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Mesh Optimization for the Quasicontinuum Method: A Generalization of VALE

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The current formulation of the Quasicontinuum (QC) method relies on a static triangulation of the reference crystal configuration. This computational mesh needs to encompass a wide range of spatial resolutions, from fully atomistic at defect cores, to continuum-like in defect-free regions. Moreover, it must continously adapt to the structure of the deformation field, so as to return the least possible potential energy for a fixed number of nodes. To this end, the mesh adaption process has been usually governed by empirical indicators. We present an extension of the Variational Adaptive Lagrangian-Eulerian (VALE) method into the QC context. In the spirit of VALE, the computational mesh is factored directly into the description of the energetics of the crystal. Therefore, the potential energy minimizer determines not only the equilibrium configuration of the crystal, but also the optimal configuration of the computational mesh. We apply the VALE-QC method to the investigation of early stages of plastic deformation during nano-indentation.

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