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A body-force formulation for analyzing adhesive interactions with special considerations for handling symmetry

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ABSTRACT

Adhesive interactions between particles are important in situations ranging from technological applications like atomic force microscopy to the initial stages of planet formation. In this work, we present a body force formulation with first-order convergence rate for the finite element analysis of adhesive interactions due to van der Waals force, which overcomes the restrictions of the commonly used surface force formulation. Though the classical Newton–Raphson method offers second-order convergence, substantial reduction in the computational cost per iteration justifies the use of present method in this case. First we discuss the general formulation, which is later modified for special cases like handling symmetry. We present a convenient implementation for reflective symmetry formulation, which can be easily extended to problems with any number of planes of symmetry. The axisymmetric formulation developed in this work provides significant computational benefits compared to a full three-dimensional formulation. The comparison of the results of our analyses with analytical solutions is provided for a number of benchmark problems. We also provide a comparison among general, reflective-symmetry and axisymmetric formulations in terms of accuracy and computational speed.

1. Introduction

Adhesion due to van der Waals interaction is of special interest in studies ranging from technological applications like atomic force microscopy [2] to the initial phase of planet formation [10]. It manifests in the origin of friction and wear [44] as well as in various biological processes including locomotion [31]. Such a wide-ranging significance has attracted extensive research on adhesive interactions in the form of theoretical [25], experimental [18], and computational [26,45] studies. Computational studies can help to bridge the gap between theoretical predictions and experimental observations by reducing the simplifications required for developing theoretical models, while not having all the complexities associated with experiments. In this work, we present a computational model for analyzing the adhesive interactions between two elastic particles.

Computational studies on adhesive contact mechanics commonly use finite element method for the analysis [26,45]. Such studies usually assume van der Waals force causing adhesion to be a surface force due to its steep gradient. This results in considerable computational advantages. For example, even commercial finite element software can be used for the analysis by suitably modifying the contact or other existing elements [26,12]. Sauer and Li [39,41] have developed an improved surface force formulation based on volumetric integration, various aspects of which are discussed in detail by Sauer and coworkers later [42,14]. They demonstrated its applicability by studying interaction between asperities for understanding the origin of friction [41,37] and many other important problems. However, when the size of the particles becomes very small or the adhesion becomes very strong, the surface force approximation becomes inaccurate. In addition, the inherent assumptions like uniform density assumption involved in developing a surface force model are not strictly valid when the deformation is large [42]. In all such situations, it is necessary to use a body force model considering the van der Waals force to be distributed over the volume of interacting particles [9,4].

Cho and Park [9] were the first to use the body force formulation for the finite element analysis of adhesive contact problems. They studied the interaction between an elastic body and rigid half-space in a quasi-static setting by making suitable modifications in Abaqus. Sauer and Li [40] extended the concept, and proposed a general framework for multiscale contact mechanics based on atomic interactions. The same researchers [36,38,39] developed the complete Newton–Raphson formulation of the body force model of adhesive interaction between elastic bodies. Even though this formulation offers quadratic convergence, it was observed that the implementation is computationally very costly due to the need for six levels of

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integration in analysis of a three-dimensional problem and the loss of sparsity of stiffness matrix, in addition to the involved numerical computations required for finding each elemental stiffness matrix term. Hence, the emphasis of those studies was on developing an improved surface force model suitable for moderately large problems. Fan et al. [11] have compared the body force and surface force models and concluded that the computational efficiency and coarse-mesh accuracy of the surface force model are better than those of the body force model. However, in cases like problems dealing with small particles or strong adhesion, it is necessary to use a body force model [42] employing a fine mesh.

In this paper, we present a formulation with first-order convergence rate for the finite element analysis of adhesive interactions between two elastic particles. Both the van der Waals and the short-range steric repulsion forces are modeled as body forces in this formulation. Due to the computational reasons mentioned above, we do not attempt to use the classical Newton–Raphson approach. Though our scheme with first-order convergence rate results in an increase in the number of iterations required, the reduction in computational cost per iteration justifies the use of such a formulation. We have discussed the development of the general formulation first and then the special cases like symmetry considerations. We present a convenient approach for handling reflective symmetry, which can be extended to any number of planes of symmetry as well as to repetitive symmetry situations. The axisymmetric formulation developed in this work offers significant computational advantages over the three-dimensional formulation. For the sake of completeness and consistency of notations, the outline of the entire formulation is given, though the general formulation is derivable from previous studies [36,38]. The formulation is implemented in a large deformation finite element code, incorporating stress–displacement hybrid elements [22]. A number of case studies are presented to validate and demonstrate the use of this formulation, and the computational aspects are also discussed.

2. Modeling and formulation

2.1. Force interaction between two volume elements

Let the potential of interaction between a pair of atoms in the interacting solids is represented by the $n-6$ *Lennard–Jones* potential:

$$V = -\frac{C}{r^6}+\frac{D}{r^n} \tag{1}$$

where r is the distance between the atoms and C and D are material constants. The first term in the above equation represents the attractive *van der Waals* force and second term is an approximation to the short-range *steric repulsion*. By adding potential of interaction between all pairs of constituent atoms (*pairwise addition*), we get the potential of interaction between two volume elements in the solid bodies:

$$V_{\mathrm{vol}} = \left(-\frac{C}{r^6}+\frac{D}{r^n}\right)\beta_1\beta_2\ \mathrm{d}\Omega_1\ \mathrm{d}\Omega_2 \tag{2}$$

where β_1 and β_2 represent the number of atoms in first and second volume elements ($\mathrm{d}\Omega_1$ and $\mathrm{d}\Omega_2$) respectively. The magnitude and sign of the force between two elemental volumes as shown in Fig. 1 is obtained by taking the gradient of the volumetric potential with the separation:

$$f_{\mathrm{int}} = -\frac{\partial V_{\mathrm{vol}}}{\partial r} = \left(-\frac{6C}{r^7}+\frac{nD}{r^{n+1}}\right)\beta_1\beta_2\ \mathrm{d}\Omega_1\ \mathrm{d}\Omega_2 \tag{3}$$

This force has a line of action connecting the two volume elements as shown in the figure. Utilizing the Hamaker constant defined as

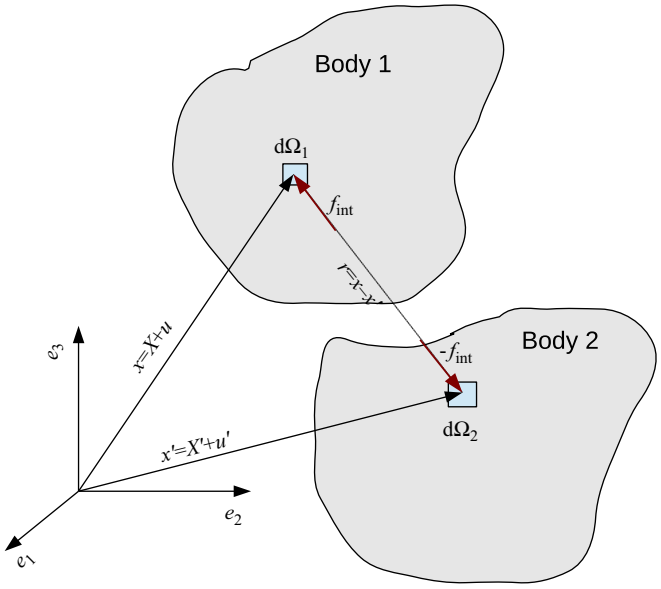

Fig. 1. Schematic diagram showing the force interaction between two volume elements. The net force at any point in a body should be obtained by integrating such elemental forces due to all the volume elements in the other body.

$A_{\mathrm{H}} = \pi^2 C\beta_1\beta_2$ [6,19] and a repulsion constant $A_{\mathrm{R}} = \pi^2 D\beta_1\beta_2$ [46] we get

$$f_{\mathrm{int}} = \left(-\frac{6A_{\mathrm{H}}}{\pi^2 r^7}+\frac{nA_{\mathrm{R}}}{\pi^2 r^{n+1}}\right)\mathrm{d}\Omega_1\ \mathrm{d}\Omega_2 \tag{4}$$

The body force per unit volume at any point in one body can be obtained by an integration over the other body. It may be noted that both the magnitude and the direction of interaction force depend on the locations of the volume elements, and hence vary during the integration. This integration is performed numerically within the finite element program as explained in the next section.

The Hamaker constant can be obtained from dielectric constants of the materials, and the values for interaction between various materials have been measured or estimated [6]. Hence the use of Hamaker constant in the above formulation helps to get rid of the inaccuracies associated with the pairwise additivity assumption. Given the value of n and *equilibrium* interatomic separation r_0, A_{R} and A_{H} can be related as [20]

$$A_{\mathrm{R}} = \frac{A_{\mathrm{H}}D}{C} = \frac{6A_{\mathrm{H}}(r_0)^{n-6}}{n} \tag{5}$$

The work of adhesion per unit area (w) can be expressed in terms of the Hamaker constant and the repulsion constant as [29,3,21]

$$w = \frac{(n-6)A_{\mathrm{H}}}{12(n-4)\pi z_0^2} \tag{6}$$

where z_0 is the equilibrium separation between two infinite plates without any external loads:

$$z_0 = \left(\frac{12A_{\mathrm{R}}}{(n-2)(n-3)A_{\mathrm{H}}}\right)^{1/6} \tag{7}$$

2.2. Finite element formulation

The body force at a point in body 1 due to a volume element in body 2 is obtained as given in Eq. (4). Hence the total body force vector at $\mathrm{d}\Omega_1$ due to body 2 can be obtained by summing up the contributions from all the finite elements in body 2, where the contribution from each finite element is obtained by numerical integration using Gauss quadrature method. The body force at any point in body 2 due to body 1 also can be obtained similarly. These