Multiscale modeling for crystalline materials: a comprehensive study in statics and dynamics

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Preprint no. 2024-07

Abstract

Computational materials science plays a crucial role in advancing new and improved materials. To leverage the advantages of local and nonlocal methods and aid in the advancement of predictive capabilities for materials, multiscale models have been introduced. Many such methods have been proposed to overcome computational challenges in accuracy and efficiency.

In this work, a symmetric and consistent blended force-based Atomistic-to-Continuum scheme for 1D atomistic chains is created. The conditions for the well-posedness of the underlying model are established by analyzing an optimal blending size and blending type to ensure the stability for the blended force-based operator. Several numerical experiments are presented to test and confirm the theoretical findings.

Then, a Peridynamics-to-Peridynamics model is created to model a bimaterial bar in one dimension. Peridynamics naturally allows for the simulation of crack propagation in its model due to its use of integro-differentials and time derivatives instead of the spatial derivatives typical of classical models. We prove the conservation laws, derive the dispersion relation, and estimate the coefficient of reflection near the interface for this nonlocal-to-nonlocal problem. We then investigate optimal interaction kernel for the cross-material interaction to reduce spurious reflection artifacts.

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