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An accurate force–displacement law for the modelling of elastic–plastic contacts in discrete element simulations

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ABSTRACT

This paper presents an accurate model for the normal force–displacement relationship between elastic–plastic spheres in contact for use in discrete element method (DEM) simulations. The model has been developed by analysing the normal force–displacement relationship between an elastic–perfectly plastic sphere and a rigid surface using the finite element method (FEM). Empirical relationships are found that relate the parameters of the new model to material properties. This allows the model to be used in the DEM for direct simulation of well characterised elastic–plastic materials without fitting parameters to experimental results. This gives the model an advantage over models in the literature for which fitting to experimental results is required. The implementation of the model into an existing DEM code is discussed and validated against the results from FEM simulations. The new model shows a good match to the FEM results and the DEM implementation correctly distinguishes between the loading, unloading and re-loading phases of contact between two spheres.

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1. Introduction

Granular materials are of vital importance in many industrial and natural processes. For example they are widespread in the pharmaceutical industry [1] and natural processes such as avalanches and tidal mud flows [2]. The difficulty and expense of large-scale experiments involving granular flows and the lack of any over-arching physical laws to describe them means that they are ideally suited to computational study. To that end, computational modelling of granular systems has increased significantly in recent years [3], particularly using the discrete element method (DEM). The main advantage of DEM is that it gives information on the microscopic scale of individual particles, which can be used to explore the relationship between macro- and microscopic properties in granular materials.

Soft-sphere DEM was originally developed by Cundall and Strack [4]. Particle deformation is modelled as an overlap of the particles for every collision of a pair of particles. Simple models are used to relate this overlap, or displacement, to the forces acting on each particle. Newton's second law is then used to calculate accelerations that are integrated over small time-steps to determine the new velocities and positions of the particles. The nature of a model and its parameterisation directly affect the accuracy of a DEM simulation.

Models are usually designed for smooth particles of regular rounded shape and they provide force-displacement laws that account for both normal and tangential interactions. For elastic contacts, the Hertz [5] and Mindlin–Deresiewicz [6] models are the most common means to account for the normal and tangential components when the two contributions can be uncoupled. Their range of application and validity has been verified by detailed finite element (FEM) simulations and experiments conducted using elastic spheres [7,8]. However, most materials exhibit some form of energy dissipation, either viscoelastic or plastic, and these models are not able to describe these behaviours. A number of both normal and tangential models have been developed for viscoelastic and elastic–plastic materials and these are summarised in a number of review papers [9–13].

Zheng et al. [14] have recently developed a comprehensive viscoelastic model with both normal and tangential components that compares well to the results obtained using detailed FEM simulations. The model is an improvement on previous models not only because it is accurate but also because it has parameters that can be derived directly from material properties.

Elastic–plastic models are complex because they have to take into account the transition between elastic and plastic behaviour and between loading, unloading and reloading stages. Most of the models that have been developed use a piecewise approach to the different stages—that is different force–displacement relationships are used for elastic, elastic–plastic and unloading behaviours.

It has been shown in FEM simulations and experiments [15,16] that the relationship between the force and displacement is non-linear for

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elastic materials and for elastic–plastic materials immediately after the plastic yield displacement. However, a number of models use linear relationships between displacement and force because they are less computationally expensive to calculate thus allowing the simulation of larger systems using DEM. These include the recent models of Thakur et al. [17] and Pasha et al. [18], which also include adhesive forces, and the older Walton–Braun model [19], recently extended for cyclic loading [20]. Broadly speaking these models and the models of Luding [21] and Walton and Johnson [22] use linear springs, characterised by an appropriate stiffness, for each part of the force–displacement relationship. For the Thakur model stiffness values needed for a specific material are found by comparing the results of DEM simulations to experiment and calibrating the stiffnesses appropriately [23]. This requires experiments to be carried out for every material to be simulated. Similar procedures are required to find the stiffness values for the other models or alternatively the models can be fitted directly to experimental results [9,20].

The Thornton [24] model has three constituent parts: non-linear elastic loading and unloading and linear plastic loading

$$F = \begin{cases} -k\delta^{3/2}, & \dot{\delta} \geq 0 \wedge \delta < \delta_y \\ -\left(k\delta_y^{3/2} + \pi \cdot p_y \cdot R^*\left(\delta - \delta_y\right)\right), & \dot{\delta} \geq 0 \wedge \delta > \delta_y \\ -\left(k_{un}(\delta - \delta_{min})^{3/2}\right), & \dot{\delta} < 0. \end{cases} \quad (1)$$

The first part is the Hertz elastic model, where $k = 4/3E^*\sqrt{R^*}$. This gives the force up to a yield displacement

$$\delta_y = R^*\left(\frac{\pi p_y}{2E^*}\right)^2. \quad (2)$$

The second part is plastic, where p_y is the contact yield stress. Using the von Mises criterion, p_y can be calculated from the yield stress, σ_y, using $p_y = A_y[\nu]\sigma_y$ where $A_y[\nu]$ depends exclusively on the material's Poisson's ratio, ν [25]. Alternatively the plastic loading is often fitted to experimental or computational results using p_y as an adjustable parameter [9,26] rather than as a theoretically determined parameter. The third part is elastic unloading where $k_{un} = 4/3E^*\sqrt{R^*_{un}}$ is the elastic unloading constant. It is the Hertzian constant with the effective radius, R^*, replaced by the effective radius of unloading, R^*_{un} to account for the flattening of the contact due to the permanent plastic deformation. It is assumed that the ratio of the effective radii is equal to the ratio of the maximum elastic force and the actual maximum force. Thus, R^*_{un}, is

$$R^*_{un} = R^*\frac{k\delta^{3/2}_{\max}}{F_{\max}}. \quad (3)$$

The non-adhesive version of the Tomas model [27] is similar to the Thornton model. It uses the Hertz elastic model up to the same yield displacement. Above this displacement the loading relationship contains a parameter, the contact area coefficient, that represents the ratio of the plastically deformed area to the total deformed area. This parameter is 0 for perfectly elastic deformation and 1 for plastic deformation (at which point the loading relation is given by the same linear expression as in the Thornton model). Increasing this parameter with displacement allows the Tomas model to capture the non-linear nature of the force response in the intermediate elastic–plastic regime between pure elastic and pure plastic loading. In recent work [16,28] a fitting parameter is added to this loading relation in order to fit it to experimental results.

The original Tomas model is used with a Hertzian model for unloading [27], similar to the Thornton model but with an unchanged radius of curvature, appropriate for 'healing' contacts [29]. It is also used with an adapted radius of curvature [28] based on the work of Stronge [30] with an additional adjustable parameter to allow fitting to experimental results.

The Vu-Quoc and Zhang model [15] and the Li–Wu–Thornton (LWT) model [31] were developed using FEM simulations. They are both significantly more complex than the models previously considered and both models have to be solved numerically to obtain the force for a given displacement. This means that at every time-step numerous iterations have to be carried out for every collision in order to calculate the forces, making them computationally expensive.

There are also a number of force–displacement models in the tribology literature [32–35]. These are designed for much larger relative displacements than typically seen in DEM in order to model high force impacts, often of a single spherical object onto a near-rigid flat. These models include the analytical Brake model [32] and the empirical Jackson and Green model [33].

The Brake model has four parts: Hertzian elastic loading, elastic–plastic loading, purely plastic loading and elastic unloading. The plastic loading is linear and given by the product of the contact pressure and area. The elastic–plastic loading, between the yield displacement δ_y and the displacement at the onset of fully plastic loading, δ_p, is given by cubic Hermite polynomials. These depend on a series of derived parameters including δ_y and δ_p as well as the forces at these displacements and their derivatives. δ_p is related to the material hardness, H. The form of the unloading relation is the same as that in the Thornton model above with different expressions for R^*_{un} and δ_{min}, which depend on the type of loading at the maximum displacement.

The Jackson and Green (JG) model has two parts: Hertzian elastic loading and plastic loading. The plastic loading relation was determined empirically from FEM simulations and the parameters are directly related to the material properties. The original model does not contain unloading but it can be used [32,36] in conjunction with the unloading model of Etison et al. [37] or an empirical model fitted to the FEM results of Jackson et al. [38]. Unlike the Brake, Thornton and Vu-Quoc and Zhang models that use the Hertz elastic model up to the yield displacement given by Eq. (2), the JG model uses the Hertz elastic model up to 1.9 times the yield displacement (called the 'critical interference' by Jackson and Green).

Many of the models discussed suffer from limitations including the need for calibrating or fitting parameters to time consuming experiments for each material to be simulated, computational expense or being unable to replicate the non-linear nature of the force response. In this paper a new normal force–displacement model for spherical elastic–perfectly plastic particles that addresses some of these limitations is presented. It has been developed using detailed FEM simulations. Relationships between forces and displacements are derived for the loading, unloading and re-loading stages of the contact interactions and can be implemented into DEM without the need for complex numerical methods. The model has parameters that can be derived directly from material properties that have been independently characterised and is designed for small relative displacements common in DEM. It is compared with the Thornton model and the Brake and JG models.

2. Finite element simulations

2.1. Method

3D FEM simulations of the normal impact of a deformable elastic–perfectly plastic sphere on a rigid surface are carried out in order to investigate in detail the behaviour of the sphere when in contact with the surface. By symmetry the collision of a sphere with a rigid flat is the same as a collision of two identical spheres with the same material properties. The simulations are carried out using Abaqus software package [39]. Only a small portion of the sphere, which can be seen in Fig. 2, is simulated because the contact area is very localised. The contact radius obtained during the FEM simulations is much smaller than all other dimensions and, therefore, the remote boundaries do not affect the solution. This is the method employed by Zheng et al. [14] and they show that using a portion instead of the whole sphere has very little impact on the results of the

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