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Uniform accuracy of the quasicontinuum method

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The accuracy of the quasicontinuum method is studied by reformulating the summation rules in terms of reconstruction schemes for the local atomic environment of the representative atoms. The necessary and sufficient condition for uniform first-order accuracy and, consequently, the elimination of the "ghost force" is formulated in terms of the reconstruction schemes. The quasi-nonlocal approach is discussed as a special case of this condition. Examples of reconstruction schemes that satisfy this condition are presented. Transition between atom-based and element-based summation rules are studied.

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I. INTRODUCTION

The quasicontinuum (QC) method[1–3] is one of the most successful multiscale techniques for simulating static properties of crystalline solids. It combines continuum and atomistic descriptions of solids in a rather seamless way, thus allowing for an efficient description of the system with accuracy comparable to that of the atomistic model but at a much smaller cost. This is implemented in the setting of a piecewise linear finite element method through two main steps: kinematically by introducing representative atoms (rep-atoms) to reduce the number of degrees of freedom in regions where the atomic displacement is smooth; energetically by introducing the simplified summation rule based on the so-called Cauchy-Born (CB) hypothesis to approximately compute the total energy of the system. According to whether CB rule is used, the computational domain is divided into local and nonlocal regions. In the local region the summation is done element-wise using CB rule. This corresponds to a continuum approach of nonlinear elasticity with the stored energy functional obtained from CB rule. Full atom summation is used in the nonlocal region. In addition, QC uses an adaptive mesh refinement strategy in order to adaptively select the representative atoms and decide whether a more continuum-like or atomistic-like approach should be used locally.

QC is a typical example of a multiscale method that uses multiple levels of physical descriptions, here the atomistic and continuum models of the system. Such a methodology raises questions regarding their accuracy and stability. For QC, this problem is manifested by the existence of the so-called "ghost force" At the equilibrium state the forces on the atoms are not zero, thus the equilibrium state is no longer at equilibrium in a QC description. This is a typical problem for such an energy-based multi-physics methodology, shared, for example, by all the QM-MM methods that combine quantum mechanics and molecular mechanics descriptions (see, for example, Ref. 4). Even though such forces can always be corrected by hand (for example, by introducing some dead load, as is suggested in Ref. 3), typically such correction schemes are not done at the level of the energy. One exception is the work of Shimokawa *et al.*[5] which we will return to later.

The issue of "ghost force" is just one aspect of the problem of accuracy. More generally, what we need is a framework under which issues of accuracy for such coupled methodologies using multi-levels of physical descriptions can be discussed. This is the main purpose of this series of papers. In this first paper, we will focus on QC with classical atomistic models. In subsequent papers, we will discuss QM-MM as well as nonlocal QC methods using various models of quantum mechanics, such as the tight-binding model and density functional theory.

As we will see later, there are two sources of inconsistency between the continuum and the atomistic models when computing the total energy in QC. One is that the continuum approach using the Cauchy-Born rule is purely local, depending only on the nearest vertices on the finite element mesh, whereas the full-atom summation is usually nonlocal depending on the range of the atomic interaction. The other is that the continuum approach is naturally an element-based summation rule, whereas the full-atom summation is more naturally associated with each of the atoms. Our strategy in this paper is to treat the two problems separately, by introducing two interfaces where the two transitions take place, a local/nonlocal interface and an atom-based/element-based interface. The second interface is inside the local region. Between the two interfaces, we will introduce an atom-based summation rule which is a natural modification of the continuum approach based on the Cauchy-Born rule.

In this paper, we will introduce a way of calibrating the local truncation error in nonlocal QC. We will discuss how one can achieve uniform first-order accuracy by modifying the way energy is computed at the local-nonlocal interface. As we will demonstrate, this problem can be reduced to that of a reconstruction problem: At the local/nonlocal interface, how do we reconstruct the local environment in order to compute the energy of the representative atoms? We will formulate a condition, which is both necessary and sufficient, on the reconstruction scheme in order to guarantee that the local truncation error is uniformly first order. This condition can be roughly stated as follows: If we group together pairs of atoms that in the equilibrium configuration lie on the same line and with the same distance apart, then for uniformly deformed configurations, the dependence of their reconstructed positions on any other fixed atom cancels out. The quasi-nonlocal reconstruction scheme can be viewed as a simplified form of this condition (which is then sufficient but no longer necessary) in which each pair of atoms form their own group. Our extension of this condition puts together the pairs of atoms that are co-linear and with the same distance apart. We will then discuss a general reconstruction scheme under which the local truncation error is uniformly first order. In the end, we will show briefly that for finite-range atomic potentials, one can, in principle, sum the energy exactly in $O(N_{\text{rep}})$ cost, bypassing the CB rule and thus eliminating the errors in the summation step.

II. THE QUASICONTINUUM METHOD

We start with a brief review of the QC method and notations used in the following sections. QC starts with an underlying atomistic model of the material which is considered to be accurate. This could, in principle, be a quantum-mechanics based description such as a tight-binding model or models based on the density functional theory (DFT), but in the present paper we will focus on atomistic models using empirical potentials.

We denote by $\boldsymbol{y}_i$ and $\boldsymbol{x}_i$ the positions of the ith atom in the deformed and undeformed configurations, respectively. For simple crystalline solids, the undeformed state can be represented as the collection of points with the form

$$\boldsymbol{x} = n_1\boldsymbol{A}_1 + n_2\boldsymbol{A}_2 + n_3\boldsymbol{A}_3, \tag{1}$$

where $\boldsymbol{A}_1$, $\boldsymbol{A}_2$, and $\boldsymbol{A}_3$ are the basis vectors, and n_1, n_2, and n_3 are integers. The displacement vector for the ith atom is defined as

$$\boldsymbol{u}_i = \boldsymbol{y}_i - \boldsymbol{x}_i. \tag{2}$$

The total energy of the system can be written as a sum over the energy of each atom,

$$E^{\text{tot}}(y) = \sum_{i=1}^{N} E_i(\boldsymbol{y}) = \sum_{i=1}^{N} E_i(\{\boldsymbol{y}_1,\boldsymbol{y}_2, \ldots ,\boldsymbol{y}_N\}), \tag{3}$$

where E_i is the energy associated with the ith atom, which depends on the positions of the other atoms in the deformed configuration and has finite range, N is the number of total atoms in the solid.

If some external load is applied to the system, the total energy of the system can be written as

$$\Phi(\boldsymbol{y}) = E^{\text{tot}}(\boldsymbol{y}) - \sum_{i=1}^{N} \boldsymbol{f}_i\boldsymbol{y}_i, \tag{4}$$

where $-\boldsymbol{f}_i\boldsymbol{y}_i$ is the work done by the external load $\boldsymbol{f}_i$ on atom i.

The actual displacement of the atoms can, in principle, be found by minimizing the above total energy functional. In practice, this is often very expensive and uninformative: Not only is the computational cost quite large, the information of interest is often buried together with a huge amount of uninteresting data. In QC, one makes the observation that in regions where the atomic displacement is rather smooth, there is no need to include the position of every atom as an independent degree of freedom, since the deformation in these regions can be represented with satisfactory accuracy by a much smaller set of representative atoms. This idea is implemented in QC through a set of kinematic constraints—reducing the number of degrees of freedom by introducing representative atoms (rep-atoms) and represent the displacement of all other atoms in terms of the displacement of the representative atoms.

Representative atoms are selected using an adaptive mesh refinement procedure over finite element meshes. The representative atoms are vertices of the underlying triangulation. Piecewise linear finite elements are used. This restricts the method to first order accuracy.

The kinematic constraint for the displacement of the atoms is given by:

$$\boldsymbol{u}^h(\boldsymbol{x}_i) = \sum_{j=1}^{N_{\text{rep}}} S_j(\boldsymbol{x}_i)\boldsymbol{u}_j, \tag{5}$$

where $S_j(\boldsymbol{x})$ is the basis function of the underlying finite element space associated with the jth rep-atom, and N_{rep} is the number of rep-atoms, $N_{\text{rep}} \ll N$.

The total energy of such a system is now a function of the positions (displacements) of the rep-atoms only. However, to compute this energy by direct summation using the original atomistic model would still require visiting all the atoms. QC bypasses this by introducing approximate summation rules.

A. Element-based summation rule

In QC, the computational domain is divided into *local* and *nonlocal* regions according to the smoothness of the displacement field $\boldsymbol{u}^h$. Inside the nonlocal region where deformation is large, all the atoms are rep-atoms, hence the energy associated with these atoms can be computed using direct summation.

Inside the local region, the total energy is computed element-wise by using the Cauchy-Born rule on each element. For simple crystals, the CB rule works as follows (there is a simple generalization to complex crystals, see Refs. 6 and 7): Let $F = \nabla \boldsymbol{u}$ be the deformation gradient tensor of a uniform deformation, and $E_0(F)$ be the energy of the unit cell in a deformed lattice when its lattice vectors are deformed according to F,

$$\boldsymbol{a}_i = F\boldsymbol{A}_i. \tag{6}$$

Here $\boldsymbol{a}_i$ and $\boldsymbol{A}_i$ are the lattice vectors in the deformed and undeformed configurations, respectively. The strain energy density at F is given by

$$W_{\text{CB}}(F) = \frac{E_0(F)}{\Omega_0}, \tag{7}$$

where Ω_0 is the volume of the unit cell in the equilibrium state. The total energy associated with an element is simply this energy density evaluated at the deformation gradient associated with this element (F_e) and multiplied by the volume of this element (Ω_e). The total potential energy in the local region is simply the sum of the energies on each element,

$$E^{\text{local}} = \sum_{e=1}^{N_{\text{element}}} \Omega_e W_{\text{CB}}(F_e). \tag{8}$$

The total potential energy of the system for the QC method is the sum of the energy of the local and nonlocal regions,

$$E_{\text{QC}}^{\text{tot}} = E^{\text{local}} + E^{\text{nonlocal}}. \tag{9}$$

This formulation of the summation rule introduces an inconsistency across the local/nonlocal interface: The energy in the local region is computed for each element, whereas the energy in the nonlocal region is naturally computed for each rep-atom. Formally, the energy of the local region can be rewritten as a sum over all the rep-atoms:

$$E^{\text{local}} = \sum_j \omega_j E_j^{\text{el}}, \tag{10}$$

where the energy associated with each local atom is defined as

$$E_j^{\text{el}} = \frac{1}{\omega_j} \sum_e \omega_{j,e} W_{\text{CB}}(F_e). \tag{11}$$

One possible way to obtain the weights $\omega_{j,e}$ is using Voronoi diagram associated with the triangulation. ω_j is the total weight,

$$\omega_j = \sum_e \omega_{j,e}. \tag{12}$$

However, transition between these two formulations may also introduce inconsistency at the interface where this transition takes place.

B. Cluster-based summation rule

Knap and Ortiz[8] proposed an alternative way of approximating the energy by introducing a class of summation rules using clusters of atoms. The energy function is sampled on clusters (neighborhoods) of the rep-atoms. Each cluster may be regarded as a representative crystal where the state and behavior of the crystal are sampled.[8] More specifically, denote by C_j the cluster around the jth rep-atom, E_j^{cluster} is approximated by

$$E_j^{\text{cluster}} = \frac{1}{|C_j|} \sum_{k \in C_j} E_k, \tag{13}$$

where $|C_j|$ is the number of atoms in the cluster C_j, and E_k is the atomic energy of the kth atom (not necessarily a rep-atom). Then the local energy is computed as

$$E = \sum_j \omega_j E_j^{\text{cluster}}. \tag{14}$$

The clusters are chosen so that they are separated from each other.

This summation rule introduces an approximation to the energy and forces in the local region. This approximation can be improved by increasing the cluster size.

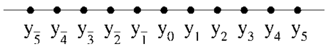

FIG. 1. 1D chain.

C. General summation rules

In general, the energy of the system can be expressed as

$$E_{\text{QC}}^{\text{tot}} = \sum_j \omega_j E_j. \tag{15}$$

In this form, the problem reduces to the computation of E_j. The element-based and cluster-based summation rule are examples of different choices of E_j, using CB rule and cluster sampling, respectively. The energy associated with each rep-atom E_j depends on the local environment of the rep-atom. Therefore, the real issue is how to reconstruct the local environment of each rep-atom. Well inside the nonlocal region, this is not a problem since, naturally, we will use the exact positions of nearby atoms, each of which is a rep-atom. But in the local region and on the interface between the two regions, one needs to reconstruct the relative atomic positions with respect to the rep-atom.

The error in QC comes from two main sources. In the local region the error comes mainly from the kinematic constraint and the CB rule used. This source of error can be understood following the work of E and Ming.[7,9] More interesting is the error introduced at the interface of the local and nonlocal region, where the "ghost forces" are. As is well-known and is shown again below, both the element-based and the cluster-based summation rule will, in general, introduce the so-called "ghost forces", i.e., the forces on the rep-atoms are not zero in the undeformed state.

III. THE ISSUE OF GHOST FORCE

Let us start with simple examples to illustrate the issue of "ghost forces". We will first show that element-based summation rule generates "ghost forces". This is a manifestation of the inconsistency between the summation rules used in the local and nonlocal regions.

Consider a one-dimensional chain shown in Fig. 1. Let atom 0 be the interface between the local and nonlocal regions, with the local region on the right and the nonlocal region on the left. For simplicity, we also assume that all atoms are rep-atoms. We will also assume that the atoms interact with each other with a pairwise potential. It is easy to see that if the interaction is limited to the nearest neighbors, CB is the same as direct summation. In this case, the element-based summation rule is exact, and there is no ghost force. However, if the interaction range contains the second nearest neighbors, according to the summation rule, we have

$$E_{\bar{3}} = \frac{1}{2}\left(V(r_{\bar{5}\bar{3}}) + V(r_{\bar{4}\bar{3}}) + V(r_{\bar{3}\bar{2}}) + V(r_{\bar{3}\bar{1}})\right),$$

$$E_{\bar{2}} = \frac{1}{2}\left(V(r_{\bar{4}\bar{2}}) + V(r_{\bar{3}\bar{2}}) + V(r_{\bar{2}\bar{1}}) + V(r_{\bar{2}0})\right),$$

$$E_{\bar{1}} = \frac{1}{2}\left(V(r_{\bar{3}\bar{1}}) + V(r_{\bar{2}\bar{1}}) + V(r_{\bar{1}0}) + V(r_{\bar{1}1})\right),$$

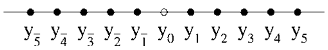

FIG. 2. 1D chain with cluster-based summation rule.

$$E_0 = \frac{1}{2}(V(r_{\bar{2}0}) + V(r_{\bar{1}0}) + V(r_{01}) + V(2r_{01})),$$

$$E_1 = \frac{1}{2}(V(2r_{01}) + V(r_{01}) + V(r_{12}) + V(2r_{12})),$$

$$E_2 = \frac{1}{2}(V(2r_{12}) + V(r_{12}) + V(r_{23}) + V(2r_{23})). \tag{16}$$

Therefore, the forces on the atoms with index $\bar{1}$, 0, and 1 are given by

$$f_{\bar{1}} = - V'(r_{\bar{3}\bar{1}}) - V'(r_{\bar{2}\bar{1}}) + V'(r_{\bar{1}0}) + \frac{1}{2}V'(r_{\bar{1}1}),$$

$$f_0 = - V'(r_{\bar{2}0}) - V'(r_{\bar{1}0}) + V'(r_{01}) + 2V'(2r_{01}),$$

$$f_1 = - \frac{1}{2}V'(r_{\bar{1}1}) - 2V'(2r_{01}) - V'(r_{01}) + V'(r_{12}) + 2V'(2r_{12}). \tag{17}$$

In the equilibrium state, we have

$$f_{\bar{1}} = - \frac{1}{2}V'(2\delta),$$

$$f_0 = V'(2\delta),$$

$$f_1 = - \frac{1}{2}V'(2\delta), \tag{18}$$

where $\delta = x_1 - x_0$ is the lattice constant.

From this example, we see that ghost force arises due to the asymmetry in calculating the energies in the local and nonlocal regions. The energy associated with the atom indexed by $\bar{1}$ depends on $\boldsymbol{y}_1$, but the energy associated with the atom indexed by 1 does not depend on $\boldsymbol{y}_{\bar{1}}$.

Similarly, cluster-based summation rule also generates "ghost force." Consider a one-dimensional chain shown in Fig. 2. Let us assume that all the atoms except atom 0 are rep-atoms with cluster size 1, i.e., the cluster for each rep-atom contains simply the rep-atom itself. Assume that the atoms interact via a pairwise potential whose interaction range is limited to the nearest neighbors. According to the cluster-based summation rule, we have

$$E_{\bar{1}} = \frac{1}{2}\left(V(r_{\bar{2}\bar{1}}) + V\left(\frac{1}{2}r_{\bar{1}1}\right)\right),$$

$$E_1 = \frac{1}{2}\left(V\left(\frac{1}{2}r_{\bar{1}1}\right) + V(r_{12})\right),$$

$$E_2 = \frac{1}{2}(V(r_{12}) + V(r_{23})),$$

$$E_3 = \frac{1}{2}(V(r_{23}) + V(r_{34})). \tag{19}$$

It is clear that $\omega_{\bar{1}} = \omega_1 = \frac{3}{2}$ and $\omega_i = 1$ for $i \neq \pm 1$. When the system is at equilibrium, the force acting on atom 1 is

$$f_1 = - \frac{1}{2}V'(\delta). \tag{20}$$

Thus, by symmetry

$$f_{\bar{1}} = \frac{1}{2}V'(\delta). \tag{21}$$

This is a "ghost force." However, it is expected that the "ghost force" decreases as cluster size increases.

At the heart of the matter, the existence of "ghost force" is a manifestation of the well-known problem of compatibility between different physical descriptions at the interface. The problem discussed here is the simplest of its kind. Next we discuss how such "ghost forces" can be eliminated and uniform accuracy can be achieved by using more sophisticated summation rules.

IV. THE QUASI-NONLOCAL METHOD

In order to overcome the difficulty with "ghost forces," Shimokawa etc.[5] introduced the notion of quasi-nonlocal atoms at the local-nonlocal interface. The concept of quasi-nonlocal atoms is very simple: In the energy computation, these atoms act as local atoms when interacting with local atoms and as nonlocal atom when interacting with nonlocal atoms. Therefore quasi-nonlocal atoms are limited to a neighborhood of the interface between the local and nonlocal regions.

Let us revisit the 1*D* chain example using the formulation of quasi-nonlocal atoms, see Fig. 1. Again we assume pairwise potential V with second nearest neighbor interaction. Now atom 0 and 1 are quasi-nonlocal atoms. All the atoms on the left are nonlocal atoms and those on the right are local atoms. The energy associated with atom 0 can be written as

$$E_0 = \frac{1}{2}(V(r_{\bar{2}0}) + V(r_{\bar{1}0}) + V(r_{01}) + V(2r_{01})), \tag{22}$$

which is the same as that of an interface atom in the QC method. However, the energy associated with atom 1 is now

$$E_1 = \frac{1}{2}(V(r_{\bar{1}1}) + V(r_{01}) + V(r_{12}) + V(2r_{12})), \tag{23}$$

which is different from that in the QC method—there the term $V(r_{\bar{1}1})$ is replaced by $V(2r_{01})$. The energies associated with the local and nonlocal atoms are calculated in the same way as in the original QC method. It is easy to show that this eliminates the "ghost forces."

In order to eliminate "ghost force" using the quasi-nonlocal approach, the size of the interaction range has to be limited. More precisely, the interaction range is limited to second, third, fourth, fourth, and third nearest neighbors for 1*D*, 2*D* triangular, 3*D* h.c.p., f.c.c., and b.c.c. lattices, respectively.[5]

V. GENERAL CONSIDERATIONS OF ACCURACY

The existence of "ghost force" is just one manifestation of the lack of accuracy at the interface between different levels of physical description. Our goal is to introduce quantitative measures to calibrate the accuracy at the such interfaces and to construct coupling methods that are uniformly accurate.

Definition 1. Consider a crystal with displacement $\boldsymbol{u}_i=\boldsymbol{u}(\boldsymbol{x}_i)$ where $\boldsymbol{u}$ is a smooth function, i.e., $\boldsymbol{y}_i=\boldsymbol{x}_i+\boldsymbol{u}_i$. Let $\boldsymbol{u}^h$ be the piecewise linear interpolation of $\boldsymbol{u}$ over the finite element triangulation used in QC, and $\boldsymbol{y}_i^h=\boldsymbol{x}_i+\boldsymbol{u}_i^h$. Let $\boldsymbol{f}_\alpha(\boldsymbol{y})$ be the force on rep-atom α computed from the full atomistic model, and let $\boldsymbol{f}_\alpha^{\mathrm{QC}}(\boldsymbol{y}^h)$ be the force on rep-atom α computed using QC. We say that the local truncation error of QC is uniformly first order, if

$$\left\| \boldsymbol{f}_\alpha(\boldsymbol{y}) - \frac{\boldsymbol{f}_\alpha^{\mathrm{QC}}(\boldsymbol{y}^h)}{\omega_\alpha} \right\| \leq C\delta, \tag{24}$$

where δ is the largest diameter of the elements and $\|\cdot\|=\max_\alpha\{\cdot\}$ is the L^∞ norm (maximum norm) of discrete functions defined on the finite element mesh.

Remark. We can similarly define "locally uniform first order accuracy" by restricting the L^∞ norm to a subset of the whole mesh. In particular, we will be interested in locally uniform first order accuracy at local/nonlocal interface.

The next lemma plays the role of the well-known Bramble-Hilbert lemma in approximation theory.

Lemma 2. *The condition (24) is equivalent to requiring that for uniformly deformed state,* $\boldsymbol{f}_\alpha^{\mathrm{QC}}=0$.

Proof. Necessity is obvious. For sufficiency, consider a fixed α. Let $\boldsymbol{u}^{h,\alpha}$ be the uniform deformation determined by atom α:

$$\boldsymbol{u}^{h,\alpha}(\boldsymbol{x}) = \boldsymbol{u}^h(\boldsymbol{x}_\alpha) + \nabla \boldsymbol{u}^h(\boldsymbol{x}_\alpha)\cdot(\boldsymbol{x}-\boldsymbol{x}_\alpha) \tag{25}$$

and

$$\boldsymbol{y}_i^{h,\alpha} = \boldsymbol{x}_i + \boldsymbol{u}_i^{h,\alpha}. \tag{26}$$

As discussed in Ref. 7, we have

$$|\boldsymbol{f}_\alpha(\boldsymbol{y}) - \boldsymbol{f}_\alpha(\boldsymbol{y}^{h,\alpha})| \leq C\delta, \tag{27}$$

since $|\boldsymbol{y}-\boldsymbol{y}^{h,\alpha}|$ is locally second-order and the interaction has finite range. By a similar argument, we also have

$$\frac{1}{\omega_\alpha}|\boldsymbol{f}_\alpha^{\mathrm{QC}}(\boldsymbol{y}^h) - \boldsymbol{f}_\alpha^{\mathrm{QC}}(\boldsymbol{y}^{h,\alpha})| \leq C\delta. \tag{28}$$

From the assumption, we know that $\boldsymbol{f}_\alpha^{\mathrm{QC}}(\boldsymbol{y}^{h,\alpha})=0$, since by its definition, $\boldsymbol{y}^{h,\alpha}$ is a uniformly deformed state. Also, we have $\boldsymbol{f}_\alpha(\boldsymbol{y}^{h,\alpha})=0$ due to the symmetry of the potential. Therefore, (24) follows from (27) and (28). □

As we have seen earlier, computing the energy for the system is equivalent to computing E_i for each rep-atom. For this purpose, it suffices to reconstruct the local environment of each rep-atom. We can then compute the associated energy using the atomic potential. The summation rules we have discussed in this paper all correspond to specific reconstruction schemes for the environment of the rep-atoms.

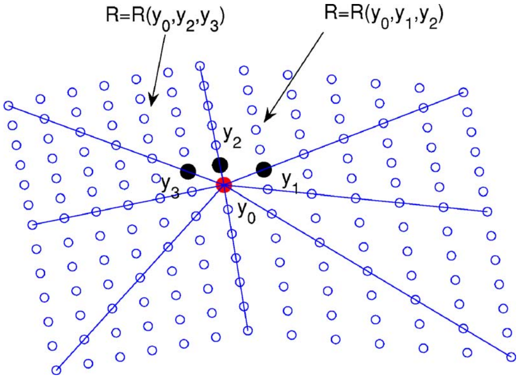

FIG. 3. (Color online) Modified reconstruction scheme based on the CB rule.

We denote by $\boldsymbol{R}_j(k)$ the reconstruction of the relative position of the atom k with respect to the atom j. Well inside the nonlocal region, reconstruction is not a problem: We may simply use the exact position of nearby rep-atoms. We denote the reconstruction scheme using the exact position as $\boldsymbol{R}_j^a(k)=\boldsymbol{y}_k-\boldsymbol{y}_j$. Inside the local region and at the local-nonlocal interface, one needs to reconstruct the relative atomic positions with respect to the rep-atom.

The reconstruction scheme that corresponds to the element-based summation rule is as follows. To compute E_j, for each element e whose vertices contain j, we use the local deformation gradient F_e to reconstruct the positions of nearby atoms, by assuming that the system is locally under uniform deformation. We denote the relative position of atom k with respect to j by $\boldsymbol{R}_{j,e}^{\mathrm{CB}}(k)$, since it depends on the rep-atom j as well as the element e considered.

For our purpose, it is helpful to consider the following reconstruction scheme associated with a rep-atom, which is obtained by combining the reconstruction schemes from the surrounding elements. This is done as follows. The whole space is divided into sectors by extending the surrounding elements of the rep-atom radially. If the atom k is located in the sectorial extension of element e, we define the reconstruction of the position of atom k by $\boldsymbol{R}_{j,e}^{\mathrm{CB}}(k)$, see Fig. 3. In this way, we define a modified reconstruction operator, $\boldsymbol{R}_j^{\mathrm{CB}}$, which only depends on atom j but not on the element.

This reconstruction scheme also corresponds to a summation rule: Once the local environment of the rep-atom is constructed, one can compute the energy associated with that rep-atom by direct summation. We call this summation rule the atom-based summation rule.

The quasi-nonlocal approach also corresponds to a modification of the reconstruction scheme corresponding to the original QC method: For a quasi-nonlocal atom i, we define

$$\boldsymbol{R}_i^{\mathrm{QN}}(j) = \begin{cases} \boldsymbol{R}_i^a(j), & \text{if } j \text{ is nonlocal atom,} \\ \boldsymbol{R}_i^{\mathrm{CB}}(j), & \text{otherwise.} \end{cases} \tag{29}$$

The reconstruction operators for other atoms are kept unchanged.

To better understand the reconstruction scheme, let us revisit the 1D chain example, Fig. 1. We will focus on the reconstruction operator $\boldsymbol{R}_0$ and $\boldsymbol{R}_1$, since atom 0 and 1 are quasi-nonlocal atoms. When atom 1 is considered,

$$\boldsymbol{R}_1^{\mathrm{QN}}(\bar{1}) = \boldsymbol{R}_1^{a}(\bar{1}) = \boldsymbol{y}_{\bar{1}} - \boldsymbol{y}_1, \tag{30}$$

since atom 1 is a quasi-nonlocal atom and atom $\bar{1}$ is nonlocal. However, in the original QC method,

$$\boldsymbol{R}_1^{\mathrm{CB}}(\bar{1}) = 2(\boldsymbol{y}_0 - \boldsymbol{y}_1). \tag{31}$$

Therefore, the term $V(2r_{01})$ appears in the energy formulation. As we have shown, the reconstruction scheme for quasi-nonlocal approach eliminates the "ghost forces."

The origin of the "ghost force" and inconsistency comes from two sources. One is the difference in the reconstruction schemes: Inside the local region, the reconstruction operator only depends on the nearest neighbor rep-atoms. The other is the difference between the atom-based and the element-based summation rules. To better understand the nature of each of these two inconsistencies, we will introduce two interfaces on which the two transitions take place separately: The transition between the atomistic and CB-based reconstruction takes place on the local/nonlocal interface, and there is an additional interface inside the local region on which the transition between the atom-based and the element-based summation rules takes place.

VI. ACCURACY AT THE LOCAL/NONLOCAL INTERFACE

We first discuss accuracy at the local/nonlocal interface. Without loss of generality, we will assume that each atom is a rep-atom.

A. Geometrically consistent reconstruction schemes

We now discuss the general condition on the reconstruction scheme which guarantees uniform accuracy in the local/nonlocal interface region. From Lemma 2, we see that this condition has to be invariant under uniform deformation, namely if the condition holds for a reconstruction scheme at the equilibrium state, it continues to hold at any uniformly deformed state. Observe that under uniform deformation, even though some symmetries of the crystal are broken, the translational and point inversion symmetry are preserved. Therefore, we will divide all the atom pairs $\langle i,j\rangle$ into different groups accordingly: The vectors connecting the pairs within each group will have the same distance R_n and are parallel to the same direction τ_m in equilibrium. Notice that the pairs $\langle i,j\rangle$ and $\langle j,i\rangle$ are generally different. It is clear that this grouping is invariant under uniform displacement.

Definition 3. The reconstruction scheme is geometrically consistent if for all k, n, and m,

$$\sum_{\substack{|\boldsymbol{r}_i(j)|=R_n \\ \boldsymbol{r}_i(j)\parallel\tau_m}} \mathrm{sgn}(\boldsymbol{r}_i(j)\cdot\tau_m)\frac{\partial \boldsymbol{R}_i(j)}{\partial \boldsymbol{y}_k} = 0, \tag{32}$$

where $\boldsymbol{r}_i(j)=\boldsymbol{x}_j-\boldsymbol{x}_i$ denotes the relative position of atom j with respect to atom i in the equilibrium state.

This condition depends only on the geometry of the crystal. We will consider the class of potentials that satisfy the following conditions:

(1) the potentials are invariant under translation: For every constant vector $\boldsymbol{r}$,

$$E_i(\boldsymbol{y}) = E_i(\boldsymbol{y}+\boldsymbol{r}), \tag{33}$$

where $\boldsymbol{y}+\boldsymbol{r}=\{\boldsymbol{y}_1+\boldsymbol{r},\boldsymbol{y}_2+\boldsymbol{r},\cdots,\boldsymbol{y}_N+\boldsymbol{r}\}$.

(2) the potentials are invariant under point inversion with respect to the equilibrium lattice points:

$$E_i(\boldsymbol{y}) = E_i(I_j(\boldsymbol{y})), \tag{34}$$

where I_j defined by $I_j(\boldsymbol{y})=\{2\boldsymbol{y}_j-\boldsymbol{y}_1,2\boldsymbol{y}_j-\boldsymbol{y}_2,\cdots,2\boldsymbol{y}_j-\boldsymbol{y}_N\}$ is the inversion operator with respect to atom j.

These conditions are satisfied by all the well-known potentials such as the Lennard-Jones potential, Morse potential, EAM potentials,[10,11] Tersoff potential,[12] Stillinger-Weber potential,[13] etc.

Next, we show that if the reconstruction scheme satisfies this condition, then the resulting QC method is locally uniform first order accurate at the local/nonlocal interface.

Proposition 4. *If the reconstruction scheme is geometrically consistent, the resulting QC is locally uniform first order accurate at the local/nonlocal interface.*

Proof. Using Lemma 2, we only have to show that in uniformly deformed states, the forces acting on the atoms all vanish. We consider the force acting on atom k,

$$\begin{aligned} f_k &= \frac{\partial E^{\mathrm{tot}}}{\partial \boldsymbol{y}_k} = \sum_i \frac{\partial E_i}{\partial \boldsymbol{y}_k} = \sum_{i,j}\frac{\partial E_i}{\partial \boldsymbol{y}_j}\frac{\partial \boldsymbol{R}_i(j)}{\partial \boldsymbol{y}_k} \\ &= \sum_{n,m}\sum_{\substack{|\boldsymbol{r}_i(j)|=R_n \\ \boldsymbol{r}_i(j)\parallel\tau_m}} \left[\mathrm{sgn}(\boldsymbol{r}_i(j)\cdot\tau_m)\frac{\partial E_i}{\partial \boldsymbol{y}_j}\right]\cdot\left[\mathrm{sgn}(\boldsymbol{r}_i(j)\cdot\tau_m)\frac{\partial \boldsymbol{R}_i(j)}{\partial \boldsymbol{y}_k}\right]. \end{aligned} \tag{35}$$

According to the symmetry of the interacting potentials (33) and (34) for fixed n,m,

$$B_{n,m} = \mathrm{sgn}(\boldsymbol{r}_i(j)\cdot\tau_m)\frac{\partial E_i}{\partial \boldsymbol{y}_j}$$

is independent of i and j in the uniformly deformed states. We have

$$f_k = \sum_{n,m} B_{n,m}\sum_{\substack{|\boldsymbol{r}_i(j)|=R_n \\ \boldsymbol{r}_i(j)\parallel\tau_m}} \mathrm{sgn}(\boldsymbol{r}_i(j)\cdot\tau_m)\frac{\partial \boldsymbol{R}_i(j)}{\partial \boldsymbol{y}_k} = 0. \tag{36}$$

The last equality follows from (32).

Next we show that geometric consistency is also a necessary condition for local uniform first order accuracy at the local/nonlocal interface.

Proposition 5. *If for any potential satisfies (33) and (34), the local truncation error is of uniform first order at the local/nonlocal interface, then the reconstruction scheme must be geometrically consistent.*

Proof. Suppose that the condition (32) is not satisfied. Then there exist k, n', and m', such that

$$\sum_{\substack{|\boldsymbol{r}_i(j)|=R_{n'}\\ \boldsymbol{r}_i(j)\parallel\tau_{m'}}} \operatorname{sgn}(\boldsymbol{r}_i(j)\cdot\tau_{m'})\frac{\partial \boldsymbol{R}_i(j)}{\partial \boldsymbol{y}_k} \neq 0. \tag{37}$$

According to the same logic as in the proof of Proposition 4,

$$\boldsymbol{f}_k = \sum_{n,m} B_{n,m} \sum_{\substack{|\boldsymbol{r}_i(j)|=R_{n}\\ \boldsymbol{r}_i(j)\parallel\tau_{m}}} \operatorname{sgn}(\boldsymbol{r}_i(j)\cdot\tau_{m})\frac{\partial \boldsymbol{R}_i(j)}{\partial \boldsymbol{y}_k}, \tag{38}$$

where $B_{n,m}=\operatorname{sgn}(\boldsymbol{r}_i(j)\cdot\tau_m)\frac{\partial E_i}{\partial \boldsymbol{y}_j}$. By choosing a pairwise potential,

$$V_{ij} = \begin{cases} |\boldsymbol{y}_j - \boldsymbol{y}_i|, & |\boldsymbol{r}_i(j)| = R_{n'}, \boldsymbol{r}_i(j) \parallel \tau_{m'}, \\ 0, & \text{otherwise}, \end{cases} \tag{39}$$

which certainly satisfies the condition (33) and (34), we have

$$B_{n,m} = \begin{cases} \operatorname{sgn}(\boldsymbol{r}_i(j)\cdot\tau_m)\dfrac{\boldsymbol{y}_j - \boldsymbol{y}_i}{|\boldsymbol{y}_j - \boldsymbol{y}_i|}, & n=n', m=m', \\ 0, & \text{otherwise}, \end{cases} \tag{40}$$

which is indepent of i and j in the uniformly deformed state. Therefore,

$$\boldsymbol{f}_k = B_{n',m'} \sum_{\substack{|\boldsymbol{r}_i(j)|=R_{n'}\\ \boldsymbol{r}_i(j)\parallel\tau_{m'}}} \operatorname{sgn}(\boldsymbol{r}_i(j)\cdot\tau_{m'})\frac{\partial \boldsymbol{R}_i(j)}{\partial \boldsymbol{y}_k} \neq 0. \tag{41}$$

□

B. Analysis of the quasi-nonlocal method

The quasi-nonlocal approach is a special case of the general consideration. To understand the connection, let us introduce the following definition.

Definition 6. The reconstruction scheme satisfies the reciprocity condition if

$$\frac{\partial \boldsymbol{R}_i(j)}{\partial \boldsymbol{y}_k} = \frac{\partial \boldsymbol{R}_j(i)}{\partial \boldsymbol{y}_k}, \quad \forall\, k \neq i,j. \tag{42}$$

In the example of the $1D$ chain, according to the notion of quasi-nonlocal atom, we have $\boldsymbol{R}_1(\bar{1})=\boldsymbol{y}_{\bar{1}}-\boldsymbol{y}_1$ and $\boldsymbol{R}_{\bar{1}}(1)=\boldsymbol{y}_1-\boldsymbol{y}_{\bar{1}}$, therefore,

$$\frac{\partial \boldsymbol{R}_1(\bar{1})}{\partial \boldsymbol{y}_0} = 0 = \frac{\partial \boldsymbol{R}_{\bar{1}}(1)}{\partial \boldsymbol{y}_0}. \tag{43}$$

However, in the original QC method, since $\boldsymbol{R}_1(\bar{1})=2\boldsymbol{y}_0-2\boldsymbol{y}_1$, the reciprocity condition is violated.

From the definition, it is obvious that if the reconstruction scheme satisfies the reciprocity condition, it is geometrically consistent. The difference is that in the reciprocity condition, each group contains only two pairs of atoms, namely the pairs $\langle i,j\rangle$ and $\langle j,i\rangle$.

Proposition 7. *If the reciprocity condition holds, the resulting QC is locally uniform first order accurate at the local/nonlocal interface.*

Proof. This is a corollary of Proposition 4. □

The quasi-nonlocal reconstruction scheme uses the positions of the nearest neighbor atoms to reconstruct the relative position of other atoms. Therefore, the method is limited to case that along each line, the interaction only involves the second nearest neighbors. If the interaction range is larger, for example if it involves the third nearest neighbors along a line, the reciprocity condition is violated. In Fig. 1, the reconstruction of atom 3 starting from atom 0 will use the position of atom 1. However, the reconstruction of atom 0 from atom 3 does not involve atom 1, since it is not the nearest neighbor of atom 3. Consequently, for the reciprocity condition to hold, the interaction range is limited to second, third, fourth, fourth, and third nearest neighbors for $1D$, $2D$ triangular, $3D$ h.c.p., f.c.c., and b.c.c. lattices, respectively.

C. Examples of geometrically consistent reconstruction scheme

To find reconstruction schemes that are geometrically consistent, instead of using either $\boldsymbol{R}_i^a(j)$ or $\boldsymbol{R}_i^{\mathrm{CB}}(j)$, we allow linear combinations of $\boldsymbol{R}_i^a(j)$ and $\boldsymbol{R}_i^{\mathrm{CB}}(j)$,

$$\boldsymbol{R}_i(j) = C_i(j)\boldsymbol{R}_i^a(j) + (1 - C_i(j))\boldsymbol{R}_i^{\mathrm{CB}}(j), \tag{44}$$

where the $C_i(j)$'s are the coefficients to be determined. The original QC and the quasi-nonlocal approach corresponds to the case when $C_i(j)$ equals to either 0 or 1. We further require that away from the interface, in the local region, $C_i(j)=0$ in accordance with the CB rule and in the nonlocal region, $C_i(j)=1$ in accordance with the atomistic reconstruction. Using these boundary conditions, we can solve the linear equation system (32) to determine the coefficients $C_i(j)$. We now consider some examples.

First we go back to the example of the $1D$ chain, see Fig. 1. We will limit ourselves to interactions that involve upto the fifth nearest neighbors. We do not need to specify τ_m here since there is only one direction. For the nth nearest neighbors of atom i, we let

$$\boldsymbol{R}_i(i \pm n) = C_i(i \pm n)\boldsymbol{R}_i^a(i \pm n) + (1 - C_i(i \pm n))\boldsymbol{R}_i^{\mathrm{CB}}(i \pm n). \tag{45}$$

For boundary conditions, we let $C_i(j)=1$ for $i<-5$ and $C_i(j)=0$ for $i>5$. This leaves a sufficiently wide transition region for interactions that involve upto the fifth nearest neighbors.

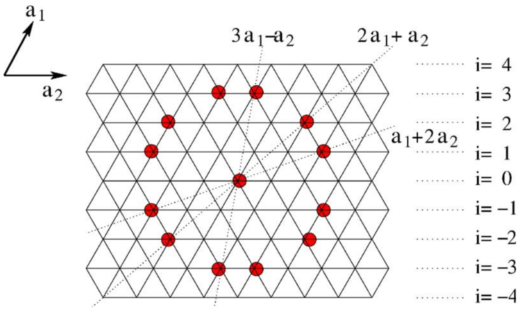

FIG. 4. (Color online) 2D triangular lattice, $\boldsymbol{a}_1=(1/2,\sqrt{3}/2)$ and $\boldsymbol{a}_2=(1,0)$.

TABLE I. Coefficients for 1D chain.

R_n	C_{-5}^-	C_{-5}^+	C_{-4}^-	C_{-4}^+	C_{-3}^-	C_{-3}^+	C_{-2}^-	C_{-2}^+	C_{-1}^-	C_{-1}^+	C_0^-	C_0^+	C_1^-	C_1^+	C_2^-	C_2^+	C_3^-	C_3^+	C_4^-	C_4^+	C_5^-	C_5^+
First	1	1	1	1	1	1	1	1	1	1	1	0	1	0	0	0	0	0	0	0	0	0
Second	1	1	1	1	1	1	1	1	1	1	1	0	1	0	0	0	0	0	0	0	0	0
Third	1	1	1	1	1	1	1	1	1	2/3	1	0	1	0	1/3	0	0	0	0	0	0	0
Fourth	1	1	1	1	1	1	1	5/6	1	1/2	1	0	1	0	1/2	0	1/6	0	0	0	0	0
Fifth	1	1	1	1	1	9/10	1	7/10	1	2/5	1	0	0	0	3/5	0	3/10	0	1/10	0	0	0

There is more than one solution of (32). Table I shows one set of possible solution with high symmetry. For simplicity, we have replaced the notations $C_i(i-n)$ and $C_i(i+n)$ by C_i^- and C_i^+, respectively. Note that the coefficients for $n=1,2$ is nothing but the corresponding values used in the quasi-nonlocal approach.

As a second example, we look at the $2D$ triangular lattice, see Fig. 4. In this example, we assume that the interface is along the $\boldsymbol{a}_2$ direction and is labeled $i=0$. The bottom half uses the atomistic model and top half uses the continuum model. By translational symmetry, the set of coefficients are invariant along the interface. Now there are different directions for the same bond length. We plotted three directions of bonds connecting the fourth nearest neighbors, and the other three can be obtained by reflection with respect to $\boldsymbol{a}_1+\frac{1}{2}\boldsymbol{a}_2$.

Table II shows the coefficients along each direction for different interaction ranges. Again, we select only one solution for each case here. As expected, up to the third nearest neighbor, the coefficients are the same as the corresponding values in the quasi-nonlocal formulation.

In Table III we give the coefficients for the face-centered cubic (f.c.c.) lattice structure. One of the {111} planes is taken to be the interface, see Fig. 5. Every atom on the same (111) plane has the same set of coefficients.

Let us look at the fifth nearest neighbors of the atom i. They stay on five layers of (111) planes which are labeled by *ABCAB* from top to bottom, consistent with the fact that f.c.c. lattices have *ABC* packing. There are only two different types of directions in the current case. All the other possible directions can be reached by rotation with respect to the [111] direction and shift according to a vector within the (111) plane. Along each direction, the atoms that interact with atom i are labeled by counting the number of layers separating them.

Again one can see that the coefficients we choose in Table III up to the fourth nearest neighbor are the same as the corresponding values in the quasi-nonlocal approach.

VII. TRANSITION BETWEEN ATOM-BASED AND ELEMENT-BASED SUMMATION

In the analysis presented above, we have assumed for simplicity that every atom in the system is a rep-atom. In practice, this is, of course, not the case. In order to reduce the computational cost, the element size should become larger where the deformation is smoother. The summation rule used in the last section essentially uses the local environment of rep-atoms (which are vertex atoms) to determine the energy. However, for large element, the environment of the vertex atoms is not representative and the summation rules discussed will introduce large errors. Instead bulk atom (the atom inside the element) dominates and we should use

TABLE II. Coefficients for 2D triangular lattice.

R_n	τ	C_{-4}^-	C_{-4}^+	C_{-3}^-	C_{-3}^+	C_{-2}^-	C_{-2}^+	C_{-1}^-	C_{-1}^+	C_0^-	C_0^+	C_1^-	C_1^+	C_2^-	C_2^+	C_3^-	C_3^+	C_4^-	C_4^+
First	(0,1)	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0
First	(1,0)	1	1	1	1	1	1	1	1	1	0	1	0	0	0	0	0	0	0
Second	(1,1)	1	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0
Second	(2,−1)	1	1	1	1	1	1	1	1	1	0	1	0	0	0	0	0	0	0
Third	(0,2)	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0
Third	(2,0)	1	1	1	1	1	1	1	1	1	0	1	0	0	0	0	0	0	0
Fourth	(1,2)	1	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0
Fourth	(2,1)	1	1	1	1	1	1	1	1	1	0	1	0	0	0	0	0	0	0
Fourth	(3,−1)	1	1	1	1	1	1	1	2/3	1	0	1	0	1/3	0	0	0	0	0
Fifth	(0,3)	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0
Fifth	(3,0)	1	1	1	1	1	1	1	1	1	0	1	0	1	0	0	0	0	0
Sixth	(2,2)	1	1	1	1	1	1	1	1	1	0	1	0	0	0	0	0	0	0
Sixth	(4,−2)	1	1	1	1	1	5/6	1	1/2	1	0	1	0	1/2	0	1/6	0	0	0
Seventh	(1,3)	1	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0
Seventh	(3,1)	1	1	1	1	1	1	1	2/3	1	0	1	0	1/3	0	0	0	0	0
Seventh	(4,−1)	1	1	1	1	1	5/6	1	1/2	1	0	1	0	1/2	0	1/6	0	0	0

TABLE III. Coefficients for 3D f.c.c. lattice.

R_n	No. of layer	C_{-2}^-	C_{-2}^+	C_{-1}^-	C_{-1}^+	C_0^-	C_0^+	C_1^-	C_1^+	C_2^-	C_2^+
First	0	1	1	1	1	0	0	0	0	0	0
First	1	1	1	1	1	1	0	1	0	0	0
Second	1	1	1	1	1	1	0	1	0	0	0
Third	0	1	1	1	1	1	0	0	0	0	0
Third	1	1	1	1	1	1	0	1	0	0	0
Third	2	1	1	1	1	1	0	1	0	0	0
Fourth	0	1	1	1	1	1	0	0	0	0	0
Fourth	2	1	1	1	1	1	0	1	0	0	0
Fifth	1	1	1	1	1	1	0	1	0	0	0
Fifth	2	1	1	1	1	1	0	1	0	0	0

element-based summation rule. Therefore, we need to consider a second problem, which is the transition between atom-based summation rule, which is more appropriate for atoms near the local-nonlocal transition region, to element-based summation rule, which is more appropriate well inside the local region

Let us first examine the effect of changing one rep-atom from atom-based summation to element-based summation. Since the transition occurs in the local region, we can assume without loss of generality that the interaction is limitted to the nearest neighbor (in fact, the positions of the other neighboring atoms depend on the the nearest neighbors since the CB reconstruction is adopted). We illustrate the issue by considering a $2D$ triangular lattice and the case that every atom is a rep-atom. As shown in Fig. 6, the energy associated with atom 0 is changed from atom-based summation to element-based summation. For the atom-based summation, the energy of atom 0 is

$$E_0 = V(\boldsymbol{y}_0;\boldsymbol{y}_1,\boldsymbol{y}_2,\boldsymbol{y}_3,\boldsymbol{y}_4,\boldsymbol{y}_5,\boldsymbol{y}_6), \tag{46}$$

where V is the potential. For the element-based summation, the energy is computed element-wise, and can be written as

$$E_0^{\mathrm{el}} = \frac{1}{6}\sum_k E_{0,e_k}, \tag{47}$$

where E_{0,e_k} is the energy associated with the element e_k. To compute that energy, we use the three vertices of that element to determine the positions of all the atoms. It is easy to check that

$$\frac{\partial E_0^{\mathrm{el}}}{\partial \boldsymbol{y}_0} = \frac{\partial E_0}{\partial \boldsymbol{y}_0} = 0. \tag{48}$$

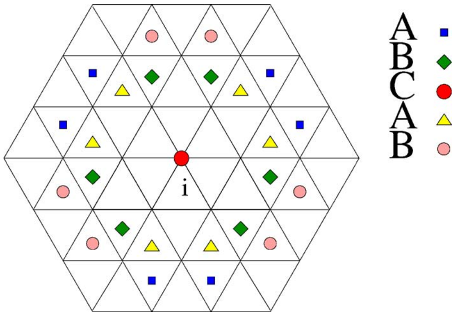

FIG. 5. (Color online) f.c.c. lattice.

To compute the force acting on atom 1, we observe that only E_{0,e_1} and E_{0,e_6} depend on the position y_1,

$$E_{0,e_1} = V(\boldsymbol{y}_0;\boldsymbol{y}_1,\boldsymbol{y}_2,\boldsymbol{y}_0-\boldsymbol{y}_1+\boldsymbol{y}_2,2\boldsymbol{y}_0-\boldsymbol{y}_1,2\boldsymbol{y}_0-\boldsymbol{y}_2,\boldsymbol{y}_0+\boldsymbol{y}_1-\boldsymbol{y}_2);$$

$$E_{0,e_6} = V(\boldsymbol{y}_0;\boldsymbol{y}_1,\boldsymbol{y}_0+\boldsymbol{y}_1-\boldsymbol{y}_6,2\boldsymbol{y}_0-\boldsymbol{y}_6,2\boldsymbol{y}_0-\boldsymbol{y}_1,\boldsymbol{y}_0-\boldsymbol{y}_1+\boldsymbol{y}_6,\boldsymbol{y}_6).$$

Therefore,

$$\frac{\partial E_0^{\mathrm{el}}}{\partial \boldsymbol{y}_1} = \frac{2}{3}V_6' + \frac{1}{3}V_3' + \frac{1}{3}V_5' \neq V_6' = \frac{\partial E_0}{\partial \boldsymbol{y}_1}, \tag{49}$$

where

$$V_i' = \frac{\partial E_0}{\partial \boldsymbol{y}_i}. \tag{50}$$

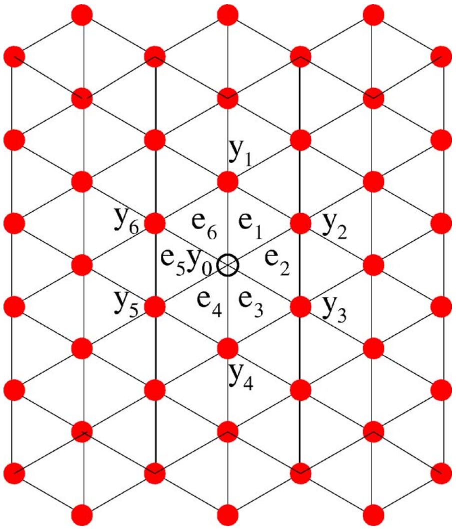

FIG. 6. (Color online) All atoms except atom 0 (the circle one) use atom-based summation, while atom 0 uses element-based summation.

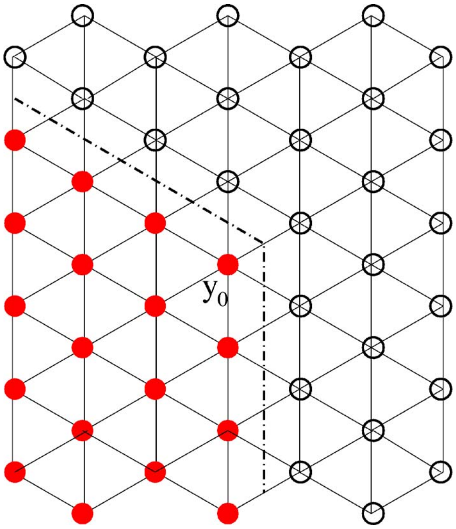

FIG. 7. (Color online) Solid atoms use atom-based summation, while circle atoms use element-based summation.

By symmetry, if the energy of atom 0 changes from atom-based summation to element-based summation, the nearest neighbors of atom 0 will be subject to a nonzero force, even if the system is at equilibrium. Here, we demonstrate that the inconsistency between atom-based summation and element-based summation introduces another source of error in the computation of the force, i.e., a source of "ghost force." This will pose a restriction on the geometry of the interface of transition from atom-based summation to element-based summation. If the interface has a corner, for example as shown in Fig. 7. According to the above calculation, it is obvious that the force acting on atom 0 is not zero, since the third nearest neighbors of atom 0 adopt element-based summation.

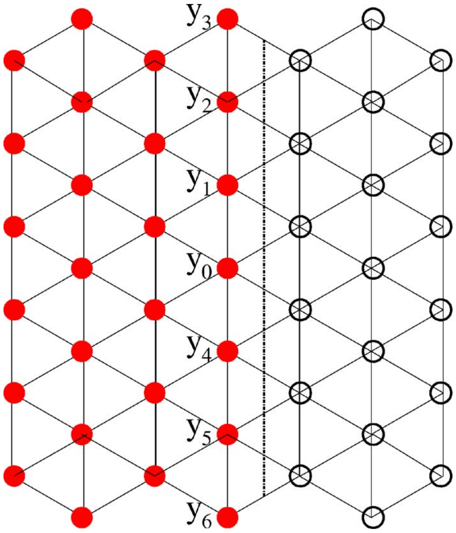

FIG. 8. (Color online) Flat interface. Solid atoms use atom-based summation, while circle atoms use element-based summation.

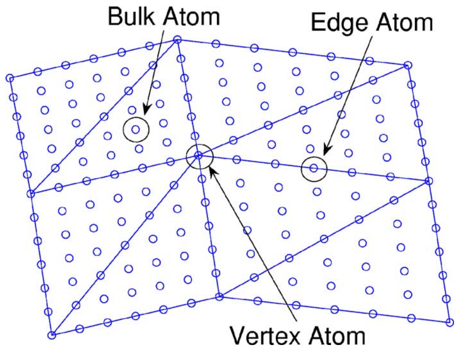

FIG. 9. (Color online) Illustration of different atoms.

One possible solution to this problem is to use special planes for this interface, as shown in Fig. 8. One can show that in this case, the force on each atom is zero if the system is under uniform deformation.

VIII. ACCURACY OF ELEMENT-BASED SUMMATION RULE IN THE LOCAL REGION

In this section we discuss the accuracy of the element-based summation rule inside the local region.

A. Piece-wise linear approximation of the displacement field

Under the assumption that the displacement field is piece-wise linear, the CB rule makes an additional error by treating every atom inside the element as having the same local environment as the bulk atoms. As illustrated in Fig. 9, atoms in an element can be divided into bulk atoms, edge atoms, and vertex atoms in $2D$. For the $3D$ case, we have bulk atoms, surface atoms, edge atoms, and vertex atoms according to their relative position within one element. Without loss of generality, we will consider the $2D$ case where only bulk, edge, and vertex atoms appear.

First we examine the error of the energy calculation for an edge atom. To estimate the magnitude of this error, let us first consider a simplified problem shown in Fig. 10. The crystal is homogeneously deformed with different deformation gradients F_1 and F_2 on both sides of the interface. Denote by τ the tangent direction of the interface. Then we have

$$F_1\tau = F_2\tau. \tag{51}$$

Now we calculate the energy of a strip with width L_{strip}. Formally, the difference between the energy with full atomistic calculation and that with the CB rule is

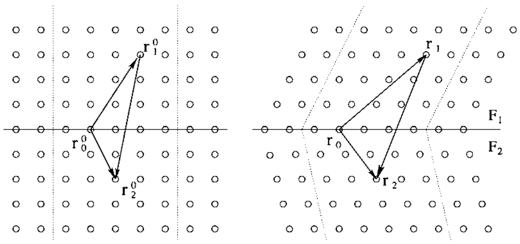

FIG. 10. Edge atoms.

$$\Delta E^{\text{strip}} = E^{\text{strip}} - E_1^{\text{tot,CB}} - E_2^{\text{tot,CB}}, \tag{52}$$

where E^{strip} is full atomistic energy of the strip, the last two terms are the energy computed using CB rule for the two regions, respectively. Although all three terms in the above expression are infinite, the energy difference ΔE^{strip} is finite, and only depends on atoms whose distance at the deformed state to the interface are smaller than the cut-off distance R_c of the empirical potential. For any atom i, say in the top half of the crystal, the distance between i and a neighbor j in the other half crystal is

$$\boldsymbol{R}_i^a(j) = F_1\boldsymbol{r}_0(i) - F_2\boldsymbol{r}_0(j) = F_1\boldsymbol{r}_i(j) + (F_2 - F_1)\boldsymbol{r}_0(j), \tag{53}$$

where $\boldsymbol{y}_0$ is some arbitrary point on the interface. However, CB rule calculates this distance using the deformation gradient F_1,

$$\boldsymbol{R}_{i,1}^{\text{CB}}(j) = F_1\boldsymbol{r}_i(j). \tag{54}$$

For any fixed j, we can select $\boldsymbol{y}^0$ such that $|\boldsymbol{r}_0(j)|$ has the minimum value, which is always smaller than the cut-off distance R_c. As a consequence, we get

$$|\boldsymbol{R}_i^a(j) - \boldsymbol{R}_{i,1}^{\text{CB}}(j)| \leqslant C_0\|F_2 - F_1\|. \tag{55}$$

Thus the error in calculating the energy of atom i can be estimated as

$$\begin{aligned}|\Delta E_i^{\text{strip}}| &= |E_i(\{\boldsymbol{R}_i^a(j)\}) - E_i(\{\boldsymbol{R}_{i,1}^{\text{CB}}(j)\})| \\ &\leqslant C_0 \max\left|\frac{\partial E_i}{\partial \boldsymbol{y}_j}(\{F_1\boldsymbol{r}_i(j)\})\right| \cdot \|F_2 - F_1\|.\end{aligned} \tag{56}$$

Notice here that the coefficient in front of $\|F_2 - F_1\|$ depends on the deformed state instead of the reference state.

Now we have

$$|\Delta E^{\text{edge}}| \leqslant C(F_1, F_2)\|F_2 - F_1\|N_{\text{edge}}, \tag{57}$$

where

$$C(F_1, F_2) \tag{58}$$

$$= C_0 \max\left\{\left|\frac{\partial E_i}{\partial \boldsymbol{y}_j}(\{F_1\boldsymbol{r}_i(j)\})\right|, \quad \left|\frac{\partial E_i}{\partial \boldsymbol{y}_j}(\{F_2\boldsymbol{r}_i(j)\})\right|\right\} \tag{59}$$

depends on the deformed state instead of the reference state and N_{edge} is the number of atoms near the interface.

In the same spirit of the CB rule, we can define the density of energy error due to the edge

$$W_{\text{CB}}^{\text{edge}} = \frac{\Delta E^{\text{strip}}}{L_{\text{strip}}}. \tag{60}$$

Thus, the energy correction along the bulk part of edges can be estimated as

$$\Delta E^{\text{edge}} = L_{\text{edge}} W_{\text{CB}}^{\text{edge}}, \tag{61}$$

where L_{edge} is the length of the edge.

A similar estimate can be derived for the vertex atoms,

$$|\Delta E^{\text{vertex}}| \leqslant C(F_1, \ldots, F_N) \sum_{\substack{i,j=1 \\ i \neq j}}^{N_{\text{vertex}}} \|F_i - F_j\|. \tag{62}$$

Again the coefficient $C(F_1, \ldots, F_N)$ depends on the deformed state.

This procedure of estimating the error due to edge and vertex atoms also suggests a way to calculate the "exact" atomistic energy of an element

$$E^{\text{tot},h} = E^{\text{bulk}}N^{\text{bulk}} + \sum_{\text{edge}} \Delta E^{\text{edge}} + \sum_{\text{vertex}} \Delta E^{\text{vertex}}. \tag{63}$$

Since the number of edges and vertices are proportional to the number of rep-atoms in the system, the complexity of this exact summation rule still proportional to the number of rep-atoms N_{rep}.

B. Higher order approximation of the displacement field

QC uses piecewise linear functions to approximate the displacement field $\boldsymbol{u}$, the error of this approximation is second order in displacement and first order in deformation gradient,

$$\|\boldsymbol{u}^h - \boldsymbol{u}\| \leqslant C\delta^2, \tag{64}$$

where δ is the largest diameter of the elements, C is a constant that depends only on $\boldsymbol{u}$. The approximation of the energy is second order,[7]

$$|E^{\text{tot},h} - E^{\text{tot}}| \leqslant C\delta^2, \tag{65}$$

and the accuracy of the forces is the first order,

$$\|\boldsymbol{f}^h - \boldsymbol{f}\| \leqslant C\delta. \tag{66}$$

Other than using piecewise linear function to approximate the displacement field, we can also use higher order piecewise polynomials. In this case, the simple summation rule used in local QC with the help of the CB rule does not apply since the displacement field is not uniform on each element. One can construct an alternative way of calculating the energy of the element using some quadrature rules as suggested in Ref. 14. What one needs is the energy density at the quadrature points of the elements and the energy associated with the element is obtained using the quadrature rule. The energy density at the quadrature points can be obtained using CB rule.

IX. CONCLUSION

The problem of accuracy across the interface where two different physical models are coupled together is the most common and most important problem in multiscale, multiphysics modeling. QC provides one of the simplest settings for understanding this problem. As we discussed earlier, there are two sources of inconsistency between summation rules using the CB rule and full atom summation. One is that the CB-based summation is purely local, depending only on the nearest neighbor rep-atoms. The other is that the CB-based summation is an element-based strategy, whereas the full atom summation is more naturally associated with each of the atoms. These two problems are treated separately in this paper by introducing two interfaces where the two transitions take place, a local/nonlocal interface and an atom-based/element-based interface. The second interface is inside the local region. The inconsistency at the local/nonlocal interface can be reformulated in terms of the geometric compatibility of the reconstruction schemes, and we have found the necessary and sufficient condition for locally uniform first-order accuracy at the local/nonlocal interface. This condition is geometric in nature. It contains the quasi-nonlocal approach as a special case and it guarantees the elimination of the "ghost forces." The atom-based/element-based interface is another subtle problem. Consistency at this interface depends not only on the geometry of the underlying lattice but also on the triangulation used in QC. We have understood this problem in various cases but we have not found a general condition for consistency at this interface.

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