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A multiscale quasicontinuum method for lattice models with bond failure and fiber sliding

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ABSTRACT

Structural lattice models incorporating trusses and beams are frequently used to mechanically model fibrous materials, because they can capture (local) mesoscale phenomena. Physically relevant lattice computations are however computationally expensive. A suitable multiscale approach to reduce the computational cost of large-scale lattice computations is the quasicontinuum (QC) method. This method resolves local mesoscale phenomena in regions of interest and coarse grains elsewhere, using only the lattice model. In previous work, a virtual-power-based QC framework is proposed for lattice models that include local dissipative mechanisms. In this paper, the virtual-power-based QC method is adopted for lattice models in which bond failure and subsequent frictional fiber sliding are incorporated – which are of significant importance for fibrous materials such as paper, cardboard, textile and electronic textile. Bond failure and fiber sliding are nonlocal dissipative mechanisms and to deal with this nonlocality, the virtual-power-based QC method is equipped with a mixed formulation in which the kinematic variables as well as the internal history variables are interpolated. Previously defined summation rules can still be used to sample the governing equations in this QC framework. Illustrative examples are presented.

1. Introduction

Structural lattice models and discrete networks using trusses and beams are often used for the mechanical modeling of fibrous materials with discrete fibers and yarns at the mesoscale and microscale [23,36,21,41,13,39,55,45,51]. They are typically used to model biological materials [2,11,47,24,1], paper networks [8,3,33,46,29] and textiles [27,42,58,9,10,6]. The discrete elements in lattice models naturally represent the discrete fibers and yarns of these materials. Therefore, lattice models intrinsically capture discrete mechanical phenomena that occur at the mesoscale or microscale, such as fiber fracture, failure of interfiber bonds and fiber sliding. Even global phenomena such as large rotations of yarns are naturally incorporated in lattice models, whereas these are complex to include in continuum descriptions of fibrous materials [38,50].

Also the mechanical microscale behavior of other materials, for which a discrete representation seems not directly relevant, are nowadays often modeled with lattice models and discrete networks. Reasons are the simplicity and intrinsic discreteness of lattice models and the ability to capture highly anisotropic behavior. Failure of concrete is for instance regularly modeled using lattice models [12,32], whereas they are also used to investigate polymer behavior [37,40,26,56] and delamination of thin films [52].

A disadvantage is the computational cost for physically relevant macroscale lattice computations [32], since lattice models are constructed at the level of the mesoscale or microscale. Consequently, macroscale lattice computations have a large

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number of degrees of freedom (DOFs) which makes their governing equations inefficient to solve. The second cause of large computational costs is the computational effort to construct the large number of governing equations.

Multiscale techniques can be adopted to increase the efficiency of large-scale structural lattice computations. Stylianopoulos and Barocas [47] have used a classical homogenization scheme for a lattice model of a collagen network. Classical homogenization schemes are able to capture macroscale properties such as the effective stiffness from the mesoscale lattice model, but they are unable to capture local discrete events such as the fracture of an individual fiber. Individual failure events are important to include in mechanical models because they are the precursors of macroscale failure of fibrous materials. In another multiscale approach, continuum descriptions in coarse domains are coupled to lattice models in regions of interest. This is for instance used by Ha-Minh et al. [20] to model ballistic impact of a woven textile. Failure of discrete fibers and bonds can be modeled by such a multiscale scheme in regions where the lattice model is used. Disadvantages are that the required continuum models for fibrous materials are not trivial to formulate (as mentioned before) and the non-trivial procedures to couple continuum regions to discretely resolved lattice regions.

Other multiscale approaches that are promising for structural lattice models (using trusses and beams) are frameworks that increase the efficiency of atomistic lattice computations. Like structural lattice models, atomistic lattice models include discrete interactions. Several of these [14,54,16] also combine continuum descriptions with lattice models, also involving a considerable complexity. The quasicontinuum (QC) method [48] however, only relies on the lattice model and is successfully used for atomistic lattice computations [49,34,35,30,31]. Conveniently, a continuum description is thus not required. Several QC methods still require a coupling procedure for the internal interface between coarse domains and fully resolved domains of interest – due to the use of the Cauchy–Born rule which is local [48,49,43,44]. However, some avoid this internal interface [28,15,18,5,7]. A number of QC methodologies are therefore potentially convenient for structural lattice models and discrete networks. In the study of Beex et al. [4] a QC approach without internal interface has been developed to deal with (conservative) structural lattice models.

In the recent work of Beex et al. [7], a QC framework has been proposed that is based on the virtual-power statement of non-conservative structural lattice models since many structural lattice models include dissipation. This is in contrast to other QC methods [15,4,5] developed for conservative atomistic lattice models that are based on energy minimization and cannot deal with dissipative lattice models. Using a virtual-power approach, non-conservative lattice forces can be directly inserted in the QC framework of Beex et al. [7]. This has been shown for a structural lattice model with elastoplastic trusses.

The aim of this work is to extend the approach to be able to deal with interfiber bond failure and subsequent frictional fiber sliding.

The failure of interfiber bonds (and subsequent fiber sliding) is an important cause of failure of fibrous materials. Different studies have been carried out to investigate bond failure in paper networks [22,25,19,33,29]. Bond failure for a nonwoven glass structure was modeled by Ridruejo et al. [39] and fiber sliding (i.e. slippage) in textiles was investigated by Zhu et al. [57]. Here, a refined version of the lattice model for bond failure and subsequent fiber sliding of Wilbrink et al. [53] is used. Instead of the small-sliding formulation of Wilbrink et al. [53], we use an expression for the energy stored in the lattice that allows for large sliding displacements. Furthermore, our model is rate-dependent instead of the rate-independent case considered by Wilbrink et al. [53].

The same type of linear interpolation is used for the sliding displacements (internal history variables) as for the regular displacements (kinematic variables). Consequently, the summation rule of Beex et al. [6], in which only one internal sampling point in each interpolation triangle is selected, can still be used. The extension of the virtual-power-based QC framework is validated by comparing the results of multiscale QC examples, in which bond failure and subsequent fiber sliding occur, to the results of direct lattice computations.

The outline of the paper is as follows. First the lattice model of Wilbrink et al. [53] is reformulated, including a viscous dissipation and an energy expression that allows for large sliding displacements. In the subsequent section, the main principles of the virtual-power-based QC method are considered, as well as the incorporation of the lattice model for bond failure and fiber sliding. In Section 4, multiscale examples are shown and their results are compared to those of the direct lattice computations. Finally, conclusions and recommendations are presented in Section 5.

2. Lattice thermodynamics for bond failure and fiber sliding

QC frameworks increase the efficiency of lattice computations by means of interpolation of the displacements and summation rules to approximate the governing equations instead of resolving them exactly – this is discussed in more detail in the next section. Using summation rules, the potential energy (in this framework the virtual-power) of only a small number of lattice points (so-called sampling points) is determined, instead of determining the potential energy (or virtual-power) of all lattice points. Structural lattice models must be thermodynamically consistent so that no errors occur in the potential energy (or virtual-power) of these sampling points. The reason is that the error in a sampling point is also present in the lattice points that are represented by the sampling point. This can result in a poor accuracy. The formulation of a thermodynamically consistent structural lattice model including bond failure and fiber sliding is therefore first considered along the lines of Germain [17], as well as a possible solution strategy.

The lattice model considered in this study is an equidistant X-braced network with linear elastic trusses, see Fig. 1. It can be observed that in general every lattice point (i.e. a truss node) is connected to eight neighboring points. Lattice points are