Journal of the Mechanics and Physics of Solids 64 (2014) 154–169

Contents lists available at ScienceDirect

Journal of the Mechanics and Physics of Solids

journal homepage: www.elsevier.com/locate/jmps

A multiscale quasicontinuum method for dissipative lattice models and discrete networks

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ARTICLE INFO

Article history:
Received 23 January 2013
Received in revised form
26 September 2013
Accepted 20 November 2013
Available online 1 December 2013

Keywords:
Multiscale
Quasicontinuum method
Lattice model
Virtual power
Dissipation

ABSTRACT

Lattice models and discrete networks naturally describe mechanical phenomena at the mesoscale of fibrous materials. A disadvantage of lattice models is their computational cost. The quasicontinuum (QC) method is a suitable multiscale approach that reduces the computational cost of lattice models and allows the incorporation of local lattice defects in large-scale problems. So far, all QC methods are formulated for conservative (mostly atomistic) lattice models. Lattice models of fibrous materials however, often require non-conservative interactions. In this paper, a QC formulation is derived based on the virtual-power of a non-conservative lattice model. By using the virtual-power statement instead of force-equilibrium, errors in the governing equations of the force-based QC formulations are avoided. Nevertheless, the non-conservative interaction forces can still be directly inserted in the virtual-power QC framework. The summation rules for energy-based QC methods can still be used in the proposed framework as shown by two multiscale examples.

1. Introduction

Structural lattice models and discrete networks that include trusses or beams are frequently used to represent discrete microstructures of fibrous materials (Bronkhorst, 2003; Clyne et al., 2005; Zohdi and Powell, 2006; Stylianopoulos and Barocas, 2007; Ridruejo et al., 2010; Silberstein et al., 2012; Beex et al., 2013; Wilbrink et al., 2013). Likewise, for investigating the mechanical responses of other materials, e.g. concrete and polymers, lattice models and discrete networks are often applied (Lilliu and Van Mier, 2003; Cusatis et al., 2003; Ostoja-Starzewski and Wang, 2006; Rinaldi et al., 2008; Kim and Buttlar, 2009; Zhao, 2012). The advantage of discrete models is that they naturally incorporate discrete phenomena occurring in meso- and microstructures of many materials. Individual microscale events such as fiber failure and bond failure, precursors for macroscale failure, can be readily incorporated in lattice models, whereas these they are not easily included in continuum models. Even the incorporation of global mechanisms such as large rotations may lead to relatively complex continuum models and finite element implementations (Peng and Cao, 2005; Ten Thije et al., 2007), whereas they are naturally captured by truss networks.

A clear disadvantage of lattice models is the required computational effort for large-scale physically relevant models. This large computational cost essentially results from the construction of the lattice model at the meso- or microscale. Consequently, if lattice models are being used for macroscopic computations, a large number of lattice points is involved. First, this leads to a large number of degrees of freedom (DOFs) making the system of equations computationally expensive

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0022-5096/$ - see front matter
http://dx.doi.org/10.1016/j.jmps.2013.11.010

to solve. Secondly, the construction of the system of equations is computationally expensive because all lattice points must be visited for this (Beex et al., 2011).

A suitable approach to reduce the computational cost of structural lattice models is the quasicontinuum (QC) method. The QC method was originally developed for the reduction of atomistic lattice models by Tadmor et al. (1996a) and has been widely used to investigate phenomena such as intergranular fracture (Miller et al., 1998) and nanoindentation (Tadmor et al., 1996b; Knap and Ortiz, 2001; Kulkarni et al., 2008). In a previous study (Beex et al., 2011) the applicability of the QC method has been demonstrated for structural lattice models of fibrous materials that employ elastic trusses. An overview of several QC frameworks is given by Miller and Tadmor (2002).

The benefit of the QC method is its intrinsic multiscale character, allowing the accurate incorporation of local lattice defects in large-scale problems. This is not trivially possible with multiscale methods that are based on computational homogenization (Stylianopoulos and Barocas, 2007). Moreover, the QC method entirely relies on the microstructural lattice topology, unlike approaches as those of Xiao and Belytschko (2004) and Fish et al. (2007), that need a continuum description in addition to the discrete model. This is an advantage, since continuum descriptions for fibrous materials tend to be complex to formulate (Peng and Cao, 2005). Another advantage is that a number of QC frameworks (Knap and Ortiz, 2001; Eidel and Stukowski, 2009; Beex et al., 2011, submitted for publication) do not require a handshaking region or coupling procedure between fully resolved domains (in which the exact lattice model is recovered) and coarse domains (in which an approximation is made). Several other multiscale approaches require such a coupling procedure (Shenoy et al., 1999; Xiao and Belytschko, 2004; Fish et al., 2007; Ha-Minh et al., 2011).

The QC method introduces two remedies to reduce the computational cost of lattice models. First, interpolation is applied to the displacements of the lattice points to reduce the number of DOFs and thus reducing the size of the governing set of equations. In coarse regions, the interpolation triangles are large so that many lattice points are interpolated. In regions of interest, e.g. around lattice defects, the exact lattice model is captured by refining the interpolation such that every lattice point corresponds to a point of the interpolation triangulation (so-called representative point or reppoint).

Secondly, so-called summation rules are used in the QC method to ensure that only a small, selective number of lattice points (so-called sampling points) needs to be visited to construct the governing equations, instead of all lattice points. To obtain an accurate solution, all lattice points in the fully resolved regions are sampling points, while in the coarse regions only a small number of points is used (see for instance the studies of Zhang and Gunzburger, 2010; Beex et al., 2011 and Beex et al., submitted for publication).

Most QC formulations are based on minimizing the total potential energy of the interpolated system (Tadmor et al., 1996a; Miller et al., 1998; Shenoy et al., 1999; Eidel and Stukowski, 2009). Also the QC formulation of Beex et al. (2011), developed for structural lattice models with elastic interactions only, uses this ansatz. Depending on the application, such an elastic description is adequate (Delincé and Delannay, 2004; Sharma and Sutcliffe, 2004; Gonella and Ruzzene, 2008; Hatami-Marbini and Picu, 2009; Zeman et al., 2011). For many applications however, more advanced descriptions of lattice interactions are required that include dissipation in the lattice interactions by e.g. using plasticity (Kato et al., 1997; Desphande et al., 2001; Arnoux et al., 2002; Bronkhorst, 2003; Chen and Baker, 2003; Mohr, 2005; Doyoyo and Hu, 2006; Silberstein et al., 2012; Beex et al., 2013; Wilbrink et al., 2013) or damage (Cusatis et al., 2003). In these cases, a straightforward minimization of the potential energy can no longer be employed since the dissipation leads to non-conservative interactions. Energy-based QC formulations are thus inadequate for structural lattice models with dissipative interactions.

Existing force-based QC formulations may be appropriate alternatives. The QC formulations that depart from a force-equilibrium however (Knap and Ortiz, 2001; Kulkarni et al., 2008), also appear to be energetically inconsistent for conservative systems. This has been shown by Eidel and Stukowski (2009) for the widely used cluster QC approach of Knap and Ortiz (2001).

The aim of this study is therefore to develop an energetically consistent QC formulation for non-conservative lattice models. Our point of departure for this forms a virtual-power statement (Germain, 1973) in which the non-conservative forces can be directly inserted. As a result, the framework is equivalent to energy minimization for conservative lattices, but its applicability is broader.

Another advantage of using the virtual-power statement is that summation rules proposed in energy-based QC formulations can directly be used in the proposed QC methodology. In this study, the summation rule for atomistic lattice models as presented by Beex et al. (submitted for publication) is used to reduce the computational efforts of the considered lattice model.

The outline of this paper is as follows. In Section 2 the thermodynamics of structural lattice models with dissipative interaction forces are formulated. The lattice model of interest is discussed here as well. In Section 3, the virtual-power-based QC formulation is introduced and applied to an elastoplastic lattice model consisting of an equidistant X-braced truss network with elastoplastic interactions. This fairly simple lattice model is chosen in order to show the possibilities of the framework. In Section 4 two multiscale numerical examples are simulated to evaluate the accuracy and efficiency of the virtual-power-based QC method and to illustrate some of key features for fibrous materials.

2. Structural lattice models with non-conservative interactions

It is useful to formulate structural lattice models, as adopted in the QC method, on a thermodynamic basis. The reason is that most QC methods are based on energy-minimization and that thermodynamical inconsistencies in sampling points are carried over to their corresponding lattice points. These inconsistencies can significantly contribute to the inaccuracy of the