# How to obtain constitutive relations about stress and density from DEM simulations

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**Abstract**
Fine, cohesive-frictional powders are the subject of this study. The behavior under isotropic compression is examined for different material properties involving, friction, rolling-resistance, and contact-adhesion. From a single simulation, the constitutive relation for the density-pressure relation can be extracted. The examined powders show an interesting behaviour: the compaction slows down for moderate stresses and then accelerates for higher pressures.

## 1 Introduction

Fine, cohesive-frictional powders show peculiar flow behavior since several contact forces are equally important [1]. Friction, rolling-resistance, and contact-adhesion are active at the same time and lead to macroscopic cohesion and macroscopic friction that is not proportional to the microscopic contact parameters. Besides many experiments, Molecular Dynamics (MD) or Discrete Element Models (DEM), which solve the equations of motion for all particles in a system, are used to understand these granular media [2,3]. While experiments and continuum theory deal with macroscopic material parameters, for the particle simulations, the (microscopic) contact forces are the only physical laws that have to be defined beforehand, see Ref. [2] for details on the contact models.
For powders, as an example, the particle properties and interaction laws are inserted into a discrete particle molecular dynamics and lead to the collective behavior of the dissipative, frictional, adhesive many-particle system. From the particle simulation, one can extract, e.g., the coordination number or the pressure of the system as a function of density, but also velocity gradient, viscosity and other macroscopic material properties. For cohesionless particles many simulations were performed for various deformation modes, like oedometric or isotropic compression, pure shear or triaxial shear. For cohesive powders the amount of literature us much smaller, so that we focus first on the simplest mode of deformation, namely *isotropic compression*, and postpone shear simulations to a later study.
In the following, normal interactions, like adhesion and elasto-plastic contact deformations are used as well as friction, rolling- and torsion resistance in tangential direction. Examples of a compression test are presented for which some of the contact model parameters are varied so that the compaction process is affected [4]. Of special interest are quantities like porosity or density, plotted against the applied pressure. The functional behavior between density and pressure is an important ingredient for many constitutive models, however, with many open questions remaining.

## 2 Discrete Element Method DEM

Particle simulations are referred to as discrete element models (DEM). For details see Ref. [2]. The elementary units of granular materials are mesoscopic grains, which deform under stress. Since the realistic modeling of the deformations of the particles is much too complicated, we relate the interaction force to the overlap of two particles in normal direction and to the displacement in tangential direction. Details of the simulation method and of the contact models are described in [2].

## 3 Compaction Simulations

In this section, a compression test is presented, where the particles are initially positioned on a square-lattice in a cubic system with periodic boundary conditions, in order to avoid wall effects. The system is first allowed to evolve to a disordered state, by attributing random velocities to all particles. The density is increased by slowly increasing the particle size while the system volume is kept constant. During the simulation, the particles are thus slowly growing and quantities like density, coordination number, energy and pressure can be reported.

The systems examined in the following contain $N$=1728 particles with equal radii $a$. In the simulations, the radii change with a constant rate $g_r = 0.2$, relative to the radius, if not explicitly specified. The growth is stopped when a target volume fraction is reached. The contact model parameters used are described in detail in Ref. [4]. The choice of numbers and units is such that the particles correspond to spheres with initial radius $a_0 = 5$ μm, growing up to a maximum radius 11.7 μm at the maximal volume fraction 0.75.

### 3.1 Compression rate

When compressing the system (by growing the particles) the first quantity of interest is the density (or volume fraction). The second quantity is the pressure that is reached during compression, plotted as a function of the volume fraction, see Fig. 1. Note that we plot the dimensionless pressure that is approximately the average overlap relative to the particle size, i.e., a dimensionless pressure of 0.1 corresponds to a contact deformation of about 10%.

During compression, the pressure remains at a very small level, until it starts to increase strongly and nonlinearly from a certain volume fraction on. There are two regimes: (i) an initial, nonlinear regime for small pressures, and (ii) an almost linear regime for higher pressures.

The slow simulations (red lines) lead to a somewhat smaller pressure than the fast simulations (green lines), showing the dynamic effect of the rather fast compression rate 0.2.

After the maximal density is reached, the compression is reversed, i.e., the particles are shrinking with rate -0.2 (blue line). The un-loading branch follows the linear branch (ii) of pressure and does not reproduce the non-linear regime (i) for small pressures. Interestingly, the pressure displays negative values during un-loading, due to the

attractive tensile forces that become active. The negative stress peak corresponds to the maximal isotropic tensile strength of the powder, after it had reached the maximal density.

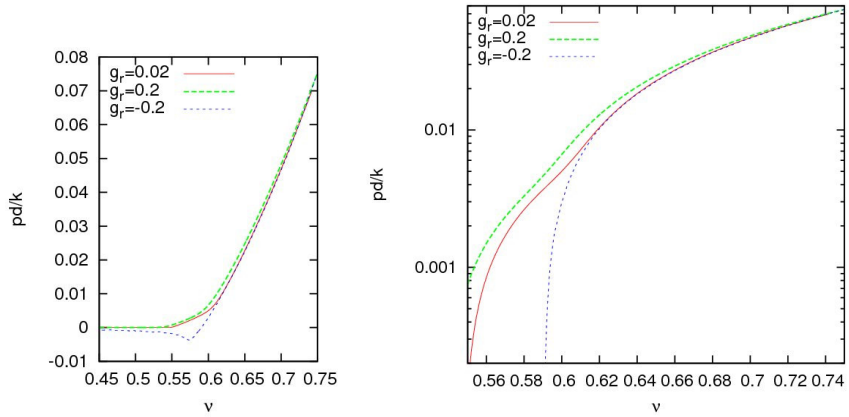


**Fig.1:** Dimensionless pressure $pd/k$, with $d=2a$, and $k$ the spring stiffness of the normal contact force model, plotted as function of the density for simulations with coefficients of friction $\mu=1$ and rolling-resistance coefficient $\mu_r=0.01$. The growth rate is given in the inset, where the negative value corresponds to unloading after the maximal density was reached. The left plot is linear in pressure while the right plot is logarithmic to better visualize the small pressure values.

## 3.2 Parameter study

In the following, the friction coefficient $\mu$ and the rolling- and torsion-resistance coefficients $\mu_r=\mu_o$ are varied. According to the growing procedure, the volume fraction is increased, i.e., the pore-number $e$ is decreased, as plotted against the pressure in Fig. 2 for various simulations.

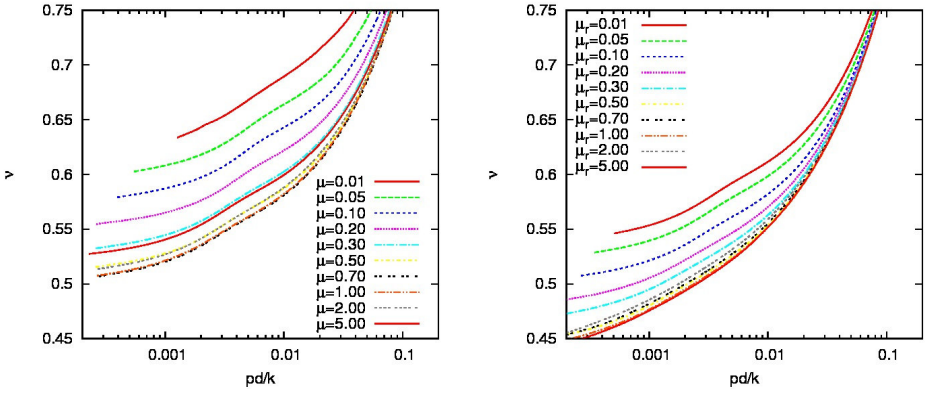


**Fig.2:** Volume fraction plotted against pressure for data with $g_r=0.2$ and kinetic to potential energy ratio below 0.1. The values of the friction coefficient are varied at constant $\mu_r=0.1$ (Left), and the values of rolling- and torsion-coefficients are varied at constant $\mu=1$ (Right).

From the left panel in Fig.2 one can conclude that small friction coefficients are always related to rather high densities, i.e., small pore numbers. Larger and larger friction coefficients, however, are not always sufficient to guarantee a lower and lower packing

density, i.e., higher and higher pore number. The simulations almost collapse for $\mu \sim 1$ and for stronger friction, interestingly, the pore number decreases, i.e. the density increases.
From the right panel, one observes similarly that larger and larger rolling- and torsion-resistance lead to smaller densities, i.e., larger pore-numbers. On the other hand, extremely high rolling- and torsion-coefficients do not necessarily lead to much lower densities. The simulations do not change much anymore for $\mu_r > 0.5$.
The reason for this behavior is a different reorganization dynamics. Increasing the friction (rolling resistance) coefficients, allows for higher pore numbers, however, above a certain value, the packing is not stabilized further and finds other deformation modes to collapse: If sliding is avoided (very large $\mu$), the packing still can roll into denser positions. Similarly, when rolling is avoided, the packing can slide into denser configurations.

## 4. Summary and Conclusion

The present study contains isotropic compression tests of adhesive, frictional, rough powder particles. While adhesion is not varied here, both friction and rolling-resistance coefficients are changed systematically. All other parameters are chosen with exemplary values, since the full set of contact models involves a too large number of parameters.
Very likely, some of the particle- and contact-properties are less important for macroscopic physical properties than others. The most relevant parameters still have to be identified and their interplay and origin from microscopic mechanisms has to be better understood.
Eventually, the quantitative validation of the simulation contact models and the corresponding parameters is the issue. The existence of low packing fractions in adhesive, frictional fine powders is one of the challenges for DEM simulations. Validation of DEM by experiments is possible then and – in reverse – the mechanisms during compaction can be examined in more detail (and better understood) by DEM.

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