Implementation and Verification of an Algorithm for Deformable Discrete Particles in the YADE DEM Software

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ABSTRACT

The simulation of granular matter, especially the handling of deformable particles is a topical issue in the field of material science and engineering [1]. The compaction of powders and pellets is widely used, e.g. in metallurgical and pharmaceutical processes [2]. We present the implementation of a volume redistribution algorithm [3,4] for particle deformation in the discrete element software YADE [5]. The obtained data are compared with experimental data.

The deformation is handled during the algorithm with a mass relocation model. In the discrete element method (DEM) the forces on every particle are calculated in dependence of the virtual overlap of the interacting particles. Usually the volume of the overlapping area is neglected in DEM. This assumption is not valid for large deformations of soft particles. To overcome the problem, the mass of the overlapping volume is redistributed by the here presented algorithm evenly over the non-contacting particle surface, resulting in a slightly enlarged spherical particle. The volume of the overlap is in this case approximated as spherical cap. This volume is recalculated numerically in every time step and for every particle/particle and particle/wall contact.

Even large particle overlaps can be handled in a physically correct way and without the loss of volume and consequently for a constant particle density, without the loss of mass. The obtained data for porosity and stresses on the packing of particles are more reliable compared to the data without using the deformation algorithm.

This way, it is possible to describe the deformation of e.g. rubber spheres for adequately large compressions sufficiently. Since the mass relocation algorithm is independent from material specific parameters, a wide range of applications is possible. Even the applicability of this model to foam bubbles will be discussed.

Furthermore the possibilities of the expandability of the open-source DEM framework YADE is presented. A comparison of the performance of different implementation strategies is given next to the validation of the code by experimental data and limits of the procedure.

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