Variationally-based Quasicontinuum Method for Elasto-Plastic Lattices

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ABSTRACT

In the last two decades, significant accomplishments have been made in the development of discrete materials models. The flexibility offered by these models, however, comes at the expense of increased computational costs. This is mainly due to the fact that many problems are of a *multi-scale nature*, since the application scale is much larger than that of the discrete links. An approach to overcome this obstacle is offered by the QuasiContinuum (QC) method, proposed by Tadmor *et al.* [3] for crystalline lattices. The method itself consists of two steps. First, *interpolation*, based on a number of selected representative particles, constrains the displacements of the remaining particles in the network. In the regions of interest, the discrete model is fully resolved, whereas fewer representative particles are employed elsewhere. Second, *summation*, in which the governing equations of the reduced model are determined by collecting the contributions from sampling particles, works in analogy to numerical integration in the finite element method.

Since its introduction in 1996, QC has been mostly applied to atomistic structures interacting via long-range *conservative* potentials. Only recently, Beex *et al.* [1] have demonstrated that the approach is also applicable to discrete material models, typically governed by the nearest-neighbor *dissipative* interactions. The goal of this contribution is to reconcile and rationalize the development by Beex *et al.*, based on the virtual-power statements, in a suitable variational framework.

Our formulation builds on the theory of *energetic solutions* for the rate-independent evolution, developed by Mielke and co-workers [2]. In this framework, the mechanical system is described by *stored* and *dissipated* energies and the evolution of the system is provided by the conditions of energetic stability and energy equality. For QC methods, the basic scheme must be complemented with the approximation and summation steps, defining the *coarse-grained* stored and dissipated energies. Using a benchmark example from [1], we demonstrate that the original formulation by Beex *et al.* delivers an energy-consistent evolution. In addition, we show that despite the significant dimension reduction and time savings achieved by the QC method, the errors in stored and dissipated energies due to interpolation and summation are rather low.

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REFERENCES

[1] L. A. A. Beex, R. H. J. Peerlings, and M. G. D. Geers. A multiscale quasicontinuum method for dissipative lattice models and discrete networks. *Journal of the Mechanics and Physics of Solids*, 64:154–169, (2014).

[2] A. Mielke. Evolution of rate-independent systems. *Handbook of Differential Equations: Evolutionary Equations*, volume 2, pages 461–559. Elsevier B.V., Amsterdam, The Netherlands, (2005).

[3] E. B. Tadmor, M. Ortiz, and R. Phillips. Quasicontinuum analysis of defects in solids. *Philosophical Magazine A*, 73(6):1529–1563, (1996).