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Implicit frictional-contact model for soft particle systems

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ABSTRACT

We introduce a novel numerical approach for the simulation of soft particles interacting via frictional contacts. This approach is based on an implicit formulation of the Material Point Method, allowing for large particle deformations, combined with the Contact Dynamics method for the treatment of unilateral frictional contacts between particles. This approach is both precise due to the treatment of contacts with no regularization and artificial damping parameters, and robust due to implicit time integration of both bulk degrees of freedom and relative contact velocities at the nodes representing the contact points. By construction, our algorithm is capable of handling arbitrary particle shapes and deformations. We illustrate this approach by two simple 2D examples: a Hertz contact and a rolling particle on an inclined plane. We also investigate the compaction of a packing of circular particles up to a solid fraction well above the jamming limit of hard particles. We find that, for the same level of deformation, the solid fraction in a packing of frictional particles is above that of a packing of frictionless particles as a result of larger particle shape change.

1. Introduction

Granular materials are of crucial importance in industrial transformation processes dealing with powders and grains as well as in geological flows and applications involving geomaterials (soils, rocks and concrete) (Nedderman, 1992; Jaeger and Nagel, 1996; Turner and Schuster, 1996). These materials present a complex pressure-dependent, density-dependent and rate-dependent mechanical behavior, which has attracted extensive modeling effort in different communities (Wood, 1990; Nedderman, 1992; Radjai et al., 2004; GDR-MiDi, 2004). Granular materials present also a broad range of characteristics related to the shapes and size distributions of their constitutive particles (Herrmann et al., 2003; Donev et al., 2004; Antony and Kuhn, 2004; Voivret et al., 2007; Azéma et al., 2009; Azéma and Radjai, 2010; CEGEO et al., 2012). Most recent fundamental research has focused on the scale-up of mechanical properties from the scale of particles and their interactions, characterized by a disordered microstructure and highly inhomogeneous stress transmission (Radjai et al., 1998; Kruyt, 2003; Majmudar and Behringer, 2005; Agnolin and Roux, 2007a; Richefeu and El Youssoufi, 2009).

Granular materials have been mainly modeled as a collection of undeformable particles. The elastic deformations are assumed to be concentrated at the contact points, and thus described as a function of the rigid-body degrees of freedom of the particles (Cundall and Strack, 1979; Matuttis et al., 2000; Radjai and Richefeu, 2009). This *hard-particle* approximation is

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the physical ground of the popular Discrete Element Method (DEM) for the simulation of granular materials composed of model particles interacting via frictional contacts (Cundall and Strack, 1979). The numerical strategies based on DEM have the advantage of being robust. They include (1) Molecular Dynamics (MD), with an explicit time-stepping scheme based on force laws with strain variables derived from rigid-particle degrees of freedom (Cundall and Strack, 1979; Matuttis et al., 2000), and (2) Contact Dynamics (CD), which employs an implicit-type time integration scheme based on contact laws expressing the mutual exclusions of the particles and their Coulomb-like frictional behavior (Moreau, 1994; Jean, 1998; Radjai and Dubois, 2011).

The material behavior of the particles may be accounted to some extent in DEM through the force laws. In particular, the Hertz law and its generalization to frictional particles involve the elastic moduli and coefficient of friction of the particles Agnolin and Roux (2007a,b). Moreover, to first order in contact deflection δ, the latter may be replaced by the overlap between two undeformable spherical particles (Leroy, 1985). This approximation holds as far as the average stress p is small compared to Young's modulus E of the particles. In many applications, however, this approximation is too crude, and the particles may undergo large elastic or inelastic deformations. For example, metallic powders are mostly composed of soft particles that may deform plastically without rupture (Rabinowicz, 1965). In the same way, many products in pharmaceutical and food industries are *soft-particle* materials. This broad class of materials may be further extended to colloidal pastes, vesicles, microgels and many suspensions if particle sizes below 1 μm are considered (Cruz et al., 2002; Cloitre et al., 2003; Bonnecaze and Cloitre, 2010). All such materials may undergo volume change as a consequence of particle rearrangements, as in hard-particle materials. But what makes them different is their property of volume change by particle shape and size change under moderate external loads. This leads to enhanced space filling compared to hard particles in which the packing fraction cannot exceed the random close packing (RCP) limit (Berryman, 1986; Torquato et al., 2000). The compaction, shear behavior and other rheological properties of soft-particle systems beyond this "jamming" limit have remained largely unexplored.

For realistic modeling of soft-particle materials at large deformations, it is necessary to combine a continuum representation of the particles, allowing for their deformation according to a prescribed constitutive model, with appropriate frictional contact conditions between particles. In this regard, a promising framework is provided by meshless models that have already been applied to problems of solid mechanics involving large deformations. One of these numerical models is now mostly known as Material Point Method (MPM) (Guilkey and Weiss, 2003). The MPM is a mixed method combining the Eulerian and Lagrangian descriptions of the material. The Lagrangian description consists in representing each body by a collection of material points, and the Eulerian description is based on a background computational mesh. The information carried by material points is projected onto the background mesh, where equations of motion are solved. The mesh solution is then used to update the material points. The MPM brings together the advantages of Eulerian and Lagrangian methods by avoiding the distortion of Lagrangian mesh and tracking the boundaries of bodies. This method has also been applied to granular materials (Bardenhagen et al., 2000a; Cummins and Brackbill, 2002).

In particle systems, the kinematic constraints and stresses arising from unilateral contacts between particles and the bulk deformations of the particles are strongly coupled. While the contacts play the role of boundary conditions for the resolution of continuum equations in each particle, the evolution of contacts is determined by particle deformations. In MPM, the use of the same set of continuous shape functions in both mappings (the mapping from material points to mesh nodes and vice versa) naturally results in sticking (no interpenetration and no slip) contact scheme and thus no interpenetration occurs. With the use of a single-valued velocity to update the positions of material points, the sticking contact between two different bodies can be handled automatically at no additional computational cost using the original MPM, and no contact surface detection is required, but the contacting objects may not separate. For this reason, it is necessary to define different body velocities at the nodes and to implement frictional contact laws independently from MPM.

This issue has been addressed by several authors. Bardenhagen et al. (2000a, 2001) extended the original MPM to account for the unilateral nature of contact. In this algorithm, a contact occurs if the material points of different bodies are projected onto the same nodes of the background mesh, and the contact force is associated with the difference between the mass-center velocity of the particles and the node velocity, reflecting the constraints arising from contact. To release the no-slip contact algorithm in MPM, (Hu and Chen, 2003) proposed a multi-mesh mapping scheme, i.e. material points of each body lie in an individual background mesh rather than in the common one. In this procedure, the normal velocity of a material points at the contact surface is calculated in the common background mesh while the tangential velocity is found from the corresponding information in respective individual meshes. In their scheme, normal acceleration is set to be the same if material points of different bodies are mapped on the same node. However, in this algorithm the friction between different bodies is ignored because the tangential velocities of different bodies are assumed to be independent. Another multi-mesh contact algorithm for MPM was proposed by Pan et al. (2008). In this approach, the contact condition is similar to that of Bardenhagen et al. (2000a, 2001). It allows for fast contact search between bolides. However, contrary to the previous contact algorithms, both normal and tangential velocities of each particle at the contact surface are calculated in the respective individual meshes.

In this paper, an implicit MPM procedure is proposed for the simulation of deformable particles in association with the CD method for the treatment of frictional contacts between particles. Our procedure is implemented in a manner that the contact variables (velocity, force, etc.) are computed simultaneously with bulk variables (stresses, strains, etc.). We validate our algorithm by considering simple single-particle problems involving one contact, namely Hertz contact between a particle and a rigid platen and rolling of a particle on an inclined plane. We briefly present these examples, and compare the