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A quasicontinuum theory for the nonlinear mechanical response of general periodic truss lattices

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Abstract

We present a framework for the efficient, yet accurate description of general periodic truss networks based on concepts of the quasicontinuum (QC) method. Previous research in coarse-grained truss models has focused either on simple bar trusses or on two-dimensional beam lattices undergoing small deformations. Here we extend the truss QC methodology to nonlinear deformations, general periodic beam lattices, and three dimensions. We introduce geometric nonlinearity into the model by using a corotational beam description at the level of individual truss members. Coarse-graining is achieved by the introduction of representative unit cells and an affine interpolation analogous to traditional QC. General periodic lattices defined by the periodic assembly of a single unit cell are modeled by retaining all unique degrees of freedom of the unit cell (identified by a lattice decomposition into simple Bravais lattices) at each macroscopic point in the simulation, and interpolating each degree of freedom individually. We show that this interpolation scheme accurately captures the homogenized properties of periodic truss lattices for uniform deformations. In order to showcase the efficiency and accuracy of the method, we perform simulations to predict the brittle fracture toughness of multiple lattice architectures and compare them to results obtained from significantly more expensive discrete truss simulations. Finally, we demonstrate the applicability of the method for nonlinear elastic truss lattices undergoing finite deformations. Overall, the new technique shows convincing agreement with exact, discrete results for most lattice architectures, and offers opportunities to reduce computational expenses in structural lattice simulations and thus to efficiently extract the effective mechanical performance of discrete networks.

Keywords: truss lattice, multiscale modeling, homogenization, finite elements, fracture

1. Introduction

Extracting the effective response of materials with engineered microstructures has been a focus of attention for decades, most recently revived by powerful small-scale fabrication techniques of additive manufacturing. The theoretical foundation for the micromechanical modeling of metamaterials began probably with the calculation of the effective, homogenized moduli of periodic linear elastic composites (Hill, 1963). Various extensions of homogenization theory followed, including probabilistics and wave propagation (Bensoussan et al., 1978) as well as nonlinearity (Geymonat et al., 1993). An excellent overview of mechanical, acoustic, and electrical properties of various microstructured materials (including trusses, foams, honeycombs, and natural materials) was presented in (Gibson and Ashby, 1997). Periodic truss networks are particularly appealing as metamaterials, since their effective, macroscale performance can be linked to the truss geometry and lattice topology. For example, the mechanical properties of truss lattices vary greatly depending on the nodal connectivity of trusses, which stems from the disparity in bending stiffness vs. stretching stiffness of slender beams. Gibson and Ashby (1997) introduced the notion of *stretching-dominated* lattices (which have homogenized elastic constants that scale with the axial, stretching stiffness of an individual strut) and *bending-dominated* lattices (which have at least one elastic constant that scales with the bending stiffness of a

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strut). The effective Young's modulus E^* of an isotropic lattice with relative density $\bar{\rho} = V_{\text{struts}}/V_{\text{UC}}$ (volume of the solid material in the unit cell divided by the volume of the unit cell) was thus derived as

$$E^* \sim E\bar{\rho}^\alpha, \quad (1)$$

with E denoting Young's modulus of the constituent material. For stretching-dominated lattices, $\alpha = 1$, whereas for bending-dominated lattices $\alpha = 3$ or $\alpha = 2$ in 2D or 3D, respectively. Unfortunately, comparable scaling laws for nonlinear truss properties or the failure behavior of truss lattices are hard to find and generally involve numerical methods.

The prospect of designing metamaterials with drastically different macroscopic properties has led to a significant amount of research into predicting the effective linear, nonlinear, and failure behavior of lattice architectures by modeling representative volume elements; see, e.g., (Berger et al., 2017; Fan et al., 2009; Gurtner and Durand, 2014; Hutchinson and Fleck, 2006; Okumura et al., 2004; Pal et al., 2016; Tancogne-Dejean et al., 2016; Tankasala et al., 2017; Vigliotti and Pasini, 2012b; Vigliotti et al., 2014). Others have used hierarchical multiscale modeling techniques (mainly FE^2) to simulate truss lattices (Asada et al., 2009; Vigliotti and Pasini, 2012a).

Imperfection sensitivity, flaw tolerance, and fracture toughness of truss lattices have been investigated via expensive discrete lattice simulations (Choi and Sankar, 2005; Cui et al., 2011; Fleck and Qiu, 2007; Romijn and Fleck, 2007; Thiyyagasundaram et al., 2011; Quintana Alonso and Fleck, 2007, 2009; Schmidt and Fleck, 2001; Slepian and Ayzenberg-Stepanenko, 2002; Symons and Fleck, 2008; Tankasala et al., 2015). Lipperman et al. (2007) used the representative cell method (Ryvkin and Nuller, 1997) to develop inexpensive brittle fracture toughness models of periodic truss lattices (mainly in 2D). Recent advances in manufacturing techniques have enabled the experimental characterization of fracture properties (Quintana-Alonso et al., 2010; OMasta et al., 2017), of the nonlinear compressive response (Meza et al., 2017, 2014; Bauer et al., 2016; Zheng et al., 2014), and of the imperfection sensitivity (Montemayor et al., 2016) of 3D truss lattices.

As the sheer number of truss members contained in such truss lattices disqualifies brute-force modeling techniques (where every truss member is modeled as a structural element) due to extreme computational expenses, many have turned to hierarchical multiscale methods like FE^2 (Feyel and Chaboche, 2000; Feyel, 2003). However, those do not apply when there is highly localized deformation, such as in fracture, since the separation of scales breaks down. Therefore, we here use an extension of the quasicontinuum (QC) method – a concurrent multiscale technique originally developed to efficiently model atomic crystals (Tadmor et al., 1996). The QC method is based on interpolation and energy sampling rules used to drastically reduce the number of degrees of freedom (dofs) and the computational costs associated with evaluating the mechanical quantities of interest in coarse-grained regions, while fully resolving all dofs and capturing the exact mechanics in regions of interest. Most implementations of the QC method interpolate the dofs in the coarse-grained regions by selecting representative sites (called representative atoms in the traditional QC method), creating a triangulation of those sites, and using piecewise affine interpolation of the dofs within each element. When it comes to sampling the mechanical quantities (such as energy and forces) in the coarse-grained regions, various methods have been proposed including local, Cauchy-Born-type approximations (Tadmor et al., 1996), force- and energy-based summation rules (Eidel and Stukowski, 2009), cluster sampling (Knap and Ortiz, 2001), numerical quadrature (Gunzburger and Zhang, 2010), and combinations of Cauchy-Born and nonlocal sampling rules (Amelang et al., 2015).

More recently, the QC method has been extended to model simple truss lattices (Beex et al., 2011). Initial studies assumed the truss members to behave as linear elastic springs; later extensions included inelasticity and failure of truss members (Beex et al., 2014d,c; Kochmann and Amelang, 2016; Rokoš et al., 2016) as well as Euler-Bernoulli beam connections to model stretching and bending of truss members (Beex et al., 2014a). Concepts were further paired with the eXtended Finite Element Method (XFEM) to track the propagation of cracks in the lattice (Rokoš et al., 2017). While these extensions of the QC method have been proven effective for basic lattices, the method has only been applied to simple Bravais lattices in 2D with truss members modeled either as nonlinear springs (thus neglecting beam bending) or as Euler-Bernoulli beams (excluding finite rotations).

Here, we extend the QC methodology for truss lattices in various directions: the presented method applies to more complex *multi-lattice* systems in *three dimensions* which have previously been out of reach. The QC method used is fully nonlocal, i.e., no conceptual distinction is made between fully-resolved and coarse-grained regions, allowing us to *adaptively refine* the mesh on the fly. Furthermore, we use *corotational beams* to model individual truss members,

so we accurately capture geometrically nonlinear phenomena. As a major difference to effective continuum theories of truss lattices – see e.g. Triantafyllidis and Bardenhagen (1993); Chen et al. (1998); Wang and Cuitiño (2000); Desmoulins and Kochmann (2017) – the presented QC technique locally retains full, discrete truss resolution where needed (e.g., near a crack tip) and seamlessly coarsens into a continuum description away from those regions, hence not assuming a separation of scales.

The remainder of this contribution is organized as follows. Section 2 outlines the new QC formulation for nonlinear 3D multi-lattice systems, followed by a series of numerical simulations highlighting the applicability of the method as well as the linear and nonlinear performance of various stretching- and bending-dominated lattice topologies. Section 3 reports three benchmark tests that isolate various key features of the method: first, Section 3.1 assesses the accuracy of the method by calculating the linear elastic moduli of various 2D and 3D truss lattice topologies using general meshes and different levels of coarsening. Second, Section 3.2 investigates the performance of the method when predicting the brittle fracture toughness for various 2D lattice topologies, similar to the boundary layer method introduced by Schmidt and Fleck (2001). Third, Section 3.3 discusses coarse-grained indentation simulations with adaptive refinement on 3D lattices undergoing nonlinear deformations. Finally, Section 4 concludes this investigation.

2. Variational quasicontinuum for nonlinear 3D truss networks

2.1. Problem statement

We consider truss lattices, i.e., cellular networks composed of beams and beam junctions (referred to as *nodes* in the following), which are produced by periodically repeating a *unit cell* (UC) along directions $\mathcal{B} = \{\mathbf{a}_1, \dots, \mathbf{a}_d\}$ with basis vectors $\mathbf{a} \in \mathbb{R}^d$ in d dimensions. We define a lattice Ω through the set of nodes, $\mathcal{P}$, and the set of truss members, $\mathcal{E}$, i.e., $\Omega = \{\mathcal{P}, \mathcal{E}\}$. For convenience, we decompose the body of interest into a set of UCs. We define a unit cell at a location $\mathbf{X}_u$ (in the undeformed configuration) by the set of points, $\mathcal{P}_u$, that lie inside the volume spanned by vectors $\mathcal{B}$ and centered at $\mathbf{X}_u$ (see Fig. 1a), i.e.,

$$\mathcal{P}_u = \left\{ \mathbf{X} \in \mathcal{P} \mid \mathbf{X} = \sum_{i=1}^d \mathbf{X}_u + t_i \mathbf{a}_i, \quad t_i \in \left(-\frac{1}{2}, \frac{1}{2}\right) \text{ for } i = 1, \dots, d \right\}, \quad (2)$$

further by the set of truss members that connect the points in $\mathcal{P}_u$ to each other, $\mathcal{E}_u$, and by the set of truss members interacting with points in neighboring unit cells, $\mathcal{E}_u^n$. Then, the unit cell is defined as $\Omega_u = \{\mathcal{P}_u, \mathcal{E}_u, \mathcal{E}_u^n\}$.

For simple Bravais lattices (e.g., triangle or diamond), each UC consists of only a single node with connections only to nodes in neighboring UCs (i.e., $\mathcal{E}_u = \{\emptyset\}$), as shown in Fig. 1(a,b) for the diamond lattice. More complex

Figure 1: (a) Example definition of a UC Ω_u based on its node(s) (solid circle) and its connecting beams $\mathcal{E}_u^n$ (in this case $\mathcal{E}_u = \emptyset$). Further shown are examples of (b) a simple Bravais lattice (diamond) and (c) a multi-lattice (hexagon, composed of two simple Bravais lattices) and their corresponding UCs and UC dofs. The dofs of all nodes inside each UC are retained with $\varphi = \{x, \theta\}$ denoting both translational and rotational dofs.

lattices (e.g., kagome or hexagon) are created with UCs consisting of multiple distinct nodes (see the hexagonal lattice in Fig. 1c). By adopting terminology from atomistics (Dobson et al., 2007), UCs with multiple unique nodes are referred to as multi-lattices, whose set of nodes can be described by n_B Bravais lattices, each defined by the same basis $\mathcal{B}$ but shifted relative to one another by shift vectors $\mathbf{S}^\alpha$ ($\alpha = 1, \dots, n_B$). Consequently, the complete point set of a multi-lattice can be written as

$$\left\{ \mathbf{X} \in \mathbb{R}^d \mid \mathbf{X} = \sum_{j=1}^d c_j \mathbf{a}_j^\alpha + \mathbf{S}^\alpha, \quad c_j \in \mathbb{Z}, \quad 1 \leq \alpha \leq n_B \right\}. \quad (3)$$

It should be noted that all previous modeling of trusses using the QC method has focused on a single Bravais lattice, while this formulation extends to multi-lattices.

As the truss network undergoes finite deformations, we track the generalized deformed position of each node (including both translations and rotations) by a mapping $\boldsymbol{\varphi}(\mathbf{X}) = \{\mathbf{x}, \boldsymbol{\theta}\}$. Rotational degrees of freedom $\boldsymbol{\theta}$ are required for beam lattices subjected to bending, and from various available options we choose rotation vectors parametrized by $2d - 3$ variables (described in detail in Section 2.4). We denote all generalized dofs of a unit cell located at $\mathbf{X}_i$ by $\tilde{\boldsymbol{\varphi}}(\mathbf{X}_i) = \{\boldsymbol{\varphi}^0(\mathbf{X}_i), \dots, \boldsymbol{\varphi}^{n_B}(\mathbf{X}_i)\}$; see Fig. 1.

Assuming a variational constitutive model, the strain energy of a truss member $e \in \mathcal{E}$ connecting the two nodes initially at $\mathbf{X}_i$ and $\mathbf{X}_j$ is given by $W_e = W(\boldsymbol{\varphi}_i, \boldsymbol{\varphi}_j)$ ¹ and the total potential energy of a finite-size truss network follows as

$$\mathcal{I} = \sum_{e \in \mathcal{E}} W_e - \mathcal{L}, \quad (4)$$

with $\mathcal{L}$ being the external force potential. Using the decomposition of the domain into unit cells as described above, the energy can be rewritten as a sum over the unit cells

$$\mathcal{I} = \sum_{\Omega_u \in \Omega} W_u(\tilde{\boldsymbol{\varphi}}_u, \tilde{\boldsymbol{\varphi}}_{N(u)}) - \mathcal{L}, \quad W_u = \sum_{e \in \mathcal{E}_u} W_e + \frac{1}{2} \sum_{e \in \mathcal{E}_u^n} W_e, \quad (5)$$

where W_u is the total energy of the UC (composed of energy of truss members $\mathcal{E}_u$ fully within Ω_u and of truss members $\mathcal{E}_u^n$ connecting to neighboring unit cells, the latter weighted by 1/2 to avoid double-counting), and $\tilde{\boldsymbol{\varphi}}_{N(u)}$ are the generalized dofs of the neighboring unit cells. Finally, the solution of a quasistatic BVP is obtained from minimizing $\mathcal{I}$ subject to essential boundary conditions².

In problems involving very large numbers of individual truss members, solving for the positions of each and every node in (5) becomes prohibitively expensive, which is why the goal of our truss QC framework is the identification of approximate minimizers of (5) in a numerically efficient manner.

2.2. Quasicontinuum approximation

In the spirit of the original QC method for atomic lattices (Tadmor et al., 1996) and its extension to simple truss networks (Beex et al., 2014a), we approximate the deformation of a truss lattice by a reduced set of dofs. However, instead of reducing the dofs by selecting representative nodes (analogous to the introduction of representative atoms in the original QC method), we choose a set of $N_{\text{rep}} \ll N$ *representative unit cells* (in the following called *repUCs*, not to be confused with representative volume elements or unit cells commonly used in homogenization), which retain all of their dofs.

While the dofs of the repUCs are retained, the dofs of the remaining UCs are obtained from interpolation as in the original QC method:

$$\tilde{\boldsymbol{\varphi}}(\mathbf{X}_u) = \sum_{a=1}^{N_{\text{rep}}} N_a(\mathbf{X}_u) \tilde{\boldsymbol{\varphi}}_a \quad (6)$$

¹In general, this methodology is agnostic to the strain energy density of a truss member, W_e , and any beam model whose strain energy depends on the nodal translations and rotations can be used. For all beam models used in this paper, we assume slender beams, thus neglecting higher-order corrections needed for non-slender lattices (i.e., shear deformation, finite-sized nodes, etc.); see Meza et al. (2017) for a discussion.

²Note that the extension to dynamic problems is, in principle, analogous and makes use of the action principle (which renders the total Lagrangian stationary). It is, however, beyond the scope of this contribution and comes with the same challenges as dynamic QC methods.

Figure 2: Illustration of the interpolated dofs and the recovery of nodal dofs within individual UCs from the interpolation: (a) shows a mesh of coarse-grained/macroscale elements whose vertices are repUCs that carry dofs $\tilde{\varphi}$. (b) Within an element K , the dofs $\tilde{\varphi}$ are interpolated by evaluating the shape functions at each UC location, e.g., X_i or X_j (in the reference configuration). (c) Dofs $\{\varphi^0, \varphi^1\}$ of the two nodes within each UC are recovered from the interpolated repUC dofs.

with some suitable shape functions $N_a(\mathbf{X})$, and the corresponding dofs of the repUCs, $\tilde{\varphi}_a$. In the following, we use linear interpolation on a Delaunay-triangulated mesh. The simplices of the Delaunay-triangulated mesh will be referred to as *coarse-grained* or *macroscopic elements* in order to differentiate them from the beam elements used to model the individual truss members within the UCs. Note that the shape functions are evaluated at the location X_u of UC u (in the reference configuration), and not at the exact positions of each individual node inside the UC; see Fig. 2. This means that some unit cells that lie inside - but near the edge - of some macroscopic element K can contain some nodes that lie outside of K , but still use the shape functions of K to interpolate the dofs (since the node is contained in a UC that lies within K ; see Fig. 3).

2.3. Sampling rule

The above quasicontinuum approximation reduces the number of dofs from $(2d-3) \times n_b \times N$ to $(2d-3) \times n_b \times N_{\text{rep}}$, whereas the efficient calculation of the total energy $\mathcal{I}$ in (5) necessitates the introduction of sampling rules (also referred to as summation rules) akin to quadrature in finite elements (FE). To this end, we select $N_s \ll N$ sampling unit cells such that

$$\mathcal{I} \approx \mathcal{I}^h = \sum_{s=1}^{N_s} w_s W_s - \mathcal{L}_s \quad (7)$$

Figure 3: Depiction of the QC interpolation and optimal summation rule applied to a 2D hexagon lattice. The blue UCs at the vertices of the mesh are the repUCs (which are also sampling unit cells with $w_s = 1$), and the red UC at the center of the element is the Cauchy-Born sampling UC. The dofs of the gray shaded UCs belong to the highlighted element (K) and are hence interpolated from the dofs of the blue repUCs.

with weights w_s akin to quadrature rules, and $\mathcal{L}_s$ is the sampled external force potential. Various summations rules have been introduced for atomistic and truss-based QC – see e.g. (Knap and Ortiz, 2001; Eidel and Stukowski, 2009; Gunzburger and Zhang, 2010; Beex et al., 2014b; Amelang et al., 2015). In the following, we use a variant of the first-order optimal summation rule proposed in Amelang et al. (2015) modified by features from the central summation rule of Beex et al. (2014b). The optimal rules were chosen since they were shown to produce smallest force artifacts and energy approximation errors for atomistic QC. Here, we briefly cover only the key aspects of the chosen summation rule; the reader is referred to Amelang et al. (2015) for a more in-depth discussion.

The sampling UCs in the summation rule used here are chosen such that all repUCs are also sampling UCs with a weight of $w_{\text{rep}} = 1$ (Beex et al., 2014b). An additional sampling site is placed at the barycenter of each macroscopic simplicial element in non-fully-resolved regions. Unlike in Beex et al. (2014b), the barycenter sampling UC here uses the Cauchy-Born rule (Amelang et al., 2015) to compute the dofs of its neighbors, irrespective of whether or not the neighboring sites are located within the same macroscopic element. The Cauchy-Born sampling UC attempts to approximate the energy of the remaining non-repUCs in the macroscopic element, and is given a weight of

$$w_{s,\text{inner}} = \frac{V_e}{V_{UC}} - \sum_{i=1}^{d+1} w_i, \quad (8)$$

where V_e and V_{UC} are the volumes of the macroscopic element and of the UC, respectively, and $w_i \leq w_{\text{rep}}$ is the i^{th} repUC's weight contribution³ to the element. Fig. 3 shows an example lattice with the QC interpolation (2.2) paired with sampling UCs of the optimal summation rule described here.

2.4. Corotational beam formulation

As individual truss members may undergo finite rotations while sustaining axial and bending loads, we resort to a corotational beam formulation based on Crisfield (1990), which is reviewed here to the extent necessary for subsequent discussions. For a detailed description of the beam elements used, the reader is referred to Crisfield (1990, 1997). Dealing with finite rotations in 2D is relatively straightforward: a single rotation variable θ can be used to represent the rotation. However, in 3D there are many choices for parametrizing rotations including rotation matrices, quaternions and rotation vectors. For our corotational formulation, we consider the rotation vector $\boldsymbol{\theta} = \theta \hat{\mathbf{e}}$ which corresponds to a rotation with magnitude $\theta = |\boldsymbol{\theta}|$ around the axis defined by the unit vector $\hat{\mathbf{e}}$. It can be converted to a rotation matrix $\mathbf{R}(\boldsymbol{\theta})$ through an exponential mapping using Rodrigues' formula (for $\theta \neq 0$)

$$\mathbf{R}(\boldsymbol{\theta}) = \exp(\mathbf{S}(\boldsymbol{\theta})) = \mathbf{I} + \frac{\sin \theta}{\theta} \mathbf{S}(\boldsymbol{\theta}) + \frac{1 - \cos \theta}{\theta^2} \mathbf{S}(\boldsymbol{\theta})^2, \quad (9)$$

where $\mathbf{S}(\boldsymbol{\theta})$ is the skew-symmetric matrix ($\theta_i = \theta \hat{\mathbf{e}}_i$ denoting the i^{th} Cartesian component of $\boldsymbol{\theta}$)

$$\mathbf{S}(\boldsymbol{\theta}) = \begin{bmatrix} 0 & -\theta_3 & \theta_2 \\ \theta_3 & 0 & -\theta_1 \\ -\theta_2 & \theta_1 & 0 \end{bmatrix}. \quad (10)$$

By inversion of (9), one arrives at the logarithmic mapping

$$\boldsymbol{\theta} = \log(\mathbf{R}(\boldsymbol{\theta})). \quad (11)$$

The 2D and 3D corotational beam description of Crisfield (1990) is based on an element frame that continuously rotates with the underlying beam element. The nonlinearity introduced in the element comes solely from the finite rotation of the element frame, while the underlying linear Euler-Bernouli model assumes small deflections with respect to the rotating frame (see Fig. 4 for all definitions used in the following).

³The weight contribution of a repUC at $\mathbf{X}$ to the element is defined by the fraction of the volume of a circle (sphere in 3D) centered at $\mathbf{X}$ that lies inside the element. In other words, the weight contribution is the angle (solid angle in 3D) divided by 2π (4π in 3D). In 2D, since the angles of all triangles sum up to $\pi/2$, the sum in (8) is $1/2$. However, since tetrahedra do not have the same property, the sum is different for each element. Amelang et al. (2015) provides a detailed discussion.

The kinematics of the corotational beams is described using three different configurations of the beam: the reference, undeformed, and deformed configurations (see Fig. 4). The reference configuration is taken as an undeformed Euler-Bernouli beam element that is oriented along the positive x -axis in the global coordinate system. The undeformed configuration represents the beam with its orientation at the start of the simulation, and can be defined by the rotation $\mathbf{R}^{ru}$, where the superscript ru signifies the rotation from the (r)eference configuration to the (u)ndeformed configuration. The deformed configuration represents the beam subjected to arbitrarily large displacements and rotations at the current step in the simulation. The deformed configuration is defined by the deformed nodal positions $\mathbf{x}_i$ and global rotations $\mathbf{R}_i^{rd}$ of each node i , where the superscript signifies the rotation from the (r)eference configuration to the (d)eformed configuration. The global rotations can also be represented by the rotation from the undeformed configuration to the deformed configuration $\mathbf{R}_i^{ud}$ which is related to the other rotation matrices through

$$\mathbf{R}_i^{rd} = \mathbf{R}_i^{ud} \mathbf{R}^{ru}. \quad (12)$$

Using the global positions and rotations of each node, the beam element's orientation $\mathbf{R}^b = [\mathbf{r}_1^b, \dots, \mathbf{r}_d^b]$ is defined as an average rotation of the beam. In both 2D and 3D, the latter is defined by introducing $\mathbf{r}_1^b$ as the unit vector pointing from node 1 to node 2, i.e.,

$$\mathbf{r}_1^b = \frac{\mathbf{x}_2 - \mathbf{x}_1}{|\mathbf{x}_2 - \mathbf{x}_1|}. \quad (13)$$

For the 2D corotational beam, the second axis $\mathbf{r}_2^b$ simply follows from a rotation of $\mathbf{r}_1^b$ by $\pi/2$. For the 3D corotational beam, the second and third axes are defined with the help of the average rotation matrix

$$\mathbf{R}^{av} = \mathbf{R}(\theta^{av}) \mathbf{R}_1^{ud} \quad \text{with} \quad \theta^{av} = \frac{\log(\mathbf{R}_2^{rd}) - \log(\mathbf{R}_1^{rd})}{2}. \quad (14)$$

With the column representation $\mathbf{R}^{av} = [\mathbf{r}_1^{av}, \mathbf{r}_2^{av}, \mathbf{r}_3^{av}]$, the remaining two axes of the beam coordinate system are defined as

$$\mathbf{r}_2^b = \mathbf{r}_2^{av} - \frac{\mathbf{r}_2^{av} \cdot \mathbf{r}_1^b}{2} (\mathbf{r}_1^b + \mathbf{r}_1^{av}), \quad \mathbf{r}_3^b = \mathbf{r}_3^{av} - \frac{\mathbf{r}_3^{av} \cdot \mathbf{r}_1^b}{2} (\mathbf{r}_1^b + \mathbf{r}_1^{av}). \quad (15)$$

This definition of a beam element's frame results in a coordinate system that is not necessarily orthogonal, but the deviation from orthogonality is small and therefore generally neglected (see Crisfield (1990) for a discussion). Lastly, we use the global rotation at each node and the beam coordinate system to define the local (assumed to be small)

Figure 4: Kinematics of the 3D corotational beam: the linear Euler Bernouli beam rotates with the element frame $\mathbf{R}^b$, and has small angle deflections at each node. Superscripts r , u , d , and b stand for the (r)eference, (u)ndeformed, (d)eformed, and (b)eam configuration, respectively.

rotations. This is done by realizing that the global rotations of each node can be described by a small local rotation around the undeformed configuration $\mathbf{R}_i^{\text{loc}}$, followed by the large rotation of the beam element (i.e., $\mathbf{R}_i^{\text{rd}} = \mathbf{R}^b \mathbf{R}_i^{\text{loc}}$). This gives the definition of the local rotation matrices and the corresponding local rotation vectors as, respectively,

$$\mathbf{R}_i^{\text{loc}} = (\mathbf{R}^b)^T \mathbf{R}_i^{\text{rd}}, \quad \boldsymbol{\theta}_i^{\text{loc}} = \log(\mathbf{R}_i^{\text{loc}}). \quad (16)$$

Since this representation describes the large global rotations in terms of small local rotations composed with a rigid body rotation, the energy of a corotational beam element is given by the classical energy of an Euler-Bernouli beam subject to the local rotations and the stretching of the beam axis in the reference configuration:

$$W_b = \frac{1}{2} \left(\frac{EA}{L_0} u_{\text{ax}}^2 + [\boldsymbol{\theta}_1^{\text{loc}}, \boldsymbol{\theta}_2^{\text{loc}}] \mathbf{D} \begin{bmatrix} \boldsymbol{\theta}_1^{\text{loc}} \\ \boldsymbol{\theta}_2^{\text{loc}} \end{bmatrix} \right), \quad (17)$$

where in 2D and 3D, respectively,

$$\mathbf{D} = \frac{1}{L_0} \begin{bmatrix} 4EI_2 & 2EI_2 \\ 2EI_2 & 4EI_2 \end{bmatrix}, \quad \mathbf{D} = \frac{1}{L_0} \begin{bmatrix} GJ & 0 & 0 & -GJ & 0 & 0 \\ 0 & 4EI_2 & 0 & 0 & 2EI_2 & 0 \\ 0 & 0 & 4EI_3 & 0 & 0 & 2EI_3 \\ -GJ & 0 & 0 & GJ & 0 & 0 \\ 0 & 2EI_2 & 0 & 0 & 4EI_2 & 0 \\ 0 & 0 & 2EI_3 & 0 & 0 & 4EI_3 \end{bmatrix}. \quad (18)$$

E and G are the base material's Young and shear moduli, respectively, I_2 and I_3 are the beam's area moments of inertia around the the y - and z -axes, J is the polar moment of inertia of the beam, L_0 is the undeformed length of the beam, and $u_{\text{ax}} = |\mathbf{x}_2 - \mathbf{x}_1| - L_0$ is the axial displacement.

To capture the global rotations of each node, the rotation $\mathbf{R}^{\text{ru}}$ is stored in each element, so only the rotation from the undeformed to the deformed configuration must be parametrized. In 2D, this is accomplished by storing the scalar rotation angle θ ; in 3D, we choose the rotation vector $\boldsymbol{\theta}^{\text{rd}}$. It should be noted that the affine interpolation of our QC method calls for caution when choosing the parametrization (e.g., the linear interpolation of rotation matrices is not permissible as it does not necessarily result in a rotation matrix).

One difference between the formulation of Crisfield (1990) and ours is the updating of the rotation vectors $\boldsymbol{\theta}^{\text{rd}}$. Theirs used forces that are conjugate to the spatial spin variables $\mathbf{v}$, which correspond to an infinitesimal rotation superimposed onto the global rotation matrix, requiring a non-additive update of the form

$$\mathbf{R}(\boldsymbol{\theta}^{i+1}) = \mathbf{R}(\delta \mathbf{v}) \mathbf{R}(\boldsymbol{\theta}^i). \quad (19)$$

Here, however, we follow Battini and Pacoste (2006) in using additive updates of the global rotational degrees of freedom, i.e., $\boldsymbol{\theta}^{i+1} = \boldsymbol{\theta}^i + \delta \boldsymbol{\theta}$. We note that the change from multiplicative updates to additive updates did not change the equilibrium solution nor the convergence properties when applied to the numerical benchmark tests from Crisfield (1990). The forces and stiffness matrices conjugate to the additive rotation vector updates with the 3D corotational beam element are computed using finite differences.

2.5. Adaptive refinement

A key benefit of the fully-nonlocal QC method over other concurrent scale-bridging techniques is that no conceptual distinction is made between the fully-resolved and coarse-grained regions, allowing for automatic adaptive refinement of the discretization down to the fully-resolved limit. Note that we here constrain ourselves to adaptive refinement without coarsening (see the discussion in Tembhekar et al. (2017)). Adaptivity thus requires a refinement criterion and a geometric refinement algorithm. We generally identify a coarse-grained element K for refinement if it passes the refinement criterion

$$V(K)^{1/d} f(\mathbf{F}_K) > r_0, \quad (20)$$

where $V(K)$ is the volume of element K in d dimensions, $f(\mathbf{F}_K)$ is a metric depending on the deformation gradient inside the element (averaged over all Bravais lattices in the multilattice; each of which is constant by the affine interpolation), and r_0 defines the refinement threshold. The refinement metric is chosen based on the lattice architecture

and the problem to be simulated. For the subsequent simulations, we use the refinement criterion

$$f(\mathbf{F}) = I_2(\mathbf{F}) = \frac{1}{2} \left((\text{tr } \mathbf{F})^2 - \text{tr}(\mathbf{F}^2) \right) \quad (21)$$

The second invariant criterion was already used in the traditional QC method of atomistic lattices (Knap and Ortiz, 2001), where it quantifies the amount of shear inside the element ultimately leading to dislocation nucleation/motion (so that r_0 was related to the Burgers vector). Here, this criterion is chosen for the brittle fracture toughness simulations in Section 3.2, because it was previously shown that shear bands may emanate from the notch tip. It is also used in Section 3.3 as a general measure of the localized deformation.

Once all coarse-grained elements have been identified for refinement, we apply a longest-edge bisection algorithm (Tembhekar et al., 2017) to insert new repUCs with the complicating constraint that all repUCs are to be located on valid lattice sites. To this end, we insert a new repUC at that vacant UC location nearest to the mid-point of the longest edge of each element to be refined. Once all new repUCs have been created, we recreate the element connectivity. Finally, nodal dofs of newly inserted repUCs are computed by interpolation from the previously existing mesh.

2.6. Numerical considerations

The above truss QC framework was implemented in an in-house computational framework for general, nonlinear periodic truss networks. The solutions to the following quasistatic BVPs are found as the minimizers of the QC-approximated energy (7), using solvers and optimization techniques provided by PETSC/TAO (Balay et al., 1997, 2017a,b). As in traditional QC, the global force vector and global tangent matrix are given by differentiating the global energy with respect to the repUC DOFs, and are not presented here in detail. Since the affine shape functions used to interpolate the dofs of the UCs have compact support, vectors and matrices are sparse with non-zero components stemming from repUCs used to interpolate the dofs of the sampling UC and its neighbors. The detailed algorithms can be found in Appendix A.

The computational efficiency of this (and all other) QC methods stems from their kinematic constraints and energy approximation techniques, viz. from the reduced number of degrees of freedom (which reduces the cost of solving the system of equations) and the reduced number of energy sampling points (which reduces the cost of force and stiffness matrix calculations). The fraction of the dofs of the QC method compared to the fully resolved case is the repUC density, and as such, the repUC density can be used directly to estimate the speed-up of the linear solve portion of the code (depending on how the linear solve algorithm scales with the number of unknowns). On the other hand, the force and stiffness calculations involve a sum over all sampling unit cells, which is a superset of all repUCs, meaning the computational savings for these actions are not quite as large as the computational savings in the linear solve. The exact speed-up, however, strongly depends on the chosen algorithmic implementation and, especially, the chosen solver and mesh adaptation scheme. It is important to note that the QC coarse-graining comes with a tremendous reduction in the number of degrees of freedom. Therefore, irrespective of the computational speed-up as compared to a fully-resolved simulation, the present method is highly valuable as it allows going to far larger systems than what is possible with full resolution (especially in 3D).

2.7. Comparison with FE^2 and classical homogenization

The truss QC theory described above was specifically designed to accurately capture the response of truss lattices both in the fully-resolved limit and in the limit of large coarse-grained elements. In the fully-resolved limit, all dofs of all nodes/UCs are retained and the energy of each truss member is calculated exactly, so that the lattice is described exactly⁴. However, when coarse-grained elements are large so that a separation of scales applies between the macroscopic BVP and the underlying unit cell, it is less obvious that our QC method accurately captures the truss response. Therefore, we here discuss how the chosen QC theory equipped with affine interpolation in the coarse-grained regions compares to other multiscale modeling techniques.

⁴By *exactly* we refer to exact agreement with a discrete simulation fully resolving each individual truss member. The particular choice of the underlying discrete truss description is not the topic here. It is assumed that the corotational beam formulation used to represent the truss lattice members is adequate (it can easily be replaced by alternative constitutive or kinematic descriptions on the individual beam level).

The macroscale boundary value problem of a heterogeneous body Ω with statistically homogeneous microstructure (represented by an RVE Ω_{UC}) aims to identify the deformation mapping or displacement field as the minimizer of the total potential energy

$$\mathcal{I}[\mathbf{u}] = \int_{\Omega} W\left(\frac{\mathbf{x}}{\epsilon}; \nabla \mathbf{u}\right) dV - \ell(\mathbf{u}) \quad (22)$$

subject to essential boundary conditions on $\partial\Omega$. Here, W denotes the strain energy density as a function of position $\mathbf{x}$ and the displacement gradient, ℓ is the linear potential of external forces, and ϵ is the size of the RVE. That is, we have

$$\mathbf{u} = \arg \min \{ \mathcal{I}[\mathbf{u}] \mid \mathbf{u} \in H_0^1(\Omega) \}, \quad (23)$$

where $H_0^1(\Omega) \subset H^1(\Omega)$ is the set of functions satisfying the Dirichlet boundary conditions.

Since the material's constitutive response fluctuates on the scale of $\mathbf{y} = \mathbf{x}/\epsilon$ whereas the boundary value problem (i.e., the geometry and any loading) varies on the scale of $\mathbf{x}$, one ideally seeks a solution following the asymptotic expansion

$$\mathbf{u}_{\epsilon}(\mathbf{x}) = \mathbf{u}(\mathbf{x}) + \epsilon \mathbf{v}\left(\mathbf{x}, \frac{\mathbf{x}}{\epsilon}\right) + O(\epsilon^2). \quad (24)$$

Within linear elasticity, closed-form solutions are feasible as unique minimizers of the convex optimization problem (see [Cioranescu and Donato \(1999\)](#) for a detailed discussion of homogenization in linear elasticity).

Where this is not analytically feasible, multiscale techniques like FE^2 have become prominent solutions ([Feyel and Chaboche, 2000](#); [Miehe and Koch, 2002](#); [Feyel, 2003](#)). For example, one may assume a separation of scales ($\epsilon \ll 1$) and decouple the macro-problem from the microscale constitutive behavior via the homogenized variational problem

$$\mathcal{I}[\mathbf{u}] = \int_{\Omega} W^*(\nabla \mathbf{u}) dV - \ell(\mathbf{u}), \quad (25)$$

whose homogenized energy density is computed from the UC as

$$W^*(\xi) = \inf \left\{ \frac{1}{|\Omega_{UC}|} \int_{\Omega_{UC}} W(\mathbf{y}, \xi + \nabla \mathbf{v}) dV \mid \mathbf{v} \in V(\Omega_{UC}) \right\}, \quad (26)$$

with $V(\Omega_{UC}) \subset H^1(\Omega_{UC})$ being the set of all H^1 -functions on Ω_{UC} whose boundary conditions are chosen according to one of several frequently used options including, e.g., affine or periodic boundary conditions. If $W(\mathbf{y}, \cdot)$ lacks quasiconvexity, then microstructures may form and W^* presents a relaxed energy density (since it includes only a single UC, it does not in general agree with the quasiconvex hull).

Note that in the homogenized case, irrespective of the type of boundary conditions chosen at the UC level, the overall solution is continuous only at the macroscale, i.e., $\mathbf{u}$ is continuous but one cannot construct an asymptotic solution of the type (24), because neither smoothness nor continuity of $\mathbf{v}$ is guaranteed at the macroscale. Therefore, constructing solutions (24) by using $\mathbf{u}$ from (25) and $\mathbf{v}$ from (26) results in solutions not within $H_0^1(\Omega)$ and therefore themselves not minimizers of (23). This lack of conformity of displacements can be seen by looking at the displacements across macro-elements in an FE^2 method with linear interpolation at the macroscale. At the edge ∂K_{12} between two elements K_1, K_2 , we have $\mathbf{u}^{K_1}(\mathbf{x}) = \mathbf{u}^{K_2}(\mathbf{x})$ but $\mathbf{v}^{K_1}(\mathbf{x}) \neq \mathbf{v}^{K_2}(\mathbf{x})$, since $\mathbf{v}(\mathbf{x})$ depends on $\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$ which is not necessarily the same in K_1 and K_2 . The non-conforming nature of displacements means that the approximate solution obtained from FE^2 does not lie in the desired space of the multiscale problem, see (23), and the upper-bound property of the approximation is lost. In linear elasticity, the difference between the minima of (22) and (25) with periodic boundary conditions on the microscale is $O(\epsilon^{1/2})$, so the error is minimal when there is a separation of scales ([Cioranescu and Donato, 1999](#)).

The goal of the QC discretization outlined here is to create a *conforming* displacement field that retains all dofs of the (discretized) fine-scale governing equation where necessary, while matching homogenization theory in coarse regions. The conforming nature of the underlying displacement field allows us to retain the upper-bound property of the original problem (i.e., up to the energy approximation by summation rules), unlike other multiscale methods. It is obvious from the construction of the approximation that all dofs of the fine-scale problem are resolved where necessary and – as will be shown in Section 3.1 – the fact that all dofs of the UC are retained as macro-variables enables us to match linear homogenization theory for uniform macroscopic deformations.

When linear homogenization theory does not apply (or more specifically, when $W(\mathbf{y}, \cdot)$ lacks quasiconvexity), the homogenized energy density W^* is the lowest energy produced by solving the UC problem (26) over an infinite number of UCs (Geymonat et al., 1993), i.e.,

$$W^*(\xi) = \inf_{k \in \mathbb{N}} \left\{ \inf \left\{ \frac{1}{|\Omega_{UC}^k|} \int_{\Omega_{UC}^k} W(\mathbf{y}, \xi + \nabla \mathbf{v}) dV \mid \mathbf{v} \in V(\Omega_{UC}^k) \right\} \right\}, \quad (27)$$

where Ω_{UC}^k denotes an RVE comprising k unit cells. For example, when performing FE^2 for a homogenized treatment of truss lattices that undergo buckling, multiple UCs in the microscale BVP were shown to result in a lower homogenized energy density and a more accurate description of the underlying truss (Vigliotti et al., 2014). In principle, enlarging the UC size in our QC framework can also capture longer-wave length buckling modes in the coarse-grained regions. However, the BVPs in this paper are such that buckling and other strong nonlinearities occur in localized domains of the simulation, where full resolution is ensured by adaptivity before the onset of buckling. We note that changing the UC size in the coarse-grained regions is not as straightforward as in FE^2 methods where a BVP is solved at each quadrature point since the QC method imposes kinematic constraints from the macroscale (and no BVP is solved on the microscale).

3. Numerical Examples

3.1. Benchmark test: elastic moduli

Since the linear elastic moduli of a periodic lattice generally emerge from affine states of deformation (depending on lattice architecture possibly with shifts in between affinely strained multiple Bravais lattices) (Vigliotti and Pasini, 2012b), the multi-lattice truss QC formulation introduced above is expected to reproduce exactly the effective, homogenized elastic moduli of, in principle, arbitrary lattice topologies. However, as was already observed in atomic lattices (Amelang et al., 2015), the unstructured coarse-graining of the QC methodology introduces errors that depend on the mesh quality and the choice of the summation rule to approximate the strain energy, cf. (7). In particular, meshes that undergo adaptive refinement involve a wide spread in element size and quality. Therefore, it is essential to verify the accuracy of the above truss QC scheme before proceeding to more advanced boundary value problems. As a worst-case scenario, we consider random meshes generated by randomly selecting repUCs from the UCs within a lattice filling the macroscopic shape of a cube. Of course, any sensible refinement algorithm, including the one described here, will not result in random meshes but in gradually refined meshes of superior quality. The generation of random meshes is therefore viewed as a worst-case scenario in terms of mesh quality. If a method performs well here, it is expected to perform even better on adaptively refinement meshes. If a method fails here, then it cannot be expected to perform well with adaptive refinement or in general unstructured meshes.

In order to understand how the method performs at various levels of coarsening, we compute the elastic moduli of a variety of 2D and 3D lattices, using meshes of various repUC densities (where by *repUC density* we denote the ratio of repUCs to total UCs in the simulation). Specifically, we present the elastic moduli of the following lattices: square, hexagon, triangle, kagome, and star-shaped lattices in 2D, and cubic, cuboctahedron, and a bcc lattice with nearest-neighbor connectivity in 3D (see Fig. 5). Since the purpose of this simulation is to investigate the method in the linear elastic regime, standard Euler-Bernouli beam elements **with linearized kinematics** are used to model the individual truss members.

For each lattice, the elastic moduli are computed by first affinely applying pure-shear, volumetric, and uniaxial states of strain to the translational dofs of the periphery of a finite-size lattice. To avoid complications because of unknown boundary conditions to be applied to the rotational dofs for given states of affine straining, we evaluate the strain energy for the elastic modulus extraction only in an inner block of the simulation domain (see Fig. 6). This way, potential boundary effects are ensured to have decayed through a peripheral region towards the center of the block.

The affine displacements applied to the translational dofs of the repUCs in the periphery for the three load cases are given by

$$\mathbf{x}^{shear} = \begin{bmatrix} 1 & \varepsilon & 0 \\ \varepsilon & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \mathbf{X}, \quad \mathbf{x}^{vol} = \begin{bmatrix} 1 + \frac{\varepsilon}{3} & 0 & 0 \\ 0 & 1 + \frac{\varepsilon}{3} & 0 \\ 0 & 0 & 1 + \frac{\varepsilon}{3} \end{bmatrix} \mathbf{X}, \quad \mathbf{x}^{uni} = \begin{bmatrix} 1 + \varepsilon & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \mathbf{X} \quad (28)$$

Figure 5: UCs of lattices with (a) square, (b) hexagon, (c) kagome, (d) triangle, (e) star-shaped 2D, (f) cubic, (g) cuboctahedron, and (h) BCC architecture.

in 3D, and

$$\mathbf{x}^{shear} = \begin{bmatrix} 1 & \varepsilon \\ \varepsilon & 1 \end{bmatrix} \mathbf{X}, \quad \mathbf{x}^{vol} = \begin{bmatrix} 1 + \frac{\varepsilon}{2} & 0 \\ 0 & 1 + \frac{\varepsilon}{2} \end{bmatrix} \mathbf{X}, \quad \mathbf{x}^{uni} = \begin{bmatrix} 1 + \varepsilon & 0 \\ 0 & 1 \end{bmatrix} \mathbf{X} \quad (29)$$

in 2D. The cube is mechanically equilibrated, after which the average strain energy of the inner block of the simulation domain (see Fig. 6) is computed as a weighted sum over the sampling UCs according to the sampling rules introduced above. Since the simulation is linear elastic, the energy is quadratic in the macroscopic strains, and the relation between the elastic modulus and the energy is

$$\lambda = \frac{2E_b}{V_b \varepsilon^2}, \quad (30)$$

where λ represents the shear, volumetric, or uniaxial strain elastic modulus, respectively, for the three above load cases. E_b is the total energy of the sampling sites inside the inner block, $V_b = w_s V_{UC}$ is the volume represented by the sampling sites with V_{UC} the volume of a single UC, and ε is the applied strain in (28) and (29).

In order to understand how the method performs at various levels of coarsening, the elastic moduli of each lattice were computed on meshes of various repUC densities from 0-100%. In addition, each simulation was repeated for two different beam slenderness ratios expressed through the relative density, viz., $\bar{\rho} = 1\%$ (slender beams) and $\bar{\rho} = 20\%$ (thicker beams). **The relative densities reported here are calculated by summing the volumes of the individual beam elements, i.e., neglecting any overlapping volumes at nodes, which is negligible at low relative densities. For a discussion of the error in relative density due to this assumption and analytical expressions for accurate relative densities of lattices, we refer the reader to Meza et al. (2017).** Each combination of lattice topology, relative density, and repUC density was performed on 20 different randomly generated meshes, where the overall size of each simulation was adjusted to keep a similar number of repUCs in all simulations.

The errors in the elastic moduli computed using truss QC (compared to the elastic moduli obtained from fully-resolved simulations) are summarized in Fig. 7. Overall, our truss QC method with optimal summation rule does an excellent job at predicting the elastic moduli in the fully-resolved limit (repUC density of 100%) and in the large-element limit (vanishing repUC density). Simulations with intermediate repUC densities show errors, with apparent variations between different lattice topologies and relative densities. Largest errors (all less than 6%) appear above

Figure 6: Representative, randomly coarse-grained truss QC simulations in 2D and 3D for the elastic constant calculation: (left) a coarse-grained hexagon lattice with 30% repUC density and (right) a bcc lattice with 10% repUC density. Affine boundary conditions are applied to the translational dofs on the outer faces of the block, and the energy of all sample UCs inside the yellow box are used to calculate the elastic modulus (the large region in between removes any boundary layer effects).

repUC densities above 60%, which in 3D amounts to regions being close to fully refined and which also agrees with observations found on random atomistic QC discretizations (Amelang et al., 2015). Indeed, it can be expected that simulations with a slightly coarsened mesh and an approximate summation rule do not perfectly match the fully resolved data, as the energy-based QC summation rules are known to generate force artifacts that lead to errors. Simulations on uniformly coarsened meshes produce the exact elastic constants for all configurations tested, again analogous to atomistic QC (Amelang et al., 2015). This confirms that the errors in Fig. 7 are expected to be larger than those occurring in most simulations with more structured, better conditioned meshes.

Finally, in order to isolate the error source, the above simulations were performed with an exact energy summation (i.e., UC positions are still being interpolated but the total energy is calculated exactly from all UCs in the simulation). Across all tested relative densities, lattice topologies, and repUC densities, this yields the exact elastic constants, which shows that the errors reported Fig. 7 can be solely attributed to the approximation of the energy, and not the QC interpolation scheme.

3.2. Fracture toughness of brittle truss lattices

Calculating the fracture toughness of truss lattices is a prime example to demonstrate the efficiency and accuracy of the truss QC method. Unlike prior techniques, truss QC allows us to restrict full resolution to those regions of interest near the crack tip while efficiently coarse-graining the remaining domain, thus easily admitting the application of remote boundary conditions.

We base our investigation on a coarse-grained version of boundary layer analysis proposed by Schmidt and Fleck (2001) to compute the brittle fracture toughness of multiple lattice topologies, and we compare the results to those obtained by brute-force discrete lattice calculation. Boundary layer analysis consists of applying displacements corresponding to the K -field of an equivalent continuum to the periphery of a large, notched lattice. Since the lattices are not necessarily isotropic, the expressions for the K -field displacements of anisotropic media from Sih et al. (1965) are used (not written out here for conciseness). Brittle fracture is assumed to occur when the maximum tensile stress of any beam near the notch tip reaches the tensile strength of the constituent material within the linear elastic regime (so that Euler-Bernoulli beams with linearized kinematics can be used to model individual truss members).

For comparison, Schmidt and Fleck (2001) conducted boundary layer analyses on circular meshes with a radius of about $85l$; Quintana Alonso and Fleck (2007) and Romijn and Fleck (2007) used square meshes with dimensions $600l \times 600l$ and Tankasala et al. (2015) used square meshes with dimensions $500l \times 500l$, where l is the length of

Figure 7: Errors in the linear elastic bulk, shear, and uniaxial moduli of 2D (*left*) and 3D (*right*) lattices at 20% (solid markers) and 1% (hollow markers) relative density, computed by coarse-grained truss QC simulations with the optimal summation rule and random repUC selection for each level of repUC density. Markers correspond to the average error from 20 randomly coarsened meshes, and the bars represent the standard deviations of the errors.

a beam in the lattice (all beams in the lattices have the same length). Here, we start with an initial fully-resolved region of $16l \times 16l$, surrounded by six regions of six cells, each region coarsened by a factor of two compared to the previous region for total grid size of $768l \times 768l$ (see Fig. 8). We use the adaptive refinement described in Section 2.5. The refinement tolerance is repeatedly decreased, thereby increasing the total number of dofs in the simulation. The maximum tensile stress near the notch tip and the total energy of the system are monitored for convergence of the

Figure 8: Coarse-grained kagome lattice in 2D with a pre-existing crack undergoing mode-I loading, simulated by truss QC with adaptive mesh refinement as compared to a fully-resolved simulation. The colors correspond to the (normalized) maximum tensile stresses in the beams.

simulation. Fully-resolved simulations were performed for comparison.

We perform coarse-grained simulations of the triangle, hexagon, kagome, and star-shaped truss lattices undergoing Mode I loading. Following others that have performed boundary layer analysis, we use the elastic constants of [Quintana-Alonso et al. \(2010\)](#) for the triangle, kagome, and hexagon lattices, which correspond to a first-order approximation of the homogenized elastic constants in terms of slenderness ratio (i.e., higher-order bending terms are neglected for stretching-dominated lattices). For the star-shaped lattice, which has not been studied before, we use the first order approximation of the elastic constants which we calculated. For the exact elastic constants for each lattice, see [Appendix B](#).

Figs. 9 and 10 illustrate the convergence of the maximum tensile stress and of the total energy of the system towards the exact values obtained from fully-resolved simulations. Apparently, the accuracy of the coarse-grained

and adaptively refined simulations drastically varies based on lattice topology and relative density; and one generally expects the error to decrease with increasing repUC density. The unrefined *kagome* lattice simulations show large errors in the maximum tensile stress and energy, which are greatly reduced by the adaptive refinement of the mesh while still using only a small fraction of all dofs in the lattice. Furthermore, the refinement procedure fully refines the mesh along the shear bands that emanate from the crack tip in the fully-resolved simulation (see Fig. 8). This demonstrates the effectiveness of the adaptive QC method. While the coarse-grained simulation displays significant errors (because boundary-layer effects coming from the crack tip interfere with the coarse regions), the refinement technique enlarges the fully-resolved region only where necessary and effectively reduces the error. The *triangle* lattice shows small errors in the energy and maximum stress even in the unrefined case, suggesting that the boundary layer effects from the crack tip are highly local, so that no refinement is needed.

The star and hexagon lattices show considerable errors for the unrefined mesh. Interestingly, while the error decreases as the mesh is refined, the errors do not decrease to reasonably small values as in the previous cases, which we explain as follows. The *hexagon* lattice has a bending-dominated Young's modulus ($E \sim \bar{\rho}^3$) and a stretching-dominated bulk modulus ($\kappa \sim \bar{\rho}$), meaning that for low relative densities the effective response is nearly incompressible (see Appendix B). We thus attribute the large errors reported for the hexagon lattice to a phenomenon similar to volumetric locking in FE, where linear elements tend to drastically overpredict the energy of nearly incompressible materials. In the coarse-grained regions of our simulations, the QC method behaves close to a continuum with the homogenized elastic constants of the periodic lattice, so that the linear interpolation of the dofs in the coarse-grained QC elements results in the same phenomenon. While the FE community uses higher-order elements and reduced integration to mitigate this issue, similar techniques for the QC method will need to be developed in order to create accurate coarse-grained models of trusses with nearly incompressible effective elastic moduli.⁵

The challenges with the *star-shaped* lattice cannot be explained by volumetric locking, since both bulk and Young moduli of the effective continuum are bending-dominated. However, when the beams are slender, they act as if they are inextensible, since all macroscopic deformation can be accommodated by the bending of individual beams, which comes with significantly lower strain energy. The fact that we considerably overpredict the energy of the star-shaped lattice (and that the discrepancy increases as we decrease the relative density) suggests that the linear interpolation of the dofs of each individual Bravais lattice does not allow the multi-lattice to accommodate the macroscopic deformation without the stretching of beams. In other words, if we think of the beams as inextensible members, then the linear interpolation described in Section 2.2 leaves the lattice overconstrained for non-uniform deformation (recall that in Section 3.1 we showed that this interpolation performs well for uniform deformation). It is hypothesized that higher-order elements, additional enrichment shape functions, or special summation rules that mimic reduced integration in FE could be used to mitigate these issues, but the investigation of these topics is out of the scope of this study.

It should be noted that the excellent prediction of the elastic constants for the hexagon and star-shaped lattices in Section 3.1 and the overprediction of the energy (and therefore, the stiffness) of the lattices in this section do not contradict each other. The elastic constants simulations showed that the proposed kinematic constraints were able to match the true solution for uniform deformations, while alternative formulations may be preferable for more complex non-uniform deformations. This is analogous to how fully-integrated standard Lagrangian FE passes the patch test, but can massively overpredict the stiffness of incompressible materials undergoing more complicated deformations.

3.3. Indentation tests

In order to test the full nonlinear capabilities of truss QC, we perform adaptive indentation simulations on 2D and 3D multi-lattices. Indentation is chosen because it features highly localized deformation, buckling of beams in compression, a non-trivial onset of localization, and it has been used as a standard benchmark in classical QC (Kochmann and Amelang, 2016). We use the nonlinear corotational beams described in Section 2.4. The indenter is modeled using an energetic penalty, viz. by applying an external force potential

$$\mathcal{L}_s = \sum_{s=1}^{N_s} w_s \sum_{p \in \Omega_s} \kappa (|\mathbf{x}_p - \mathbf{x}_c| - R)^3 \quad (31)$$

⁵Higher-order interpolation within the present QC scheme is not straightforward due to the selection of representative and sampling sites from the set of actual lattice sites; see e.g. Beex et al. (2014a) for a quadratic QC interpolation.

Figure 9: Convergence of the maximum strut tensile stress near the notch tip (*left*) and of the total energy (*right*) as compared to the fully-resolved simulation for coarse-grained truss QC fracture simulations of a (a,b) kagome lattice, (c,d) triangle lattice, (e,f) hexagon lattice in 2D. Insets visualize the adaptively refined QC representation at the indicated repUC densities.

Figure 10: Convergence of the maximum strut tensile stress near the notch tip (*left*) and of the total energy (*right*) as compared to the fully-resolved simulation for coarse-grained truss QC fracture simulations of a star-shaped lattice in 2D. Insets visualize the adaptively refined QC representation at the indicated repUC densities.

where κ is a force constant, and R and $\mathbf{x}_c$ are the radius and center of the spherical indenter, respectively. The QC representation is fully-resolved where there is contact between the truss and the indenter, so the external force represents a penalty for each node in the truss lattice that penetrates the spherical indenter. It should be noted that while the contact between the truss nodes and the indenter is modeled, the contact between individual truss members is not taken into account (and not significant in the shown examples).

For comparison purposes, the 2D and 3D indentation simulations were repeated with the following settings:

- fully-resolved with corotational beams,
- fully-resolved with linear Euler-Bernoulli beams,
- truss QC with corotational beams, no refinement,
- truss QC with corotational beams, adaptive refinement.

The fully-resolved simulations with corotational beams are the highest fidelity model, and are thus used as the “exact” solution. Simulations with linear beam elements are used to demonstrate the drastic difference in predicted behavior when geometric nonlinearity is taken into account. Lastly, the two coarse-grained simulations are used to demonstrate the accuracy of truss QC and to show the importance of adaptive refinement.

The adaptive refinement technique of Section 2.5 with criterion (21) is used to enhance the QC approximation as the simulation advances. Energy minimization at each load step is carried out using the Toolkit for Advanced Optimization (TAO) (Munson et al., 2012). Specifically, we find the solution by a Newton line search method with a direct solver computing the search direction at each iteration, paired with the line search algorithm of Moré and Thuente (1994).

In 2D, we simulate indentation into a kagome lattice with relative density $\bar{\rho} = 35\%$ ($t/l \approx 0.20$ where t is the thickness of the truss member), which is tessellated to fill a square of side length $240l$ (see Fig. 11). This results in a lattice with roughly 35,000 nodes and 107,000 corotational beam elements. The coarse-grained mesh is created by having an initially fully-resolved region of size $32l \times 32l$ where the indenter makes contact, and gradually coarsening away to fill the domain resulting in a mesh with roughly 1,900 nodes ($\approx 5.3\%$ of the fully-resolved simulation). The indenter has radius $R = 60l$ and indents into the lattice a distance of $20l$ over 50 equal load steps. The refinement algorithm uses a tolerance of $r_0 = 0.075l$.

The obtained load-displacement curve is found in Fig. 12. The indenter force (F) is normalized with respect to Young’s modulus E and truss length l , while the indenter displacement (d) is normalized with respect to the truss length l . Comparing the fully-resolved corotational beam simulations to the **simulations using Euler-Bernoulli beams**

Figure 11: Initial geometry for the fully-resolved (*left*) and coarse-grained (*right*) 2D kagome lattice before indentation.

with linearized kinematics illustrates that significant geometric nonlinearity occurs during the simulation, justifying the use of corotational beams. Furthermore, the difference between the unrefined and refined truss QC simulations portrays the need for adaptive mesh refinement as the deformation becomes more severe. Most importantly, the refined truss QC simulation shows convincing agreement with the exact solution, even at significant indentation depths. The adaptively refined simulation behaves slightly stiffer than the fully-resolved simulations, which is expected since the interpolation was chosen such that truss QC overpredicts the energy of the exact solution.

Fig. 12 shows the repUC density of the simulation during refinement along with snapshots of the coarse-grained truss at various load steps. Those snapshots indicate that geometric nonlinearity in the simulation is to a considerable part due to the buckling of truss members underneath the indenter; adaptive refinement expands the fully-resolved region as necessary to capture this localized buckling.

In 3D, a kagome lattice with relative density $\bar{\rho} = 10\%$ ($r/l \approx 0.122$ where r is the radius of the truss member with circular cross-section) is tessellated to fill a cube of side length $35l$ (see Fig. 13). This results in a lattice with roughly 44,000 nodes and 130,000 corotational beam elements. The truss QC simulation starts with a mesh containing 1,600 nodes ($\approx 3.5\%$ of the fully-resolved simulation). The indenter has radius $R = 5l$ and indents into the lattice a distance of $6l$ over 50 equal load steps. Refinement uses a tolerance of $r_0 = 0.04l$.

The 3D results – while being similar to those results of the 2D lattice above – demonstrate the power of the 3D truss QC theory and implementation. The normalized load-displacement curve and the adaptive refinement results are shown in Fig. 14. Significant nonlinearity is observed in the simulation, as seen, e.g., from the drops in the load-

Figure 12: (a) Normalized load-displacement curves for the indentation into a 2D kagome lattice, (b) the repUC density as the simulation progresses, and the final deformed configurations of the (c) fully-resolved Euler-Bernouli beam, (d) fully-resolved corotational beam, and (e) adaptively refined corotational beam simulations. The colors of beams correspond to the maximum tensile stress in each beam normalized by Young's modulus.

displacement curve, which correspond to the buckling and collapse of struts beneath the indenter. Like in the case of the 2D lattice, adaptive refinement is necessary and successful in accurately predicting the response of the lattice. The adaptive truss QC simulation agrees well with the exact solution (even though not quite as well as in 2D). However, the main features of the simulation such as the initialization of buckling near the indenter and the general post-buckling behavior match well.

4. Conclusions

We have extended the quasicontinuum method to describe multi-lattice truss lattices in 2D and 3D by introducing a new interpolation scheme by which the dofs of each Bravais lattice in the multi-lattice are retained at the macroscale and are interpolated in coarse-grained regions. We have also introduced geometrically nonlinear deformation into the

Figure 13: (a) Initial geometry for the fully-resolved and (b) coarse-grained truss QC of a 3D kagome lattice before indentation.

truss QC methodology by using corotational beams for the description of individual truss members. A natural extension of the optimal summation rule of Amelang et al. (2015) to multi-lattice systems was used to efficiently sample the energy of the coarse-grained lattices. The method was numerically implemented in a parallel code with adaptive mesh refinement to automatically improve the resolution of the QC discretization where necessary and to capture localized deformation. We have tested this framework's ability to correctly model the effective elastic properties of various 2D and 3D lattices by uniformly deforming coarse-grained truss lattice blocks and comparing the effective elastic constants to those predicted by homogenization theory. When using an exact summation rule (where every UC in the simulation is a sampling UC), we found that the interpolation was able to exactly match the homogenization theory for all coarsened meshes. When the interpolation was paired with the optimal summation rule on randomly coarsened samples, small, acceptable errors were present in the predicted behavior in moderately coarsened meshes due to energy sampling errors that arise in all known sampling rules for the QC method. Furthermore, we tested the new truss QC theory and the adaptive refinement routine with more complex deformations by performing coarse-grained versions of Boundary Layer Method simulations, which were previously used to predict the brittle fracture toughness of various lattice topologies. The proposed QC method performs excellently for the triangle and kagome lattices; the maximum stress near the notch tip and total energy of the system matches the fully-resolved simulations within a few percent, while using only a small fraction of the dofs. **The hexagon and star-shaped lattices did not show such agreement with the fully-resolved simulations. This disagreement is attributed to the fact that the linear interpolation of dofs in the coarse-grained regions requires the lattice to deform through stretching of individual truss members when the lattices undergo nonuniform deformation. Due to the large strain energy difference in stretched vs. bent beams, that phenomenon may cause a significant overprediction of the energy of bending-dominated lattices.** Higher-order interpolation, additional enrichment functions, or reduced integration strategies will be explored in future studies to mitigate those errors. Lastly, we tested the fully capabilities of the new methods by indentation simulations on 2D and 3D kagome (multi-)lattices with nonlinear corotational beams to model individual truss members, and adaptive refinement to improve the mesh as the deformation becomes severe. We found that both the inclusion of geometric nonlinearity and adaptive mesh refinement was necessary to match the behavior seen in the fully-resolved nonlinear simulations. Most importantly, we found that the coarse-grained simulations matched the fully-resolved simulations

Figure 14: Normalized load-displacement curve for the indentation of a 3D kagome lattice (top left), the repUC density as the simulation progresses (top right), and the slices of the final deformed configurations of the fully-resolved (bottom left) and adaptively refined (bottom right) simulations with average axial strain contours.

well while only using a fraction of the dofs. We note that the presented method is sufficiently general to be extended to other discrete systems not necessarily of truss or lattice type (in fact, every representative unit cell can be decoupled into a set of (possibly many) Bravais lattices if each unique master node is considered as an independent Bravais lattice). The chosen truss application is ideal for this scheme, since the number of Bravais lattices to be considered in such fashion is relatively small, so that retaining dofs on the macroscale is sufficiently efficient, as shown in the chosen benchmark examples.

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Appendix A. Algorithmic implementation of truss QC

Algorithms 1 and 2 describe how the global force vector and global tangent matrix are assembled from the sampling unit cells. For simulations involving adaptive refinement, equilibrium is reached before any refinement takes place. After the mesh is refined, the system is solved again at the same load step. This is repeated until the system is at equilibrium and no macroscopic elements pass the refinement criterion. Algorithm 3 summarizes the steps involved in solving a load step.

Algorithm 1 Compute Global Force Vector

```

for each sampling UC  $s$  do
  for each truss element  $e$  contained inside  $s$  do
    calculate element force  $F_e$ 
    for each node  $p$  of  $e$  do
      for each repUC,  $r$ , used to interpolate DOFs of  $p$  do
         $F_r^p \leftarrow F_r^p + w_s N_r(X_p) F_e$ 
  for each neighboring UC  $n$  do
    for each truss element  $e$  connected to  $n$  do
      calculate element force  $F_e$ 
      for each node  $p$  of  $e$  do
        for each repUC  $r$  used to interpolate DOFs of  $p$  do
           $F_r^p \leftarrow F_r^p + \frac{1}{2} w_s N_r(X_p) F_e$ 

```

Algorithm 2 Compute Global Tangent Matrix

```

for each sampling UC  $s$  do
  for each truss element  $e$  contained inside  $s$  do
    calculate stiffness matrix,  $K_e$ 
    for each node  $p_1$  of  $e$  do
      for each node  $p_2$  of  $e$  do
        for each repUC  $r_1$  used to interpolate DOFs of  $p_1$  do
          for each repUC  $r_2$  used to interpolate DOFs of  $p_2$  do
             $K_{r_1, r_2}^{p_1, p_2} \leftarrow K_{r_1, r_2}^{p_1, p_2} + w_s N_{r_1}(X_{p_1})^2 K_e^{p_1, p_2}$ 
  for each neighboring UC  $n$  do
    for each truss element  $e$  connected to  $n$  do
      calculate element stiffness matrix  $K_e$ 
      for each node  $p_1$  of  $e$  do
        for each node  $p_2$  of  $e$  do
          for each repUC  $r_1$  used to interpolate DOFs of  $p_1$  do
            for each repUC  $r_2$  used to interpolate DOFs of  $p_2$  do
               $K_{r_1, r_2}^{p_1, p_2} \leftarrow K_{r_1, r_2}^{p_1, p_2} + \frac{1}{2} w_s N_{r_1}(X_{p_1}) N_{r_2}(X_{p_2}) K_e^{p_1, p_2}$ 

```

Algorithm 3 Compute a Loadstep

```

repeat
   $[U_{n+1}, residual] \leftarrow \text{Solve}(U_n)$ 
  refineMesh()
until  $residual < tolerance$ 

```

Appendix B. Effective elastic constants of periodic truss lattices

For comparison, we here report the homogenized stiffness tensors of the various 2D truss lattices in Voigt notation as functions of the relative density $\bar{\rho}$. These stiffness tensors were calculated by solving the unit cell problem with periodic boundary conditions, i.e., we compute

$$\mathbb{C}_{ijkl} = \frac{W}{\partial \varepsilon_{ij} \partial \varepsilon_{kl}} \quad (\text{B.1})$$

where

$$W(\varepsilon) = \inf_{U, \theta} \left\{ \frac{1}{|\Omega_{\text{UC}}|} \sum_{e \in \mathcal{E}} W_e(U, \theta) \mid U^+ - U^- = \varepsilon(X^+ - X^-), \theta^+ - \theta^- = 0 \right\} \quad (\text{B.2})$$

where + and – represent nodes on opposite sides of the UC boundary $\partial\Omega_{UC}$, $(X^+ - X^-)$ is the vector that points from the – side to the + side between pairs of boundary nodes, $\mathbf{U}$ and $\boldsymbol{\theta}$ denote the vectors of displacement and rotational dofs, respectively. The thus obtained effective stiffness tensors of the lattice architectures in this study are listed below (with E denoting the base material's Young modulus and $\bar{\rho}$ the relative density). Unfortunately, the analogous expressions for the 3D truss lattices could not be computed in closed form due to their complexity.

Appendix B.1. Triangle lattice

$$\mathbb{C}_{\text{Voigt}} = \begin{pmatrix} \frac{E\bar{\rho}(\bar{\rho}^2+36)}{96} & -\frac{E\bar{\rho}(\bar{\rho}^2-12)}{96} & 0 \\ -\frac{E\bar{\rho}(\bar{\rho}^2-12)}{96} & \frac{E\bar{\rho}(\bar{\rho}^2+36)}{96} & 0 \\ 0 & 0 & \frac{E\bar{\rho}(\bar{\rho}^2+12)}{96} \end{pmatrix}$$

Appendix B.2. 2D kagome lattice

$$\mathbb{C}_{\text{Voigt}} = \begin{pmatrix} \frac{E\bar{\rho}(\bar{\rho}^2+18)}{48} & -\frac{E\bar{\rho}(\bar{\rho}^2-6)}{48} & 0 \\ -\frac{E\bar{\rho}(\bar{\rho}^2-6)}{48} & \frac{E\bar{\rho}(\bar{\rho}^2+18)}{48} & 0 \\ 0 & 0 & \frac{E\bar{\rho}(\bar{\rho}^2+6)}{48} \end{pmatrix}$$

Appendix B.3. Square Lattice

$$\mathbb{C}_{\text{Voigt}} = \begin{pmatrix} \frac{E\bar{\rho}}{2} & 0 & 0 \\ 0 & \frac{E\bar{\rho}}{2} & 0 \\ 0 & 0 & \frac{E\bar{\rho}^3}{4} \end{pmatrix}$$

Appendix B.4. Hexagon lattice

$$\mathbb{C}_{\text{Voigt}} = \begin{pmatrix} \frac{E\bar{\rho}(9\bar{\rho}^2+4)}{4(3\bar{\rho}^2+4)} & \frac{E\bar{\rho}(4-3\bar{\rho}^2)}{4(3\bar{\rho}^2+4)} & 0 \\ \frac{E\bar{\rho}(4-3\bar{\rho}^2)}{4(3\bar{\rho}^2+4)} & \frac{E\bar{\rho}(9\bar{\rho}^2+4)}{4(3\bar{\rho}^2+4)} & 0 \\ 0 & 0 & \frac{3E\bar{\rho}^3}{6\bar{\rho}^2+8} \end{pmatrix}$$

Appendix B.5. Star lattice

$$\mathbb{C}_{\text{Voigt}} = \begin{pmatrix} \frac{8E\bar{\rho}^3}{16\bar{\rho}^2+25} & 0 & 0 \\ 0 & \frac{8E\bar{\rho}^3}{16\bar{\rho}^2+25} & 0 \\ 0 & 0 & \frac{E\bar{\rho}^3}{\bar{\rho}^2+100} \end{pmatrix}$$