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Particle Technology: Basics + Modeling …

Stefan Luding, MSM, ET, MESA+, UTwente, NL

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JMBC course
Particle Technology
for PhD+MSc students

April 29 – May 03, 2019
University of Twente
Enschede, The Netherlands

Contact:
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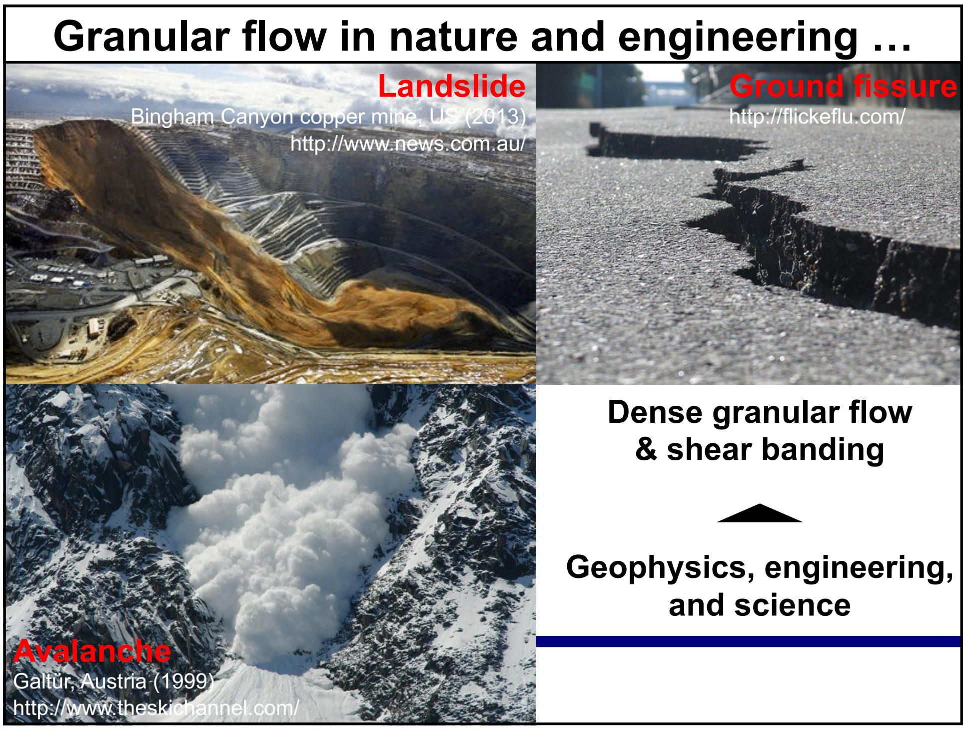
DEM 8

8th International Conference on Discrete Element Methods

July 22-26, 2019
University of Twente
Enschede,
The Netherlands



Granular flow in nature and engineering …

Landslide
Bingham Canyon copper mine, US (2013)
http://www.news.com.au/

Ground fissure
http://flickeflu.com/

Avalanche
Galtür, Austria (1999)
http://www.theskichannel.com/

Dense granular flow & shear banding

▲

Geophysics, engineering, and science

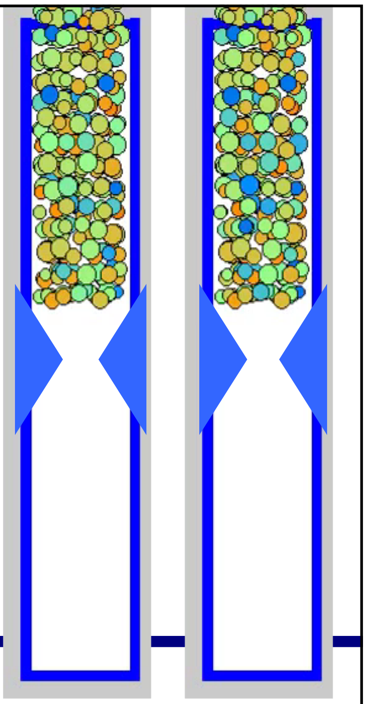
Physics: Why are granular materials interesting?

They exhibit different phase.

Particle systems

sometimes FLUID
sometimes SOLID
sometimes BOTH

un-jamming:
fluid <==> solid

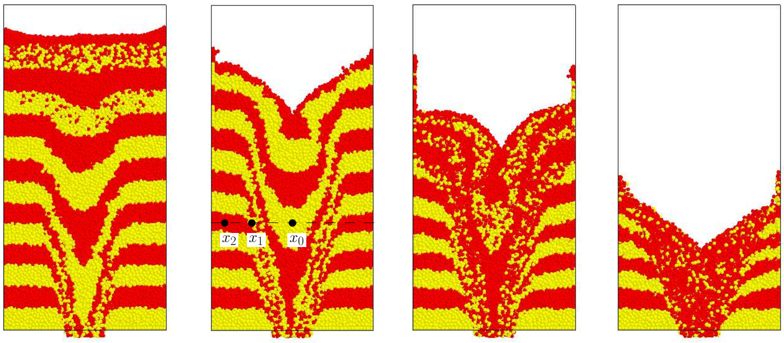


Why granular materials are so important?

- 2nd only to water as the most handled material in global industry.
- 40% of industrial plant efforts are wasted.
- 10% of the energy consumed in the world.

Test case: Silo flow model

Silo flow model with internal flow pattern is used

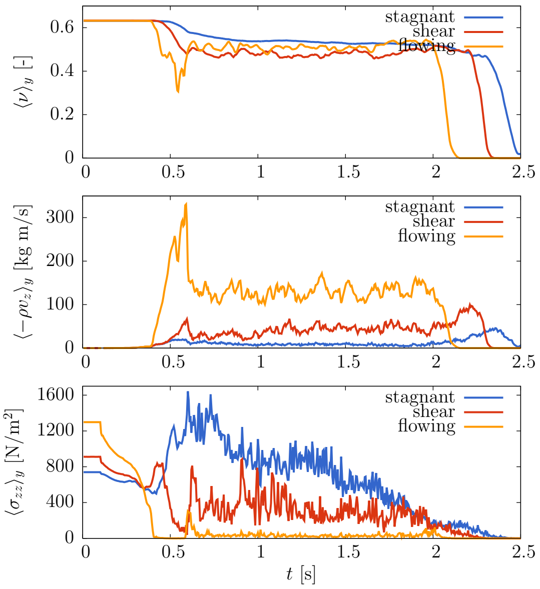


(a) t=0.745s (b) t=1.200s (c) t=1.490s (d) t=2.240s

T. Weinhart, C. Labra, et al., Powder Technol., 2016

Test case: Silo flow model

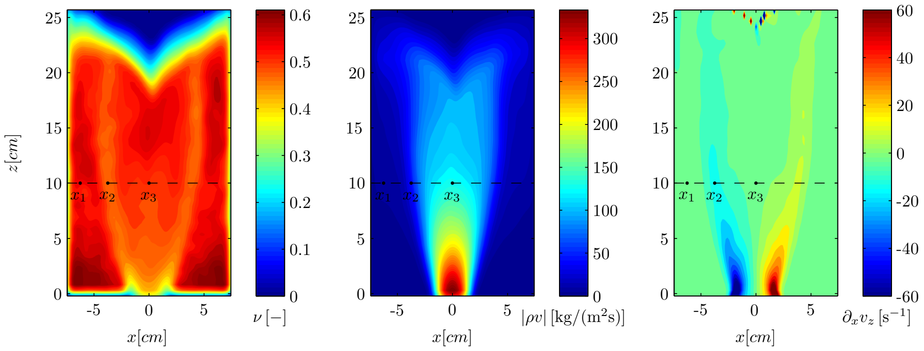
Horizontal variation:



T. Weinhart, C. Labra, et al., Powder Technol., 2016

Test case: Silo flow model

Horizontal variation – different fields:



Multi Scale – from Particles to Continuum – HOW?

For fluids and solids this can be done

For particles and their contacts,
i.e. granular materials and powders,
use: discrete approaches for fluid- & solid-like behavior

Micro-Macro transition
to derive constitutive relations for continuum theory
and applications with FEM/CFD

Example 1: Vibration => Leidenfrost

N. Rivas,
MSM, 2011

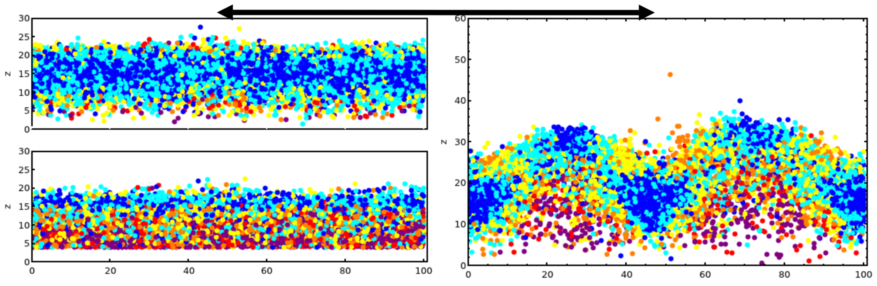
Example 2: Vibration => Fingering

N. Rivas,
MSM, 2011

VIBRATED SHALLOW BOX

“From colliding particles to a hydrodynamic description of granular matter” N. Rivas

Transition

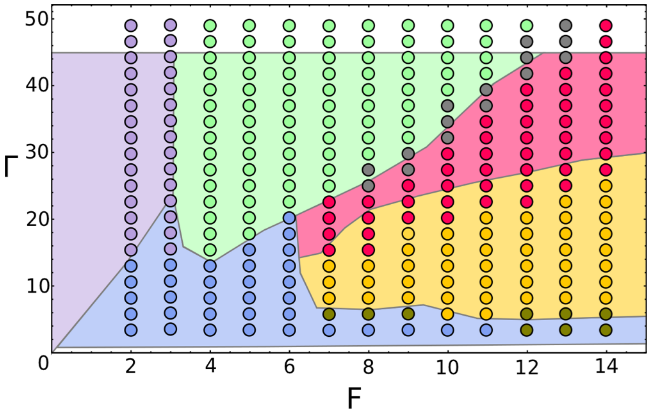


Experimental
Analytical
Simulations: - Molecular Dynamics (ED, DEM)
- Granular Hydrodynamics Solver

VIBRATED SHALLOW BOX

"From colliding particles to a hydrodynamic description of granular matter" N. Rivas

ED SIMULATIONS



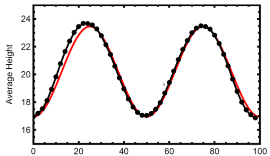
—background from *P. Eshuis*, et al. Physics of Fluids, 2007

VIBRATED SHALLOW BOX

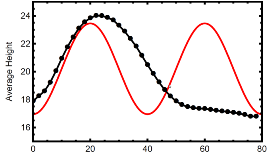
"From colliding particles to a hydrodynamic description of granular matter" N. Rivas

ED SIMULATIONS

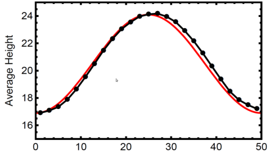
Lx = 100



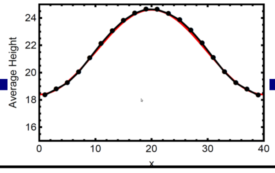
Lx = 80



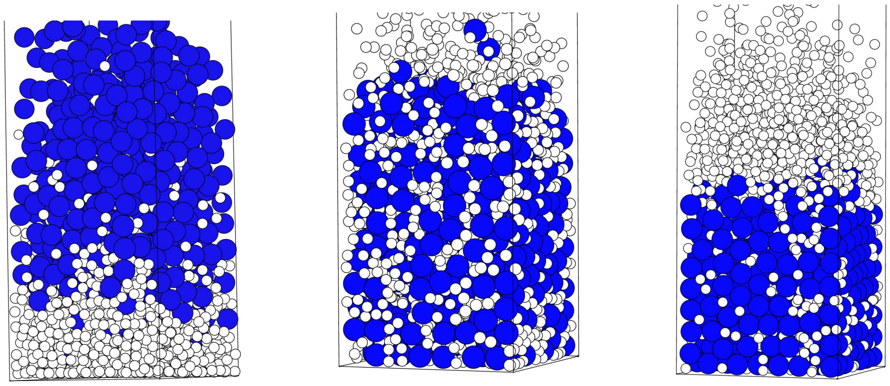
Lx = 50



Lx = 40

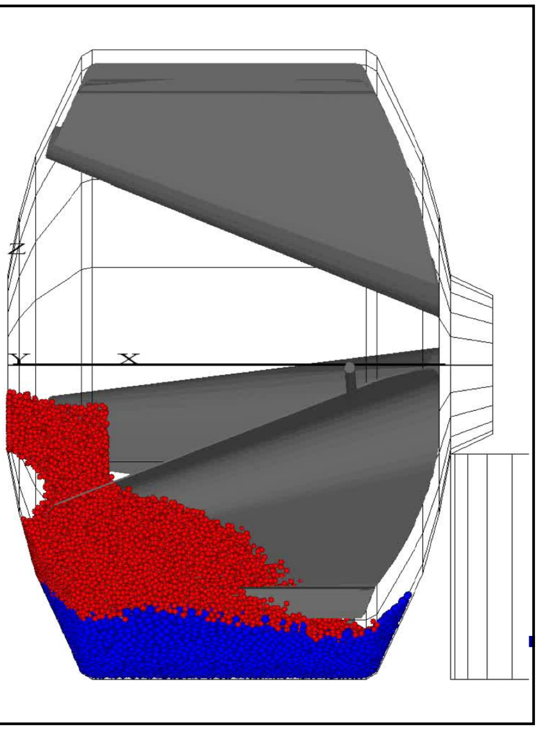


Example: Segregation/Mixing



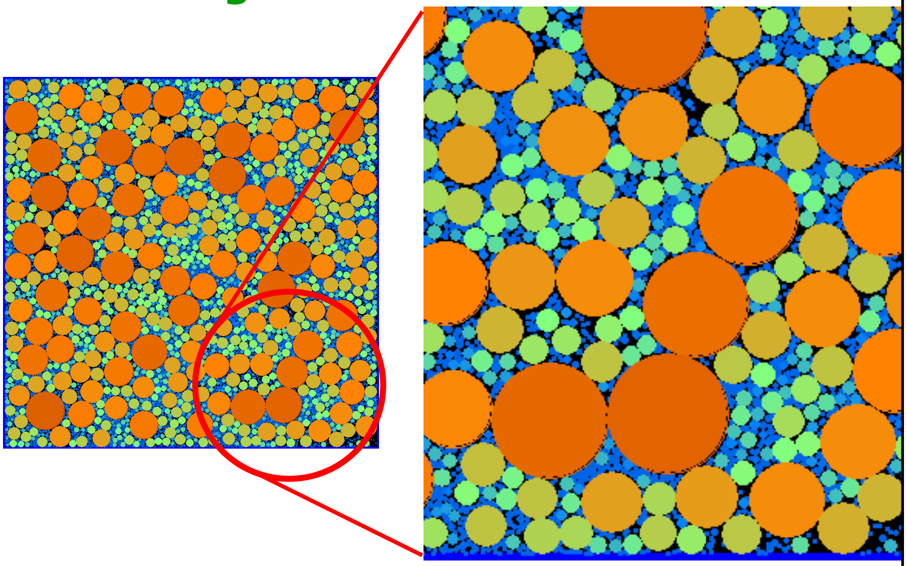
P. V. Quinn, D. Hong, SL, PRL 2001

Example: Mixing



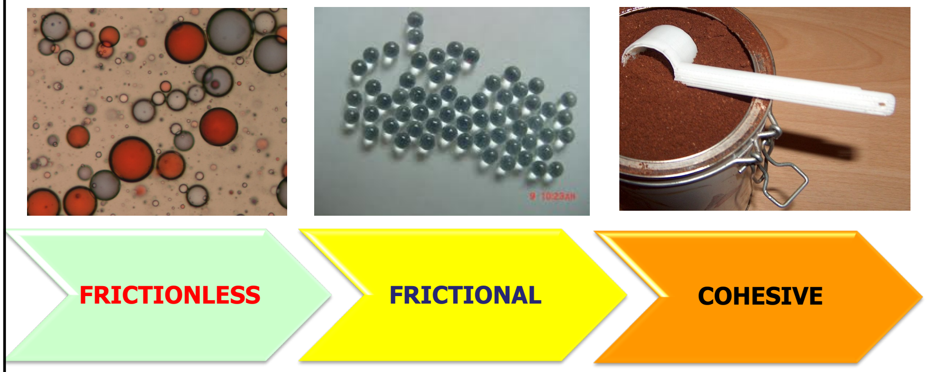
A. Gupta et al., MSM, 2010

Challenge: DEM with realistic sizes



… highly polydisperse powders

Our Approach: MATERIALs



FRICTIONLESS

FRICTIONAL

COHESIVE

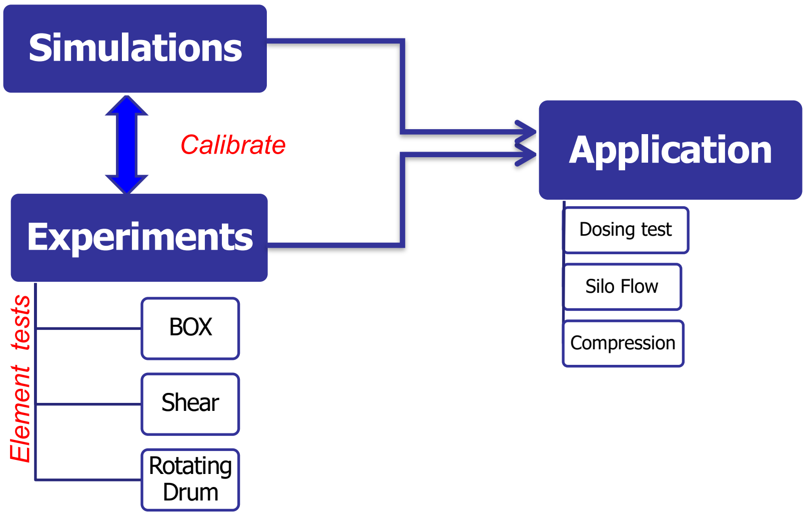
F. Goncu, CRAS, 2010
O. I. Imole et al KONA, 2013
N. Kumar et al Particuology (2013)
N. Kumar et al. Acta Mechanica (2014)

V. Magnanimo (2011-13)
O. I. Imole et al (to be submitted and in preparation, 2014)

S. Luding et al. (2001-13)

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

PARDEM Overview/Philosophy



Simulations

Calibrate

Experiments

Element tests

- BOX
- Shear
- Rotating Drum

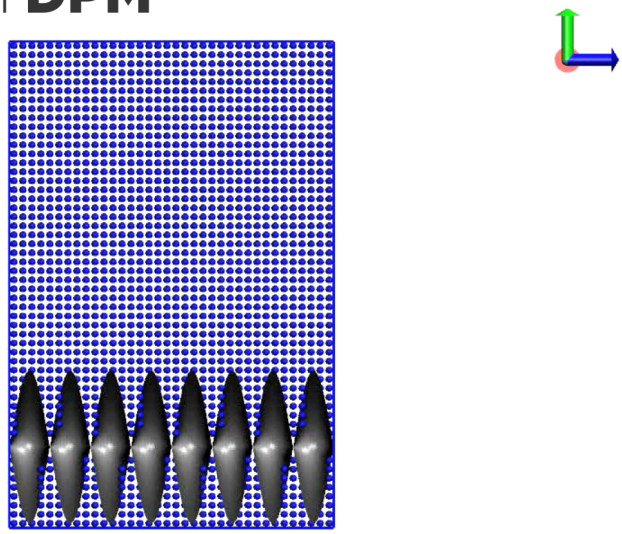
Application

- Dosing test
- Silo Flow
- Compression

MERCURYDPM

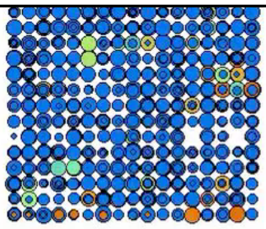
Open source

Based on:
- HGrid
- MicroMacro



Dosing application example …

MERCURYDPM



Open source

Based on:
- HGrid
- MicroMacro

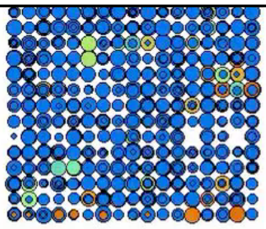
flowable powder

© Marco Ramaioli, Nestle

(screw hidden)

Dosing application example …

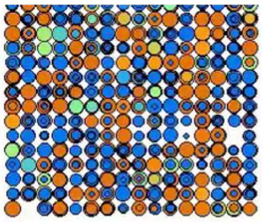
MERCURYDPM



Open source

Based on:
- HGrid
- MicroMacro

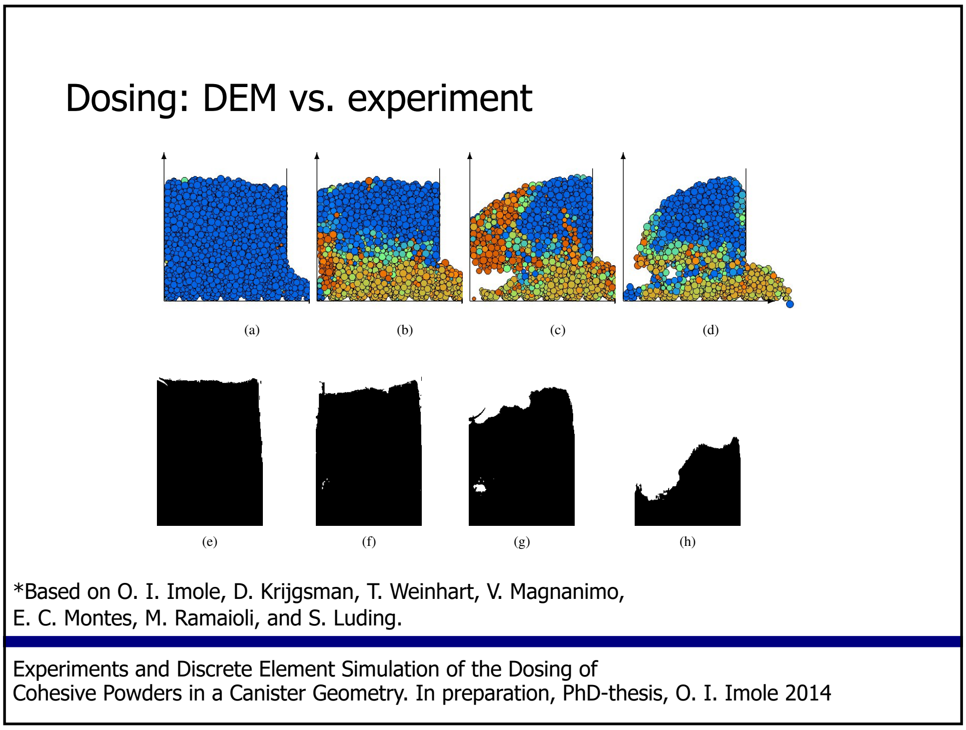
flowable powder vs.
sticky, chunky powder



(screw hidden)

O. I. Imole, MSM, 2013

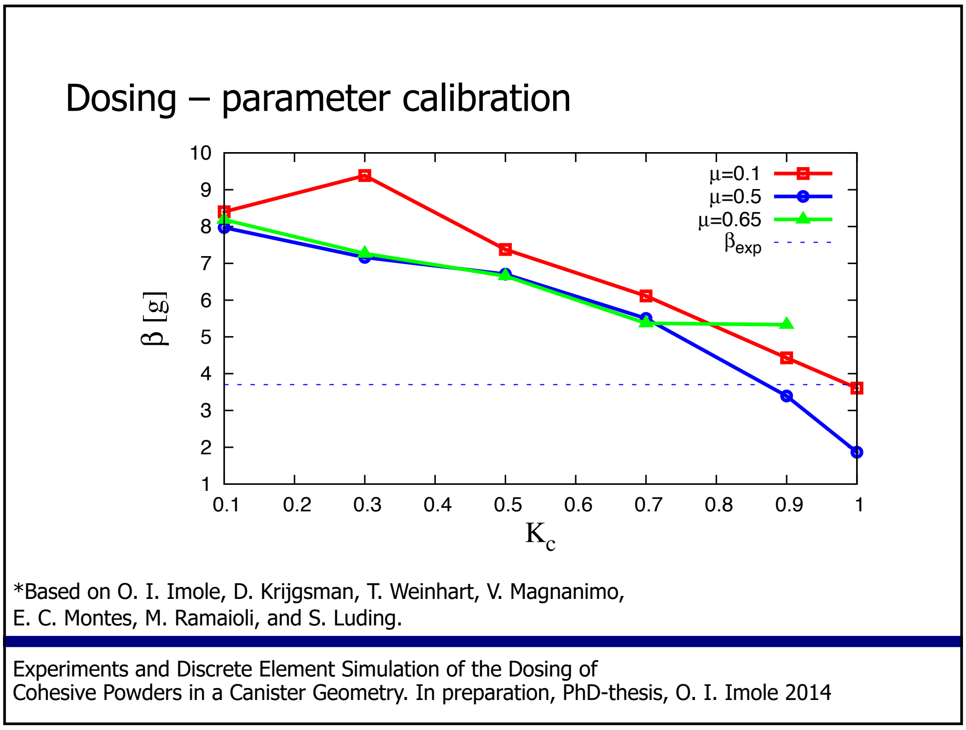
Dosing application example …



Dosing: DEM vs. experiment

*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. 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.

Experiments and Discrete Element Simulation of the Dosing of
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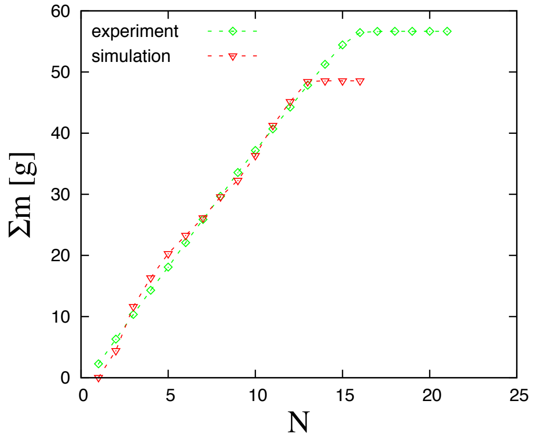
Dosing: DEM vs. experiment



*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. In preparation, PhD-thesis, O. I. Imole 2014

Software used …

See talk by T. Weinhart,
Thu 11:20, M&S=StPetersbg.

- DEMSolutions/EDEM
- YADE
- DCS Comp.
- MercuryDPM
- and others

MERCURYDPM

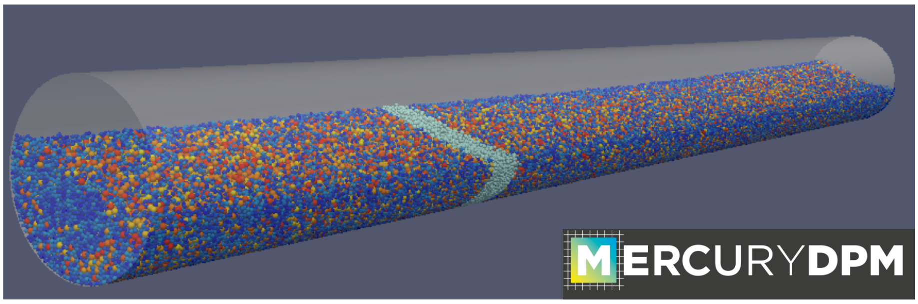
unique features:
- open-source (really ;-)
- HGrid for largely different particle sizes
- mercuryCG for coarse-graining to continuum
- analytical complex geometry-support
- parallel, etc.

See talk by A.R. Thornton, Tue 15:20, Mixing=Shanghai

So far: Nothing about parallelization in this talk …

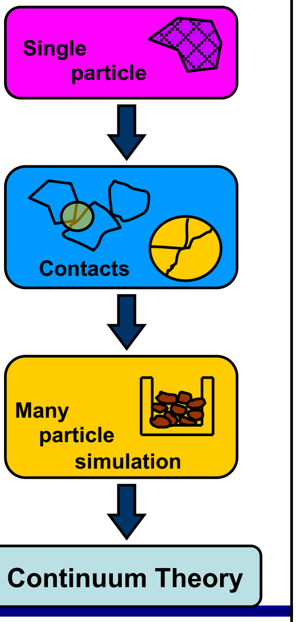
A) There are serial ED algorithms that **not** parallelize

B) Standard MD/DEM does parallelize very well …



Overview Particles&Continuum

- Introduction
- Contact models
- Many particle simulation
- Local micro-macro
- Continuum Theory


Single particle

Contacts

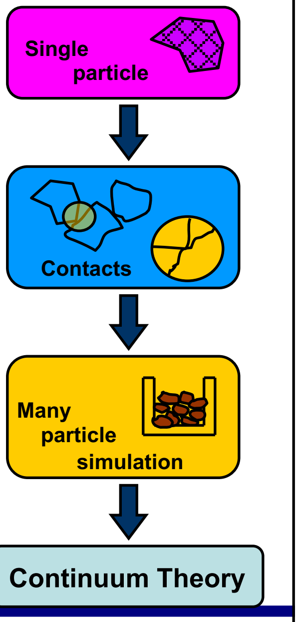
Many particle simulation

Continuum Theory

Goal:

Large Scale systems
Applications

Continuum Theory



Single particle

Contacts

Many particle simulation

Continuum Theory

Continuum theory

mass conservation:

$$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x_i}\left(\rho u_i\right) = 0$$

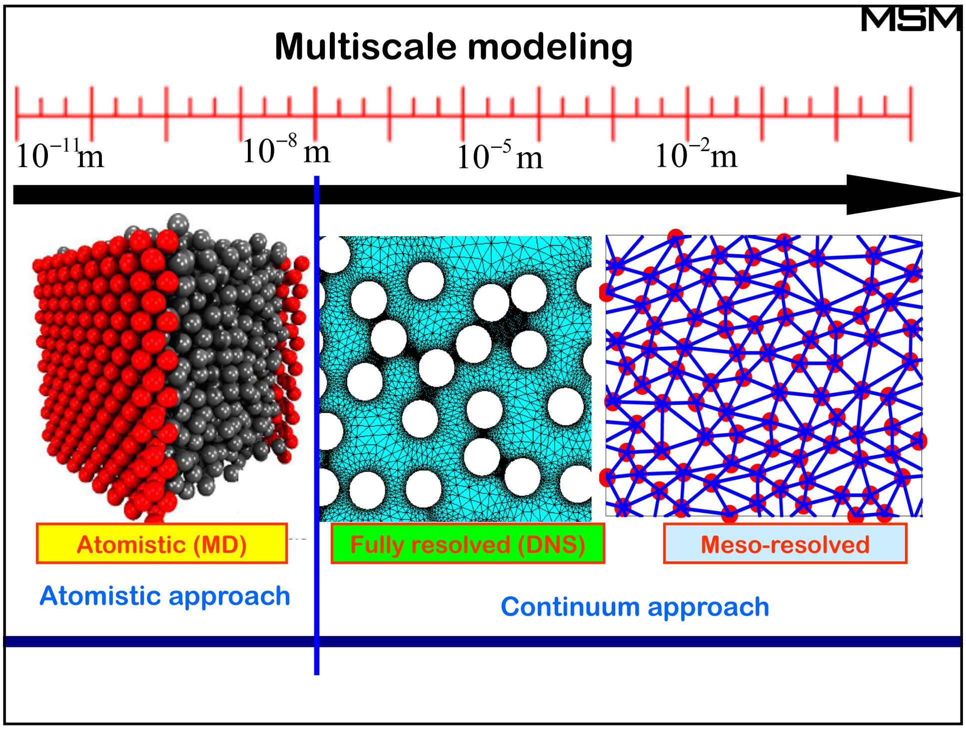
momentum conservation:

$$\frac{\partial}{\partial t}\left(\rho u_i\right) + \frac{\partial}{\partial x_k}\left(\rho u_i u_k\right) = -\frac{\partial}{\partial x_i} P + \frac{\partial}{\partial x_j}\sigma_{ij}^{\mathrm{dev}} + \rho g_i$$

energy balance:

$$\frac{\partial}{\partial t}\left(\tfrac{1}{2}\rho u^2 + \tfrac{1}{2}\rho v^2\right) = -\frac{\partial}{\partial x_k}\left[\rho u_k\left(\frac{P}{\rho} + \tfrac{1}{2}u^2 + \tfrac{1}{2}v^2\right) - u_i \sigma_{ik}^{\mathrm{dev}} - K\frac{\partial}{\partial x_k}\left(\tfrac{1}{2}\rho v^2\right)\right] + \rho u_i g_i - I$$

- **Pressure *P***
- **Shear Stress** $\sigma_{ij}^{\mathrm{dev}}$
- **Energy Dissipation Rate *I***



Multiscale modeling

10^{-11}m 10^{-8} m 10^{-5}m 10^{-2}m

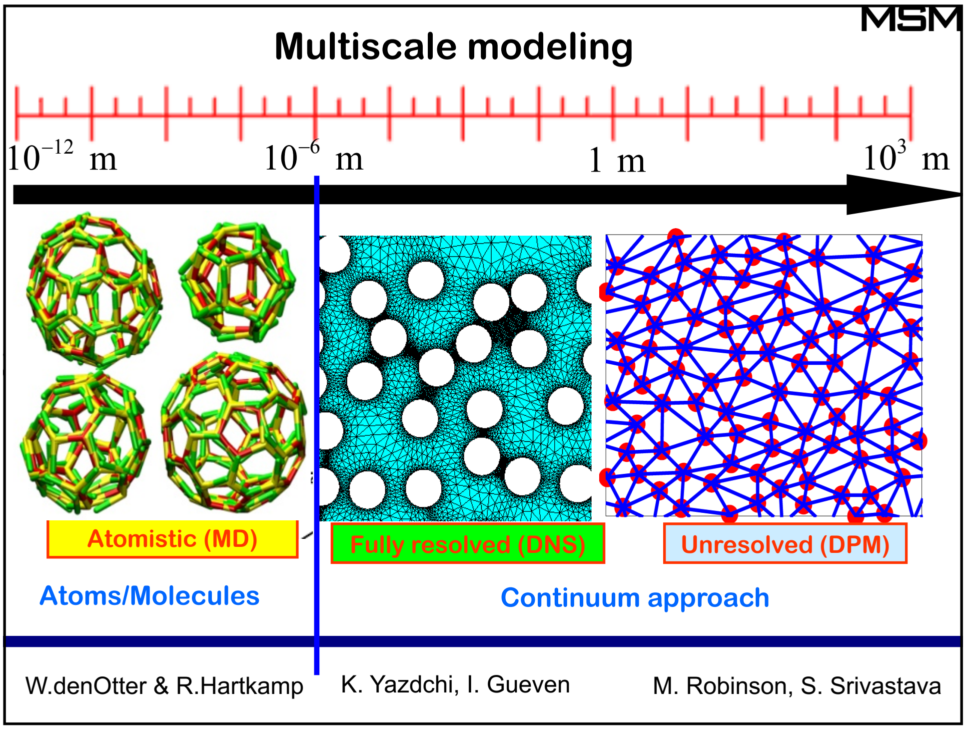
Atomistic (MD)

Fully resolved (DNS)

Meso-resolved

Atomistic approach

Continuum approach



Multiscale modeling

10^{-12} m 10^{-6} m 1 m 10^{3} m

Atomistic (MD)

Fully resolved (DNS)

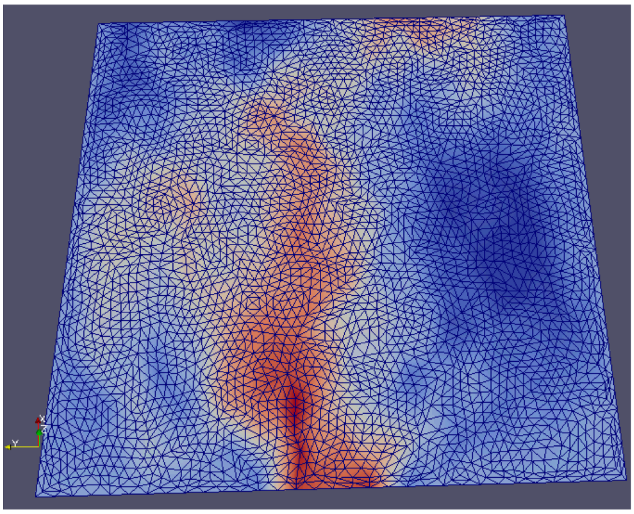
Unresolved (DPM)

Atoms/Molecules

Continuum approach

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

Example: Fluidization DEM-FEM



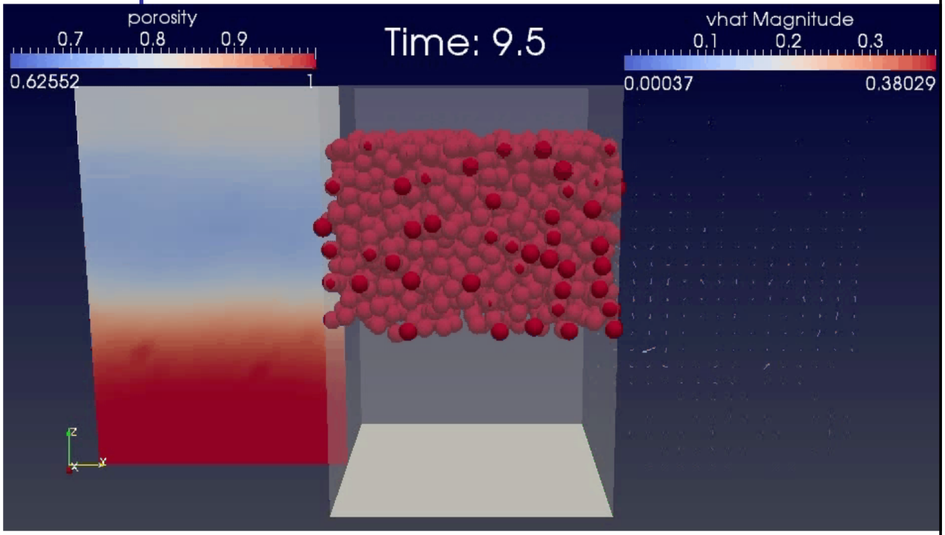
Fluidization on moving mesh with 800 particles (with gravity)

Set of Realistic Fluid-Particle Parameters

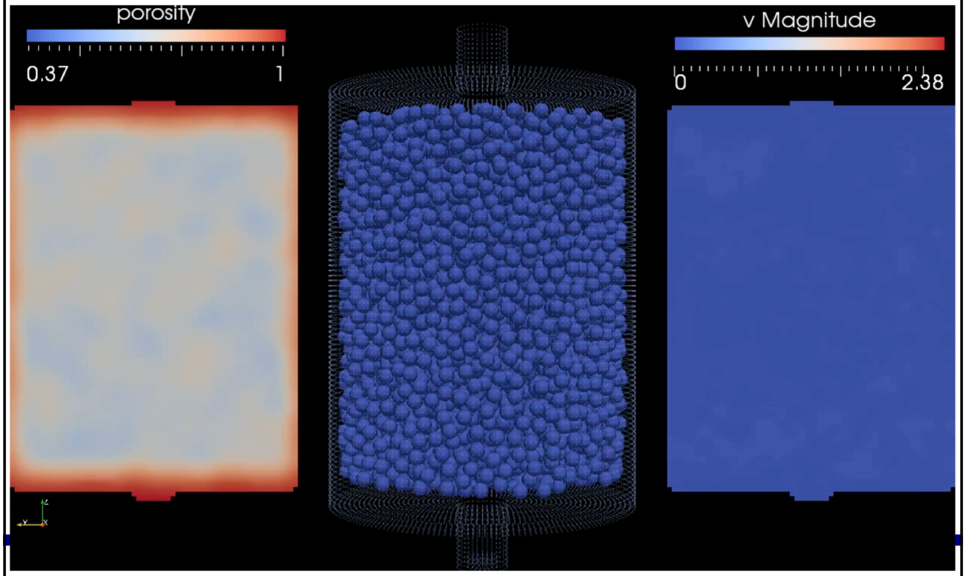
- Three different fluids used to provide a range of particle Reynolds Numbers
- Parameters based on air, water and 10% glycerol-water solution

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

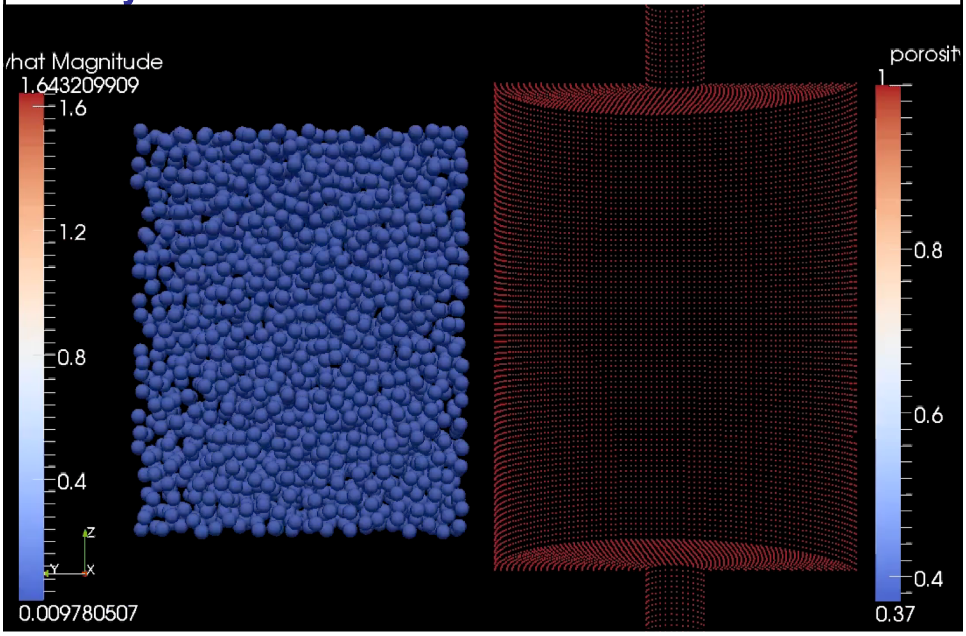
Multiple Particle Sedimentation – SPH Results



Wet Start



Dry Start

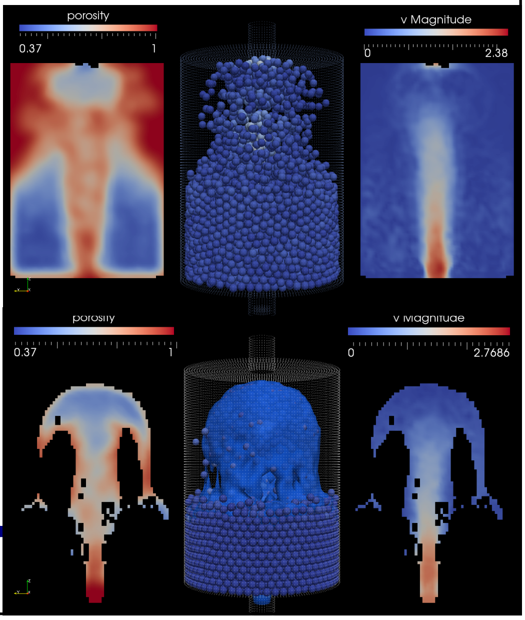


Simulation of powder dispersion by a liquid jet

- 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).

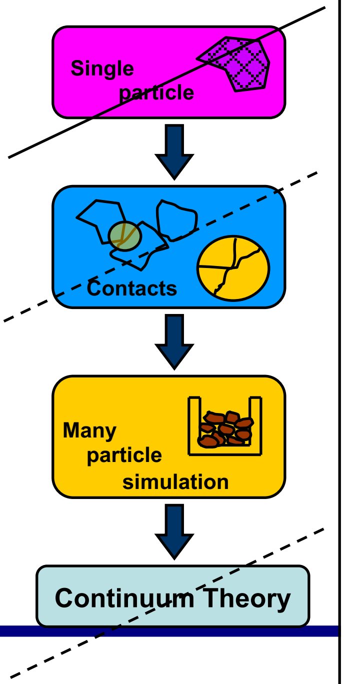
TODO:
Gas-phase not modelled yet;
Surface tension not modeled yet;
Polydisperse particles ..

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



Overview

- Introduction
- Contact models
- Many particle simulation
- Local micro-macro
- Continuum Theory
- … Anisotropy


Single particle

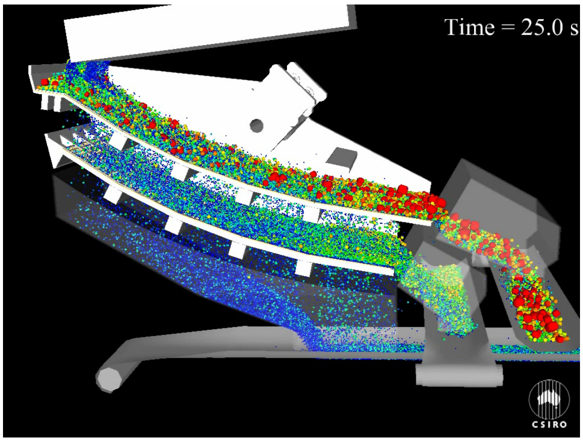
Contacts

Many particle simulation

Continuum Theory

Two deck banana screen (6g)

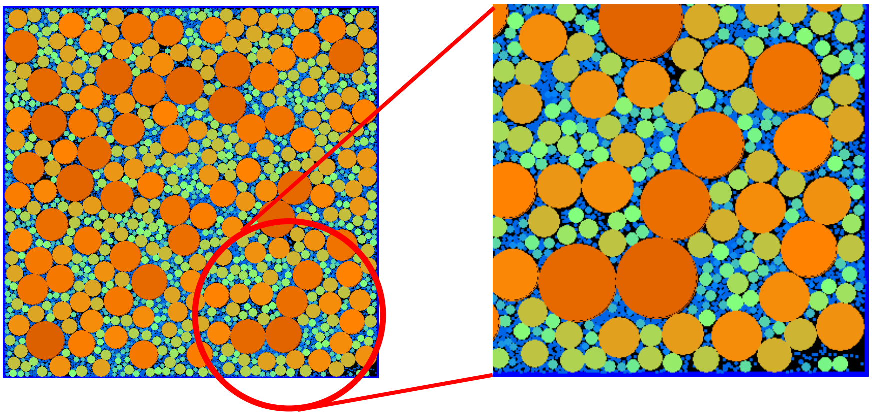
Colour By size



- Top deck bed is dense and coherent (not dilated with little saltation)
  - Clear reduction in finer (blue) material along the top deck

Examples are provided on courtesy of Paul Cleary, CSIRO, Australia.

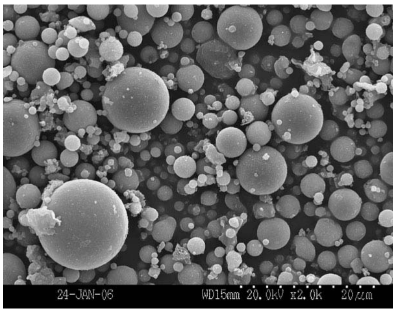
Challenge: DEM with realistic sizes



… highly polydisperse powders

Challenge:

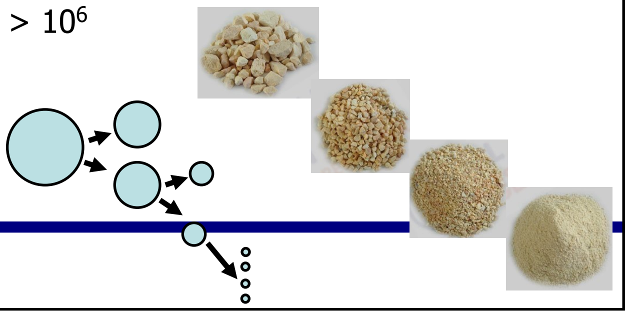
Fast contact detection between particles with strongly different sizes



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

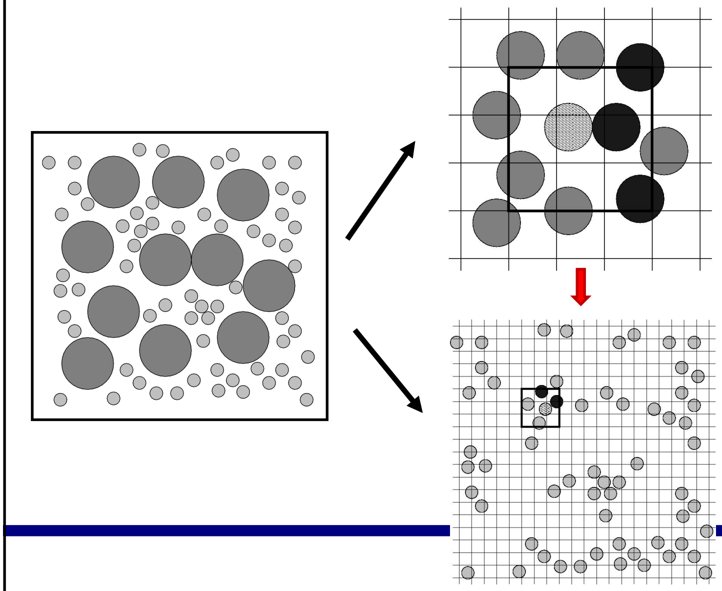
Size ratio >> 10
Number of particles > 10^6

- **Breakage / Grinding**
- **Granulation**



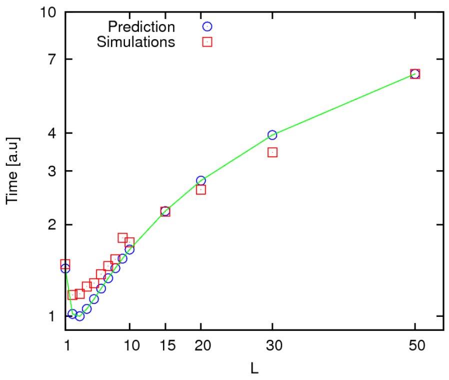
Hierarchical grid: fast, robust & flexible

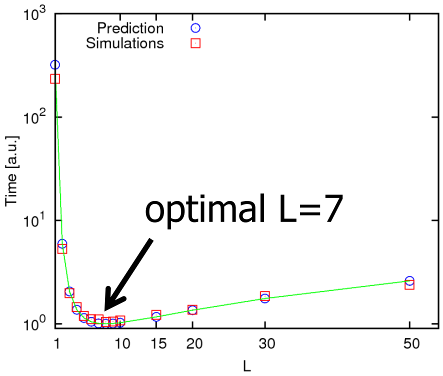
example: L=2 level grid

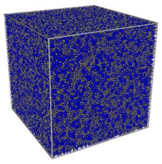


Analytical prediction vs Simulations

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

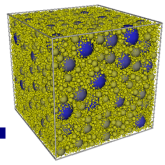






$\boxed{L^* \cong 2}$

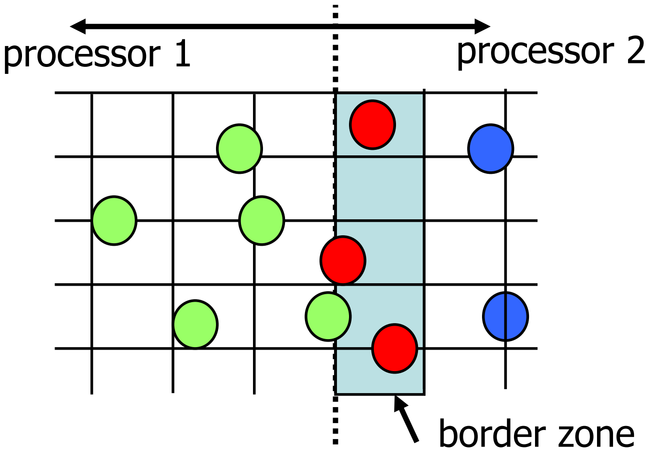
uniform size



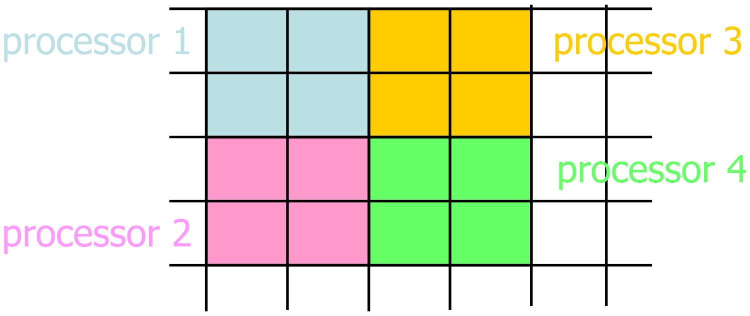
$\boxed{L^* > 2}$

uniform volume

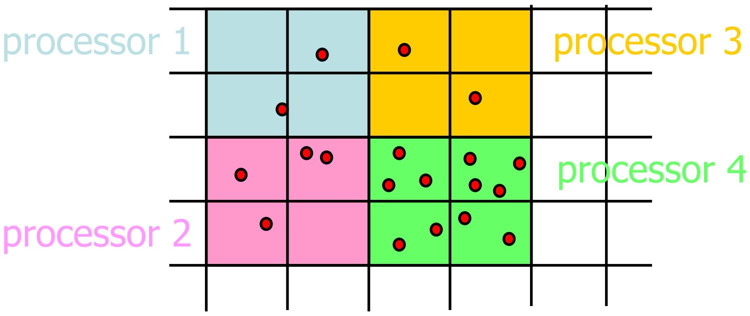
Parallelization – communication



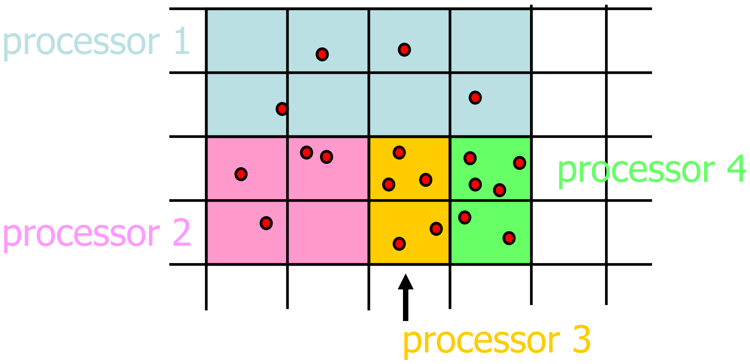
Parallelization – load balancing



Parallelization – load balancing

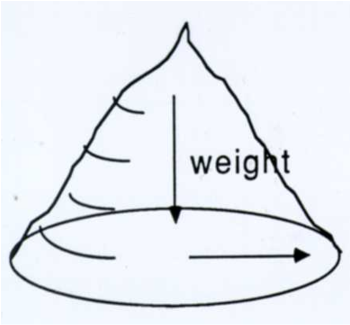


Parallelization – load balancing

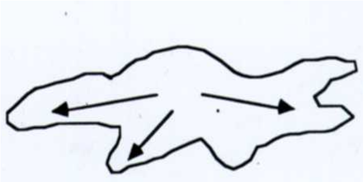


Powder and Liquid Flow (differences)

Inherent Yield Stress



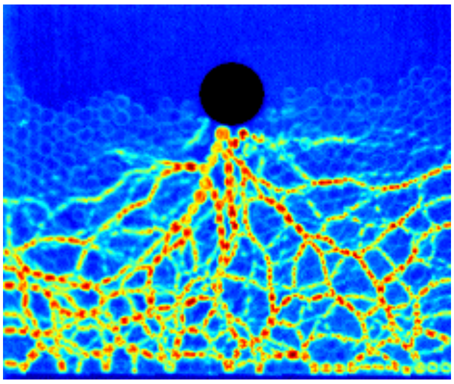
Powders heap

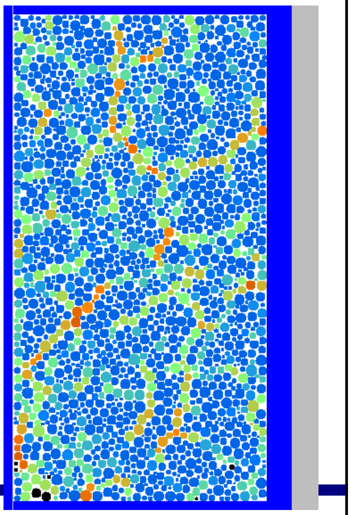


Liquid spreads

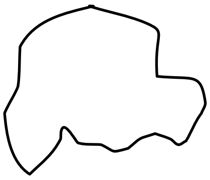
Yield stress = resistance against flow

Dense particle systems: experiments - simulations

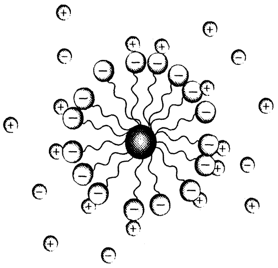




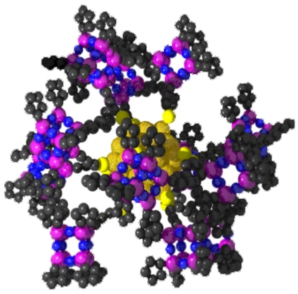
Particle Interactions



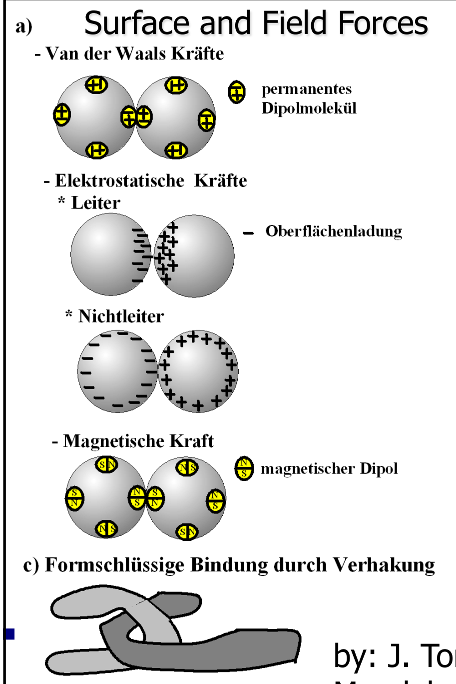
Mechanical
(d_p>10µm)



Chemical
(10nm<d_p<10µm)



Atomic Cluster
(d_p<10nm)



a) Surface and Field Forces

- Van der Waals Kräfte

permanentes Dipolmolekül

- Elektrostatische Kräfte
  - * Leiter

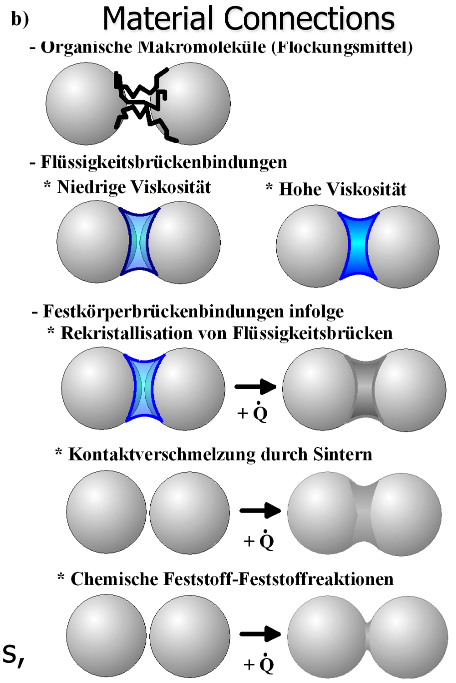
Oberflächenladung

  - * Nichtleiter

- Magnetische Kraft

magnetischer Dipol

c) Formschlüssige Bindung durch Verhakung



b) Material Connections

- Organische Makromoleküle (Flockungsmittel)
- Flüssigkeitsbrückenbindungen
  - * Niedrige Viskosität
  - * Hohe Viskosität
- Festkörperbrückenbindungen infolge
  - * Rekristallisation von Flüssigkeitsbrücken
  - * Kontaktverschmelzung durch Sintern
  - * Chemische Feststoff-Feststoffreaktionen

by: J. Tomas,
Magdeburg

How to model Contacts?

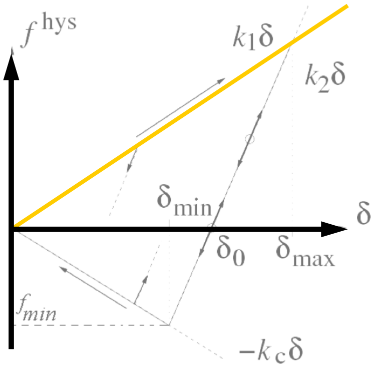
Atomistic/Molecular …

Continuum theory + Contact Mechanics

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

Contact Modeling

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



Linear Contact model

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

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

Linear Contact model

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

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

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

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

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

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

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

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

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

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

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

Time-scales

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

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

$t_n < t_c$

↑

time between contacts

↓

$t_n > t_c$

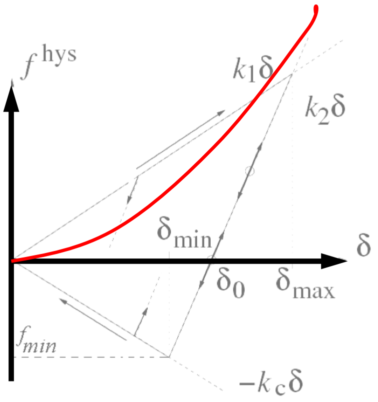
different sized particles

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

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

experiment T

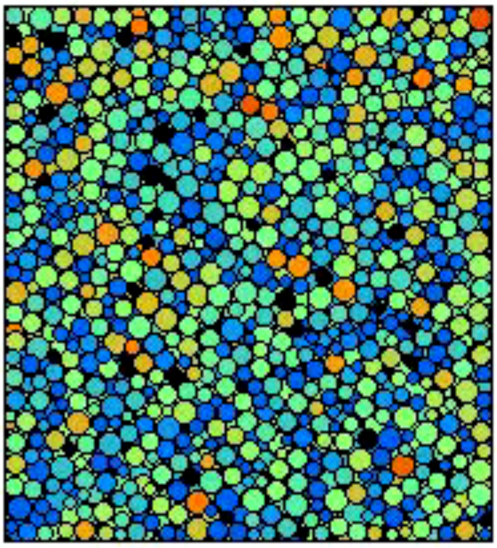
http://www2.msm.ctw.utwente.nl/sluding/PAPERS/coll2p.pdf



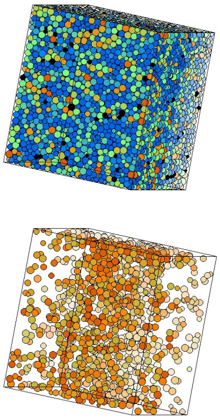
Hertz Contact model

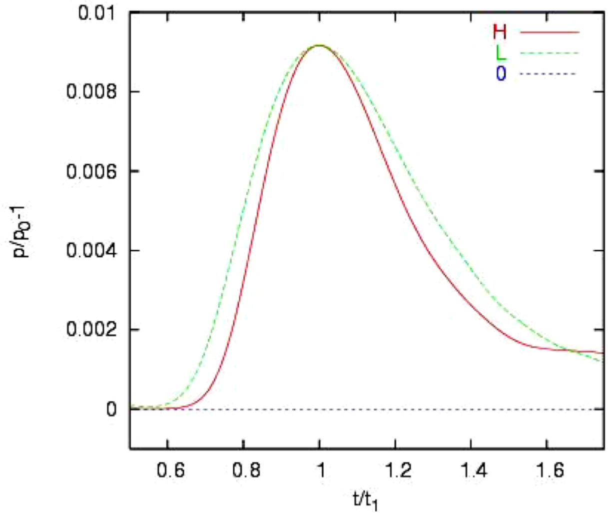
- **simple ☺**
- **non-linear**
- **easy to implement**

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



Sound





P-wave shape and speed

The picture can't be displayed.