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An adhesive contact mechanics formulation based on atomistically induced surface traction

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ABSTRACT

In this work, we have developed a novel multiscale computational contact formulation based on the generalized Derjuguin approximation for continua that are characterized by atomistically enriched constitutive relations in order to study macroscopic interaction between arbitrarily shaped deformable continua. The proposed adhesive contact formulation makes use of the microscopic interaction forces between individual particles in the interacting bodies. In particular, the double-layer volume integral describing the contact interaction (energy, force vector, matrix) is converted into a double-layer surface integral through a mathematically consistent approach that employs the divergence theorem and a special partitioning technique. The proposed contact model is formulated in the nonlinear continuum mechanics framework and implemented using the standard finite element method. With no large penalty constant, the stiffness matrix of the system will in general be well-conditioned, which is of great significance for quasi-static analysis. Three numerical examples are presented to illustrate the capability of the proposed method. Results indicate that with the same mesh configuration, the finite element computation based on the surface integral approach is faster and more accurate than the volume integral based approach. In addition, the proposed approach is energy preserving even in a very long dynamic simulation.

1. Introduction

Contact that occurs at the interface between different continuum objects transmits forces. Classical (Hertz) contact between deformable bodies under large deformations has been extensively studied in computational contact mechanics, all of which are mainly focused on contact between large-scale objects governed by the principles of continuum mechanics and the no-penetrability condition [1,2]. With the increasing demand in nano-engineering and nano-science, the treatment of adhesive contact at nano/micro scale is becoming more and more important. The applications of small scale contact interaction range from nanoindentation [3–5], flexible nanotubes [6,7], MEMS design [8], atomic force microscopy [9–11], DNA strands and proteins [12], dynamic droplet spreading [13,14], to the contact/adhesion/crawling of living cells [15,16].

The adhesive contact phenomena at small scale can be modeled by several theoretical models, such as Johnson, Kendall and Roberts (JKR) model [17] and Derjaguin, Muller and Toporov (DMT) model [18]. Finite element based numerical methods have also be employed in modeling the adhesive/contact [19]. These analytical or numerical models have been successfully

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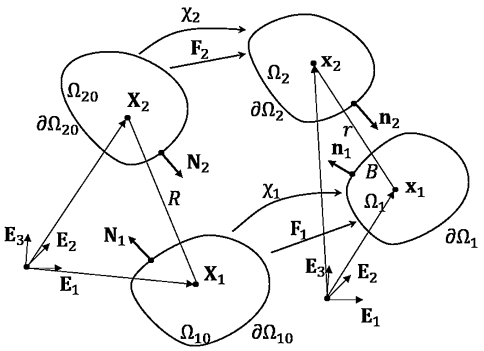

Fig. 1. Continuum description of the contact model.

applied to a lot of areas, but they have their intrinsic limitations, by either assuming infinitesimal deformations, contacting bodies with special geometries, or requiring one of the contacting body to be rigid, which substantially simplifies the computational treatment. Microscopically, the contact interaction of two bodies originates from the inter-body interaction of individual atoms or molecules. In principle, one can always directly simulate the problem using molecular dynamics [20–22], which essentially treats all participating atoms as classical objects whose motions are governed by the Newton's second law. But due to the intrinsic limitations [20], most of the studies using molecular dynamics mainly focus on the general principles, instead of practical applications in nano-engineering.

An appropriate model for describing such small scale contact/adhesion, should incorporate the microscopic interactions of the underlying atoms/molecules, formulate in nonlinear continuum mechanics framework, and at the same time maintain low computation cost. Similarly to classic Barrier contact method [1,23], one can characterize the small scale contact by introducing the inter-body interaction potentials between atoms/molecules into the total potential energy of the system. One of the advantages of this method is that it does not require any large penalty constant, such that the contact stiffness matrix of the system is in general well-conditioned. However, if one directly applies the body to body atomistic interaction potential to the system, the computational cost would be so large that no practical engineering problem can be solved. In this work, the double-layer volume integral describing the contact interaction (energy, force vector, matrix) is converted into a double-layer surface integral through a mathematically consistent approach that employs the divergence theorem and a special partitioning technique. Based on resulting surface formulation, a novel multiscale computational contact model is developed. We want to mention that the contact model developed here works for problems in both two and three dimensional space. A similar approach is accomplished in [24,25] for two-dimensional problem with certain physical assumptions.

The proposed contact model is formulated in the framework of nonlinear continuum mechanics and implemented for both quasi-static and explicit dynamic analysis. Results show that with the same mesh configuration, the proposed surface integral approach is faster and more accurate than the one directly applies the volume integral. The dynamic simulation of impact of the two cylinders within a rigid frame reveals that the proposed model is energy preserving in a long time dynamic simulation.

The paper is organized into five sections. In Section 2, the problem description of the multiscale contact model is presented in the framework of nonlinear continuum mechanics. In Section 3, the conversion from the double-layer volume integral to a double-layer surface integral for the contact model is presented. Section 4 deals with the Galerkin weak formulation of the proposed contact model. In Section 5, the details of finite element implementation for both quasi-static and dynamic cases of the multiscale contact model are being discussed. In Section 6, several numerical examples are presented with some discussions are provided. Finally in Section 7, we close the presentation by making a few remarks.

2. Problem description

We are considering two interacting bodies 1 and 2, as shown in Fig. 1. Subjected to certain boundary conditions (not shown in the figure) and the inter-body contact interactions, the two bodies originally occupying the physical domains Ω_{10}, Ω_{20} deform and evolve to Ω_1, Ω_2 in the current configuration. Correspondingly, the boundaries (surfaces) and unit out-normals of the two bodies change from $\partial\Omega_{10}$, $\partial\Omega_{20}$ and $\mathbf{N}_1$, $\mathbf{N}_2$ to $\partial\Omega_1$, $\partial\Omega_2$ and $\mathbf{n}_1$, $\mathbf{n}_2$.

If the system is conservative, the total potential energy of the system can be written as,

$$\Pi^{total} = \sum_{I=1}^{2} \left(\Pi^{int,I} + \Pi^{ext,I} \right) + \Pi^{C}, \tag{1}$$

where $\Pi^{int,I}$ is the internal elastic energy, $\Pi^{ext,I}$ is the external potential energy and Π^{C} represents the interaction potential energy due to the adhesive contact. In general, the internal elastic energy