A unified approach to computational contact problems at multiple length scales using adaptive homogenization of nanoscale contact

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Abstract

We present a novel computational contact formulation suitable for contact-interaction problems at different length scales ranging from the nanometer scale to macroscopic length scales. The proposed model is an advancement of a recently developed contact model that combines the approaches of molecular mechanics and continuum mechanics [1], [2]. This recent model is based on the coarse-graining of the discrete, interatomic interactions, like the Lennard-Jones potential, into an effective continuum contact formulation which can be implemented efficiently within a computational contact framework like the finite element method. It allows the accurate description of contact problems at atomistic scales as they occur in nanoindentation [3] and carbon nanotube interaction [1]. While, in principle, the model proposed in [1] can be applied to macroscopic problems, its formulation becomes computationally inefficient at large length scales. This motivates a modified formulation which aims to restore efficiency, while maintaining accuracy for increasing scales.

The new research presented here offers such a formulation. It is based on a second level of coarse-graining which is constructed from a Gaussian distribution on a logarithmic scale. The Gaussian distribution is used to homogenize the fine-scale contact forces into effective, coarse-scale forces. The degree of this homogenization is variable and can thus be chosen such that a balance between accuracy and efficiency of the resulting model is achieved over varying length scales. Thus an adaptive computational contact model is obtained, based on atomistic interactions, that is suitable to simulate contact problems at a wide range of different length scales using a single unified model. The novel contact model is contrasted with classical computational contact approaches developed for macroscopic contact problems, like the penalty, Lagrange multiplier, barrier and cross-constrained method [4]. We highlight the insights gained from atomistically-based contact modelling which help to better understand and improve macroscopic contact modelling both conceptually and computationally. The proposed computational contact model is illustrated by several numerical examples.

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