Molecular Dynamics Simulation of Cohesive Granular Materials

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1 Introduction

The experimental motivation for this study are recent publications on cohesive granular materials [2–4,10]. Our central question is, in which regime and by which mechanism the the movement of grains changes from movement of independent particles to a movement of small clusters with increasing cohesion. Cohesion introduces an additional length scale, so that the effects become size-dependent. The cohesive force acting on a volume element of size $l \times l \times l$ is proportional to its surface, or $\propto l^2$. The repulsive force generated by the mass of the volume element is $\propto l^3$. The strength of the cohesion and the density of the particles determine the size for which repulsion and cohesion are in equilibrium for a certain characteristic length d.

2 Simulation Method

The idea was to model the cohesive force on the particle level, without any macroscopic modeling. The particles are represented by polygons to allow arbitrary shape and size dispersions. They move according to phenomenological interactions in a molecular dynamics simulation.

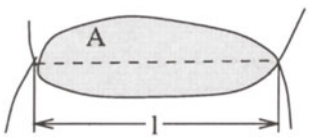

Fig. 1. Undeformed (full line) and deformed (dashed line) particles in a contact. The force resulting from the deformation is assumed to be proportional to the area overlap of the colliding particles. The penetration depth is exaggerated in comparison to simulations with realistic parameters.

The repulsive contact force in normal direction is proportional to the particle overlap and to Young's modulus. The overlap represents the deformation of the overlapping polygons in the "real world". Additional damping in normal

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direction as well as a model for static friction in tangential direction [7] are also present. The implementation of static friction is indispensable for the heap formation, without static friction the grains behave like a fluid. For the simulations presented in this article, a friction coefficient of $\mu = 0.6$ and Young's modulus of Y$= 4 \cdot 10^7$ N/m was used.

The cohesion was modeled proportional to the contact length (see Fig. 1) and chosen proportional to a cohesion parameters k_{coh}. In two dimensions, k_{coh} has the units [N/m], so that the attractive force F_{coh} is proportional to the contact length l:

$$F_{\mathrm{coh}} = k_{\mathrm{coh}} \cdot |l|. \tag{1}$$

Further details on the model can be found in [11].

3 Setup of the Simulation

The simulation is performed with the so-called "draining-crater method" [5]. An upper vessel filled with cohesive granulate is emptied via an outlet, see Figs 2 and 3. The outcome for angle of repose, correlation time etc. is studied in dependence of the cohesion.

The simulation was performed using particles which had about the same diameter as the experiment [10,2,3]. The box size in the experiments was about 80-250 particle diameters, in our simulation it was about 160-200 particle diameters. The size of the outlet was about 12-25 particles in the experiment and 12-40 particles in the simulation. One series of measurements was taken with mono-disperse regular polygons with 15 faces, one series with a poly-disperse mixture, and a linear distribution of the radius within the interval $[0.75 \cdot r, 1.25 \cdot r]$. Another series was taken with the same size dispersion, but with regular polygons with 63 faces to monitor the effect of size dispersion and particle shape. All series give consistent data for medium to strong cohesion. For weak cohesion, the mono-disperse grains have a strong tendency to order on a triangular grid which dominates the entire physics of the system. In the simulation, the static and dynamic friction coefficients were chosen as $\mu_{\mathrm{stat.}} = \mu_{\mathrm{dyn.}} = 0.6$, Young's modulus was $Y = 10^7$ N/m, the particle diameter was 1 mm for the mono-disperse, and 0.6-1 mm for the poly-disperse particles. The time step for the simulations was dt$=0.2 \cdot 10^{-5}$ s, the density was 5000 kg/m^2.

We computed the angle of repose ϕ of the material in the upper vessel by calculating the two-dimensional analogue from [10] so that

$$\tan\phi = 2 \cdot \frac{\text{area}}{\text{base length}^2}. \tag{2}$$

The advantage of calculating ϕ from the area below the slope is that it yields an integral criterion. This smoothes out any effects from jagged surfaces of the slopes, which are typical for strongly cohesive materials such as in Fig. 3. Different layers of the grains during initialization of the particles are denoted by different shadings. For non-cohesive materials like in Fig. 2, the angle of repose