An Accurate and Efficient Blended Quasicontinuum Energy

Predictive Simulation and Design of Materials by Quasicontinuum and Accelerated Dynamics Methods

Mitchell Luskin
University of Minnesota
206 Church St SE, Minneapolis, MN 55455

Abstract

The quasicontinuum energy (QCE) of [2] directly couples an atomistic model to a volume-based finite element continuum model based on the Cauchy-Born strain energy density. QCE reproduces the atomistic energy density for a uniformly deformed lattice simply by modifying the volume of the tetrahedra at the boundary of the atomistic region. The atomistic and Cauchy-Born energies give zero net forces for a uniformly deformed lattice by symmetry, but the symmetry is broken in the QCE atomistic-to-continuum interface and QCE does not thus satisfy the *patch test*.

The development of patch test consistent quasicontinuum energies for multi-dimensional crystalline solids modeled by many-body potentials remains a challenge. We propose that by blending the atomistic and corresponding volume-based Cauchy-Born continuum models of QCE in an interfacial region with thickness of a small number k of blended atoms, a blended quasicontinuum energy (BQCE) can be developed that significantly improves the accuracy of QCE. To define our blended quasicontinuum energy, we let $\beta : \Omega \to [0,1]$ be a blending function and define

$$\mathcal{E}^{\beta}(y) := \sum_{\text{atomistic}} \beta_j \mathcal{E}^a_j(y) + \sum_{T \in \mathbb{T}} \nu^{\beta}_T W(\nabla y|_\ell)$$

where $\mathcal{E}^a_j(y)$ is the energy of atom j, $W(F)$ is the Cauchy-Born strain energy density, ∇y_T is the deformation gradient on the triangle T, and where ν^{β}_T is explicitly given by the blending function and the triangulation $\mathbb{T}$ in the continuum region [3]. The BQCE energy can be implemented for any decomposition of three-dimensional space into tetrahedra, and a code for the BQCE energy can be developed by simply suppressing the coarsening in the blending interface of an existing QCE code. Our initial numerical tests have demonstrated that the BQCE energy is the most accurate atomistic-to-continnum coupling energy that has been implemented to date.

We have proven for a one-dimensional chain that the ℓ^2 strain error for the QCE energy, which has low order $O(\varepsilon^{1/2})$ where ε is the atomistic length scale, can be reduced by a factor of $k^{3/2}$ for an optimized blending function [3]. The QCE energy has been shown to suffer from a $O(1)$ error in the critical strain at which the lattice loses stability [1]. We have proven that the critical strain error of BQCE can be reduced by a factor of k^2 for an optimized blending function [3], thus demonstrating the accuracy of the BQCE energy near lattice instabilities such as crack growth.

References

[1] M. Dobson, M. Luskin, and C. Ortner. Accuracy of quasicontinuum approximations near instabilities. *Journal of the Mechanics and Physics of Solids*, 58:17411757, 2010. arXiv:0905.2914v2.

[2] E. B. Tadmor, M. Ortiz, and R. Phillips. Quasicontinuum analysis of defects in solids. *Philosophical Magazine A*, 73(6):1529–1563, 1996.

[3] B. Van Koten and M. Luskin. Analysis of energy-based blended quasicontinuum approximations, 2011. arXiv:1008.2138v3 [math.NA].