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Green's function techniques for atomic-scale static and dynamic contact

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Contact mechanical calculations are important for computing interaction forces and pressure distributions below contacting and sliding bodies. Traditional approaches rely on continuum elasticity and cannot capture the dynamical response of a material. We here show how to construct Green's functions for atomic solids in the static limit and how to extend those techniques to dynamical contact problems. This allows the computation of the surface mechanical response of systems effectively consisting of billions of atoms.

Keywords (from 3 to 5 max): surface lattice Green's functions, boundary element method, contact mechanics

1. Introduction

Mechanical contacts occur in many technical and biological systems, and they determine our experience with the surrounding through touch or when walking. Contact is governed by a balance between the energy gained when making intimate atomic contact and the deformation energy required for surfaces to conform. Sophisticated analytical and computational continuum models have been developed over the last century that accurately describe the deformation energy and contact in the static limit. Those numerical models typically map the subsurface deformation on the surface degrees of freedom, leading to a boundary-element formulation of the surface's small-strain elastic response. Continuum boundary-element formulations have also been developed for the dynamic (typically viscoelastic) response of a surface within the last decade. Atomic-scale boundary element formulations have a much shorter history, starting with the pioneering work by Campana & Müser [1], later extended by one of us [2]. Atomic-scale dynamic contact methods have not yet been described in the literature.

2. Methods & Discussion

We present a new dynamic contact Green's function method for solving time-dependent contact mechanics problems in atomistic settings. In a semi-infinite system, modes with in-plane wavevectors $\sim q$ are excited at the surface and propagate into the bulk. Surface modes disperse through phonon coupling into the continuum of three dimensional wavevectors in the bulk and do not return to the surface. Modes are effectively damped as they move away from the interface. Our approach is motivated by the simple observation that large q modes propagate the shortest distance into solids, while small q modes persist over large ranges and times.

We describe the entire system by a single Hamiltonian and the only approximation is to neglect anharmonic terms in the substrate. Many other atomistic/coupling schemes introduce ghost forces or cannot be described by a single Hamiltonian. Previous applications of the Green's function approach have also neglected some forces near the elastic/explicit boundary leading to violations of Newton's third law and ghost forces when interactions extend beyond nearest layers.

The static Green's function can be efficiently calculated using transfer matrix or renormalization group techniques [2]. Fourier transforming in the plane of the substrate reduces the problem to a one-dimensional coupling between N layers for each in-plane wave vector q. The method is applicable to pair or many-body potentials (such as embedded-atom method or bond-order potentials) as long as the interaction is short-ranged.

For the full dynamic response of the system, we solve the lattice dynamical equation that arises from the harmonic approximation for the bulk atoms. Since modes are viscously damped with a damping coefficient $\sim q$, small q modes propagate further into the solid than large q modes. For each (surface)-q, we can therefore treat the bulk solid up to large depth for small q but small depth for large q [3]. This reduces the computational effort for solving the dynamical problem from N^3 N to N^3 ln N.

The static and dynamic contact methods are demonstrated on typical contact mechanics problems (Hertz, rough surfaces) as well as collision (coefficient of restitution) and dynamic friction problems.

3. Dedication

Mark O. Robbins, mentor and friend to both of us, was directly involved in the development of the techniques described here.

4. References

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