

RECENT ADVANCES IN QUASICONTINUUM AND OTHER ATOMISTIC/CONTINUUM METHODS

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ABSTRACT

Atomistic-continuum bridging methods such as the Quasicontinuum (QC) method have proven to be very powerful techniques for micromechanical simulations of deformation processes. The combination of atomistic resolution and continuum description allows rigorous calculations of deformation fields across a wide range of length scales, seamlessly bridging them. Many examples exist in the literature where these coupling methods have been successful in studying processes such as nanoindentation, nanovoid deformation, crack propagation, grain boundary processes, fundamental dislocation junction properties, etc. However, many challenges still remain, such as generalizations of QC to finite temperature, improving sampling techniques for highly non-convex energy landscapes, treatment of free surfaces, quantifying coarse graining force and energy calculations, consistent error estimation and adaptive meshing techniques, etc. In this minisymposium, we aim to provide a forum to present and exchange research results featuring contributions on advancing the QC method or other atomistic/continuum methods.

REFERENCES

- [1] Tadmor, E.B., Ortiz, M., and Phillips, R. Quasicontinuum analysis of defects in solids, *Philosophical Magazine A*, 1996, 73, 1529-1563.
- [2] <http://qcmethod.org/>