Molecular Dynamics Simulation of cohesive Granular Materials

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1 Introduction

The experimental motivation for the study were recent publications on cohesive granular materials [10,2–4]. Our central question was, in which regime and how the the movement of grains would change from movement of independent particles to a movement of small clusters with increasing cohesion. Cohesion introduces an additional lengthscale in granular materials, 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 arbitray shape and size dispersions and they move according to phenomenological interactions in a molecular dynamics simulation.

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 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 Youngs 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:

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

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

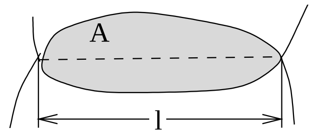

Fig. 1. Undeformed (full line) and deformed (dashed line) particles in a contact. The force resulting from the deformation is assumed to be proportional to the area overlap of the colliding particles. The penetration depth is exaggerated in comparison to simulations with realistic parameters.

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.

3.1 Weak cohesion

For no or weak cohesion $< 0.005N/m$ single particles flow through the outlet. The slopes of the heap above and below the the flow through the outlet are straight and smooth, the irregularities are of the size of up to two particle diameters. The good mixing is indicated by the colors of the particles.

Heaps built from a point source with non- or weakly cohesive polydisperse material show a pressure dip in the middle of the heap. For monodisperse non-cohesive particles, there is no pressure minimum [11], but the pressure distribution is similar to that of a regular packing of particles like the one in [9].

3.2 Strong cohesion

For strong cohesion $> 0.005N/m$ not single particles but whole clusters leave the outlet. The slopes of the resulting heaps above and below the outlet are ragged and rounded. The suppression of mixing is indicated by layers of particles of the same color.

For strongly cohesive materials even heaps built from a point source with monodisperse particles exhibits a pressure minimum, see Fig. 5.

4 Implications for the modeling of cohesion and friction

Fig. 6 (left) shows an increased correlation time between neighboring particles. The time correlation between particles is measured as the percentage of

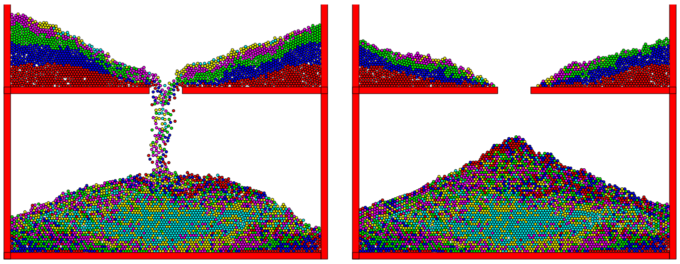

Fig. 2. Snapshots of the outflow with weak cohesion (left) and final configuration ($k_{\mathrm{coh}} = 4 * 10^5$ N/m)
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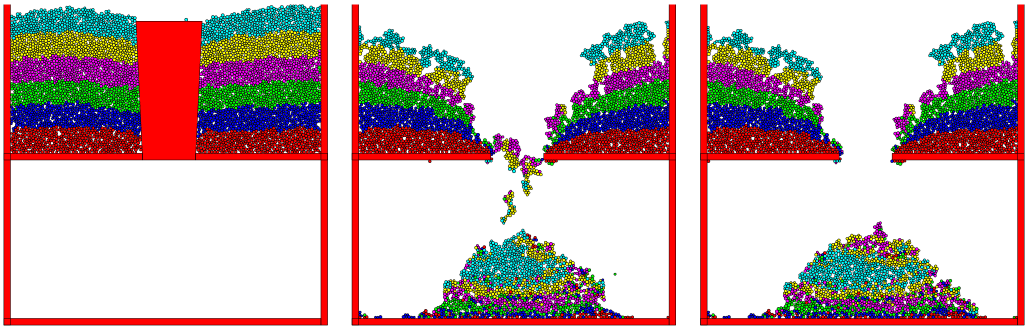

Fig. 3. Snapshot of the starting configuration before the stopper is removed (left), outflow of particle clusters and the final configuration with ragged surfaces (right) for strong cohesion ($k_{\mathrm{coh}} = 2 * 10^3$ N/m).

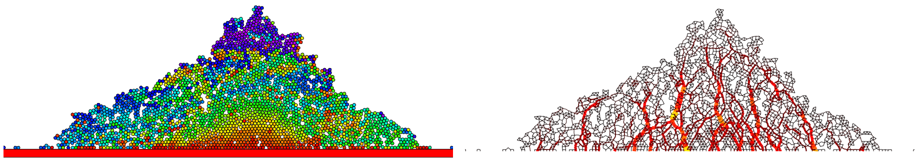

Fig. 4. Heap made from cohesive particles (left) and the corresponding force network (right).

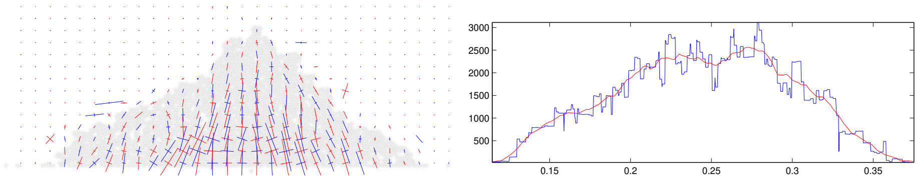

Fig. 5. Stress distribution (left) and pressure distribution at the bottom of the heap (right)

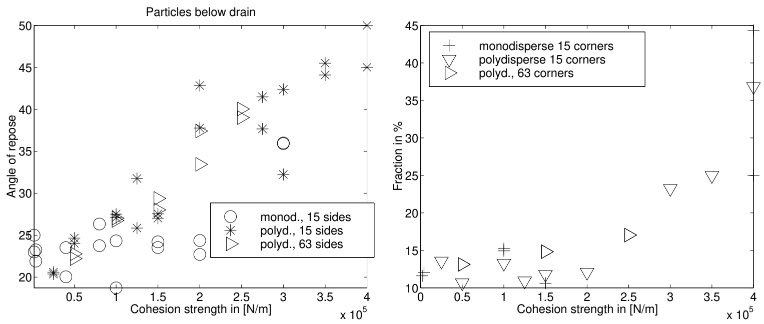

Fig. 6. Left: Angle of repose in the lower box of Fig. 3. Right: Percentage of particles which were nearest neighbors at the beginning of the simulation and less than 1 particle diameter spaced at the end in the lower box (see Fig. 3) Statistics for next nearest neighbors give similar, but more noisy data.

particles which were nearest neighbors at the beginning of the simulations and within 1 average particle diameter at the end of the simulation. The data indicates as well the cluster movement as well as the suppressed mixing observed in Fig. 3 for strong cohesion.

The graphic view of this correlation means that the particles are "chained together" (see Fig. 7) by the cohesive forces. Actually, this is reminiscent to simulations of non-spherical particles made from connected round particles [8]. In the same way, an attempt was used in modeling "rough" particles via connected spheres to mimic static friction [12].

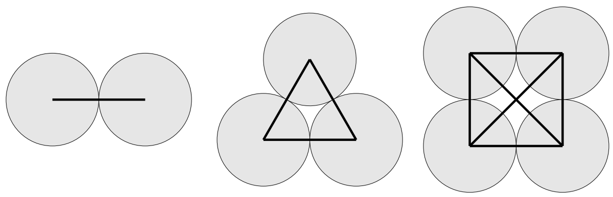

Fig. 7. Modeling of "rough" granular materials as Polymers of "smooth" round monomers. The coupling can either be done by constraints like in [8] or with "soft" springs [12].

In powder technology, the strength of the cohesion is classified by a single parameter together with the the surface roughness of the grains. This parameter is independent from the angle of repose, as proposed by Carr [6] see e.g. Ref., [1]. That the static friction for bulk solids can be independent of the particle roughness is already mentioned in the textbook by Rabinowicz [13]. This means that roughness/cohesion on the one hand is distinct from friction on the other hand. For systems of connected spherical particles, namely dimers, also a linear increase of the angle of repose on a rough surface was observed.

From our cohesive modeling and the approach of [6], one can reinterpret the results from [8,12] as the modeling of rough and/or cohesive granular materials without static friction. The smallest angle of repose was well below 20 degrees (14 degrees for dimers in [8] on a rough bottom, 14 degrees for particles made from 5 balls in [12] in a drum), which is definitely below the angles which were observed by us and experimentally in [10] of about 22 degrees. Therefore, “rough” or “connected smooth” particles without Coulomb friction can be expected to behave very much like cohesive particles without friction. As cohesion and particle roughness cannot be distinguished by macroscopic parameters, we propose our modeling of cohesion also to mimic an effective “roughness” of grains in computer simulations without implementing additional geometric information for the particles.

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