Mesoscale modeling of particles and particles in fluids

- Multi-Scale (Models) and
- Continuum Theory (Applications)
- Jamming and un-jamming

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Introduction

Dense granular flow & shear banding

Geophysics, engineering, and science

Overview

Introduction

Contact models

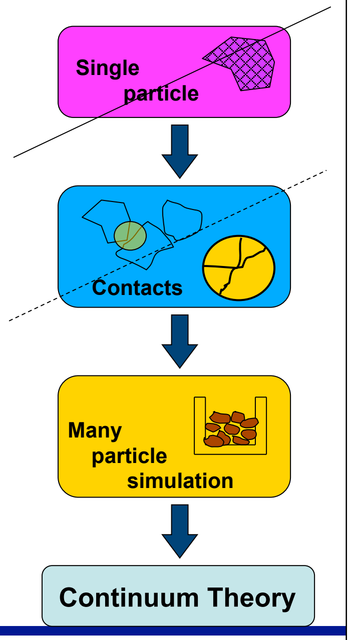
Many particle simulation

Local micro-macro

Continuum Theory

… model with anisotropy

Particles & Fluids



From particles to continuum theory

1. particles/powders – discrete ingredients
2. fluid- and solid-like constitutive relations

– multiple scales (from nano-meter to meters)
– from particles+contacts to application scale …

Scales:
+ particle modeling (DEM) -> micro-scale
--
+ continuum modeling -> macro-scale

From particles to continuum theory

1. particles/powders – discrete ingredients
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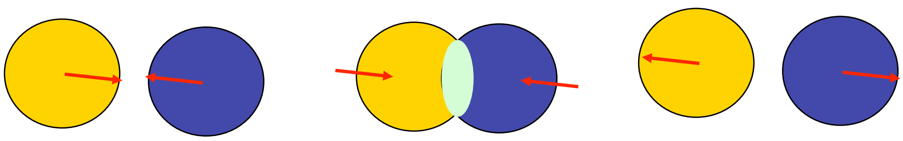
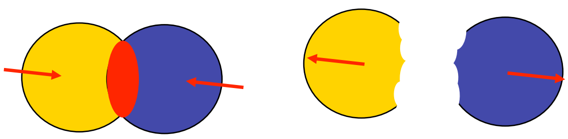
– multiple scales (from nano-meter to meters)
– from particles+contacts to application scale …

Scales:
+ particle modeling (DEM) -> micro-scale
-- (stochastic) plastic events => meso-scale
+ continuum modeling -> macro-scale

Elastic spheres (idealized)

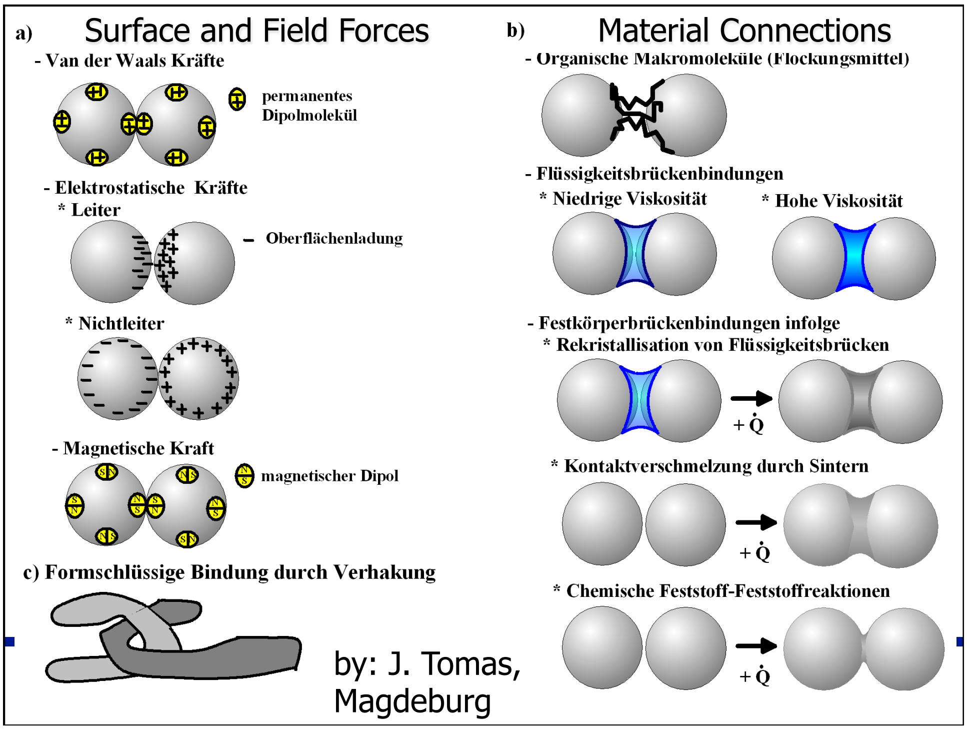


Elasto-plastic spheres (realistic)



Before During After

Mostly use idealized non-plastic particles …



2P+MD+DEM Literature

(http://www2.msm.ctw.utwente.nl/sluding/publications.html)

[1] 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]

[2] S. Luding, *Cohesive frictional powders: Contact models for tension* Granular Matter 10(4), 235-246, 2008 [http://www2.msm.ctw.utwente.nl/sluding/PAPERS/LudingC5.pdf]

[3] 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]

[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]

Linear Contact model

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

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

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

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

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

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

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

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

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

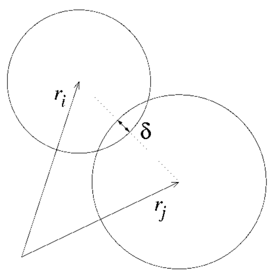
$$\dot{\delta}(t) = \frac{v_0}{\omega}\exp(-\eta t)\left[-\eta\sin(\omega t) + \omega\cos(\omega t)\right]$$

contact duration $\boxed{t_c = \pi/\omega}$

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

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

Discrete particle model

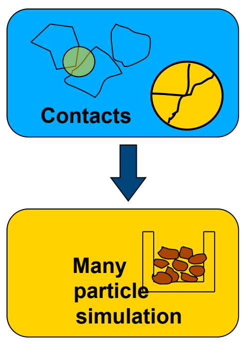


Equations of motion

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

Forces and torques:

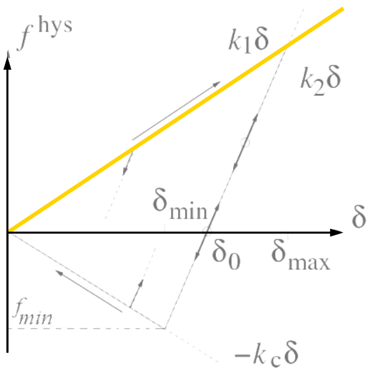
$$\vec{f}_i = \sum_c \vec{f}_i^{\,c} + \sum_w \vec{f}_i^{\,w} + m_i g$$



Contact if Overlap > 0

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

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



Linear Contact model

- (really too) simple ☺
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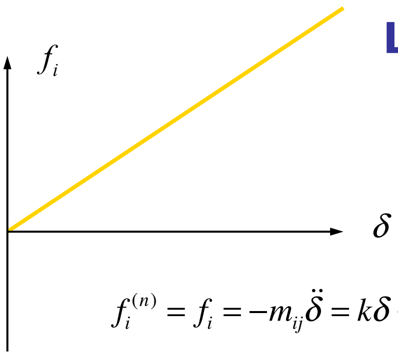
$$f_i^{hys} = \begin{cases} k_1\delta & \text{for un-/re-loading} \\ & \end{cases}$$



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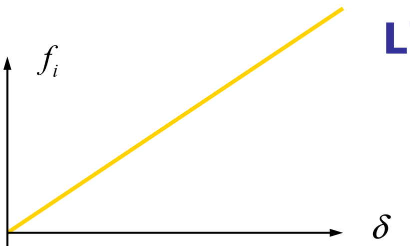
rel. velocity $\dot{\delta} = -\left(\vec{v}_i - \vec{v}_j\right)\cdot\hat{n}$

acceleration $\ddot{\delta} = -\left(\vec{a}_i - \vec{a}_j\right)\cdot\hat{n}$

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

Linear Contact model



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rel. velocity $\dot{\delta} = -\left(\vec{v}_i - \vec{v}_j\right)\cdot\hat{n}$

acceleration $\ddot{\delta} = -\left(\vec{a}_i - \vec{a}_j\right)\cdot\hat{n} = -\left(f_i / m_i - f_j / m_j\right) \overset{\vec{f}_j = -\vec{f}_i}{=} -\frac{1}{m_{ij}}\vec{f}_i\cdot\hat{n}$

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

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Linear Contact model

- comments/problems

restitution coefficient
Always >= 0

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

Forces negative
⇔ adhesion

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

=> Reconsider definition of *t_c* ...

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

Linear Contact model

	particle-particle	particle-wall
elastic freq.	$\omega_0 = \sqrt{k/m_{ij}}$	$\omega_0^{wall} = \sqrt{k/m_i} = \omega_0/\sqrt{2}$
eigen-freq.	$\omega = \sqrt{\omega_0^2 - \eta^2}$	$\omega^{wall} = \sqrt{\omega_0^2/2 - \eta^2/4}$
visc. diss.	$\eta = \dfrac{\gamma}{2m_{ij}}$	$\eta^{wall} = \dfrac{\gamma}{2m_i} = \dfrac{\eta}{2}$
contact duration	$\boxed{t_c = \pi/\omega}$	$\boxed{t_c^{wall} = \pi/\omega^{wall} > t_c}$
restitution coeff.	$r = \exp(-\eta t_c)$	$r^{wall} = \exp(-\eta^{wall} t_c^{wall})$

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

Time-scales

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

contact duration $\boxed{t_c = \pi/\omega}$ $\quad t_c^{wall} = \pi/\omega^{wall} > t_c$

$t_n < t_c$

↑

time between contacts

↓

$t_n > t_c$

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

experiment T

Time-scales

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

contact duration $\boxed{t_c = \pi / \omega}$

$t_n < t_c$

different sized particles

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

time between contacts

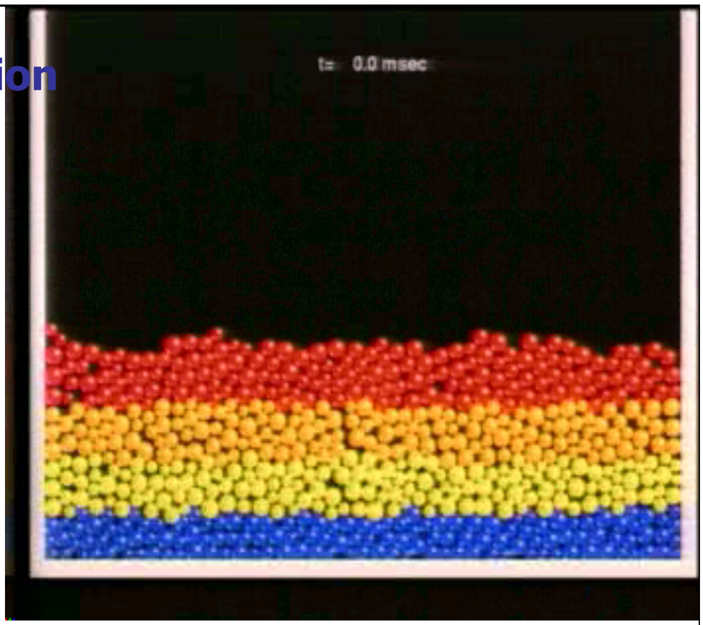
$t_n > t_c$

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

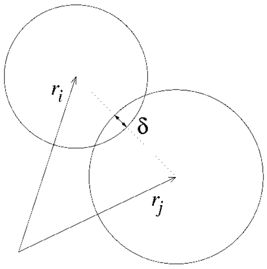
experiment T

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

Convection



Discrete particle model



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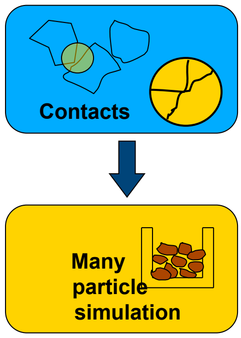

Contact if Overlap > 0

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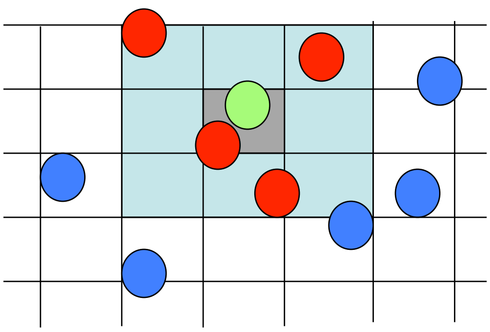
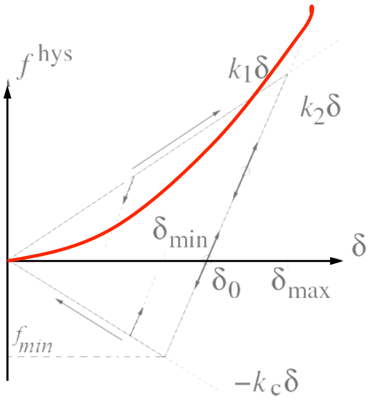
Normal $\hat{n} = \vec{n}_{ij} = \frac{\left(\vec{r}_i - \vec{r}_j\right)}{\left|\vec{r}_i - \vec{r}_j\right|}$

Algorithmic trick(s) for speed-up

- Linked cells neighborhood search O(1) (*short range forces*)



- Linked cells update after 10-100 time-steps O(*N*)



Hertz Contact model

- simple ☺
- non-linear
- easy to implement

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

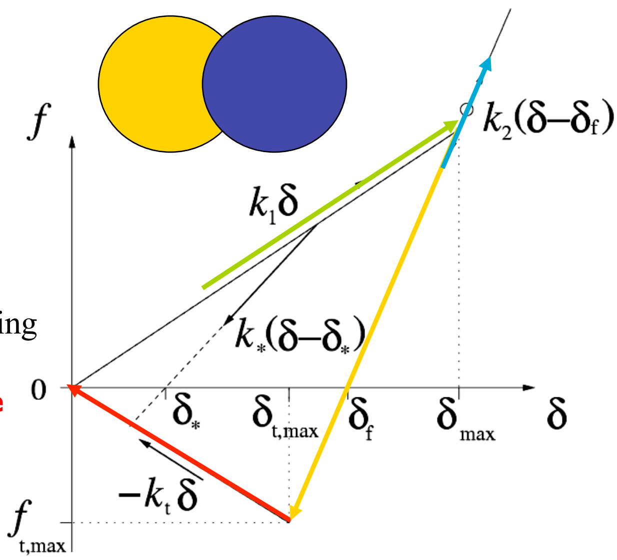
Contacts

1. loading
transition to stiffness: k_2

2. unloading

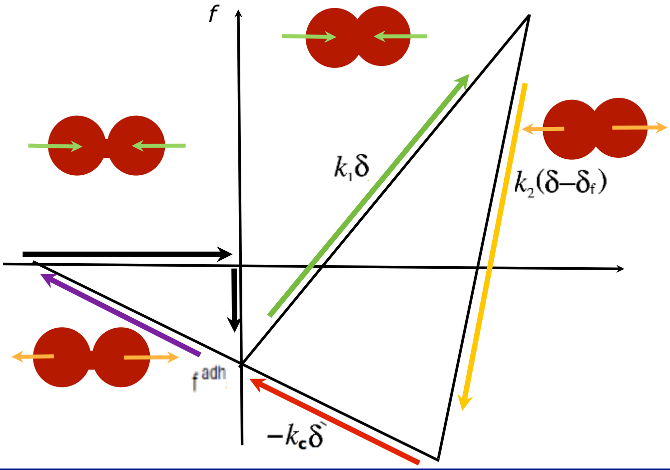
3. re-loading
elastic un/re-loading stiffness: k_2

4. tensile failure
max. tensile force

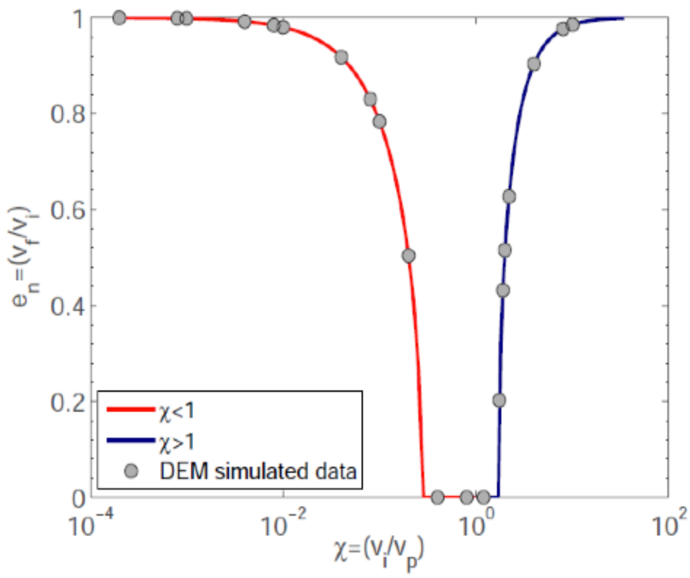


Irreversible elasto-plastic adhesive contacts

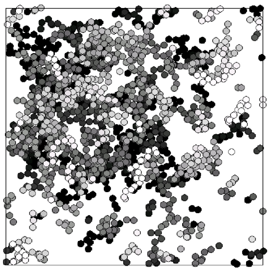
- Loading
  Plastic def.
- Unloading
  "elasto-plastic"
- Re-loading
  "elastic"
- Cohesion
- Long-range
  forces ...

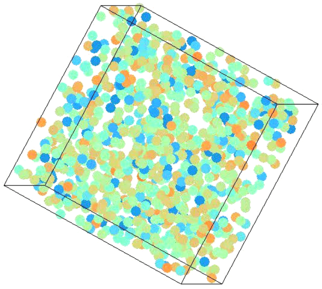


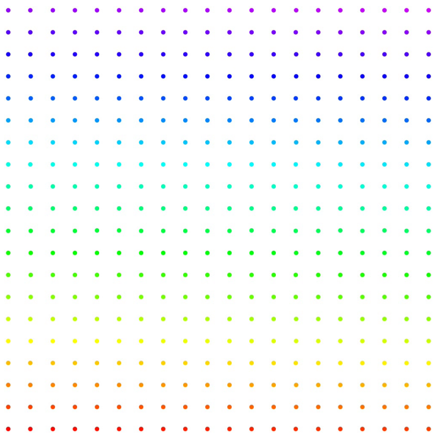
Coefficient of Restitution (analytical)



Attractive forces …

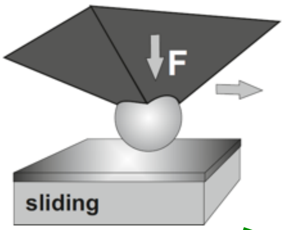


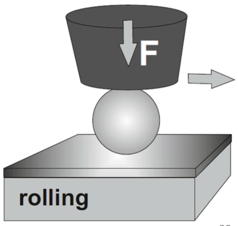


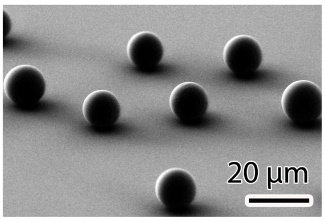


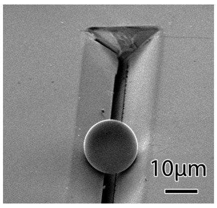
Mostly ignore dry and wet attraction … see later …

Nano-indenter -> contacts

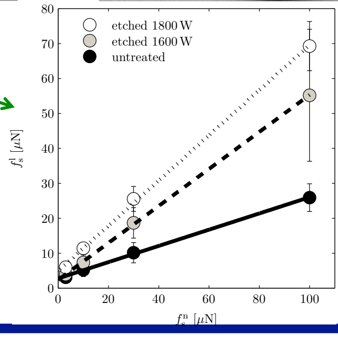






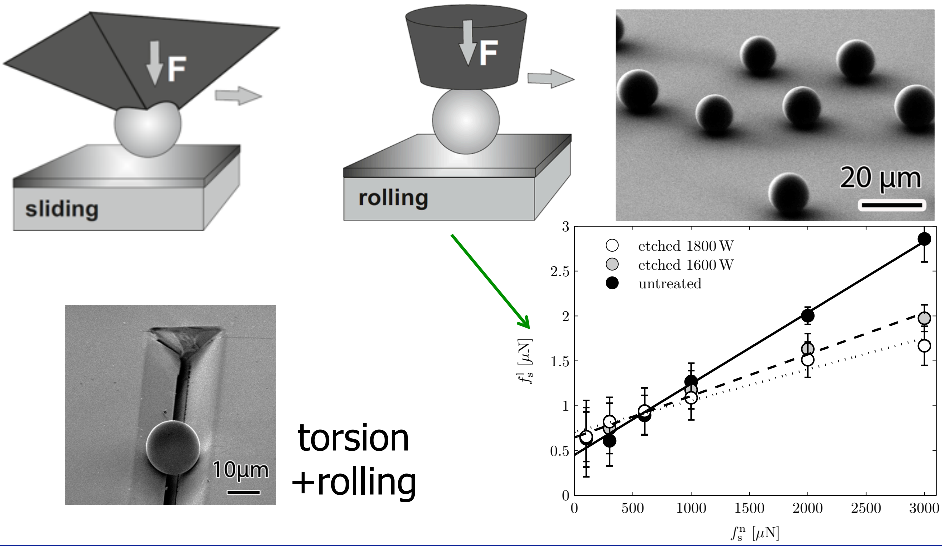


torsion
+rolling



R. Fuchs, T. Weinhart, et al. Granular Matter, 2014

Nano-indenter -> contacts



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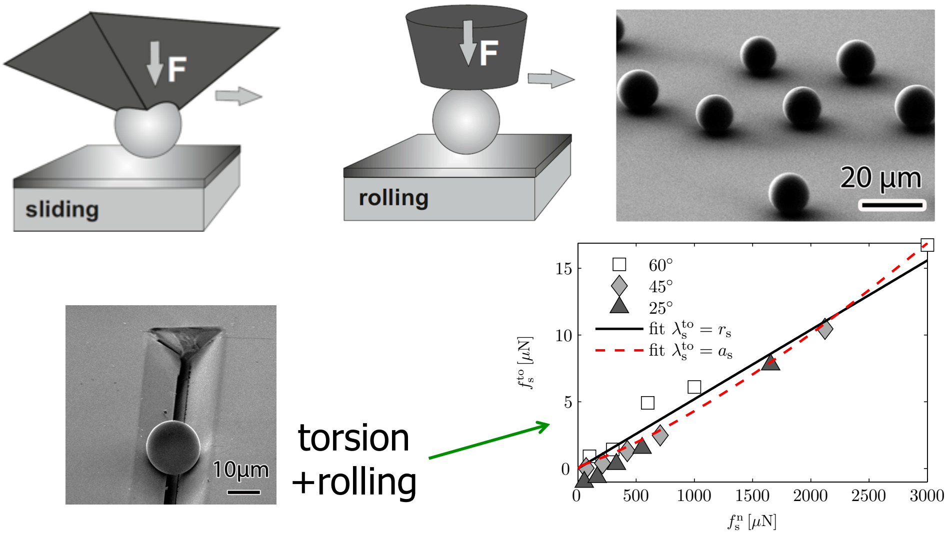

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Tangential contact model

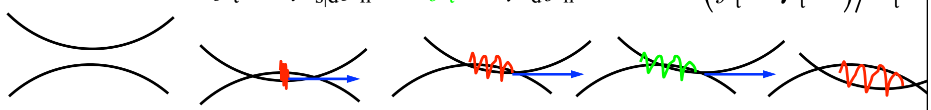
- Static friction - spring
- Dynamic friction - dashpot

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

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

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

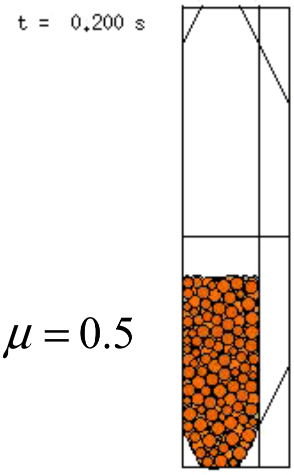
sliding: $f_{\mathrm{t}}^{0} > \mu_{\mathrm{s|d}} f_{\mathrm{n}}$ $f_{\mathrm{t}} = \mu_{\mathrm{d}} f_{\mathrm{n}} \hat{t}$ $\vartheta = (f_{\mathrm{t}} + \gamma_{\mathrm{t}}\dot{\vartheta}') / k_{\mathrm{t}}$



before contact static dynamic static

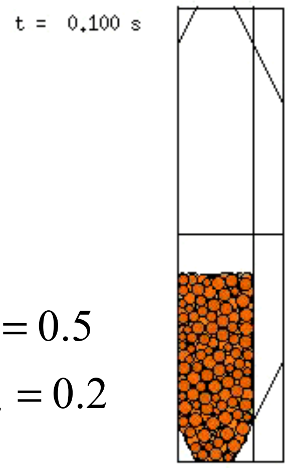
Flow with friction & rolling resistance

$\mu = 0.5$



$\mu = 0.5$

$\mu_r = 0.2$



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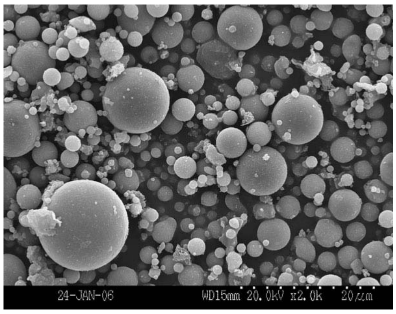
Challenge:

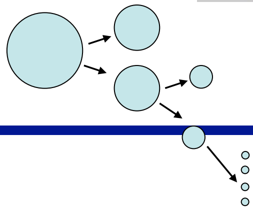
Fast contact detection between particles with strongly different sizes



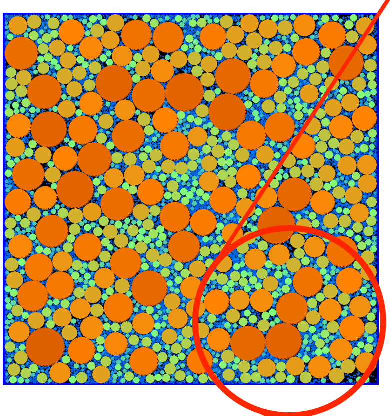
fly ash sample at 2000x magnification,
University of Kentucky, CAER

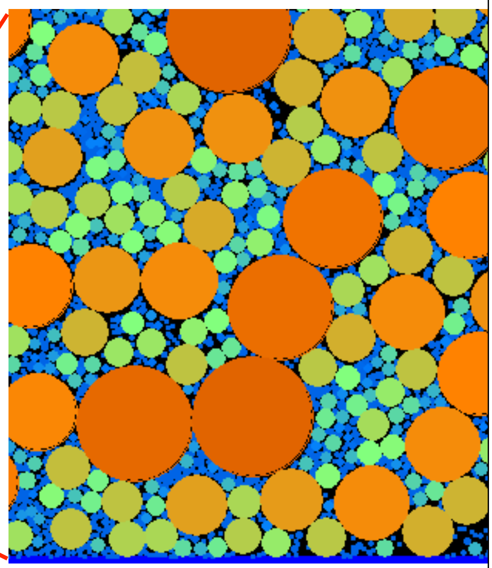
Size ratio >> 10
Number of particles > 10^6

- Breakage / Grinding
- Concrete …
- Aerosols/Smog
- Food Powders



Particles with wide size-distributions

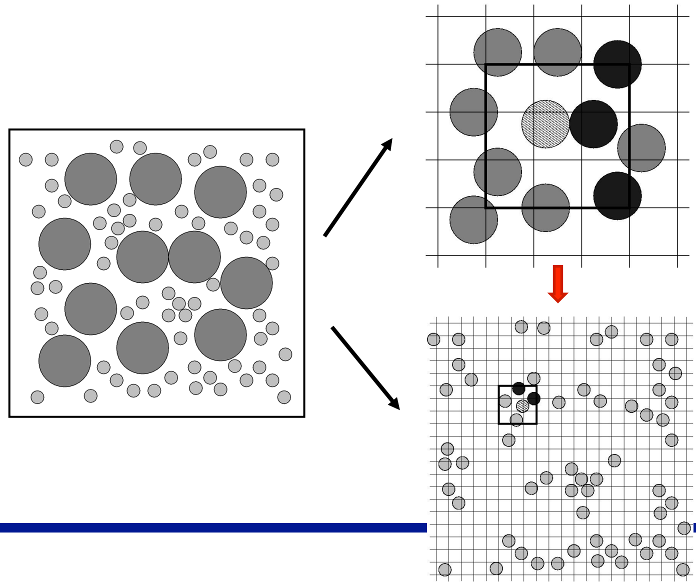




Mostly ignored, use some to avoid crystallization

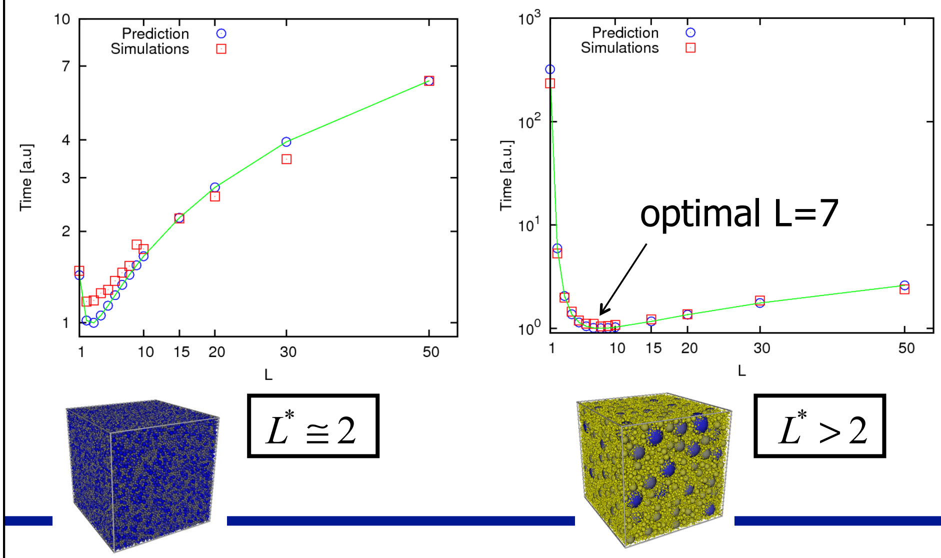
Hierarchical grid: fast, robust & flexible

example: L=2 level grid



HGRID: Analytical prediction vs Simulations

$$T = NL(m_L + K)$$



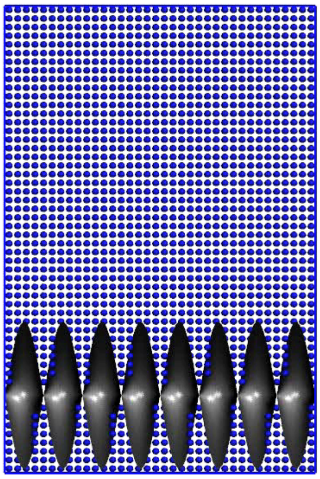
uniform size

uniform volume

MERCURYDPM

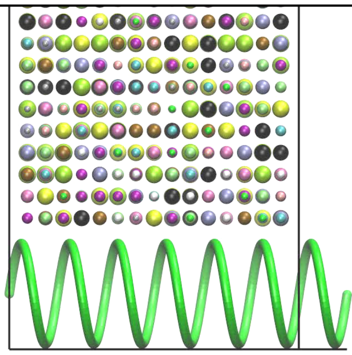
Open source
(mercurydpm.org)

Based on:
- HGrid (contacts)
- MicroMacro (tools)



Dosing application example …

MERCURYDPM



Open source

Based on:
- HGrid
- MicroMacro

**flowable powder vs.
sticky, chunky powder**

O. I. Imole, MSM, 2013

Dosing application example …

MERCURYDPM

Open source

Based on:
- HGrid
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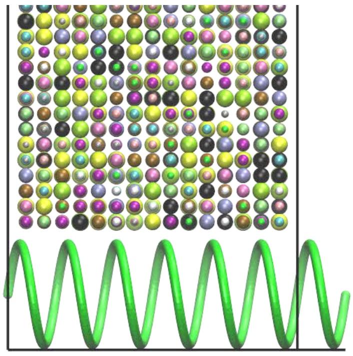
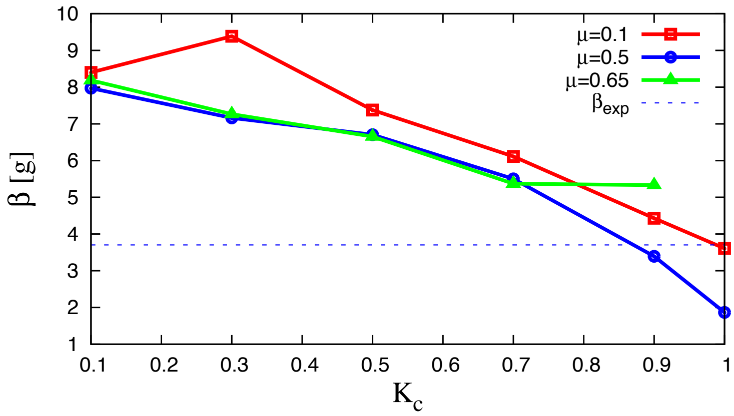
flowable powder vs.
sticky, chunky powder



O. I. Imole, MSM, 2013

Dosing application example …

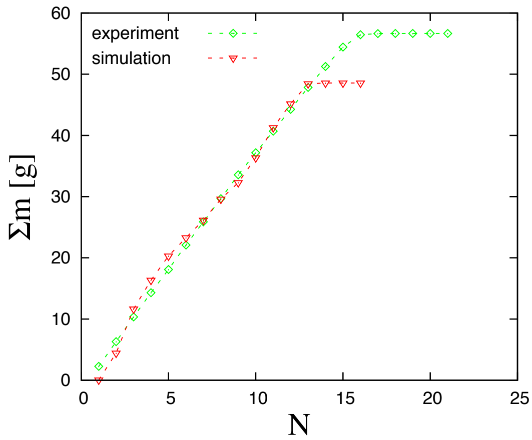
Dosing – parameter calibration



*Based on
O. I. Imole, D. Krijgsman, T. Weinhart, V. Magnanimo, E. C. Montes, M. Ramaioli, and S. Luding.

Experiments and Discrete Element Simulation of the Dosing of Cohesive Powders in
a Canister Geometry. submitted to Powder Techn. 2014 & PhD-thesis, O. I. Imole 2014

Dosing: DEM vs. experiment



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Experiments and Discrete Element Simulation of the Dosing of Cohesive Powders in a Canister Geometry, Powder Technology 2016 & PhD-thesis, O. I. Imole 2014

Software used …

- DEMSolutions/EDEM
- DCS Computing/LIGGGHTS
- MercuryDPM
- and some others

Software used …

- DEMSolutions/EDEM
- DCS Computing/LIGGGHTS
- MercuryDPM
- and some othe

MERCURYDPM

unique features:
- open-source (really ;-)
- HGrid for largely different particle sizes
- mercuryCG for coarse-graining to continuum
- analytical complex geometry-support
- etc.

Software used …

- DEMSolutions/
- DCS Computin
- MercuryDPM
- and some other

MERCURYDPM

MercuryLab

- Mercury*Cloud*
- Training
- Consulting
- Support

Software used …

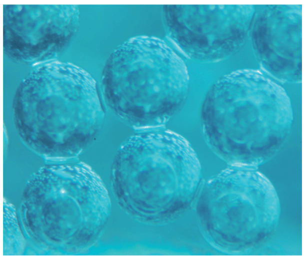
- DEMSolutions/E
- DCS Computing
- MercuryDPM
- and some other

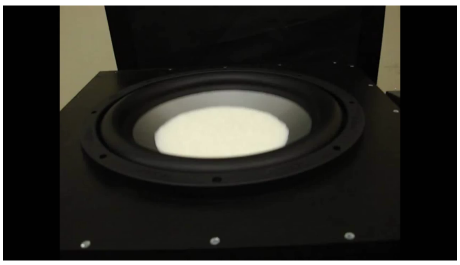
MERCURYDPM

MercuryLab

- Mercury*Cloud* no need to buy hardware/pay on demand
- Training you still need someone who understands ☺
- Consulting … or you order the full service
- Support

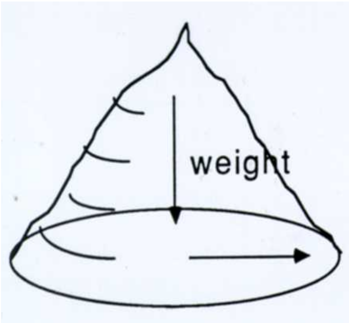
Granular Matter:
shear thin/thick fluid? or plastic solid?

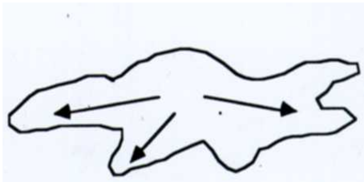




Powder and Liquid Flow (differences)

Inherent Yield Stress



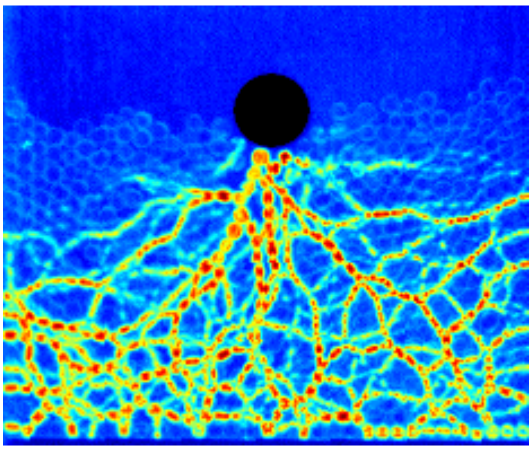


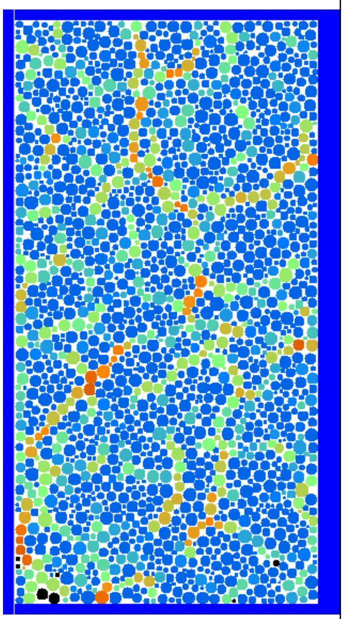
Powders heap

Liquid spreads

Yield stress = resistance against flow

Dense particle systems:





experiments - simulations

Biaxial box element test

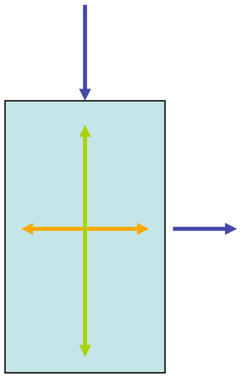
- Top wall: strain controlled

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

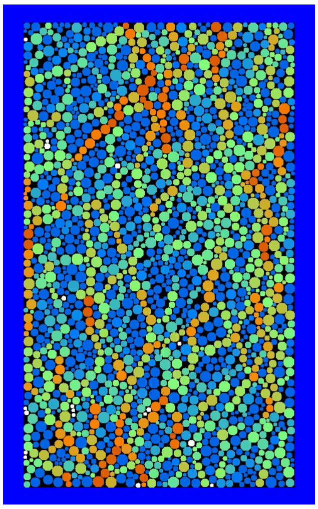
- Right wall: stress controlled

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

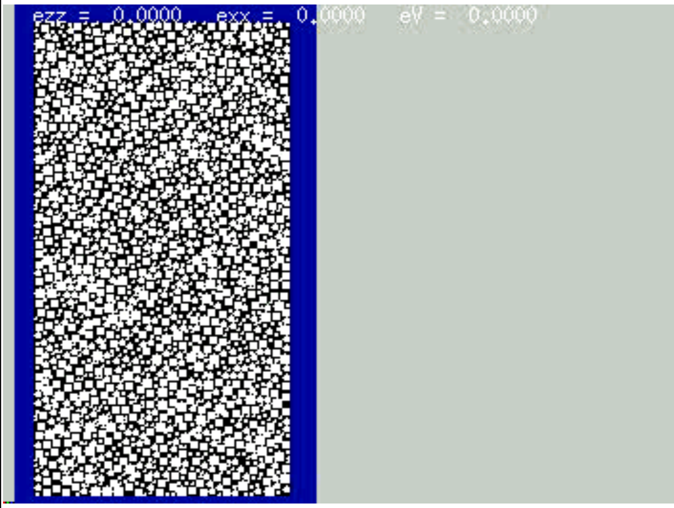
- Evolution with time … ?



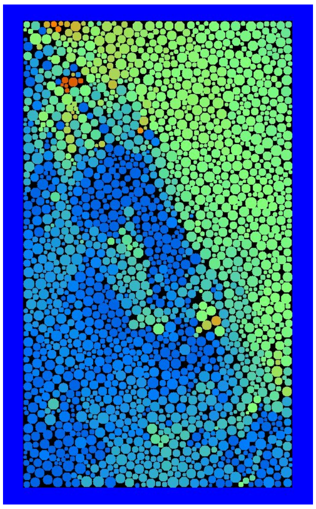
Bi-axial box (stress chains)



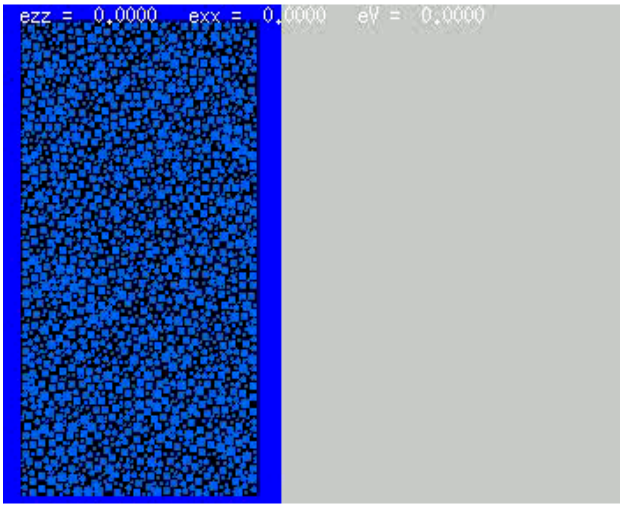
Bi-axial box (stress chains)



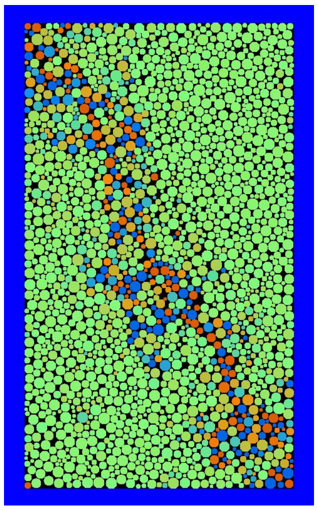
Bi-axial box (kinetic energy)



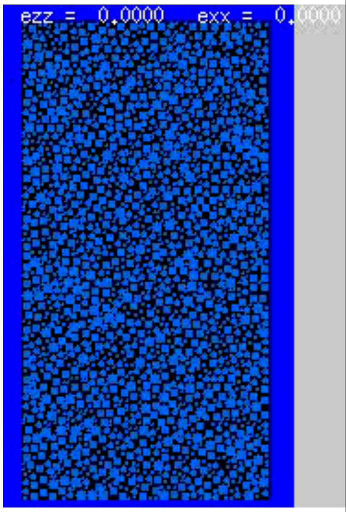
Bi-axial box (kinetic energy)



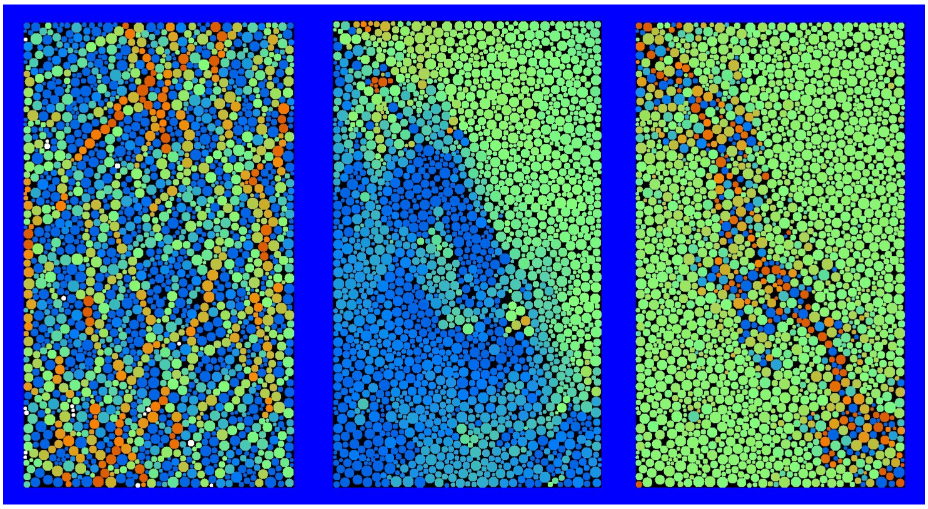
Bi-axial box (rotations)



Bi-axial box (rotations)

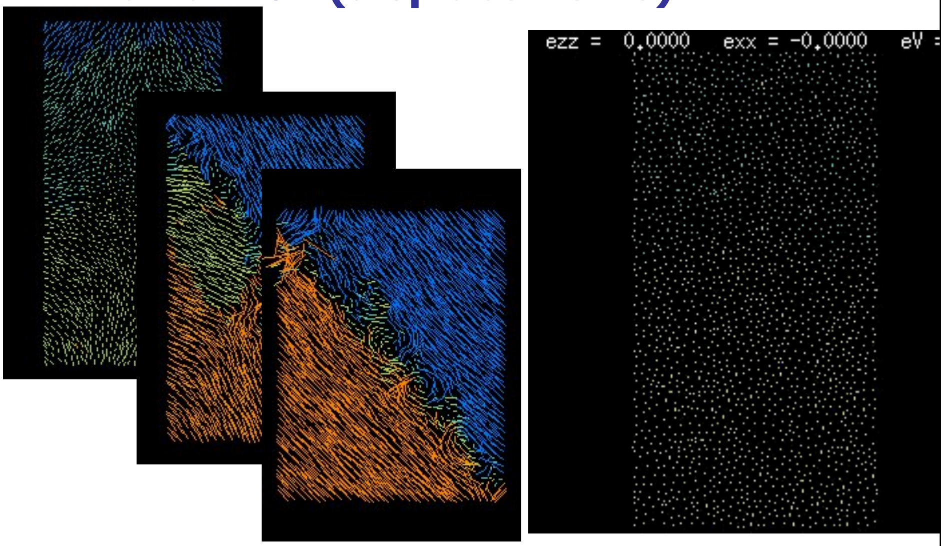


Multiple micro-mechanisms

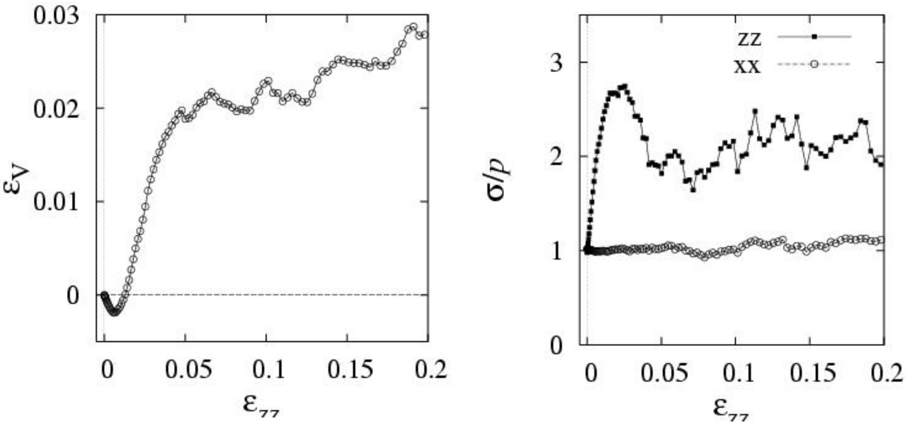


inhomogeneity & anisotropy, instabilities & structures, rotations

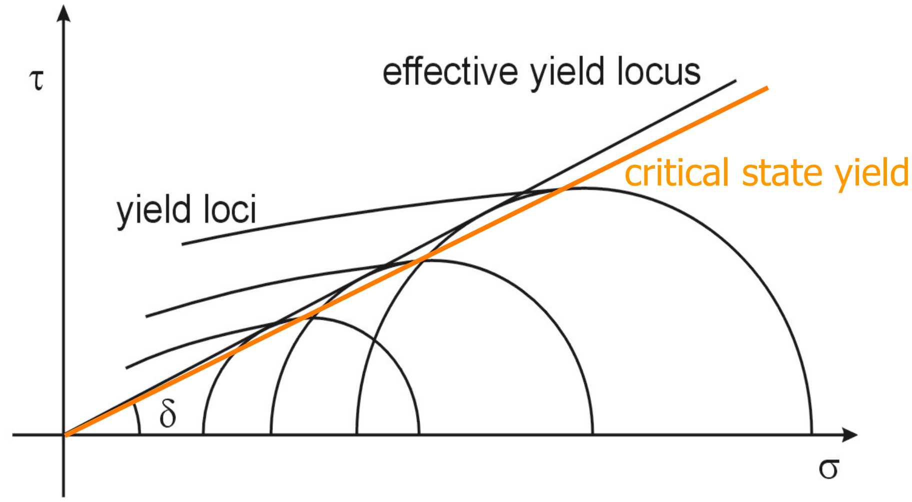
Bi-axial box (displacements)



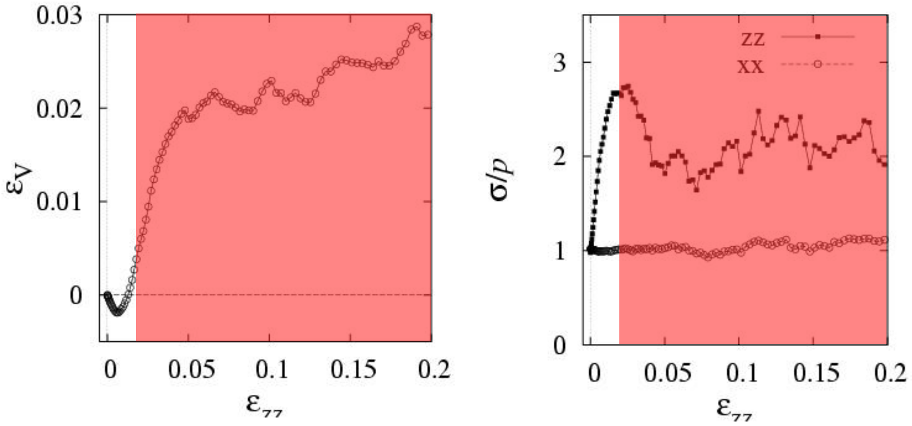
Bi-axial compression with p_x=const.



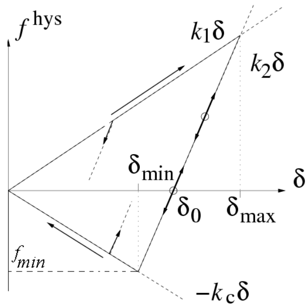
Yield loci

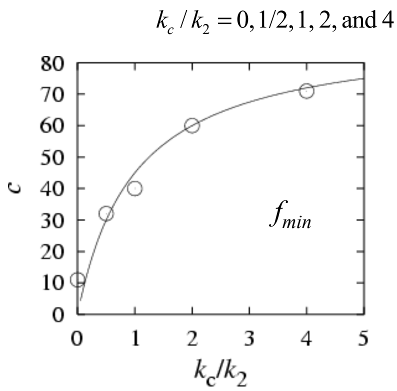


Bi-axial compression with p_x=const.



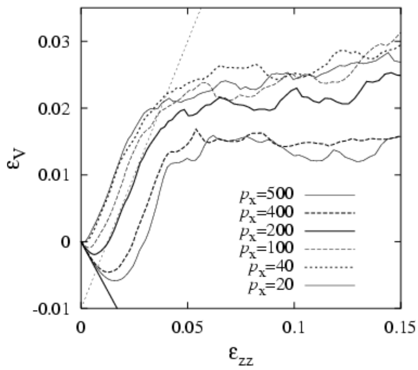
Micro-macro for cohesion

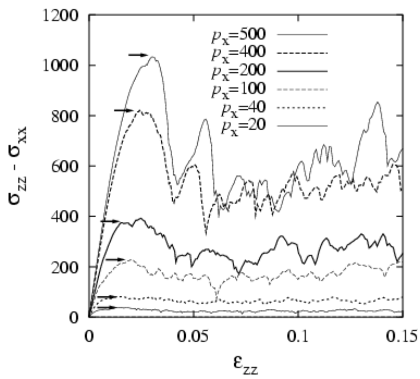




micro adhesion: f_{min} macro cohesion $c = c_0 \dfrac{1 - k_1/k_2}{1 + k_2/k_c}$

Pressure dependence

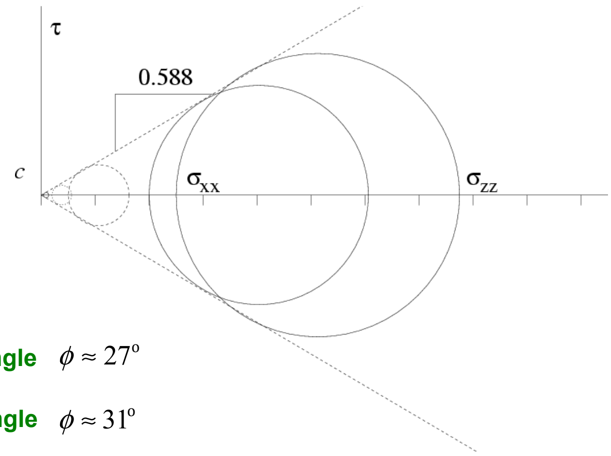




Results for friction μ=0.5 and different p_x and k_c=0

Friction – no cohesion

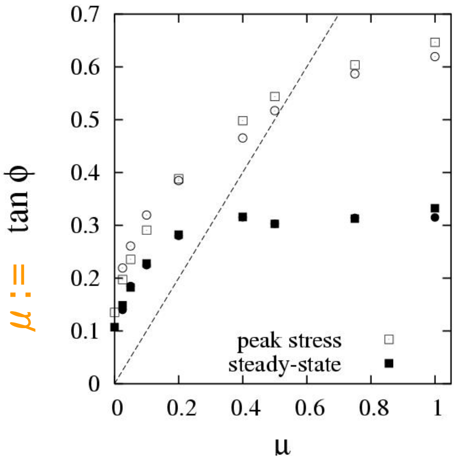
$k_c = 0$ and $\mu = 0.5$



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

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

Micro-macro for friction



prepared μ_p=0

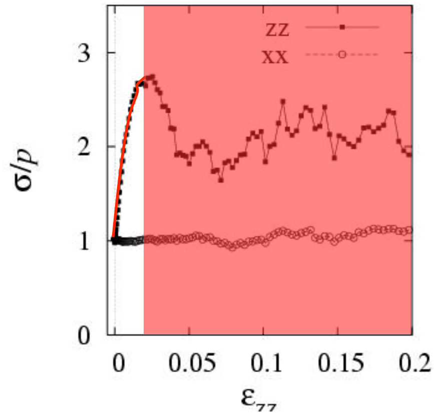
prepared μ_p=0.5

steady-state shear

micro contact-friction μ_p macro friction-angle μ

An-isotropy (in absence of friction&cohesion)

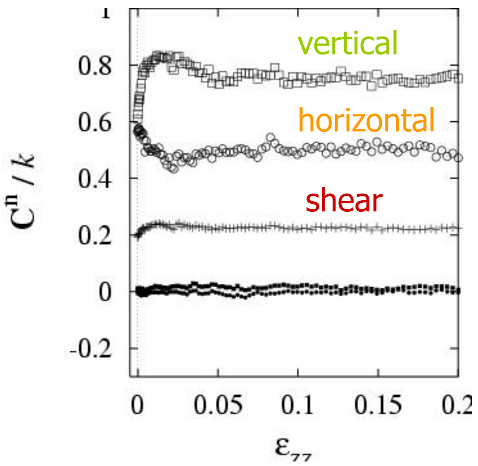
in stress

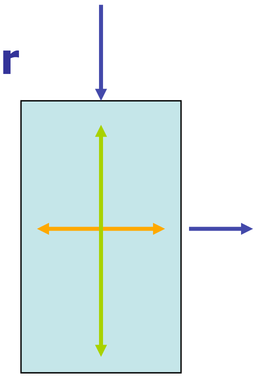


An-isotropy (Stress)

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

Stiffness/structure tensor





Different moduli:

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

An-isotropy (Stress & Structure)

~ elastic Modulus

Macro-Friction

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

$$\frac{\partial}{\partial \varepsilon_D} A = \beta_F \left(A_{\max} - A \right)$$

An-isotropy (Stress & Structure)

~ elastic Modulus

Macro-Friction

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

$$\frac{\partial}{\partial \varepsilon_D} A = \beta_F \left(A_{\max} - A \right)$$

max. anisotropy

Anisotropy evolution rate

An-isotropy (Stress & Structure)

~ elastic Modulus (*G*/*p*)

Macro-Friction

plastic prob.

$$\frac{\partial}{\partial \varepsilon_D} s_D = \beta_s \left(s_{\max} - s_D \right) = \beta_s s_{\max} \left(1 - \pi_D \right)$$

$$\frac{\partial}{\partial \varepsilon_D} A = \beta_F \left(A_{\max} - A \right)$$

max. anisotropy

Anisotropy (structural) evolution rate

Constitutive model – elastic-plastic, incr.

quasi-static, scalar (in the biaxial box eigen-system)

$$\delta\sigma_V = B\varepsilon_V + A\left(1-\pi_D\right)\varepsilon_D$$

$$\delta\sigma_D = A\varepsilon_V + G\left(1-\pi_D\right)\varepsilon_D$$

and: evolution of microstructure (isotropic) …

$$\frac{\partial}{\partial \varepsilon_V}\phi_c \vdots B \vdots G \neq 0$$

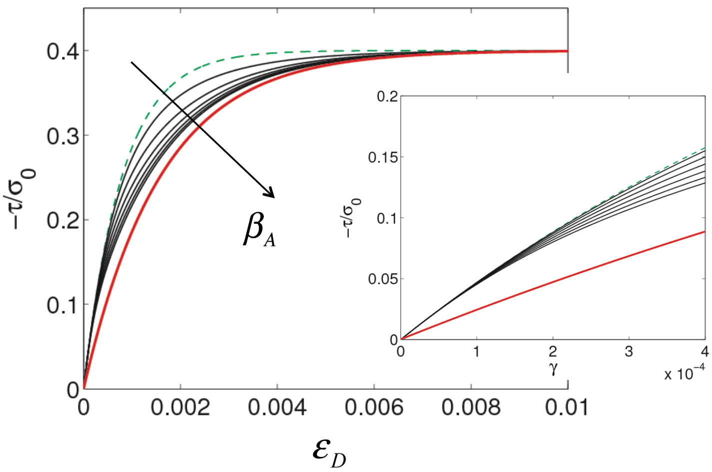
and: evolution of microstructure (deviator) …

$$\frac{\partial}{\partial \varepsilon_D} A = \beta_A\left(A_{\max} - A\right)$$

… based on homogeneous element test DEM data
(for finite strain)

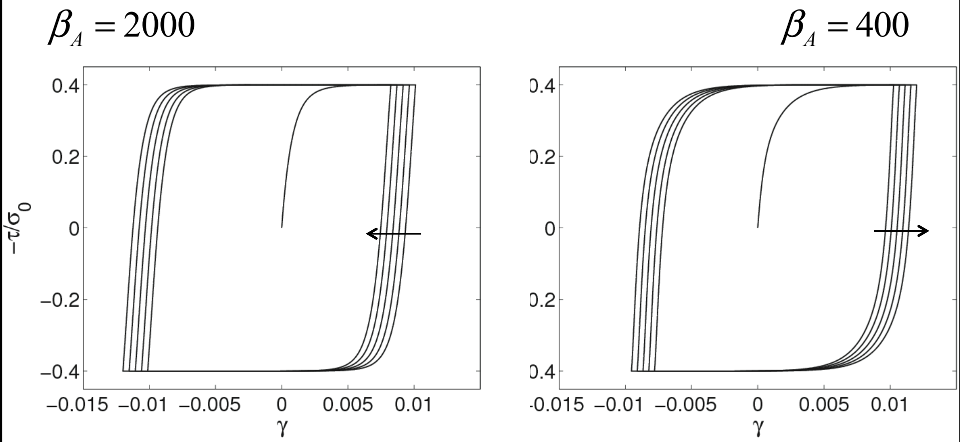
Constitutive model – shear stress

(scalar in the biaxial box eigen-system)

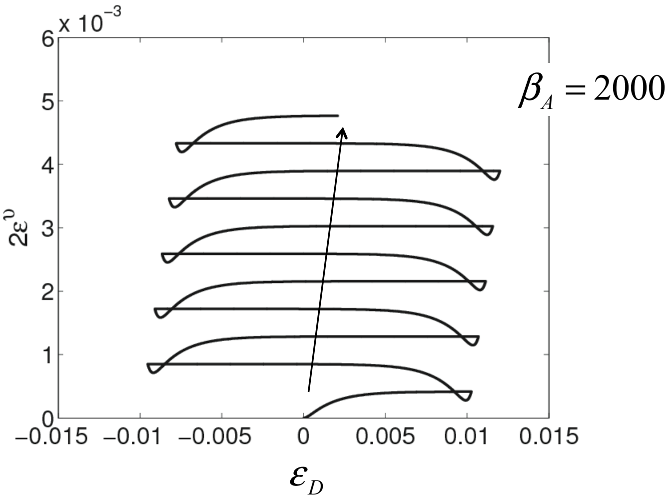


Constitutive model – cyclic loading

(in the biaxial box eigen-system)

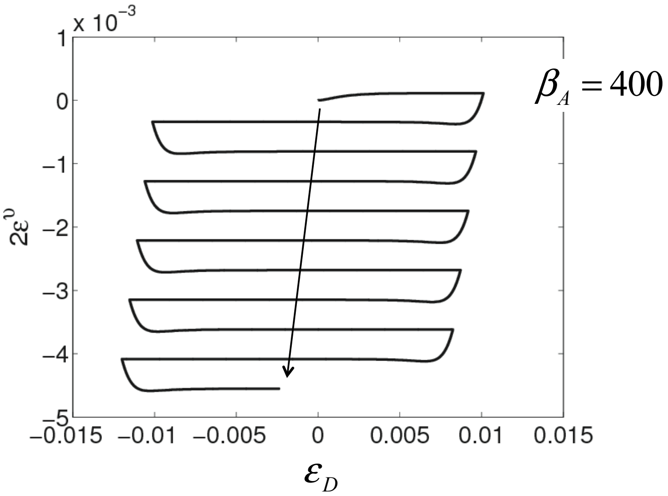


Constitutive model – scalar: dilatancy



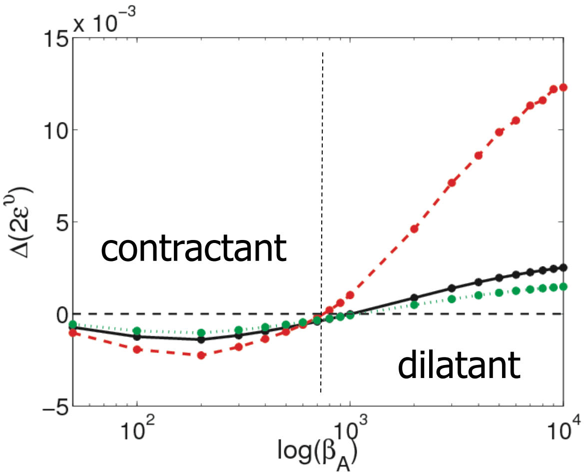
… for fast structural evolution

Constitutive model – scalar: contractancy



... for slow structural evolution

Constitutive model – anisotropy rate



Constitutive model – scalar, anisotropic

Cross-coupling of isotropic and deviatoric parts

and

Interplay between:
shear stress (rate) G/p and anisotropy (rate) β_A

$G/p > \beta_A$: contractant, collapsing material
$G/p < \beta_A$: dilatant, "hardening" material

Calibration: Elastic Moduli (3D)

Constitutive behavior of an **anisotropic** material described **incrementally** as

$$\begin{bmatrix} \delta P^* \\ \delta\sigma^*_{\rm dev} \end{bmatrix} = \begin{bmatrix} B & A_1 \\ A_2 & G^{\rm oct} \end{bmatrix} \begin{bmatrix} 3\delta\varepsilon_{\rm v} \\ \delta\varepsilon_{\rm dev} \end{bmatrix}$$

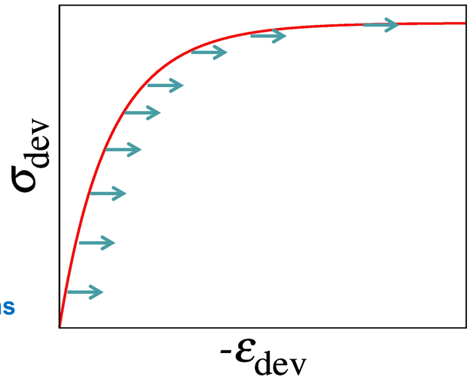
$$(B, A_1, A_2, G^{\rm oct}) = \mathcal{F}(\mathbf{F}, \boldsymbol{\sigma}) = \mathbb{F}(F_{\rm v}, F_{\rm dev}, P, \sigma_{\rm dev})$$

Stress – Strain

Preparation: ISO+SHEAR (dev)

Purely deviatoric perturbations
(amplitude ?)

Similarly, purely isotropic perturbations



N. Kumar et al. Acta Mechanica, (2014)
Luding and Perdahcioglu *CIT* (2011), Magnanimo and Luding, *Granular Matter* (2011)

Constitutive model with structural anisotropy

$$\delta P^* = 3B\delta\varepsilon_{\rm v} + \boxed{A_1} S_\sigma \delta\varepsilon_{\rm dev},$$
$$\delta\sigma^*_{\rm dev} = 3\boxed{A_2}\delta\varepsilon_{\rm v} + G^{\rm oct} S_\sigma \delta\varepsilon_{\rm dev},$$
$$\delta F_{\rm dev} = \beta_F \operatorname{sign}(\varepsilon_{\rm dev}) F^{\max}_{\rm dev} S_F \delta\varepsilon_{\rm dev}$$

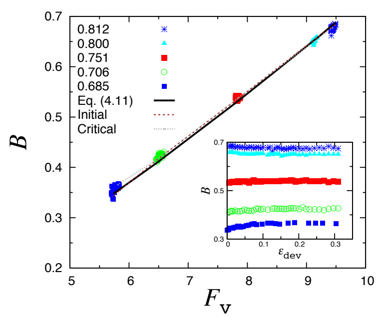
+ other terms (3D, not shown)

with probability for elastic deformation: $S := (1 - \pi_D)$

Due to $\boldsymbol{A_1}$ and $\boldsymbol{A_2}$, the model provides a **cross coupling** between the two types of stress and strain in the model

Need to define: **initial state and deformation path = history**

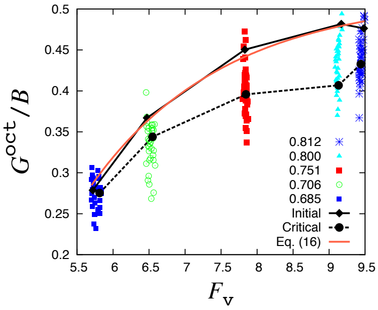
Constitutive model – calibration
Direct moduli (B,G,A) probing …



$B = b_0 F_V$

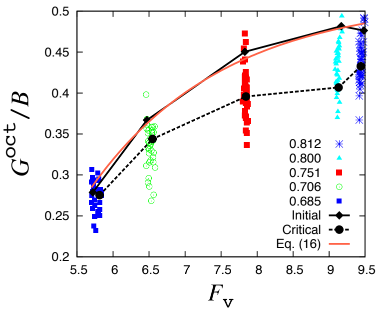
(with isotropic F_V)

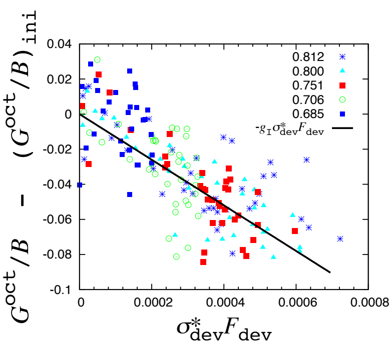
Constitutive model – calibration
Direct moduli (B,G,A) probing …



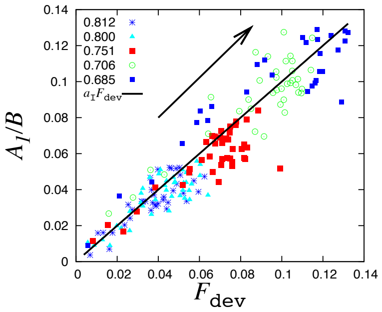
$G = B\ g(F_V)$

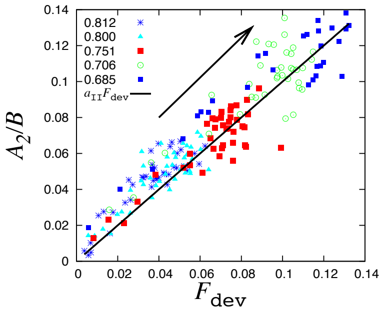
Constitutive model – calibration
Direct moduli (B,G,A) probing …





Constitutive model – calibration
Direct moduli (B,G,A) probing …





A_1=A_2 =: A

Constitutive model – calibration (elastic)
Direct moduli (B,G,A) probing …

Bulk Modulus: $B = b_0 F_V$

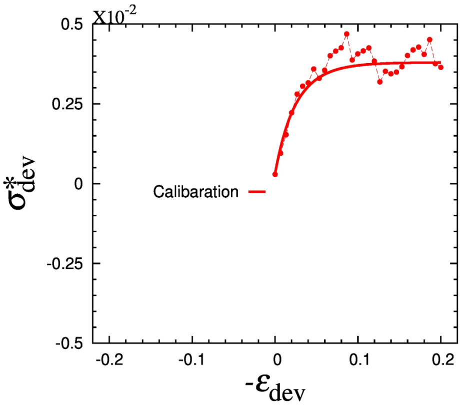
Shear Modulus: $G = B\, g(F_V)\, [1-\sigma^*_{dev} F_{dev}]$

Anisotropy Modulus: $A = B\, F_{dev}$

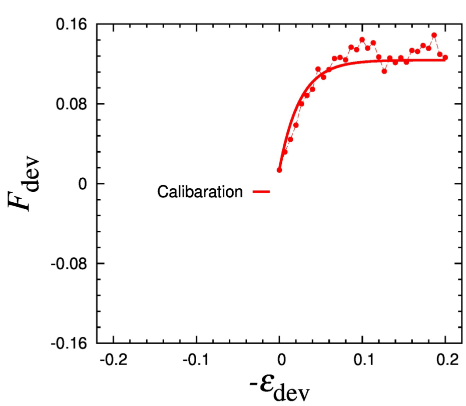
with actual microstructure $F_{V\,(iso)}$ and $F_{dev(iatoric)}$

Calibration (volume conserving shear -- loading)

Initial state: **isotropic volume fraction 0.71;** Deformation path: **shear loading**



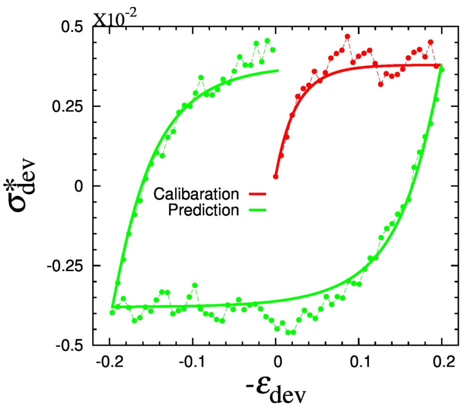
Shear Stress



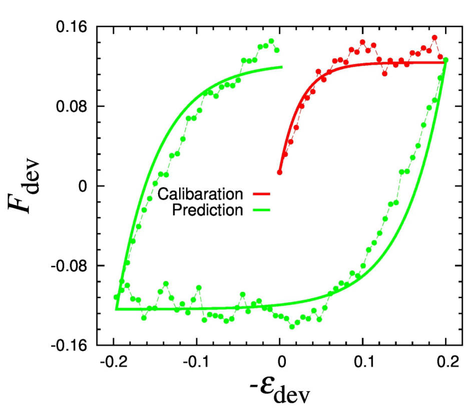
Deviatoric Fabric

Validation (volume conserving cyclic shear)

Initial state: **isotropic volume fraction 0.71;** Deformation path: **cyclic (pure) shear**



Shear Stress



Deviatoric Fabric

- Initial state after one cycle is **anisotropic**
- **Soft response** during strain reversals well predicted by the model

does global averaging make sense?

micro-macro for various deformation modes

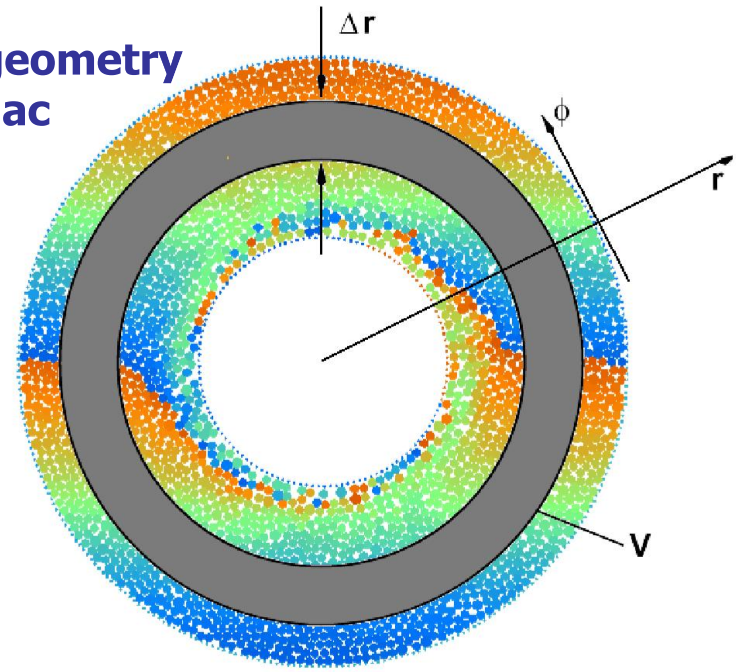
- (visco)-elasticity
- yield stress
- anisotropy

But: inhomogeneity must be ignored

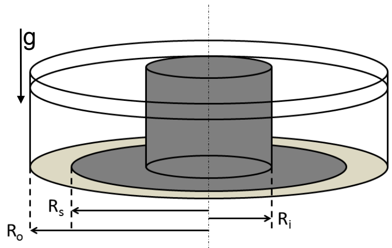
Instead: **advantages of local averaging:**

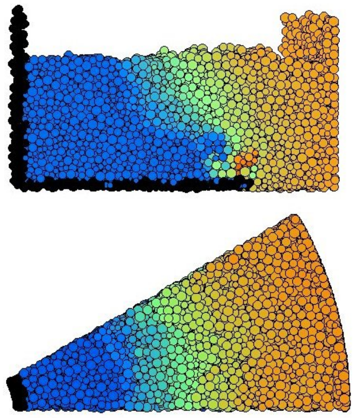
- shearband position known!
- long time-averaging -> slow+fast
- space-averaging -> small resolution

Ring geometry mic-mac



Split bottom ring-shear cell: Simulation setup



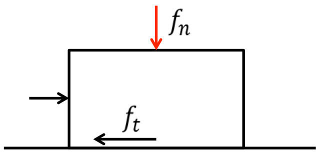


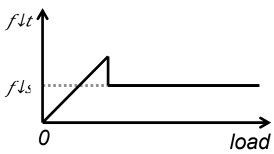
- polydisperse particles of average size 1.1 mm and width of size distribution 0.1892
- wide and stable shear band
- no side wall effects!

Fenistein, D. and Hecke, M. V. 2003. Kinematics – wide shear zones in granular bulk flow. Nature 425, 256--256

Coulomb's law of friction (global vs. local)

Rigid body



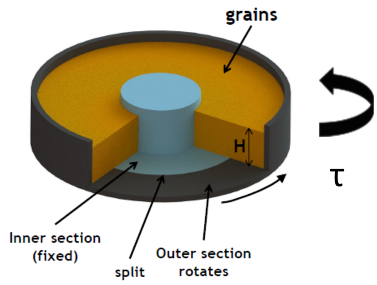


Sliding friction

$$f_s = \mu f_n$$

Granular flow

Filled with grains:

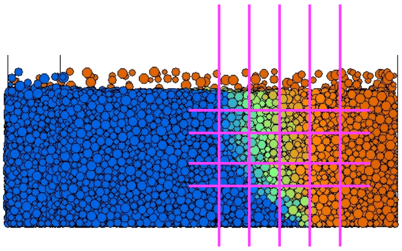


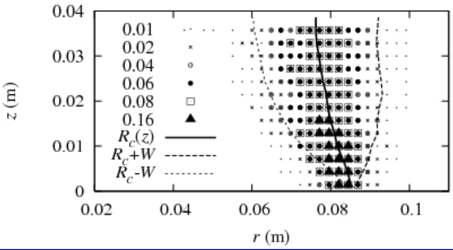
Pressure induced due to gravity P

$$\tau = \mu P$$

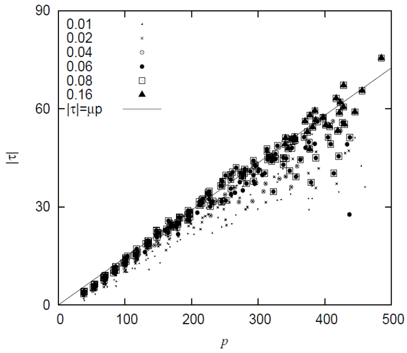
Shear Band

local mic-mac averaging =>





Constitutive relations



Local quantities

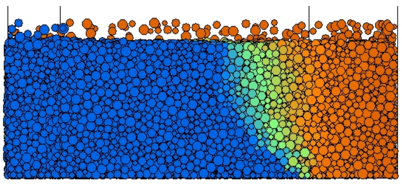
shear rate $\dot{\gamma}$

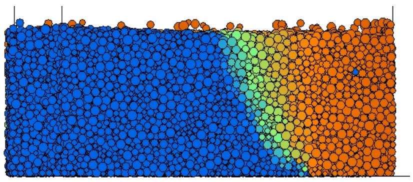
shear stress τ

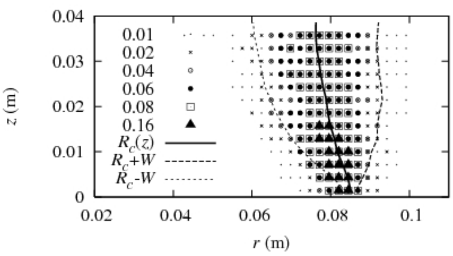
pressure P

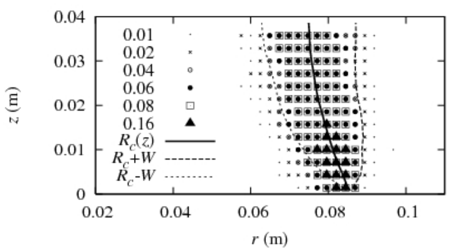
others ρ, ϕ, F

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



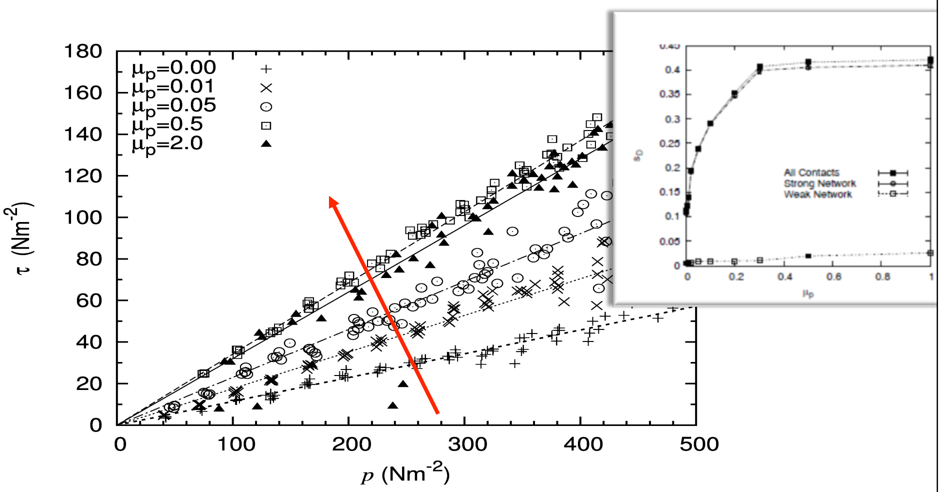






no friction friction

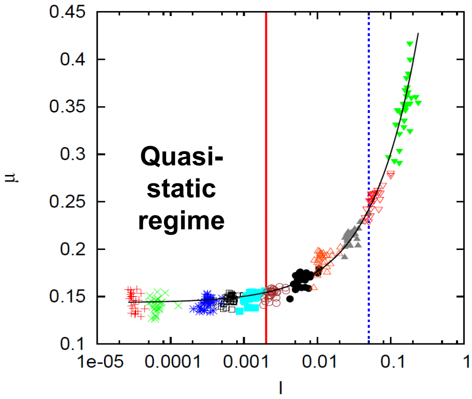
macro-Friction vs. micro-friction

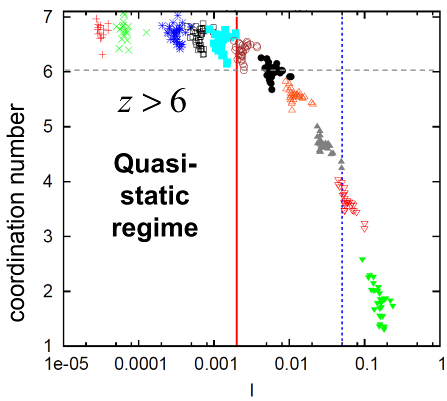


The slope of termination locus increases with friction (non-linear)

Rigid particles – effect of strain-rate

macro-friction coefficient **coordination number**



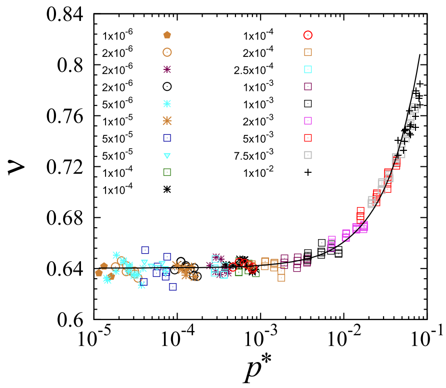


Macro-Friction coefficient

Fitting $\mu(I) = \mu_0 + aI^{\alpha}$ $\alpha \approx 1$

Density dependence on stiffness and gravity

In quasi-static, rigid regime: $\nu(I=0, P^*=0) \approx \nu_0$



Volume fraction in quasi-static regime

Fitting $\nu(P^*) = \nu_0 - a_\nu I + b_\nu P^{*\beta} \quad \beta \approx 0.50$

Macroscopic friction - rheology

Time scales

$$\tau_s = 1/\dot{\gamma} \qquad \tau_c = \sqrt{m/k_n}$$

$$\tau_g = \sqrt{\bar{d}/g} \qquad \tau_P = \sqrt{\bar{m}/P\bar{d}} \qquad \kappa = \tau_P/\tau_g$$

Dimensionless numbers

Inertial number $\quad I = \tau_P/\tau_s$

"Softness" parameter $\quad P^* = \left(\tau_c/\tau_P\right)^2$

Friction coefficient

$$\mu(I) = \mu_0 + aI + \ldots$$

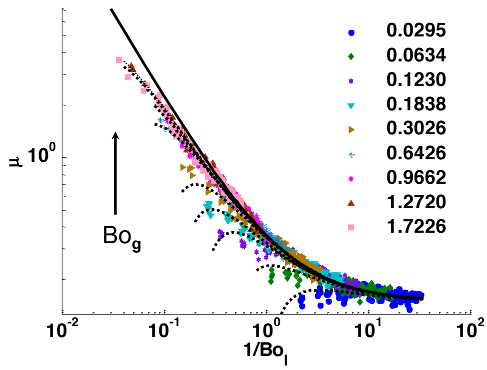
$$\mu(P^*) = \mu_0 - b\left(P^*\right)^{1/2}$$ **in quasi-static regime**

Rheology updates

Micro Parameters	Status
$\mu_p \rightarrow \mu$	Done
k_n, g $\rightarrow P^* \rightarrow \mu$	Done

Present focus: cohesion! dry & wet
$f_c \rightarrow Bo \rightarrow \mu$

Local rheology (macro-friction) depends on pressure: from weak to strong cohesion



$$\mu = \mu_o + \beta_1 Bo_l + \beta_2 Bo_l^{\ 2}$$

where $\mu_o = 0.15,\ \ \beta_1 = 0.22$

- **Local friction coefficient is non-linearly varying in the large Bo_l limit and approaches constant values for small Bo_l**
- **Control parameter: local Bond number with higher order correction**

Recent News (multiplicative rheology)

Dependence on stiffness and cohesion in inertial flow states

$$\mu(I, P^*, Bo_l) = \left(\mu_0 + \frac{\mu_\infty - \mu_0}{1 + I_0/I}\right)\left(1 - b\sqrt{P^*}\right) f(Bo_l)$$

with: $I = \dot{\gamma} d / \sqrt{P/\rho}$ and dim.-less compressibility/stress P^*

Outlook

Local constitutive relations?
… including granular temperature?
via the Reynolds stress or kinetic pressure? P_k ?

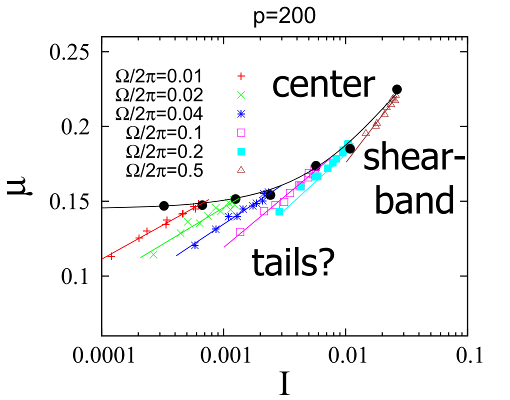
Rheology updates

Micro Parameters	Status
$f_c \rightarrow Bo \rightarrow \mu$	Done
$\mu_p \rightarrow \mu$	Done
k_n, $g \rightarrow P^* \rightarrow \mu$	Done
Small I correction $\rightarrow \mu$	in progress

Quasistatic Flow

Dependence on stiffness (gravity) in inertial flow states

$$\mu(I,P^*) = \mu_0 + aI^\alpha - bP^{*\beta} \ \ ?$$



Very small strain rate: $\mu\left(I < I^*, p^*\right) = \mu_0^{\text{local}}\left(p^*\right)\left[1 - \alpha \ln\left(I/I^*\right)\right]$

[Koval et al. PRE 2009]

Most recent news: granular temperature

Dependence on stiffness and dynamic T_g (inertial & static)

$$\mu(I,P^*,Bo_l,I_k) = \left(\mu_0 + \frac{\mu_\infty - \mu_0}{1 + I_0/I}\right) f_{P^*}(P^*) f_{Bo_l}(Bo_l) \frac{1}{1 + 1/\beta(\phi) I_k}$$

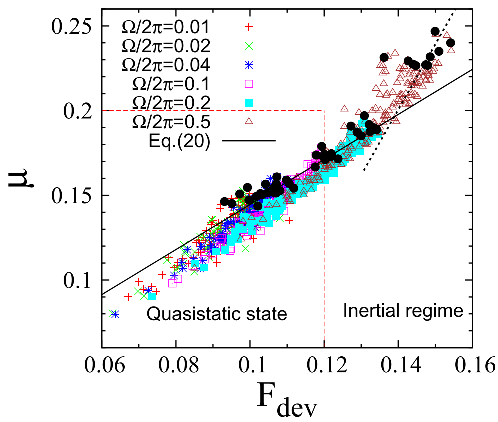
with: kinetic $I_k = \dot{\gamma} d \Big/ \sqrt{P_k/\rho} = I\sqrt{P/P_k}$; kinetic stress P_k

Outlook

Local constitutive relations, in 3D – and fully tensorial?

Rheology – stress-fabric relation

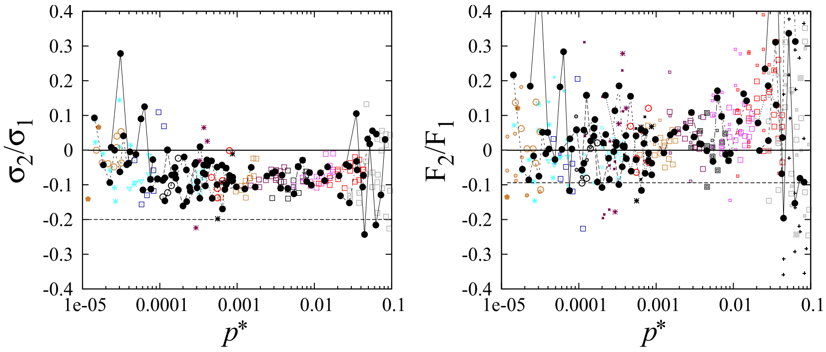
Fully tensorial 3D => … in progress …



A. Singh et al., NJP 2015

Rheology – stress-fabric relation

Fully tensorial 3D => … in progress …



A. Singh et al., NJP 2015

Summary

micro-macro **constitutive model**
based on homogeneous DEM

memory/history => micro-structure evolution
plastic/relaxation events ⇔ stochastic?

ISO+DEV => three! **moduli** (3D +axial)

macro:
incremental stress (structure) – strain relations

=> **prediction** of macro flow behavior ...

... but what about fluctuations?

Constitutive model
scalar! ... **how about the fluctuations?**

Isotropic stress $0 = \delta\sigma_V = 2B\varepsilon_V + AS\,d\gamma$

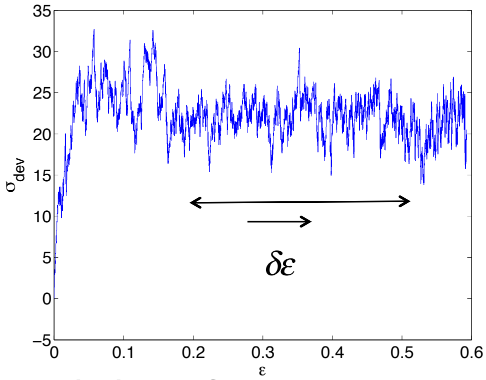
Deviatoric stress $0 = \delta\sigma_D = A\varepsilon_V + 2GS\,d\gamma$

Anisotropy $0 = \delta A = \beta_A\left(A^{\max} - A\right)\left|d\gamma\right|$

probability for:
- elastic events $S = 1 - \sigma_D / \sigma_D^{\max} = 1 - \pi_D$
- plastic events π_D

$\varepsilon_V \mid d\gamma$

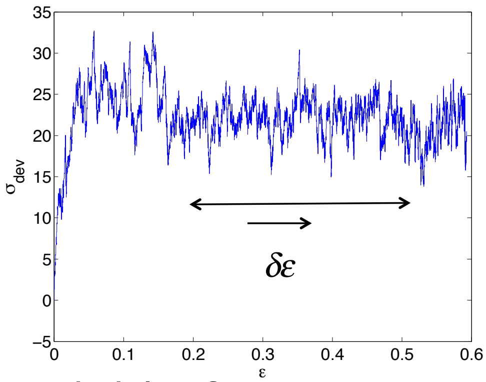
Constitutive model <= fluctuations?

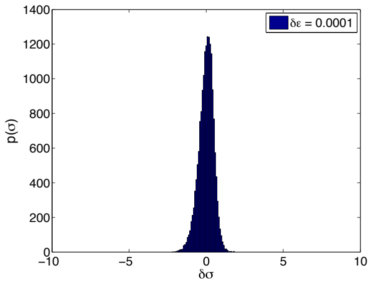


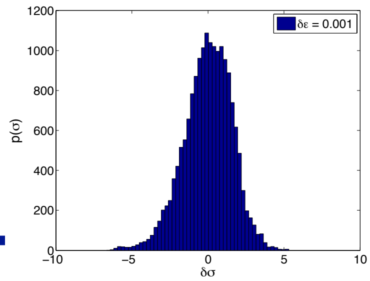
probability for:

- elastic events $S = 1 - \pi_D$
- plastic events π_D

Constitutive model <= fluctuations?



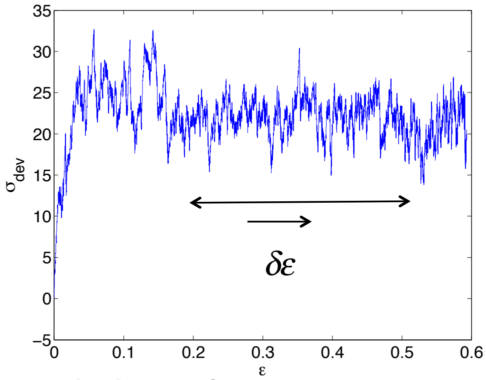


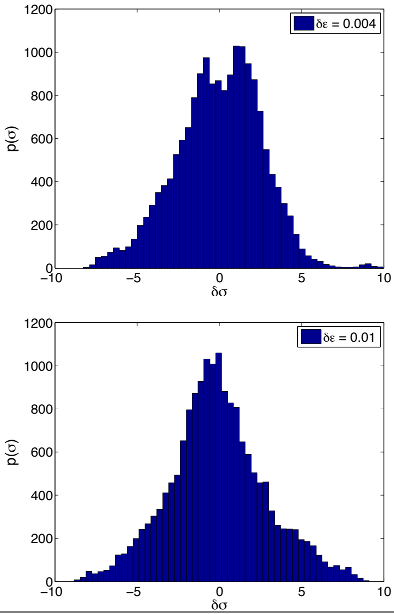


probability for:

- elastic events $S = 1 - \pi_D$
- plastic events π_D

Constitutive model <= fluctuations?



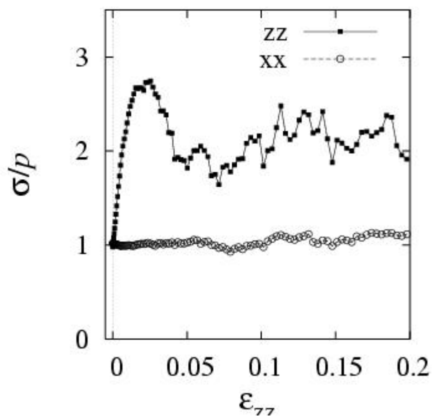


probability for:

- elastic events $S = 1 - \pi_D$
- plastic events π_D

How to model?

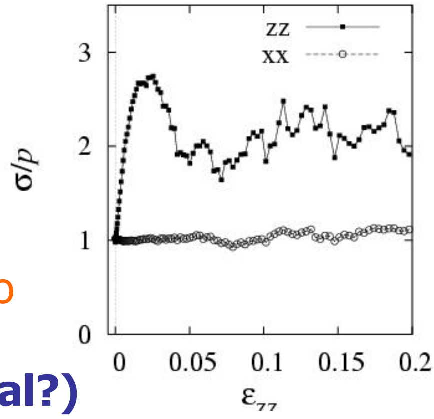
1 – critical state
2 – fluctuations
3 – anisotropy …



Minimal constitutive model?

How to model?

1 – critical state
2 – ~~fluctuations~~
3 – anisotropy …



lost by time/ensemble averaging/micro-macro

Minimal (too minimal?) constitutive model?

THE UNIVERSITY *of* EDINBURGH

UNIVERSITY OF TWENTE.

Influence of coarse graining parameters on the analysis of DEM simulation results

Carlos Labra, Thomas Weinhart, Jin Y. Ooi and Stefan Luding

Powder Technology, in press, April 2016

Outline

- Introduction
- Temporal and spatial coarse graining
- Silo flow example
  - Influence of coarse graining parameters
  - Shear band identification and development
  - Bulk stress interpretation
- Conclusion

Temporal-spatial coarse graining

- Define the macro-density using a coarse-graining function:

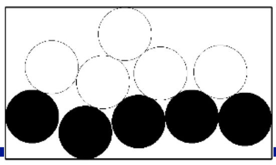
$$\rho(\mathbf{r}) = \sum_{\mathbf{i=1}}^{\mathbf{N}} \mathbf{m_i}\varphi(\mathbf{r} - \mathbf{r_i})$$

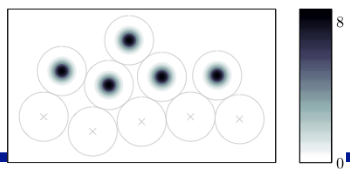
- Define velocity sι ∂ρ/∂t + ∇ · (ρV) = 0, is satisfied:

$$\mathbf{V} = \mathbf{p}/\rho, \text{ where } \mathbf{p} = \sum_{i=1}^{N} m_i \mathbf{v}_i \varphi(\mathbf{r} - \mathbf{r}_i)$$

- weight funct

$$\varphi(\mathbf{r}) = \frac{1}{(\sqrt{2\pi}w)^3} \exp\left(-\frac{|\mathbf{r} - \mathbf{r}_i|^2}{2w^2}\right)$$



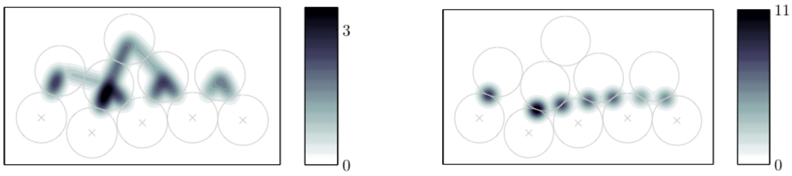


Density ρ for a 2D-Gaussian coarse-graining function. w = d/8.

Temporal-spatial coarse graining

- Define stress and wall drag such that momentum balance is sati

$$
\begin{aligned}
\boldsymbol{\sigma}^k &= -\textstyle\sum_{i=1}^{N} m_i \mathbf{v}'_i \mathbf{v}'_i \varphi(\mathbf{r}-\mathbf{r}_i) \\
\boldsymbol{\sigma}^c &= -\textstyle\sum_{c_{ij}} \mathbf{f}_{ij}\mathbf{r}_{ij} \int_0^1 \varphi(\mathbf{r}-(\mathbf{r}_i+s\mathbf{r}_{ij}))ds \\
&\quad -\textstyle\sum_{w_{ik}} \mathbf{f}_{ik}\mathbf{a}_{ik} \int_0^1 \varphi(\mathbf{r}-(\mathbf{r}_i+s\mathbf{a}_{ij}))ds \\
\mathbf{t} &= -\textstyle\sum_{w_{ik}} \mathbf{f}_{ik}\varphi(\mathbf{r}-\mathbf{c}_{ik})
\end{aligned}
$$

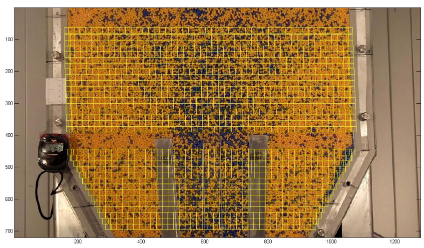


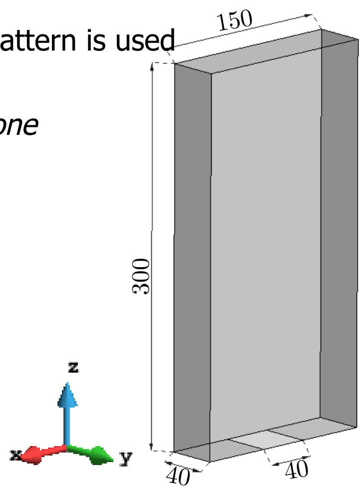
Weinhart, T., Thornton, A.R., Luding, S., Bokhove, O., From discrete particles to continuum fields near a boundary. Granular Matter 14(2), 289-294 (2012)

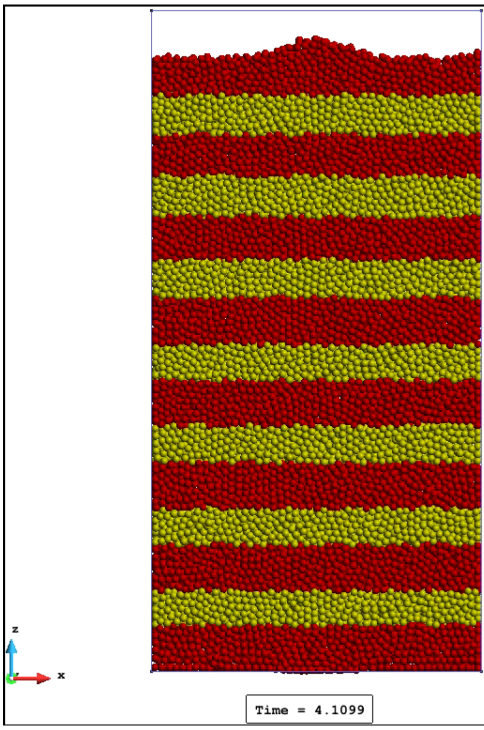
Test case: Silo flow model

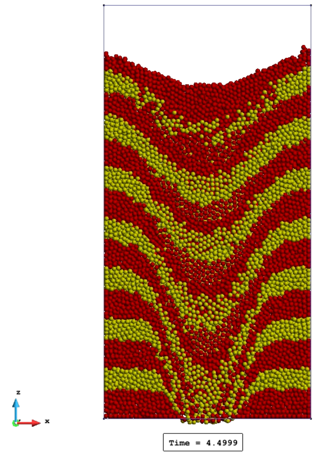
Silo flow model with internal flow pattern is used

- *Stagnant zone – core flow*
- *High shear-rate localization zone*
- *Fast core flow zone*



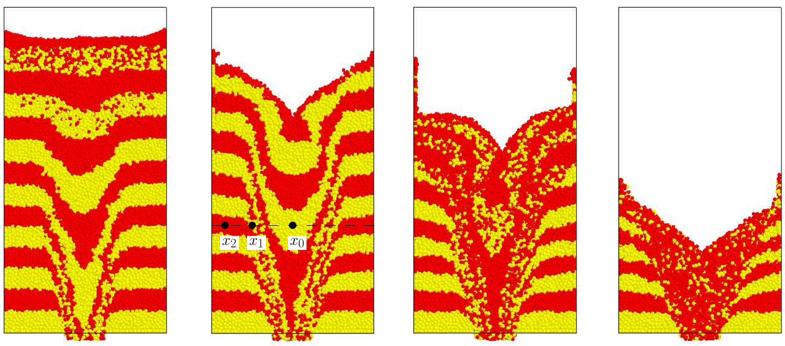






Test case: Silo flow model

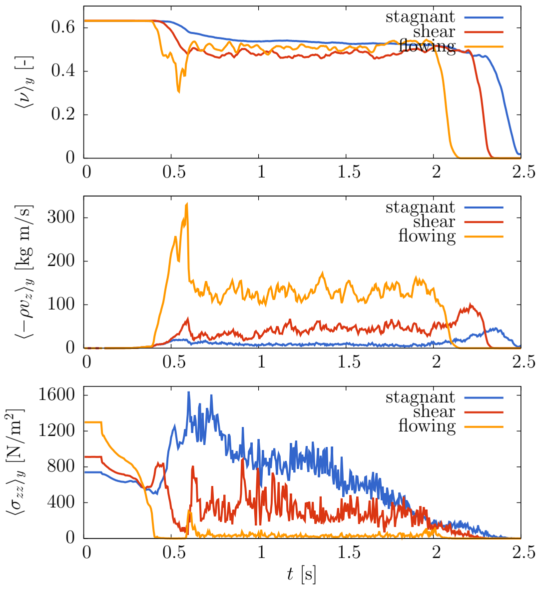
Silo flow model with internal flow pattern is used



(a) t=0.745s (b) t=1.200s (c) t=1.490s (d) t=2.240s

Test case: Silo flow model

Horizontal variation:



shear band – which field?

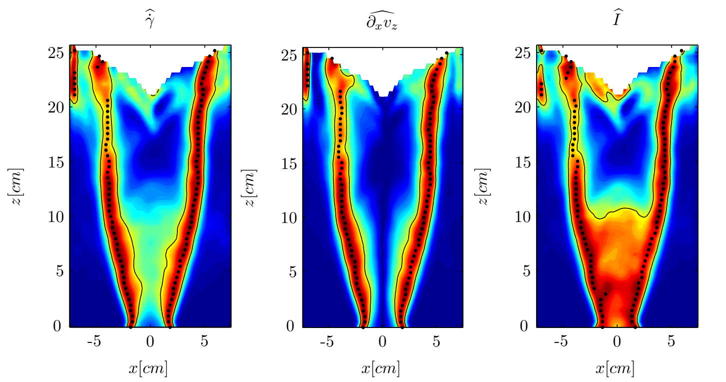
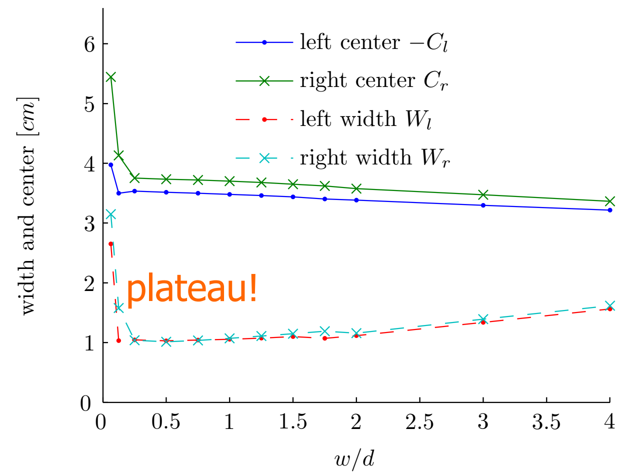
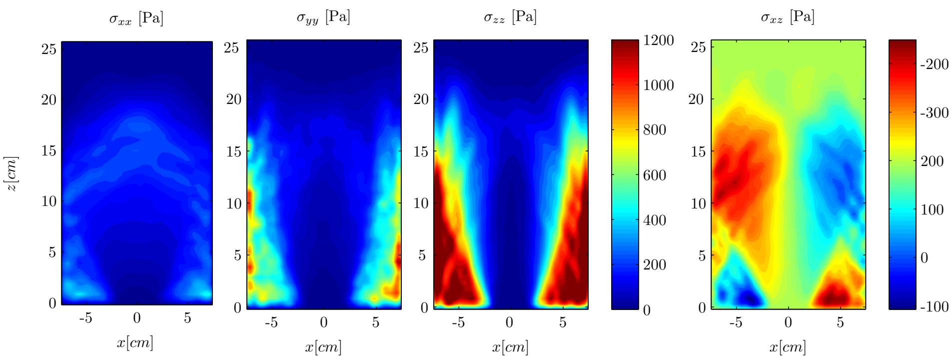


Figure 12: Tensorial shear rate $\dot{\gamma}$, horizontal shear rate $\partial_x v_z$, and inertial number $I = \frac{\dot{\gamma} d}{\sqrt{p/\rho_p}}$ scaled onto the interval $[0, 1]$ by its maximum at each height, see (16). Data for $\nu < 0.1$ (white area on the top) is not considered. Dots denote the maxima of the depicted values in the left and right half of the domain, black contours denote demarcation of the shear band where the scaled value is less than a tolerance ($tol = 0.6$). All values averaged over y and $1 \leq t \leq 1.4$ for $w = d$.

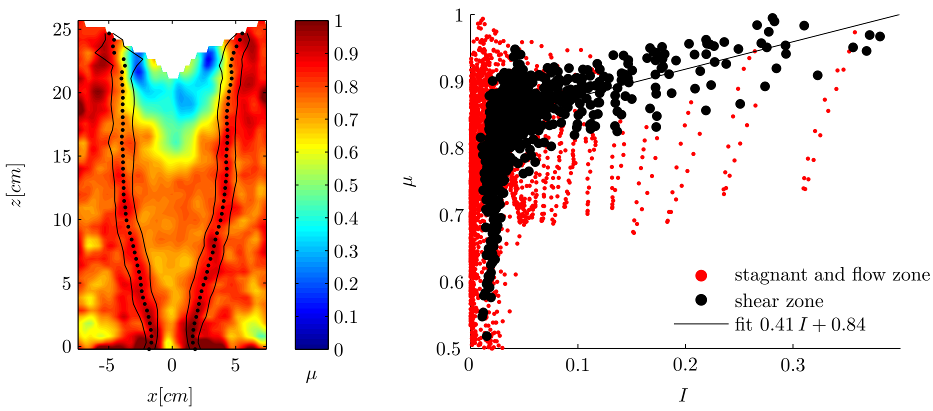
shear band – which w (CG-width)?



stress components



Shear stress ratio (macro-friction) … in the bulk and on the wall

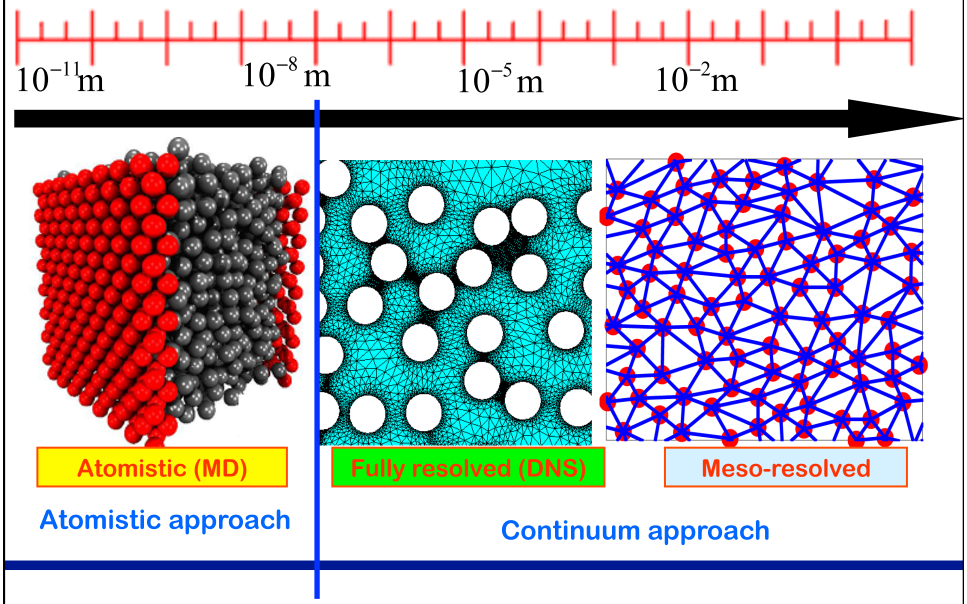


Micro-macro: coarse-graining

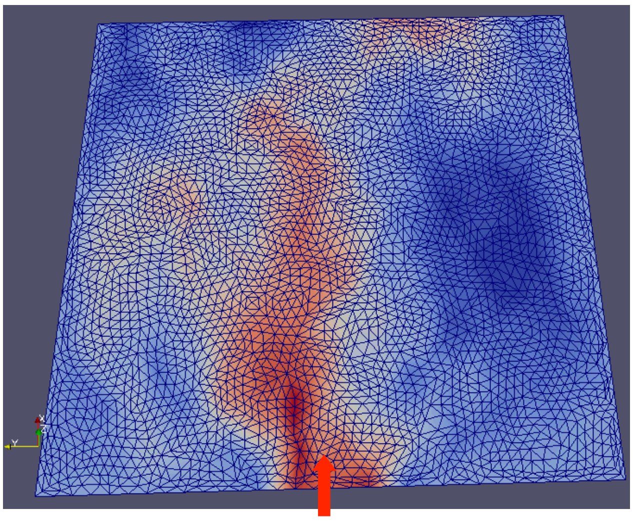
- micro-macro CG applied to silo flow example
- Influence of CG parameters analysed (width and time-window)
  - Macro-variables should be independent of both temporal and spatial averaging scale.
- Study of shear band development
  - Shear band defined as above average vertical shear in each horizontal slice
  - Better use objective tensor norms or other invariants relative to local state
- Study of bulk and wall stress
  - Anisotropic normal bulk stresses with signs of force chains & arches
  - Wall supports most of the bulk mass (due to high microscopic wall friction)e
- Next? use those results from DEM for your purpose!

PARDEM

Multiscale modeling of particles in a fluid



Example: Fluidization DEM-FEM Mesoscale

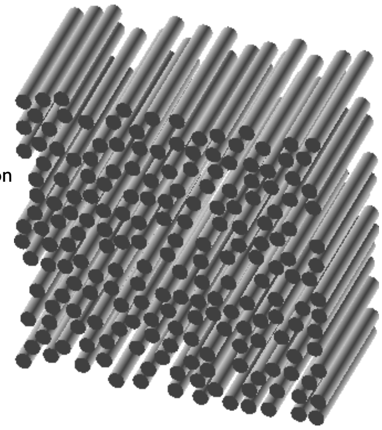


Fluidization on moving mesh with 800 particles (with gravity)

Why fibrous media?

- Composite materials
- Collides and suspensions
- Filtration & separation
- Geophysics & soil science
- Biological tissues
- Polymer membranes
- ➢ **Drag/permeability**
- Fluidized beds
- Rheology
- …

Flow direction



K. Yazdchi et al., IJMF 37(8), 2011-2013.

Fluid-Particle micro-macro

- Characterization of microstructure
  - ➢ Geometrical/Orientational/Network
- From micro to macro properties (permeability)
- Darcy's law – upscaling the transport equations

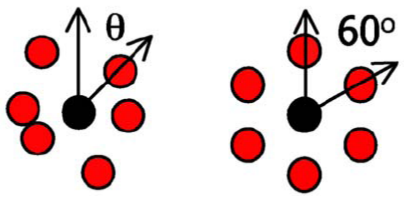
Microstructure

orientation angles

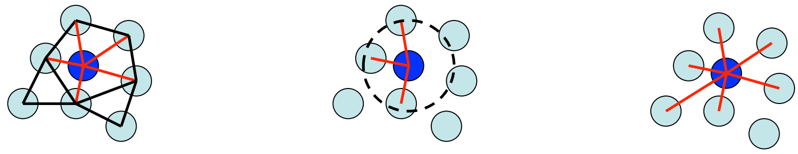
Z. Wang et al., J. Chem. Phys., 134, 2011.

$$\psi_6^{global} = \frac{1}{N}\left|\sum_{k=1}^{N}\frac{1}{n_k}\sum_{j=1}^{n_k} e^{6i\theta_{kj}}\right|$$

✓ $$\psi_6^{local} = \frac{1}{N}\sum_{k=1}^{N}\frac{1}{n_k}\left|\sum_{j=1}^{n_k} e^{6i\theta_{kj}}\right|$$



How to find the neighbors?



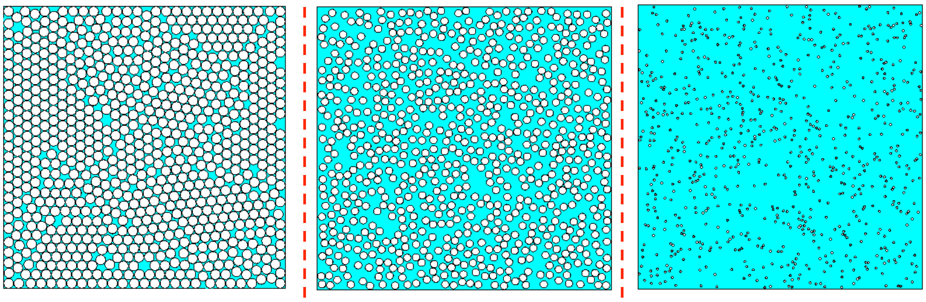
Delaunay edges | Cutoff radius | 6 near-neighbors

Content

- Characterization of microstructure
- From micro to macro properties (permeability)

Permeability-Porosity

dense ~0.4 **moderate** ~0.8 **dilute**



Lubrication?	Carman-Kozeny	Cell method
$\frac{K}{d^2}=C\left(\sqrt{\frac{1-\varepsilon_c}{1-\varepsilon}}-1\right)^{2.5}$	$\frac{K}{d^2}=\frac{1}{\psi_{CK}}\frac{\varepsilon^3}{(1-\varepsilon)^2}$	$\frac{K}{d^2}=\frac{1}{32\phi}\left(\ln\left(\frac{1}{\phi}\right)-\frac{3}{2}+2\phi-\frac{\phi^2}{2}\right)$

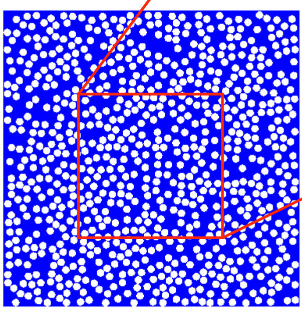
$\phi = 1-\varepsilon$

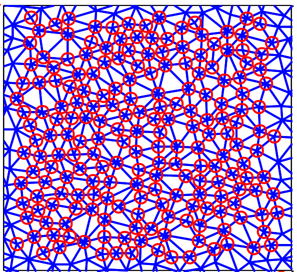
K. Yazdchi et al., Composites Part A 43(11), 2012.

Microstructural model

$\varepsilon = 0.6,\ \delta_{\min} = 0.05d,$

Monte Carlo

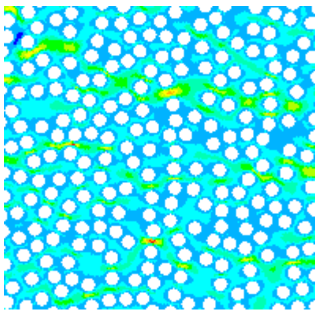


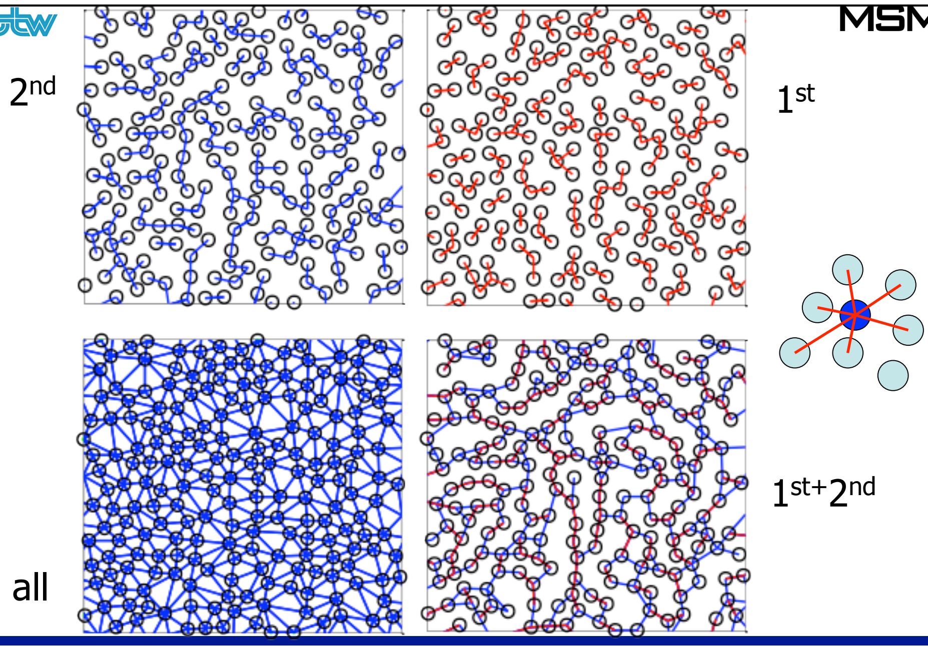


DT edges?

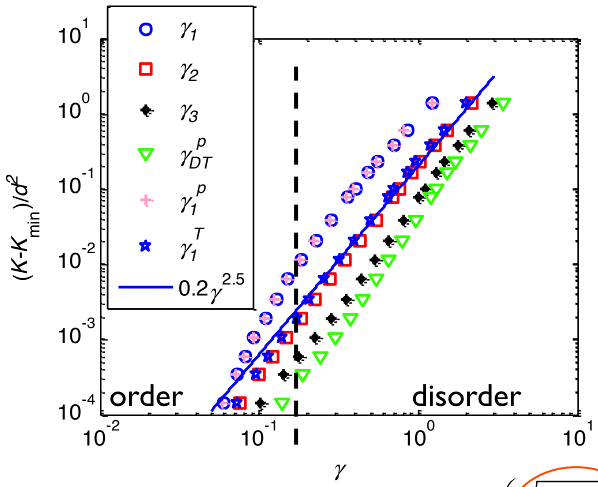
$$\gamma = \frac{\langle r_{ij}\rangle - d}{d} = \frac{\langle \Delta \rangle}{d}$$

$$\boxed{K/d^2 \propto \gamma?}$$





Microstructural model



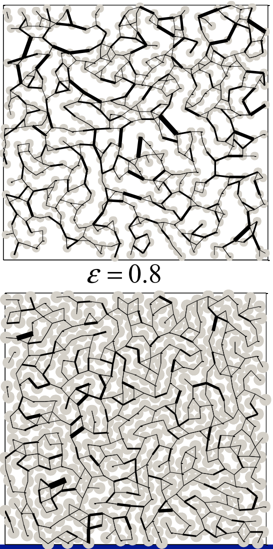
$$\gamma = \frac{\langle r_{ij} \rangle - d}{d} = \frac{\langle \Delta \rangle}{d}$$

$$\boxed{\frac{K}{d^2} \propto \gamma^{\alpha}}$$

Lubrication: $\frac{K}{d^2} = C\left(\sqrt{\frac{1-\varepsilon_c}{1-\varepsilon}} - 1\right)^{2.5} \rightarrow \Delta / d = \gamma$

229

Microstructural model

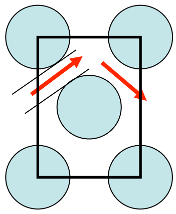


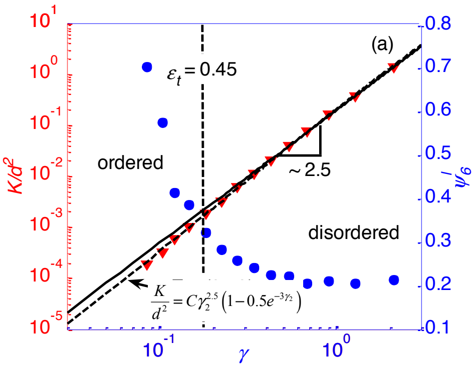
$\varepsilon = 0.8$

$\varepsilon = 0.4$

Lubrication theory:

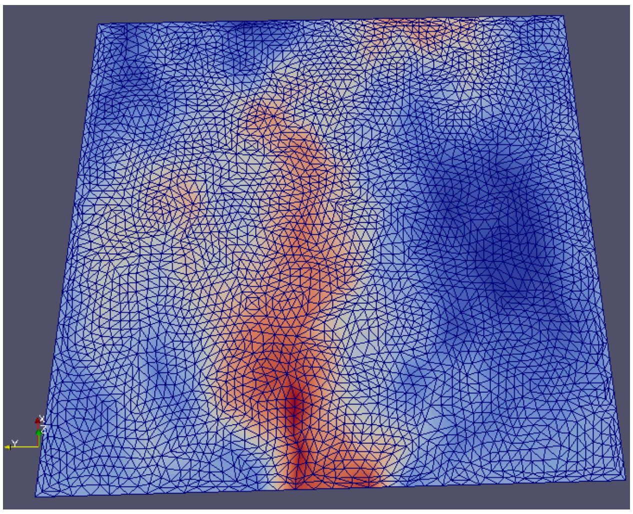
$$\frac{K}{d^2} = C\left(\sqrt{\frac{1-\varepsilon_c}{1-\varepsilon}} - 1\right)^{2.5} = C\gamma^{2.5}$$





Shortest Delaunay edges
(or 2nd nearest neighbor distances)

Example: Fluidization DEM-FEM



Fluidization on moving mesh with 800 particles (with gravity)

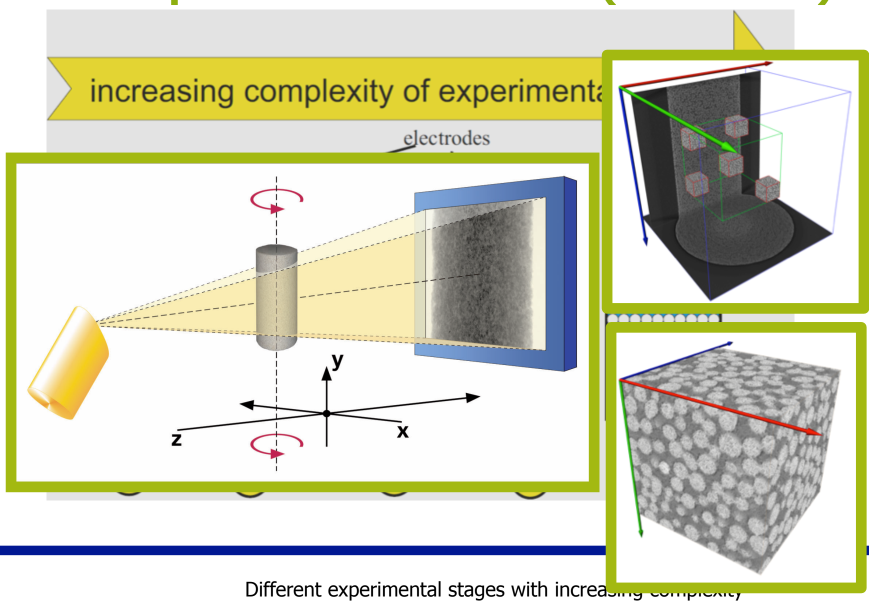
sintered model porous media beds

- **sintered mono- & weakly polydisperse glass beads:**
- **porosity: $\varphi \approx 0.12 - 0.38$**
- **different glass bead diameters: $d_p = 0.4 - 8$ mm**
- **cylindrical samples, different (d_b = 25, 30 & 50 mm)**

(Ref.: I. Gueven, in preparation)

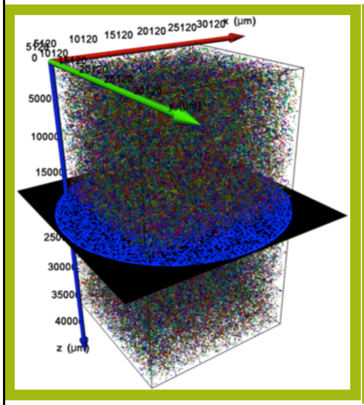
d_p = 0.6-0.8mm **d_p = 3.0mm** **d_p = 5.0mm** **d_p = 8.0 mm**

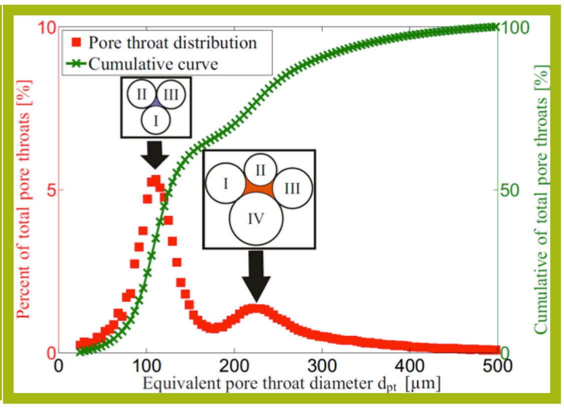
3D multiphase flow + CT-scan (FOM-Shell)



Different experimental stages with increasing complexity

results – pore throat distribution

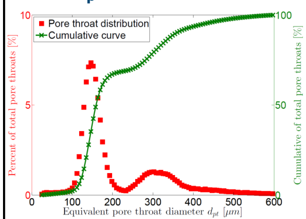




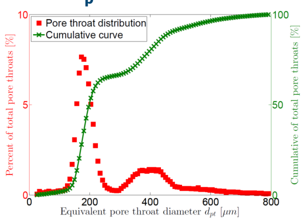
Investigated subvolume for pore throat analysis with dimensions of 1300 (x) X 1300 (y) X

results – pore throat size distribution and correlation to permeability

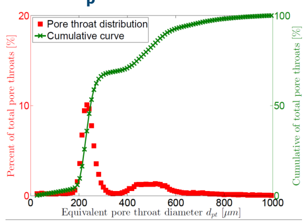
- d_p = 0.6 – 0.8 mm



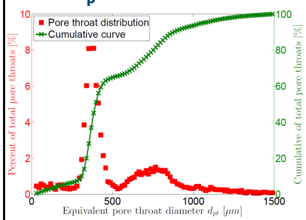
- d_p = 0.8 – 1.0 mm



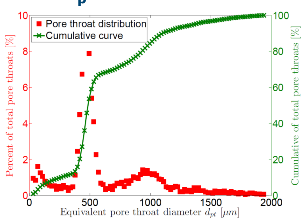
- d_p = 1.0 – 1.2 mm



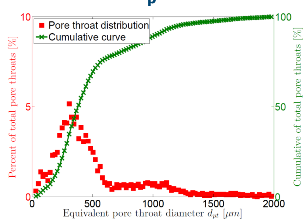
- d_p = 1.5 – 2.0 mm



- d_p = 2.0 – 2.5 mm



- d_p = 3.0 mm

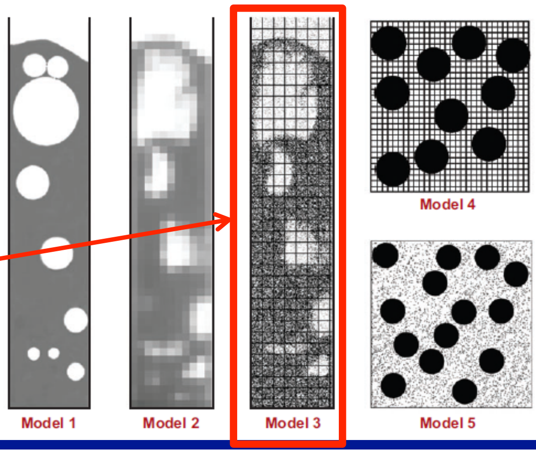


Pore throat distribution of different sintered glass bead packages obtained from subvolumes

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

Length scale of interest determines simulation method

Fluid resolution > particle diameter



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.

Fluid-particle simulation – multiscale …
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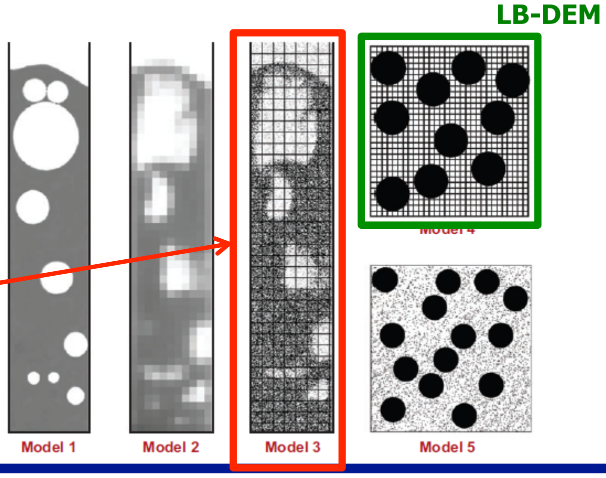

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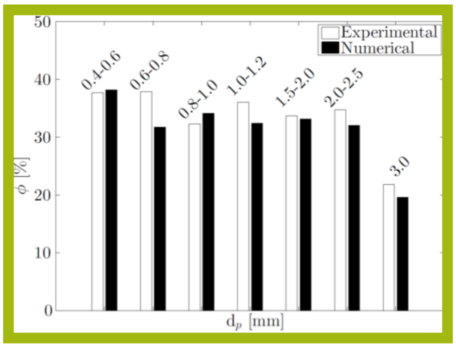
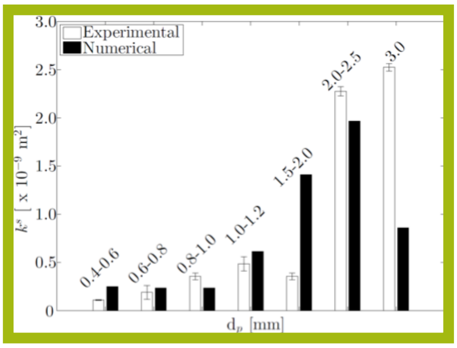
results - porosity & permeability

- porosity
- permeability





Numerical and experimental determined porosity (left) and permeability (right) values for sintered glass bead samples showing different particle diameter

permeability ← →pore throat

results - porosity & permeability

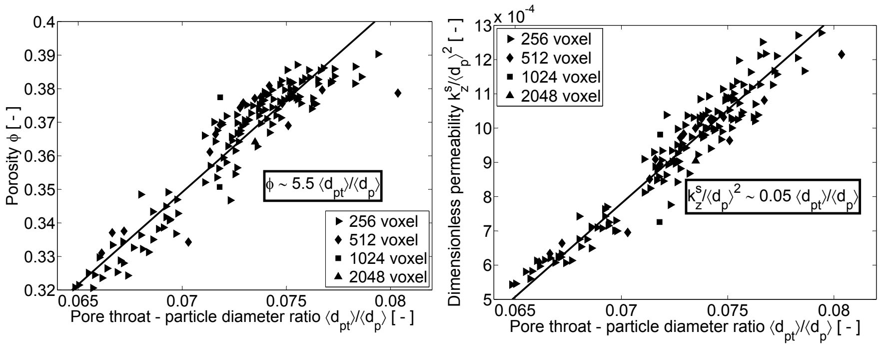
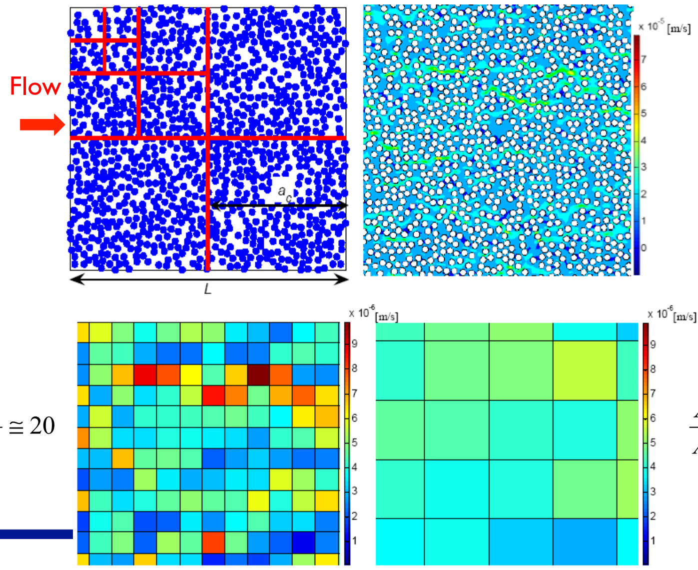


Figure 2.17: Porosity (left) and dimensionless permeability (right) in dependence on the mean pore throat diameter normalized to the mean particle diameter. Both, the porosity ϕ and normalized intrinsic permeability $k_z^s/\langle d_{pt}^2\rangle$, show linear dependency on the normalized mean pore throat diameter $\langle d_{pt}\rangle/\langle d_p\rangle$.

permeability ← →pore throat

Upscaling => Uniform averaging cells

Average horizontal velocity at $\varepsilon = 0.6$



$\frac{A_c}{A_p} \cong 20$

$\frac{A_c}{A_p} \cong 160$

Fluid solved by SPH (Smooth Particle Hydrodynamics)

Locally Averaged Navier Stokes Equations

- Anderson and Jacksons (1967) derived locally averaged Navier Stokes equations (AVNS)
- Solid particle distribution is converted to a smooth porosity field (Ref.: M. Robinson et al. 2012-2014)

$$\frac{\partial(\bar{\rho})}{\partial t} + \nabla \cdot (\bar{\rho}\mathbf{u}) = 0$$

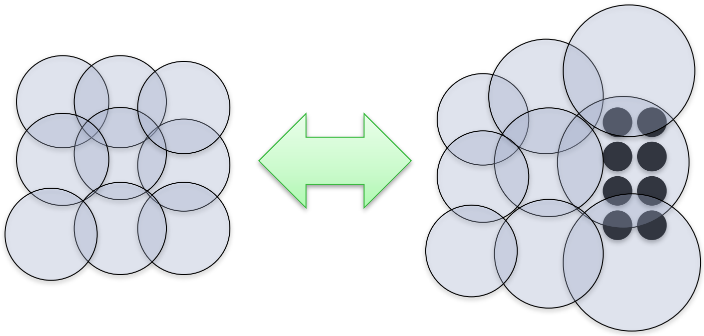
$$\bar{\rho}\left(\frac{\partial \mathbf{u}}{\partial t} - \mathbf{u} \cdot \nabla \mathbf{u}\right) = -\nabla P + \nabla \cdot \tau - n\mathbf{f}_i + \bar{\rho}\mathbf{g}$$

Define a superficial density

$$\bar{\rho}_a = \varepsilon_a \rho_a = \sum_b m_b W_{ab}$$

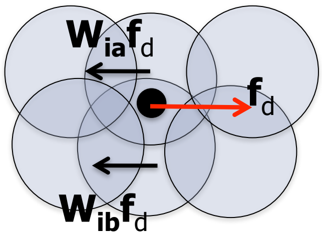
Variable resolution fluid solver

- SPH resolution (smoothing length h) depends on density
- Therefore, resolution coupled to porosity ($h \approx \varepsilon^{-1/3}$)
- Retains accuracy, as particles increase effective viscosity but inhibits turbulent flow



M. Robinson, M. Ramaioli, S. Luding, MSM, IJMF, 2013

Fluid-Particle Drag Force



- Force on DEM particle due to fluid:

$$\mathbf{f}_i = V_p(-\nabla P + \nabla \cdot \tau) + \mathbf{f}_d$$

- Where $\mathbf{f}_d$ is the drag force model
  - Stokes drag (creeping flow, single particle)
  - Di Felice (1994) drag model (higher Re, multiple particles)

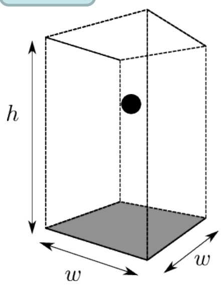
- Drag force calculated on each DEM particle
- Particle drag force then interpolated to surrounding SPH particles
- Constructed so that Newton's third law is satisfied

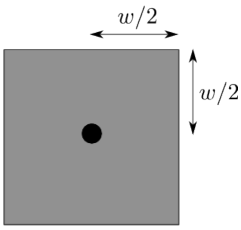
M. Robinson, M. Ramaioli, S. Luding, MSM, IJMF, 2013

3D Sedimentation Test Cases - Validation

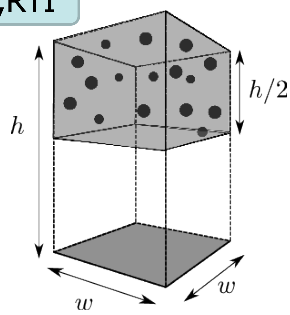
1. **Single Particle Sedimentation (SPS)**
2. **Sedimentation of a constant porosity block (CPB)**
3. **Rayleigh Taylor Instability (RTI)**

SPS





CPB,RTI



M. Robinson, M. Ramaioli, S. Luding, MSM, IJMF, 2013

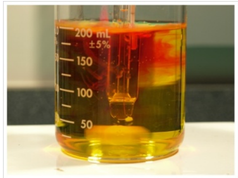
Set of Realistic Fluid-Particle Parameters

- Particle properties chosen to match glass beads used in dispersion cell experiments
- Contact law – linear spring dashpot
  - Very low stiffness to speed up calculations – particle collisions not important here

Property	Value
Density	2500 kg/m^3
Diameter	1x10^{-4} m
Spring Stiffness	1x10^{-4} kg/s^2
Damping	0 kg/s

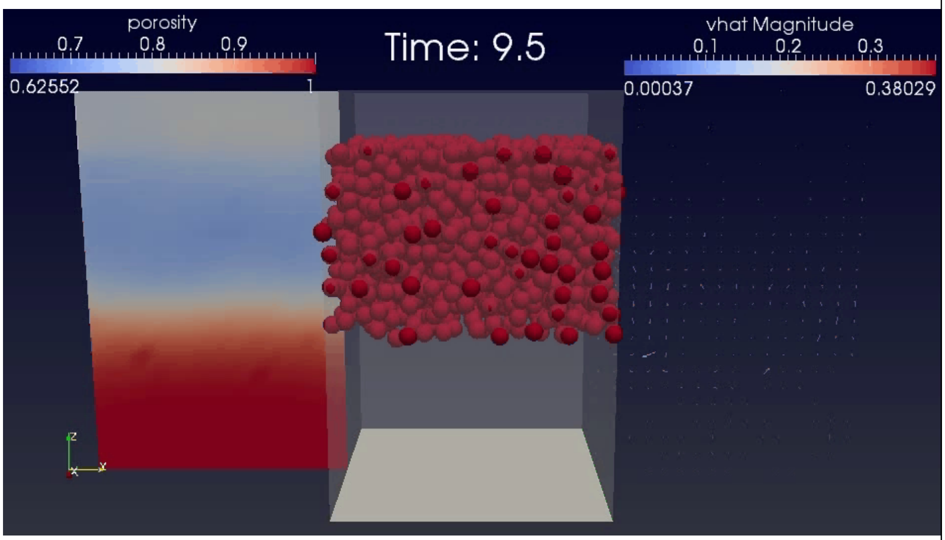
Set of Realistic Fluid-Particle Parameters

- Three different fluids used to provide a range of particle Reynolds Numbers
- Parameters based on air, water and 10% glycerol-water solution

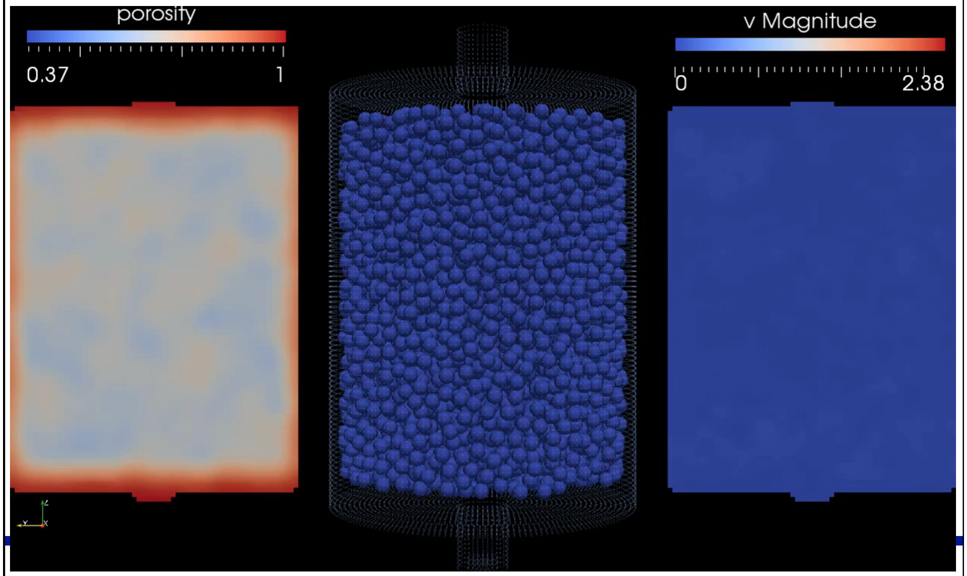


Property	Air	Water	Glycerol-water
Density	1.18 kg/m^3	1000 kg/m^3	1150 kg/m^3
Viscosity	1.86x10^{-5} Pa·s	8.9x10^{-4} Pa·s	8.9x10^{-3} Pa·s
Re_p	0.65 – 3.19	0.15 – 0.85	0.002 – 0.011

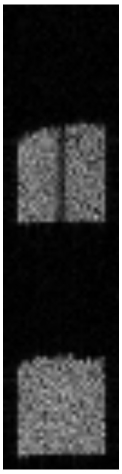
Multiple Particle Sedimentation – SPH Results

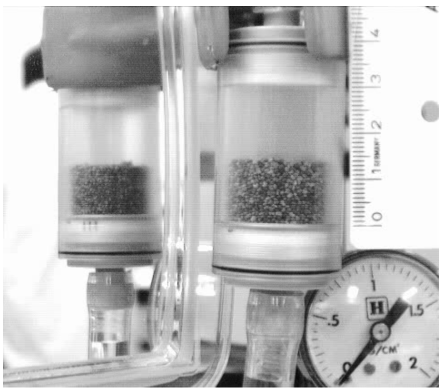


Wet Start

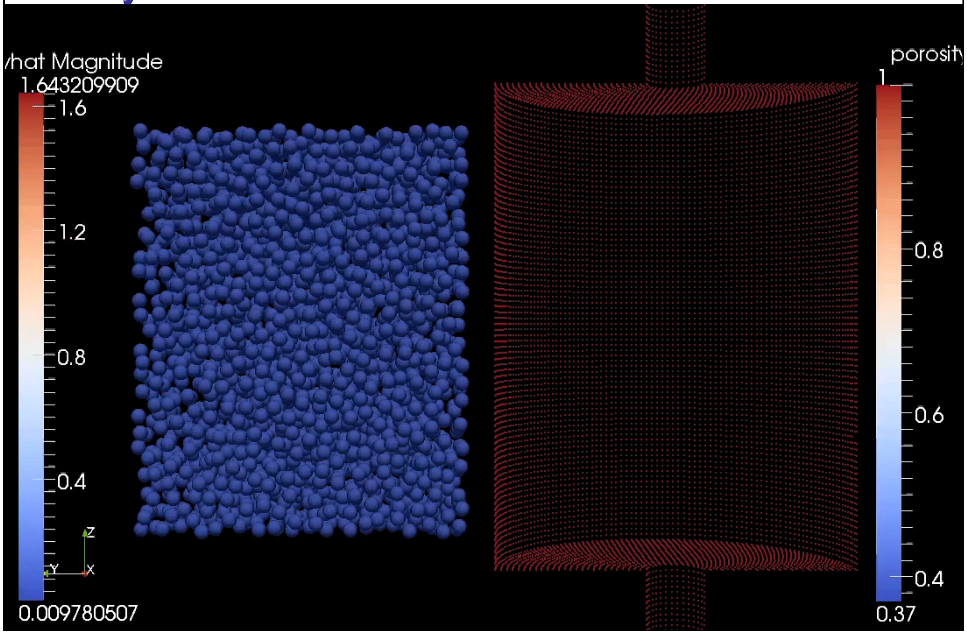


Dry Start





Dry Start

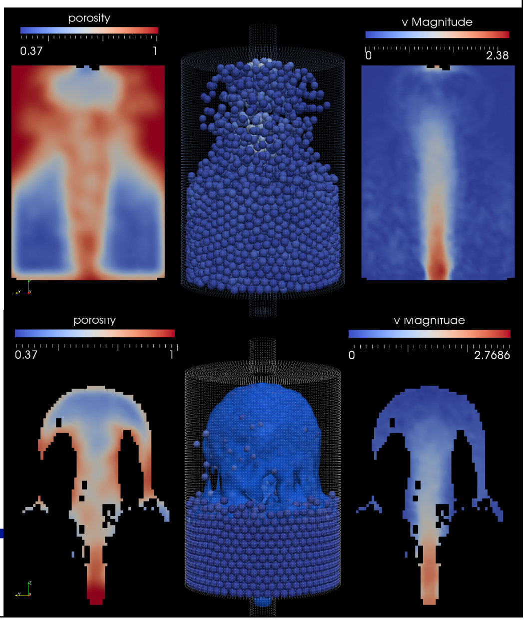


Simulation of powder dispersion by a liquid jet

- Application: Particle dispersion
  (collaboration with Nestle)
- Method: SPH-DEM
- Results:
  - **Wet** – Recovers quanitative features from experiment: Jet, dispersion …
  - **Dry** – Fails to recover some major features (e.g. bed lift regime).

TODO:
Surface tension not modeled yet.
Second phase not modeled yet.
Different size particles …

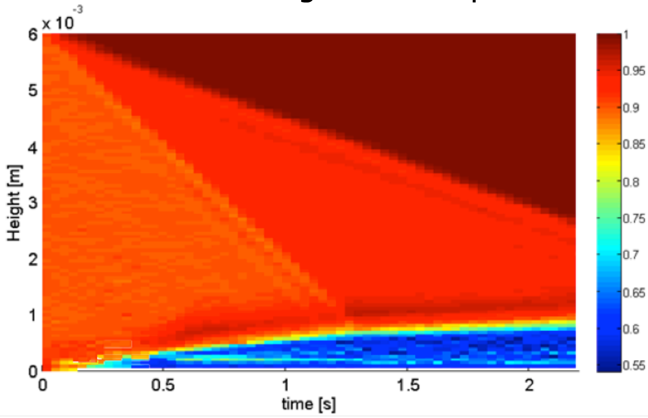
M. Robinson, M. Ramaioli,
S. Luding, MSM, PG2013



Multi-species DEM-SPH model

- G. Raso (MSc thesis, Univ. Calabria, UT)

Test/validation case 4: Homogeneous 2-species sedimentation



More multi-scale models?
… using micro-macro techniques

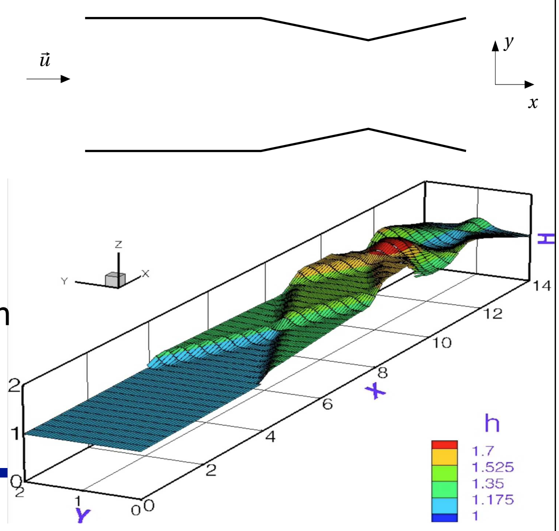
- Constitutive models for soils and powders (dry)
  - with (strain) evolution of micro-structure (anisotropy)
- Constitutive models for wet&cohesive particle systems
  - interaction between micro-structure, cohesion&perm.
- Constitutive models for multi-phase systems
  - mixing vs. segregation (not shown)
  - one => two => many species/phases

Plug those into your continuum solver ☺
… no DEM needed?

Shallow flow equations (3D->2D)

- D. Tunuguntla (PhD-thesis 2015)

- calibrated by DEM
- boundary conditions
- multi-species mixing & segregation
- erosion & sedim.



Shallow flow equations (3D->2D)

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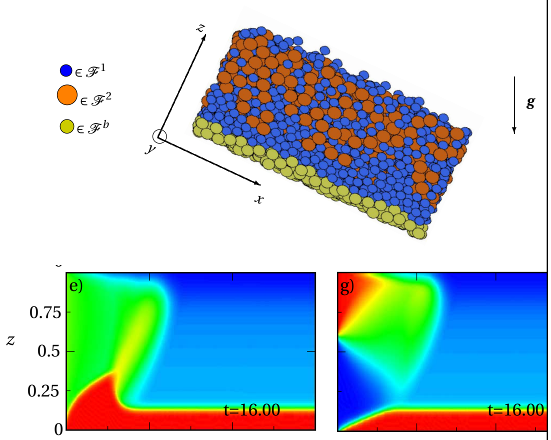

PARDEM

- DEM – increasingly popular for modelling particulate systems on the PARticle scale
- Initially a scientific tool to investigate and qualitatively understand particulate solid behaviour and phenomena
- Increasing use of DEM for quantitative simulation based design and optimisation of engineering systems
- One major obstacle for widespread adoption: lack of **validation and model calibration** methodologies
- Also require well trained R&D engineers to exploit the full potential of DEM

PARDEM

T-MAPPP => session this afternoon ☺

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- Initially a scientific tool to investigate and qualitatively understand particulate solid behaviour and phenomena
- Increasing use of DEM for quantitative simulation based design and optimisation of engineering systems
- One major obstacle for widespread adoption: lack of **validation and model calibration** methodologies
- Also require well trained R&D engineers to exploit the full potential of DEM

Constitutive model
scalar! (in the biaxial box eigen-system)

Isotropic stress $\delta p = \delta\sigma_V = 2B\varepsilon_V + AS\,d\gamma$

Deviatoric stress $\delta\tau = \delta\sigma_D = A\varepsilon_V + 2GS\,d\gamma$

Anisotropy $\delta A = \beta_A\left(A^{\max} - A\right)|d\gamma|$

stress-isotropy $S = 1 - \sigma_D / \sigma_D^{\max} = 1 - s_D / s_D^{\max}$

Isotropic|deviatoric strain increment $\varepsilon_V \mid d\gamma$

B … Bulk-, *G* … Shear-, *A* … Anisotropy-Modulus

Constitutive model
scalar! …

Isotropic stress $\delta p = \delta\sigma_V = 2B\varepsilon_V + AS\,d\gamma$

Deviatoric stress $\delta\tau = \delta\sigma_D = A\varepsilon_V + 2GS\,d\gamma$

Anisotropy $\delta A = \beta_A\left(A^{\max} - A\right)|d\gamma|$

probability for:
- elastic events $S = 1 - \sigma_D / \sigma_D^{\max} = 1 - \pi_D$
- plastic events π_D

$\varepsilon_V \mid d\gamma$

Constitutive model
scalar! … but where is the time-scale?

Isotropic stress $\delta p = \delta\sigma_V = 2B\varepsilon_V + AS\,d\gamma$

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probability for:
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- plastic events π_D

$\varepsilon_V \mid d\gamma$

Constitutive model
scalar! … but where is the time-scale?

Isotropic stress $\delta p = 2B\varepsilon_V + AS\,d\gamma - 1/\tau_p\, p\,dt$

Deviatoric stress $\delta\sigma_D = A\varepsilon_V + 2GS\,d\gamma - 1/\tau_D\, \sigma_D\,dt$

Anisotropy $\delta A = \beta_A\left(A^{\max} - A\right)\left|d\gamma\right| - 1/\tau_A\, A\,dt$

$\varepsilon_V \mid d\gamma$

Constitutive model

$$S = 1 - \sigma_D / \sigma_D^{\max} = 1 - s_D / s_D^{\max}$$

scalar! ... **but where is the time-scale?**

Isotropic stress $\quad \delta p = 2B\varepsilon_V + \cancel{AS}\, d\gamma - \frac{1}{\tau_p} p\, dt$

Deviatoric stress $\quad \delta\sigma_D = \cancel{A}\varepsilon_V + 2G\cancel{S}\, d\gamma - \frac{1}{\tau_D} \sigma_D\, dt$

~~Anisotropy~~ $\quad \cancel{\delta A = \beta_A \left(A^{\max} - A\right)\left|d\gamma\right| - \frac{1}{\tau_A} A\, dt}$

Isotropic?

$\varepsilon_V \mid d\gamma$

Constitutive model

scalar! ... **but where is the time-scale?**

Isotropic stress $\quad \delta p = 2B\varepsilon_V - \frac{1}{\tau_p}\left(p - p_c\right) dt$ *

Deviatoric stress $\quad \delta\sigma_D = 2G\, d\gamma - f\sigma_D\, dt$

*Krijgsman & Luding, P&G 2013

$\varepsilon_V \mid d\gamma$

Constitutive model
scalar! … but where is the time-scale?

Isotropic stress $\delta p = 2B\varepsilon_V - \frac{1}{\tau_p}(p - p_c)\,dt$

Deviatoric stress $\delta\sigma_D = 2G\,d\gamma - f\sigma_D\,dt$

fluidity (Nguyen et al. 2011, Kamrin/Koval 2012)
… with an evolution equation by its own … $f \propto \dot{\gamma}$?

Steady (critical) state: $2\frac{G}{f}\dot{\gamma} = \sigma_D^{\max} = \alpha G$

$\varepsilon_V \mid d\gamma$

Constitutive model
scalar! … but where is the time-scale?

$S = 1 - \frac{\sigma_D}{\sigma_D^{\max}} = 1 - \frac{s_D}{s_D^{\max}}$

Isotropic stress $\delta p = 2B\varepsilon_V + AS\,d\cancel{\gamma} - \frac{1}{\tau_p}(p - p_c)\,dt$

Deviatoric stress $\delta\sigma_D = \cancel{A}\varepsilon_V + 2G\cancel{S}\,d\gamma - \frac{1}{\tau_D}\sigma_D\,dt$

~~Anisotropy~~ $\cancel{\delta A = \beta_A\left(A^{\max} - A\right)|d\gamma| - \frac{1}{\tau_A}A\,dt}$
Isotropy?

Granular Solid Hydrodynamics
GSH-type formulation (M. Liu 2003-2015)

$\varepsilon_V \mid d\gamma$

Constitutive model
scalar! … but where is the time-scale?

Isotropic stress $\delta p = 2B\varepsilon_V - \frac{1}{\tau_p}(p - p_c)\,dt$

Deviatoric stress $\delta\sigma_D = 2G\,d\gamma - \frac{1}{\tau_D}\sigma_D\,dt$

different relaxation times for p and s_D $\frac{1}{\tau} \propto T_g \propto \dot{\gamma}$?

Granular Solid Hydrodynamics
GSH-type formulation (M. Liu 2003-2011)

$\varepsilon_V \mid d\gamma$

Constitutive model isotropic! …
… in the critical state!

$S = 1 - \sigma_D / \sigma_D^{\max} = 1 - s_D / s_D^{\max}$

Deviatoric stress (Luding) $0 = 2GS\,d\gamma$

Deviatoric stress (GSH) $0 = 2G\,d\gamma - \frac{1}{\tau_D}\sigma_D\,dt$

relaxation rate

viscosity

GSH-type formulation (M. Liu 2003-2015) $\varepsilon_V \mid d\gamma$

Constitutive model isotropic! …
… in the critical state!

Deviatoric stress (Luding) $0 = 2G\left(1 - {s_D}/{s_D^{\max}}\right)d\gamma$

Deviatoric stress (GSH) $0 = 2G\,d\gamma - {1}/{\tau_D}\,\sigma_D^{\max}\,dt$

relaxation rate ${1}/{\tau_D} = \frac{2G}{\sigma_D^{\max}}\dot{\gamma} = \frac{2G/p}{s_D^{\max}}\dot{\gamma}$

app. viscosity $\eta = {\sigma_D^{\max}}/{\dot{\gamma}} = 2G\tau_D$

GSH-type formulation (M. Liu 2003-2015) $\varepsilon_V \mid d\gamma$

Constitutive model – back anisotropy scalar! … with plastic and relaxation term

Isotropic stress $\delta p = AS d\gamma - {1}/{\tau_p}\left(p - p_c\right)dt$

Deviatoric stress $\delta\sigma_D = 2G\,S\,d\gamma - {1}/{\tau_D}\,\sigma_D\,dt$

with probability for elastic deformations:

$$S = 1 - {\sigma_D}/{\sigma_D^{\max}} = 1 - {s_D}/{s_D^{\max}} = 1 - {s_D}/{\mu\left(I, P^*, Bo\right)} = 1 - \pi_D$$

$\varepsilon_V \mid d\gamma$

Constitutive model – back anisotropy scalar! ... **with plastic and relaxation term**

Isotropic stress $\delta p = AS d\gamma - \frac{1}{\tau_p}(p - p_c)\,dt$

Deviatoric stress $\delta\sigma_D = 2G\,S\,d\gamma - \frac{1}{\tau_D}\sigma_D\,dt$

steady state => $0 = 2G\left(1 - \frac{s_D}{s_D^{\max}}\right)d\gamma - \frac{1}{\tau_D}\sigma_D\,dt$

... => $0 = 2G\left(1 - \frac{\sigma_D}{\mu p}\right)d\gamma - \frac{1}{\tau_D}\sigma_D\,dt$

$$\sigma_D = 2G\dot\gamma \big/ \left(2G\dot\gamma/\mu p + 1/\tau_D\right) = \mu p \big/ \left(1 + \mu p \big/ \left(2\tau_D G\dot\gamma\right)\right)$$

Constitutive model – back anisotropy scalar! ... **with plastic and relaxation term**

Isotropic stress $\delta p = AS d\gamma - \frac{1}{\tau_p}(p - p_c)\,dt$

Deviatoric stress $\delta\sigma_D = 2G\,S\,d\gamma - \frac{1}{\tau_D}\sigma_D\,dt$

fluidity in steady state => $1/g := \sigma_D/\dot\gamma\, p = 1\big/\left(\dot\gamma/\mu + p/2G\tau_D\right)$

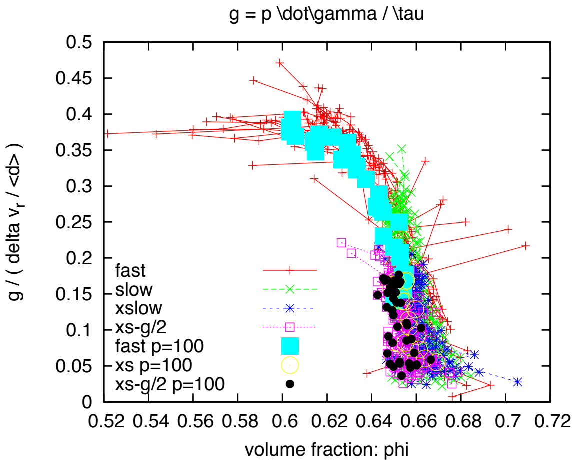
$= \mu\big/\left(\dot\gamma + \mu p\big/\left(2G\tau_D\right)\right)$

$\tau_D = d\big/\sqrt{T_g} = d/\delta v$

$= \tau_D\mu\big/\left(\dot\gamma\tau_D + \mu p\big/(2G)\right)$

(for small $\dot\gamma\tau_D$) $\approx 2G\tau_D\big/(p) = 2G\tau_D / B\varepsilon_V$

Constitutive model – back anisotropy scalar! ... with plastic and relaxation term



$$\tau_D = d/\sqrt{T_g} = d/\delta v$$

fluidity in s.s.: $$g\tau_D := p\dot{\gamma}\tau_D / \sigma_D = \left(\dot{\gamma}\tau_D/\mu + p/(2G)\right)$$

Time-scales (summary)

- Contact duration tc
- inverse shear rate ts
- Time between collisions tn
- inverse dissipation rate td
- inverse isotropic pressure-change rate
- inverse anisotropic stress-change rate
- *Relaxation time = f(tc,tn,ts,td)?*
- *Non-co-linearity relaxation?*

Interaction of time-scales?

Constitutive model
scalar! … **but where is the time-scale?**

$$S = 1 - \sigma_D / \sigma_D^{\max} = 1 - s_D / s_D^{\max}$$

How to measure, e.g., time-scale τ_D

Deviatoric stress $\delta\sigma_D = 2G\,S d\gamma - \frac{1}{\tau_D}\sigma_D\,dt$

stop! $\dot{\sigma}_D = -\frac{1}{\tau_D}\sigma_D$ $\quad \frac{1}{\tau_D(t)} \propto T_g$

$\dot{T}_g = -I$

Constitutive model – co-linear?
scalar! … **but where is the time-scale?**

How to measure, e.g., non-colinearity ϕ_σ

Relaxation model: $\delta\phi_\sigma = \tfrac{1}{2}d\gamma_s - \frac{1}{\tau_\phi}(\phi_\sigma - \phi_\varepsilon)\,dt$

in general non-colinear (also for *A*)!

Note the difference between γ_s and γ

Summary micro-macro

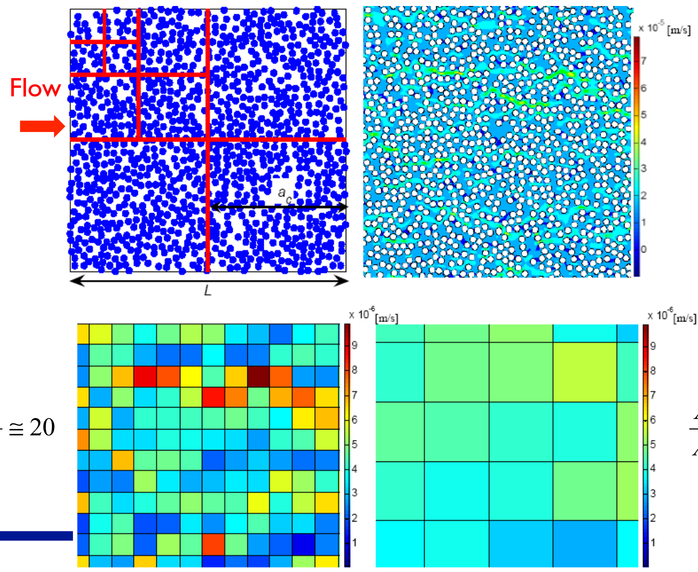
- Micro-/Macro-Flow Rheology
  - micro-mechanics&fluctuations … macro-flow
  - micro-contact-friction … macro-friction-angle
  - relation between fluctuations and macro-response?

- Non-Newtonian Rheology (Anisotropy, Micro-polar?)

- **Does global averaging make sense anyway?**
… spatial (size-effects) vs. temporal (plastic events)

Upscaling => Uniform averaging cells

Average horizontal velocity at $\varepsilon = 0.6$



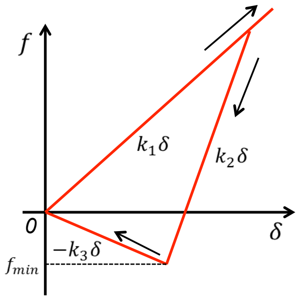
$\frac{A_c}{A_p} \cong 20$ $\frac{A_c}{A_p} \cong 160$

Questions?

Questions?
micro-structure?
meso-models?

Effect of particle's cohesion (dry)

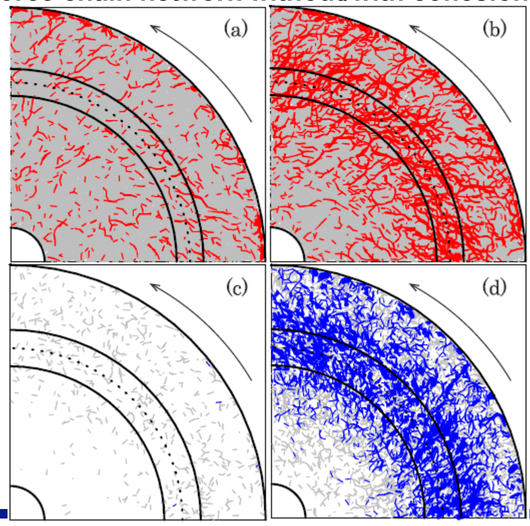
Cohesive contact model



The local Bond number

$$B_O = \frac{f_{\min}}{\langle f \rangle}$$

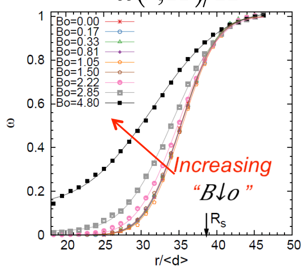
Force chain network without/with cohesion



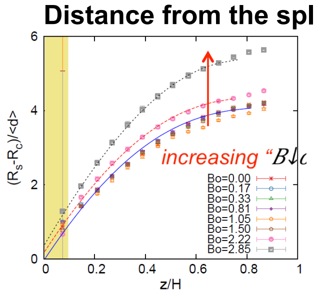
$B_O = 0.33$ $B_O = 2.85$

Effect of particle's cohesion (dry)

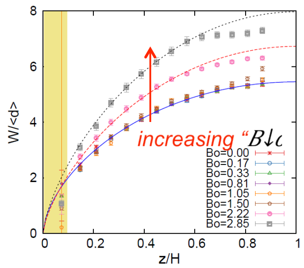
$\omega(r,H)/\Omega$



Distance from the split



Width

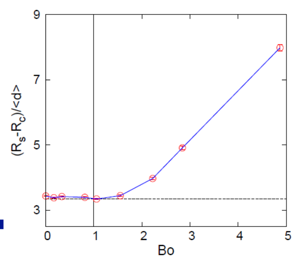


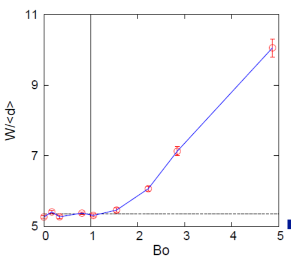
$B_O < 1$

Effect of cohesion is suppressed.

$B_O > 1$

The difference increases with Bo.

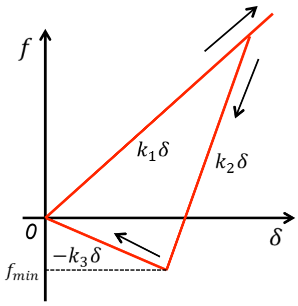




[A. Singh, V. Magnanimo, K. Saitoh, and S. Luding, PRE, 2014]

Effect of particle's cohesion (dry)

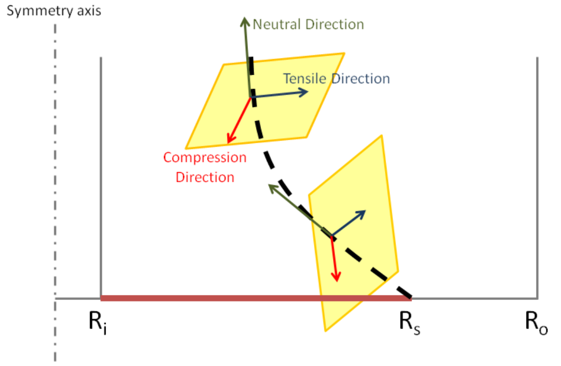
Cohesive contact model



The local Bond number

$$B_O = \frac{f_{\min}}{\langle f \rangle}$$

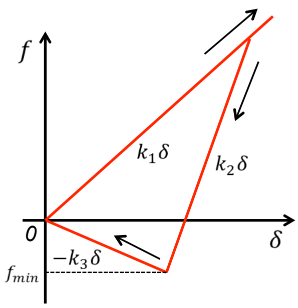
Force network anisotropy with cohesi



[A. Singh, V. Magnanimo, K. Saitoh, and S. Luding, PRE, 2014]

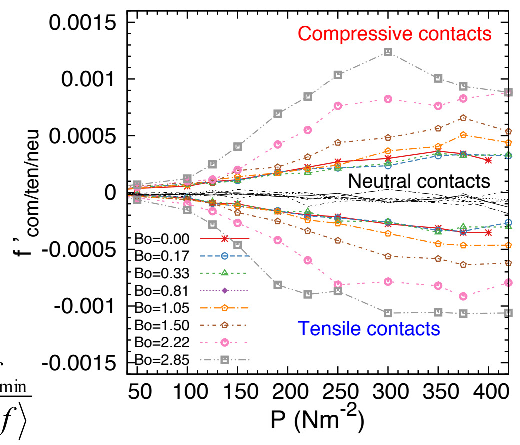
Effect of particle's cohesion (dry)

Cohesive contact model



Local Bond number $B_O = \frac{f_{\min}}{\langle f \rangle}$

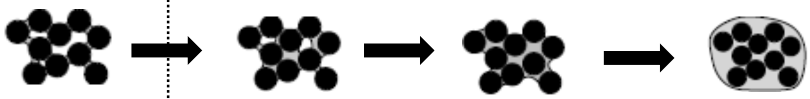
Force network anisotropy + cohesion



[A. Singh, V. Magnanimo, K. Saitoh, and S. Luding, PRE, 2014]

Wet Granular Material

State of wet granular material is defined by the bulk saturation (**S***) of the materials i.e. the ratio of the liquid volume to void volume (liquid volume + confined air volume)



Pendular
0.05 < S* < 0.3

Funicular
0.3 < S* < 0.9

Capillary
S* > 0.9

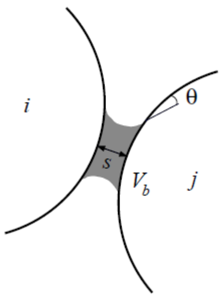
Suspension
S* = 1.0

Capillary forces/ Cohesion active between the particles

No capillary forces between the particles

Mitarai N. and Nori F. , 2006. *Wet Granular Materials.* Adv. Phys. 55, 1 - 45

Willett's model for capillary forces between spheres



Capillary bridge force between the particles:

$$fc_{ij} = \frac{2\pi\gamma R\cos(\theta)}{1 + 1.05\bar{S} + 2.5\bar{S}^2}$$

where $\bar{S} = S\sqrt{\frac{R}{V_b}}$

θ — *Contact Angle of the liquid*

γ —***Surface tension***

R — *Mean harmonic radius of contact particles*

V_b — *Liquid Bridge Volume*

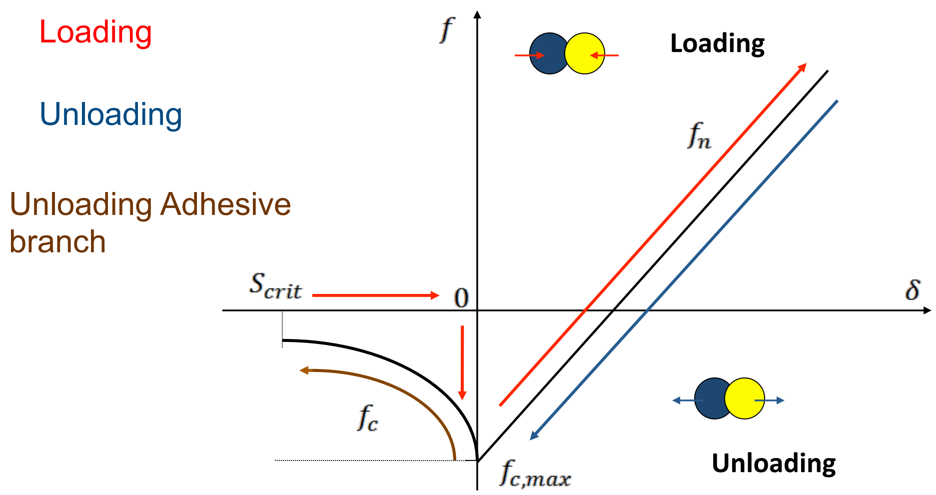
S —*Separation Distance*

The bridge rupture distance is defined by:

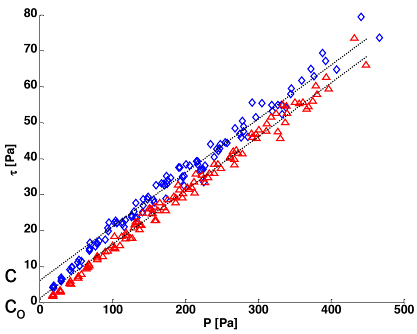
$$S_c = \left(1 + \frac{\theta}{2}\right) V_b^{1/3}$$

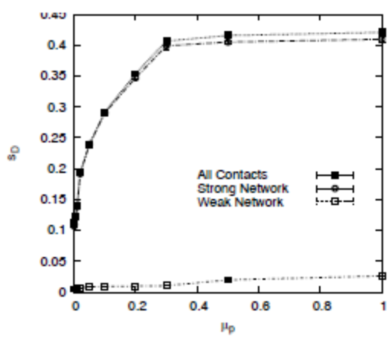
Willett, C.D., Adams, M.J., Johnson S.A. and Seville J.P.K.. 2000. *Capillary Bridges between Two Spherical Bodies.* Langmuir 16, 9396-9405

Liquid bridge + Linear contact model



Friction and cohesion (wet)





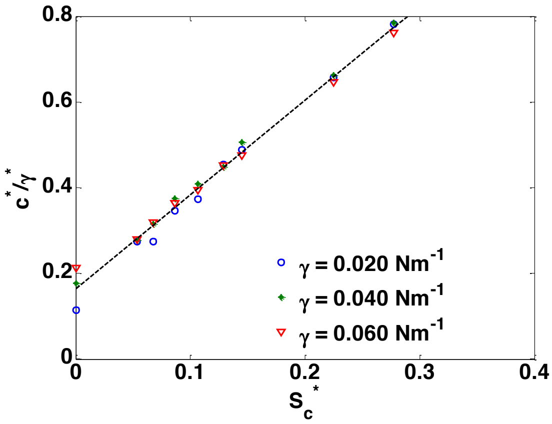
Dry: $\tau = \mu P,$

Cohesive: $\tau = \mu P + c, c_o = c(V_b = 0)$

μ: Macroscopic friction coefficient
c: Macroscopic cohesive strength

Singh, A., Magnanimo, V. and Luding S., 2014, Effect of friction on the force distribution in sheared granular materials, Proc. of NUMGE2014.8

Micro-macro correlation for liquid bridge model



$$\frac{c^*}{\gamma^*} = aS_c^* + b,$$

$$a \approx 2.6$$

$$b \approx 0.16 \approx \frac{c_o^*(\gamma)}{\gamma^*}$$

$$c^* = \frac{c}{f_g / d_p^2}, \gamma^* = \frac{\gamma}{f_g / d_p}, S_c^* = \frac{S_c}{d_p}$$

f_g: gravitational force on single particle
d_p: mean diameter of particle

Roy, S., Singh, A., Weinhart, T. and Luding S., 2015, Micro-macro Transition and Simplified Contact Models for Wet Granular Materials, Journal of CPM.9

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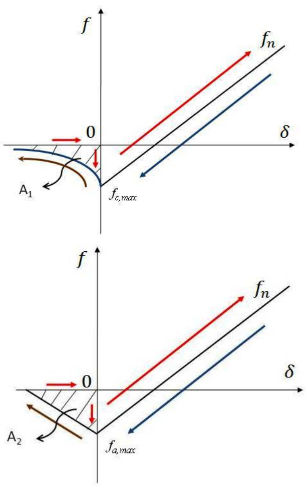
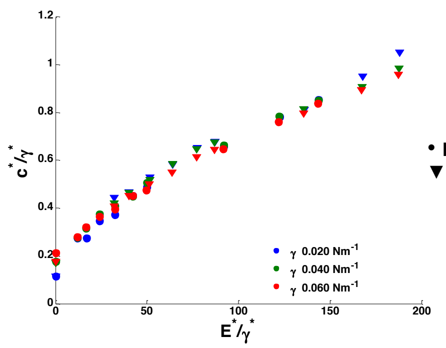
Simplified linear contact model for wet particles





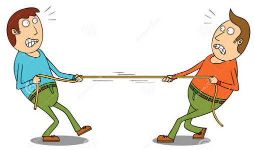
- liquid bridge model
- ▼ linear model

Key Parameters for equal cohesion:
- **Adhesive Energy E**
- **Maximum adhesive force which is linearly proportional to the surface tension of liquid**

Roy, S., Singh, A., Weinhart, T. and Luding S., 2015, Micro-macro Transition and Simplified Contact Models for Wet Granular Materials, Journal of CPM.

Local Rheology for wet granular materials: slow shear and cohesion

$$Bo_l = \frac{f_c^{\max}}{\langle f(P^*) \rangle} = \frac{2\pi R\gamma\cos\theta}{\langle f(P^*) \rangle}$$



$f_c^{\max}$: Maximum adhesive force

$\langle f(P^*) \rangle$: Mean normal repulsive force at a given height of the shear cell

$$P^* = Pd_p{}^2 / f_c^{\max}$$

$$Bo_g = \frac{f_c^{\max}}{\langle f(P_{\max}^*) \rangle}$$

$$\mu = f(Bo, P^*)?$$

- Control parameter: Bond number, pressure
- Global Bond number $\mathbf{Bo_g}$ is experimentally measurable quantity

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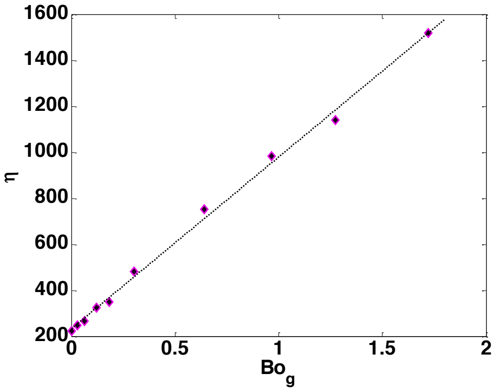
1

Global Apparent Viscosity from Weak to Strong Cohesion



$$\eta = \eta_o + \eta' Bo_g$$

η_o : **Viscosity for dry materials (232 Pa.s^{-1})**

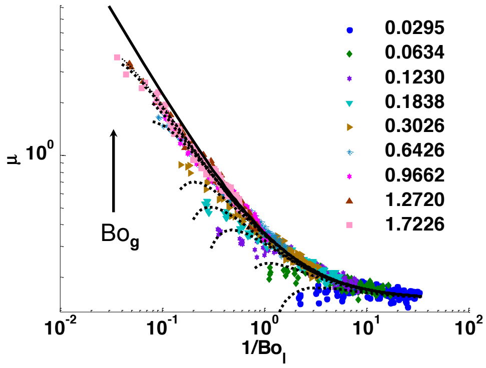
$\eta' \approx 747$ Pa.s^{-1}

Bo_g : **Global Bond number**

$$\eta^* = \frac{\eta}{\eta_o + \eta' Bo_g}$$

where $Bo_g = \frac{f_c^{\max}}{\langle f(P_{\max}^*) \rangle}$

Local rheology (macro-friction) depends on pressure: from weak to strong cohesion



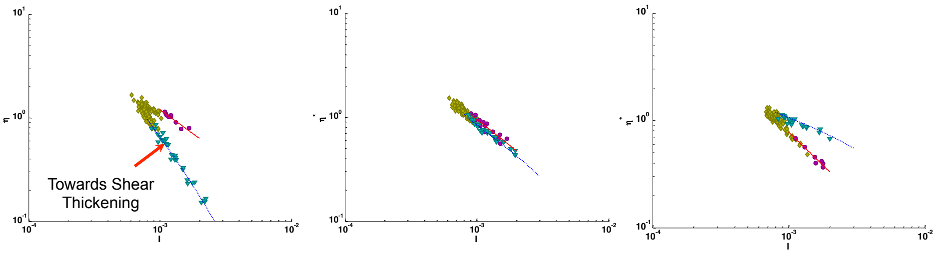
$$\mu = \mu_o + \beta_1 Bo_l + \beta_2 Bo_l^{\,2}$$

where $\mu_o = 0.15,\ \beta_1 = 0.22$

- **Local friction coefficient is non-linearly varying in the large *Bo_l* limit and approaches constant value under small *Bo_l* limit**
- **Control parameter: local Bond number with higher order correction**

Local rheology (apparent viscosity): from weak to strong cohesion

Weak cohesion | Moderate cohesion | Strong cohesion



$$I = \frac{\dot{\gamma}\, d_p}{\sqrt{P/\rho}}, \quad \eta = \frac{\tau}{\dot{\gamma}}$$

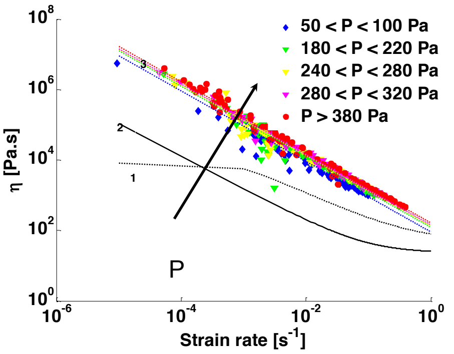
d_p : mean particle diameter

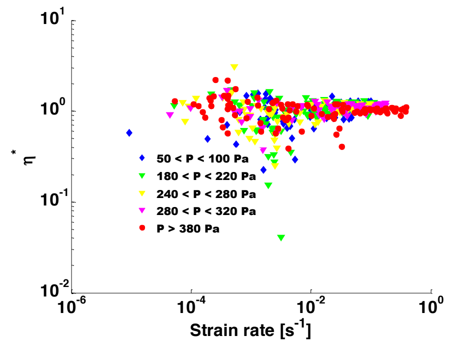
ρ : particle density

Red: P > 380 Pa
Green: 100 < P < 380 Pa
Blue: P < 100 Pa

- Non-Newtonian behavior of granular materials with shear thinning
- Towards shear thickening for increasingly cohesive materials
- Control parameters: Inertial number and Bond number

Shear Thinning: Wet Granular Materials





1. **Bird-Carreau fit (dry)**
2. **Herschel-Bulkley fit (dry)**
3. **$\mu(Bo_l)$ rheology fit**

$$\eta^* = \frac{\eta}{\mu(I, P_m^*, Bo_l) P_m / \dot{\gamma}}$$

New:
Bond number dependent rheology

Rheology of wet granular materials

Prediction of the non-linear apparent viscosity (S. Roy et al.)

Summary:

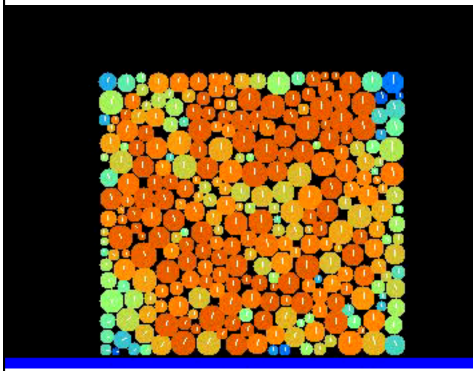
- *Four* local dimensionless numbers are the controlling parameters (μ_p, I, P^*, Bo_l)
- Existing $\mu(I)$ and $\mu(I, P^*)$ rheology for quasistatic flow – *embedded* … extended

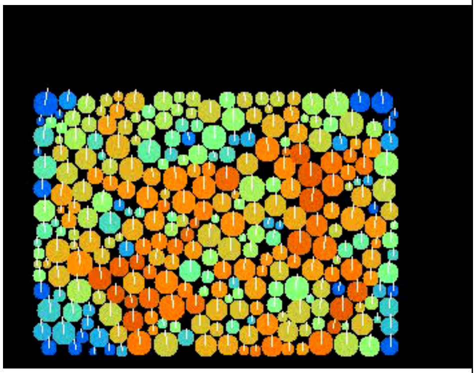
Our own contribution:

- Both friction and (apparent) viscosity increase with cohesion (surface tension)
- Under small pressure,
  the viscosity changes from strong shear thinning to less shear thinning

Powder chunks -> examples

Vibration test





p=100 *p*=10