Summation rules for a fully-nonlocal energy-based quasicontinuum method

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Abstract

The quasicontinuum (QC) method coarse-grains crystalline atomic ensembles in order to bridge the scales from individual atoms to the micro- and mesoscales. A crucial cornerstone of all QC techniques, summation or quadrature rules efficiently approximate the thermodynamic quantities of interest. Here, we investigate summation rules for a fully-nonlocal, energy-based QC method to approximate the total Hamiltonian of a crystalline atomic ensemble by a weighted sum over a small subset of all atoms in the crystal lattice. Our formulation does not conceptually differentiate between atomistic and coarse-grained regions and thus allows for seamless bridging without domain-coupling interfaces. We review traditional summation rules and discuss their strengths and weaknesses with a focus on energy approximation errors and spurious force artifacts. Moreover, we introduce summation rules which produce no residual or spurious force artifacts in centrosymmetric crystals in the large-element limit under arbitrary affine deformations in two dimensions (and marginal force artifacts in three dimensions), while allowing us to seamlessly bridge to full atomistics. Through a comprehensive suite of examples with spatially non-uniform QC discretizations in two and three dimensions, we compare the accuracy of the new scheme to various previous ones. Our results confirm that the new summation rules exhibit significantly smaller force artifacts and energy approximation errors. Our numerical benchmark examples include the calculation of elastic constants from completely random QC meshes and the inhomogeneous deformation of aggressively coarse-grained crystals containing nano-voids. In the elastic regime, we directly compare QC results to those of full atomistics to assess global and local errors in complex QC simulations. Going beyond elasticity, we illustrate the performance of the energy-based QC method with the new second-order summation rule by the help of nanoindentation examples with automatic mesh adaptation. Overall, our findings provide guidelines for the selection of summation rules for the fully-nonlocal energy-based QC method.

Keywords: atomistics, quasicontinuum, multiscale modeling, error analysis

1. Introduction

The state of the art in material modeling offers highly-accurate methods for each individual scale, from density functional theory (DFT) and molecular dynamics (MD) at the lower scales all the way up to continuum theories for the macroscale. Unfortunately, a wide gap exists due to a lack of models applicable at the mesoscale, where the continuum hypothesis fails yet atomistic techniques exceed computational limitations. Mastering this gap is key to understanding such diverse open problems as the response of nanoporous and nanostructured metals, the effective properties of nano- and micro-scale structures, or the underlying mechanisms of material failure. Therefore, there is urgent need for techniques that bridge across scales in order to accurately describe, to thoroughly understand, and to reliably predict the mechanics and physics of solids.

The *quasicontinuum* (QC) method was introduced to bridge from atomistics to the continuum by coarse-graining the atomistic description of crystalline solids (Tadmor et al., 1996; Miller et al., 1998; Phillips et al., 1999). Such spatial coarse-graining reduces the number of degrees of freedom by introducing geometric constraints, thereby making the lower-scale accuracy efficiently available for larger-scale simulations, see (Tadmor et al., 1996; Izvekov and Voth,

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2005; Suryanarayana, 2011; Iyer and Gavini, 2011). Coarse-graining strategies offer a number of advantages over domain-coupling methods: (i) the model is solely based on the lower-scale constitutive description and hence comes with superior accuracy (in contrast to domain coupling methods, there is no need for an oftentimes phenomenological constitutive law in the coarse-grained domain); (ii) the transition from fully-resolved to coarse-grained is seamless (no approximate hand-shake region is required between different domains); (iii) depending on the chosen technique, model adaptation can efficiently reduce computational complexity.

In the QC approach, this is achieved by three integral components: *geometric constraints* (which interpolate lattice site positions from the positions of a reduced set of representative atoms), *summation rules* or *sampling rules* (which avoid the computation of thermodynamic quantities from the full atomistic ensemble), and *model adaptation* schemes (which localize atomistic resolution and thereby efficiently minimize degrees of freedom). To date, numerous QC flavors have been developed which mainly differ in the choice of how the aforementioned three aspects are realized. For example, geometric constraints in the original QC method (Tadmor et al., 1996; Shenoy et al., 1998; Knap and Ortiz, 2001) were enforced by affine interpolation on a finite element mesh. More recent versions have explored higher-order polynomial shape functions (Park and Im, 2008; Kwon et al., 2009) as well as meshless interpolation using smoothed-particle approaches (Yang and Xiao, 2005; Xiao and Yang, 2007) or local maximum-entropy shape functions (Kochmann and Venturini, 2014). Specific adaptation techniques will not be discussed here.

Summation rules have become an essential component of the QC method (even though they are sometimes not referred to as such). While the introduction of geometric constraints reduces the number of degrees of freedom, summation rules are required to efficiently reduce the number of lattice sites to be considered e.g. in the computation of energies and forces. To this end, the thermodynamics of the full atomistic ensemble are approximated by those of a small set of carefully-chosen lattice sites (in the following referred to as *sampling atoms*), comparable to quadrature rules commonly used in the finite element method. To seamlessly bridge from atomistics to the continuum without differentiating between atomistic and coarse-grained regions, we make use of a fully *non-local QC* approximation without entire elements being represented by the Cauchy-Born rule as commonly done in local QC (Tadmor et al., 1996; Marshall and Dayal, 2013). Summation rules now differ by the choice of (i) sampling atom locations and (ii) sampling atom weights. Successful examples of summation rules introduced previously include node-based cluster summation (Knap and Ortiz, 2001) with sampling atoms located in clusters around repeatoms, and quadrature-type summation (Gunzburger and Zhang, 2010; Yang et al., 2013) with sampling atoms chosen nearest to Gaussian quadrature points with or without the repeatoms included as sampling atoms. Furthermore, element-based summation rules have been introduced in the non-local QC context (Gunzburger and Zhang, 2010; Yang et al., 2013) and have demonstrated superior accuracy over traditional cluster-based summation schemes (Iyer and Gavini, 2011). Recently, Beex et al. (2014) studied a first-order quadrature rule which is similar in spirit and contained as a special case within the new summation rules reported here. Many summation rules have been introduced to mediate particular QC deficiencies (e.g. cluster rules were introduced to remove zero-energy modes in force-based QC (Knap and Ortiz, 2001)) or by borrowing schemes from related models (e.g. finite element quadrature rules (Gunzburger and Zhang, 2010)).

Summation rules can either approximate the energy of the system (Eidel and Stukowski, 2009) or the forces experienced by repeatoms (Knap and Ortiz, 2001). Systematic mathematical error and stability analyses of node-based cluster summation rules have highlighted the deficiencies of force-based QC schemes and have advocated the energy-based QC formulation (Luskin and Ortner, 2009; Dobson et al., 2010a,b,c) due to its conservative structure. Moreover, the proper convergence of energy-based QC techniques was shown recently for harmonic lattices (Espanol et al., 2013). Therefore, in the following we choose an energy-based QC formulation. We note that, although we focus on the QC method applied to atomistic ensembles, the same technique can be used e.g. in coarse-graining Density Functional Theory (Suryanarayana et al., 2013) as well as in multiscale structural mechanics (Beex et al., 2011).

Here, we compare various summation rules for the energy-based QC method in a unified scheme based on *sampling atoms* whose locations and weights differ between the various rules. To assess the accuracy of each scheme, we carry out a comprehensive analysis of spurious force artifacts in one and two-dimensions. Based on our findings, we introduce a class of summation rules with minimal approximation errors and marginal or vanishing residual force artifacts in centrosymmetric lattices. The remainder of this paper is structured as follows: Section 2 reviews the fundamentals of the QC method and introduces our nonlocal energy-based formulation. Section 3 briefly discusses summation rules. Section 4 studies errors and force artifacts in one dimension, followed by two- and three-dimensional analyses in Sections 5 and 6, respectively. Numerical examples of energy errors and force artifacts are reported in Section 7. Sections 8 and 9 summarize numerical benchmark simulations, before Section 10 concludes our analysis.

2. The quasicontinuum method

2.1. Quasicontinuum approximation of an atomic ensemble

In classical mechanics, an atomistic ensemble containing N atoms is uniquely described by how their positions $\mathbf{q} = \{\mathbf{q}_1, \dots, \mathbf{q}_N\}$ and momenta $\mathbf{p} = \{\mathbf{p}_1, \dots, \mathbf{p}_N\}$ with $\mathbf{p}_i = m_i \dot{\mathbf{q}}_i$ evolve with time t . m_i is the mass of atom i , and dots denote material time derivatives. The system's Hamiltonian is defined by

$$\mathcal{H}(\mathbf{q}, \mathbf{p}) = \sum_{i=1}^N \frac{|\mathbf{p}_i|^2}{2m_i} + V(\mathbf{q}), \quad (1)$$

where the first term accounts for the kinetic energy and the second term represents the potential energy of the ensemble with V denoting a suitable atomic interaction potential. The time evolution of the system is given by Hamilton's equations, yielding Newton's equations of motion for atoms $i = 1, \dots, N$, viz.

$$m_i \ddot{\mathbf{q}}_i = \mathbf{f}_i(\mathbf{q}) = -\frac{\partial V}{\partial \mathbf{q}_i}(\mathbf{q}), \quad (2)$$

where $\mathbf{f}_i(\mathbf{q})$ is the total force acting on atom i (the notion of conservative forces is implicit in the fact that forces are assumed to derive from a potential V). We note that V can, in principle, depend on both positions and momenta, which is necessary e.g. when using the quasiharmonic approximation to mimic conditions of quasistatic finite temperature (Tadmor et al., 2013). For conciseness, we here restrict our analysis to position-dependent potentials; the extension to include momenta is straight-forward. Furthermore, we limit our analysis to crystalline solids in which the ground state atomic positions agree with sites of a Bravais lattice and the interaction potential most commonly has the additive decomposition

$$V(\mathbf{q}) = \sum_{i=1}^N E_i(\mathbf{q}) \quad (3)$$

with E_i being the energy of atom i . Note that some authors prefer to distinguish between external and internal forces by introducing external forces $\mathbf{f}_{i,\text{ext}}$ on atoms $i = 1, \dots, N$ so that

$$\mathbf{f}_i(\mathbf{q}) = \mathbf{f}_{i,\text{ext}}(\mathbf{q}_i) - \frac{\partial V}{\partial \mathbf{q}_i}(\mathbf{q}). \quad (4)$$

Ideally (and in any reasonable physical system), such external forces are conservative and derive from an external potential $V_{\text{ext}}(\mathbf{q})$ and we may combine internal and external forces into a single potential, which is tacitly assumed in the following. Examples of conservative external forces include gravitation, long-range Coulombic interaction, or multi-body interactions often realized by artificial potentials, see e.g. (Kelchner et al., 1998) for indentation.

Because of computational costs, it is generally not feasible to apply the above framework to simulate long-range elastic effects, even for short-range interatomic potentials. However, except in the vicinity of lattice defects and flaws, the local environment of nearby atoms in a crystal lattice is almost identical up to translation. Therefore, the *quasicontinuum* (QC) *approximation* replaces the full atomistic ensemble by a reduced set of $N_h \ll N$ representative atoms (or *repatoms* for short) having positions $\mathbf{x}(t) = \{\mathbf{x}_1(t), \dots, \mathbf{x}_{N_h}(t)\}$. The approximate current position $\mathbf{x}_i^h$ and momentum $\mathbf{p}_i^h$ of atom i are obtained by interpolation:

$$\mathbf{q}_i \approx \mathbf{q}_i^h = \sum_{a=1}^{N_h} N_a(\mathbf{X}_i) \mathbf{x}_a, \quad \mathbf{p}_i \approx \mathbf{p}_i^h = m_i \dot{\mathbf{x}}_i^h = m_i \sum_{a=1}^{N_h} N_a(\mathbf{X}_i) \dot{\mathbf{x}}_a \quad \text{for } i = 1, \dots, N. \quad (5)$$

$N_a(\mathbf{X}_i)$ is the shape function of repatom a evaluated at the position $\mathbf{X}_i$ of lattice site i in the reference configuration. As an essential feature, this coarse-graining scheme locally recovers the exact atomic ensemble when all atoms are turned into repatoms (shape functions are chosen to satisfy the Kronecker property $N_a(\mathbf{X}_b) = \delta_{ab}$ for all $1 \leq a, b \leq N_h$ with δ_{ij} denoting Kronecker's delta). In the following, we will restrict our analysis to an affine interpolation on a Delaunay triangulated mesh as in the traditional QC method.

The introduction of geometric constraints (5) has reduced the total number of independent degrees of freedom from $d \times N$ in d dimensions to $d \times N_h$. Consequently, the reduced Hamiltonian $\mathcal{H}^h$ of the coarse-grained system, now involving approximate positions $\mathbf{q}^h = \{\mathbf{q}_1^h, \dots, \mathbf{q}_N^h\}$ and momenta $\mathbf{p}^h = \{\mathbf{p}_1^h, \dots, \mathbf{p}_N^h\}$, only depends on positions and momenta of the repatoms through (5):

$$\mathcal{H}^h(\mathbf{x}, \dot{\mathbf{x}}) = \sum_{i=1}^N \frac{|\mathbf{p}_i^h|^2}{2m_i} + V(\mathbf{q}^h). \quad (6)$$

Instead of solving for the positions and momenta of all N lattice sites, the QC approximation allows us to update only the positions and momenta of the N_h repatoms, which requires to compute forces on repatoms. These are obtained from the potential energy by differentiation, which yields the force on repatom k :

$$\mathbf{F}_k(\mathbf{x}) = -\frac{\partial V(\mathbf{q}^h)}{\partial \mathbf{x}_k} = \sum_{j=1}^N \mathbf{f}_j^h(\mathbf{q}^h) N_k(\mathbf{X}_j) \quad \text{with} \quad \mathbf{f}_j^h(\mathbf{q}^h) = -\frac{\partial V(\mathbf{q}^h)}{\partial \mathbf{q}_j^h} = -\sum_{i=1}^N \frac{\partial E_i(\mathbf{q}^h)}{\partial \mathbf{q}_j^h}. \quad (7)$$

$\mathbf{f}_j^h(\mathbf{q}^h)$ denotes the total force acting on atom j . A common approximation for non-conservative external forces is

$$\mathbf{F}_{k,\text{ext}}(\mathbf{x}) = \sum_{j=1}^N \mathbf{f}_{j,\text{ext}}(\mathbf{q}^h) N_k(\mathbf{X}_j), \quad (8)$$

so that the overall force on repatom k can be written as

$$\mathbf{F}_k(\mathbf{x}) = \sum_{j=1}^N \left(\mathbf{f}_{j,\text{ext}}(\mathbf{q}^h) - \frac{\partial V(\mathbf{q}^h)}{\partial \mathbf{q}_j^h} \right) N_k(\mathbf{X}_j) = \sum_{j=1}^N \mathbf{f}_j^h(\mathbf{q}^h) N_k(\mathbf{X}_j), \quad (9)$$

where $\mathbf{f}_j^h(\mathbf{q}^h)$ is the total force on atom j . Note that in an infinite Bravais lattice in the absence of external loading the forces on all atoms vanish, i.e. $\mathbf{f}_i^h(\mathbf{q}^h) = \mathbf{0}$, so that the forces on all repatoms vanish as well ($\mathbf{F}_k = \mathbf{0}$). This implies that the kinematic QC approximation itself does not introduce any force artifacts on repatoms.

2.2. Summation rules and spurious force artifacts

Even though the number of degrees of freedom has been reduced from $d \times N$ to $d \times N_h$ by selecting repatoms, the calculation of repatom forces still requires computing the forces between all N atoms and their on average N_b neighbors located within each atom's radius of interaction. These $\mathcal{O}(N \times N_b)$ operations become computationally not feasible for realistically-sized systems (in principle, summations in (9) can be reduced to the support of the shape functions but even this is prohibitively expensive in large elements). Therefore, *summation rules* have been introduced to replace the sum over index i in (3) or (9) by a weighted sum over N_s carefully-chosen *sampling atoms*. Consequently, the total potential energy is approximated by

$$V(\mathbf{q}^h) = \sum_{i=1}^N E_i(\mathbf{q}^h) \approx \tilde{V}(\mathbf{q}^h) = \sum_{\alpha=1}^{N_s} w_\alpha E_\alpha(\mathbf{q}^h), \quad (10)$$

where w_α is the weight of sampling atom α . Physically, w_α defines the number of atoms represented by sampling atom α . Because the summation rule is applied to the Hamiltonian, (10) is commonly referred to as an *energy-based* summation rule. The force experienced by repatom k is obtained by differentiation in analogy to (7), i.e.

$$\tilde{\mathbf{F}}_k(\mathbf{x}) = -\frac{\partial \tilde{V}(\mathbf{q}^h)}{\partial \mathbf{x}_k} = -\sum_{\alpha=1}^{N_s} w_\alpha \sum_{j=1}^{N_b} \frac{\partial E_\alpha(\mathbf{q}^h)}{\partial \mathbf{q}_j^h} N_k(\mathbf{X}_j). \quad (11)$$

Now, repatom force calculation has been reduced to $\mathcal{O}(N_s \times N_b)$ operations. The selection of sampling atoms and the calculation of sampling atom weights aims for a compromise between maximum accuracy (ideally $N_s = N$ and $w_\alpha = 1$) and maximum efficiency (requiring $N_s \ll N$ and $w_\alpha \gg 1$).

Summation rules on the energy level not only reduce computational complexity but also give rise to *force artifacts*, see e.g. (Eidel and Stukowski, 2009) for a recent discussion. By rewriting (11) without neighborhood truncations as

$$\tilde{\mathbf{F}}_k(\mathbf{x}) = - \sum_{\alpha=1}^{N_s} w_{\alpha} \sum_{j=1}^N \frac{\partial E_{\alpha}(\mathbf{q}^h)}{\partial \mathbf{q}_j^h} N_k(\mathbf{X}_j) = \sum_{j=1}^N \left(- \sum_{\alpha=1}^{N_s} w_{\alpha} \frac{\partial E_{\alpha}(\mathbf{q}^h)}{\partial \mathbf{q}_j^h} \right) N_k(\mathbf{X}_j), \quad (12)$$

and comparing with (9), we notice that the term in parentheses in (12) does not equal force $\mathbf{f}_j^h$ and hence does not vanish in general even if $\mathbf{f}_j^h = \mathbf{0}$ for all atoms (unless the set of sampling atoms is chosen to agree with the full atomic ensemble, i.e. $N_s = N$ and $w_{\alpha} = 1$). As a consequence, the QC representation with energy-based summation rules shows *residual forces* on repatoms in the undeformed ground state which are non-physical. Note that for uniform QC meshes these residual forces disappear due to symmetry because the sum in parentheses in (12) cancels pairwise when carrying out the full summation. Residual forces therefore only appear in spatially non-uniform meshes, see also (Iyer and Gavini, 2011). In the original QC method (Tadmor et al., 1996) where atomistic and coarse-grained regions (treated by a local Cauchy-Born formulation) are spatially separated, such forces only appear at the interface between atomistic and continuum regions and were called *ghost forces* (Miller et al., 1998; Shenoy et al., 1998). In non-local, energy-based schemes – as discussed here – the analogous forces are known as spurious or residual forces (Eidel and Stukowski, 2009). In contrast to previous studies, we would like to explicitly differentiate between residual and spurious forces. *Residual forces* are force artifacts in the undeformed configuration which can be removed by computing those forces and subtracting them as dead loads from all repatom forces in subsequent calculations, similarly to the method of ghost-force correction, see e.g. (Shenoy et al., 1998). In contrast, we denote by *spurious forces* those erroneous forces that arise in the deformed configuration from the introduction of summation rules. Even though residual and spurious forces are conservative in the energy-based scheme, they are non-physical and can typically be quantified in defect-free infinite systems.

To avoid residual forces, Knap and Ortiz (2001) introduced *force-based summation rules* which do not approximate the Hamiltonian but the repatom forces explicitly, i.e. the summation rule is applied directly to (7), giving

$$\mathbf{F}_k(\mathbf{x}) = \sum_{i=1}^N \mathbf{f}_i^h(\mathbf{q}^h) N_k(\mathbf{X}_i) \approx \tilde{\mathbf{F}}_k(\mathbf{x}) = \sum_{\alpha=1}^{N_s} w_{\alpha} \mathbf{f}_{\alpha}^h(\mathbf{q}^h) N_k(\mathbf{X}_{\alpha}). \quad (13)$$

Consequently, the force-based formulation does not produce any residual forces because $\mathbf{f}_{\alpha}^h(\mathbf{q}^h) = \mathbf{0}$ in an undeformed infinite crystal (they become apparent, though, when considering finite-sized crystals with free surfaces). Yet, this approximation gives rise to a new problem: the force-based method is non-conservative; ergo, there is no energy potential from repatom forces derive. This has a number of drawbacks including slow convergence or convergence to non-physical equilibrium states, numerical instability and loss of accuracy (Luskin and Ortner, 2009; Dobson et al., 2010a,b,c; Ortner, 2011), see e.g. (Eidel and Stukowski, 2009; Miller and Tadmor, 2009; Iyer and Gavini, 2011) for discussions. Further, for dynamic or finite-temperature QC, force-based summation rules cannot be used to simulate systems in the microcanonical ensemble (of course, this does not rule out the use of alternative ensembles). Finally, repatom masses, required for dynamic simulations, are not uniquely defined since there is no effective kinetic energy potential when using force-based summation rules. In contrast, energy-based summation rules lead to conservative forces, to strictly-symmetric stiffness matrices, and to only the six admissible zero eigenvalues even for purely nodal summation rules as shown by (Eidel and Stukowski, 2009). For all those reasons, we focus on energy-based summation rules. Note that in the following we neglect thermal fluctuations and consider only zero temperature. For finite-temperature QC extensions see e.g. (Shenoy et al., 1999b; Hai and Tadmor, 2003; Dupuy et al., 2005; Tang et al., 2006; Kulkarni et al., 2008; Marian et al., 2010; Tadmor et al., 2013; Venturini et al., 2014) and references therein. These approaches can be applied to the spatial coarse-graining techniques discussed here; yet, they go beyond the scope of this paper.

The above coarse-graining framework is sufficiently general for most types of crystalline solids. For example, the Embedded Atom Method (EAM) of Daw and Baskes (1984) defines the interatomic potential energy of a collection of N atoms by

$$E_i(\mathbf{q}) = \mathcal{F}(\rho_i) + \frac{1}{2} \sum_{\substack{j=1 \\ j \neq i}}^N \Phi(r_{ij}), \quad \rho_i = \sum_{j=1}^N f(r_{ij}). \quad (14)$$

The pair potential $\Phi(r_{ij})$ represents the energy due to electrostatic interactions between atom i and its neighbor j whose distance is given by $r_{ij} = |\mathbf{r}_{ij}|$ and $\mathbf{r}_{ij} = \mathbf{q}_i - \mathbf{q}_j$. ρ_i denotes the (approximated) effective electron density which atom i senses due to its neighboring atoms. $f(r_{ij})$ is the electron density at site i due to atom j as a function of their distance r_{ij} . $\mathcal{F}(\rho_i)$ accounts for the energy release upon embedding atom i into the local electron density ρ_i .

Although all subsequent examples will be restricted to quasistatics, we would like to point out that the aforementioned fully-nonlocal energy-based QC formulation provides consistent repatom masses, which are required e.g. for finite-temperature simulations (Tadmor et al., 2013; Venturini et al., 2014). The total kinetic energy of the atomic ensemble (approximated by the QC interpolation scheme) is given by

$$\frac{1}{2} \sum_{i=1}^N m_i (\dot{\mathbf{q}}_i^h)^2 = \frac{1}{2} \sum_{i=1}^N m_i \left| \sum_{a=1}^{N_h} N_a(X_i) \dot{\mathbf{x}}_a \right|^2 = \frac{1}{2} \sum_{a=1}^{N_h} \sum_{c=1}^{N_h} \dot{\mathbf{x}}_a \cdot \left(\sum_{i=1}^N m_i N_a(X_i) N_c(X_i) \right) \dot{\mathbf{x}}_c, \quad (15)$$

where the term in parentheses may be interpreted as components M_{ac}^h of a consistent mass matrix $\mathbf{M}^h$. In avoidance of solving the global system during time stepping, one may use particle-mass lumping, cf. (Knap and Ortiz, 2001). Applying the energy-based summation rule to the kinetic energy (analogously to the approximation of the potential energy) yields a consistent approximation of the kinetic energy with the consistent mass matrix components

$$M_{ac}^h = \sum_{i=1}^N m_i N_a(X_i) N_c(X_i) \approx \tilde{M}_{ac}^h = \sum_{b=1}^{N_s} w_b m_b N_i(X_b) N_j(X_b). \quad (16)$$

3. General framework of summation rules

We consider energy-based summation rules applied to a crystalline lattice that is coarse-grained by the QC approximation using an affine interpolation. The total potential energy is approximated by (10) and repatom forces by (11). Specific summation rules differ by the selection of the N_s sampling atoms and by the calculation of their weights w_α . The choice of sampling atoms is, in principle, independent of the choice of repatoms. Fig. 1 schematically illustrates four types of summation rules previously introduced by the QC community.

In the *nodal* summation rule the set of sampling atoms agrees with the set of repatoms ($N_s = N_h$). In avoidance of the significant energy approximation errors and resulting force artifacts, *cluster* summation rules were introduced which choose sampling atoms as lattice sites located in spherical clusters around repatoms (Knap and Ortiz, 2001; Eidel and Stukowski, 2009). Increasing the cluster radius r_c to include more shells of atoms increases the accuracy but also significantly raises computational expenses since the number of atoms per cluster scales with $O(r_c^3)$. Eidel and Stukowski (2009) showed that to reduce errors and force artifacts to a reasonable level clusters must be chosen sufficiently large to overlap, which incurs high computational expenses. The main deficiency of all node-based summation rules is the error made by approximating the energy of many lattice sites well within an element by those at or near the vertices. As a remedy, *element quadrature* summation rules take sampling atoms as those lattice sites closest to quadrature points of the finite element mesh using e.g. Gauss-Lobatto quadrature (Gunzburger and Zhang, 2010; Yang et al., 2013). *Quadrature* summation rules sample over all repatoms plus quadrature-type lattice sites comparable to

Figure 1: Various types of summation rules introduced by the QC community: nodal, cluster, quadrature-type, and element quadrature rules. Small open circles represent lattice sites, solid black circles are repatoms, and open large circles are sampling atoms. Except in element quadrature, all summation rules include the repatoms in the set of sampling atoms in order to naturally bridge to full atomistics.

stress-point integration in particle methods (Xiao and Yang, 2007). In addition, one can formulate mixed summation rules having clusters around repatoms or quadrature-type sites, or around both (Gunzburger and Zhang, 2010). Further summation rules have been proposed which identify unique atomic neighborhoods for all lattice sites within a given element and compute the exact energy by weighting their energies (Yang et al., 2014). While this approach effectively removes force artifacts, it is computationally much more expensive due to large numbers of sampling atoms. It is also difficult to generalize since each geometrically-different element requires a different summation rule. We therefore exclude this method from our analysis.

For brevity, we identify summation rules by two numbers: n_{Cl} , the number of shells included in clusters around repatoms, and n_{Q} , the number of quadrature-type sampling atoms per element (we do not consider clusters around sampling atoms for reasons explained later). Hence, a summation rule is characterized by the pair $(n_{\text{Cl}}, n_{\text{Q}})$, cf. Fig. 1. To seamlessly bridges to full atomistics, we will not conceptually differentiate between local and non-local elements. Therefore, we exclude element quadrature rules of type $(-, n_{\text{Q}})$ from our numerical examples because they do not include repatoms in the set of sampling atoms so that **some assumptions and a special algorithmic treatment may be required to recover full atomistics**. All other schemes can **transition seamlessly without explicitly differentiating between atomistic and coarse-grained regions** by ultimately having all lattice sites being repatoms and sampling atoms.

We specifically focus on quadrature-type summation rules which have been neglected in numerical QC realizations in the past. Gunzburger and Zhang (2010) showed that quadrature-type summation has, for the same accuracy, lower complexity than cluster-based approximation schemes. Luskin and Ortner (2009) reported that cluster summation rules lead to inconsistent and inaccurate QC approximations when used with non-uniform meshes and that increasing the cluster size does not resolve this problem. However, element-based summation rules e.g. using clusters around quadrature points Gunzburger and Zhang (2010), though not passing the patch test, show significantly smaller errors than node-based cluster summation rules, which decay with element size for sufficiently large elements (Iyer and Gavini, 2011). Unfortunately, to date all error analyses in this context have been limited by one or more of the following: (i) one-dimensional or at most two-dimensional scenarios, (ii) small numbers of repatoms, (iii) simplistic interatomic potentials, and (iv) only uniform repatom spacings or individual mesh interfaces were considered instead of complex geometries with aggressive coarse-graining and non-regular repatom distribution. Therefore, our goal is a general assessment of the accuracy of the various energy-based summation rules with realistic potentials in severely non-uniform meshes containing large numbers of lattice sites in two and three dimensions.

In most previous schemes, weights have been computed by solving a more or less complicated system of equations to satisfy two main requirements. First, in the full atomistic limit ($N_h \rightarrow N$) we must recover the correct energy, i.e. we must have $w_\alpha \rightarrow 1$. Second, weights were chosen such that the summation rule is zeroth- and first-order consistent to guarantee convergence with mesh refinement. Here, we propose to compute weights w_α from the volumes Ω_α of Voronoi cells in a tessellation based on the set of all sampling atoms, i.e. $w_\alpha = \rho \Omega_\alpha$ with ρ being the effective atomic density (which is uniformly constant for a pristine single crystal). By defining $\rho = 1/\Omega_0$ with Ω_0 the Voronoi cell volume of each atom in an undeformed perfect single crystal and by choosing an interpolation scheme that satisfies the Kronecker property $N_a(\mathbf{x}_b) = \delta_{ab}$ (such as affine interpolation), we ensure the correct atomistic limit. Computing weights in this way bears a number of advantages: (i) the computation of weights is computationally feasible for any spatial distribution of sampling atoms and does not require further approximations (e.g. differentiating between small and large elements); (ii) the computation of weights is independent of the chosen interpolation scheme and is therefore generally applicable, e.g. to meshless interpolations (Kochmann and Venturini, 2014); (iii) the resulting summation rules satisfy zeroth- and first-order consistency (approximately in case of cluster rules), which supports convergence with h -refinement; for details, see the discussion in (Kochmann and Venturini, 2014). For cluster summation rules we assign a unique weight to each cluster, i.e. we tessellate the $N_{s,\text{Cl}}$ cluster center atoms, where each cluster center α is surrounded by a set $n_{\text{C}}(\alpha)$ of cluster atoms. Then, weights are given by $w_\alpha = w_{\alpha,\text{tess.}}/|n_{\text{C}}(\alpha)|$, i.e. by the weight obtained from dividing the tessellated volumes by the number of atoms within each cluster. A quick calculation for this case shows that it is first-order consistent only if every cluster center $\mathbf{X}_\alpha$ is located at the geometric average of all atoms contained within its cluster. In centrosymmetric lattices, this can generally be assumed to hold (unless in very distorted meshes or near full atomistic resolution). Knap and Ortiz (2001) computed cluster weights by enforcing zeroth- and first-order consistency explicitly (or an approximate version thereof via lumping), which, however, we do not consider here due to the enormous computational expenses of solving a linear system for all weights.

In the following, we will investigate the accuracy of several (old and new) energy-based summation rules to assess their accuracy with respect to three crucial aspects: (i) What is the *approximation power* of the summation rule, i.e.

Figure 2: Overview of summation rules in one dimension. Small open circles represent lattice sites, closed circles denote repatoms, and large open circles denote sampling atoms. Weights w_i (one for each sampling atom) are obtained from tessellation.

how well does it approximate the total energy? (ii) To what extent do *force artifacts* arise from the summation rule in non-uniform meshes? (iii) Does the summation rule offer *seamless bridging* to full atomistics?

4. Analysis of summation rules in one dimension

In avoidance of the geometric complexity of higher dimensions, [Eidel and Stukowski \(2009\)](#) and [Iyer and Gavini \(2011\)](#) compared the accuracy of selected energy- and force-based summation rules by studying a representative one-dimensional example. Here, we will follow a similar approach and investigate the approximation power and force artifacts of various summation rules of type (n_C, n_Q) in one dimension as shown in Fig. 2. In particular, we include quadrature summation rules which were not included previously. Of course, the one-dimensional example will not accurately capture the physical reality, yet it allows us to draw important conclusions in a clean and instructive manner, which will lead to improved summation rules in higher dimensions.

4.1. Energy approximation error

Consider the one-dimensional chain of atoms schematically shown in Fig. 3a, which consists of two semi-infinite atomic chains with uniform atomic spacing l and repatom spacings $n_1 l$ and $n_2 l$ to the left and right of an interface repatom, respectively. Both sides of the interface are assumed to undergo **affine deformations** changing atomic spacings into $F_1 l$ and $F_2 l$. The radius of interaction of the atomic potential is assumed to involve n_b neighbors. We assume that both elements are sufficiently large, i.e. $n_1, n_2 \gg n_b$. Because linear interpolation results in affine deformation on either side of the interface, atoms located at distances greater than or equal to n_b from the interface have the same energy E_1 (to the left of the interface) or E_2 (to its right), see Fig. 3b. The energy of the $(2n_b - 1)$ atoms near the

Figure 3: a) Example of an interface in a one-dimensional chain of atoms: two semi-infinite atomic chains with repatom spacings $n_1 l$ and $n_2 l$ to the left and right of the interface repatom, respectively. Atoms to the left and right of the interface (originally at equal distances l) experience uniform **deformation gradients** F_i resulting in atomic spacings $F_1 l$ and $F_2 l$, respectively. b) Schematic illustration of the energy per atom along the one-dimensional chain. We note that, here and in the following, the exact form of the energy in the transition between elements depends essentially on the potential and the deformation gradients inside the elements; the shown close-to-linear transition from E_1 to E_2 is only schematic (observable e.g. in a 1D Lennard-Jones crystal with $F_1 = 0.95$, $F_2 = 1.08$ and fourth-nearest neighbor interactions).

interface deviates from these two values; we denote their average energy per atom by $\bar{E}_0$. Therefore, the two elements adjacent to the interface have the exact total energy (counting repatoms as belonging half to each adjacent element)

$$V_{\text{exact}} = \left(n_1 - n_b + \frac{1}{2}\right) E_1 + \left(n_2 - n_b + \frac{1}{2}\right) E_2 + (2n_b - 1) \bar{E}_0. \quad (17)$$

In the *nodal summation rule* (0, 0) of Fig. 2a sampling atoms coincide with repatoms, and sampling atom weights to the left and to the right the interface are n_1 or n_2 , respectively. The interface repatom has weight $(n_1 + n_2)/2$. The interface lattice site is assumed to have energy E_0 which may deviate from the average of its neighbors, $\bar{E}_0$. The approximate total energy of the two interface elements is now given by

$$\tilde{V}_{(0,0)} = \frac{n_1}{2} E_1 + \frac{n_2}{2} E_2 + \frac{n_1 + n_2}{2} E_0. \quad (18)$$

Only in the unstrained ground state (i.e. when $F_1 = F_2 = 1$ and therefore $E_1 = E_2 = E_0 = \bar{E}_0$) the approximate energy becomes exact, i.e. $\tilde{V} = V_{\text{exact}}$. In the limit of large elements ($n_1, n_2 \rightarrow \infty$), the nodal rule leads to the relative error

$$\left| \frac{\tilde{V}_{(0,0)} - V_{\text{exact}}}{V_{\text{exact}}} \right| = \left| \frac{\frac{1}{2} (E_0 - E_1)n_1 + (E_0 - E_2)n_2 - (2\bar{E}_0 - E_1 - E_2)(2n_b - 1)}{(n_1 - n_b + \frac{1}{2}) E_1 + (n_2 - n_b + \frac{1}{2}) E_2 + (2n_b - 1) \bar{E}_0} \right| \rightarrow \left| \frac{\frac{1}{2} (E_1 - E_0) + (E_2 - E_0) \frac{n_2}{n_1}}{E_1 + E_2 \frac{n_2}{n_1}} \right| = O(1),$$

a deficiency of this type of summation rule that was already pointed out by Iyer and Gavini (2011). The error persists in uniform meshes (i.e. if $n_1 = n_2$) and only vanishes if **deformation gradients** are uniform ($F_1 = F_2$). Physically, this can be expected since the energies of inner-element lattice sites are misrepresented by the energy of the interface sampling atom.

For a *nodal cluster summation rule* ($n_{\text{Cl}}, 0$) shown in Fig. 2b, the above derivation equally applies except that E_0 must be replaced by the energy average of all atoms in the cluster around the interface repatom. Therefore, $|E_0 - \bar{E}_0|$ decreases with increasing cluster radius and vanishes if $n_c \geq n_b$. However, the above scaling for large elements still applies so that the approximation error of all node-based summation rules in the large-element limit is significant.

Next, suppose an *element quadrature rule* of lowest order $(-, 1)$ as shown in Fig. 2c. Sampling atoms are located at element centers and therefore have weights n_1 or n_2 . The approximate total energy of the two elements simply becomes

$$\tilde{V}_{(-,1)} = n_1 E_1 + n_2 E_2 \quad (19)$$

and the relative energy error assumes the form (with abbreviation $n_i \sim n_1, n_2$)

$$\left| \frac{\tilde{V}_{(-,1)} - V_{\text{exact}}}{V_{\text{exact}}} \right| = \left| \frac{(2n_b - 1) \left[\frac{1}{2} (E_1 + E_2) - \bar{E}_0 \right]}{(n_1 - n_b + \frac{1}{2}) E_1 + (n_2 - n_b + \frac{1}{2}) E_2 + (2n_b - 1) \bar{E}_0} \right| = O\left(\frac{1}{n_i}\right). \quad (20)$$

Figure 4: Schematic view of a one-dimensional mesh interface separating elements of two different sizes, along with atomic energies and deformation gradients arising from a displacement of the central repatom.

As the element size increases ($n_1, n_2 \gg n_b$), quadrature summation rules hence approximate the total energy of the coarse-grained ensemble with increasing accuracy. This result, of course, also holds true for higher-order quadrature rules $(-, n_Q)$ as well: as long as elements are sufficiently large, increasing the number of quadrature atoms per element, n_Q , does not alter the approximated energy since all inner-element quadrature atoms will contribute the same energy. The same applies if clusters were added around quadrature atoms.

Finally, *quadrature summation rules* $(0, n_Q)$ as shown in Fig. 2d-e combine element quadrature and nodal summation rules, i.e. the set of sampling atoms includes all repatoms as well as n_Q equally-spaced quadrature-type sampling atoms per element. In this case, all sampling atoms to the right and to the left of the interface have weights $n_i/(n_Q + 1)$ ($i = 1, 2$, respectively) and the interface sampling atom has weight $(n_1 + n_2)/(2(n_Q + 1))$. The approximate total energy of the two interface-adjacent elements follows as

$$\tilde{V}_{(0, n_Q)} = \frac{2n_Q + 1}{2(n_Q + 1)} (n_1 E_1 + n_2 E_2) + \frac{n_1 + n_2}{2(n_Q + 1)} E_0 \quad (21)$$

and the large-element limit shows that the relative energy error is

$$\left| \frac{\tilde{V}_{(0, n_Q)} - V_{\text{exact}}}{V_{\text{exact}}} \right| \rightarrow \frac{1}{n_Q + 1} \left| \frac{\tilde{V}_{(0, 0)} - V_{\text{exact}}}{V_{\text{exact}}} \right| = O(1). \quad (22)$$

Consequently, for quadrature summation rules all qualitative conclusions drawn above for the nodal summation rule apply with the total error reduced by a factor of $n_Q + 1$.

It is important to note that all of the aforementioned summation rules produce the exact energy if the entire crystal is affinely deformed so that $F_1 = F_2$ and hence $E_1 = E_2 = E_0 = \bar{E}_0$. This can be expected since the summation rules are zeroth-order consistent and therefore reproduce a constant field exactly. In summary, the only summation rule with vanishing energy approximation error in large elements is based on element quadrature which, however, we exclude from our fully-nonlocal QC investigation for the following reasons.

The envisioned nonlocal QC formulation does not methodologically differentiate between fully-atomistic and coarse-grained regions and therefore can adaptively adjust the mesh resolution locally in a fully-automatic fashion. There is no notion of an interface between the two regions, and the transition is seamless. Of course, the local/nonlocal QC framework can also bridge to full atomistic resolution by refining elements down to the terminal atomistic level, see e.g. (Prudhomme et al., 2006; Ortner and Shapeev, 2013). However, repatoms in local/nonlocal QC are treated fundamentally differently in atomistic and coarse-grained regions (e.g. the construction of deformed neighborhoods or the calculation of repatom forces, etc. follow different algorithms in those two regions). The presented fully-nonlocal formulation does not differentiate between local and nonlocal elements, and it does not switch from an element-based formulation to a node-based formulation in the atomistic limit – in fact, our QC implementation applies the same algorithms to all repatoms. For all these reasons, we exclude element-based quadrature rules in the following.

4.2. Residual forces

Residual forces are a good indicator of spurious force artifacts. They arise when summation rules are applied to spatially non-uniform meshes. Consider the one-dimensional chain of atoms shown in Fig. 4. If the interface repatom

is displaced by u to its new position x_0 with all other repatoms fixed, the two elements adjacent to the interface experience **deformation gradients** that are linked by

$$n_1 F_1 + n_2 F_2 = n_1 + n_2 \quad \Rightarrow \quad dF_2 = -\frac{n_1}{n_2} dF_1. \quad (23)$$

The force on the interface repatom becomes

$$\tilde{F}_0 = -\frac{\partial \tilde{V}}{\partial x_0}(F_1, F_2) = -\frac{\partial \tilde{V}}{\partial F_1} \frac{\partial F_1}{\partial x_0} - \frac{\partial \tilde{V}}{\partial F_2} \frac{\partial F_2}{\partial x_0} = -\left(\frac{\partial \tilde{V}}{\partial F_1} - \frac{n_1}{n_2} \frac{\partial \tilde{V}}{\partial F_2} \right) \frac{\partial F_1}{\partial x_0} \quad (24)$$

with $\tilde{V}$ denoting the approximated total energy determined from the sampling atoms located in the two adjacent elements only (for an affine interpolation, only lattice sites in these two elements are affected by x_0). For all of the aforementioned summation rules, we can further expand

$$\tilde{F}_0 = -\frac{1}{n_1 l} \left[\frac{\partial \tilde{V}}{\partial E_1} \frac{\partial E_1}{\partial F_1} - \frac{n_1}{n_2} \frac{\partial \tilde{V}}{\partial E_2} \frac{\partial E_2}{\partial F_2} + \frac{\partial \tilde{V}}{\partial E_0} \left(\frac{\partial E_0}{\partial F_1} - \frac{n_1}{n_2} \frac{\partial E_0}{\partial F_2} \right) + \frac{\partial \tilde{V}}{\partial E_L} \frac{\partial E_L}{\partial F_1} - \frac{n_1}{n_2} \frac{\partial \tilde{V}}{\partial E_R} \frac{\partial E_R}{\partial F_2} \right], \quad (25)$$

where we used that $F_1 n_1 l = n_1 l + u$ so that $\partial F_1 / \partial x_0 = \partial F_1 / \partial u = 1/(n_1 l)$. Here, E_L and E_R are the energies of the repatoms to the left and to the right of those elements adjacent to the interface, respectively.

When considering forces on repatoms in an affinely-strained ground state (with initially uniform lattice **deformation gradient** F) and elements being sufficiently large ($n_1, n_2 \geq 2n_b$) so that E_1 and E_2 arise from uniform straining by F_1 and F_2 , respectively, we have

$$\left. \frac{\partial E_1}{\partial F_1} \right|_{F_1=F} = \left. \frac{\partial E_2}{\partial F_2} \right|_{F_2=F}. \quad (26)$$

Because of symmetry in the one-dimensional setting and, again, if elements are sufficiently large, we also have

$$\left. \frac{\partial E_0}{\partial F_1} \right|_{F_1=F} = \left. \frac{\partial E_0}{\partial F_2} \right|_{F_2=F} = \left. \frac{\partial E_L}{\partial F_1} \right|_{F_1=F} = \left. \frac{\partial E_R}{\partial F_2} \right|_{F_2=F}. \quad (27)$$

Further, note that $\partial V / \partial E_0 = w_0$ is the weight of the sampling atom at the interface and $\partial V / \partial E_i = w_{i,\text{total}}$ is the sum of all weights of sampling atoms in element i (not including sampling atoms on repatom positions). w_L and w_R are the weights of the repatoms to the left and to the right of the interface, respectively. Overall we thus arrive at the residual force on the interface repatom in an affinely-strained ground state:

$$\tilde{F}_0 = -\left[\frac{w_{1,\text{total}}}{n_1} - \frac{w_{2,\text{total}}}{n_2} \right] \frac{1}{l} \left. \frac{\partial E_1}{\partial F_1} \right|_{F_1=F} + w_0 \frac{n_1 - n_2}{n_1 n_2} \frac{1}{l} \left. \frac{\partial E_0}{\partial F_1} \right|_{F_1=F} + \left[\frac{w_R}{n_2} - \frac{w_L}{n_1} \right] \frac{1}{l} \left. \frac{\partial E_L}{\partial F_1} \right|_{F_1=F}. \quad (28)$$

For an interatomic potential of the Embedded Atom Method (Daw and Baskes, 1984) we can further specify

$$\left. \frac{\partial E_1}{\partial F_1} \right|_{F_1=F} = \frac{\partial}{\partial F_1} \left[\sum_{i=1}^{n_b} \Phi(F_1 i l) + \mathcal{F} \left(2 \sum_{i=1}^{n_b} \phi(F_1 i l) \right) \right] \Big|_{F_1=F} = l \sum_{i=1}^{n_b} i \left[\Phi'(F i l) + 2\mathcal{F}'(\rho_0) \phi'(F i l) \right], \quad (29)$$

where

$$\rho_0 = 2 \sum_{i=1}^{n_b} \phi(F i l) \quad (30)$$

is the effective electron density of an atom in an atomic chain uniformly deformed by F . Analogously, we have

$$\left. \frac{\partial E_0}{\partial F_1} \right|_{F_1=F} = \left. \frac{\partial E_L}{\partial F_1} \right|_{F_1=F} = \frac{\partial}{\partial F_1} \left[\sum_{i=1}^{n_b} \frac{1}{2} \Phi(F_1 i l) + \sum_{i=1}^{n_b} \frac{1}{2} \Phi(F_1 i l) + \mathcal{F} \left(\sum_{i=1}^{n_b} \phi(F_1 i l) + \sum_{i=1}^{n_b} \phi(F_1 i l) \right) \right] \Big|_{F_1=F} = \frac{1}{2} \left. \frac{\partial E_1}{\partial F_1} \right|_{F_1=F}. \quad (31)$$

Figure 5: Approximated energy of a periodic one-dimensional QC chain described by a Lennard-Jones potential vs. the displacement u of the central repatom for five different discretizations (see schematics) using the nodal summation rule $(0, 0)$. Non-uniform meshes only show residual forces if elements are sufficiently small (e.g. see the two bottom left examples whose energy minimum is not at $u = 0$ compared to all other examples which do not exhibit a residual force).

Altogether, this results in

$$\tilde{F}_0 = \frac{n_1 \left(w_{2,\text{total}} + \frac{1}{2}w_0 + \frac{1}{2}w_R \right) - n_2 \left(w_{1,\text{total}} + \frac{1}{2}w_0 + \frac{1}{2}w_L \right)}{n_1 n_2} \frac{1}{l} \frac{\partial E_1}{\partial F_1} \Big|_{F_1=F}. \quad (32)$$

The undeformed ground state of the crystal lattice is characterized by an energy minimum with respect to the atomic spacing, so that (29) and thus (32) must vanish in the undeformed lattice, i.e. when $F = 1$. Therefore, in a one-dimensional non-uniform QC chain with affine interpolation and sufficiently-large elements none of the summation rules will produce residual forces. In reality, however, marginal numerical errors of the lattice spacing are sufficient to render (32) non-zero and thus to produce residual forces. If the chain undergoes uniform affine deformation with $F_1 = F_2 = F$, all lattice sites (in the exact atomistic scenario) should still be force-free but (32) will produce forces on repatoms, a clear indication of spurious forces.

Let us evaluate these spurious forces in the large element limit for the above summation rules applied to an affine deformation with gradient $F \neq 1$. For the *nodal rule* $(0, 0)$, there are no quadrature-type sampling atoms within elements ($w_{1,\text{total}} = w_{2,\text{total}} = 0$) and the weights of sampling atoms at repatom locations are given by $w_L = n_1$, $w_R = n_2$, and $w_0 = (n_1 + n_2)/2$. Insertion into (32) yields the spurious force on the interface repatom arising from the nodal summation rule:

$$\tilde{F}_0^{(0,0)} = \frac{n_1^2 - n_2^2}{4 n_1 n_2} \frac{1}{l} \frac{\partial E_1}{\partial F_1} \Big|_{F_1=F}. \quad (33)$$

Apparently, the spurious force at the mesh interface only disappears if the mesh is uniform ($n_1 = n_2$). The addition of clusters containing n_c lattice sites around repatoms does not change this conclusion as long as elements are sufficiently large (i.e. if $n_1, n_2 \geq 2n_b$ and $n_1, n_2 \geq n_c$).

Eidel and Stukowski (2009) presented the one-dimensional example of a chain of two periodically-repeated elements of different sizes as shown in Fig. 5. For small element sizes, including those analyzed in (Eidel and Stukowski, 2009), the energy obtained from a nodal summation rule is no longer minimal in the undeformed ground state but the crystal can seemingly reduce its energy by displacing the central repatom by u . Fig. 5 illustrates the energy vs. u for various element sizes in the undeformed ground state using a Lennard-Jones potential (with $n_b = 4$). Here we point out that, for element sizes $n_1, n_2 \geq 2$, the energy landscape becomes symmetric and all residual forces vanish.

Element quadrature rules $(-, n_Q)$ choose sampling atoms within elements and do not include repatoms in the set of sampling atoms, i.e. we have $w_0 = w_L = w_R = 0$ and $w_{i,\text{total}} = n_i$. Therefore, the residual force (32) is reduced to

$$\tilde{F}_0^{(-,n_Q)} = \frac{n_1 n_2 - n_2 n_1}{n_1 n_2} \frac{1}{l} \frac{\partial E_1}{\partial F_1} \Big|_{F_1=F} = 0. \quad (34)$$

Consequently, element quadrature rules do not produce residual forces in large elements for any choice of $\mathbf{F}$. This is exactly why the local QC region of [Tadmor et al. \(1996\)](#) does not produce any residual forces (if elements are sufficiently large, it does not make a difference if one uses the Cauchy-Born rule or computes the energy of an actual inner-element lattice site based on its affinely-deforming local neighborhood).

Finally, *quadrature summation rules* of type $(0, n_Q)$ lead to weights

$$w_L = \frac{n_1}{n_Q + 1}, \quad w_R = \frac{n_2}{n_Q + 1}, \quad w_{i,\text{total}} = n_i \frac{n_Q}{n_Q + 1}, \quad w_0 = \frac{w_L + w_R}{2} = \frac{n_1 + n_2}{2(n_Q + 1)}, \quad (35)$$

which in turn result in the following residual force at the interface:

$$\tilde{F}_0^{(0, n_Q)} = \frac{n_1^2 - n_2^2}{4 n_1 n_2 (n_Q + 1)} \frac{1}{l} \frac{\partial E_1}{\partial F_1} \Big|_{F_1 = F} = \frac{1}{n_Q + 1} \tilde{F}_0^{(0,0)}(x_0). \quad (36)$$

Like the energy approximation error, the residual force is reduced by the addition of quadrature sampling atoms; yet, it only vanishes in uniform meshes with $n_1 = n_2$ or in the undeformed ground state ($\mathbf{F} = \mathbf{F}_0$).

4.3. Optimal summation rule

Based on the above insight, let us conceive a summation rule which does not exhibit spurious force artifacts in any affinely-deformed non-uniform QC mesh ($n_1 \neq n_2$) in one dimension. To allow for seamless bridging to full atomistics (and to avoid computational expenses of clusters), we assume a quadrature rule $(0, x)$ whose set of sampling atoms includes all repatoms and x additional inner-element sampling atoms. According to (32), vanishing forces require

$$w_{2,\text{total}} + \frac{1}{2}w_0 + \frac{1}{2}w_R = n_2 \quad \text{and} \quad w_{1,\text{total}} + \frac{1}{2}w_0 + \frac{1}{2}w_L = n_1. \quad (37)$$

From all possible solutions, the simplest is to assign the same weight w_{rep} to each sampling atom at a repatom location. To maintain zeroth-order consistency, we choose the remaining sampling atom weights accordingly. This results in

$$w_0 = w_L = w_R = w_{\text{rep}}, \quad w_{i,\text{total}} = n_i - w_{\text{rep}}. \quad (38)$$

Obviously, the choice (38) makes (32) vanish. Therefore, this summation rule does not produce any residual or spurious forces for arbitrary affine **deformation gradients** $\mathbf{F}$. We note that the recent summation rule proposed by [Beex et al. \(2014\)](#) forms a special case of this scenario by defining $w_{\text{rep}} = 1$. Here instead, we identify w_{rep} by minimizing the energy approximation error. In analogy to our previous derivations, we obtain the total energy of the two interface-adjacent elements as

$$\tilde{V} = w_{\text{rep}} E_0 + \left(n_1 - \frac{1}{2}w_{\text{rep}}\right) E_1 + \left(n_2 - \frac{1}{2}w_{\text{rep}}\right) E_2 \quad (39)$$

so that the relative energy error of the two elements becomes

$$\left| \frac{\tilde{V}_{(0,x^*)} - V_{\text{exact}}}{V_{\text{exact}}} \right| = \left| \frac{(2n_b - 1 - w_{\text{rep}})(E_1 + E_2) + 2(E_0 w_{\text{rep}} - \bar{E}_0(2n_b - 1))}{2 V_{\text{exact}}} \right|. \quad (40)$$

Hence, the relative energy error in large elements is minimal if

$$w_{\text{rep}} = 2n_b - 1, \quad (41)$$

which leads to

$$\left| \frac{\tilde{V}_{(0,x^*)} - V_{\text{exact}}}{V_{\text{exact}}} \right| = (2n_b - 1) \left| \frac{E_0 - \bar{E}_0}{V_{\text{exact}}} \right| = O\left(\frac{n_b}{n_i}\right). \quad (42)$$

This relative energy error is bounded and decreases rapidly as elements become larger than the radius of atomic interactions. The error scales with the difference between the interface atom's energy and the average energy of all lattice sites within its radius of interaction. For many EAM-type potentials (in particular for most pair potentials) we have $E_0 \approx \bar{E}_0$, so that the error is marginal. We note that one can even force the energy error to vanish by replacing

Figure 6: Schematic view of the new summation rule: sampling atoms at repatom locations have identical weights w_{rep} , whereas quadrature-type sampling atoms within elements have element-size-dependent weights w_{inner} . The energy is constant within elements and only varies within the radius of interaction of repatoms; all affected lattice sites are represented by the sampling atoms at repatom locations. As in Fig. 3, the exact form of the energy in the transition between elements depends on the potential and the elements' deformation gradients; the shown close-to-linear transition is only schematic (observable e.g. in a 1D Lennard-Jones crystal at moderate strains).

sampling atoms on repatoms by clusters of sampling atoms around repatoms containing $2n_b - 1$ lattice sites, in which case we automatically recover $\bar{E}_0 = E_0$.

Finally, it is important to note that the exact location of the quadrature-type sampling atoms in this new scheme is irrelevant, as long as these are contained well within elements so their neighboring lattice sites undergo an affine deformation of Cauchy-Born type. Also, the number of such sampling atoms is irrelevant (since they all contribute the same energy) and it is sufficient to choose only one such sampling atom. This implies furthermore that we do not even have to specify an actual lattice site for the sampling atom location (as commonly done in quadrature schemes where Gaussian quadrature point-nearest lattice sites are chosen, cf. (Beex et al., 2014)). One might as well introduce one (fictitious) sampling atom per element which undergoes affine Cauchy-Born deformation and whose weight is defined by $w_{i,\text{total}}$ from (38) with (41). We will refer to this summation rule in the following as $(0, 1^*)$.

The new summation rule $(0, 1^*)$ allows for a clean physical interpretation as schematically shown in Fig. 6: each repatom is turned into a sampling atom which represents all lattice sites within the radius of interaction of the repatom (these lattice sites are well represented by the repatom because their interactions reach into the adjacent element). All remaining lattice sites within an element are represented by a single quadrature-type sampling atom which undergoes the same affine deformation as all inner-element lattice sites.

5. Analysis of summation rules in two dimensions

5.1. Force artifacts in two dimensions

Inspired by the one-dimensional analysis, we proceed to review summation rules in two dimensions with the ambition to derive a similar summation rule with vanishing force artifacts and minimal energy approximation error in the limit of large elements. Let us consider an arbitrarily coarse-grained patch of simplicial (linear, triangular) elements in two dimensions and assume that all elements are sufficiently large such that all neighboring lattice sites within the circle of interaction of any repatom are contained within elements adjacent to that repatom only. Such a scenario is shown in Fig. 7a, where five triangular elements meet at the central repatom. Suppose a quadrature summation rule of type $(0, 1)$ whose set of sampling elements contains all repatoms as well as one additional sampling atom per element located within the element (whose atomic neighborhood undergoes an affine deformation in the Cauchy-Born sense due to the large element sizes). We assume an atomic lattice in the undeformed ground state so that the neighborhoods of all sampling atoms are identical. The lattice can, in principle, be of any type; the only assumption we will introduce here is that it satisfies centrosymmetry. This includes e.g. all cubic lattices such as bcc and fcc and therefore the vast majority of metals and ceramics. Our goal is to derive the spurious or residual force acting on the central repatom due to the non-uniform QC mesh. The affine interpolation scheme ensures that only the positions of lattice sites in the adjacent elements (shown in light gray) are affected by a displacement $\mathbf{u}$ of the central repatom from its original position $\mathbf{X}_0$ to the new position $\mathbf{x}_0 = \mathbf{X}_0 + \mathbf{u}$. Fig. 7a illustrates only one example element patch; in the following, we will generalize our analysis to an arbitrary number of n_e adjacent elements defined by n_e repatoms surrounding the central repatom.

Figure 7: Example of a non-uniform patch of triangular elements that result in a residual force on the central repatom 0: a) patch of elements with repatoms at element vertices (large solid circles), sampling atoms at vertices and within elements (large open circles), and neighboring lattice sites (small dots) contained within the dashed circles of interaction around each sampling atom. Lattice sites in dark gray regions lie outside the patch; their position remains unaffected by the motion of the central repatom. b) Recombination of all neighboring lattice sites within the radii of interaction of those repatoms on the vertices of elements 1 and 2 into equivalent semi-circles of interaction.

The total (approximated) potential energy affected by the position $\mathbf{x}_0$ of the central repatom is thus given by

$$\tilde{V} = \sum_{e=1}^{n_e} w_{e,\text{inner}} E_{e,\text{inner}} + \sum_{i=1}^{n_e} w_i E_{i,\text{vertex}} + w_0 E_0, \quad (43)$$

where $E_{e,\text{inner}}$ denotes the energy of the sampling atom located inside element e , $E_{i,\text{vertex}}$ is the energy of outer repatom i , and E_0 is the energy of the central repatom. $w_{e,\text{inner}}$ and w_i denote the weights of those sampling atoms within elements and those on element vertices, respectively. **We assume that** quadrature-type sampling atoms are chosen sufficiently far away from element edges so that $E_{e,\text{inner}}$ results from Cauchy-Born deformation. The force on the central repatom,

$$\tilde{\mathbf{F}}_0(\mathbf{x}_0) = -\frac{\partial \tilde{V}}{\partial \mathbf{x}_0}(\mathbf{x}_0), \quad (44)$$

is determined by differentiation. When using linear interpolation, each element e undergoes an affine deformation characterized by a deformation gradient $\mathbf{F}_e$ (with $F_{iJ} = x_{i,J}$). For conciseness, let us denote by $\mathcal{S}$ the set of all lattice sites contained within a neighborhood of interaction, and $\mathbf{R}_j$ ($j \in \mathcal{S}$) is the distance vector from the central atom to its neighboring lattice site j . For an EAM potential this leads to

$$E_{e,\text{inner}} = \sum_{j \in \mathcal{S}} \frac{1}{2} \Phi(|\mathbf{F}_e \mathbf{R}_j|) + \mathcal{F}(\rho_e), \quad \rho_e = \sum_{j \in \mathcal{S}} \phi(|\mathbf{F}_e \mathbf{R}_j|). \quad (45)$$

Consequently, we obtain

$$\frac{\partial E_{e,\text{inner}}}{\partial \mathbf{x}_0} = \frac{\partial E_{e,\text{inner}}}{\partial \mathbf{F}_e} \cdot \frac{\partial \mathbf{F}_e}{\partial \mathbf{x}_0} = \sum_{j \in \mathcal{S}} \left[\frac{1}{2} \Phi'(|\mathbf{F}_e \mathbf{R}_j|) + \mathcal{F}'(\rho_e) \phi'(|\mathbf{F}_e \mathbf{R}_j|) \right] \frac{\mathbf{F}_e \mathbf{R}_j \otimes \mathbf{R}_j}{|\mathbf{F}_e \mathbf{R}_j|} \cdot \frac{\partial \mathbf{F}_e}{\partial \mathbf{x}_0}. \quad (46)$$

For the sampling atoms located on repatom positions on the outer vertices of the patch of elements, the energy calculation is more involved because only those neighboring lattice sites contained within the light-gray adjacent elements depend on the position $\mathbf{x}_0$ (while those atoms in the dark-gray regions are independent of $\mathbf{x}_0$). Taking for

example the top sampling atom (1) whose neighbors are contained in elements 1 and 2, we have

$$E_{1,\text{vertex}} = \sum_{j \in \mathcal{S}_1^1} \frac{1}{2} \Phi(|\mathbf{F}_1 \mathbf{R}_j|) + \sum_{j \in \mathcal{S}_2^1} \frac{1}{2} \Phi(|\mathbf{F}_2 \mathbf{R}_j|) + \sum_{j \in \mathcal{S}_{\text{ex}}^1} \frac{1}{2} \Phi(|\mathbf{F}_{\text{ex}} \mathbf{R}_j|) + \mathcal{F} \left[\sum_{j \in \mathcal{S}_1^1} \phi(|\mathbf{F}_1 \mathbf{R}_j|) + \sum_{j \in \mathcal{S}_2^1} \phi(|\mathbf{F}_2 \mathbf{R}_j|) + \sum_{j \in \mathcal{S}_{\text{ex}}^1} \phi(|\mathbf{F}_{\text{ex}} \mathbf{R}_j|) \right], \quad (47)$$

where $\mathcal{S}_e^j = \mathcal{S}^j \cap E_e$ is the set of neighbors of repatom j contained in element e , and $\mathcal{S}_{\text{ex}}^j = \mathcal{S}^j \setminus \bigcup_{e=1}^{n_e} E_e$ are those neighboring lattice sites located outside the patch of elements (E_e denotes the set of all lattice sites in element e). $\mathbf{F}_{\text{ex}}$ is the (generally not constant) deformation gradient acting on the lattice sites not contained in the patch of elements. Consequently, we see that

$$\begin{aligned} \frac{\partial E_{1,\text{vertex}}}{\partial \mathbf{x}_0} &= \frac{\partial E_{1,\text{vertex}}}{\partial \mathbf{F}_1} \cdot \frac{\partial \mathbf{F}_1}{\partial \mathbf{x}_0} + \frac{\partial E_{1,\text{vertex}}}{\partial \mathbf{F}_2} \cdot \frac{\partial \mathbf{F}_2}{\partial \mathbf{x}_0} \\ &= \sum_{e=1}^2 \sum_{j \in \mathcal{S}_e^1} \left[\frac{1}{2} \Phi'(|\mathbf{F}_e \mathbf{R}_j|) + \mathcal{F}'(\rho_1) \phi'(|\mathbf{F}_e \mathbf{R}_j|) \right] \frac{\mathbf{F}_e \mathbf{R}_j \otimes \mathbf{R}_j}{|\mathbf{F}_e \mathbf{R}_j|} \cdot \frac{\partial \mathbf{F}_e}{\partial \mathbf{x}_0} \end{aligned} \quad (48)$$

with

$$\rho_1 = \sum_{j \in \mathcal{S}_1^1} \phi(|\mathbf{F}_1 \mathbf{R}_j|) + \sum_{j \in \mathcal{S}_2^1} \phi(|\mathbf{F}_2 \mathbf{R}_j|) + \sum_{j \in \mathcal{S}_{\text{ex}}^1} \phi(|\mathbf{F}_{\text{ex}} \mathbf{R}_j|). \quad (49)$$

Analogously, the energies (and their derivatives) of all sampling atoms on the outer vertices can be computed. Finally, the energy of the sampling atom located at the position of the central repatom involves neighboring lattice sites in all adjacent elements. Here we have

$$E_0 = \left[\sum_{e=1}^{n_e} \sum_{j \in \mathcal{S}_e^0} \frac{1}{2} \Phi(|\mathbf{F}_e \mathbf{R}_j|) \right] + \mathcal{F}(\rho_0), \quad \rho_0 = \sum_{e=1}^{n_e} \sum_{j \in \mathcal{S}_e^0} \phi(|\mathbf{F}_e \mathbf{R}_j|) \quad (50)$$

and consequently

$$\frac{\partial E_0}{\partial \mathbf{x}_0} = \sum_{e=1}^{n_e} \frac{\partial E_0}{\partial \mathbf{F}_e} \cdot \frac{\partial \mathbf{F}_e}{\partial \mathbf{x}_0} = \sum_{e=1}^{n_e} \sum_{j \in \mathcal{S}_e^0} \left[\frac{1}{2} \Phi'(|\mathbf{F}_e \mathbf{R}_j|) + \mathcal{F}'(\rho_0) \phi'(|\mathbf{F}_e \mathbf{R}_j|) \right] \frac{\mathbf{F}_e \mathbf{R}_j \otimes \mathbf{R}_j}{|\mathbf{F}_e \mathbf{R}_j|} \cdot \frac{\partial \mathbf{F}_e}{\partial \mathbf{x}_0}. \quad (51)$$

The total force acting on the central repatom is now given by inserting (46), (48), and (51) into

$$\tilde{\mathbf{F}}_0(\mathbf{x}_0) = - \left[\sum_{e=1}^{n_e} w_{e,\text{inner}} \frac{\partial E_{e,\text{inner}}}{\partial \mathbf{x}_0} + \sum_{i=1}^{n_e} w_i \frac{\partial E_{i,\text{vertex}}}{\partial \mathbf{x}_0} + w_0 \frac{\partial E_0}{\partial \mathbf{x}_0} \right] \quad (52)$$

Let us determine the spurious/residual force acting on the central repatom in a uniformly strained configuration with deformation gradient $\mathbf{F}_0$ applied to every element (e.g. in the undeformed ground state we have $\mathbf{F}_0 = \mathbf{I}$). Under these conditions, the residual force is given by

$$\tilde{\mathbf{F}}_0 = - \sum_{e=1}^{n_e} \left[\frac{\partial \tilde{V}}{\partial \mathbf{F}_e} \right]_{\mathbf{F}_e = \mathbf{F}_0} \cdot \frac{\partial \mathbf{F}_e}{\partial \mathbf{x}_0}, \quad (53)$$

where

$$\frac{\partial \tilde{V}}{\partial \mathbf{F}_e} = \sum_{e=1}^{n_e} w_{e,\text{inner}} \frac{\partial E_{e,\text{inner}}}{\partial \mathbf{F}_e} + \sum_{i=1}^{n_e} w_i \frac{\partial E_{i,\text{vertex}}}{\partial \mathbf{F}_e} + w_0 \frac{\partial E_0}{\partial \mathbf{F}_e}. \quad (54)$$

First, consider only those contributions from a particular element e ; e.g. take element 2 whose deformation gradient $\mathbf{F}_2$ is applied to atomic spacings in the circles of interactions of repatoms 0, 1 and 2 and of the sampling atom located

inside element 2 (see Fig. 7). Therefore, we obtain

$$\begin{aligned} \left[\frac{\partial \widetilde{V}}{\partial \mathbf{F}_2} \right]_{\mathbf{F}_2=\mathbf{F}_0} &= \left[w_{2,\text{inner}} \frac{\partial E_{2,\text{inner}}}{\partial \mathbf{F}_2} + w_1 \frac{\partial E_{1,\text{vertex}}}{\partial \mathbf{F}_2} + w_2 \frac{\partial E_{2,\text{vertex}}}{\partial \mathbf{F}_2} + w_0 \frac{\partial E_0}{\partial \mathbf{F}_2} \right]_{\mathbf{F}_2=\mathbf{F}_0} \\ &= w_{2,\text{inner}} \sum_{j \in \mathcal{S}} \left[\frac{1}{2} \Phi'(|\mathbf{F}_0 \mathbf{R}_j|) + \mathcal{F}'(\rho_0) \phi'(|\mathbf{F}_0 \mathbf{R}_j|) \right] \frac{\mathbf{F}_0 \mathbf{R}_j \otimes \mathbf{R}_j}{|\mathbf{F}_0 \mathbf{R}_j|} \\ &\quad + \sum_{\alpha=0}^2 w_\alpha \sum_{j \in \mathcal{S}_2^\alpha} \left[\frac{1}{2} \Phi'(|\mathbf{F}_0 \mathbf{R}_j|) + \mathcal{F}'(\rho_0) \phi'(|\mathbf{F}_0 \mathbf{R}_j|) \right] \frac{\mathbf{F}_0 \mathbf{R}_j \otimes \mathbf{R}_j}{|\mathbf{F}_0 \mathbf{R}_j|} \end{aligned} \quad (55)$$

with

$$\rho_0 = \sum_{j \in \mathcal{S}} \phi(|\mathbf{F}_0 \mathbf{R}_j|). \quad (56)$$

The individual segments of the circles of interactions, $\mathcal{S}_2^1$, $\mathcal{S}_2^2$, and $\mathcal{S}_2^0$ are shown in Fig. 7b. For a centrosymmetric lattice, these three segments can be recombined as shown in Fig. 7b: by translating segments $\mathcal{S}_2^1$ and $\mathcal{S}_2^2$ to the central repatom and reflecting $\mathcal{S}_2^1$ about the latter (due to centrosymmetry), we see that

$$\mathcal{S}_2^1 \cup \mathcal{S}_2^2 \cup \mathcal{S}_2^0 = \mathcal{S}_{1/2}, \quad (57)$$

i.e. the three segments recombine to half the circle of interaction denoted by $\mathcal{S}_{1/2}$. How exactly the circle is split in half is irrelevant due to centrosymmetry (see e.g. the two equivalent semi-circles shown in Fig. 7b) because (55) is independent of the sign of all $\mathbf{R}_j$. In other words, summing over all lattice site neighbors within any semi-circle of interaction will yield the same result in (55) as long as all lattice sites within that semi-circle experience the same affine deformation.

Note that the energy of a single atom in a lattice that is affinely deformed by a deformation gradient $\mathbf{F}_0$ is given by

$$E(\mathbf{F}_0) = \sum_{j \in \mathcal{S}} \frac{1}{2} \Phi(|\mathbf{F}_0 \mathbf{R}_j|) + \mathcal{F}(\rho_0), \quad \rho_0 = \sum_{j \in \mathcal{S}} \phi(|\mathbf{F}_0 \mathbf{R}_j|) \quad (58)$$

and the first Piola-Kirchhoff stress tensor of the Cauchy-Born continuum follows as (Ericksen, 1984; Tadmor et al., 1996)

$$\mathbf{P}(\mathbf{F}_0) = \frac{\partial E}{\partial \mathbf{F}} \Big|_{\mathbf{F}=\mathbf{F}_0} = \sum_{j \in \mathcal{S}} \left[\frac{1}{2} \Phi'(|\mathbf{F}_0 \mathbf{R}_j|) + \mathcal{F}'(\rho_0) \phi'(|\mathbf{F}_0 \mathbf{R}_j|) \right] \frac{\mathbf{F}_0 \mathbf{R}_j \otimes \mathbf{R}_j}{|\mathbf{F}_0 \mathbf{R}_j|}. \quad (59)$$

Here it becomes apparent that summing only over the semi-circle of interaction gives the same result due to centrosymmetry (replacing any of the $\mathbf{R}_j$ by $-\mathbf{R}_j$ in (59) does not alter the result), so that we might as well write

$$\mathbf{P}(\mathbf{F}_0) = 2 \sum_{j \in \mathcal{S}_{1/2}} \left[\frac{1}{2} \Phi'(|\mathbf{F}_0 \mathbf{R}_j|) + \mathcal{F}'(\rho_0) \phi'(|\mathbf{F}_0 \mathbf{R}_j|) \right] \frac{\mathbf{F}_0 \mathbf{R}_j \otimes \mathbf{R}_j}{|\mathbf{F}_0 \mathbf{R}_j|}, \quad (60)$$

where, as before, $\mathcal{S}_{1/2}$ denotes any semi-circle of interaction. If the single-crystalline atomic lattice is in its undeformed ground state (i.e., $\mathbf{F}_0 = \mathbf{I}$), we know that the energy is minimized and therefore

$$\mathbf{P}(\mathbf{I}) = \sum_{j \in \mathcal{S}} \left[\frac{1}{2} \Phi'(|\mathbf{R}_j|) + \mathcal{F}'(\rho_0(\mathbf{I})) \phi'(|\mathbf{R}_j|) \right] \frac{\mathbf{R}_j \otimes \mathbf{R}_j}{|\mathbf{R}_j|} = \mathbf{0}. \quad (61)$$

A comparison shows that the term in (55) associated with the inner sampling atom (i.e. the term multiplying $w_{2,\text{inner}}$) must vanish in the undeformed ground state. The remaining terms, however, cannot vanish for arbitrary element geometries, unless one chooses $w_1 = w_2 = w_0$ so that the remaining terms recombine into a sum over the semi-circle of interaction. In other words, if the weights assigned to sampling atoms at repatom locations depend on the element size and geometry (as is commonly the case in nodal, cluster, or traditional quadrature rules), force artifacts will be unavoidable in non-uniform QC meshes, even in the large-element limit. If the mesh is uniform and sampling atoms

are uniformly spaced, these forces vanish due to uniform repatom weights. The observed spurious force artifacts also imply a significant approximation error of the total potential energy due to the summation rules. **As shown in one dimension**, the local QC formulation based on Cauchy-Born kinematics does not suffer from these forces because it uses $w_i = 0$ for all repatoms. Yet, **it requires to switch from an element-based to a node-based formulation when transitioning to fully-atomistic resolution and to treat atomistic and coarse-grained regions fundamentally differently.**

5.2. Optimal summation rule in two dimensions

Based on the above observations, let us introduce a quadrature summation rule $(0, 1^*)$ with vanishing spurious forces in the large-element limit in two-dimensional non-uniform QC meshes under affine deformation. To this end, we adopt the concept discussed in one dimension: we assign the same weight to all sampling atoms at repatom locations, i.e.

$$w_0 = w_1 = \dots = w_{n_e} = w_{\text{rep}}. \quad (62)$$

In this case, the force (53) on the central repatom simplifies dramatically because the sums over all repatom neighbors recombine into semi-circles of interaction as discussed above, cf. Fig. 7b. After insertion of all derivatives analogously to (55), (53) turns into

$$\tilde{\mathbf{F}}_0 = - \sum_{e=1}^{n_e} \left(w_{e,\text{inner}} + \frac{1}{2} w_{\text{rep}} \right) \left[\sum_{j \in S} \left[\frac{1}{2} \Phi'(|\mathbf{F}_0 \mathbf{R}_j|) + \mathcal{F}'(\rho_0) \phi'(|\mathbf{F}_0 \mathbf{R}_j|) \right] \frac{\mathbf{F}_0 \mathbf{R}_j \otimes \mathbf{R}_j}{|\mathbf{F}_0 \mathbf{R}_j|} \right] \cdot \frac{\partial \mathbf{F}_e}{\partial \mathbf{x}_0}. \quad (63)$$

By comparison of (61) and (63), we conclude that in the undeformed ground state ($\mathbf{F}_0 = \mathbf{I}$) no residual forces exist in arbitrary non-uniform meshes (with sufficiently large elements).

Let us proceed to identify sampling atom weights that do not produce spurious forces in any affinely-deformed state with $\mathbf{F}_0 \neq \mathbf{I}$. To this end, we exploit the fact the deformation gradients $\mathbf{F}_e$ within the n_e elements in (63) are not independent, since they all result from the central repatom moving to the new location $\mathbf{x}_0$ while the other repatoms are held fixed. For any simply-connected two-dimensional region Ω with area A_Ω whose outer boundary is deforming affinely according to an imposed deformation gradient $\mathbf{F}_0$, the average deformation gradient within Ω must satisfy

$$\int_{\Omega} \mathbf{F} \, dA = \int_{\Omega} \text{Grad} \, \mathbf{x} \, dA = \int_{\partial\Omega} \mathbf{x} \otimes \mathbf{N} \, dA = \int_{\partial\Omega} \mathbf{F}_0 \mathbf{X} \otimes \mathbf{N} \, dA = \int_{\Omega} \mathbf{F}_0 \, \text{Grad}(\mathbf{X}) \, dA = \int_{\partial\Omega} \mathbf{F}_0 \, dA = \mathbf{F}_0 A_\Omega. \quad (64)$$

For a discrete patch of n_e simplicial elements (as in Fig. 7) with constant deformation gradients $\mathbf{F}_e$ and areas A_e ($i = 1, \dots, n_e$) one can show the analogous condition,

$$\sum_{e=1}^{n_e} A_e \mathbf{F}_e = \mathbf{F}_0 A. \quad (65)$$

An immediate consequence is that

$$\sum_{e=1}^{n_e} A_e \frac{\partial \mathbf{F}_e}{\partial \mathbf{x}_0} = \mathbf{0}. \quad (66)$$

By using (66), we can make (63) vanish for an arbitrary $\mathbf{F}_0$ by extending (62) into

$$w_0 = w_1 = \dots = w_{n_e} = w_{\text{rep}} \quad \text{and} \quad w_{e,\text{inner}} = A_e - \frac{1}{2} w_{\text{rep}} \quad (67)$$

such that

$$\tilde{\mathbf{F}}_0 = - \left[\sum_{j \in S} \left[\frac{1}{2} \Phi'(|\mathbf{F}_0 \mathbf{R}_j|) + \mathcal{F}'(\rho_0) \phi'(|\mathbf{F}_0 \mathbf{R}_j|) \right] \frac{\mathbf{F}_0 \mathbf{R}_j \otimes \mathbf{R}_j}{|\mathbf{F}_0 \mathbf{R}_j|} \right] \cdot \sum_{e=1}^{n_e} A_e \frac{\partial \mathbf{F}_e}{\partial \mathbf{x}_0} = \mathbf{0}. \quad (68)$$

It is important to note that, if weights are chosen according to (67), not only do residual forces in the undeformed ground state vanish but also in any other uniformly strained configuration. Consequently, the new weights (67) ensure that an arbitrary non-uniform QC mesh (of sufficiently large elements) produces zero forces on all repatoms under affine deformation. This is the first (nonlocal) QC summation rule with these features.

Figure 8: a) Schematic illustration of the weights of sampling atoms at repatom sites (dark gray regions) and of quadrature-type sampling atoms for the $(0, 1^*)$ rule applied to a two-dimensional triangular QC mesh (quadrature-type sampling atoms need not be actual lattice sites). b) Color-plot showing the energy of each lattice site in a deformed QC mesh whose affine interpolation results in constant energies within elements with deviations near element boundaries.

We still have not defined w_{rep} , the weight of individual repatoms. Inspired by the one-dimensional analysis, we aim to minimize the energy approximation error by choosing weights such that each sampling atom at a repatom site represents all those lattice sites within an *effective interaction distance* r_{eff} whose energy is best represented by that of the repatom. The exact value of r_{eff} can be determined by numerical experiments and will be reported later for specific examples (a detailed analysis will be reported elsewhere). Thus we have $w_{\text{rep}} = \pi r_{\text{eff}}^2 \rho$ with atomic density ρ . The sampling atom within each element thus represents all remaining lattice sites not represented by the sampling atoms at nodes. Fig. 8a illustrates the weights of the new summation rule in two dimensions in a non-uniform QC mesh. Fig. 8b shows the distribution of the energy per lattice site in a QC discretization with affine interpolation, clearly showing constant energies within elements with variations near the element boundaries. This completes the $(0, 1^*)$ summation rule in two dimensions.

We note that, like in one dimension, the exact location of the inner-element sampling atom is irrelevant as long as its entire neighborhood of interaction is contained within the element. As a matter of fact, we might as well introduce a sampling atom at a fictitious lattice site with a pristine single-crystalline neighborhood deformed by the Cauchy-Born rule according to the element's deformation gradient. Numerically, the Cauchy-Born neighborhood of a fictitious sampling atom can be realized by the same setup by introducing fictitious neighboring lattice sites. In case such neighborhoods reach outside an element, the positions of all neighboring lattice sites is obtained by affine extrapolation. Thus, rule $(0, 1^*)$ combines local QC with energy-based nodal QC.

5.3. Optimal summation rule of second order in two dimensions

The $(0, 1^*)$ summation rule introduced above admits extensions of higher order. In $(0, 1^*)$, the inner-element sampling atom represents all inner-element lattice sites except those within the effective interaction radius of repatoms. Let us consider the new $(0, 1^*)$ rule as a first-order summation rule (zeroth being the original local QC technique with $(-, 1)$, relying solely on the Cauchy-Born rule for each element). A second-order summation rule follows by adding sampling atom on element edges, one such sampling atom per element edge to represent all those lattice sites on and near the element edges (having semi-spheres of interaction within both elements adjacent to the edge). This second-order scheme will be denoted by $(0, 1^*, 3^*)$ and is shown in Fig. 9d. In sufficiently large elements, we now choose the following repatom weights to minimize energy errors in analogy to the first-order rule $(0, 1^*)$:

$$w_0 = w_1 = \dots = w_{n_e} = w_{\text{rep}} = \pi r_{\text{eff}}^2, \quad w_{i,\text{edge}} = L_i r_{\text{eff}} \quad \text{and} \quad w_{e,\text{inner}} = A_e - \frac{1}{2} w_{\text{rep}} - \sum_{i=1}^3 \frac{w_{i,\text{edge}}}{2} \quad (69)$$

In addition to our previous definitions, $w_{i,\text{edge}}$ denotes the weight of a sampling atom at an element edge of length L_{edge} . The final sum is over all three element edges of element e . Key to understanding spurious force artifacts is

the fact that neighboring lattice sites of each sampling atom on an element edge contain a complete semi-circle of neighbors in either of the two adjacent elements. As explained before, due to centrosymmetry these do not produce residual forces in sufficiently large elements (i.e., when each semi-circle undergoes an affine deformation).

Spurious force artifacts are derived in analogy to the previous case and result in

$$\begin{aligned} \tilde{\mathbf{F}}_0 = & - \sum_{e=1}^{n_e} \left(w_{e,\text{inner}} + \frac{1}{2} w_{\text{rep}} \right) \left[\sum_{j \in S} \left[\frac{1}{2} \Phi'(|\mathbf{F}_0 \mathbf{R}_j|) + \mathcal{F}'(\rho_0) \phi'(|\mathbf{F}_0 \mathbf{R}_j|) \right] \frac{\mathbf{F}_0 \mathbf{R}_j \otimes \mathbf{R}_j}{|\mathbf{F}_0 \mathbf{R}_j|} \right] \cdot \frac{\partial \mathbf{F}_e}{\partial \mathbf{x}_0} \\ & - \sum_{e=1}^{n_e} \left(\sum_{i=1}^3 \frac{w_{i,\text{edge}}}{2} \right) \left[\sum_{j \in S} \left[\frac{1}{2} \Phi'(|\mathbf{F}_0 \mathbf{R}_j|) + \mathcal{F}'(\rho_0) \phi'(|\mathbf{F}_0 \mathbf{R}_j|) \right] \frac{\mathbf{F}_0 \mathbf{R}_j \otimes \mathbf{R}_j}{|\mathbf{F}_0 \mathbf{R}_j|} \right] \cdot \frac{\partial \mathbf{F}_e}{\partial \mathbf{x}_0}, \end{aligned} \quad (70)$$

where the final term contains a sum over all three edges adjacent to element e . If weights are chosen according to (69), then (70) reduces to (68) which vanishes in affinely-deformed meshes. Therefore, the second-order scheme $(0, 1^*, 3^*)$ comes with the same properties as its first-order counterpart: spurious force artifacts vanish in sufficiently large elements for any affine deformation of the non-uniform QC mesh. However, the energy approximation error is considerably reduced by appropriately representing all edge-nearest lattice sites. **We note that similar approaches to the second-order summation rule have been introduced in the context of cohesive zone modeling of fracture (Zeng and Li, 2010) as well as in atomistic-to-finite-element coupling techniques (Shan and Nackenhorst, 2010).**

6. Extension to three dimensions and the full range of element sizes

In three dimensions, the analysis is analogous to the two-dimensional one presented above with one crucial difference. In two dimensions, we could devise an optimal summation rule with vanishing force artifacts and minimal approximation errors because – with the proper choice of summation rule weights – the contributions from all inner angles of each triangular element recombined into a semi-circle of interaction, cf. (57). In three dimensions, the four solid angles within each tetrahedral element unfortunately do *not* recombine into a semi-sphere of interaction in general. In fact, the sum of all four solid angles in a tetrahedron is not constant and depends on the exact geometry, see e.g. (Masket, 1957). For example, let α_i ($i = 1, \dots, 6$) denote the six dihedral angles between pairs of tetrahedral faces. The sum of all four solid angles ϕ_i ($i = 1, \dots, 4$) amounts to

$$\sum_{i=1}^4 \phi_i = 2 \sum_{i=1}^6 \alpha_i (\text{rad}) - 4\pi (\text{sr}). \quad (71)$$

Consider a regular tetrahedron in which all dihedral angles are $\arccos(1/3)$, so that the above sum of all four solid angles yields $12 \arccos(1/3) - 4\pi \approx 2.21$. Now, let the height of the tetrahedron shrink to zero, in which case the sum of all four solid angles must approach that of a hemisphere, viz. 2π . Ergo, the sum of all four solid angles within a tetrahedron is geometry-dependent, which is why the neighboring lattice sites of the four repatoms within an element do not recombine into a hemisphere of interaction. Spurious and residual forces will thus depend on the specific element geometry and there exists no general quadrature summation rule that removes all residual forces. However, any reasonable QC discretization will aim to (and any useful remeshing technique should) avoid large element coordination numbers. In this case, we can accept small errors and extend the new summation rule to 3D.

As before, every sampling atom at the location of a repatom is assigned the same weight, now $w_{\text{rep}} = 4\pi/3 r_{\text{eff}}^3 \rho$, which represents the number of lattice sites within the effective interaction distance of the atomic potential. In addition, each element receives one quadrature-type sampling atom feeling affine neighborhood changes in large elements. When using fictitious sampling atoms and the Cauchy-Born rule, this scheme agrees with the classical local QC model (Tadmor et al., 1996) enriched by sampling atoms at element vertices. This analogy, however, breaks down with decreasing element size where, ultimately, the original QC formulation would switch to non-local QC while we maintain the same non-local structure.

To this end, we generalize the summation rule $(0, 1^*)$ to elements of arbitrary sizes. Similar in spirit to the truncation of overlapping clusters (Knap and Ortiz, 2001; Eidel and Stukowski, 2009), we define sampling atom weights as follows. When effective interaction spheres of sampling atoms on element vertices overlap, their weights

Figure 9: Schematic illustration of the weight computation for arbitrary element sizes using summation rule $(0, 1^*)$: a) fully atomistic (all sampling atoms have the same weight $w_i = 1$); b) overlapping circles of interaction in intermediate-sized elements are split to determine weights; c) in large elements sampling atoms at element vertices have the same weights again. The inner-element quadrature atom can either be treated by the Cauchy-Born rule or by applying its actual atomic neighborhood (which may reach into adjacent elements if elements are not large). d) Second-order summation rule $(0, 1^*, 3^*)$.

are obtained by removing the overlapping regions and splitting weights equally, cf. Fig. 9. As before, the inner-element sampling atom's weight is given by the remaining lattice sites according to

$$w_{e,\text{inner}} = V_e - \sum_{i=1}^4 w_i \geq 0 \quad (72)$$

with V_e the total number of lattice sites in element e . This three-dimensional $(0, 1^*)$ scheme locally reduces to full atomistics as the element size decreases. Whether or not the inner-element sampling atom should be computed using its actual atomic neighborhood or a fictitious Cauchy-Born neighborhood will be discussed by the aid of numerical examples in Section 7. We will see that the Cauchy-Born rule is generally better suited to represent the collections of inner-element lattice sites rather than picking a specific lattice site and its actual neighborhood. This can be expected from our analyses in one and two dimensions which demonstrated vanishing residual and spurious forces in affinely deformed crystals if the inner-element sampling atoms experienced affine neighborhood deformations (which would not be the case when picking actual lattice sites so that neighbors reach into adjacent elements). Figure 10 shows the sampling atom weights of a non-uniform QC mesh in two dimensions; the 3D scenario is analogous but hard to visualize.

We note that this summation rule automatically satisfies zeroth-order consistency because all sampling atom weights add up to the total number of lattice sites. As long as elements are sufficiently large (or fully atomistic), the scheme also satisfies first-order consistency, cf. (Kochmann and Venturini, 2014). The same applies in the limit of full atomistics. However, there is a narrow intermediate regime of element sizes on the order of the interatomic interaction radius where first-order consistency is not guaranteed.

Similarly to 2D, we can devise higher-order summation rules, e.g. the second-order rule $(0, 1^*, 4^*)$ with one additional sampling atom on each element face, or the third-order scheme $(0, 1^*, 4^*, 6^*)$ with one additional sampling atom on each element face and edge. However, the latter becomes computationally quite expensive and our numerical examples in the following section will demonstrate the benefits of the first- and second-order summation rules.

7. Numerical examples

7.1. Residual forces in non-uniform meshes

Let us demonstrate the performance of the new summation rule for the fully-nonlocal energy-based QC formulation by a few selected examples in two and three dimensions. We deliberately include two-dimensional examples for better visibility of the phenomena of interest. As a first performance metric for the various summation rules of type $(n_{\text{Cl}}, n_{\text{Q}})$, we illustrate residual forces (i.e. non-physical spurious force artifacts in the undeformed ground state)

Figure 10: Illustration of sampling atom weights for a) the first-order rule $(0, 1^*)$ and b) the second-order rule $(0, 1^*, 3^*)$ for a non-uniform 2D mesh that is gradually coarse-grained around an atomistic region in the bottom left corner. Blue circles denote weights of sampling atoms at repatom locations, white regions represent weights assigned to inner-element sampling atoms, and red regions show weights of sampling atoms on edges in the second-order rule. Small dots illustrate sampling atom locations (blue are those on repatom sites, red at barycenters, and green are those at edge midpoints).

in non-uniform QC meshes. Fig. 11 shows residual forces arising at sharp interfaces in a QC mesh that is rapidly coarse-grained from full atomistic resolution in four steps with coarsening factors of 2, modeled by the extended Finnis-Sinclair potential of Dai et al. (2006) for pure Cu. Shown are residual forces for the nodal summation rule $(0, 0)$, cluster summation rule $(3, 0)$ (each 3-shell cluster contains 54 lattice sites), classical quadrature summation rules with one and three sampling atoms per element, and the new summation rules of first and second order. In addition, we compare results obtained with and without using the Cauchy-Born rule for all non-repatom sampling atoms. It becomes apparent that the new schemes perform much better than the shown previous schemes, while being much more efficient than e.g. the cluster rule due to the small number of sampling atoms. As can be expected, the second-order scheme is superior to the first-order scheme, producing smaller residual forces and confining these to only those repatoms adjacent to the full atomistic region. Similarly, the application of the Cauchy-Born rule for inner-element sampling atoms appears to be beneficial. While this does not affect the energies and forces in atomistic or in sufficiently large elements, it does affect those small elements in between. The benefits of the Cauchy-Born rule can be explained by the restoration of symmetry in each element by application of the Cauchy-Born rule: without the Cauchy-Born rule, every quadrature-type sampling atom must be placed on an actual lattice site to define its atomic neighborhood. In small elements, this sampling atom can significantly move away e.g. from the element's barycenter, depending on the element geometry. The resulting (non-affinely deforming) neighborhoods produce forces in the undeformed configuration (and introduces force artifacts in the undeformed configuration). To allow for a fair comparison, we have also included the traditional quadrature rule $(0, 3)$ with sampling atoms not tied to actual lattice sites, see Fig. 11e. Even in this case, the superior performance of the new schemes is apparent.

Similarly, Fig. 12 compares residual forces arising in a non-uniform QC mesh with diffuse mesh interfaces. Again, the new summation rules perform significantly better, showing residual forces of much smaller magnitude and at fewer locations. Here, the second-order scheme surprisingly shows larger forces which arise from the strong geometric irregularities of the randomized mesh. Overall, the new summation rules confine residual forces to a small band of element sizes right above full atomistics and below elements exceeding $2n_b - 1$ lattice sites per side, as can be expected from our analysis. Thus, the ghost forces observed in the traditional local/non-local QC are effectively smeared over a regime of element sizes (rather than being localized at the sharp interface between atomistic and coarse-grained regions). Yet, the new scheme allows us to treat the entire domain in exactly the same manner without explicitly differentiating between local and non-local repatoms or elements.

Residual forces are a good and intuitive indicator for the performance of a summation rule. Yet, the best metric is the error of the total energy when approximated by a specific summation rule as compared to summing over all lattice sites. Fig. 13 illustrates this energy error in a new way. We randomly move repatoms into a (non-equilibrated)

Figure 11: Residual forces at sharp mesh interfaces in two dimensions for various summation rules (coarsening factor of 2 at each interface), using the extended Finnis-Sinclair potential of (Dai et al., 2006) for Cu. The color code of arrows reflects the magnitudes of residual forces (in arbitrary units); small dots represent repatoms (blue) and additional sampling atoms (red/green).

deformed state. Next, we compute the exact energy of each lattice site by considering its local atomic neighborhood as obtained from the QC interpolation. For each lattice site we then compare the obtained exact energy to that of the sampling atom which it is represented by in a summation rule. Fig. 13 shows the thus-obtained relative errors. Note that because approximated and exact energies are computed from the same atomic positions, the shown energy errors are merely due to the summation rules and free from approximation errors incurred by the affine QC interpolation. These results confirm that the new scheme assigns weights such that the total energy error is considerably reduced.

To quantify the total error in those graphics, Fig. 14a shows the average energy approximation error per atom for the different summation rules (in particular, results of Fig. 13 were obtained with a normalized random displacement of 0.2 and are included in Fig. 14). Using the same meshes of Fig. 13 with sharp interfaces, we plot the average

Figure 12: Residual forces at diffuse mesh interfaces in two dimensions for various summation rules (repatom positions of Fig. 11 have been perturbed randomly), using the extended Finnis-Sinclair potential of (Dai et al., 2006) for Cu; the color code reflects residual force magnitudes.

energy error of all lattice sites in the crystal with increasing (randomized) displacements of all repatoms from their equilibrium positions. Fig. 14a repeats the analysis for diffuse interfaces. It becomes apparent that the new schemes of first and second order offer a considerable improvement over all other schemes, yielding errors that are significantly lower, especially close to the undeformed configuration. While the residual forces shown above only applied to the undeformed configuration, these results here demonstrate that the new scheme also performs best in deformed meshes, resulting in lower energy errors and thus in reduced spurious forces.

The same qualitative conclusions drawn above also apply to three dimensions. Fig. 15 demonstrates residual forces in non-uniform QC meshes with diffuse interfaces in three dimensions for the same summation rules discussed above. Here, nodal cluster and quadrature rules reduce residual force artifacts more effectively than in two dimensions; yet, the new summation rules are again shown to be superior to all others. Both the new first and second-order schemes

Figure 13: Approximation error introduced by the summation rules on the energy level for a QC mesh with sharp interfaces. After application of the affine QC interpolation, we compare the exact energy of each lattice site to that of the associated sampling atom.

reduce force artifacts to small elements right above atomistic resolution, as can be expected from our analysis. The energy approximation errors show exactly the same trends discussed above for two dimensions (for conciseness and because of visualization difficulties we omit further 3D results here).

8. Elastic benchmark simulations in three dimensions

The QC method is primarily used to approximate long-range elastic fields. In the immediate vicinity of defects, full atomistic refinement turns our non-local QC scheme into lattice statics with no approximation errors or residual forces. Therefore, we concentrate on scenarios where the repeat spacing is larger than the atomistic limit. Moreover, once plastic microstructure starts to form, simulation results show statistical deviations (even fully-atomistic results are not exactly reproducible in general due to numerical noise). Therefore, our quantitative benchmark examples in this section will concentrate on elastic deformation. Results beyond the onset of plasticity will be compared qualitatively to solutions obtained from lattice statics in Section 9. In all examples, we compare the following types of summation rules:

- (0, 0): a purely nodal summation rule,
- $(n_{cl}, 0)$: nodal cluster summation rules with n_{cl} shells of clusters,
- $(0, n_Q)$: quadrature summation rules with n_Q quadrature-type sampling atoms per element,
- $(0, 1^*)$: new first-order summation rule,
- $(0, 1^*, 4^*)$: new second-order summation rule.

Figure 14: Average relative energy error per atom in the 2D QC meshes of Fig. 13 containing a) sharp and b) diffuse interfaces. Repatoms are displaced randomly by a fraction of the distance to their nearest neighbor repatom (this fraction is shown as the normalized random displacement). Both graphics use the same legend to identify the various summation rules; errors are shown on a logarithmic scale.

Note that, as before, we exclude pure element quadrature rules from our analysis, since they require a **switching mechanism from the local element-based formulation to the non-local node-based description in the limit of full atomistics**. Here, we focus only on fully-nonlocal QC schemes that seamlessly bridge across all element sizes. Furthermore, in the case of quadrature summation rules, general three-dimensional examples require numerical compromises: quadrature summation rules define their sampling atom locations within elements as lattice sites closest to Gauss-Lobatto quadrature points (commonly used in the finite element method). Of course, the existence of a lattice constrains the choice of quadrature-atom locations. In the following, if several lattice sites are located at the same distance from a quadrature point, we make a random choice. If no such lattice site exists within an element (or if the only ones coincide with already existing sampling atoms), then no new sampling atom is inserted. Also, for higher-order quadrature rules we identify quadrature-type sampling atoms within each element in a random order.

8.1. Elastic constants in randomly coarse-grained copper single crystals

To assess the total error introduced by the various summation rules, we compute elastic constants in three-dimensional QC representations of an infinite fcc copper single-crystal modeled by the extended Finnis-Sinclair potential of Dai et al. (2006). Affine boundary conditions are applied remotely to a large coarse-grained crystalline ensemble whose repatom locations are chosen randomly from the entire set of lattice sites. This qualifies as a worst-case scenario of severely non-uniform meshes of poorest quality. We define the (repatom) *density* of a QC mesh as the ratio of the number of repatoms to the total number of lattice sites contained in the sample. For each chosen value of density, the specific distribution of the randomly-chosen repatoms affects the results. Therefore, multiple realizations of each system size and summation rule choice are required to reliably determine mean relative errors and standard deviations (all errors are calculated against (theoretically) exact elastic constants obtained from a fully-atomistic description). Fig. 16 illustrates example distributions of repatoms for four different densities along with the associated QC meshes. In order to guarantee a minimum number of repatoms inside the sample (especially for densities below 1%) system sizes are chosen to increase with decreasing density. Any reasonable summation rule must reproduce the exact results in uniformly coarse-grained samples (and all summation rules studied here do so within numerical tolerances). As representative examples, we investigate the four more traditional summation rules shown in Fig. 17 along with the new summation rule of first order. It is important to note that the reported errors of the elastic constants stem from two main sources (besides numerical noise). On the one hand, the QC approximation, i.e. the affine interpolation of atomic positions, leads to errors. On the other hand, the summation rule introduces energy approximation errors which, in turn, lead to residual and spurious force artifacts that relax the sample to an incorrect minimum of the (approximated) total potential energy. Together, these result in the total error of the non-local, energy-based, quasistatic QC method.

Elastic constants are determined from the curvature of the energy landscape. To this end, we incrementally apply

Figure 15: Residual forces in non-uniform QC meshes with diffuse interfaces for various summation rules in three dimensions (the new summation rules use the Cauchy-Born rule for non-repatom sampling atoms). As before, the color code reflects residual force magnitudes (in arbitrary units).

average strains to the sample and compute the energy of the relaxed configuration. The three-dimensional computational domain consists of a buffer region surrounding the actual sample core (which is orders of magnitude larger than the potential cut-off radius) to avoid surface effects in the core. Average infinitesimal strain tensors ϵ are enforced by affinely deforming all repatoms in the remote buffer region, linking all deformed and undeformed positions ($\mathbf{x}_i$ and $\mathbf{X}_i$, respectively) by $\mathbf{x}_i = (\mathbf{I} + \epsilon)\mathbf{X}_i$. To obtain elastic constants, we apply strains $\epsilon = \gamma \xi$ where γ is increased incrementally from $\gamma_{\min} = -0.02$ to $\gamma_{\max} = +0.02$ in steps of $\Delta\gamma = 0.0005$. Negative values of γ are included to account for crystal anharmonicity. A fifth-order polynomial is fitted to the calculated energy landscape $\tilde{V}(\epsilon)$, and elastic constants specific to each deformation mode are extracted from the curvature of the energy landscape in the unstrained state (i.e. at $\gamma = 0$). Acknowledging the cubic symmetry of fcc copper, we specifically compute the effective bulk modulus

$$B = \frac{1}{9\Omega} \left. \frac{\partial^2 \tilde{V}(\gamma \xi_B)}{\partial \gamma^2} \right|_{\gamma=0} \quad \text{with} \quad \xi_B = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad (73)$$

Figure 16: Example repatom distributions in randomly coarse-grained crystals for four different repatom densities: a) 50%, b) 20%, c) 5%, and d) 0.12%. The right half of each cube illustrates tetrahedral elements used for interpolation and shown on the surface of the cube, the left half shows repatom locations (black dots represent repatoms, solid white lines are element edges).

the shear modulus

$$\mu = C_{44} = \frac{1}{4\Omega} \left. \frac{\partial^2 \tilde{V}(\gamma \xi_\mu)}{\partial \gamma^2} \right|_{\gamma=0} \quad \text{with} \quad \xi_\mu = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad (74)$$

and the uniaxial elastic constant

$$C_{11} = \frac{1}{\Omega} \left. \frac{\partial^2 \tilde{V}(\gamma \xi_E)}{\partial \gamma^2} \right|_{\gamma=0} \quad \text{with} \quad \xi_E = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad (75)$$

where Ω denotes the volume of the core domain. For a detailed derivation of these relations see e.g. (Venturini, 2010).

Figs. 18(a)-(c) illustrate the relative error of the three elastic constants obtained from the various summation rules vs. repatom density. A repatom density of 100% corresponds to full atomistics and is free of errors. Each point denotes the mean error of all random realizations for a specific summation rule and repatom density; the associated standard deviations are indicated by error bars. When interpreting these results, it is useful to keep in mind that repatom densities between 10% and 100% can be expected to be rare in actual simulations since these only occur in the immediate vicinity of full atomistic resolution (in elements with only a few atomic distances per edge densities are already considerably lower). Overall, the results shown in Fig. 18 admit the following conclusions:

- Uniformly coarse-grained samples reproduce all elastic constants exactly. This can be expected since equally-spaced repatoms are free of spurious forces, which results in affine deformations and hence in a uniform atomic energy which, in turn, is summed exactly by all summation rules due to zeroth-order consistency. Consequently, energies and thus elastic constants must be reproduced exactly. (Marginal errors are visible in some of the data points for uniform meshes and demonstrate the level of numerical errors to be expected from our numerical implementation.)
- For non-uniform repatom distributions, nodal summation rules of type (0,0) exhibit the largest relative errors for all three elastic constants. For densities below 10% (not shown because of the scales in graphics), the mean error appears to stabilize in the 9 – 13% range with individual realizations showing errors well above 25%, which is generally not tolerable.
- Adding clusters to the nodal summation rule considerably reduces these errors. Cluster rule (3,0) produces errors significantly below those of the nodal rule (0,0). The effect is most pronounced at high density values, as can be expected: at values of 10% the average element size is very small (side lengths of only a few atomic spacings) so that clusters tend to overlap. As reported by Eidel and Stukowski (2009), cluster sizes are most effective in this regime and can lead to significantly improved results. However, lower densities (e.g. below

Figure 17: Example distributions of sampling atoms for four different summation rules applied to the same set of repatoms: a) purely nodal (0,0), b) lowest-order quadrature (0,1), c) second-order quadrature (0,4), and d) 3-shell cluster rule (3,0). Also shown is a sample tetrahedral element with its repatoms and sampling atoms for each case. The four graphics give an impression of the different levels of computational expenses which grow with the total number of sampling atoms in the QC model.

Figure 18: Results of elastic constant calculations: a)-c) relative errors of the elastic constants (computed by the QC method using various summation rules) compared to their (theoretically) exact values obtained from full atomistics; d) relative errors vs. normalized computation times required for elastic constant calculations for the different summation rules (small percentage labels denote repatom densities; computation times are normalized by those of comparable fully-atomistic run times).

Figure 19: Distribution of element sizes in the void-expansion simulation shown on the right: without considering all fully-atomistic elements, the curves indicate what volume fraction of the entire domain is occupied by elements smaller than a particular size (normalized by the smallest (atomistic) element size, $V_0 = a_0^3/24$, shown schematically for fcc), and the fraction of the number of elements smaller than a particular size.

5%) result in larger average element sizes, for which the error rises rapidly. At very low densities near 0.1% the impact of clusters is marginal and the elastic constant error is comparable to that of the nodal summation rule.

- Of all traditional summation rules, quadrature rules of type $(0, n_Q)$ show the smallest relative errors for the entire range of densities investigated here. In particular, for quadrature rule $(0, 1)$ the relative errors of all elastic constants remain below 5% across all investigated density levels. When using quadrature rule $(0, 4)$, the relative errors remarkably remain below 1.2% throughout (for C_{11} even smaller). Interestingly, cluster summation rule $(3, 0)$ outperforms the lowest-order quadrature summation rule $(0, 1)$ only for densities larger than 5%. At lower densities (where element sizes increase), $(0, 1)$ provides considerably lower errors than the much more expensive cluster summation rule $(3, 0)$. In the dilute limit, $(0, 1)$ requires approximately $N_h + N_e$ sampling atoms (with N_e the number of elements, and we neglect the possibility of double-counting in small elements). The number of elements in simplicial 3D meshes scales roughly linearly with the number of nodes. In those meshes shown here we observe $N_e \approx 5 N_h$, which results in an approximate total number of sampling atoms of $6 N_h$. In contrast, $(3, 0)$ applied to, e.g., an fcc Cu lattice requires approximately $42 N_h$ sampling atoms (clusters do not overlap in the dilute case).
- The new first-order summation rule $(0, 1^*)$ shows noticeable errors only at repatom densities above 10%, and even these remain below 1.4% for all elastic constants. Remarkably, below densities of 10% the error becomes marginal and is comparable to the numerical errors found in uniform QC meshes. This holds true for all three elastic constants. The largest errors appear for repatom densities close to 100%, which, in an actual QC simulation, primarily affects elements in the transition region right above fully-atomistic resolution. In our general QC framework with mesh adaptation the simulation volume occupied by elements of such sizes is rather small. This is illustrated in Fig. 19 for the example of a Cu single crystal with a nano-void at its center with fully-atomistic resolution around the void and diffuse coarse-graining away from the void. Here, it is difficult to talk about an individual element's repatom density, which is why we plot the curves vs. the element volume normalized by the atomic cell size V_0 (i.e., a normalized element size of 10 implies a repatom density of $1/10 = 10\%$ if the entire domain was filled with such elements). As shown by the dotted lines, in this example about 43% of all elements have repatom densities larger than 10% (and can thus be expected to show errors in their elastic behavior on the order of 1%). Yet, due to their small volume, these elements occupy about 0.01% of the overall simulation domain (which contains a total of 42568 elements). The new second-order rule $(0, 1^*, 4^*)$ shows even lower errors in general. However, the random meshes used for the elastic constant simulations contain extremely-poor tetrahedral elements for which reasonable definitions of the weights of face-centered sampling atoms become nontrivial. This problem does not arise in reasonable meshes as those obtained e.g. from our adaptive remeshing (see Section 9).

To assess the computational cost associated with each summation rule, Fig. 18(d) shows elastic constant errors vs.

computational runtime per lattice site. Specifically, we compare the computation time required to obtain the energy curves from which C_{44} is extracted (which involves applying an average strain $\epsilon = \gamma \xi$ to the sample and relaxing the system to obtain its energy for $\gamma_{\min} < \gamma < \gamma_{\max}$). We note that in our implementation there is no algorithmic difference between the various summation rules during these steps (the initial setup of the QC representation is not considered). Therefore, the differences in runtime are a direct consequence and thus a good indicator of the varying complexity of the summation rules. Fig. 18(d) contains the same relative errors shown in Fig. 18(b) but plotted vs. the **computational run time normalized by the computation time of a comparable fully-atomistic calculation using the same code** to allow for a fair comparison (this accounts for the increasing domain size with decreasing density). The small percentage values indicate the reatom densities for reference. As can be expected, for each summation rule the computation time generally decreases with decreasing density. This is a direct consequence of the reatom count reduction, which automatically leads to a reduction of the number of sampling atoms in each scheme. **Interestingly, at high reatom densities, the new summation rule (0, 1*) – just like the cluster rule (3, 0) – is computationally more expensive than full atomistics, primarily because of the large number of sampling atoms. At lower densities, however, the graphic shows that the new rule provides the lowest errors and low computational run times.**

Overall, the quadrature summation rules (0, 1) and (0, 4) perform much better than the nodal and cluster summation rule (3, 0), showing lower errors at comparable or lower costs. If the relative error is required to remain below 3%, (0, 1) is sufficient and by far the most efficient choice. For the relative error to remain below 1%, (0, 4) is required and, again, by far the most efficient summation rule. As seen before, cluster rule (3, 0) only reduces the error in case of high reatom densities and otherwise produces large relative errors. (3, 0) is considerably (by orders of magnitude) less efficient than the pure nodal rule (0, 0). The seemingly interesting behavior for (3, 0) at large runtimes stems from overlapping clusters becoming significant at large levels of the reatom density. The new scheme (0, 1*) incurs costs that are comparable to the (0, 1) quadrature rule at lower densities. It is more expensive at high reatom densities because inner-element sampling atoms persist until their weights go to 0, whereas quadrature rules (which snap sampling atoms to actual lattice sites) produce fewer sampling atoms near the atomistic limit. At low reatom densities, the errors of (0, 1*) are so small that they can no longer be shown on the logarithmic scale while becoming less and less costly. Therefore, at low reatom densities of 1% and below, the by far most efficient and most accurate choice in our examples is the new (0, 1*) scheme.

Note that here and in some of the following examples deformation is enforced through affine boundary conditions applied to a buffer region around the actual simulation core. Since atomic potentials generally require more than next-to-nearest neighbor interactions, such a buffer region (a common technique in MD) is required to avoid parasitic surface effects by providing all required neighbors to the core region. This, of course, is only an approximation to impose a desired average remote loading. Since our QC formulation allows us to, in principle, coarse-grain aggressively to arbitrary sample sizes, it is well possible to apply those boundary conditions arbitrarily far away from the simulation core. This avoids spurious cell-size effects that can arise in atomistic calculations, see e.g. (Szajewski and

Figure 20: Examples of single-crystalline cubes of pure copper used to compare the accuracy of summation rules in three dimensions: the atomistic core with a spherical nano-void at its center is coarse-grained in multiple steps using (a) randomized diffuse and (b) sharp mesh interfaces. Affine boundary conditions of uniaxial extension are applied to all blue reatoms, while the core regions defined by all red reatoms are relaxed to equilibrium. The zoomed images show the relaxed QC regions; (b) includes example results of energy and displacement errors.

Figure 21: Example of a single-crystalline Cu nanocube with a spherical void undergoing uniaxial extension in the vertical $[100]$ direction, modeled by a non-uniform QC mesh with *sharp* interfaces. Each graphic results from a particular summation rule and illustrates the distribution of repatoms and sampling atoms (left), the displacement errors of all lattice sites compared against full atomistics (bottom), and the corresponding relative energy errors of all lattice sites (top). Errors are shown on logarithmic scales, displacement errors are shown in Angstroms. For reference, the lattice spacing in Cu is approximately 3.61 Å.

[Curtin, 2015](#)).

8.2. Local position and energy errors

QC simulations generally avoid the extreme element aspect ratios and coarsening ratios found in the random meshes of the previous section. Instead, gradual coarse-graining is favored to reduce approximation errors due to summation rules and interpolation schemes (and is automatically achieved by intelligent model adaptation). We proceed to assess the performance of the various summation rules in such meshes, where we study long-range inhomogeneous elastic deformation. The elastic constant calculations revealed the total error to be expected from a summation rule, yet it did not yield any information about where significant local errors are to be expected within a model discretized by the QC approximation.

The next example is a Cu single-crystal having a single spherical void (diameter 5 nm). The void leads to an inhomogeneous stress distribution with concentrations in the vicinity of the void. To properly resolve the void, we assign atomistic resolution to its immediate vicinity and rapidly coarse-grain away from the void in a total of six steps with coarsening ratios of roughly 2, as shown in Fig. 20. The sample is loaded at its top and bottom in uniaxial extension (affine boundary conditions are chosen to remove surface effects and mimic an infinite single crystal). The cube is stretched vertically in the $[100]$ direction and relaxed to equilibrium. Next, the relaxed positions of all lattice sites are computed from the shown QC model using its affine interpolation rules. For comparison, we also compute all exact atomic positions from a geometrically-equivalent lattice statics model with the same boundary conditions. The system contains $67.1 \cdot 10^6$ lattice sites whose interactions are modeled by two different QC meshes: one mesh containing sharp interfaces (comprising about 7,140 repatoms and 41,800 elements) and one mesh that is seamlessly

Figure 22: Example of a single-crystalline Cu nanocube with a spherical void undergoing uniaxial extension in the vertical $[100]$ direction, modeled by a non-uniform QC mesh with *diffuse* interfaces. Each graphic results from a particular summation rule and illustrates the distribution of reatoms and sampling atoms (left), the displacement errors of all lattice sites compared against full atomistics (bottom), and the corresponding relative energy errors of all lattice sites (top). Errors are shown on logarithmic scales, displacement errors are shown in angstroms.

coarse-grained by randomized, diffuse interfaces (roughly 7,130 reatoms and 42,500 elements). Therefore, in both cases the number of degrees of freedom has been reduced to about 0.01%. We deliberately limit our discussion to elastic loading in a radically coarse-grained QC model to demonstrate the approximation power of long-range elastic fields. Microstructure evolution is certainly the main application of the QC method. However, as discussed before, QC is essential in approximating long-range elastic fields while atomistic defects require locally full atomistic resolution (capabilities to study complex microstructural mechanisms will be shown in Section 9). Besides, the formation of inelastic defects automatically introduces randomness of solutions, which defeats the purpose of a one-to-one comparison of lattice site positions.

Fig. 21 illustrates the displacement errors and relative energy errors of all lattice sites compared against the exact atomistic solution for various summation rules applied to the sharp-interface QC mesh. For the nodal and cluster summation rules, displacement errors show significant values throughout all coarse-grained regions. The same trends as in previous examples are observed in both energy and displacement errors: the introduction of nodal clusters reduces the error of the nodal summation rule (0,0) with increasing cluster size, see e.g. (3,0). Quadrature summation rules reduce errors below those of cluster rules. Even the lowest-quadrature rule (0,1) produces smaller errors than the computationally much more expensive (3,0) rule in larger elements. In regions with close-to-atomistic resolution, cluster rules and quadrature rule (0,4) produce minimal errors because essentially all lattice sites are turned into sampling atoms, resulting in poor efficiency. The new summation rules (whose efficiency is comparable to (0,1) and (0,4) quadrature for the first- and second-order schemes, respectively) reveal by far the lowest errors overall with only marginal differences between the first and second-order schemes. We note that the vanishing displacement errors are not only an indication of the excellent performance of the summation rules but also confirm the general applicability of the QC approximation to represent long-range elastic fields. Also, it is important to realize that errors of the

Figure 23: Comparison of the average relative energy approximation errors of all lattice sites for the example of Fig. 20b (nanocube with a void using a QC mesh with sharp interfaces and undergoing uniaxial extension) for five different summation rules and the interatomic potentials of Table 1.

traditional summation rules do not only arise in the coarse-grained regions but propagate into the full atomistic core as well, primarily due to spurious force artifacts. Fig. 22 shows the equivalent displacement and energy errors for the diffuse QC mesh. As can be expected, errors are larger than in the case of sharp mesh interfaces but reproduce the same trends. Note that in both cases, the second-order scheme performs better than the first-order rule.

We would like to demonstrate that the new scheme performs equally well for all EAM potentials and is not tied to the specific interatomic potentials used in our examples. To this end, we compare five atomic potentials which greatly differ by their radii of interaction (see Table 1). In each case, we have determined the effective interaction radius r_w (required to determine the weights of sampling atoms) by numerical experimenting. **Specifically, we have repeated the void-expansion simulations of Fig. 22 for various effective interaction radii r_w and have chosen those values as optimal that produce the least total position error of all lattice sites in the sample. Of course, this does not guarantee that the determined radii are optimal for arbitrary simulation scenarios. However, the chosen example involves a wide range of element sizes in an unstructured mesh and was selected as a representative scenario. There is clearly room for improvement here but even this rather ad-hoc choice performs orders of magnitude better than the other summation rules. A more detailed analysis of optimal values for the effective interaction radii in particular in the presence of free surfaces can be found in (Amelang and Kochmann, 2015).**

Figs. 23 and 24 summarize the average relative energy and position errors, respectively, of all lattice sites contained in the cube with a nanovoid of Fig. 20b for five different summation rules and for all potentials listed in Table 1. The general qualitative conclusions drawn above hold for all five potentials. The new first- and second-order summation rules produce significantly smaller errors compared to nodal, cluster and traditional quadrature rules (note the logarithmic scales in both graphics).

8.3. Effect of residual force removal

In the traditional QC method as well as in general atomistic-continuum coupling schemes, force artifacts appear both as residual forces (i.e., in the undeformed configuration) and as spurious forces (i.e., errors in repatom forces in

Figure 24: Comparison of the position error per atom (average of all lattice sites) for the example of Fig. 20b (nanocube with a void using a QC mesh with sharp interfaces and undergoing uniaxial extension) for five different summation rules and the interatomic potentials of Table 1.

the deformed configuration). Various corrections have been introduced to remove such force artifacts, in particular in coarse-graining schemes that explicitly differentiate between atomistic and coarse-grained regions. There, one commonly speaks of *ghost force corrections*, see e.g. (Shenoy et al., 1999a; Ortner and Zhang, 2014). Residual forces are simple to compute, whereas spurious forces are rather difficult to determine. A misconception is that the removal of residual forces by appropriate dead loads on repatoms (determined in the undeformed, initial state) is sufficient to significantly reduce force artifacts in the deformed state **in a fully-nonlocal QC scheme**. We can use the same nano-void example to illustrate that this is indeed not the case (and that the best way to effectively remove both residual and spurious force artifacts is by minimizing energy approximation errors via optimal summation rules such as those investigated here). To this end, we take the example of Fig. 20b with different summation rules; we determine the residual forces in the undeformed state and remove those by (constant) dead loads on all repatoms. Then, we apply uniaxial extension and relax the sample in the presence of the corrective dead loads. Of course, the undeformed configuration will now be reproduced exactly but the deformed state displays the errors shown in Fig. 25. Apparently, the effect of the dead load correction (see the bottom row) is marginal and for some of the summation rules even produces larger errors than without correction. **Note that correction methods have been introduced in local/nonlocal QC, cf. (Shenoy et al., 1999a), which effectively reduce ghost forces at the local/nonlocal interfaces by recomputing corrective dead loads after each iteration step. However, this affects the conservative energy-based nature of the QC scheme, it requires special procedures for repatoms near the local/nonlocal interface, and it requires the notion of an interface (which does not exist in the fully-nonlocal formulation here).**

9. Inelasticity and the formation of microstructure

Nanoindentation is a classical example that has been subject to previous investigations by the QC method, see e.g. (Smith et al., 2001; Knap and Ortiz, 2003; Jin et al., 2008). Most previous studies considered relatively small sample and indenter sizes or incipient indentation depth. Here, we apply the presented fully non-local QC formulation with the new second-order summation rule to two- and three-dimensional single-crystalline Cu samples deforming under spherical indenters modeled by the potential of Kelchner et al. (1998). This scenario goes beyond our previous examples in various ways. On the one hand, indentation leads to significant inelastic deformation mechanisms involving dislocation nucleation and propagation. Here, the nature of the atomistic energy landscape with myriads of local minima corrupts the repeatability of results in the presence of numerical noise (due to computational parallelism). Therefore, we qualitatively compare the microstructure obtained from QC to that of full lattice statics; quantitatively we compare the load vs. indentation depth curves via statistical averaging as explained below. On the other hand, this scenario involves free surfaces which present a challenge to the QC method because of considerable force artifacts arising from the traditional summation rules. Using e.g. a cluster summation rule results in large residual forces which lead to an artificially deforming free surface. This in turn will initiate mesh adaptation and ultimately lead to atomistic refinement of the entire surface, which is prohibitively expensive. In contrast, the new second-order rule assigns sampling atoms to the faces of tetrahedral elements, which automatically takes care of free surfaces by representing all surface-nearest lattice sites by those sampling atoms on the surface. We will report details of how surfaces and interfaces can be modeled by the new scheme elsewhere; here, we will show that the second-order scheme can successfully master the combined challenges of free surfaces and microstructure formation.

potential	cut-off distance	lattice spacing	radius r_w	potential reference
Johnson potential	3.249000 Å	3.609966 Å	1.7 Å	Johnson (1989)
extended Finnis-Sinclair potential	4.320000 Å	3.609966 Å	2.4 Å	Dai et al. (2006)
Voter potential	4.961000 Å	3.614999 Å	2.5 Å	Mishin et al. (2001)
Mishin potential	5.506786 Å	3.615000 Å	2.4 Å	Mishin et al. (2001)
Mendelev potential	6.000000 Å	3.635871 Å	2.1 Å	Mendelev and King (2013)

Table 1: Overview of Cu interatomic potentials used for a comparison of approximation errors, along with their tabulated cut-off distances as well as the lattice spacing obtained from energy minimization in a perfect infinite crystal lattice (rounded to six digits). The optimal effective interaction radii r_w for the definition of sampling atom weights for the five potentials are also included.

Figure 25: Influence of removing residual forces by dead loads using by comparing errors produced by four different summation rules (a-d) without and (e-h) with removed residual forces; top halves of all graphics illustrate relative energy errors per atom, bottom halves show displacement errors of all lattice sites for the sharp-interface scenario of Fig. 20b.

While a two-dimensional setting allows for a direct comparison with full atomistics, the three-dimensional example by far exceeds our computational resources to run a comparative lattice statics simulation. Therefore, we will first illustrate results obtained in two dimensions. A Cu sample (i.e., a close-packed {111} plane modeled by the extended Finnis-Sinclair potential of Dai et al. (2006)) of dimensions 0.1×0.082 microns and containing 148,000 lattice sites is relaxed and then indented by a circular indenter with a 20 nm diameter and a force constant of 10^3 eV/Å³. The sample's bottom is constrained to suppress displacements in the vertical direction, whereas lateral edges are constrained in the horizontal direction. The quasi-static evolution of the indenter is simulated by 1,000 displacement steps at increments of 0.003 nm (i.e., each relaxation step involves about 1% of the Cu lattice spacing). Twenty realizations have been used to obtain the average force-indentation curves shown in Fig. 26. The parallel implementation of the QC method (specifically, the random order in which threads contribute to the repatom forces) leads to small random fluctuations, which in turn produce variations of the simulated results (similar to the effect of thermal fluctuations). Therefore, we show the average curve along with its standard deviation.

Overall, the QC results agree well with the lattice statics findings. In particular, the initial elastic response is identical, the first dislocation event occurs at identical indentation depths, and the general trends of the load-displacement curves show great similarities. It is worth mentioning that our QC simulation does not use a static mesh with a large atomistic region underneath the indenter. Instead, we use automatic mesh adaptation to locally refine the initial QC mesh. To this end, we use the second-invariant criterion of (Knap and Ortiz, 2001) with a tolerance of 0.1 to identify regions of refinement (i.e., we check if the second invariant of an element's deformation gradient exceeds its threshold). We then apply a complex combination of element bisection and local mesh reconstruction for mesh refinement. Further reduction of the tolerance parameter appeared to produce no significant differences in the average force-displacement curves. Fig. 27 shows the top section of the initial QC mesh as well as of the final QC representation at an indentation depth of approximately 3 nm. As becomes apparent from the final mesh, we suppress the refinement of the side and bottom faces to reduce computational expenses.

In order to better compare the forming microstructure, Fig. 28 shows the final deformed state at an indentation depth of about 3 nm, color-coded by the centrosymmetry parameter of individual atoms (Kelchner et al., 1998). For the QC solution we first determine the positions of all lattice sites from those of the repatoms via the affine QC interpolation. Then, we compute the exact centrosymmetry parameter for each atom in the interpolated configuration.

Figure 26: Indenter force vs. indentation depth for a two-dimensional Cu single crystal obtained from (a) lattice statics (full atomistic resolution) and (b) the QC method using the new second-order summation rule and automatic mesh adaptation. Shown are the mean force–displacement curves obtained from 20 simulations with standard deviations shown by the gray shading. For a direct comparison, the dashed (red) line in (b) is the average response from (a) obtained from lattice statics.

Obviously, interpolations may lead to non-centrosymmetric neighborhoods across elements, which is why Fig. 28b shows significantly more noise than the exact solution in Fig. 28a. It is important to note that this noise does not represent actual defects but simply interpolation errors that would disappear e.g. when relaxing the final QC positions without the affine interpolation constraints. Therefore, we primarily care about the qualitative agreement of the observed dislocation activity. We see that all three slip systems (in the close-packed directions of the 2D lattice) **and the exact same slip planes** are activated in both solutions; the pile-up of dislocations directly underneath the indenter agrees **qualitatively, and the core structure and size** of dislocations is identical in both simulations. Of course, we do not claim a perfect fit but the **qualitative agreement is convincing in our view**, considering that this simulation uses automatic mesh adaptation and started from the mesh of Fig. 27a. Also, unlike in many other atomistic-to-continuum coupling techniques there is no methodological differentiation between atomistic and coarse-grained regions. Clearly, in such simulations the accuracy of the chosen remeshing scheme plays a crucial role and becomes as essential as the summation rule, and there is clearly room for improvement here.

Finally, let us demonstrate the capabilities of the presented energy-based QC flavor by a three-dimensional example. Fig. 30 summarizes the evolution of dislocation loops underneath a 40 nm indenter in three dimensions, using the indenter potential of Kelchner et al. (1998) with a force constant of $10^3 \text{ eV/\AA}^3$. The maximum penetration depth is 6 nm, and the sample size is 1 micron (containing approximately 86 billion lattice sites which are represented in the final deformed state by about 5.65 million repatoms). Due to the large sample size, we do not perform comparative simulations using full lattice statics and instead only report our findings from the QC simulation. To avoid the distraction by approximation errors stemming from the remeshing scheme (and to confirm that the scheme can equally well handle sharp mesh transitions), we start with a large atomistic region, as shown in Fig. 29.

Figure 27: Top sections of the initial and final QC meshes of a nanoindentation simulation in two dimensions using automatic mesh adaptation.

Figure 28: Dislocation emission from the surface during nanoindentation simulated by (a) lattice statics and (b) the fully-nonlinear energy-based QC method with the new second-order summation rule and automatic mesh adaptation in two dimensions (see the QC meshes in Fig. 27), color-coded by centrosymmetry on a log-scale (0.07-0.7, red being highest). Noise in the QC solution stems from the affine interpolation scheme.

Figure 29: Cut through the undeformed QC mesh, view of all repatoms, and cut through the final deformed QC mesh (with void) in three dimensions.

The Cu micro-cube is initially single-crystalline and defect-free but contains a spherical void of radius 0.75 nm at a depth of 4 nm below the indented surface; such voids arise e.g. from exposure to radiation (Whitley et al., 1979). The void creates an inhomogeneous stress field with concentrations in its vicinity, which is of interest for two reasons. First, this promotes the heterogeneous nucleation and emission of dislocation loops from the void (the large indenter size would require considerably larger indentation depths to create defects in an initially defect-free crystal). Second, the interaction of the void with the free surface is an ideal scenario for the QC method since it requires to accurately capture long-range elastic fields. Void growth in infinite crystals subject to remote loading has been investigated by the QC method before, see e.g. (Marian et al., 2005, 2008; Ariza et al., 2012), but not in a macroscopic boundary value problem such as the nanoindentation scenario studied here. Results of the microstructure evolution from the initial void to the final defect network are shown in Fig. 30 (defects have been identified by the centrosymmetry parameter).

Figure 30: Zoomed-in snapshots of the microstructure evolving during 3D nanoindentation into a Cu single-crystal with an isolated nano-void at indentation depths of 0 nm, 2.1 nm, 3.0 nm, and 5.7 nm; defects are visualized by the centrosymmetry parameter (color code in arbitrary units).

10. Conclusions

We have compared various summation rules for the energy-based fully-nonlocal QC method and investigated their impact on the accuracy of results and the efficiency of simulations. Besides traditional nodal, cluster, and quadrature summation rules, we compared first- and second-order realizations of a new summation rule based on sampling atoms with optimal weights. The new scheme minimizes spurious and residual force artifacts as well as energy approximation errors compared to all other summation rules investigated here. After a theoretical study in one and two dimensions, we have demonstrated the accuracy and efficiency of the various summation rules by instructive two- and three-dimensional benchmark examples using a variety of EAM potentials. Examples include the calculation of elastic constants from fully randomized QC meshes and the comparison of energy and position errors in samples undergoing inhomogeneous deformation in the vicinity of a nano-void, using QC meshes with both sharp and randomized diffuse interfaces. Finally, we have demonstrated the applicability of the non-local QC formulation with the new second-order summation rule and with automatic mesh adaptation to the test case of nanoindentation which involves defect nucleation and microstructure evolution. In all examples, the comparison of QC results to those of full atomistics has shown convincing qualitative and quantitative agreement and, in particular, the superiority of the new second-order summation rule over the traditional QC summation rules (especially compared to the classical node-based cluster summation rules).

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atomistic core with a nanovoid

diffuse mesh interfaces

(a)

3dexamplesn2.pdf

(b)

sharp, structured mesh interfaces

(a) nodal (0,0)

3dresultsn.pdf

(b) quadrature (0,1)

(c) quadrature (0,4)

(d) cluster (3,0)

(e) new, first order (0,1*)

(f) new, second order (0,1*,4*)

(a) fully atomistic

(b) adaptive nonlocal QC

(a) cluster rule (3,0) **(b)** quadrature rule (0,4) **(c)** first-order new (0,1*) **(d)** second-order new (0,1*,4*) **(e)** cluster rule (3,0)
with correction **(f)** quadrature rule (0,4)
with correction **(g)** first-order new (0,1*)
with correction **(h)** second-order (0,1*,4*)
with correction

(a) nodal (0,0)

(b) quadrature (0,1)

(c) quadrature (0,3)

(d) new, first order (0,1*)
with Cauchy-Born

(e) new, second order (0,1*,3*)
with Cauchy-Born

(a) nodal (0,0)

(b) cluster (3,0)

(c) quadrature (0,1)

(d) quadrature (0,4)

(e) new, first order (0,1*)

(f) new, second order (0,1*,4*)

(a) nodal (0,0)

(b) cluster (3,0)

(c) quadrature (0,1)

(d) quadrature (0,4)

(e) new, first order (0,1*)

(f) new, second order (0,1*,4*)

indentation_comic.pdf

d) second-order rule (0,1*,3*)

a) nodal summation rule: (0,0) overview2n.pdf

b) nodal cluster summation rule: (1,0)

c) element quadrature summation rule: (-,1)

d) quadrature summation rule: (0,1)

e) quadrature summation rule: (0,2)

randomcoarsening2.pdf

a) 50%

b) 20%

c) 5%

d) 0.12%

(a) nodal (0,0)

(b) cluster (3,0)

(c) quadrature (0,1)

(d) quadrature (0,3)

(e) quadrature (0,3)
(sampling atoms not on lattice sites) (f) new, first order (0,1*)
without Cauchy-Born (g) new, first order (0,1*)
with Cauchy-Born (h) new, second order (0,1*,3*)
without Cauchy-Born (i) new, second order (0,1*,3*)
with Cauchy-Born

(a) nodal (0,0)

(b) cluster (3,0)

(c) quadrature (0,1)

(d) quadrature (0,3)

(e) quadrature (0,3)
(sampling atoms not on lattice sites) (f) new, first order (0,1*)
without Cauchy-Born (g) new, first order (0,1*)
with Cauchy-Born (h) new, second order (0,1*,3*)
without Cauchy-Born (i) new, second order (0,1*,3*)
with Cauchy-Born

Figure

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