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A numerical model for the deterministic analysis of adhesive rough contacts down to the nano-scale

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ABSTRACT

A numerical model based on the Multi-Level Multi-Integration technique has been developed to study the adhesion between two surfaces. The model provides a self-consistent solution of surface separation and contact pressure throughout an arbitrary surface contact (including random surface roughness) with the adhesive interactions governed by the Lennard-Jones potential. Using this approach, the behaviour of rough surfaces can be assessed with a deterministic description of the surface, and contact stresses include valid adhesive interactions between all non-contacting surface nodes. The model is first compared to similar analyses from smooth surface models, where good agreement with published results is obtained. The model is then applied to randomly rough surfaces and shows both the significant impact of roughness on adhesive behaviour and how individual surface asperities influence the loading–unloading response of adhesive contacts. Lastly, the ability of the model to investigate nano-scale contacts is assessed through comparisons with atomistic simulations previously published elsewhere. It is clearly shown that our continuum mechanics-based model, in which an atomistic configuration is represented by a discretised continuum representation of the surface using a hard-sphere atomic model, is capable of reproducing many of the features identified through detailed atomistic simulations. The suitability of the presented model for studying adhesive contacts from the nano-scale to much larger, soft contacts, where adhesive forces can alter the contact mechanics, is demonstrated. The developed modelling tool and the algorithms implemented by the authors open the possibility to perform fast and accurate calculations using a deterministic description of the roughness for a wide variety of contact conditions.

1. Introduction

The terms adhesion or adherence are used when two bodies are stuck, or attracted to one another, and require some force to be separated. Adhesive forces are the attractive forces that can occur between two surfaces and may act between any two bodies in contact, whether or not they experience complete adherence. The presence of these adhesive forces will alter the mechanics of the contact to some extent. In many situations of interest, the effect of these adhesive forces is small compared to that of other contact forces and, consequently, can be neglected. However, this is not always the case. Two commonly cited examples are contacts between compliant (e.g. rubber) materials and contacts between bodies of nanometer dimensions. In both of these situations, adhesive forces should be accounted for in any valid contact analysis. Before returning to these examples in detail, it is useful to consider the physics of adhesive forces.

The Lennard-Jones potential, conventionally used to model simple interactions between two particles (atoms) in atomistic simulations, is also often used to describe adhesive forces in contact mechanics. The model is representative of van der Waals forces and neglects the possible influences of any electrostatic and capillary forces that may exist, but is a sensible representation for many cases of interest here. The Lennard-Jones potential is commonly expressed as:

$$V = 4\varepsilon\left\{\left(\frac{r_0}{r_s}\right)^{12} - \left(\frac{r_0}{r_s}\right)^{6}\right\} \tag{1}$$

where r_s is the separation of the two particles, r_0 is the separation at which the potential is minimum and ε indicates the strength of the interaction (the minimum potential with respect to the zero potential at an infinite separation). Differentiation of this potential with respect to r results in an expression for the force between two particles. This, in turn, can be integrated over a surface area to provide an expression that is more conveniently applied to a continuum

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description of contact mechanics. Thus the pressure acting between two infinite, parallel surfaces separated by a distance z is given by:

$$p = \frac{8w}{3z_0}\left\{\left(\frac{z_0}{z}\right)^9 - \left(\frac{z_0}{z}\right)^3\right\} \tag{2}$$

where z_0 is the equilibrium separation, w the work of adhesion. The work of adhesion indicates the possible strength of adhesive forces between two materials; it is equal to the work required to separate two infinite surfaces from equilibrium to an infinite distance and expressed in units of energy per unit area. This force-separation curve is shown in Fig. 1, from which a number of observations can be made. Firstly, there is a maximum value of adhesive pressure acting between any two materials, whilst the repulsive pressure has no such limit. Secondly, the attractive force reaches a maximum at a separation of $(1/3)^{1/6}z_0$, and decreases rapidly as the separation increases, being just 4% of its peak value at a separation of $4z_0$. These two aspects alone can explain the circumstances in which adhesive forces can and cannot be neglected, irrespective of the type of contact and the examples given above.

Since the maximum adhesive force has a fundamental limit, the contribution of adhesion in a contact will be negligible if the applied pressure is significantly larger than this value. For this reason, the effect of adhesive forces is more evident in contacts for which the net force is low, which generally applies to smaller contacts, of order nanometers for most engineering materials. The limited range of surface separation for which adhesive forces are non-trivial also accounts for observations of low adhesion. For adhesive forces to be noticeable at the scale of the overall contact, a significant portion of the surfaces must be separated by distances within this range. Once again, this requires contacts of nanometer scale, since values for z_0 are of <1 nm. It is also apparent that contact between rough surfaces will have a greater distribution of surface gaps, which would suggest that rough surfaces will experience lower adhesion – a fact well-reported. However, the details of this phenomenon are perhaps more complex and will be examined in the later discussion.

Early research of adhesion in the field of contact mechanics included that of Bradley (1932) but it was in the 1970s that significant progress was made. Any review of the literature on adhesive contacts will highlight the acrimonious (Johnson, 1998) disagreement between proponents of two analytical models developed in this period, the JKR model (Johnson et al., 1971) and the DMT model (Derjaguin et al., 1975). Both models considered adhesive contact between a smooth sphere and a flat body, but with different approaches and making significantly different assumptions. The idea that the two models are both correct (or both incorrect) for different types of contact was put forward by Tabor (1977) who identified a characteristic parameter, now known as the Tabor parameter, of which one form is given by:

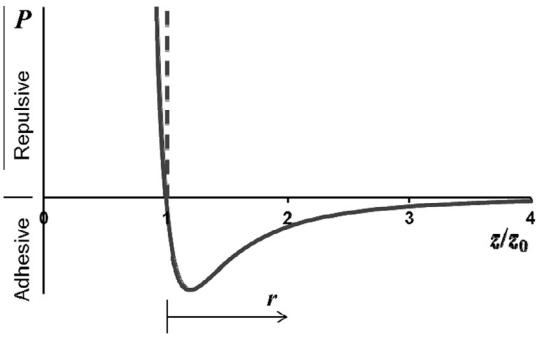

Fig. 1. Force-separation relationship for the parallel surface representation of the Lennard-Jones potential. The dashed line indicates an approximate solution for the repulsive forces.

$$\mu = \left(\frac{Rw^2}{E^{*2}z_0^3}\right)^{\frac{1}{3}}$$

where R is the radius of the sphere and E^* is the effective elastic modulus.

The JKR model was found to be representative only for contacts with a large value for the Tabor parameter ($\gg$5) and the DMT model for contacts with a small value ($\ll$0.1). This is regularly summarised by stating that the JKR model is suitable for larger, compliant contacts and the DMT for smaller, stiffer contacts. However, it must be recognised that neither model gives a full and accurate account of the contact mechanics; the assumptions made in each model become more or less valid depending upon the Tabor parameter, but each model remains an approximation of the true contact state and some local values for stress or displacement will be inaccurate. Moreover, there exists a transition region in which neither model is adequate. Muller et al. (1980) made progress in bridging the two models by removing the problematic assumptions and developing a self-consistent analysis of adhesive contact between a sphere and a flat. Greenwood later continued this approach with similar analyses to a higher level of accuracy and providing more detail of the method (Greenwood, 1997). Whilst these models seem to provide the solution to contact mechanics of smooth adhesive contacts, the complexity and numerical basis of the models hindered exploitation and alternative models were developed. Maugis applied a Dugdale-type analysis (from fracture mechanics to contact mechanics) to the problem (Maugis, 1992), replacing the true adhesive forces with a constant adhesive force acting between the surfaces at all points separated less than a critical distance. Greenwood and Johnson used a "double-Hertz" analysis to similarly simplify the solution and provide results suitable for analytical manipulation (Greenwood and Johnson, 1998). These methods may offer a step forward in analytical capabilities, but are a step back in accuracy from the Muller and Greenwood analyses, to which we will return for the development of our numerical model.

Finite element models for adhesive contact problems have also been developed, where the contact description obtained using the Lennard-Jones potential is incorporated into the framework of nonlinear continuum mechanics (Sauer and Li, 2007; Sauer and Wriggers, 2009), also in the presence of plasticity (Du et al., 2007) and within the context of multi-scale simulations, *e.g.* (Eid et al., 2011; Luan and Robbins, 2009). Alternative approaches have also been developed based on the boundary element method, which incorporates adhesion through energy minimisation (Carbone and Mangialardi, 2004; Carbone and Mangialardi, 2008).

Most of the models discussed above were developed for or applied to smooth surface contact, nominally between a sphere and a flat. Since a common justification for neglecting adhesive forces is the existence of surface roughness, a model is required that can account for the effects of surface roughness. An early and significant analysis was carried out by Fuller and Tabor (1975). Through a theoretical analysis based on an asperity model of roughness, it was shown that the adhesive influence could be described by an "adhesion parameter":

$$\theta = \frac{E^*\sigma^{\frac{3}{2}}}{\beta^{\frac{1}{2}}\Delta\gamma}$$

where β is the asperity radius, σ the *centre line average* roughness and $\Delta\gamma$ the surface energy (or work of adhesion).

This is, in effect, a ratio of the adhesive force of "lower" asperities to the elastic push of "higher" asperities. The theory was found to show reasonable agreement when fitted to experimental results. Fuller and Tabor had used the JKR model on an asperity level; Maugis repeated the analysis using the DMT model and