A GAMMA-CONVERGENCE ANALYSIS OF THE QUASICONTINUUM METHOD

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Continuum mechanics models of solids have certain limitations as the length scale of interest approaches the atomistic scale, for instance when studying defects. A possible solution in such situations is to use a pure atomistic model. However, this approach could be computational prohibited as we are dealing with million of atoms. The quasicontinuum (QC) method is a computational technique that reduces the atomic degrees of freedom. In this talk, we review two foundational steps of QC: interpolation schemes and summation rules. Using the tools of Gamma-convergence (a variational notion of convergence which, in particular, implies convergence of energy minimizers), we identify sufficient conditions on the interpolation and on the summation rules for the sequence of approximating energies to be convergent in the case of harmonic lattices. Numerical convergence studies on three-dimensional BCC crystals governed by empirical potentials are presented. The convergence properties of the numerical model bear out the results of the Gamma-convergence analysis.

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