UNIVERSITY OF TWENTE.

From micro to macro in granular matter

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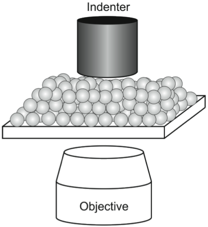
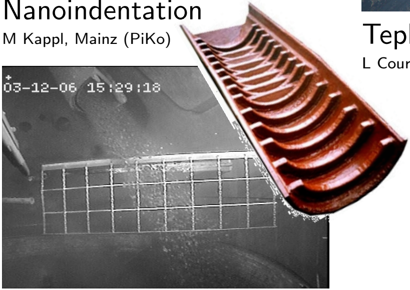
Grains in nature and industry

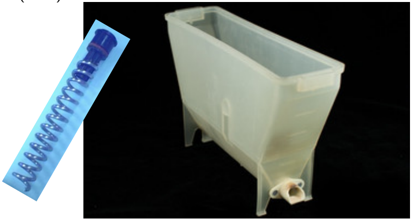


Nanoindentation
M Kappl, Mainz (PiKo)

Tephra expulsion
L Courtland (USF)



Rotating blast-furnace chute
D Tunuguntla, O Bokhove (Chorus)



Vending machine canister
K Imole (PARDEM)

Outline

1. The Discrete Particle Method (DPM)
2. The coarse graining method
3. Micro-Macro transition for free surface flows
4. Conclusions and future work

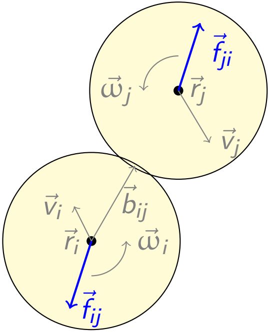
The Discrete Particle Method (DPM)

- Particles have position $\vec{r}_i$, velocity $\vec{v}_i$, angular velocity $\vec{\omega}_i$, diameter d_i, mass m_i
- Governed by Newtonian mechanics:

$$m_i \frac{d^2\vec{r}_i}{dt^2} = \vec{f}_i, \quad I_i \frac{d\vec{\omega}_i}{dt} = \vec{t}_i$$

- Contact forces and body forces:

$$\vec{f}_i = \sum_j \vec{f}_{ij} + m_i \vec{g}_i, \quad \vec{t}_i = \sum_j \vec{b}_{ij} \times \vec{f}_{ij}$$



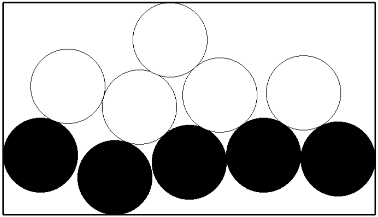
Coarse graining (CG)

Objective

Define macroscopic fields such as mass density ρ, velocity $\vec{V}$, stress $\boldsymbol{\sigma}$, ... based on particle data ($\vec{r}_i$, $\vec{v}_i$, m_i, $\vec{f}_i$, ...).

The fields should satisfy mass and momentum balance exactly.

Example: A static system of 5 fixed and 5 free particles.



Coarse graining: density ρ and mass balance

A) We define the macro-density using a coarse-graining function ϕ,

$$\rho(\vec{r}) = \sum_{i=1}^{n} m_i \phi(\vec{r} - \vec{r}_i).$$

Coarse graining: density ρ and mass balance

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$$\rho(\vec{r}) = \sum\nolimits_{i=1}^{n} m_i \phi(\vec{r} - \vec{r}_i).$$

B) We define the velocity s.t. mass balance,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{V}) = 0,$$

is satisfied:

$$\vec{V} = \frac{\vec{p}}{\rho}, \text{ where } \vec{p} = \sum_{i=1}^{n} m_i \vec{v}_i \phi(\vec{r} - \vec{r}_i).$$

Coarse graining: momentum balance

C) We define the stress s.t. momentum balance,

$$\rho \frac{D\vec{V}}{Dt} = -\nabla \cdot \boldsymbol{\sigma} + \vec{t} + \rho \vec{g},$$

is satisfied:

$$\boldsymbol{\sigma}^k = -\sum_{i=1}^{n} m_i \vec{v}_i' \vec{v}_i' \phi(\vec{r} - \vec{r}_i),$$

$$\boldsymbol{\sigma}^c = -\sum_{\text{contacts } \{i,j\}} \vec{f}_{ij} \vec{r}_{ij} \int_0^1 \phi(\vec{r} - (\vec{r}_i + s\vec{r}_{ij}))\, ds$$

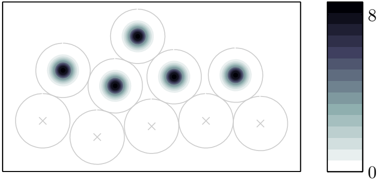
$$- \sum_{\text{wall contacts } \{i,k\}} \vec{f}_{ik} \vec{b}_{ik} \int_0^1 \phi(\vec{r} - (\vec{r}_i + s\vec{b}_{ik}))\, ds,$$

$$\vec{t} = -\sum_{\text{wall contacts } \{i,k\}} \vec{f}_{ik} \phi(\vec{r} - \vec{c}_{ik}),$$

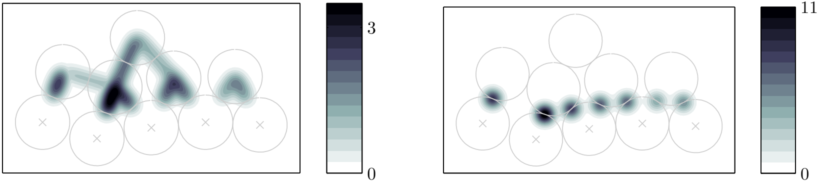
with boundary interaction force density $\vec{t}$.

Weinhart, Thornton, Luding, Bokhove, GranMat (2012) 14:289

A static system of 5 fixed and 5 free particles.



Density ρ *for 2D-Gaussian CG function of width* $w = d/8$.

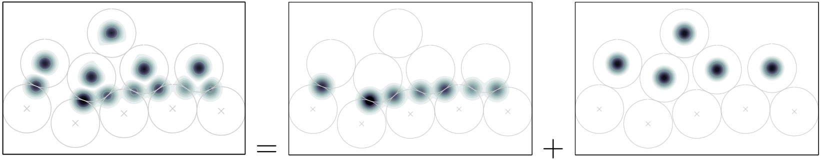


Magnitude of stress $|\boldsymbol{\sigma}|_2$ *and boundary interaction force* $|\vec{t}|_2$.

Satisfying mass and momentum balance.

- Mass balance in a static system is trivial.
- Satisfying the momentum balance in a static system requires

$$\nabla \cdot \boldsymbol{\sigma} = \vec{t} + \rho \vec{g}.$$



Magnitudes of stress divergence $|\nabla \cdot \boldsymbol{\sigma}|_2$ *(left), boundary interaction force density* $|\vec{t}|_2$ *(centre), and weight density* $|\rho \vec{g}|$ *(right).*

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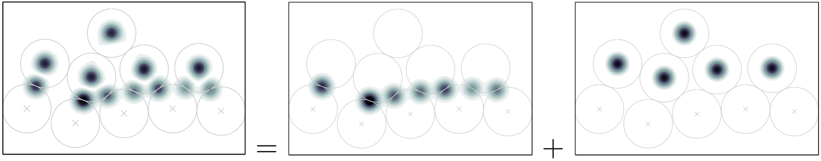

Magnitudes of stress divergence $|\nabla \cdot \boldsymbol{\sigma}|_2$ (left), boundary interaction force density $|\vec{t}|_2$ (centre), and weight density $|\rho \vec{g}|$ (right).

Important result

Mass/mom. bal. is satisfied locally for any coarse-graining function.

MercuryCG statistical toolbox

- open source: `www2.msm.ctw.utwente.nl/athornton/MD/`
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- many CG-functions: Gaussian, Heaviside, Polynomials (Lucy)
- many fields: temperature, displacement, fabric tensor, mixture drag, rotational dof, ...

** Grey items will be available in the next release*

Free-surface flows: A) flow through contraction

Glass particles flowing through a contraction

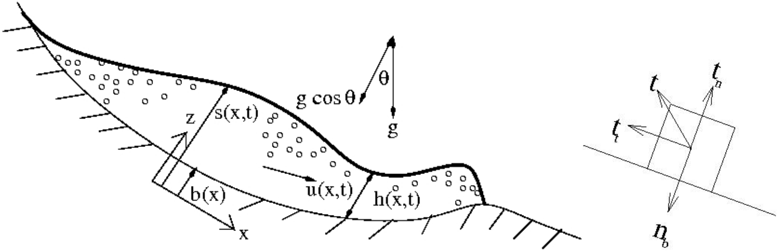
from: Vreman *et al.*, *J. Fluid Mech.* **578** (2007) 233-269

Free-surface flows: B) impingement on inclined plane

Sand particles impacting an inclined plane

from: Johnson, Gray, JFM **675** (2011) 87

The granular shallow-layer equations



Depth- and width-averaged mass/mom. balance for shallow flow:

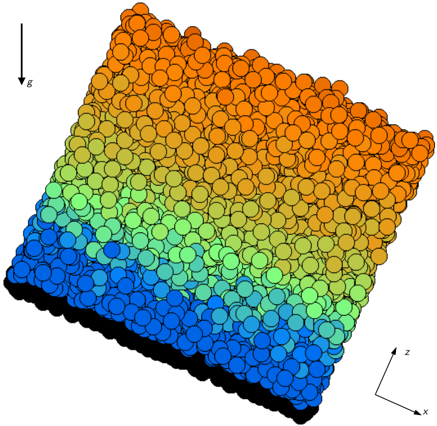
$$\frac{\partial h}{\partial t} + \frac{\partial h\bar{u}}{\partial x} = 0,$$

$$\frac{\partial}{\partial t}(h\bar{u}) + \frac{\partial}{\partial x}\left(h\alpha\bar{u}^2 + \frac{K}{2}gh^2\cos\theta\right) = gh(\sin\theta - \mu\frac{\bar{u}}{|\bar{u}|}\cos\theta),$$

Closure relations are required for velocity shape factor $\alpha = \frac{\overline{u^2}}{\bar{u}^2}$, normal stress ratio $K = \frac{\bar{\sigma}_{xx}}{\bar{\sigma}_{zz}}$, and bed friction $\mu = \frac{|t_t|}{|t_n|}$ at $z = b$.

Objective

Find closure relations $\mu(h, \bar{u})$, $\alpha(h, \bar{u})$ and $K(h, \bar{u})$
using small DPM simulations of steady uniform flow.



DPM of steady uniform chute flow over fixed-particle base, periodic in x- and y-direction, varying inclination θ and particle number N.

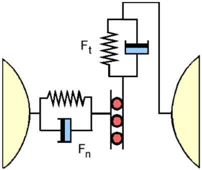
Parameters of the DPM

- Scaled s.t. diameter $d = 1$, mass $m = 1$, gravity $g = 1$.
- Linear elastic, dissipative and frictional contact forces:

$$\vec{f}_{ij} = f_{ij}^{n}\vec{n} + f_{ij}^{t}\vec{t},$$

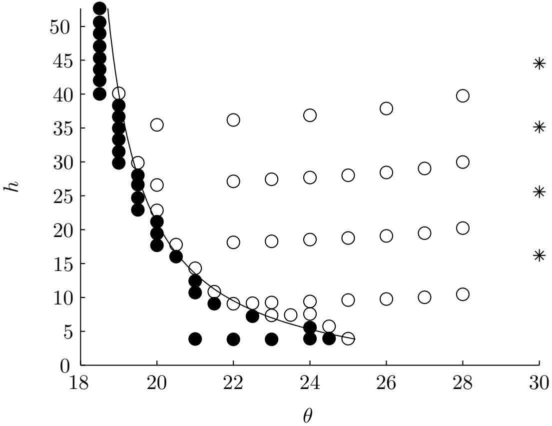
$$f_{ij}^{n} = -k_n\delta_{ij} - \gamma_n v_{ij}^{n},$$

$$f_{ij}^{t} = -min(|k_t\vec{\delta}_{ij}^{t} + \gamma_t\vec{v}_{ij}^{t}|, \mu_c f_{ij}^{n}),$$



- Collision time $t_c = 0.005\sqrt{d/g}$, restitution $r = 0.88$, friction $\mu_c = 0.5$.
- Integration (Velocity-Verlet) until $t = 2000\sqrt{d/g}$.

Three regimes: arresting $\bullet$, steady $\circ$, accellerating $*$



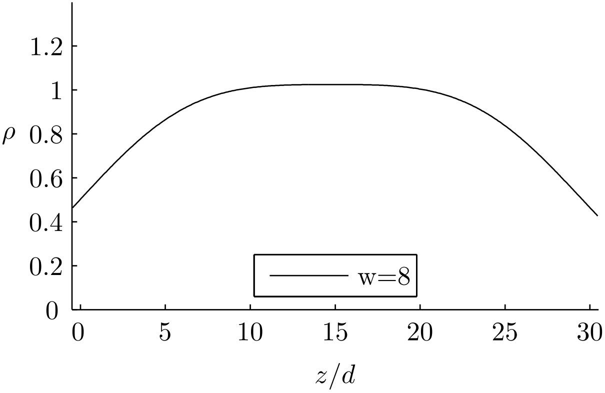
Demarkation line $h_{stop}(\theta)$ between arrested and steady flow,

fit to $h_{stop}(\theta) = {\color{blue}A}d\,\dfrac{\tan({\color{blue}\theta_2}) - \tan(\theta)}{\tan(\theta) - \tan({\color{blue}\theta_1})}$.

fit according to Pouliquen, Forterre, JFM, 2002

Choosing the right coarse-graining scale

For $h = 30$, $\theta = 28°$, we average over $x \in [0, 20]$, $y \in [0, 10]$, $t \in [2000, 2500]$ ($dt = t_c/2$) for several coarse graining widths w:



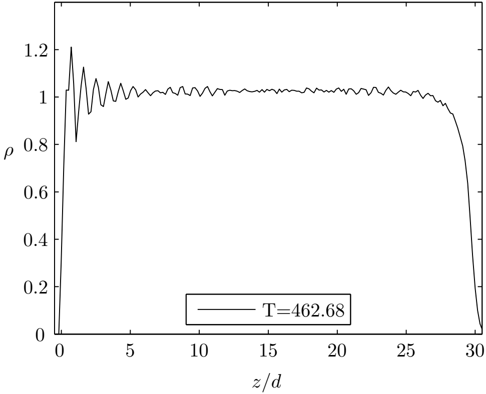
$\Rightarrow$ the larger w, the less fluctuations

$\Rightarrow$ the larger w, the more artificial smoothing.

Weinhart, Hartkamp, Thornton, Luding, Phys. Fl. (2012), submitted

Choosing the right time-interval

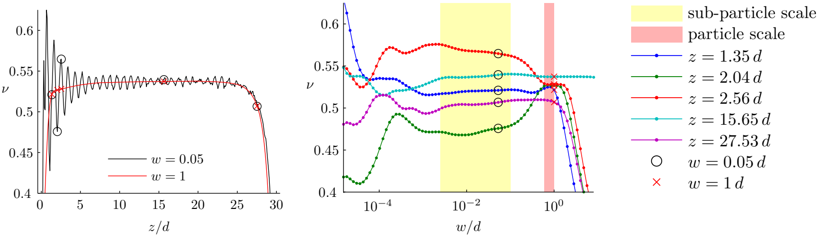
For $h = 30$, $\theta = 28^\circ$, we integrate over $t \in [2000, 2000 + T]$ ($dt = t_c/2$) for coarse graining widths $w = 0.1$:



$\Rightarrow$ the larger T, the less fluctuations

$\Rightarrow$ we choose $T = 500$.

Choosing the right coarse-graining scale



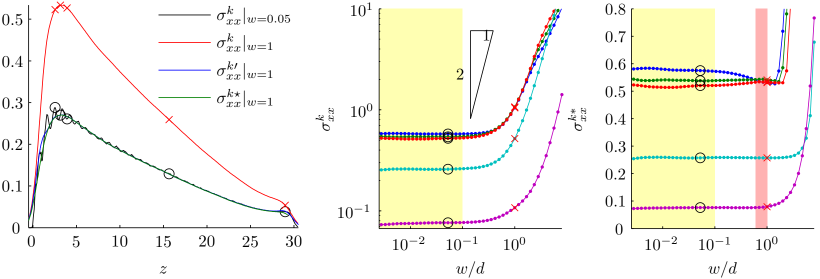
Volume fraction $\nu = \rho/\rho_p$ for varying w.

Two scale-independent ranges exist:

- sub-particle scale $0.005d < w < 0.1d$ (shows oscillations)
- particle scale $0.6d < w < d$ (only valid in bulk)

Here, we choose $w = 0.1d$.

Kinetic stress σ^k_{xx} and granular temp. T_g



- Kinetic stress is scale-dependent on the particle scale [1],

$$\sigma^k_{xx} = \sum_{i=1}^{N} m v'_{ix} v'_{ix} \mathcal{W}_i \text{ with } \vec{v}_i' = \vec{v}_i - \vec{V}(\vec{r}).$$

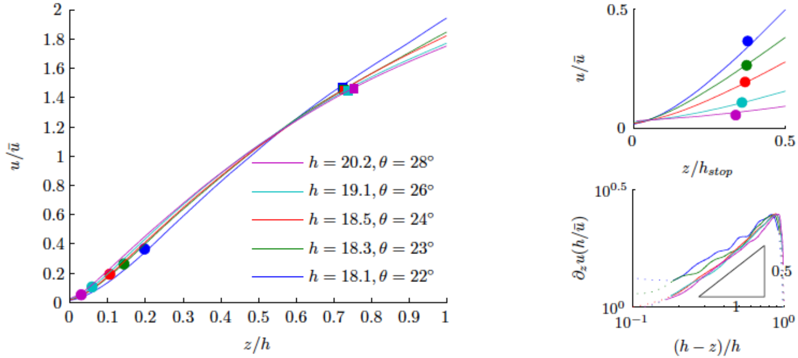
- The kinetic-theory definition is scale-independent,

$$\sigma^{k\star}_{xx} = \sum_{i=1}^{N} m v^\star_{ix} v^\star_{ix} \mathcal{W}_i \text{ with } \vec{v}_i^\star = \vec{v}_i - \vec{V}(\vec{r}_i).$$

- One can show $\sigma^k_{xx} - \rho\dot{\gamma}^2 \frac{w^2}{3} \approx \sigma^{k\star}_{xx}$.

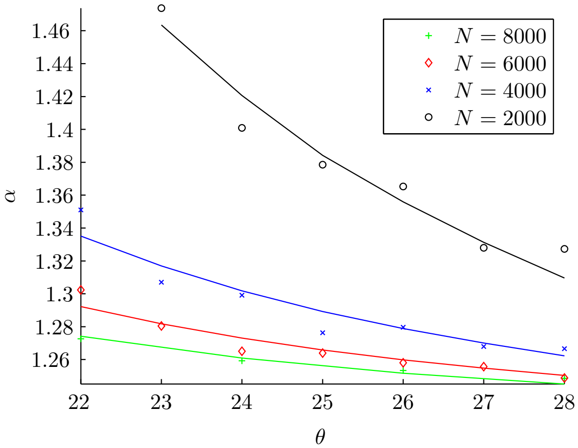
[1] Glasser, Goldhirsch, Phys Fl. 13, 407 (2001)

Closure for the velocity shape factor $\alpha = \frac{\overline{u^2}}{\bar{u}^2}$



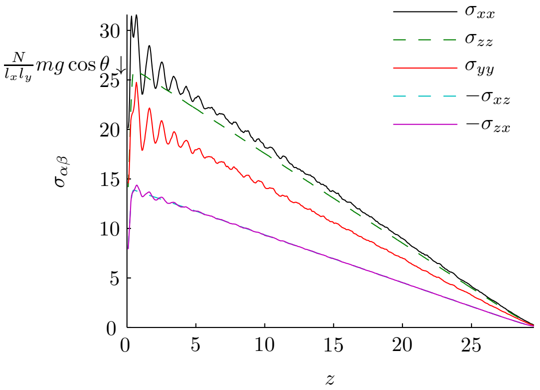
Bagnold velocity profile in bulk, quadratic near base
($z < b\, h_{stop}(\theta)/h$), linear near surface ($z > h - 5$).

Closure for the velocity shape factor $\alpha = \frac{\overline{u^2}}{\bar{u}^2}$



Shape factor $\alpha(h, \theta) = \alpha(h, \tan^{-1}(\mu))$
from simulations (markers) and fit (lines).

Closure for the normal stress ratio and bed friction



- Normal stress ratio $K = \frac{\bar{\sigma}_{xx}}{\bar{\sigma}_{zz}} \approx 1$.
- Friction $\mu = -\frac{\sigma_{xz}}{\sigma_{zz}} = \tan\theta$.

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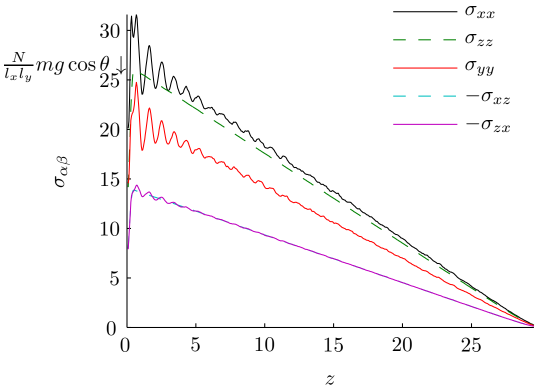
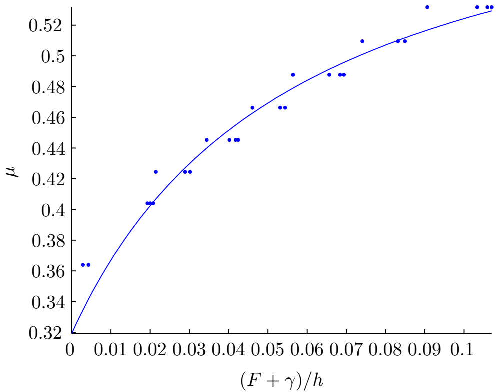


- Normal stress ratio $K = \frac{\bar{\sigma}_{xx}}{\bar{\sigma}_{zz}} \approx 1$.
- Friction $\mu = -\frac{\sigma_{xz}}{\sigma_{zz}} = \tan\theta$.
- But note: Stress is slightly asymmetric, oscillating at the boundary, and anisotropic.*

*see W, Hartkamp, Thornton, Luding, Phys. Fl. (2012) submitted

Closure for the bed friction $\mu = -\frac{\sigma_{xz}}{\sigma_{zz}}$



$$\mu(h,\bar{u}) = \tan(\theta_1) + (\tan(\theta_2) - \tan(\theta_1)) \left(1 + \frac{\beta}{Ad} \frac{h}{F+\gamma}\right)^{-1}.$$

The Micro-Macro transition

We closed the granular shallow-layer equations,

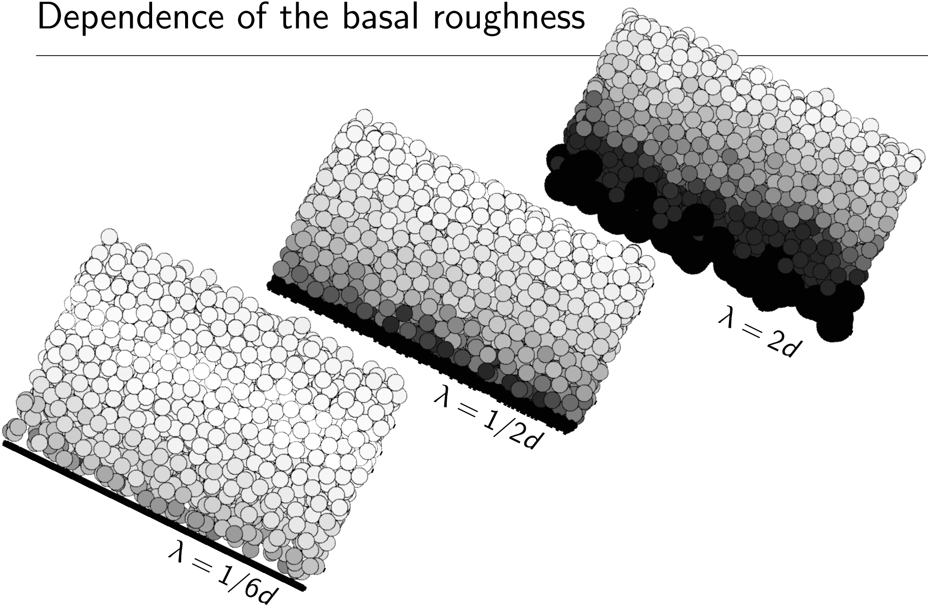
$$\frac{\partial h}{\partial t} = -\frac{\partial h\bar{u}}{\partial x},$$
$$\frac{\partial h\bar{u}}{\partial t} = -\frac{\partial}{\partial x}\left(h\,\alpha(h,\bar{u})\,\bar{u}^2 + \frac{K(h,\bar{u})}{2} g h^2 \cos\theta\right) + gh\left(\sin\theta - \mu(h,\bar{u})\frac{\bar{u}}{|\bar{u}|}\cos\theta\right),$$

for a given set of microscopic and geometric parameters.

Objective

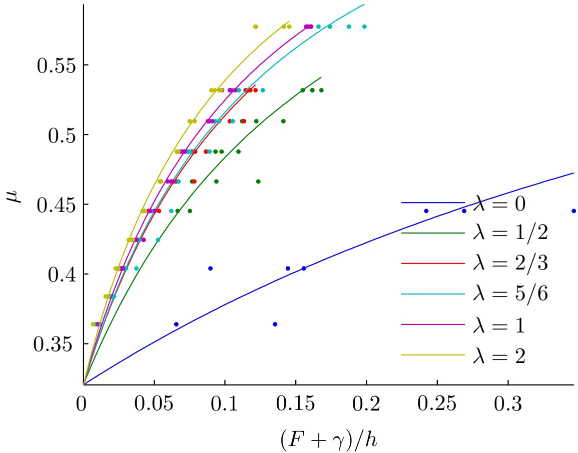
Study the dependence of the closure laws on the parameters M (the micro-macro transition).

Dependence of the basal roughness



Increasing basal roughness by increasing base particle diameter λ.

Dependence of the basal roughness



Friction increases with increasing base particle diameter λ.

Steady disordered flows fitted to $F = \beta \frac{h}{h_{stop}(\theta; \lambda=1)} - \gamma$.

Conclusions 1/2

- Coarse-grained fields are defined s.t. mass and momentum balance holds exactly, even at external boundaries.
  - W, Thornton, Luding, Bokhove, *From discrete particles to continuum fields near a boundary*, Granular Matter (2012) 14:289

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- Coarse-grained fields should be independent of CG width.

  For chute flows, two scales (sub-particle/particle) exist.

  Fluctuation velocity requires correction on particle scale.

  Objective description of stress tensor.
    - W, Hartkamp, Thornton, Luding, *Coarse-grained local and objective continuum description of 3D granular flows*, Phys. Fl. (2012) submitted

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- Micro-macro transition: Closure relations extracted from DEM. Closure depends on particle/ contact properties.
  - W, Thornton, Luding, Bokhove, *Closure Relations for Shallow Granular Flows from Particle Simulations*, Granular Matter (2012) 14:531
  - Thornton, W, Luding, Bokhove, *Frictional dependence of shallow granular flows from discrete particle simulations*, EPJ (2012).

Conclusions 2/2

- CG applied to mixtures (bidispersed flows):
  - Thornton, A.R., W, Luding, S., Bokhove, O., *Modeling of particle size segregation: Calibration using the discrete particle method,* Int. J. Mod. Phys. C 23, 1240014 (2012)
  - W, Luding, S., Thornton, A.R., From discrete particles to continuum fields in mixtures, Powders & Grains 2013, Conference Proceedings (2013), submitted

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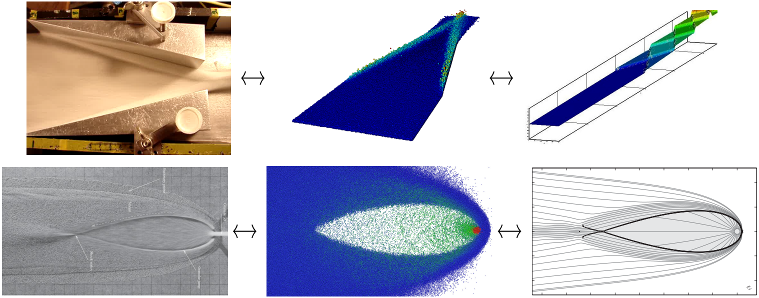
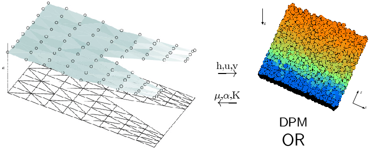
  - W, Luding, S., Thornton, A.R., From discrete particles to continuum fields in mixtures, Powders & Grains 2013, Conference Proceedings (2013), submitted
- CG applied to molecular flows
  - R. Hartkamp, A. Ghosh, T. Weinhart and S. Luding, A study of the anisotropy of stress in a fluid confined in a nanochannel", J. Chem. Phys. 137, 044711 (2012) Download

Future Work

1. Validate contact model by comparing DPM to lab-scale experiments
2. Validate closure laws by comparing FEM and DPM simulations



3. Where no closure rules are known (transient/boundary effects), a two-way multi-scale coupling is desired.



FEM for shallow-layer eqn's

DPM
OR
closure eqn's.