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Numerical Methods for Multilattices

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Among the efficient numerical methods based on atomistic models, the quasicontinuum (QC) method has attracted growing interest in recent years. The QC method was first developed for crystalline materials with Bravais lattice and was later extended to multilattices (Tadmor et al, 1999). Another existing numerical approach to modeling multilattices is homogenization. In the present paper we review the existing numerical methods for multilattices and propose another concurrent macro-to-micro method in the numerical homogenization framework. We give a unified mathematical formulation of the new and the existing methods and show their equivalence. We then consider extensions of the proposed method to time-dependent problems and to random materials.

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