

From micro to macro in granular matter

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Objective: Micro-macro transition for shallow granular flow



Experiment and DEM simulation of glass particles flowing through a contraction d = 1mm, $N \approx 400\,000$, $dt = 5\,\mu s$.

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

The continuum model for shallow granular chute flow



Depth- and width-averaging mass- & momentum balance yields the lithostatic balance, $\sigma_{zz}(z) \approx \rho g cos \theta(h-z)$, and

$$\frac{\partial h}{\partial t} + \frac{\partial h \bar{u}}{\partial x} = 0,$$
$$\frac{\partial}{\partial t} (h\bar{u}) + \frac{\partial}{\partial x} (h\alpha \bar{u}^2) + \frac{\partial}{\partial x} \left(\frac{\kappa}{2} g h^2 \cos\theta\right) = gh(\sin\theta - \mu \frac{\bar{u}}{|\bar{u}|} \cos\theta),$$

where closure relations are required for velocity shape factor $\alpha = \frac{u^2}{\bar{u}^2}$, 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 DEM simulations of steady uniform flow.



DPM of steady uniform chute flow, periodic in x- and y-direction, fixed-particle layer at the base, unrestrained surface, inclination θ .



Parameters of the DPM

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

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

$$f_{ij}^{n} = -k_{n} \delta_{ij} - \gamma_{n} \mathbf{v}_{ij}^{n},$$

$$f_{ij}^{t} = -\min(|k_{t} \vec{\delta}_{ij}^{t} + \gamma_{t} \vec{v}_{ij}^{t}|, \mu_{c} f_{ij}^{n}),$$

- collision time $t_c = 5 \cdot 10^{-3} \sqrt{d/g}$, restitution r = 0.88, friction $\mu_c = 0.5$ ($k_n = 2 \cdot 10^5$, $\gamma_n = 25$, $k_t = 2/7k_n$, $\gamma_t = \gamma_n$)
- integration with velocity verlet, $dt = t_c/50$ until t = 2000.

Statistics by coarse-graining

We define the macrosc. density using a coarse-graining function ϕ ,

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

We define the velocity field \vec{V} , s.t. it satisfies mass balance *exactly*,

$$ec{V}=ec{
ho}/
ho,\,\, ext{where}\,\,ec{
ho}=\sum_{i=1}^nm_iec{
ho}_i\phi(ec{r}-ec{r}_i).$$



Density ρ of a static system of 5 fixed and 5 free particles for a Gaussian coarse-graining function of width w = d/8.

Statistics by coarse-graining

We define the stress tensor s.t. it satisfies momentum balance exactly. Then $\vec{\sigma} = \vec{\sigma}^c + \vec{\sigma}^k$, with contact and kinetic stress

$$\begin{split} \sigma_{\alpha\beta}^{k} &= -\sum_{i=1}^{n} m_{i} v_{i\alpha}' v_{i\beta}' \phi(\vec{r} - \vec{r}_{i}), \\ \sigma_{\alpha\beta}^{c} &= -\sum_{\text{contacts } \{i,j\}} f_{ij\alpha} r_{ij\beta} \int_{0}^{1} \phi(\vec{r} - (\vec{r}_{i} + s\vec{r}_{ij})) \, ds \\ &-\sum_{\text{wall contacts } \{i,k\}} f_{ik\alpha} a_{ik\beta} \int_{0}^{1} \phi(\vec{r} - (\vec{r}_{i} + s\vec{a}_{ik})) \, ds, \end{split}$$

with branch vector \vec{a}_{ik} and fluctuation velocity $\vec{v}'_i = \vec{v}_i - \vec{V}$.



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



Demarkation line $h_{stop}(\theta)$ between arrested and steady flow, fitted to $h_{stop}(\theta) = Ad \frac{\tan(\theta_2) - \tan(\theta)}{\tan(\theta) - \tan(\theta_1)}$ (fit from Pouliquen, Forterre, 2003). Closure for the friction $\mu = \frac{|t_t|}{|t_0|} = \tan \theta$ 4 3.53 2.52 1.51 0.50 5101520 $h/h_{stop}(\theta)$ Steady flows fitted to $F = \beta \frac{h}{h_{stop}(\theta)} - \gamma$, where $F = \frac{\bar{u}}{\sqrt{g \cos \theta h}}$.

Substituting $\mu = tan(\theta)$ yields

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

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



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

Right: Shape factor $\alpha(h, \theta)$ from simulations (markers) and fit (lines). Closure for the normal stress ratio $K = \frac{\bar{\sigma}_{xx}}{\bar{\sigma}_{zz}}$



Dependence of the basal smoothness



Figure: We change the base roughness by varying the base particle diameter $0 < \lambda \leq 2$. Figure shows $\lambda = 2$.

Dependence of the basal smoothness



Figure: Fit of steady disordered flows to $F = \beta \frac{h}{h_{stop}(\theta; \lambda = 1)} - \gamma$. Froude number increases for smoother base.



Conclusions:

- Density, velocity and stress definition satisfies mass and momentum balance exactly, even at external boundaries.
 - W, Thornton, Luding, Bokhove, *From discrete particles to continuum fields near a boundary*, Granular Matter
- Discrete particle simulations were used to obtain closure rules

 $\mu(h, \bar{u}), \ \alpha(h, \bar{u}), \ K \approx 1.$

Micro-macro transition: Closure depends on the particle and contact properties, f.e. bed roughness λ , bed friction μ_b :

- W, Thornton, Luding, Bokhove, *Closure Relations for Shallow Granular Flows from Particle Simulations*, Granular Matter, submitted,
- Thornton, W, Luding, Bokhove, *Frictional dependence of shallow granular flows from discrete particle simulations*, EPL, submitted.



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Future work:

- Apply the new stress definition to bi-dispersed flows (segregation effects).
- Validate the closures for nonuniform flow (contraction, obstacles)