Particle Technology: Modeling …

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

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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

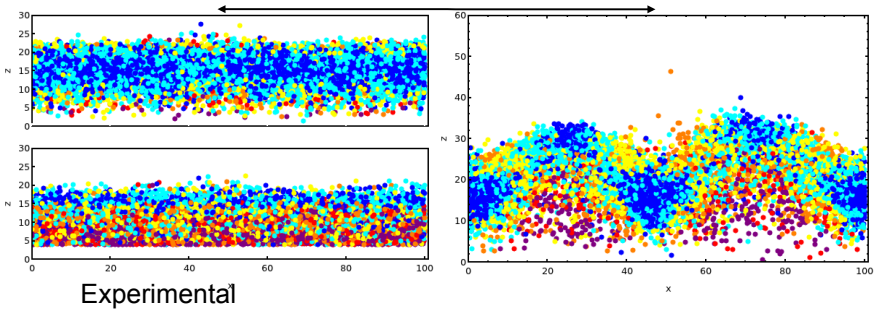
Example 1: Agitation/Vibration

N. Rivas,
MSM, 2011

VIBRATED SHALLOW BOX

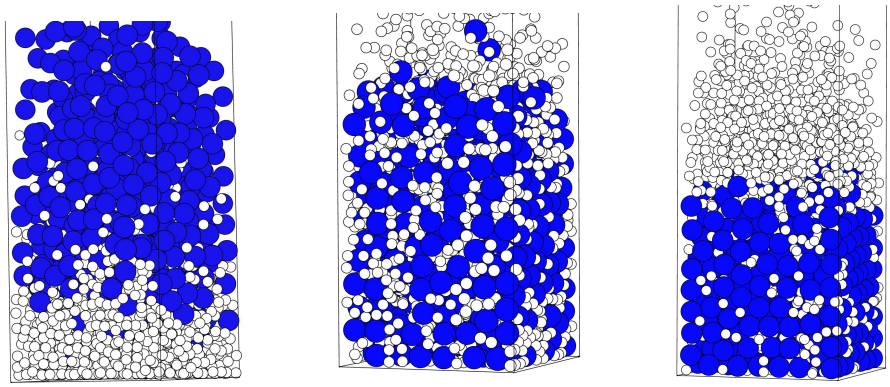
"From colliding particles to a hydrodynamic description of granular matter" N. Rivas

Transition



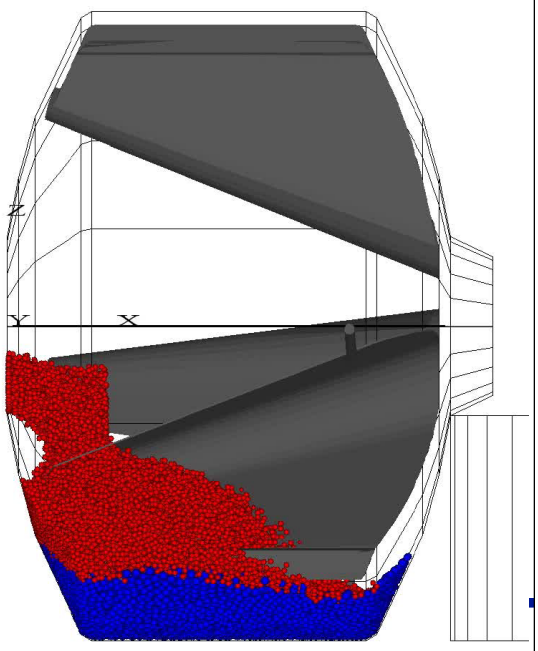
Experimental
Analytical
Simulations: - Molecular Dynamics (ED, DEM)
- Granular Hydrodynamics Solver

Example: Segregation/Mixing



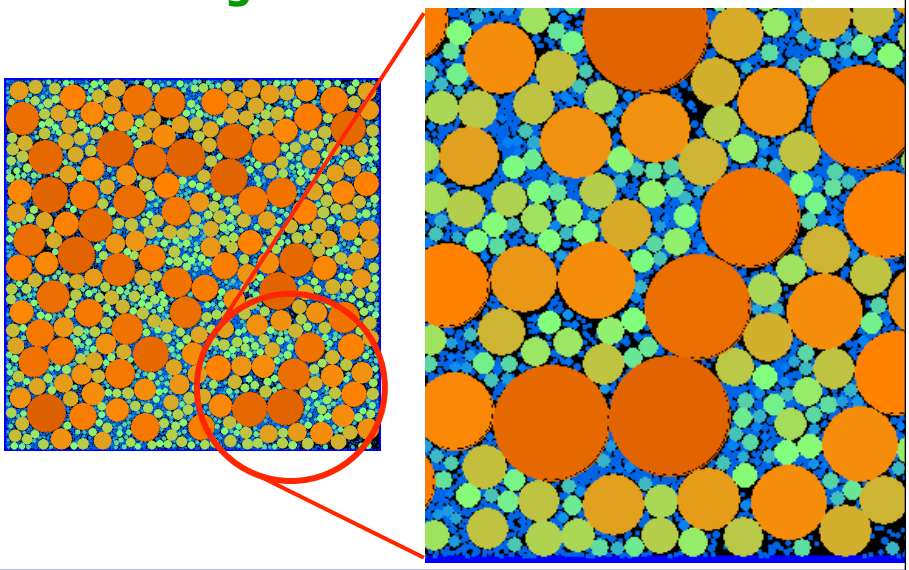
P. V. Quinn, D. Hong, SL, PRL 2001

Example: Mixing



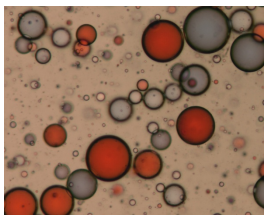
A. Gupta et al., MSM, 2010

Challenge: DEM with realistic sizes



… highly polydisperse powders

Our Approach: MATERIALs

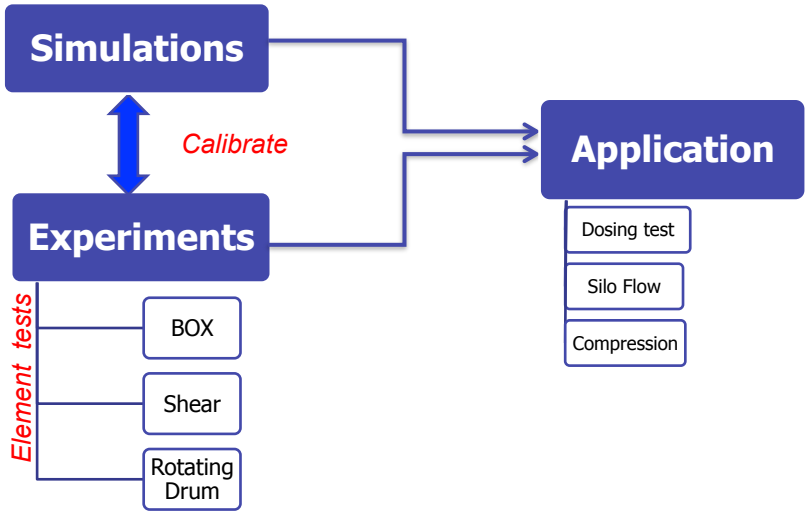


FRICTIONLESS → **FRICTIONAL** → **COHESIVE**

F. Goncu, CRAS, 2010
V. Magnanimo (2011-13)
S. Luding et al. (2001-13)
O. I. Imole et al KONA, 2013
O. I. Imole et al (to be submitted and in preparation, 2014)
N. Kumar et al Particuology (2013)
N. Kumar et al. Acta Mechanica (2014)

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

PARDEM Overview/Philosophy



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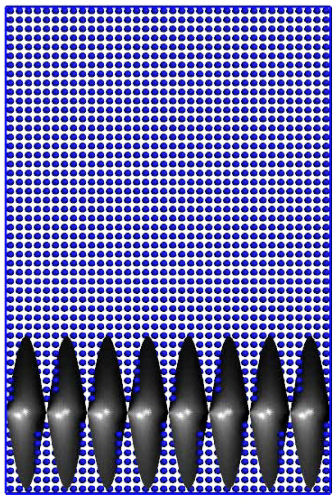
MERCURYDPM

Open source

Based on:
- HGrid
- MicroMacro



Dosing application example …

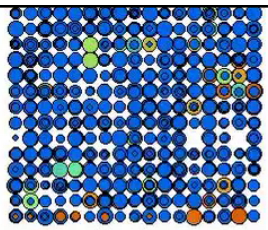
MERCURYDPM

Open source

Based on:
- HGrid
- MicroMacro

flowable powder

(screw hidden)



© Marco Ramaioli, Nestle

Dosing application example …

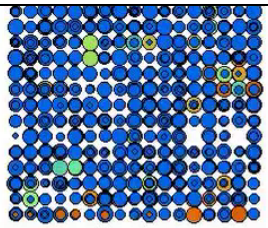
MERCURYDPM

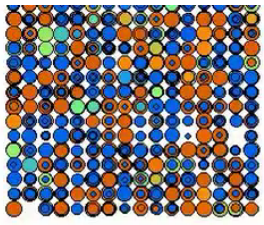
Open source

Based on:
- HGrid
- MicroMacro

flowable powder vs.
sticky, chunky powder

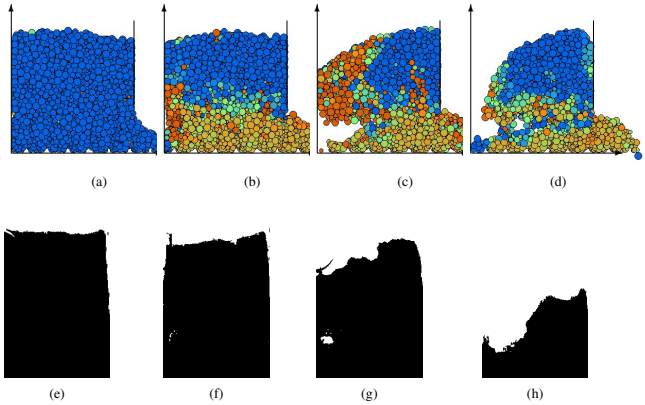
(screw hidden)





Dosing application example …

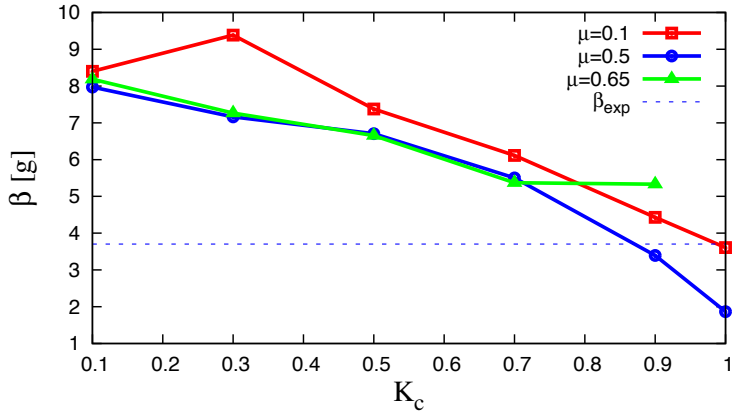
Dosing: DEM vs. experiment



*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



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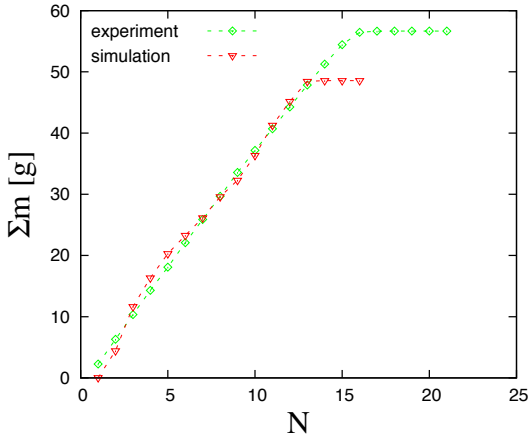
Dosing: DEM vs. experiment



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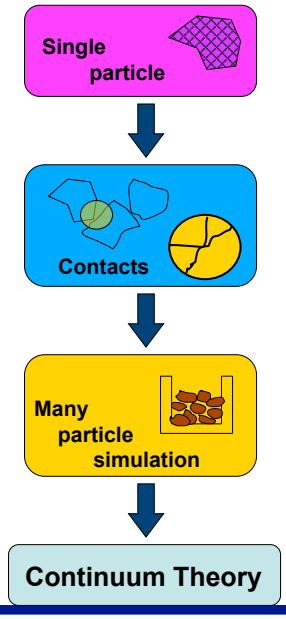
Experiments and Discrete Element Simulation of the Dosing of Cohesive Powders in a Canister Geometry. In preparation, PhD-thesis, O. I. Imole 2014

Overview Particles&Continuum

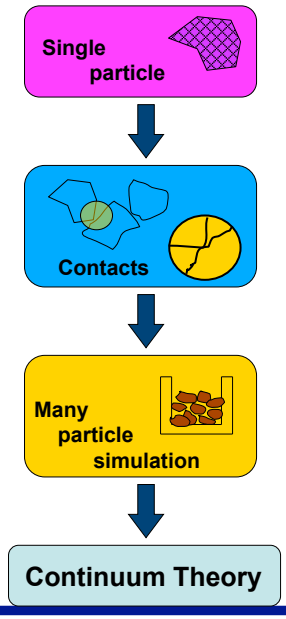
- Introduction
- Contact models
- Many particle simulation
- Local micro-macro
- Continuum Theory



Goal:

Large Scale systems
Applications

Continuum Theory



Continuum theory

mass conservation:

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

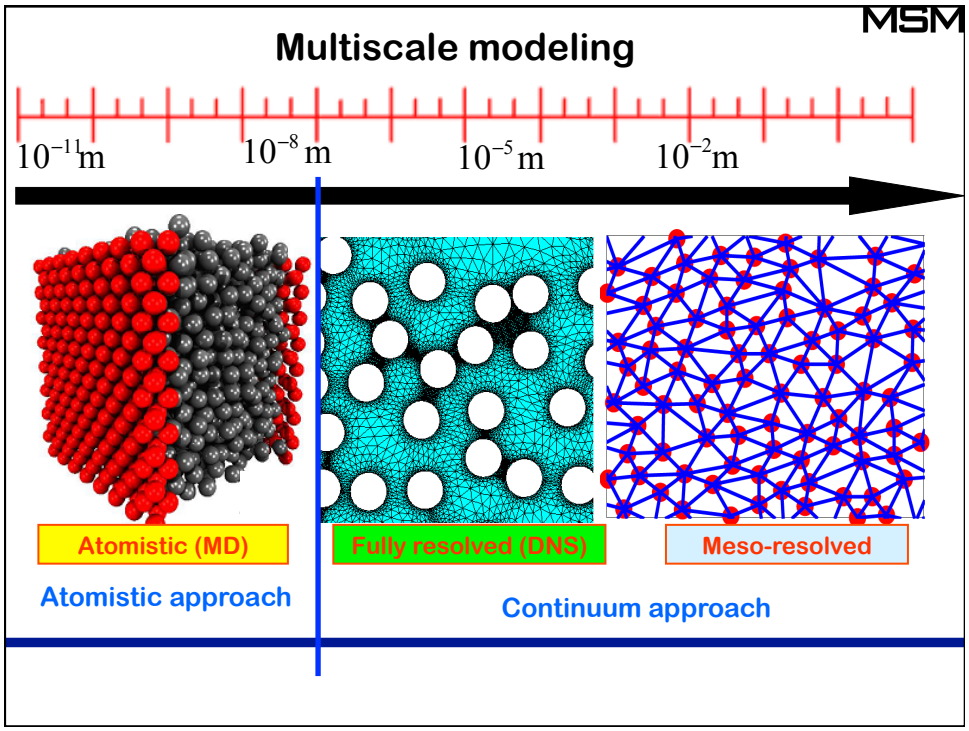
momentum conservation:

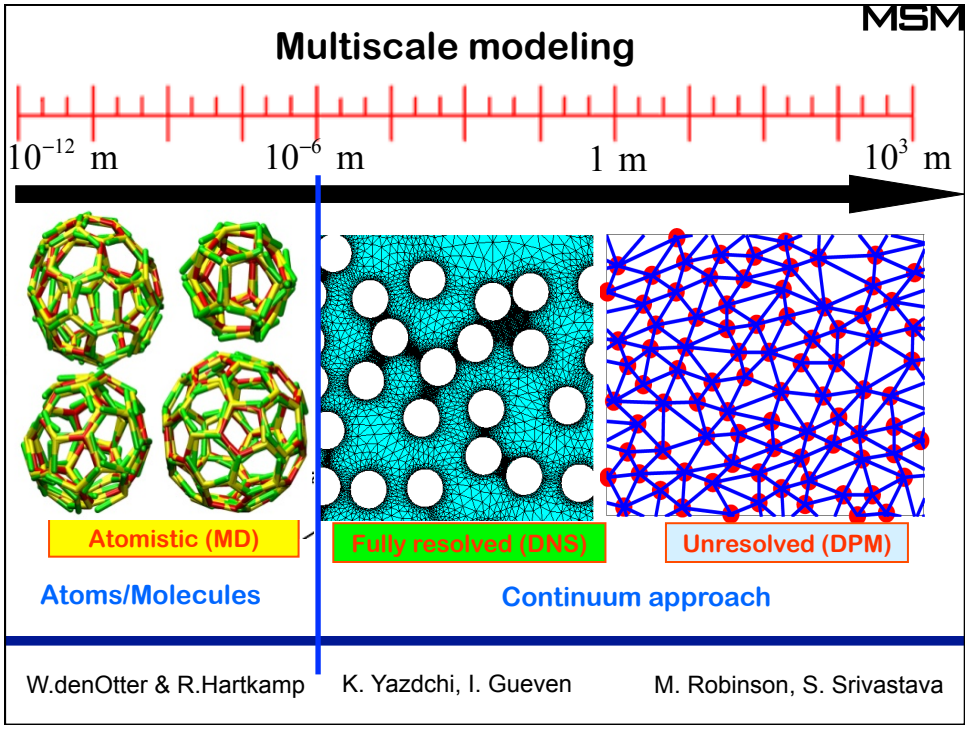
$$\frac{\partial}{\partial t}(\rho u_i)+\frac{\partial}{\partial x_k}(\rho u_i u_k)=-\frac{\partial}{\partial x_i}P+\frac{\partial}{\partial x_j}\sigma_{ij}^{\mathrm{dev}}+\rho g_i$$

energy balance:

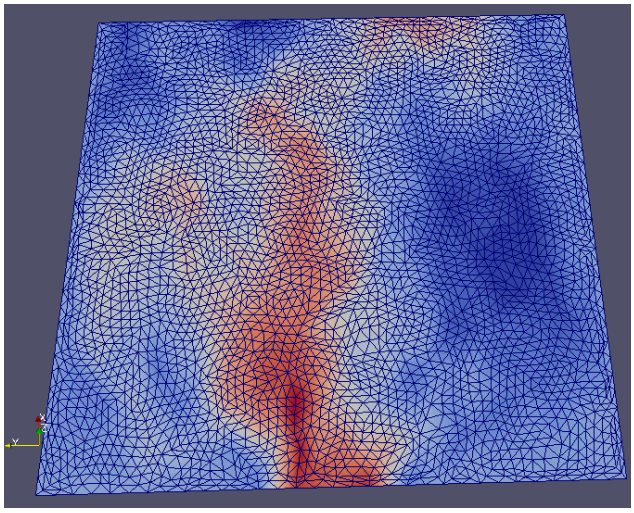
$$\frac{\partial}{\partial t}\left(\tfrac{1}{2}\rho u^2+\tfrac{1}{2}\rho v^2\right)=-\frac{\partial}{\partial x_k}\left[\rho u_k\left(\frac{P}{\rho}+\tfrac{1}{2}u^2+\tfrac{1}{2}v^2\right)-u_i\sigma_{ik}^{\mathrm{dev}}-K\frac{\partial}{\partial x_k}\left(\tfrac{1}{2}\rho v^2\right)\right]+\rho u_i g_i-I$$

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


MSM
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


MSM
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

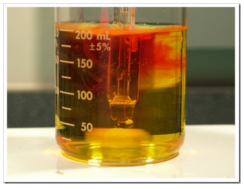
Example: Fluidization DEM-FEM



Fluidization on moving mesh with 800 particles (with gravity)

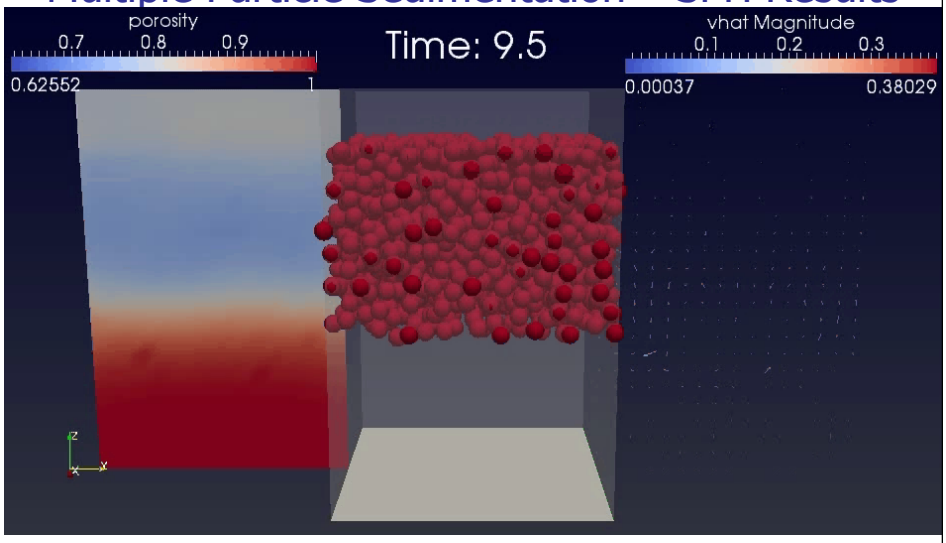
Set of Realistic Fluid-Particle Parameters

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

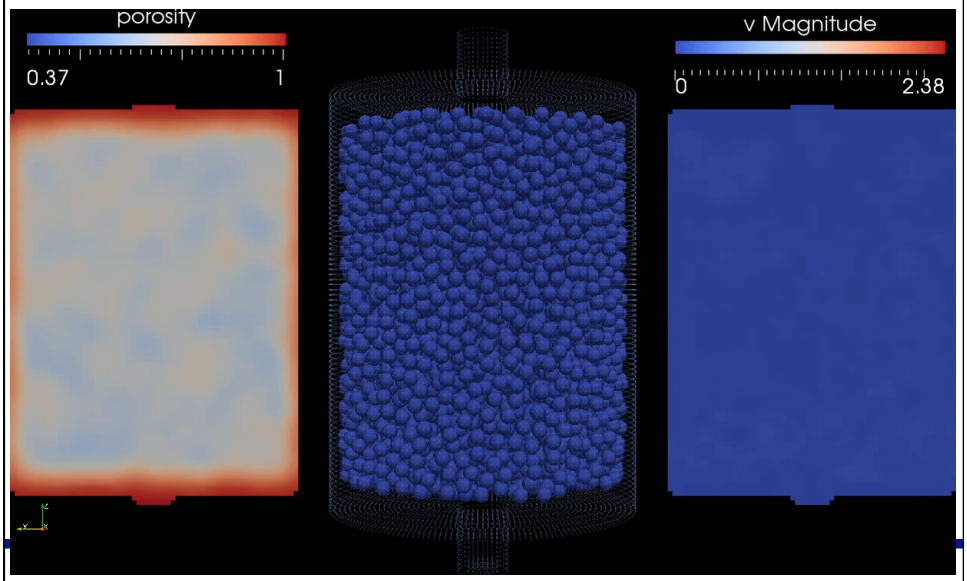


Property	Air	Water	Glycerol-water
Density	1.18 kg/m^3	1000 kg/m^3	1150 kg/m^3
Viscosity	1.86x10^{-5} Pa·s	8.9x10^{-4} Pa·s	8.9x10^{-3} Pa·s
Re_p	0.65 – 3.19	0.15 – 0.85	0.002 – 0.011

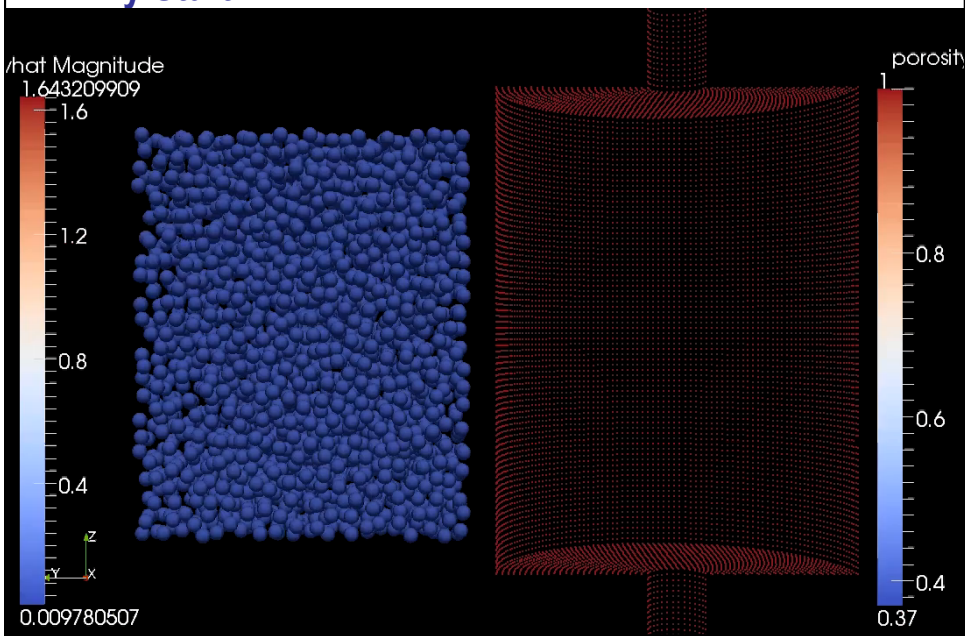
Multiple Particle Sedimentation – SPH Results



Wet Start



Dry Start

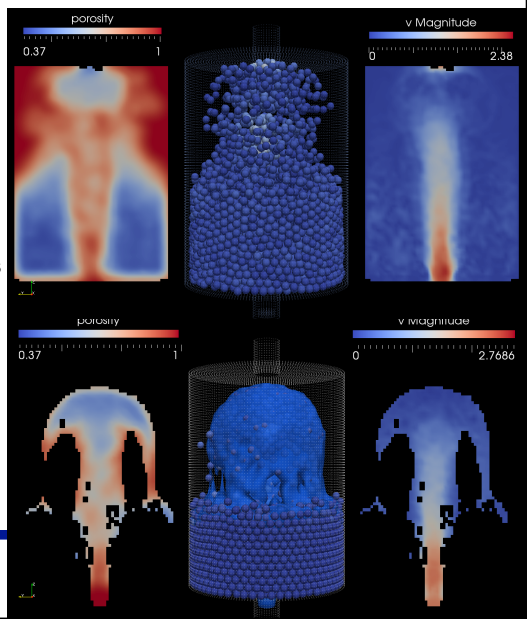


Simulation of powder dispersion by a liquid jet

- 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

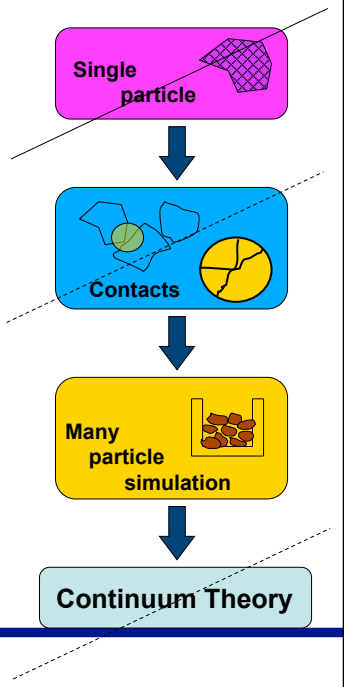
Contact models

Many particle simulation

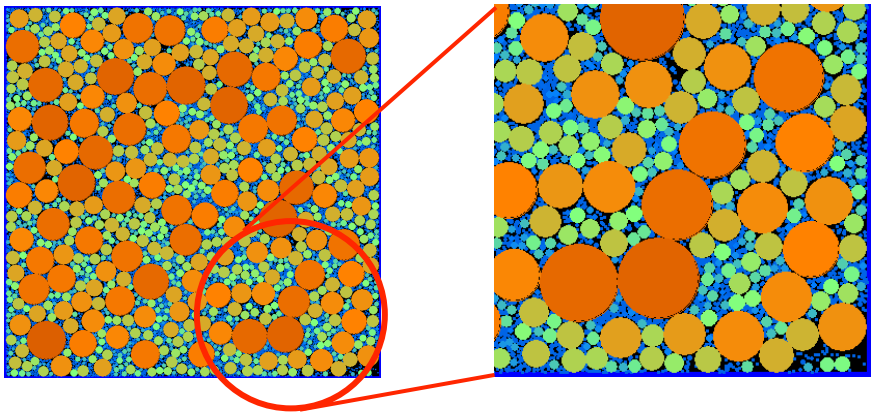
Local micro-macro

Continuum Theory

... Anisotropy



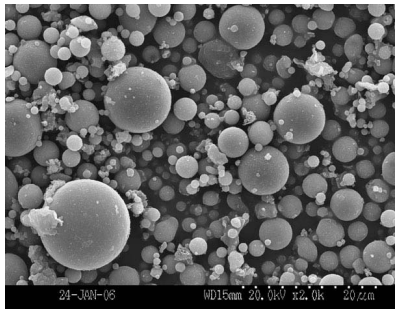
Challenge: DEM with realistic sizes



... highly polydisperse powders

Challenge:

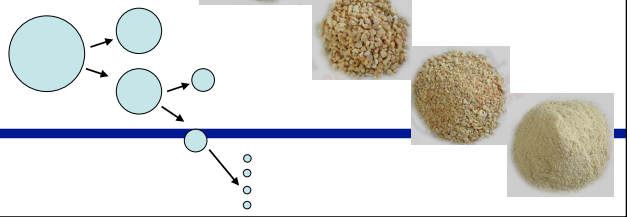
Fast contact detection between particles with strongly different sizes



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

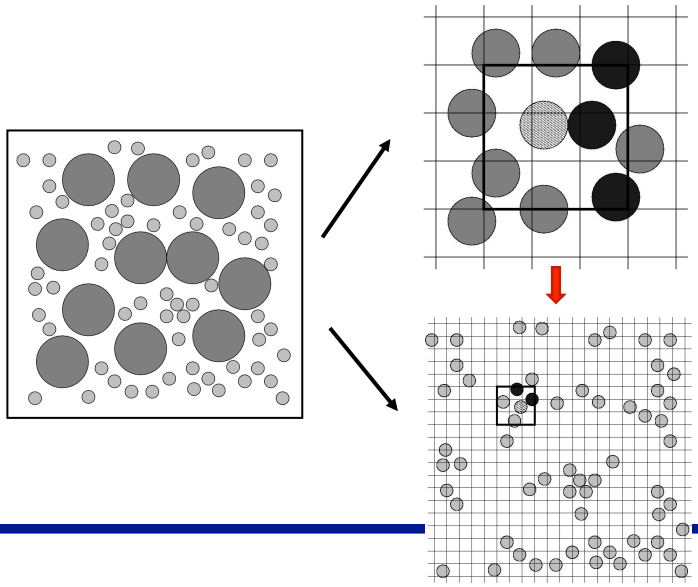
Size ratio >> 10
Number of particles > 10^6

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



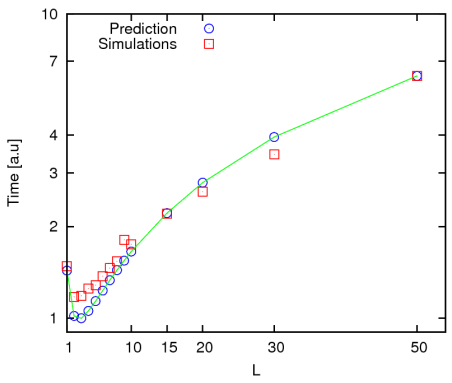
Hierarchical grid: fast, robust & flexible

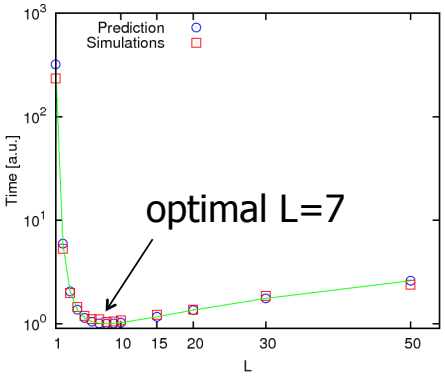
example: L=2 level grid



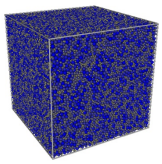
Analytical prediction vs Simulations

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



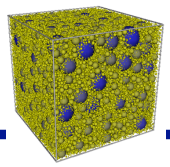


$L^* \cong 2$



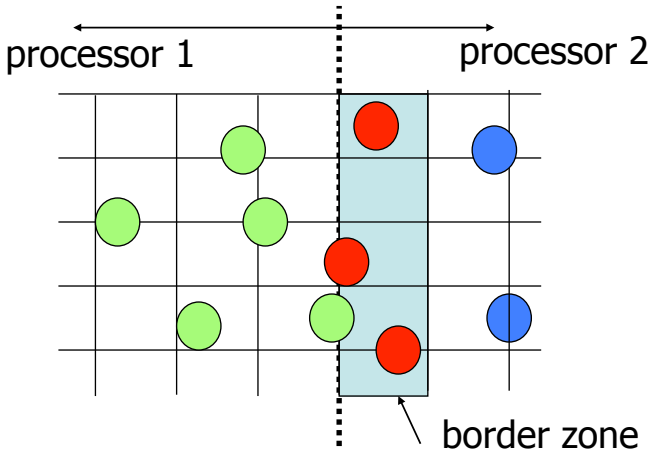
uniform size

$L^* > 2$

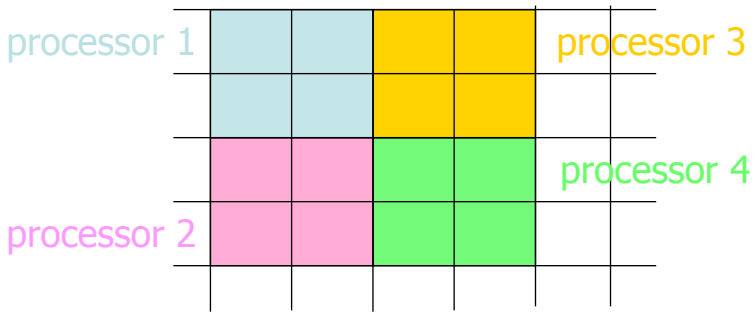


uniform volume

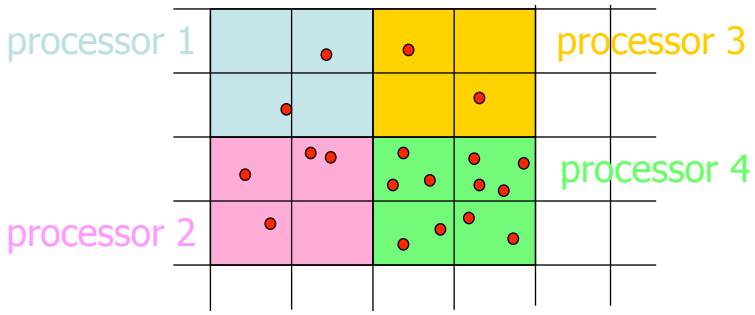
Parallelization – communication



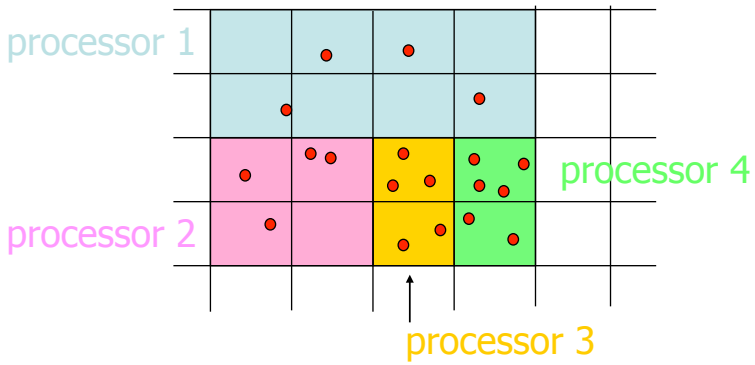
Parallelization – load balancing



Parallelization – load balancing

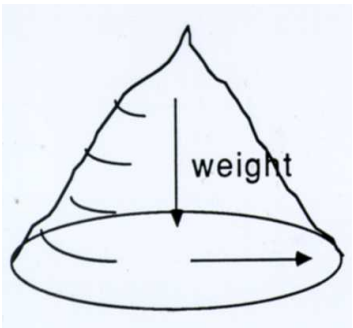


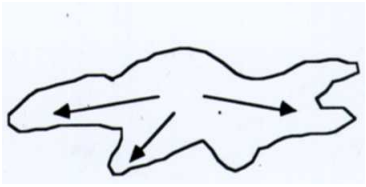
Parallelization – load balancing



Powder and Liquid Flow (differences)

Inherent Yield Stress

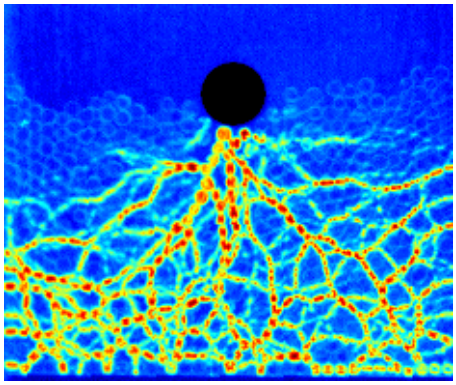


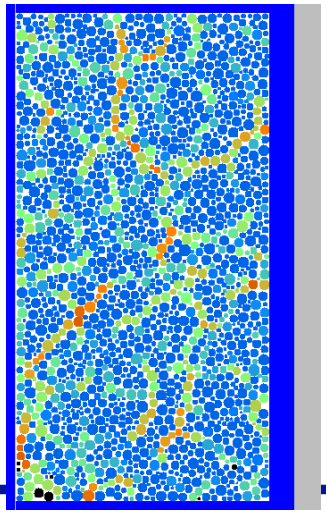


Powders heap **Liquid spreads**

Yield stress = resistance against flow

Dense particle systems: experiments - simulations





How to model Contacts?

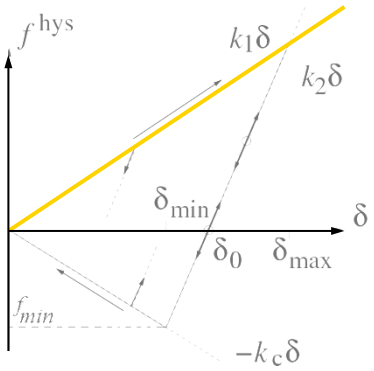
Atomistic/Molecular …

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

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

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

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

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

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

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

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

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

Linear Contact model

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

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

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

contact duration $t_c = \pi/\omega$

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

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

Time-scales

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

contact duration $t_c = \pi/\omega$

$t_n < t_c$ different sized particles $t_c^{large} > t_c^{small}$

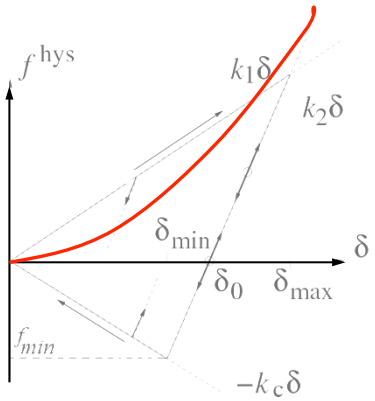
time between contacts

$t_n > t_c$

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

experiment T

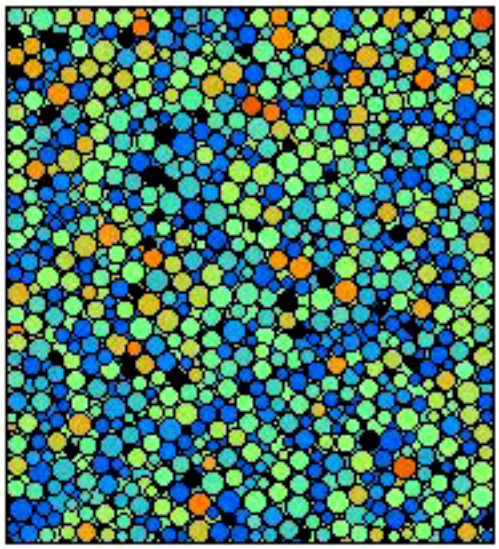
http://www2.msm.ctw.utwente.nl/sluding/PAPERS/coll2p.pdf



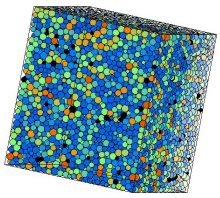
Hertz Contact model

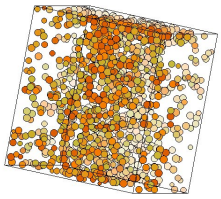
- simple ☺
- non-linear
- easy to implement

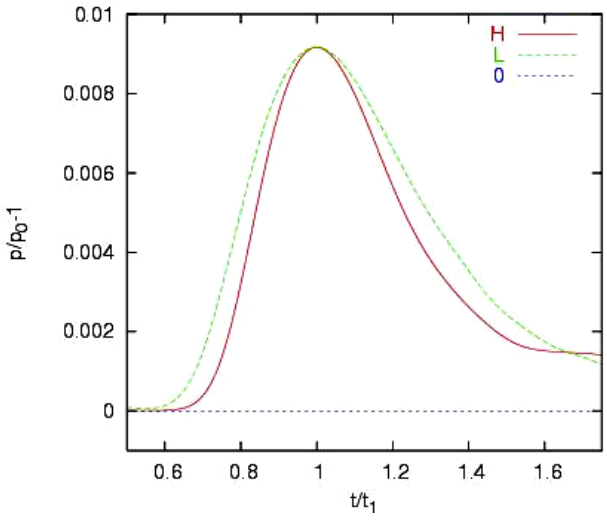
$$f_i^{hys} = \begin{cases} k_1\delta^{3/2} & \text{for un-/re-loading} \end{cases}$$



Sound







P-wave shape and speed

The image cannot be displayed. Your computer may not have