Fine-particle research

Stefan Luding, Multiscale Mechanics (MSM),
MESA+, ET, University of Twente, NL

UNIVERSITY OF TWENTE.

Fine particle-research
Fine-particle research

Stefan Luding, Multiscale Mechanics (MSM),
MESA+, ET, University of Twente, NL

UNIVERSITY OF TWENTE.

Common issues

- From micro/contact-mechanics to macro-behaviour
- Calibration and Validation
  But for which philosophy: primary or meso-particles?
- Choice of calibration tests and relevant parameters - depending on (flow) regime(s) and application.
- CPU-time when running moderate to large DEM+
- Apply modern and novel experimental techniques for additional information not available otherwise

From particles to continuum theory

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

– 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
2. fluid- and solid-like constitutive relations

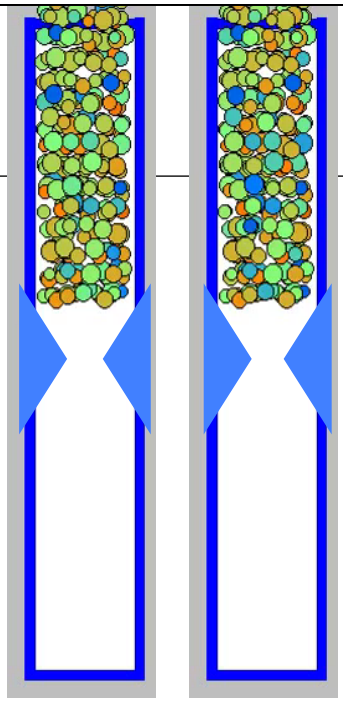
– multiple scales (from nano-meter to meters)
– from particles+contacts to application scale …

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

Particle systems

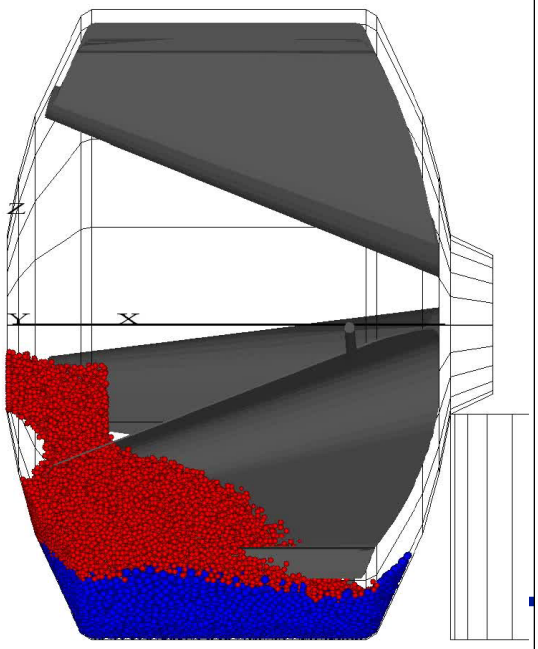
sometimes FLUID
sometimes SOLID
sometimes BOTH

un-jamming:
fluid <==> solid



msm UNIVERSITY OF TWENTE.

Example: Mixing



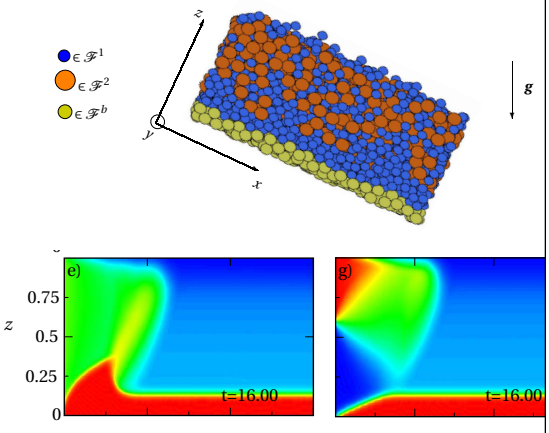
A. Gupta et al., MSM, 2010

Shallow flow continuum equations (3D->2D)

D. Tunuguntla et al. 2016

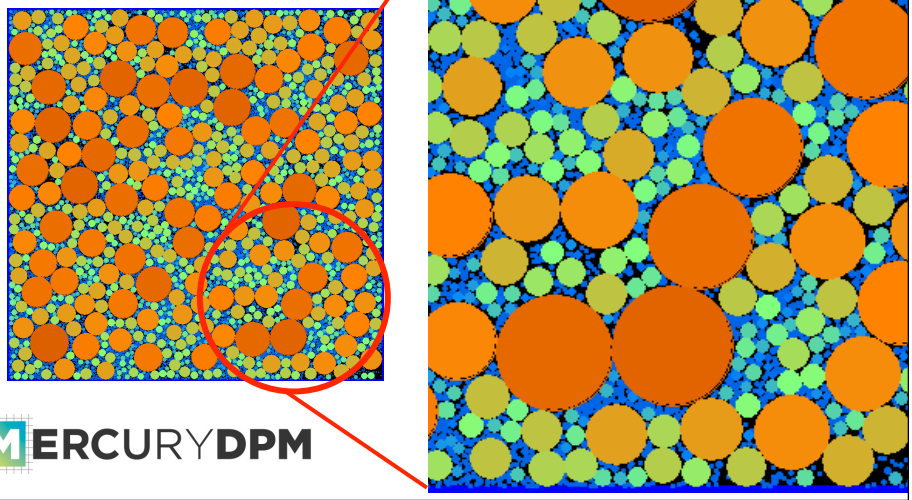
- D. Tunuguntla (PhD-thesis 2015)

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



msm UNIVERSITY OF TWENTE.

Challenge: DEM with realistic sizes => HGrid



MERCURYDPM

A. Ogarko et al., MSM, 2010-14

... highly polydisperse powders

Different MATERIALs

FRICTIONLESS → **FRICTIONAL** → **COHESIVE**

F. Goncu, CRAS, 2010
O. I. Imole et al KONA, 2013
N. Kumar et al Particuology (2013)
N. Kumar et al. Acta Mechanica (2014), GM 2016

V. Magnanimo (2011-13)
O. I. Imole et al (2014-16)

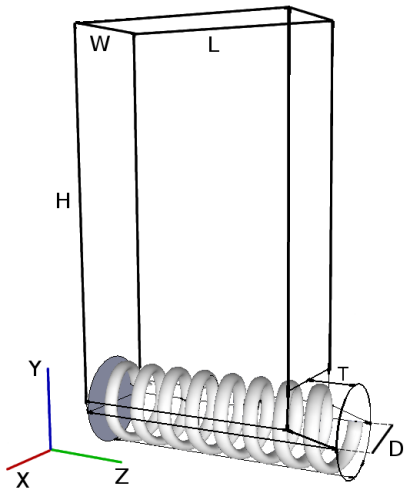
S. Luding et al. (2001-13)
A. Singh et al. (2014-16)
S. Roy et al. (2015-17)

Pictures: J. Brujic et al. Nature 460 (2009)
Dijksman, Brodu, Behringer (2013-14)

MERCURYDPM

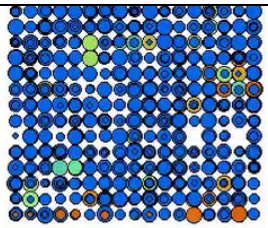
Open source

Based on:
- HGrid
- MicroMacro



Dosing application example …

MERCURYDPM



Open source

Based on:
- HGrid
- MicroMacro

flowable powder

(screw hidden)

© Marco Ramaioli, Nestle

Dosing application example …

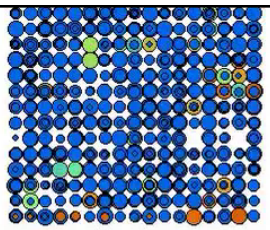
MERCURYDPM

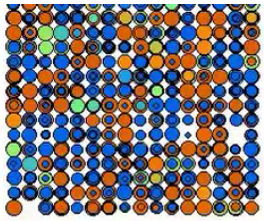
Open source

Based on:
- HGrid
- MicroMacro

flowable powder vs. sticky, chunky powder

(screw hidden)

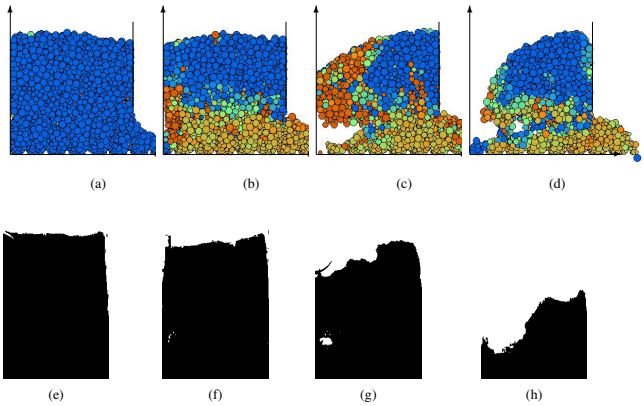




O. I. Imole, MSM, 2013

Dosing application example …

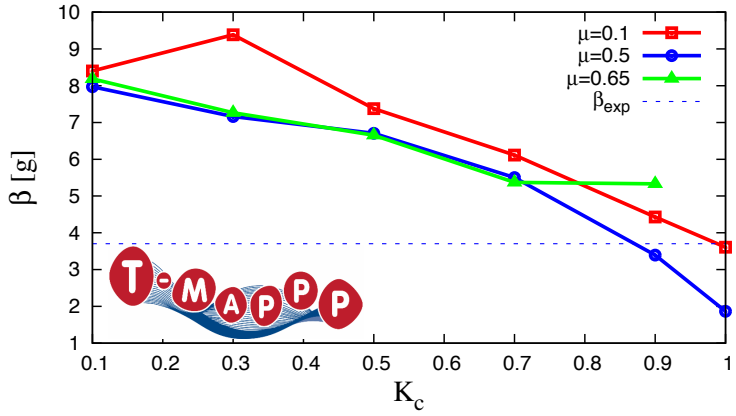
Dosing meso-rheology:
DEM vs. experiment <= Validation



*Based on O. I. Imole, D. Krijgsman, T. Weinhart, V. Magnanimo, E. C. Montes, M. Ramaioli, and S. Luding, Powder Tech, 2016.

Experiments and Discrete Element Simulation of the Dosing of Cohesive Powders in a Canister Geometry. In preparation, PhD-thesis, O. I. Imole 2014

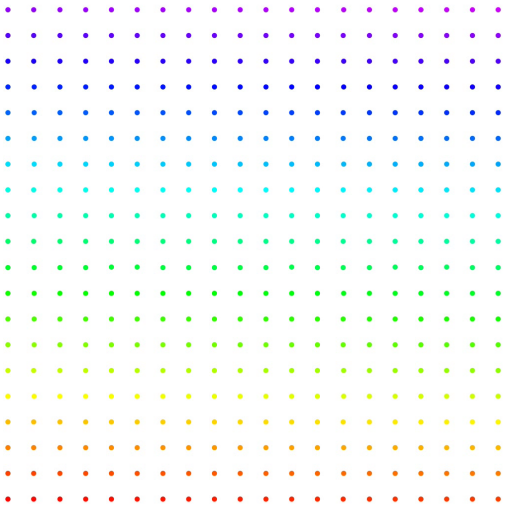
Dosing – parameter calibration



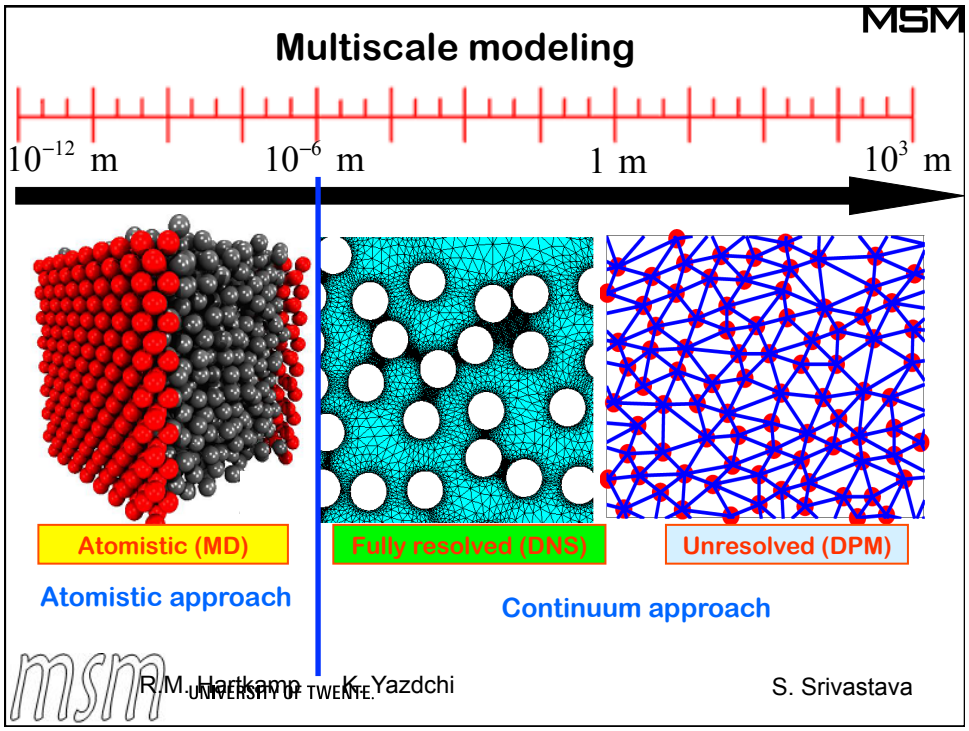
*Based on O. I. Imole, D. Krijgsman, T. Weinhart, V. Magnanimo, E. C. Montes, M. Ramaioli, and S. Luding, Powder Tech, 2016.

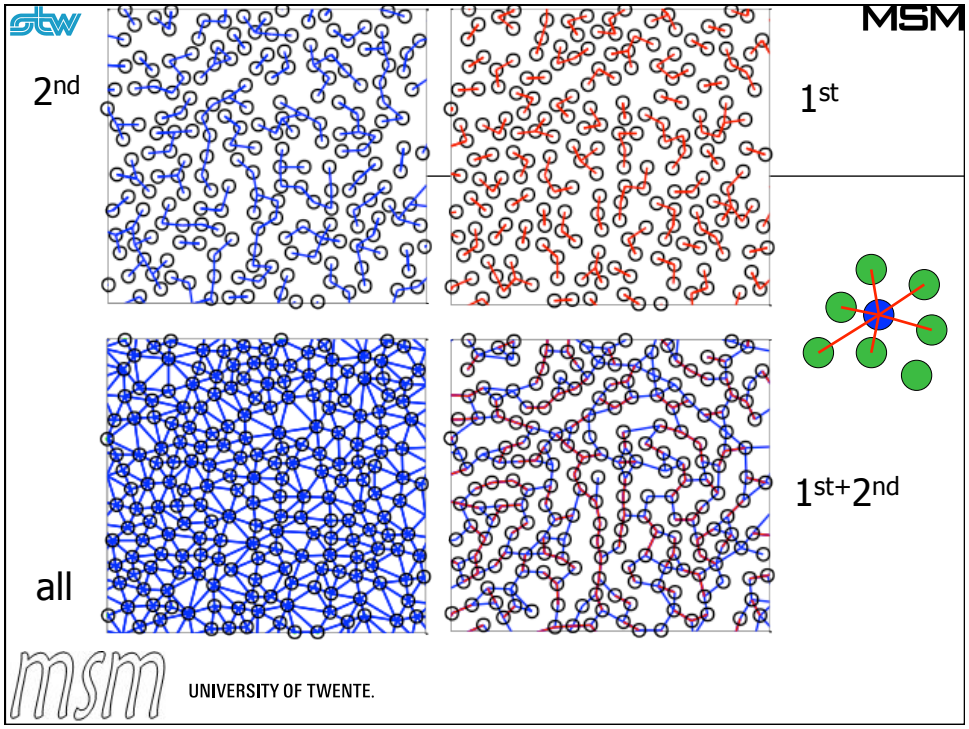
Experiments and Discrete Element Simulation of the Dosing of Cohesive Powders in a Canister Geometry. In preparation, PhD-thesis, O. I. Imole 2014

Dynamic Agglomeration

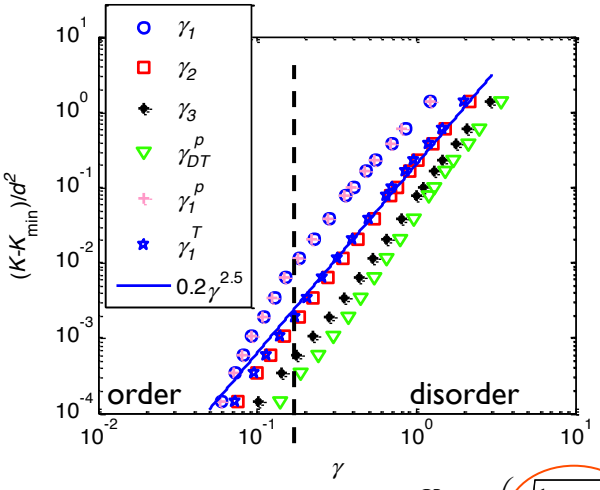


S. Gonzalez-Briones, MSM, 2010


MSM
Multiscale modeling
10^{-12} m
10^{-6} m
1 m
10^{3} m
Atomistic (MD)
Fully resolved (DNS)
Unresolved (DPM)
Atomistic approach
Continuum approach
msm
UNIVERSITY OF TWENTE.
R.M. Hartkamp
K. Yazdchi
S. Srivastava


stw
MSM
2nd
1st
all
1st+2nd
msm
UNIVERSITY OF TWENTE.

Microstructural model



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

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

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

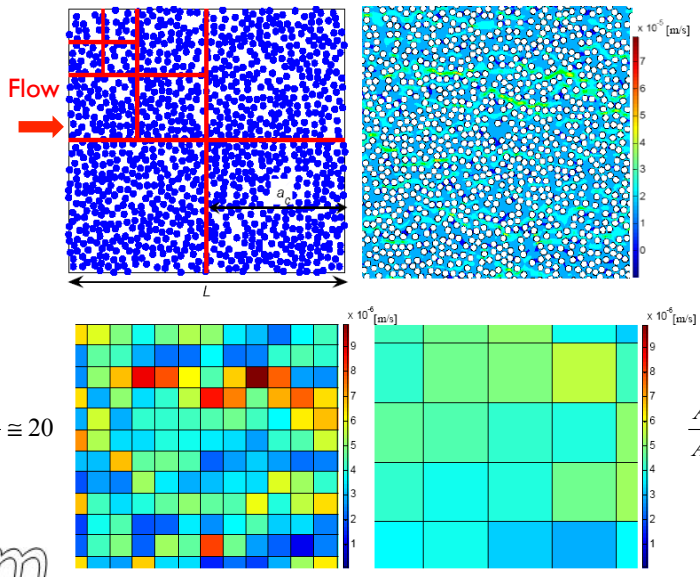
UNIVERSITY OF TWENTE.

- Characterization of microstructure
- From micro to macro properties (permeability)
- … suction
- … dispersion
- … etc

UNIVERSITY OF TWENTE.

Uniform averaging cells

Average horizontal velocity at $\varepsilon = 0.6$



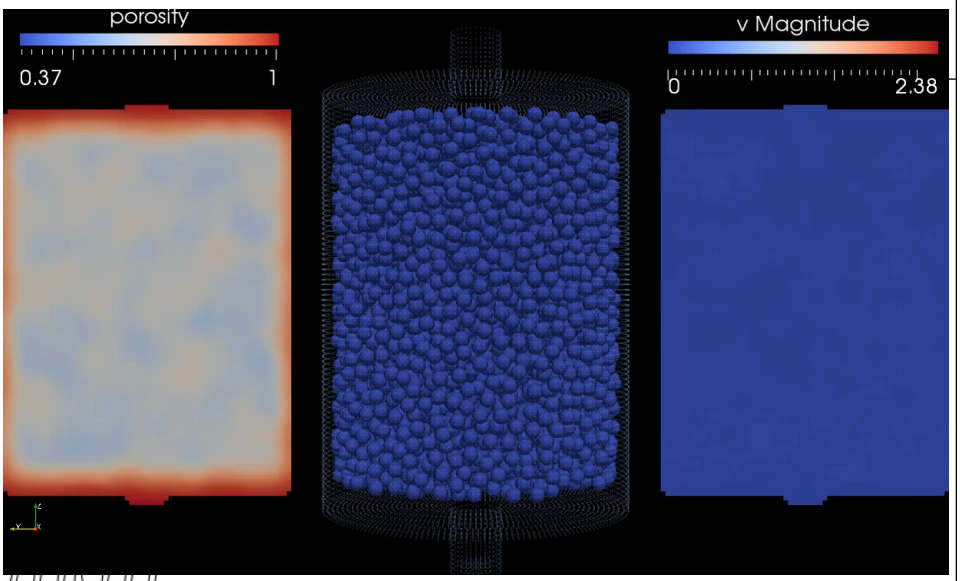
$\frac{A_c}{A_p} \cong 20$

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

UNIVERSITY OF TWENTE.

35

Liquid jet dispersion: Wet Start

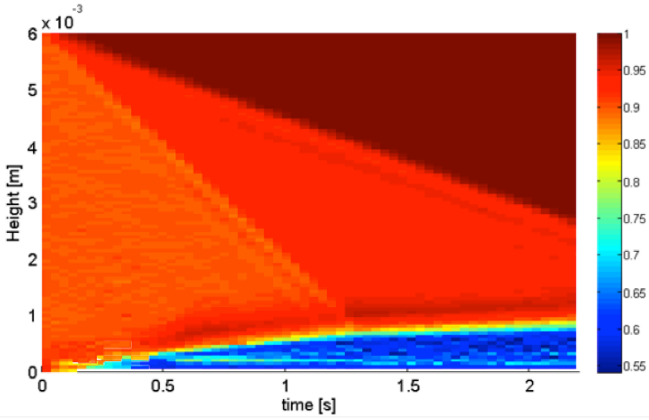


UNIVERSITY OF TWENTE.

Multi-species DEM-SPH model

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

Test/validation Homogeneous 2-species **batch sedimentation**

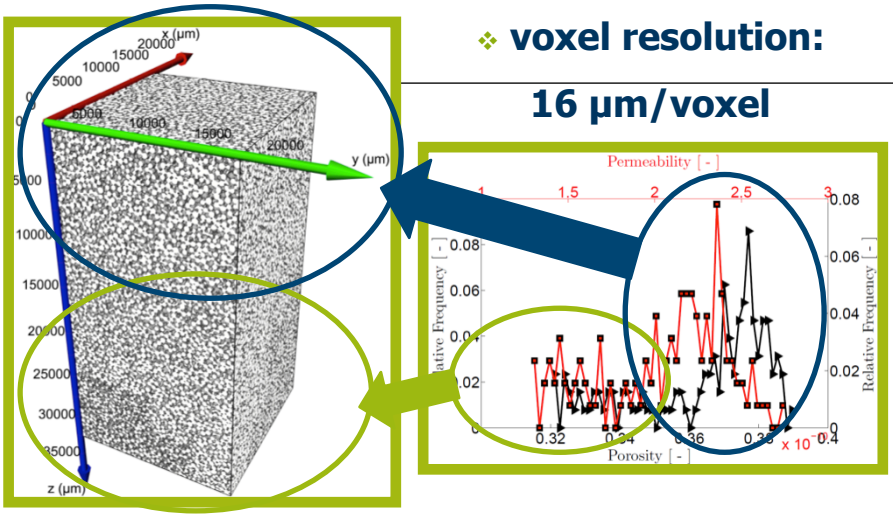


UNIVERSITY OF TWENTE.

Validate results – porosity & permeability

❖ **voxel resolution:**

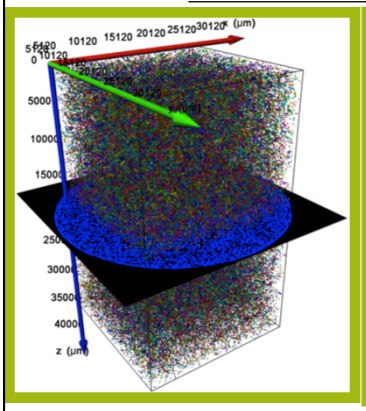
16 µm/voxel

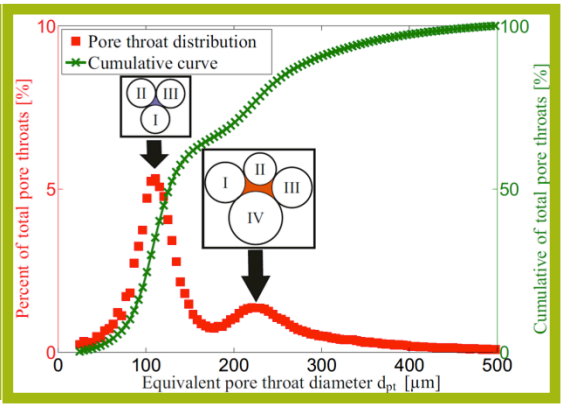


3D image data of the initial cube (left) with dimensions of 1024 (x) X 1024 (y) X 2048 (z) voxel^3 (left). Frequency distribution for porosity and permeability within the initial cuboid (right).

UNIVERSITY OF TWENTE.

results – pore throat distribution

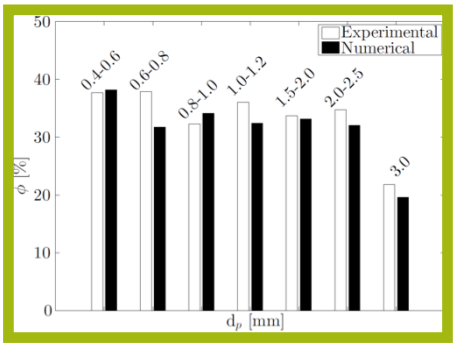


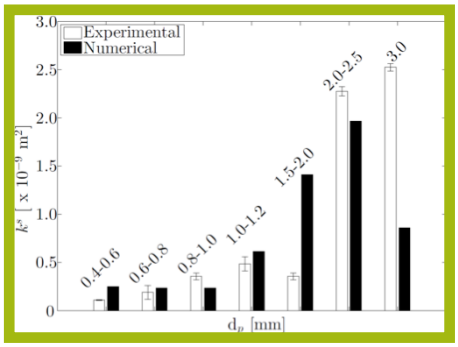


msm UNIVERSITY OF TWENTE.

Validate 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

T-MAPPP Common issues

- From micro/contact-mechanics to macro-behaviour
- Calibration and Validation
  But for which philosophy: primary or meso-particles?
- Choice of calibration tests and relevant parameters - depending on (flow) regime(s) and application.
- CPU-time when running moderate to large DEM+
- Apply modern and novel experimental techniques for additional information not available otherwise

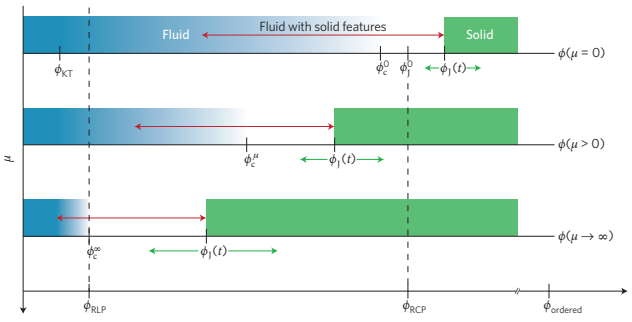
Introduction

• Granular materials are the combination of **discrete** solid (macroscopic) particles

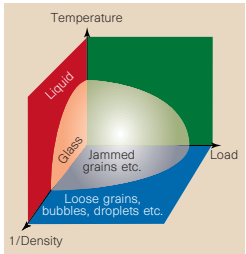
• **many interesting phenomena - can we understand them? all together?**

history-dependence, slow relaxation, creep/aging, shear-localization, "avalanches", …

fluid-solid transition => jamming "~~point~~" – **no point, but a variable! J-line!**



S. Luding, Nature, 2016



A. Liu and S. Nagel, Nature 396, 1998

Constitutive Model: With Anisotropy

Isotropy (before) + Anisotropy F_{dev}

$$\begin{aligned}
\delta P^* &= 3B\delta\varepsilon_{\mathrm{v}} + A_1 S_\sigma \delta\varepsilon_{\mathrm{dev}}, \\
\delta\sigma^*_{\mathrm{dev}} &= 3A_2\delta\varepsilon_{\mathrm{v}} + G^{\mathrm{oct}} S_\sigma \delta\varepsilon_{\mathrm{dev}}, \\
\delta F_{\mathrm{dev}} &= \beta_F \mathrm{sign}\left(\varepsilon_{\mathrm{dev}}\right) F_{\mathrm{dev}}^{\max} S_F \delta\varepsilon_{\mathrm{dev}}
\end{aligned}$$

Due to A_1 and 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 the deformation path

… then integrate the incremental evolution …

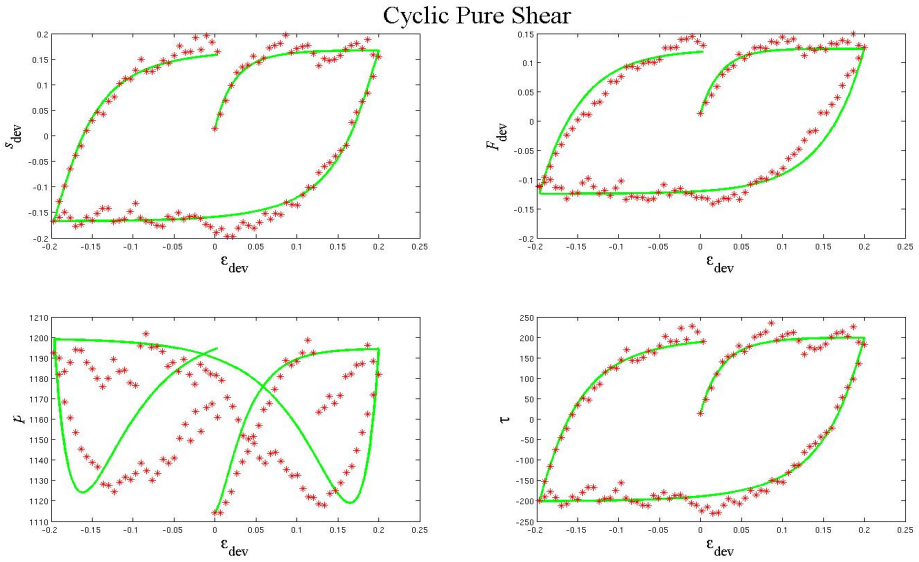
Constitutive model – calibration
Direct moduli (B,G,A) probing …

Bulk Modulus: $B = b_0 F_V$

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

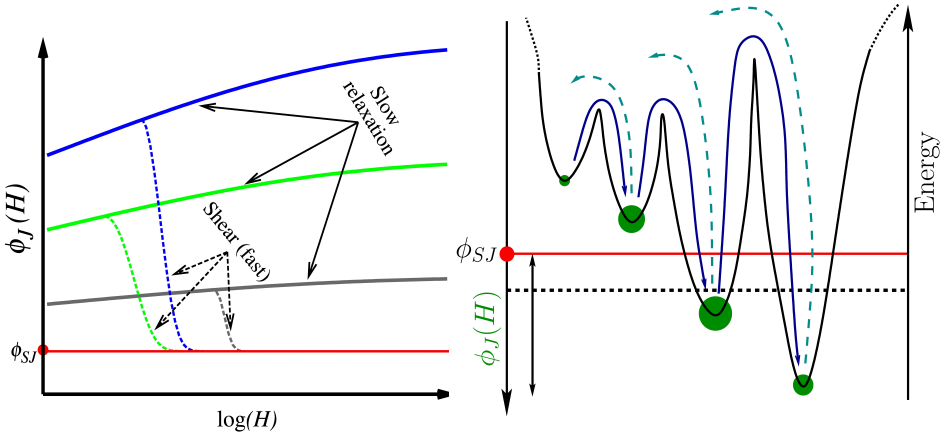
Anisotropy Modulus: $A = B F_{dev}$

Prediction (improved 2014) – Cyclic Shear



N.Kumar, S. Luding, V. Magnanimo, Acta Mechanica, 2014

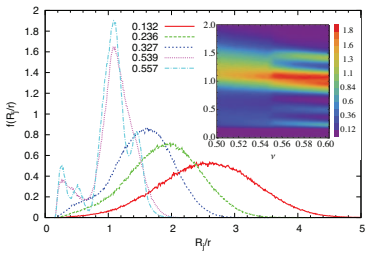
Evolution of jamming points with history

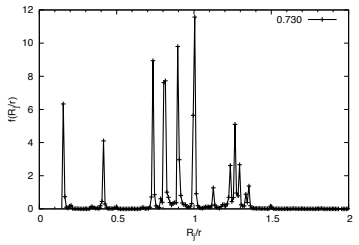


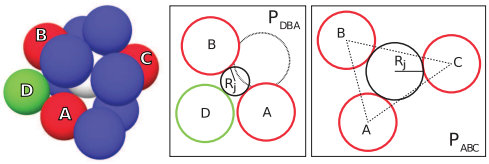
The image cannot be displayed. Your computer may not have

Meso scale stochastic physics model

Fluid with solid features ⇔ microstructure







channel/throat distribution
(4 particle correlation)
2D order in 3D !

V. Ogarko, N. Rivas, SL, JCP 2014

So much for the jamming point …

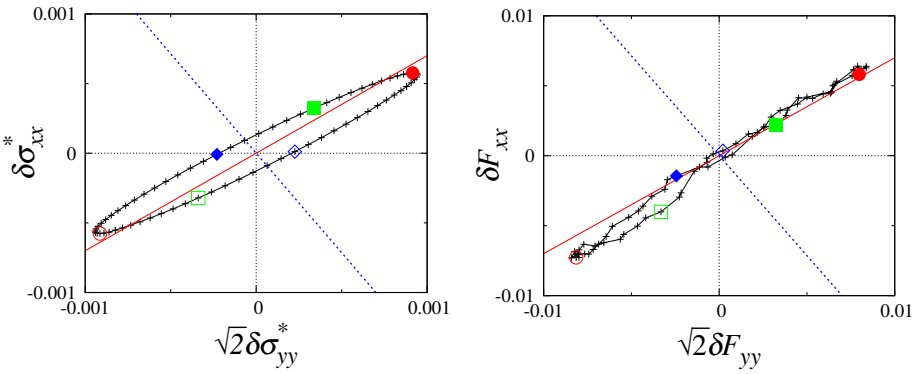
Response: jamming "point" moves!
- slow for ISO => increase
- fast for DEV => decrease
- in fluid and in solid states ⇔ **dilatancy**

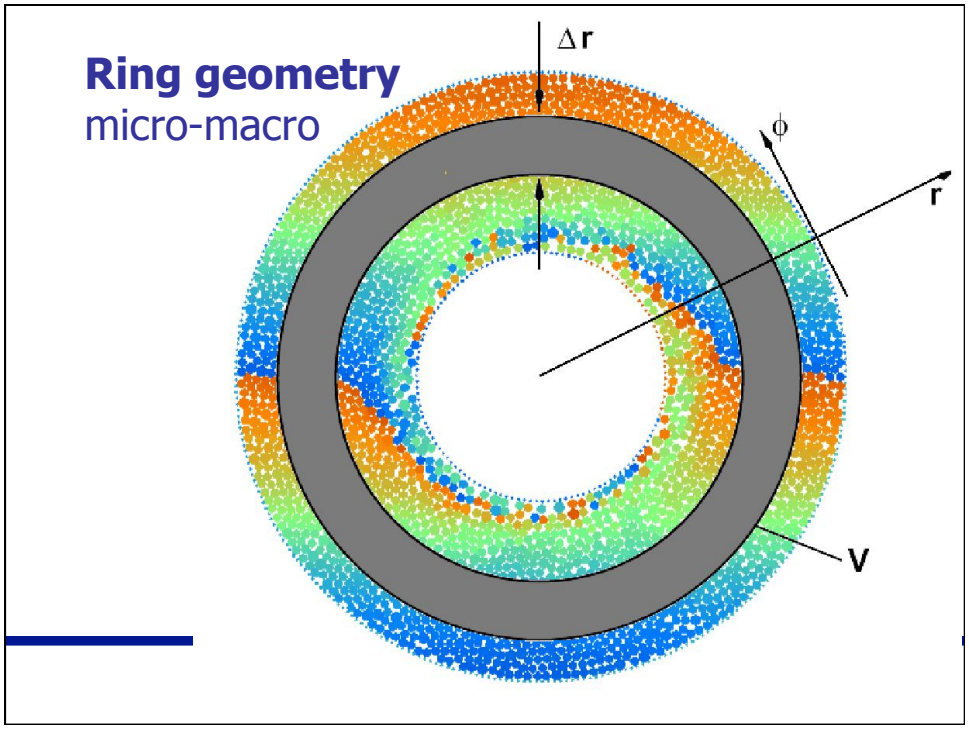
Fluid with solid features vs. flowing solid
There is not just one phase-diagram ☹

All mechanisms **without friction** (colloids/glass)
1 – friction/material changes regime/values
2 - re-entrance = shear-jamming/-thickening

Predictive power – large strain shear MACRO

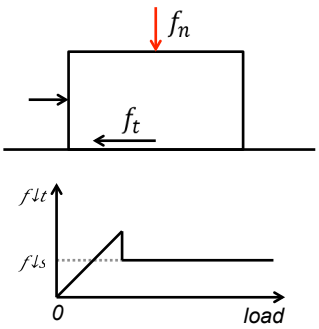
=> Failure/yield surfaces … work in progress …





Coulomb's law of friction (steady/critical state)

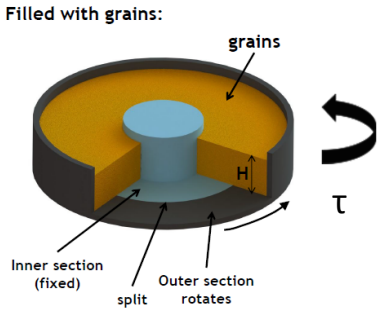
Rigid body



Sliding friction

$f_s = \mu f_n$

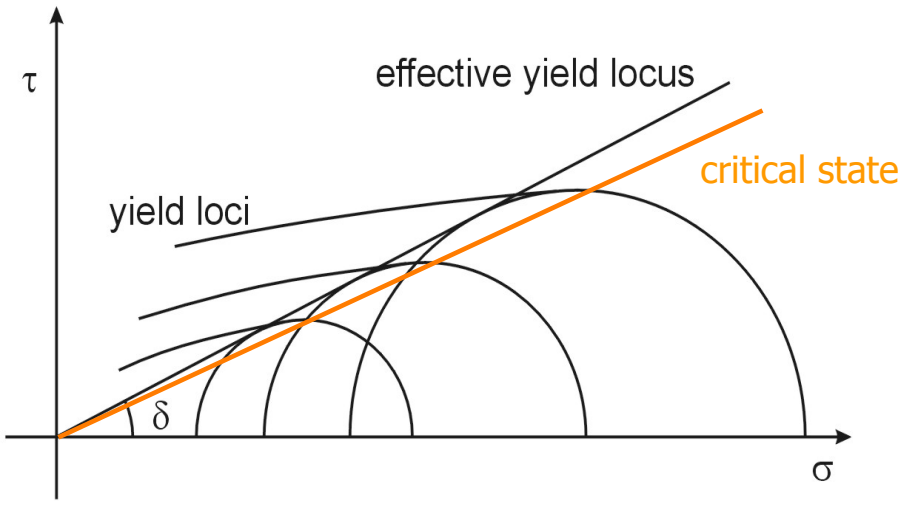
Granular flow



Pressure induced due to gravity P

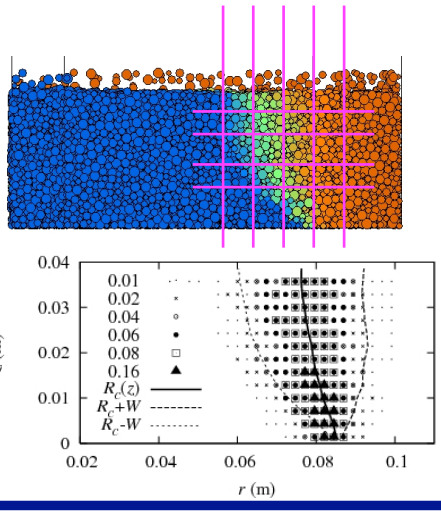
$$\tau = \mu P$$

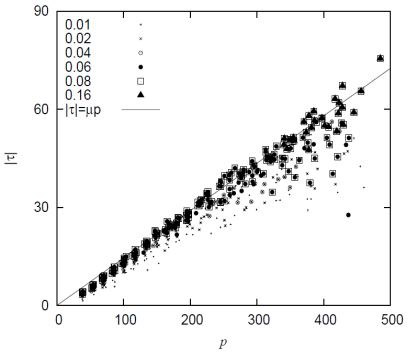
Yield loci => steady state flow



Shear Band (steady/critical state)

local mic-mac averaging => **Constitutive relations**





Local quantities

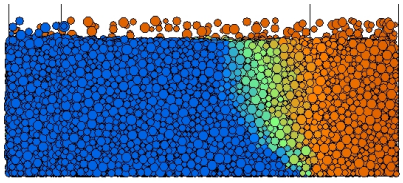
shear rate $\dot{\gamma}$

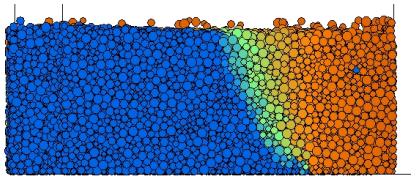
shear stress τ

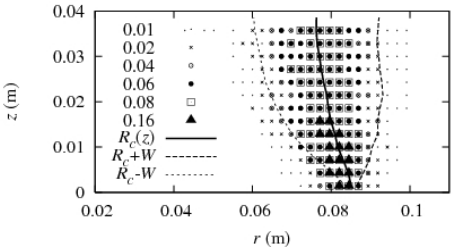
pressure P

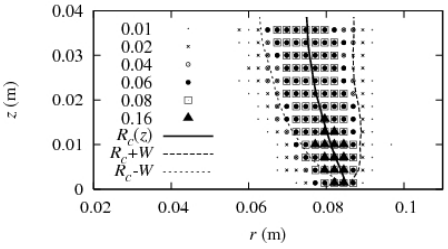
others ρ, ϕ, F

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



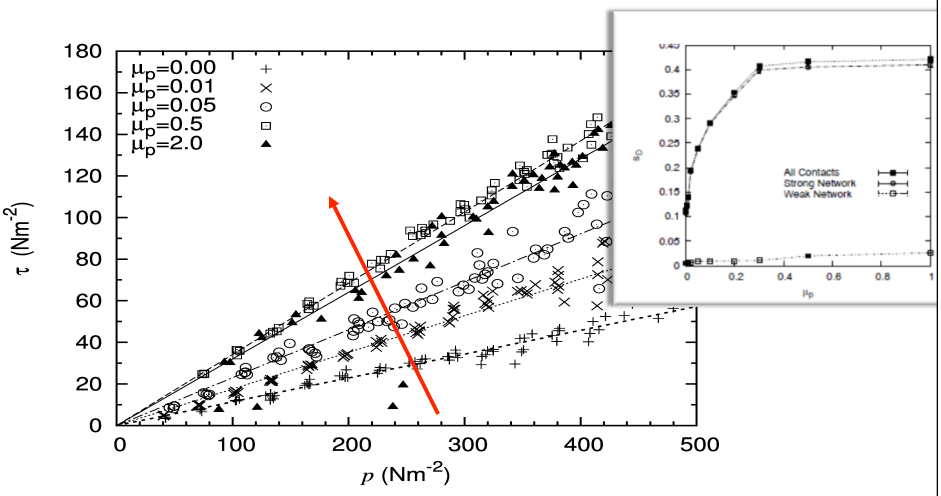






no friction friction

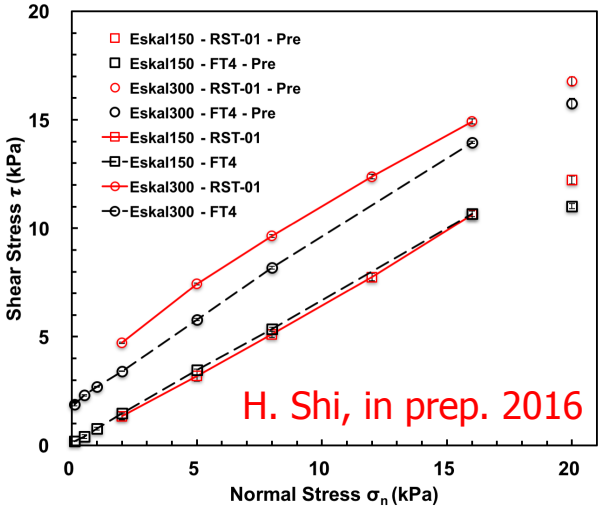
macro-friction vs. micro-friction



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

VALIDATION

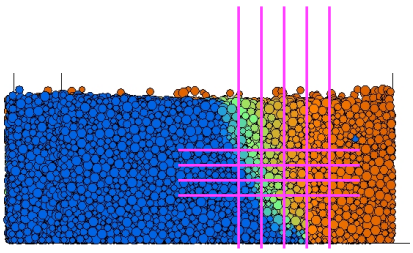
RING SHEAR TESTER AND FT4 POWDER RHEOMETER FOR DIFFERENT (LIME-STONE) POWDERS

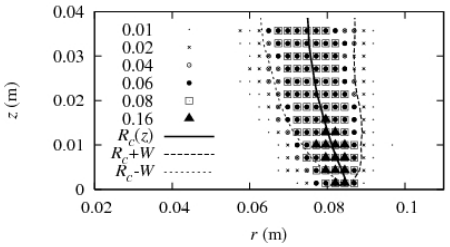


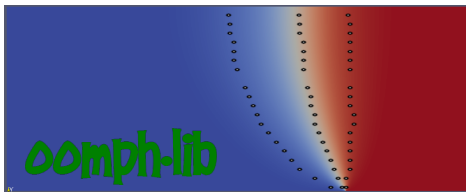
24-Jan-17

Constitutive relations => continuum solver

$\dot{\gamma}$



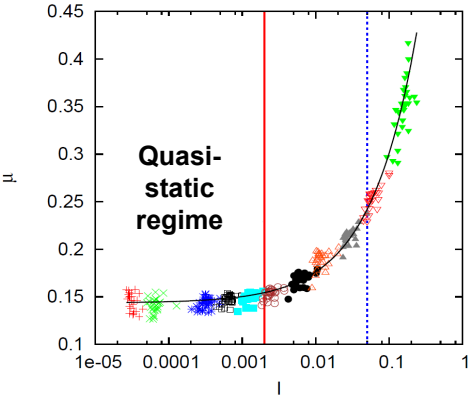




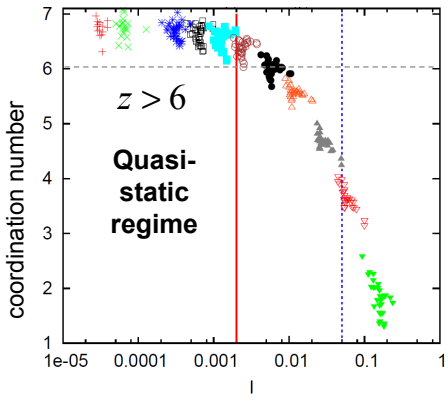
M. Schrojenstein Lantman

Rigid particles – effect of strain-rate

macro-friction coefficient



coordination number

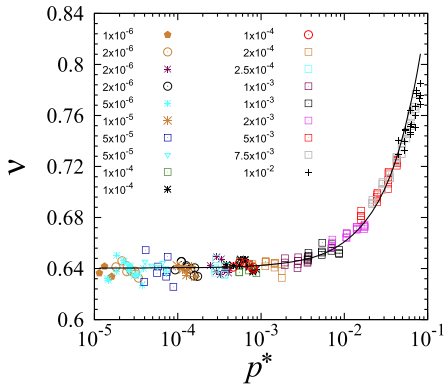


Macro-Friction coefficient $\nu(P^*) = \nu_0 - a_\nu I^\alpha$

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 $\nu(P^*) = \nu_0 + b_\nu P^{*\beta}$ $\beta \approx 1$

Macroscopic friction - rheology

Time scales

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

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

Dimensionless numbers

Inertial number $I = \tau_P/\tau_s$

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

Friction coefficient

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

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

A. Singh et al., NJP 2015

Inertial and soft flow-rheology?

Dependence on stiffness (gravity) in inertial flow states

$$\mu(I, P^*) = \mu_0 + aI^{\alpha} - bP^{*1/2}$$

$$\nu(P^*) = \nu_0 - a_\nu I + b_\nu P^*$$

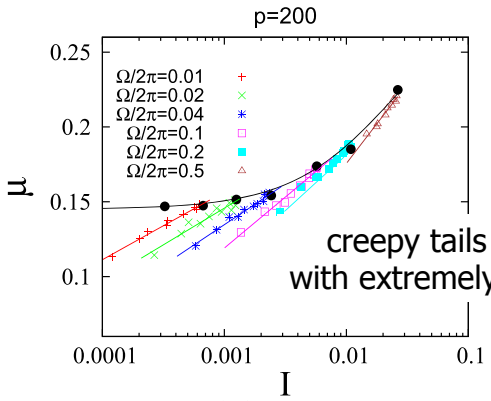
Generalized rheology:
includes dilatancy/compactancy,
as well as: slow and inertial flow regimes
for both: rigid and soft particles
and: low and high confining stress

A. Singh et al., NJP 2015

Inertial and soft flow-rheology?

Dependence on stiffness (gravity) in inertial flow states

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



creepy tails of shearbands
with extremely small strain rate

A. Singh et al., NJP 2015 $\mu\left(I < I^{\star}, p^{\star}\right) = \mu_0^{\text{local}}\left(p^{\star}\right)\left[1 - \alpha \ln\left(I/I^{\star}\right)\right]$

Recent News (multiplicative rheology)

Combined dependence on stiffness in inertial flow states

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

with: $I = \dot{\gamma} d / \sqrt{P/\rho}$ and scaled stress P^*

Outlook

Local constitutive relations at low gravity?

Recent News (multiplicative rheology)

Combined dependence on stiffness in inertial flow states

$$\mu(I, P^*, Bo_l) = \mu_0 f_I\left(I\right) f_p\left(P^*\right) f_{\text{creep}}(I)$$

with: $I = \dot{\gamma} d / \sqrt{P/\rho}$ and scaled stress P^*

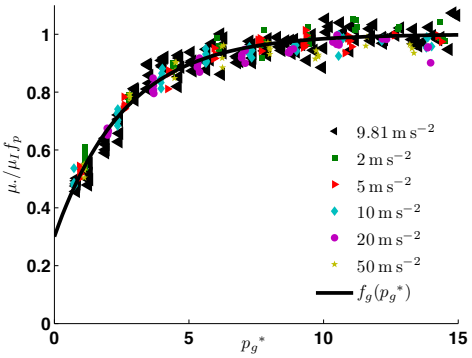
Generalized rheology

Local constitutive relations at low confining stress?
Low gravity (astrophysics) or unconfinde at free-surface

Inertial, soft, low-p flow-rheology?

Dependence on stiffness (gravity) in dry flow states (SB)

$$f_g(P^*) = 1 - a' \exp\left(-\frac{p_g^*}{p_{g0}^*}\right) \quad \text{with} \quad p_g^* = \frac{p}{\rho d g}$$



S. Roy et al., NJP 2016 (submitted)

Recent News (multiplicative rheology)

Combined dependence on stiffness in inertial flow states

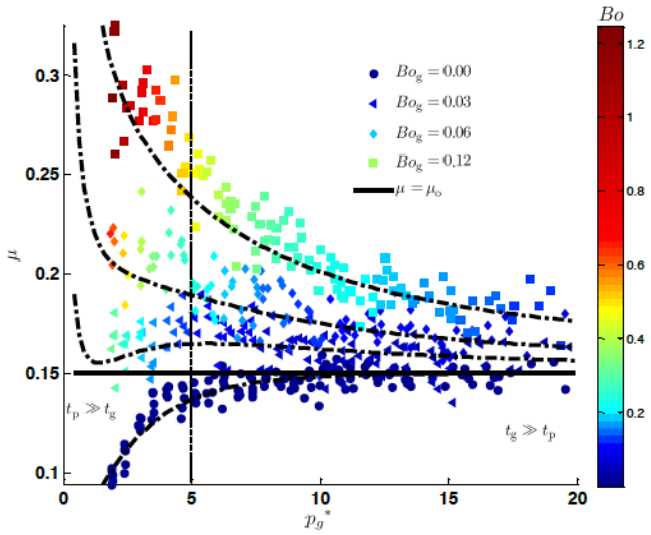
$$\mu(I, P^*, P_g^*) = \mu_0 f_I(I) f_p(P^*) f_{\text{creep}}(I) f_g(P_g^*)$$

with: $I = \dot{\gamma} d / \sqrt{P/\rho}$ and scaled stress P^*, P_g^*

Outlook

What about cohesion => Bond number Bo

Inertial, soft, low-g, cohesive flow-rheology?



S. Roy et al., DEM7, 2016

Recent News (multiplicative rheology)

Combined dependence on stiffness in inertial flow states

$$\mu(I, P^*, P_g^*, Bo) = \left(\mu_0 + \frac{\mu_\infty - \mu_0}{1 + I_0/I} \right) f_p\left(P^*\right) f_{\text{creep}}(I) f_g\left(P_g^*\right) f_c\left(Bo\right)$$

with: $I = \dot{\gamma} d / \sqrt{P/\rho}$ and scaled stress P^*, P_g^*, cohesion Bo

Outlook

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

S. Roy, 2016, submitted to NJP

Most recent news: granular temperature

Dependence on stiffness and dynamic T_g (inertial & static)

$$\mu(I, P^*, Bo_l, I_k) = \mu_0 f_I(I) f_p f_g f_c \frac{1}{1 + 1/\beta(\phi) I_k}$$

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

Conclusion

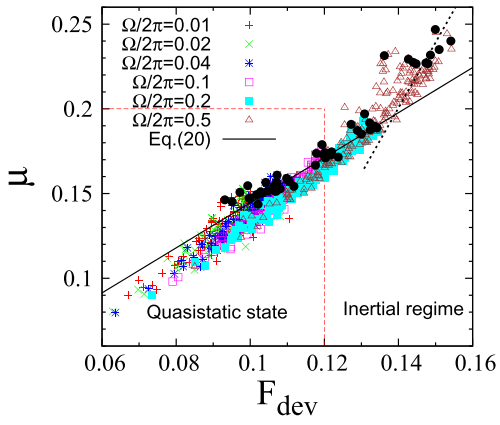
You MUST NOT neglect any of the active correction terms

Further challenges:

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

Micro-rheology – stress-fabric relation

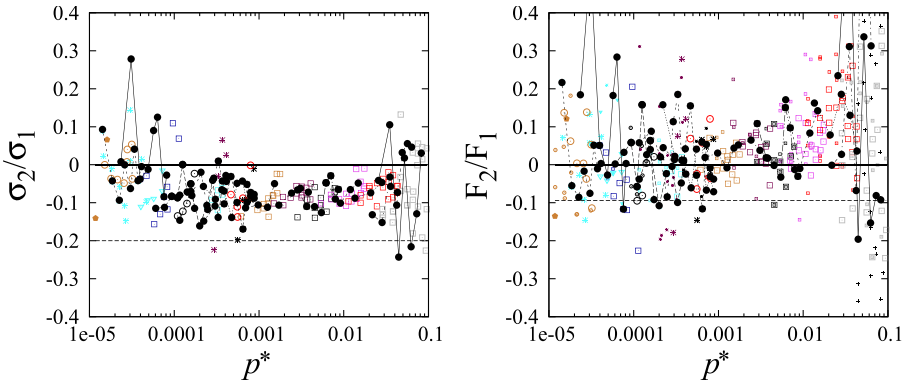
Fully tensorial 3D => … in progress …



A. Singh et al., NJP 2015

Rheology – stress-fabric relation

Fully tensorial 3D => … in progress …



A. Singh et al., NJP 2015

Common issues

- From micro/contact-mechanics to macro-behaviour
- Calibration and Validation
  But for which philosophy: primary or meso-particles?
- Choice of calibration tests and relevant parameters - depending on (flow) regime(s) and application.
- Apply modern and novel experimental techniques for additional information not available otherwise
- CPU-time when running moderate to large DEM+

Software used …

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

Software used …

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

MERCURYDPM

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

Software used …

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

- Mercury*Cloud*
- Training
- Consulting
- Support

Software used …

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

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

IFPRI Questions & Challenges

- From micro/contact-mechanics to macro-behaviour
  => achieved: micro-meso => macro/continuum
- Calibration and Validation
  But for which philosophy: primary or meso-particles?
  Needed for DEM, PBM, as well as Continuum Methods
- What is meso? Meso-particles =/= Meso-physics
  (involving fluctuations, stochastic, plastic events, …)
- Choice of calibration tests and relevant parameters - depending on (flow) regime(s) and application.
  => Best-practice guidelines and standards?