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Efficient modelling of particle collisions using a non-linear viscoelastic contact force

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ABSTRACT

In this paper the normal collision of spherical particles is investigated. The particle interaction is modelled in a macroscopic way using the Hertzian contact force with additional linear damping. The goal of the work is to develop an efficient approximate solution of sufficient accuracy for this problem which can be used in soft-sphere collision models for Discrete Element Methods and for particle transport in viscous fluids. First, by the choice of appropriate units, the number of governing parameters of the collision process is reduced to one, which is a simple combination of known material parameters as well as initial conditions. It provides a dimensionless parameter that characterizes all such collisions up to dynamic similitude. Next, a rigorous calculation of the collision time and restitution coefficient from the governing equations, in the form of a series expansion in this parameter is provided. Such a calculation based on first principles is particularly interesting from a theoretical perspective. Since the governing equations present some technical difficulties, the methods employed are also of interest from the point of view of the analytical technique. Using further approximations, compact expressions for the restitution coefficient and the collision time are then provided. These are used to implement an approximate algebraic rule for computing the desired stiffness and damping in the framework of the adaptive collision model (Kempe and Fröhlich, J. Fluid Mech. 709: 445–489, 2012). Numerical tests with binary as well as multiple particle collisions are reported to illustrate the accuracy of the proposed method and its superiority in terms of numerical efficiency.

Introduction and motivation

Particle laden flows and their numerical simulation are of major interest in a wide range of engineering applications as well as in fundamental research. A frequently used approach for the simulation of dynamic granular materials is the Discrete Element Method (DEM), cf. Cundall and Strack (1979), Hoomans et al. (1996), and Pöschel and Schwager (2005). The linear and angular momentum balance of the particles is solved to obtain their translational and rotational velocity. The hydrodynamic interaction between particles is often neglected or fluid forces are accounted for by simple empirical correlations and the particle interaction modelled using macroscopic collision models of various types. The accurate numerical modelling of the collision process, however, is crucial for the quality of the simulation in a vast regime of parameters.

Several numerical models for the collision process between particles and for the collision of particles with walls have been developed in the framework of the DEM (Kruggel-Emden et al., 2007, 2008, 2009). These models can be divided into two groups: hard-sphere models and soft-sphere models. The hard sphere approach does not aim to resolve the details of the collision process. Instead, large time steps are considered and the collisions are treated as quasi-instantaneous. The post-collisional velocities are calculated from momentum conservation between the states before and after surface contact. The reader is referred to Crowe (2006) for details. Soft-sphere models, on the other hand, usually require an excessively small time step if physically realistic material parameters are matched. In the soft-sphere approach the motion of the particles is calculated by numerically integrating the equations of motion of the particles during the collision process accounting for the contact forces acting on them. Typical for all soft-sphere models is that very small time steps must be used to ensure that for reasons of stability and accuracy the step size in time is substantially smaller than the duration of contact. The soft-sphere contact forces are usually based on linear and non-linear spring damper models, reviews of which may be found in Kruggel-Emden et al. (2007, 2008, 2009). A commonly used model for time-resolved particle interactions in numerical simulations is a Hertzian contact force in combination with a linear

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damping (Lee and Herrmann, 1993; Kruggel-Emden et al., 2007). However, in contrast to linear spring models, no closed solution exists for this equation. One is hence forced to integrate numerically with a very small time step. This issue even leads some researchers to prefer linear spring models which are much easier to evaluate (Kruggel-Emden et al., 2009).

The discussion whether the linear or the non-linear approach is to be preferred seems unsettled in the community so far (Kruggel-Emden et al., 2009), and the present paper does not aim to compare these or to advocate one or the other. Instead, the mathematical properties of the equation of damped Hertzian contact are discussed and an efficient engineering approximation is proposed so as to reduce the cost of this model. This can enhance the efficiency of DEMs employing the physically more realistic non-linear approach.

Due to the time-step reduction required by many soft-sphere models, DEM practitioners often modify the material parameters of the collision model to alleviate this problem (Hoomans et al., 1996) and allow the use of larger time steps. The idea is to make the collision process softer, hence longer in time, at the price of increased numerical overlap of particles during collisions. Obviously, the collision process cannot be lengthened arbitrarily. In particular, if the collision time becomes large compared to the free propagation kinematic time scale, the dissipation of kinetic energy may become anomalously small (Luding et al., 1994). Thus, for certain dense multiphase flows, the permissible lengthening of the collision time may only be small. The choice of the stretching factor depends on the regime considered as well as the targeted accuracy and is within the responsibility of the practitioner. Especially for large simulations, even a small increase in step size can lead to significant savings in terms of computational resources and time. The results of the present work would be of use in the implementation of such schemes.

Except for the linear models, the adjustment of parameters in the soft-sphere model is usually performed by trail and error. This is time consuming and prone to a sub-optimal choice of values. A current trend in the modelling of particulate flows is that DEMs are enhanced by representations of the viscous effects of the continuous phase around the particles, cf. Uhlmann (2005) or Kempe and Fröhlich (2012b). In this framework, hard-sphere models are inapplicable as they cannot properly account for the coupling to the surrounding viscous fluid, thus introducing substantial numerical errors (Kempe and Fröhlich, 2012a). Here, soft-sphere models are required, with the drawbacks discussed above. As a remedy, a systematic strategy was recently proposed to determine the parameters for a softened contact model (Kempe and Fröhlich, 2012a). It is based on imposing the duration of the contact between the particles during collisions according to some external constraint, such as a pre-selected time step. The coefficients in the model are then determined so as to maintain the exact restitution coefficient. This guarantees maximal physical realism under given constraints imposed by computational resources. The approach, termed Adaptive Collision Time Model (ACTM), was implemented and tested with particles in viscous fluids for single collisions (Kempe and Fröhlich, 2012a) as well as for multiple simultaneous collisions (Kempe et al., 2014).

Beyond that, the approach is very interesting for pure DEM without viscous fluid, as it provides an automated systematic approach to regularizing the collision process. Another substantial advantage of this approach is that the original physical values of the coefficients can be introduced as bounds so that the original model is obtained again in a regular limit when the collision time is sufficiently reduced. This provides optimal commodity for the user.

It should be noted, that the full collision modelling procedure for particles in viscous flow proposed by Kempe and Fröhlich (2012b), termed Adaptive Collision Model (ACM), consists not only of the ACTM but also a lubrication model and an Adaptive Tangential Force Model (ATFM). The latter accounts for the effects of tangential forces during surface contact. This issue is not addressed in the present paper, which focuses on the treatment of normal collisions in the ACTM paradigm only.

In a simulation with many particles, each collision takes place with different velocities of the collision partners. Hence, when imposing the duration of contact and the restitution coefficient, one is forced to select the model coefficients for stiffness and damping for each collision individually. If no closed solution is available, this requires an iterative procedure, as indeed used so far (Kempe and Fröhlich, 2012a). In the present paper, this is now improved by providing a direct solution to this problem, based on a systematically controlled approximation. The increased efficiency is demonstrated by suitable test cases and comparison to the original method.

The paper is structured as follows. First, an exact formal solution of the equation of motion for a normal linearly damped Hertzian collision is derived using nonlinear transformations and a parametric series expansion. Then, a rigorous calculation of the collision time and restitution coefficient is carried out. As a next step, compact analytical approximations are developed. These formulæ allow the direct computation of the physically relevant parameters, i.e. collision time and restitution coefficient, from the intrinsic material parameters. Afterwards, the inverse problem is addressed. The artificial lengthening of the collision time, while preserving the restitution coefficient, requires the computation of the appropriate stiffness and damping. Finally, numerical tests demonstrate the accuracy and efficiency of the proposed algorithm, including test runs in typical engineering settings.

Basic equation of the collision process

The situation of a normal particle–wall collision is illustrated in Fig. 1. Particle deformation during contact is represented here by the overlap of the undeformed particle with the collision partner. The equation of motion governing the surface penetration $\zeta = \zeta(t)$ during the contact phase considered here is (Kempe and Fröhlich, 2012a)

$$m_\mathrm{p}\ddot{\zeta} = -d\dot{\zeta} - k\zeta^{3/2}, \tag{1}$$

with m_p the mass of the particle, d the damping coefficient and k a stiffness parameter, the last two being material properties. The overdot represents differentiation with respect to time t. The second term on the right-hand side is the nonlinear restoring force originally derived by Hertz (1882). The first term on the right hand side of (1) corresponds to the damping, which is assumed to be linear. For $d = 0$ the behaviour is termed ideally elastic. The initial conditions at the beginning of the collision are $\zeta(t = 0) = 0$, $\dot{\zeta}(t = 0) = u_\mathrm{in}$.

Eq. (1) is more conveniently expressed in dimensionless form by defining new variables τ, z with $t = \tau t_*$ and $\zeta = z\, u_\mathrm{in} t_*$, which is tantamount to fixing the characteristic unit of velocity for the system as u_in and choosing t_* as the (at present arbitrary) unit of time. The first and second derivatives of ζ can then be expressed as

$$\dot{\zeta}(t) = u_\mathrm{in}\,\dot{z}(\tau) \tag{2}$$

and

$$\ddot{\zeta}(t) = \frac{u_\mathrm{in}}{t_*}\,\ddot{z}(\tau). \tag{3}$$

Here and in all further cases of occurrence, the overdot denotes, when applied to a dimensionless quantity, differentiation with respect to the dimensionless time τ, unless stated otherwise.