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Sound propagation in isotropically and uni-axially compressed cohesive, frictional granular solids

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ABSTRACT

Using an advanced contact model in DEM simulations, involving elasto-plasticity, adhesion, and friction, pressure-sintered tablets are formed from primary particles and prepared for unconfined tests. Sound propagation in such packings is studied under various friction and adhesion conditions. Small differences can be explained by differences in the structure that are due to the sensitivity of the packing on the contact properties during preparation history. In some cases the signals show unexpected propagation behaviour, but the power-spectra are similar for all values of adhesion and friction tested. Furthermore, one of these tablets is compressed uni-axially and under unconfined conditions and the sound propagation characteristics are examined at different strains: (i) in the elastic regime, (ii) during failure, and (iii) during critical flow: the results vary astonishingly little for packings at different externally applied strains.

1. Introduction

Granular materials in general [1–12] and especially cohesive, frictional, fine powders show a peculiar flow behaviour [13–17]. Adhesionless powder flows freely, but when adhesion due to van der Waals forces is strong enough, agglomerates or clumps form, and can break into pieces again [18–21]. This is enhanced by pressure- or temperature-sintering [22] and, under extremely strong pressure, tablets or granulates can be formed [23–26] from primary particles. Applications can be found, e.g., in the pharmaceutical industry.

The basic question is how to understand such cohesive, frictional, fine powders and whether one can use sound propagation measurements from simulations to gain additional insight. In contrast to crystalline materials [27,28], information propagation in disordered and inhomogeneous granular media is far from well understood, especially when friction and other realistic contact mechanisms are taken into account [29–31]. Understanding better the sound propagation in granular media will improve, e.g., the interpretation of ultrasound measurements in soil as a non-intrusive way to detect and measure underground structures. This has applications in archeology, seismology and – because of its cost efficiency – for the discovery and exploitation of natural resources such as ores, coal, or oil.

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Propagation of stress or sound waves through dense granular matter is the superposition of many complex phenomena, which are caused by the discrete, inhomogeneous, anisotropic and dissipative structure of this class of materials. The properties of such waves are strongly affected by phenomena like attenuation, scattering, and dispersion [32]. Ballistic pulse propagation co-exists with slower, multiply scattered coda-like signals [32,33]. The stress- and frequency-dependence of the wave propagation features are subject of ongoing discussion [32,34] in static and shaken packings as well.

Many-particle simulations methods like discrete element models (DEM) [5,35–40] complement experiments on the scale of small "representative volume elements" (RVE) [39]. Deep and detailed insight into the kinematics and dynamics of the samples can be obtained since the information about all particles and contacts is available at all times. Discrete element models require the contact forces and torques as the basic input, to solve the equations of motion for all particles in a granular system. From this, the macroscopic material properties as, among others, elastic moduli, cohesion, friction, yield strength, dilatancy, or anisotropy can be measured from such RVE tests.

The macroscopic properties are controlled by the "microscopic" contact forces and torques [32,34,41–43]. Non-linear contacts [40,44], frequency-dependence [45,46] and also scattering and attenuation in other "particle type" materials [47] have been reported.

Research challenges involve not only realistic DEM simulations of many-particle systems and their experimental validation, but also the transition from the microscopic contact properties to the macroscopic flow behaviour [15,16,39,48,49]. This so-called micro–macro transition [15,16] will allow a better understanding of the collective flow behaviour of many particle systems as a function of the particles' material and contact properties. The resulting micro-parameter based continuum description ("macroscopic") of dense granular materials can be useful for field applications (like oil discovery), since particle simulations ("microscopic") are not applicable due to the huge system sizes. Some empirical descriptions are available for dynamic and possibly non-linear deformation and propagation modes [32,34,50].

The paper is organized as follows. After introducing the simulation method in Section 2, the preparation of our samples is discussed in Section 3. Sound propagation through densely packed granular systems and its dependence on friction and adhesion is examined in Section 4.1, while sound propagation for different states of compression and failure is reported in Section 4.2. Summary and Conclusions are given in Section 5.

2. Discrete particle model

To simulate packing, failure and sound propagation in a granular material we use a discrete element model (DEM) [5,25,35–38,51]. Such simulations can complement experiments on small scale by providing deep and detailed insight into the kinematics and dynamics of the samples examined. In the following we briefly introduce the method that allows us to simulate wave propagation in (damaged) packings. The numerics and algorithms are described in text books [52–54], so that we only discuss the basic input into DEM, i.e., the contact force models and parameters. More details on the contact model can be found in Ref. [25] and references therein.

The pairwise inter-particle forces typically used are based on the overlap and the relative motion of particles. This might not be sufficient to account for the inhomogeneous stress distribution inside the particles and possible multi-contact effects. However, this simplifying assumption enables us to study larger samples of particles with a minimal complexity of the contact properties, taking into account phenomena like non-linear contact elasticity, plastic deformation, and adhesion as well as friction, rolling resistance, and torsion resistance. In the following, we will neglect rolling and torsion resistance however.

2.1. Normal contact forces

Realistic modeling of the deformations of two particles in contact with each other is already quite challenging. The description of many-body systems where each particle can have multiple contacts is extremely complex. We therefore assume our particles to be non-deformable perfect spheres. They shall interact only when in contact. We call two particles in contact when the distance of their centers of mass is less than the sum of their radii. For two spherical particles i and j in contact, with radii a_i and a_j, respectively, we define their overlap

$$\delta = (a_i + a_j) - (\boldsymbol{r}_i - \boldsymbol{r}_j) \cdot \boldsymbol{n} > 0 \quad (1)$$

with the unit vector $\boldsymbol{n} := \boldsymbol{n}_{ij} := (\boldsymbol{r}_i - \boldsymbol{r}_j)/|\boldsymbol{r}_i - \boldsymbol{r}_j|$ pointing from j to i. $\boldsymbol{r}_i$ and $\boldsymbol{r}_j$ denote the position of particles i and j, respectively.

The force on particle i, labelled $\boldsymbol{f}_i$, is modelled to depend pairwise on all particles j with which particle i is in contact, $\boldsymbol{f}_i = \sum_j \boldsymbol{f}^c_{i|j}$, where $\boldsymbol{f}^c_{i|j}$ is the force on particle i exerted by particle j at contact c. The force $\boldsymbol{f}^c_{i|j}$ can be decomposed into a normal and a tangential part, $\boldsymbol{f}^c_{i|j} = f^{\rm n}_{i|j}\boldsymbol{n} + f^{\rm t}_{i|j}\boldsymbol{t}$, where $\boldsymbol{n} \cdot \boldsymbol{t} = 0$.

To model the force $\boldsymbol{f}^c_{i|j}$ we use an adhesive, elasto-plastic, history-dependent contact law that depends on three variables only and is described in more detail in Ref. [25]: the force between two spheres is modelled to depend only on their overlap δ, the relative velocity of their surfaces, and the maximum overlap $\delta_{\max}$ this contact has suffered in the past. We will leave out the index $i|j$ from now on.

For the normal force $f^{\rm n}$ we apply a modified spring-dashpot model: the dashpot part is, as usual, a viscous damping force that depends on the normal component of the relative velocity. The spring "constant" k, however, is only temporarily constant and depends on the history of the contact, changing the force from linear in the overlap to piecewise linear: the