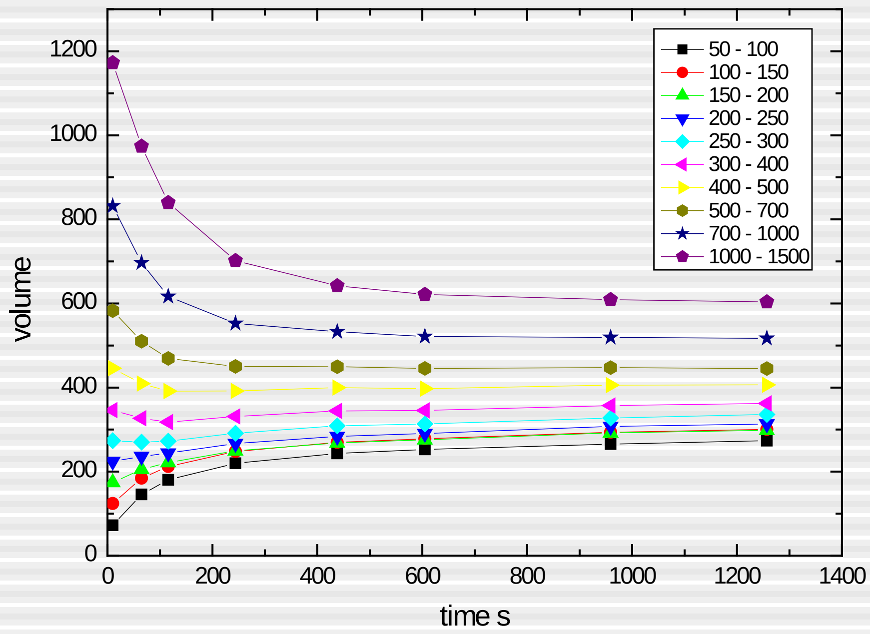
- Hysteretic effects

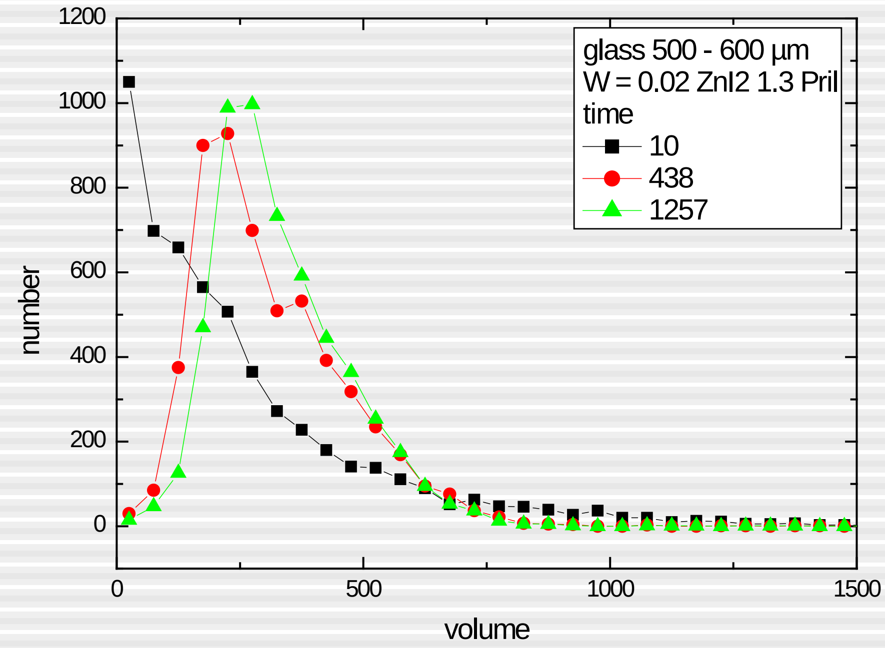
Thanks for your attention !!!

Fluid transport

(Bridge volumes measured with fast X-ray micro-tomography)

bridge volume redistributing in time after shaking a granular pile



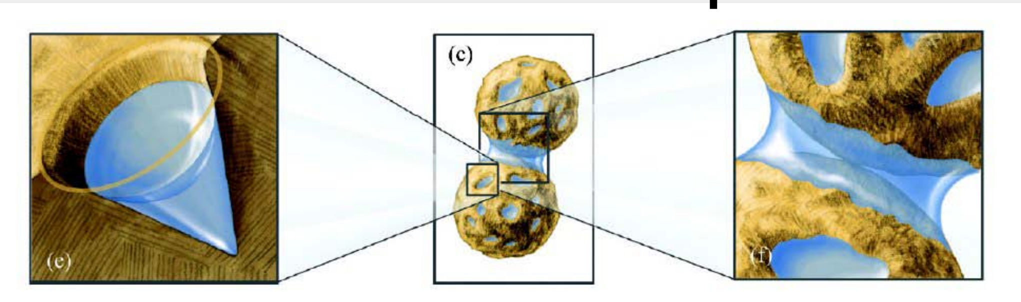


M Scheel et al. ***Phys Condens Matter*** **20: 494236 (2008)**

Find equilibration time on the order of minutes

Fluid transport

Presence of a thin liquid film on the bead surface:



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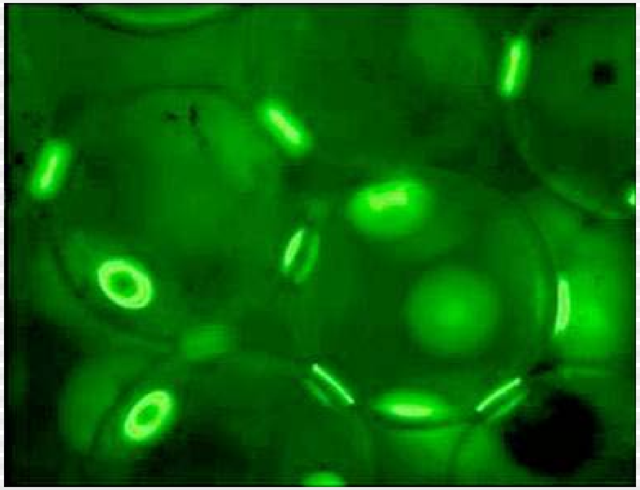
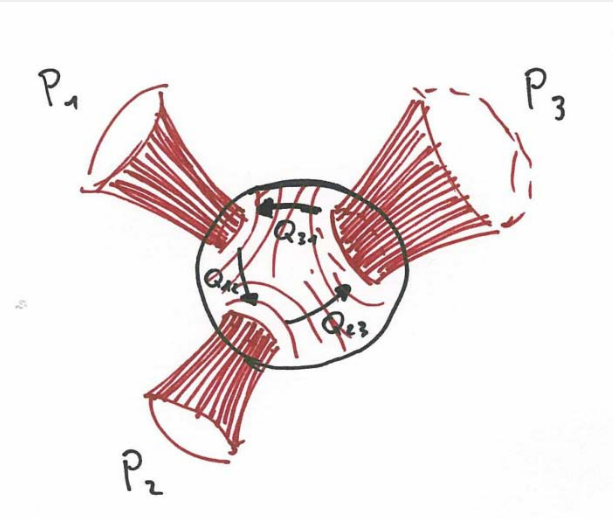
Fluid transport between liquid bridges connected to a bead



Conductance matrix

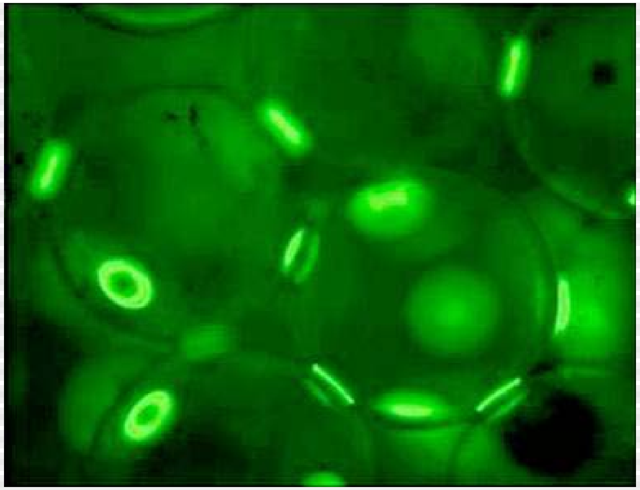
(analogy with conductivity)

$$\begin{pmatrix} Q_{11} & Q_{21} & Q_{31} & \cdots \\ Q_{12} & Q_{22} & Q_{32} & \\ Q_{13} & Q_{23} & Q_{33} & \\ \vdots & & & \ddots \end{pmatrix}$$



Fluid transport

Resolve the fluid transport across the bead surface



Darcy law

$$\vec{j} = -\mu \vec{\nabla} P$$

μ = mobility of the liquid

$$\vec{\nabla} \cdot \vec{j} = 0$$

incompressibility

$$\vec{\nabla}(\mu \vec{\nabla} P) = 0$$

μ = constant

$$\vec{\nabla}^2 P = 0$$

Laplace Beltrami operator (on a sphere geometry)

$$\frac{1}{R_0^2}\left(\frac{1}{\sin\theta}\partial_\theta \sin\theta \partial_\theta + \frac{1}{\sin^2\theta}\partial_\varphi^2\right)P = 0$$

Multi body interactions

Small liquid content:
Only bridges

fast X-ray
micro tomography

liquid content
W=0.01
bead diameter:
780 µm

M Scheel et al. *Nature Materials* 7: 189 (2008)