Numerical Quadrature in the Quasicontinuum Method with Application to Nanoindentation Simulation

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Recent research in atomistic-to-continuum coupling and in particular in the Quasicontinuum (QC) method has shown a strong interest in numerical quadrature because it largely determines the methods accuracy and efficiency, [1]-[5]. Mathematical analyses of quadrature schemes often restrict to the 1-D case of atomic chain models, to simple pair potentials and to additional ad-hoc assumptions. These simplifications make the problem tractable by analytical means or alleviate numerical analysis. Doing this, mathematics has brought new insights into concurrent multiscale modelling. However, it is not clear, whether the obtained results and conclusions of such analyses can be transferred to problems without these simplifying assumptions.

The main aim of the present contribution is the numerical analysis of different quadrature rules within the QC method in a more realistic physical setting, namely in 3-D applying EAM-potentials in paradigmatic multiscale settings of computational materials science. In particular, we compare the method proposed in [4] with the cluster-based summation rule as proposed in [1] and analyzed in [2]-[5]. The quadrature schemes are assessed in representative numerical examples like nanoindentation which showcase the influence of numerical features like numerical quadrature and (adaptive) meshing on reliable predictions of key materials and process information.

References

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