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SUMMATION RULES FOR THE QUASICONTINUUM METHOD

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The *quasicontinuum* (QC) method was introduced to seamlessly bridge from atomistics to the continuum by applying finite-element interpolation schemes to a coarse-grained atomistic ensemble, see e.g. [6, 5]. This is achieved by three integral components of the method: *geometric constraints* (which interpolate lattice site positions from the positions of a reduced set of representative atoms), *summation rules* (which avoid energy/force sampling over the full atomistic ensemble), and *model adaptation* schemes (which localize full atomistic resolution and thereby efficiently minimize degrees of freedom). To date, numerous QC flavors have been developed which mainly differ in the approximation schemes used to implement the aforementioned three aspects.

Summation rules have become a key cornerstone of every QC method because model accuracy and computational efficiency essentially rest upon evaluating all thermodynamic quantities of interest (such as energies or forces) at a very small number of carefully-chosen sampling atoms instead of the full atomistic ensemble, comparable to quadrature rules commonly used in finite elements. We have carried out and will report results from a comprehensive comparison of summation rules within the *non-local QC* formulation [7].

Summation rules now differ by the choice of (i) which lattice sites to choose as sampling atoms, and (ii) how their weights are computed. The choice of sampling atoms is, in principle, completely independent of the choice of representative atoms; there is no need (in fact it has turned out to be disadvantageous) to evaluate energies and forces only at the interpolation nodes. Successful examples of summation rules introduced previously include node-based cluster summation [3] or quadrature-type summation [2, 8] with sampling atoms chosen nearest to Gaussian quadrature points in addition to nodes in the finite element mesh. Systematic mathematical error and stability analysis of node-based cluster summation rules have highlighted the deficiencies of force-based QC schemes and have advocated for an energy-based QC formulation [4, 1]. We therefore consider only energy-based summation rules.

While many previous studies have reported simple one- or two-dimensional examples with simplified potentials to assess the accuracy of summation rules, we report the first large-scale comparative review of existing summation rules, and we propose consistent and efficient new summation rules. To this end, we summarize results obtained from representative three-dimensional examples containing millions of degrees of freedom (in turn representing billions of lattice sites) with realistic interatomic potentials. These include the computationa of elastic constants (on uniformly and completely randomly coarse-grained systems), the simulation of nano-indentation as well as nano-void expansion. Besides a careful analysis of existing summation rules, we present a new summation rule based on sampling atoms and weights based on a Voronoi tesselation, which shows a superior combination of accuracy and efficiency.

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