Quasicontinuum methods for planar beam lattices

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The quasicontinuum (QC) method is multiscale approach for lattice models that fully resolves lattice models in regions in which individual lattice events need to be captured and coarse-grains elsewhere. The QC method was originally proposed to reduce the computational costs of atomistics [1] and has so far mainly been used for this, e.g. [2-5]. Recently however, the QC method has been reformulated in terms of virtual-power to deal with (local and nonlocal) dissipation mechanisms [6,7]. In this way the QC approach can also be used for structural lattice models using dissipative springs, e.g. for electronic textile [8].

A significant amount of structural lattice models use beams, in contrast to springs, depending on the material one desires to model. Whereas the kinematic variables of spring lattices are only formed by nodal displacements, those of beam lattices consist of nodal displacements and nodal rotations. Consequently, QC approaches for beams need to deal with the nodal rotations as well. Furthermore, when planar beam lattices experience out-of-plane deformation, the nodal displacements and nodal rotations are nonlinear functions of the nodal coordinates. This means that QC approaches for beam lattices require higher-order interpolation. Consequently, standard summation rules do not suffice. This presentation will show a number of QC formulations to deal with the typical issues arising in planar beam lattices and clearly distinguishes between the error due to interpolation and the error due to summation. Finally, the QC formulation most convenient in terms of accuracy versus efficiency, is presented [9].

[1] Tadmor EB, Ortiz M, Philips R, Quasicontinuum analysis of defects in solids, Phil. Mag. A, 73 (1996) 1529-1563.
[2] Espãnol MI, Kochmann DM, Contixz S, Ortiz M, A convergence analysis of the quasicontinuum method, Multiscale Model. & Simul., 11 (2013) 766-794.
[3] Yang Q., Biyikli E, To AC, Multiresolution molecular mechanics: statics, Comput. Meth. Applied M., 258 (2013) 26-38.
[4] Kochmann DM, Venturini GN, A meshless quasicontinuum method based on local maximum-entropy interpolation, Model. Simul. Mater. Sc., 22 (2014) 034007.
[5] Yang Q., Biyikli E, To AC, Multiresolution molecular mechanics: convergence and error structure analysis, Comput. Meth. Applied M., 269 (2014) 20-45.
[6] Beex LAA, Peerlings RHJ, Geers MGD, A multiscale quasicontinuum method for dissipative lattice models and discrete networks, J. Mech. Phys. Solids., 64 (2014) 154-169.
[7] Beex LAA, Peerlings RHJ, Geers MGD, A multiscale quasicontinuum method for lattice models with bond failure and fiber sliding, Comput. Meth. Applied M., 269 (2014) 108-122.
[8] Beex LAA, Peerlings RHJ, Van Os K, Geers MGD, The mechanical reliability of an electronic textile investigated using the virtual-power-based quasicontinuum method, Mech. Mater., 80 (2015) 52-66.
[9] Beex LAA, Kerfriden P, Rabczuk T, Bordas SPA, Quasicontinuum-based multiscale approaches for plate-like beam lattices experiencing in-plane and out-of-plane deformation, Comput. Meth. Applied M., 279 (2014) 348-378.