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Implementation of rotational resistance models: A critical appraisal

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ABSTRACT

Contact models that simulate rotational resistance at particle contacts have been proposed as a means to capture the effect of shape in DEM simulations. This contribution critically explores some key issues related to the implementation of rotational resistance models; these include the need for physically meaningful model parameters, the impact of the model on the overall numerical stability/critical time increment for the DEM model, model validation, and the assessment of model performance relative to real physical materials. The discussion is centred around a rotational resistance model that captures the resistance provided by interlocking asperities on the particle surface. An expression for the maximum permissible integration time step to ensure numerical stability is derived for DEM simulations when rotational resistance is incorporated. Analytical solutions for some single-contact scenarios are derived for model validation. The ability of this type of model to provide additional fundamental insight into granular material behaviour is demonstrated using particle-scale analysis of triaxial compression simulations to examine the roles that contact rolling and sliding have on the stability of strong force chains.

Introduction

Soil grains have distinct shape characteristics, e.g., sphericity, roundness and roughness, that depend upon their production, transportation, and deposition histories as well as their mineralogical composition. Different degrees of shape irregularity result in different degrees of interlocking between soil grains. The significance of particle shape on soil behaviour has been reported in many experimental studies (e.g., Cho, Dodds, & Santamarina, 2006; Shin & Santamarina, 2013; Yang & Wei, 2012). Recent research of Payan, Khoshghalb, Senetakis, and Khalili (2016); Payan, Senetakis, Khoshghalb, and Khalili (2016) showed that particle shape has a pronounced influence on the small-strain stiffness and damping ratio of sand.

Even if very high coefficients of friction are used, the peak and critical-state angles of shearing resistance observed in DEM simulations using spherical particles are significantly below what is expected for real sand (Huang, Hanley, O'Sullivan, & Kwok, 2014; Yang, Yang, & Wang, 2012; Thornton, 2000). These differences arise because of differences in geometry between spheres and real sand grains. One approach to capture the non-spherical nature of soil grains in DEM simulations is to introduce rotational resistance at contact points between discs or spheres to simulate interlocking between irregular particles; this approach is conceptually simple and less computationally expensive than directly simulating non-spherical particles either using irregular particles or by clustering small particles. Since the pioneering work of Iwashita and Oda (1998), a number of rotational resistance models have been proposed and applied in DEM simulations in two dimensions (Jiang, Yu, & Harris, 2005; Mohamed & Gutierrez, 2010; Tordesillas & Walsh, 2002) and in three dimensions (Jiang, Shen, & Wang, 2015; Plassiard, Belheine, & Donzé, 2009; Zhao & Guo, 2014; Zhou, Wright, Yang, Xu, & Yu, 1999). Use of these models has been shown to increase the strength and dilatancy of DEM assemblies. Hence, adding rotational resistance brings the results of DEM simulations of spherical particles closer to real soil behaviour. With spherical or circular particles, rotational resistance can alternatively be achieved by bonding particles together so that a single particle has multiple degrees of freedom (e.g., Jensen, Bosscher, Plesha, & Tuncer, 1999), clumping particles so that each particle has one degree of freedom and the constituent particles are used only for

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contact detection (e.g., Thomas & Bray, 1999), or inhibiting particle rotation completely (e.g., Calvetti, 2008). These approaches have differing computational cost implications. Inhibiting rotations will not increase the computational cost of simulations, however this is an extreme model and we know some rotation takes place in real materials (e.g., Oda & Kazama, 1998). Accurately capturing the geometry of realistic grain shapes requires hundreds of sub-particles to be used to produce something approaching a realistic topology (Garcia, Latham, Xiang, & Harrison, 2009), and even then only the form of the particle shape is captured and the surface topology differs from real particles. Consequently, even where a clumping/clustering model approach is used, a contact model enabling the control of rotational resistance is advantageous to improve model fidelity.

This study explores some of the critical issues related to implementation of rotational resistance models that have been neglected in most of the prior studies in the literature. First, a model that accounts for the extent of interlocking at contacts as well as the asperity strength is briefly introduced. Focussing on this model, some crucial general implementation issues are then discussed. A general procedure to identify a numerically stable critical time step when rotational resistance is considered is detailed. Closed-form solutions pertinent to several representative particle-and-wall contacting scenarios are derived that serve to both analyse model accuracy and check the implementation in a DEM code. Finally, the model's relevance to physical materials is demonstrated in simulations of triaxial compression; how rotational resistance influences force-chain stability and hence the overall behaviour are explored.

Model description

Physical origins of rotational resistance

Both particle form (overall shape) and surface texture (presence of asperities) contribute to rotational resistance via differing mechanisms (Johnson, 1985):

(a) Deviation of the branch vector direction from the contact normal direction:

For non-spherical particles, the branch vector direction ($\overrightarrow{O_A O_B}$) is no longer coincident with the contact normal direction $\vec{f}_{\mathrm{n}}$ (Fig. 1(a)). Under such circumstances, the contact normal does not pass through the particle centroid and can impose a moment on the particle or generate a resistance to a moment applied elsewhere. This mechanism is closely related to the particle sphericity.

(b) Effect of interlocking

The non-convex, rough nature of particle surfaces produces interlocking which can be illustrated by considering the relative motion between the two gears shown in Fig. 1(b). When the two gears roll over each other, the contact force (f) at the 'teeth' induces a moment that opposes the relative rolling direction for both particles in contact. Differentiating features that define particle shape from those that define roughness is subjective; the type of micro-asperities of size ≤1 μm considered by Senetakis, Coop, and Todisco (2013) and Otsubo, O'Sullivan, Sim, and Ibraim (2015) will not measurably contribute to rotational resistance. Cavarretta, Coop, and O'Sullivan (2010) proposed a lower limit of 0.1 for measurements of roundness and so the 'teeth' considered herein can be taken as features including corners used to define roundness and large asperities that are up to 0.05D, D being a representative particle diameter. The resistance to the relative angular motion depends on 'teeth' penetration which is associated with the external force (F) acting in the normal direction. A larger F should lead to deeper penetration of two particles which thereby increases the rotational resistance. The first mechanism can only be captured when non-spherical particles are used, whereas the second mechanism can be approximated by employing rotational springs at contact points using spherical particles. It is this second type of rotational resistance that is considered here.

Model formulations

The rotational resistance model used herein is similar to the model proposed by Jiang et al. (2015). A complete description of the model is provided as Supplementary information and can be accessed through the journal website; a brief overview is given here. The interaction between two contacting particles is assumed to occur over a finite circular contact area. The contact is idealised as composed of uniformly-distributed elastic springs in both the normal and tangential directions. The mean contact stiffness ($\bar{k}_{\mathrm{n}}$ and $\bar{k}_{\mathrm{s}}$) for each of the equivalent uniformly-distributed springs is equal to its equivalent for a single spring system (k_{n} and k_{s}) divided by the modified area A', i.e., $\bar{k}_{\mathrm{n}} = k_{\mathrm{n}}/A'$, $\bar{k}_{\mathrm{s}} = k_{\mathrm{s}}/A'$, and $A' = \pi(\delta B)^2$, in which B is the radius of the contact plane and δ is a shape parameter accounting for the undulating/nonsmooth nature of the contact surface.

The rotational resistance is decomposed into a rolling component M_{r} opposing the rotational motion around the axes in the contact plane and a twisting component M_{t} counteracting the rotational motion about the contact normal. M_{r} and M_{t} are calculated according to Eq. (1):

$$\begin{cases} M_{\mathrm{r},i} = \overline{k_{\mathrm{n}}} I_i \theta_{\mathrm{r}}^i \quad \& \quad M_{\mathrm{r},i} \le \kappa f_{\mathrm{n}} R_{\mathrm{r}} \quad (i = x, y) \\ M_{\mathrm{t},i} = \overline{k_{\mathrm{s}}} J_z \theta_{\mathrm{t}}^i \quad \& \quad M_{\mathrm{t},i} \le \mu \kappa f_{\mathrm{n}} R_{\mathrm{r}} \quad (i = z) \end{cases}, \tag{1}$$

in which $I_i = \frac{\pi}{4}\left(\delta B\right)^4$ is the area moment of inertia of a circular area with respect to the ith axis in the contact plane; $J_z = \frac{\pi}{2}\left(\delta B\right)^4$ is the polar area moment of inertia with respect to the contact normal (z axis); κ a strength index, which relates the compressive strength of asperities to the normal contact force; and θ_{r}^i and θ_{t}^i are

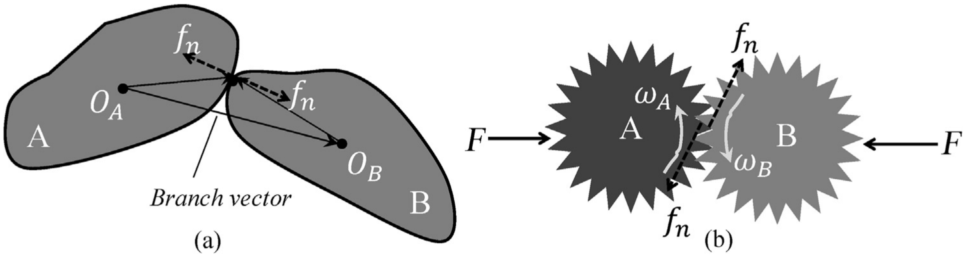

Fig. 1. Schematic of the physical origin of rotational resistance, showing (a) noncoincidence between the branch vector direction and the contact normal direction and (b) interlocking effect.

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