eXtended Variational Quasicontinuum Methodology for Modelling of Crack Propagation in Discrete Lattice Systems

Ondřej Rokoš[¶,*], Ron H. J. Peerlings[¶], Jan Zeman[†], Lars A. A. Beex[‡]

[¶] Department of Mechanical Engineering, Eindhoven University of Technology

[†] Department of Mechanics, Faculty of Civil Engineering, Czech Technical University in Prague

[‡] Faculté des Sciences, de la Technologie et de la Communication, Campus Kirchberg, Université du Luxembourg

E-mails: o.rokos@tue.nl, r.h.j.peerlings@tue.nl, jan.zeman@fsv.cvut.cz, lars.beex@uni.lu

ABSTRACT

Lattice models can be successfully used for modelling materials with discrete micro- or meso-structures, mainly because they can relatively easily incorporate non-localities, complex constitutive laws, and large fibre deformations or reorientations. Typical examples of such materials are 3D-printed structures, woven textiles, paper, foams, or concrete.

The accuracy, generality, and simplicity of discrete models come usually at the expense of excessive computational cost. This is due to the multi-scale nature of engineering problems, which require large number of interactions as the application scale is often much larger compared to the size of individual links. The Quasicontinuum (QC) methodology, introduced by Tadmor *et al.* [1], was developed to overcome this kind of limitation for conservative atomistic systems at the nano-scale. Recently, extensions towards models with dissipative interactions at the meso-scale have been developed, first based on the Coleman-Noll procedure in [2], and later based on the variational theory of energetic rate-independent systems [3].

QC, as a concurrent multiscale method, is especially suitable for modelling of damage, fracture, and crack propagation in discrete materials, mainly due to the fact that the dissipative mechanisms and nonlocalities matter most in a relatively small fracture process zone near the crack tip. Elsewhere, interpolation and coarse-graining can be used. In this presentation, the necessary extensions of variational QC towards an effective modelling of crack propagation in discrete mesoscopic systems are discussed, including the following concepts: (i) definition and geometrical description of cracks, (ii) introduction of partition-of-unity-based concepts and enrichment of the displacement interpolation, (iii) generalization of summation rule to accurately sample the incremental energy of the extended system, (iv) reconstruction of energy quantities upon mesh refinement and coarsening, and (iv) development of effective and robust mesh refinement and coarsening strategy. The efficiency and performance of the method thus obtained is demonstrated on a number of test examples.

REFERENCES

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

[2] 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).

[3] O. Rokoš, L.A.A. Beex, J. Zeman, R.H.J. Peerlings. A variational formulation of dissipative quasicontinuum methods. *International Journal of Solids and Structures*, Volumes 102-103, 15 December 2016, Pages 214–229.