

Predictive and Efficient Quasicontinuum Methods

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The development of predictive and efficient atomistic-to-continuum computational methods requires both an analysis of the error and efficiency of its many components (coupling error, model and mesh adaptivity, solution methods) as well as its integration into an efficient method capable of solving problems of technological interest. Mathematical challenges are presented by the complex energy landscape of materials with defects and microstructure, where the classical numerical analysis techniques developed for convex energy landscapes and elliptic partial differential equations is inadequate.

For crystalline materials, there are typically a few small regions with highly non-uniform structure caused by defects in the material which are surrounded by large regions where the local environment of the atoms varies slowly. The idea of the Quasicontinuum Method is to achieve accuracy similar to a fully atomistic simulation while reducing the computational complexity in regions where the strain gradient is small. It does so by selecting representative atoms as nodes for piecewise linear interpolation and by further approximating the nonlocal atomistic energy by a local strain energy density. Since the position of material defects is typically not known *a priori*, we have developed adaptive algorithms to determine where the accuracy of atomistic modeling is needed and how to coarsen the mesh in the continuum region.

There are many choices available for the interaction among the representative atoms, especially between those in the atomistic and continuum regions, which has led to the development of a variety of quasicontinuum approximations. We will present criteria for determining a good choice of quasicontinuum approximation for a given problem that considers trade-offs between accuracy and algorithmic efficiency. Our criteria are based on an analysis of the effect of the coupling error on the goal of the computation, on the integration of the quasicontinuum approximation with model and mesh adaptivity, and on the development of efficient iterative solution methods.

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