

A Quadrature-rule Type Approximation to the Quasi-Continuum Method¹

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Abstract

A quadrature-rule type approximation of the quasi-continuum method for atomistic mechanics is presented. Simple analysis and computational experiments are presented that illustrate that the new method has, for the same accuracy, lower complexity compared to not only the quasi-continuum method, but also to cluster-type approximations of that method. A discussion about some implementation issues connected to the new method is also provided.

Keywords: quasi-continuum method; atomistic models; quadrature-rule type approximation; nanoindentation; Lennard-Jones potential.

AMS subject classification: 70C20, 70-08, 65N30, 65N15

¹This work was supported by the US Department of Energy under grant number DE-FG02-05ER25698 as part of the Office of Science's "Multiscale Mathematics" program.