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A hybrid tabulation-scaling implementation of Thornton and Ning's plastic–adhesive particle contact theory

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ABSTRACT

Two novel implementations of the Thornton and Ning (TN) plastic–adhesive particle contact theory for use in numerical simulations using the discrete element method (DEM) are presented. They are both in contrast to the original TN implementation, which is indirect and requires an incremental calculation approach. First, a combined Newton–Raphson bisection (NRB) methodology, which calculates exactly the contact force in a non-incremental manner and, second, a tabulation-scaling (TS) implementation which closely approximates the elastic–adhesive unloading curve for a particle contact, resulting in a significant increase in computational speed, are described. The TS implementation is able to reproduce the total energy transferred during elastic–adhesive unloading force curves to within 3% of the exact NRB result. Since TN theory utilizes real material parameters, such as Young's modulus and adhesion energy, the TS implementation is a physically appealing and relatively fast (only slightly slower than Hertzian elastic spheres) method of performing a DEM simulation to predict the behaviour of plastic–adhesive particles. The subroutines for calculation of TN plastic–adhesive force are compatible with the open source DEM package, LIGGGHTS.

1. Introduction

The discrete element method (DEM) is now widely applied to a range of industrially important problems involving mixtures of fine adhesive powders, such as blends of drug and excipient particles used for pharmaceutical tablet compaction [1,2]. However, there are significant challenges in creating computationally tractable models that reproduce the correct physics of particle interactions. In particular, the use of a plastic–adhesive contact model, whereby particles may stick together due to their adhesion energies, and can dissipate energy during plastic deformation, may provide further insight into the potential problems of pharmaceutical tablet compaction. Unfortunately, the use of such complex contact models can greatly increase the required calculation time for DEM simulations [3].

Including the effect of plasticity in DEM simulations is a non-trivial task. Beginning with Hertz's theory of contacting elastic bodies, Stronge [4] explains how the normal force, contact radius and the work done change as the deformations transition to being elastoplastic and finally, fully plastic. This theory originates from Johnson [5] modelling the plastic zone as a hemisphere. An alternative theory of elastic–plastic particle contacts from Thornton [6] used a Hertzian contact to describe the elastic contact, and a Hertzian pressure distribution with a cutoff value for the yielded contact. This theory was extended by Li et al. [7], for rigid spheres in contact with elastic-perfectly plastic half spaces, to allow the pressure at the centre of the contact to vary with the contact radius. The effect of elastic–plastic asperities was accounted for by Chang et al. [8], and by incorporating conservation of volume into their model, they were able to more realistically calculate the contact area for rough surfaces.

The combined effects of adhesion and plasticity can be calculated especially quickly by linear contact models such as those by Luding [9] and Pasha et al. [10], but they lack a direct link between the contact model parameters and physical material properties. The contact model of Tomas [11] utilizes parameters which relate more directly to the material properties of the contacting bodies. By using parameters such as the "characteristic adhesion distance", which can be determined by the separation found in molecular interactions (Eq. (6) in Ref. [11]), the Tomas model enables prediction of behaviour for known materials. Unfortunately, not all of the model input parameters are easily obtained from common material properties, such as Young's modulus.

A theory developed by Thornton and Ning [6] offers the capability to combine the description of contact adhesion developed by Johnson, Kendall and Roberts (JKR) [5,12] with a theory proposed by Thornton and Ning for non-adhesive plastic contacts [6]. Like the original JKR theory, the Thornton and Ning (TN) theory utilizes real material parameters, such as Young's modulus and adhesion energy, giving it a more

Abbreviations: TN, Thornton and Ning; NRB, Newton–Raphson bisection; TS, tabulation-scaling.

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powerful predictive capability than alternatives which rely on experimental measurements of adhesive and plastic interactions. However, in its original implementation, it is rather complex and time-consuming to calculate.

In this paper, we present two new non-incremental procedures to calculate the TN plastic–adhesive force: first, a combined Newton–Raphson bisection (NRB) method that can be used to calculate the TN plastic–adhesive force independently of past calculations, except the unloading point (if required); second a novel tabulation-scaling (TS) procedure which is numerically stable and faster to calculate, while only losing a small amount of accuracy. A brief summary of TN theory and the original TN implementation will be presented in Section 1.1, before describing our alternative implementations in Section 2. An explanation of how TN theory is calculated by the NRB method is in Section 2.1. The numerical hygiene issues which inspired the NRB method are detailed in Sections 2.2, and 2.3 presents the TS method, which removes the need to solve computationally expensive quartic equations throughout a DEM simulation. Section 2.4 summarizes the benefits and issues with the TN, NRB and TS implementations. Section 3 contains the results from using the two new implementations of TN theory. Specifically, Section 3.1 compares the new implementations to the plastic–adhesive force curves of Thornton and Ning [6]. The error introduced into the elastic–adhesive unloading curve from using TS is explored in Section 3.2 and the computational performance is compared to a basic elastic Hertzian force in the open source DEM package LIGGGHTS [13] in Section 3.3. In Section 3.4, the relationship between the coefficient of restitution and impact velocity is explored, and results are compared to those in Ref. [6].

1.1. Thornton and Ning's plastic–adhesive contact model implementation

There are three main stages of the TN plastic–adhesive particle contact theory: elastic–adhesive loading, plastic–adhesive loading and elastic–adhesive unloading. In the original TN implementation, the contact force, P, is updated in an incremental fashion using Eq. (1), where t is the current timestep, Δt is the timestep increment, k is the contact stiffness and $\Delta\alpha$ is the change in particle overlap. In all three stages of plastic–adhesive particle contact, Eq. (1) is used, with k changing depending on the state of contact. The effective Young's modulus, E^*, and effective radius of the contact, R^*, are determined using Eqs. (5) and (6) both from Ref. [6] and are used throughout the simulation.

$$P(t+\Delta t) = P(t) + k\Delta\alpha \tag{1}$$

During elastic–adhesive loading, the initial force is described by JKR theory [5,12]. The force is calculated using Eq. (1) by setting k to $dP/d\alpha$ of Eq. (72) from Ref. [6]. The effective Hertzian force, P_1, and pull-off force, P_c, required to calculate k can be determined using Eqs. (60) and (50) both from Ref. [6], where Γ is the interface energy. Next, the contact radius, a, is updated using Eq. (59) from Ref. [6].

The contact can become plastic if the contact radius exceeds the contact radius at which yield occurs, a_y. The value of a_y is dependent on the limiting contact pressure, p_y (which is approximately equal to 2.4 times the yield stress [14]), and is determined using Eq. (65) from Ref. [6]. To update the force using Eq. (1) in the plastic contact regime, k is set to $dP_p/d\alpha$ in Eq. (69) from Ref. [6], where P_p signifies a plastic force. The contact radius during a plastic–adhesive contact is the contact radius determined by JKR theory [5,12,15]; therefore, the elastic–adhesive force is still determined at each timestep, as though yield never occurred.

The elastic–adhesive unloading force depends on the deformation history of the contact. If the contact never yields, the elastic–adhesive equations (Eqs. (72, 60, 50, 59) from Ref. [6]) are used to update the force and contact fails when overlap is equal to $-\alpha_f$ (see Eq. (49) from Ref. [6]). If the contact was in a plastic state just before unloading, then a unique elastic–adhesive regime begins, where the contact stiffness and new pull-off force are dependent on the amount of previous plastic deformation. In this paper, all future references to the elastic–adhesive unloading force refer to unloading after plastic deformation.

When elastic–adhesive unloading begins, a new effective radius is calculated, R_p^*, which can be determined using Eq. (76) from Ref. [6], where P_1^* is the effective Hertzian force at the point of unloading (acquired from the continued elastic–adhesive loading force calculations [15], and using Eq. (60) from Ref. [6]) and P^* is the plastic force at the point of unloading. To continue the force calculation in Eq. (1), k is set to $dP/d\alpha$ in Eq. (73) from Ref. [6], where the unloading pull-off force, P_{cr}, is calculated using Eq. (77) from Ref. [6], the unloading effective Hertzian force, P_{1r}, is calculated using Eq. (75) from Ref [6] and the contact radius during unloading is calculated using Eq. (74) from Ref. [6]. (It appears that R_{1r} is actually P_{1r} in the current version of Eq. (74) from Ref. [6], see [15].) It should be noted that the sign of $\pm$ in Eq. (75) from Ref. [6] is positive when elastic–adhesive unloading begins, and is negative when the unloading force reaches P_{cr} [15]. After reaching the minimum force, contact is broken when the force is equal to $\frac{-5}{9}P_{cr}$; however, contact can be re-established if reloading occurs and particle overlap is greater than α_d [15], where α_d is the larger of the two overlaps in the unloading curve when the force is equal to $\frac{-8}{9}$ P_{cr} [15]. If particle overlap increases so that P^* is exceeded, the plastic–adhesive contact regime begins again as described above. After the contact fails, the contact radius and force are held at zero until overlap is less than $-\alpha_f$.

2. New implementation of Thornton and Ning's plastic–adhesive model

2.1. Calculation details

In contrast to the original TN plastic–adhesive implementation, as described in the previous section, the present scheme is not of an incremental nature. Instead, a method which allows the direct determination of the force at any point of the contact, given its unloading history, will be described. This implementation still uses the theory set out by Thornton and Ning [6], and has the same three stages of contact. During an elastic–adhesive contact, JKR theory is used. Force determination begins with calculating the contact radius by solving Eq. (2), (originally Eq. (61) from Ref. [6]) as a quartic equation. The elastic–adhesive force is evaluated using Eq. (3) (originally Eq. (62) from Ref [6]). The elastic–adhesive contact radius and force are evaluated at every timestep during loading.

$$\alpha = \frac{a^2}{R^*} - \sqrt{\frac{2\pi\Gamma a}{E^*}} \tag{2}$$

$$P_{\text{elastic}} = \frac{4E^* a^3}{3R^*} - \sqrt{8\pi\Gamma E^* a^3} \tag{3}$$

Similarly to the TN implementation (Section 1.1), plastic deformation occurs when the elastic contact radius, a, exceeds the contact radius at which yield occurs, a_y, which is determined using Eq. (65) from Ref. [6] and the limiting contact pressure, p_y. During a plastic–adhesive loading contact, the force is determined using Eq. (4) (originally Eq. (66) from Ref. [6]). Note that the value of a is determined by solving Eq. (2).

$$P_{\text{plastic}} = \frac{4E^* a_y^3}{3R^*} - a_y\sqrt{8\pi\Gamma E^* a} + \pi p_y\left(a^2 - a_y^2\right) \tag{4}$$

The unloading regime depends on contact history, similar to the TN implementation. If the plastic–adhesive regime is never reached, Eqs. (2) and (3) are used to determine the elastic–adhesive force, until no real solutions can be found from Eq. (2). If plastic deformation preceded unloading, then a unique elastic–adhesive force is required. The