1046-74-225 **Yanzhi Zhang*** (yzhang@scs.fsu.edu), Deparment of Scientific Computing, Florida State University, 400 Dirac Science Library, Tallahassee, FL 32306-4120, and **Max Gunzburger** (gunzburg@scs.fsu.edu). *Quadrature-rule type approximations to the quasicontinuum method.*

Quasicontinuum method using representative particles provides a simplified model to study huge molecular systems. However, its calculation still involves operations over all particles so that it does not essentially reduce the computational cost. The objective of this study is to develop quadrature-rule type approximations to further simplify the quasicontinuum method. For both short and long-range interatomic interactions, the complexity of the quadrature-rule type method depends on the number of representative particles but not on the total number of particles. Numerical experiments illustrate that the quadrature-rule type method is efficient and that it preserves much of accuracy of the quasicontinuum method. In fact, for the same computational cost, the quadrature-rule type approximation produces more accurate results than the quasicontinuum method.

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