

# AN OPTIMAL ORDER ERROR ANALYSIS OF THE ONE-DIMENSIONAL QUASICONTINUUM APPROXIMATION

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ABSTRACT. We derive a model problem for quasicontinuum approximations that allows a simple, yet insightful, analysis of the optimal-order convergence rate in the continuum limit for both the energy-based quasicontinuum approximation and the quasi-nonlocal quasicontinuum approximation. The optimal-order error estimates for the quasi-nonlocal quasicontinuum approximation are given for all strains up to the continuum limit strain for fracture. The analysis is based on an explicit treatment of the coupling error at the atomistic to continuum interface, combined with an analysis of the error due to atomistic and continuum schemes using the stability of the quasicontinuum approximation.

## 1. INTRODUCTION

The quasicontinuum method (QC) denotes a class of related approximations of fully atomistic models for crystalline solids that reduces the degrees of freedom necessary to compute a deformation to a desired accuracy [6, 8, 9, 12, 13, 15–19, 21, 22, 25, 27, 28]. The derivation of a quasicontinuum method first removes atomistic degrees of freedom by using a piecewise linear approximation of the atom deformations with respect to a possibly much smaller number of representative atoms. Since atoms interact significantly with atoms beyond their nearest neighbors, a further approximation is required to obtain a computationally feasible method.

In this paper, we will analyze two QC variants that approximate the total atomistic energy by using a continuum approximation in a portion of the material called the continuum region. The deformation gradient is assumed to be slowly varying in the continuum region, making the continuum approximation accurate. The more computationally intensive atomistic model is used for the remainder of the computational domain, which is called the atomistic region. In this region, all of the atoms are representative atoms, so that there is no restriction of the types of deformations in the atomistic region. To maintain accuracy, the atomistic region must contain all regions of highly varying deformation, such as material defects. Adaptive methods that determine what portion of the domain should be assigned to the atomistic region in order to achieve the required accuracy have been considered in [1–3, 20–22, 24]. Other approaches to atomistic to continuum coupling have been developed and analyzed in [4, 23], for example.

In Section 2, we derive a model problem for QC approximations and describe the energy-based quasicontinuum (QCE) approximation and the quasi-nonlocal quasicontinuum (QNL) approximation. These two approximations use the same continuum approximation, but differ in how they

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couple the atomistic and continuum regions. We also give stability estimates for the two QC variants.

We have derived our model quasicontinuum energy from a general quasicontinuum energy by expanding each interaction to second order to be able to present a simple, but illuminating, analysis. The model differs from a standard quadratic approximation by keeping certain first-order terms. These are a source of leading-order coupling error, and reflect the behavior in the non-linear case. We have also chosen to analyze the model problem for boundary conditions given by restricting to periodic displacements to maintain the simplicity of the analysis.

The goal of this paper is to give an error analysis as the number of atoms per interval increases (the continuum limit). The residual at atoms in the coupling interface is lower order (order  $O(1/h)$  and  $O(1)$  for QCE and QNL, respectively) than the residual in either the atomistic or continuum region ( $O(h^2)$  in all cases). However, the corresponding error depends primarily on the **sum** of the residual at the atoms in the atomistic to continuum coupling interface, and this sum has the higher order  $O(h)$  due to the cancellation of the lowest order terms when the residual is summed across the interface.

In Section 3, we split the residual for the QCE approximation into the part due to the continuum approximation and the part due to coupling the atomistic and continuum regions. The stability of the QCE approximation and the  $O(h^2)$  estimate for the corresponding residual combine to give an optimal order bound on the error due to the continuum approximation. We then derive an explicit representation of the coupling error, and we observe that this error is small and decays away from the interface since the coupling residual is oscillatory, as described in the preceding paragraph. The coupling error is the leading order term in the total error, dominating the continuum approximation error.

We show that the displacement converges at the rate  $O(h)$  in the discrete  $l^\infty$  norm and the rate  $O(h^{1/p})$  in the  $w^{1,p}$  norms where  $h$  is the interatomic spacing. Our analysis extends the results of E, Ming, and Yang [14] that show that the error is  $O(1)$  in the  $w^{1,\infty}$  norm for the QCE method applied to a problem with harmonic interactions and Dirichlet boundary conditions.

In Section 4, we present the same analysis in the QNL case. Here we show that the improved order of accuracy in the coupling interface serves to nearly balance the order of the error due to the continuum approximation, and we are consequently able to give higher order optimal error estimates for the QNL approximation than for the QCE approximation. We show that the displacement now converges at the rate  $O(h^2)$  in the discrete  $l^\infty$  norm and the rate  $O(h^{1+1/p})$  in the  $w^{1,p}$  norms where  $h$  is the interatomic spacing. E, Ming, and Yang [14] have obtained  $O(h)$  estimates in the  $w^{1,\infty}$  norm for the Lennard-Jones potential and strains bounded away from the continuum limit strain for fracture. We have obtained optimal order error estimates for the discrete  $l^\infty$  and  $w^{1,p}$  norms for all strains up to the continuum limit strain for fracture.

This paper extends our analysis of the effect of atomistic to continuum model coupling on the total error in the energy-based quasicontinuum approximation [10] to include external forcing. We also now include an analysis of the quasi-nonlocal approximation.

## 2. ONE-DIMENSIONAL, LINEAR QUASICONTINUUM APPROXIMATION

We consider the periodic displacement from a one-dimensional reference lattice with spacing  $h = 1/N$ , and we denote the positions of the atoms in the reference lattice by

$$x_j := jh, \quad -\infty < j < \infty.$$

We will derive and analyze the linearization about a uniform deformation gradient  $F$  given by the deformation

$$y_j^F := jFh = ja, \quad -\infty < j < \infty, \quad (2.1)$$

which is a lattice with spacing  $a := Fh$ . We will then consider perturbations  $u_j$  of the lattice  $y_j^F$  which are  $2N$  periodic in  $j$ , that is, we will consider deformations  $y_j$  where

$$y_j := y_j^F + u_j, \quad -\infty < j < \infty,$$

for

$$u_{j+2N} = u_j, \quad -\infty < j < \infty. \quad (2.2)$$

We will often describe the perturbations  $u_j$  satisfying (2.2) as displacements (which they are if  $y_j^F$  is considered the reference lattice). We thus have that the deformation satisfies

$$y_{j+2N} = y_j + 2F, \quad -\infty < j < \infty. \quad (2.3)$$

We note that neither the reference lattice spacing  $h$  nor the uniform lattice spacing  $a$  need be the equilibrium lattice constant or the well of the interatomic potential.

**2.1. Notation.** Before introducing the models, we fix the following notation. We define the backward differentiation operator,  $D\mathbf{u}$ , on periodic displacements by

$$(D\mathbf{u})_j := \frac{u_j - u_{j-1}}{h} \quad \text{for } -\infty < j < \infty.$$

Then  $(D\mathbf{u})_j$  is also  $2N$  periodic in  $j$ . We will use the short-hand  $(D\mathbf{u})_j = Du_j$ .

For periodic displacements,  $\mathbf{u}$ , we define the discrete norms

$$\begin{aligned} \|\mathbf{u}\|_{\ell_h^p} &:= \left( h \sum_{j=-N+1}^N |u_j|^p \right)^{1/p}, \quad 1 \leq p < \infty, \\ \|\mathbf{u}\|_{\ell_h^\infty} &:= \max_{-N+1 \leq j \leq N} |u_j|, \end{aligned}$$

By including the whole period, we ensure that they are all norms (in particular,  $\|\mathbf{u}\|_{\ell_h^p} = 0$  implies  $\mathbf{u} = 0$ ). We sum over a single period to make the norms finite. We will also consider periodic functions  $u(x) : \mathbb{R} \rightarrow \mathbb{R}$  satisfying

$$u(x+2) = u(x) \quad \text{for } x \in \mathbb{R}. \quad (2.4)$$

We define corresponding continuous norms

$$\begin{aligned} \|u\|_{L^p} &:= \left( \int_{-1}^1 |u(x)|^p dx \right)^{1/p}, \quad 1 \leq p < \infty, \\ \|u\|_{L^\infty} &:= \operatorname{ess\,sup}_{x \in (-1,1)} |u(x)|. \end{aligned}$$

We let  $u'$  denote the weak derivative of the periodic function  $u$ . We note that if  $\|u'\|_{L^p} < \infty$ , then  $u(x)$  is continuous for all  $x$  in  $\mathbb{R}$  and  $u(-1) = u(1)$ . We will similarly denote higher order weak derivatives of the periodic function  $u$  as  $u''$ ,  $u'''$ , and  $u^{(4)}$ .

**2.2. Atomistic Model.** We first consider the total energy per period

$$\mathcal{E}^{tot,h}(\mathbf{y}) := \mathcal{E}^{a,h}(\mathbf{y}) - \mathcal{F}(\mathbf{y}), \quad (2.5)$$

for deformations  $\mathbf{y}$  satisfying (2.3) where the total atomistic energy per period is

$$\mathcal{E}^{a,h}(\mathbf{y}) = \sum_{j=-N+1}^N h \left[ \phi \left( \frac{y_j - y_{j-1}}{h} \right) + \phi \left( \frac{y_j - y_{j-2}}{h} \right) \right] \quad (2.6)$$

for a two-body interatomic potential  $\phi$  (assumptions on the potential are given in Section 2.5), and where the total external potential energy per period is

$$\mathcal{F}(\mathbf{y}) = \sum_{j=-N+1}^N h f_j y_j \quad (2.7)$$

for periodic dead loads  $\mathbf{f}$  such that  $f_{j+2N} = f_j$  and  $\sum_{j=-N+1}^N f_j = 0$ .

We have scaled the atomistic energy per bond in (2.6) by  $h\phi(r/h)$  and the external force per atom by  $hf_i$  in (2.7). This scaling permits a continuum limit as  $h \rightarrow 0$ . If  $y, f \in C^\infty(\mathbb{R})$  satisfy  $y(x+2) = y(x) + 2F$ ,  $y'(x) > 0$ ,  $f(x+2) = f(x)$ , and  $\int_{-1}^1 f(x) dx = 0$ ; if  $\phi(r)$  is locally Lipschitz for  $r \in (0, \infty)$ ; and if we set  $y_j = y(x_j)$  and  $f_j = f(x_j)$ , then the energy per period (2.5) converges to [5]

$$\int_{-1}^1 \left[ \hat{\phi}(y'(x)) - f(x)y(x) \right] dx \quad (2.8)$$

as  $N \rightarrow \infty$  (which implies  $h \rightarrow 0$ ), where  $\hat{\phi}(r) = \phi(r) + \phi(2r)$ . In the following, we linearize the atomistic model which leads to a corresponding linearized continuum model. This paper analyzes the convergence of two quasicontinuum approximations to the minimizer of the linearized continuum model's total energy.

**2.3. Linearized Atomistic Model.** We will henceforth consider the linearized version of the above energies while reusing the notation  $\mathcal{E}^{a,h}$  and  $\mathcal{E}^{tot,h}$ . The total atomistic energy (2.6) becomes [10]

$$\begin{aligned} \mathcal{E}^{a,h}(\mathbf{u}) := & \sum_{j=-N+1}^N h \left[ \phi'_F \left[ \frac{u_j - u_{j-1}}{h} \right] + \frac{1}{2} \phi''_F \left[ \frac{u_j - u_{j-1}}{h} \right]^2 \right. \\ & \left. + \phi'_{2F} \left[ \frac{u_j - u_{j-2}}{h} \right] + \frac{1}{2} \phi''_{2F} \left[ \frac{u_j - u_{j-2}}{h} \right]^2 \right], \end{aligned} \quad (2.9)$$

for displacements,  $\mathbf{u}$ , satisfying the periodic boundary conditions (2.2). Here  $\phi'_F := \phi'(F)$ ,  $\phi''_F := \phi''(F)$ ,  $\phi'_{2F} := \phi'(2F)$ ,  $\phi''_{2F} := \phi''(2F)$ , where  $\phi$  is the interatomic potential in (2.6). We have removed the additive constant  $2\phi(F) + 2\phi(2F)$  from the quadratic expansion of the energy, and we will remove the additive constant  $-h \sum_{j=-N+1}^N f_j y_j^F$  from  $\mathcal{F}(\mathbf{u})$  when computing the external potential of the displacement  $\mathbf{u}$ . We note that the first order terms in (2.9) sum to zero by the periodic boundary conditions and thus do not contribute to the total energy or the equilibrium equations. We keep the first order terms in the model (2.9) since they do not sum to zero when the atomistic model is coupled to the continuum approximation in the quasicontinuum energy. The

atomistic energy (2.9) has the equilibrium equations

$$(L^{a,h}\mathbf{u})_j = \frac{-\phi_{2F}''u_{j+2} - \phi_F''u_{j+1} + 2(\phi_F'' + \phi_{2F}'')u_j - \phi_F''u_{j-1} - \phi_{2F}''u_{j-2}}{h^2} = f_j, \quad (2.10)$$

$$u_{j+2N} = u_j,$$

for  $-\infty < j < \infty$ .

**2.4. Linearized Continuum Model.** For periodic  $u \in C^\infty(\mathbb{R})$  and  $u_j = u(x_j)$ , the total linearized atomistic energy

$$\mathcal{E}^{tot,h}(\mathbf{u}) := \mathcal{E}^{a,h}(\mathbf{u}) - \mathcal{F}(\mathbf{u}) \quad (2.11)$$

converges to

$$\int_{-1}^1 [W(u'(x)) - f(x)u(x)] \, dx \quad (2.12)$$

as  $N \rightarrow \infty$ , where the continuum strain energy density,  $W(\epsilon)$ , is given by

$$W(\epsilon) := [(\phi_F' + 2\phi_{2F}')\epsilon + \frac{1}{2}(\phi_F'' + 4\phi_{2F}'')\epsilon^2]. \quad (2.13)$$

The equilibrium equations (2.10) are a five-point consistent difference approximation of the equilibrium equation of the continuum model (2.12), which are

$$-(\phi_F'' + 4\phi_{2F}'')u_e'' = f, \quad (2.14)$$

$$u_e(x+2) = u_e(x),$$

for  $x \in \mathbb{R}$ .

Quasicontinuum approximations couple an approximation of the continuum model with the atomistic model. The *continuum approximation* consists of a finite element discretization of the continuum model's elastic energy. The discretization uses a continuous, piecewise linear displacement  $\mathbf{u}$  with the atom positions  $\mathbf{x}$  as nodes. The external force term is applied as a point force at each node, so that (2.12) becomes

$$\sum_{l=-N+1}^N h[W(Du_l) - f_l u_l]. \quad (2.15)$$

The continuum approximation has equilibrium equations

$$-(\phi_F'' + 4\phi_{2F}'')\frac{u_{l+1} - 2u_l + u_{l-1}}{h^2} = f_l, \quad -\infty < l < \infty,$$

$$u_{l+2N} = u_l,$$

which is a three-point consistent difference approximation of the equilibrium equations for the continuum model (2.14). In one dimension, the above is actually the standard finite difference approximation of (2.12); however, it is framed in finite element terminology for flexibility in coarsening, adaptivity, and higher dimensional modelling.

**2.5. Assumptions.** We assume that

$$\phi_F'' + 4\phi_{2F}'' > 0, \quad (2.16)$$

which implies that the total linearized atomistic energy (2.9) is positive definite (up to uniform translation of the displacement). Thus both equations (2.10) and (2.14) have a unique solution (up to uniform translation) provided that

$$\sum_{j=-N+1}^N f_j = 0. \quad (2.17)$$

For simplicity, we assume in the following that  $f$  is odd in addition to being periodic, that is,

$$f(x) = -f(-x) \quad \text{and} \quad f(x+2) = f(x) \quad \text{for} \quad -\infty < x < \infty, \quad (2.18)$$

which implies that  $f_j := f(x_j)$  satisfies

$$f_j = -f_{-j} \quad \text{and} \quad f_{j+2N} = f_j \quad \text{for} \quad -\infty < j < \infty. \quad (2.19)$$

We obtain a unique, odd periodic solution satisfying the mean value condition

$$\sum_{j=-N+1}^N u_j = 0. \quad (2.20)$$

To give nonoscillatory solutions to the equilibrium equations (2.10) (that is, to guarantee that the roots of the corresponding characteristic equation are real (3.17)), we further assume that

$$\phi_F'' > 0 \quad \text{and} \quad \phi_{2F}'' < 0. \quad (2.21)$$

The assumption (2.21) holds for potentials that allow an accurate second neighbor cut-off, such as the Lennard-Jones potential [9, 10].

**2.6. Energy-Based Quasicontinuum Approximation.** The energy-based quasicontinuum approximation (QCE) of  $\mathcal{E}^{a,h}(\mathbf{u})$  decomposes the reference lattice into an atomistic region and a coarse-grained continuum region. It computes a total energy by using the atomistic energy (2.9) in the atomistic region and by using the continuum approximation (2.15) to sum the energy of the continuum region.

For our analysis, we will consider an atomistic region defined by the atoms with reference positions  $x_j$  for  $j = -K, \dots, K$ , and a continuum region containing the remaining atoms,  $j = -N+1, \dots, -K-1$  and  $j = K+1, \dots, N$ . All atoms in the continuum region, along with the two atoms on the boundary,  $j = \pm K$  will act as nodes for the continuum approximation. The continuum region can be decomposed into elements  $(x_{(l-1)}, x_l)$  for  $l = -N+1, \dots, -K$  and  $l = K+1, \dots, N$ . (In general, elements can contain many atoms of the reference lattice, but in this paper we do not consider coarsening in the continuum region.)

To construct the contribution of the atomistic region to the total quasicontinuum energy, it is convenient to construct an energy associated with each atom by splitting equally the energy of each bond to obtain

$$\begin{aligned} \mathcal{E}_j^{a,h}(\mathbf{u}) := & \frac{h}{2} \left[ \phi_F' \left[ \frac{u_{j+1} - u_j}{h} \right] + \frac{1}{2} \phi_F'' \left[ \frac{u_{j+1} - u_j}{h} \right]^2 \right. \\ & \left. + \phi_{2F}' \left[ \frac{u_{j+2} - u_j}{h} \right] + \frac{1}{2} \phi_{2F}'' \left[ \frac{u_{j+2} - u_j}{h} \right]^2 \right] \\ & + \frac{h}{2} \left[ \phi_F' \left[ \frac{u_j - u_{j-1}}{h} \right] + \frac{1}{2} \phi_F'' \left[ \frac{u_j - u_{j-1}}{h} \right]^2 \right. \\ & \left. + \phi_{2F}' \left[ \frac{u_j - u_{j-2}}{h} \right] + \frac{1}{2} \phi_{2F}'' \left[ \frac{u_j - u_{j-2}}{h} \right]^2 \right]. \end{aligned} \quad (2.22)$$

The continuum energy (2.15) is split into energy per element  $hW(Du_l)$  where  $W$  is given in (2.13), and  $h = x_l - x_{l-1}$  is the length of the continuum element  $(x_{l-1}, x_l)$ .

To construct a quasicontinuum approximation QCE that conserves exactly the energy of atomistic model (2.9) for lattices  $y_j^F$  given by a uniform deformation gradient  $F$  (see (2.1)) the elements

$(x_{-K-1}, x_{-K})$  and  $(x_K, x_{K+1})$  on the border of the atomistic region should contribute only one half of the continuum energy associated with that element. The QCE energy is then

$$\begin{aligned} \mathcal{E}^{qce,h}(\mathbf{u}) := & \sum_{l=-N+1}^{-K-1} hW(Du_l) + \frac{1}{2}hW(Du_{-K}) + \sum_{j=-K}^K \mathcal{E}_j^{a,h}(\mathbf{u}) \\ & + \frac{1}{2}hW(Du_{K+1}) + \sum_{l=K+2}^N hW(Du_l). \end{aligned} \quad (2.23)$$

The equilibrium equations for the total QCE energy,  $\mathcal{E}^{qce,h}(\mathbf{u}) - \mathcal{F}(\mathbf{u})$ , then take the form [9, 10]

$$L^{qce,h} \mathbf{u}_{qce} - \mathbf{g} = \mathbf{f}, \quad (2.24)$$

where, for  $0 \leq j \leq N$ , we have

$$(L^{qce,h} \mathbf{u})_j = \phi_F'' \frac{-u_{j+1} + 2u_j - u_{j-1}}{h^2} + \begin{cases} 4\phi_{2F}'' \frac{-u_{j+2} + 2u_j - u_{j-2}}{4h^2}, & 0 \leq j \leq K-2, \\ 4\phi_{2F}'' \frac{-u_{j+2} + 2u_j - u_{j-2}}{4h^2} + \frac{\phi_{2F}''}{h} \frac{u_{j+2} - u_j}{2h}, & j = K-1, \\ 4\phi_{2F}'' \frac{-u_{j+2} + 2u_j - u_{j-2}}{4h^2} - \frac{2\phi_{2F}''}{h} \frac{u_{j+1} - u_j}{h} + \frac{\phi_{2F}''}{h} \frac{u_{j+2} - u_j}{2h}, & j = K, \\ 4\phi_{2F}'' \frac{-u_{j+1} + 2u_j - u_{j-1}}{h^2} - \frac{2\phi_{2F}''}{h} \frac{u_j - u_{j-1}}{h} + \frac{\phi_{2F}''}{h} \frac{u_j - u_{j-2}}{2h}, & j = K+1, \\ 4\phi_{2F}'' \frac{-u_{j+1} + 2u_j - u_{j-1}}{h^2} + \frac{\phi_{2F}''}{h} \frac{u_j - u_{j-2}}{2h}, & j = K+2, \\ 4\phi_{2F}'' \frac{-u_{j+1} + 2u_j - u_{j-1}}{h^2}, & K+3 \leq j \leq N, \end{cases}$$

with  $\mathbf{g}$  given by

$$g_j = \begin{cases} 0, & 0 \leq j \leq K-2, \\ -\frac{1}{2h} \phi_{2F}', & j = K-1, \\ \frac{1}{2h} \phi_{2F}', & j = K, \\ \frac{1}{2h} \phi_{2F}', & j = K+1, \\ -\frac{1}{2h} \phi_{2F}', & j = K+2, \\ 0, & K+3 \leq j \leq N. \end{cases} \quad (2.25)$$

For space reasons, we only list the entries for  $0 \leq j \leq N$ . The equations for all other  $j \in \mathbb{Z}$  follow from symmetry and periodicity. Due to the symmetry in the definition of the atomistic and continuum regions, we have that  $L_{i,j}^{qce,h} = L_{-i,-j}^{qce,h}$  and  $g_j = -g_{-j}$  for  $-N+1 \leq i, j \leq 0$ . To see this, we define the involution operator  $(S\mathbf{u})_j = -u_{-j}$  and observe that  $\mathcal{E}^{qce,h}(S\mathbf{u}) = \mathcal{E}^{qce,h}(\mathbf{u})$ . It then follows from the chain rule that

$$S^T L^{qce,h} S \mathbf{u} - S^T \mathbf{g} - S^T \mathbf{f} = L^{qce,h} \mathbf{u} - \mathbf{g} - \mathbf{f} \quad \text{for all periodic } \mathbf{u}.$$

Since  $S^T = S$  and the assumption (2.19) is equivalent to  $Sf = f$ , we can conclude that

$$SL^{qce,h}S = L^{qce,h} \quad \text{and} \quad Sg = g. \quad (2.26)$$

Furthermore, we can conclude that the unique mean zero solution (2.20) to the equilibrium equations (2.24) is odd. This follows from  $S^{-1} = S$  and (2.26) which together imply that  $S\mathbf{u}$  is a

solution if and only if  $\mathbf{u}$  is. Because  $S$  preserves the mean zero property, we conclude that  $\mathbf{u}_{qce}$  is odd.

**2.7. Stability of the Quasicontinuum Operator.** Our analysis of the QCE error will utilize the following stability results for the operator  $L^{qce,h}$ .

**Lemma 2.1.** *If  $\nu := \phi_F'' - 5|\phi_{2F}''| > 0$ , then*

$$h\mathbf{v} \cdot L^{qce,h}\mathbf{v} \geq \nu \|D\mathbf{v}\|_{\ell_h^2}^2. \quad (2.27)$$

*Proof.* The stability result (2.27) follows from the identity

$$\begin{aligned} \frac{1}{2}h\mathbf{v} \cdot L^{qce,h}\mathbf{v} &= \sum_{l=-N+1}^{-K-1} h\widehat{W}(Dv_l) + \frac{1}{2}h\widehat{W}(Dv_{-K}) + \sum_{j=-K}^K \widehat{\mathcal{E}}_j^{a,h}(\mathbf{v}) \\ &\quad + \frac{1}{2}h\widehat{W}(Dv_{K+1}) + \sum_{l=K+2}^N h\widehat{W}(Dv_l), \end{aligned}$$

where

$$\begin{aligned} \widehat{\mathcal{E}}_j^{a,h}(\mathbf{v}) &:= \frac{h}{2} \left[ \frac{1}{2}\phi_F'' \left[ \frac{v_{j+1} - v_j}{h} \right]^2 + \frac{1}{2}\phi_{2F}'' \left[ \frac{v_{j+2} - v_j}{h} \right]^2 \right] \\ &\quad + \frac{h}{2} \left[ \frac{1}{2}\phi_F'' \left[ \frac{v_j - v_{j-1}}{h} \right]^2 + \frac{1}{2}\phi_{2F}'' \left[ \frac{v_j - v_{j-2}}{h} \right]^2 \right] \end{aligned} \quad (2.28)$$

and

$$\widehat{W}(\epsilon) := \frac{1}{2}(\phi_F'' + 4\phi_{2F}'')\epsilon^2. \quad (2.29)$$

We then have that

$$\begin{aligned} h\mathbf{v} \cdot L^{qce,h}\mathbf{v} &\geq h \sum_{j=-N+1}^N \frac{1}{2}\phi_F'' [(Dv_{j+1})^2 + (Dv_j)^2] - h \sum_{j=-N+1}^{-K-1} 4|\phi_{2F}''| (Dv_j)^2 \\ &\quad - 2h|\phi_{2F}''| (Dv_{-K})^2 - h \sum_{j=-K}^K |\phi_{2F}''| [(Dv_{j+2})^2 + (Dv_{j+1})^2 + (Dv_j)^2 + (Dv_{j-1})^2] \\ &\quad - 2h|\phi_{2F}''| (Dv_{K+1})^2 - h \sum_{j=K+2}^N 4|\phi_{2F}''| (Dv_j)^2 \\ &\geq (\phi_F'' - 5|\phi_{2F}''|) \left[ h \sum_{j=-N+1}^N (Dv_j)^2 \right]. \quad \square \end{aligned}$$

The preceding stability Lemma 2.1 and the discrete Poincaré inequality,

$$\|\mathbf{v}\|_{\ell_h^2} \leq \frac{h}{2 \sin \frac{\pi h}{2}} \|D\mathbf{v}\|_{\ell_h^2} \leq \frac{1}{2} \|D\mathbf{v}\|_{\ell_h^2} \quad \text{if } \sum_{j=-N+1}^N v_j = 0 \quad (2.30)$$

for  $0 < h \leq 1$ , give the following stability result in the  $\|\cdot\|_{\ell_h^2}$  norm. The proof of (2.30) follows from verifying that  $(2 \sin \frac{\pi h}{2})/h$  is the smallest eigenvalue of  $D^T D$ .

**Lemma 2.2.** *If  $\nu := \phi_F'' - 5|\phi_{2F}''|$  and*

$$L^{qce,h} \mathbf{v} = \mathbf{b}, \quad (2.31)$$

where  $\sum_{j=-N+1}^N b_j = 0$ , then

$$\|D\mathbf{v}\|_{\ell_h^2} \leq \frac{1}{2\nu} \|\mathbf{b}\|_{\ell_h^2}. \quad (2.32)$$

*Proof.* The result (2.32) follows from taking the inner product of (2.31) with  $\mathbf{v}$  and then using the positive definiteness inequality (2.27) and the Poincaré inequality (2.30).  $\square$

**2.8. Quasi-nonlocal Quasicontinuum Approximation.** The quasi-nonlocal quasicontinuum approximation (QNL) is similar to the QCE approximation, but it modifies the interactions around the interface in order to remove  $\mathbf{g}$  from the elastic force. The quasi-nonlocal atoms  $\pm K, \pm(K+1)$  interact directly with any atoms in the atomistic region within the next nearest neighbor cut-off, but interact as in the continuum region with other all other atoms. That is, unlike the atomistic model and continuum approximation, the form of energy contributions for quasi-nonlocal atoms depends on the type (atomistic, continuum, or quasi-nonlocal) of the neighboring atoms. For example, the energy contribution for  $j = K$  is

$$\begin{aligned} \mathcal{E}_K^{q,h}(\mathbf{u}) := & \frac{h}{2} \left[ (\phi_F' + 2\phi_{2F}') \left[ \frac{u_{K+1} - u_K}{h} \right] + \frac{1}{2}(\phi_F'' + 4\phi_{2F}'') \left[ \frac{u_{K+1} - u_K}{h} \right]^2 \right] \\ & + \frac{h}{2} \left[ \phi_F' \left[ \frac{u_K - u_{K-1}}{h} \right] + \frac{1}{2}\phi_F'' \left[ \frac{u_K - u_{K-1}}{h} \right]^2 \right. \\ & \left. + \phi_{2F}' \left[ \frac{u_K - u_{K-2}}{h} \right] + \frac{1}{2}\phi_{2F}'' \left[ \frac{u_K - u_{K-2}}{h} \right]^2 \right] \end{aligned}$$

and the energy contribution for  $j = K+1$  is

$$\begin{aligned} \mathcal{E}_{K+1}^{q,h}(\mathbf{u}) := & \frac{h}{2} \left[ (\phi_F' + 2\phi_{2F}') \left[ \frac{u_{K+2} - u_{K+1}}{h} \right] + \frac{1}{2}(\phi_F'' + 4\phi_{2F}'') \left[ \frac{u_{K+2} - u_{K+1}}{h} \right]^2 \right] \\ & + \frac{h}{2} \left[ \phi_F' \left[ \frac{u_{K+1} - u_K}{h} \right] + \frac{1}{2}\phi_F'' \left[ \frac{u_{K+1} - u_K}{h} \right]^2 \right. \\ & \left. + \phi_{2F}' \left[ \frac{u_{K+1} - u_{K-1}}{h} \right] + \frac{1}{2}\phi_{2F}'' \left[ \frac{u_{K+1} - u_{K-1}}{h} \right]^2 \right]. \end{aligned}$$

The QNL energy is then

$$\begin{aligned} \mathcal{E}^{qnl,h}(\mathbf{u}) := & \sum_{l=-N+1}^{-K-2} hW(Du_l) + \frac{1}{2}hW(Du_{-K-1}) + \sum_{j=-K-1}^{-K} \mathcal{E}_j^{q,h}(\mathbf{u}) + \sum_{j=-K+1}^{K-1} \mathcal{E}_j^{a,h}(\mathbf{u}) \\ & + \sum_{j=K}^{K+1} \mathcal{E}_j^{q,h}(\mathbf{u}) + \frac{1}{2}hW(Du_{K+2}) + \sum_{l=K+3}^N hW(Du_l). \end{aligned} \quad (2.33)$$

The QNL equilibrium equations are

$$L^{qnl,h} \mathbf{u}_{qnl} = \mathbf{f},$$

where

$$(L^{qnl,h}\mathbf{u})_j = \phi_F'' \frac{-u_{j+1} + 2u_j - u_{j-1}}{h^2} + \begin{cases} 4\phi_{2F}'' \frac{-u_{j+2} + 2u_j - u_{j-2}}{4h^2}, & 0 \leq j \leq K-1, \\ 4\phi_{2F}'' \frac{-u_{j+2} + 2u_j - u_{j-2}}{4h^2} - \phi_{2F}'' \frac{-u_{j+2} + 2u_{j+1} - u_j}{h^2}, & j = K, \\ 4\phi_{2F}'' \frac{-u_{j+1} + 2u_j - u_{j-1}}{h^2} + \phi_{2F}'' \frac{-u_j + 2u_{j-1} - u_{j-2}}{h^2}, & j = K+1, \\ 4\phi_{2F}'' \frac{-u_{j+1} + 2u_j - u_{j-1}}{h^2}, & K+2 \leq j \leq N. \end{cases}$$

We note that the QNL energy satisfies the symmetry condition  $\mathcal{E}^{qnl,h}(S\mathbf{u}) = \mathcal{E}^{qnl,h}(\mathbf{u})$ , so the QNL operator  $L^{qnl,h}$  is defined for  $j < 0$  by the identity  $SL^{qnl,h}S = L^{qnl,h}$ . While we have successfully removed the ghost force terms  $\mathbf{g}$ , QNL is also not a consistent approximation of the continuum equations (2.14) at the interfacial atoms, such as  $j = K$  and  $j = K+1$  above. We will give a more detailed analysis of the approximation at the interface in Section 4.

Our analysis of the QNL error will utilize the following stability result for the operator  $L^{qnl,h}$ .

**Lemma 2.3.** *If  $1 \leq p \leq \infty$ ,  $\nu := \phi_F'' - 4|\phi_{2F}''| > 0$ , and*

$$L^{qnl,h}\mathbf{v} = \mathbf{b}$$

where  $\sum_{j=-N+1}^N b_j = 0$ , then

$$\begin{aligned} h\mathbf{v} \cdot L^{qnl,h}\mathbf{v} &\geq \nu \|D\mathbf{v}\|_{\ell_h^2}^2, \\ \|D\mathbf{v}\|_{\ell_h^2} &\leq \frac{1}{2\nu} \|\mathbf{b}\|_{\ell_h^2}. \end{aligned} \tag{2.34}$$

*Proof.* The proof of the stability result (2.34) follows the proof of the stability results for the QCE approximation in Lemmas 2.1 and 2.2 with the appropriate modification.  $\square$

*Remark 2.1.* The basic formulation of the QNL method removes the ghost force terms only for second-neighbor interactions in the 1D case. A longer-range matching method is proposed in [12] that removes ghost forces for longer-range interactions by extending the region near the interface which have special energies.

In 2D and 3D, there are similar restrictions on the interaction length that QNL corrects. Additional ghost forces arise when the quasicontinuum energy is extended to allow coarsening in the continuum region [12].

### 3. CONVERGENCE OF THE ENERGY-BASED QUASICONTINUUM SOLUTION

We now analyze the quasicontinuum error and obtain estimates for its convergence rate by splitting the residual into two parts. One portion contains the low order terms, has support only near the atomistic to continuum interface, and is oscillatory. The remainder is higher order, and its influence will be bounded using the stability results. We recall that the QCE solution,  $\mathbf{u}_{qce}$ , is an odd, periodic solution of

$$L^{qce,h}\mathbf{u}_{qce} = \mathbf{g} + \mathbf{f}, \tag{3.1}$$

and the continuum model solution is an odd, periodic function  $u_e(x)$  satisfying

$$-(\phi_F'' + 4\phi_{2F}'')u_e'' = f, \tag{3.2}$$

Let  $\mathbf{u}_e$  denote the vector satisfying  $u_j = u_e(x_j)$ . We will now derive estimates for the quasicontinuum error  $\mathbf{e} = \mathbf{u}_e - \mathbf{u}_{qce}$ .

It follows from the QCE equilibrium equation (3.1) that

$$L^{qce,h} \mathbf{e} = L^{qce,h} \mathbf{u}_e - L^{qce,h} \mathbf{u}_{qce} = L^{qce,h} \mathbf{u}_e - \mathbf{g} - \mathbf{f}. \quad (3.3)$$

We split the residual  $L^{qce,h} \mathbf{e}$  as

$$L^{qce,h} \mathbf{e} := \boldsymbol{\rho} + \boldsymbol{\sigma}, \quad (3.4)$$

where  $\boldsymbol{\rho}$  contains the three lowest-order residual error terms in the interface,

$$\boldsymbol{\rho} = \begin{cases} 0, & 0 \leq j \leq K-2, \\ \left( \frac{1}{2} \phi'_{2F} + \phi''_{2F} u'_{K+1/2} \right) \frac{1}{h} - \frac{1}{2} \phi''_{2F} u''_{K+1/2}, + \frac{7}{24} \phi''_{2F} u'''_{K+1/2} h, & j = K-1, \\ - \left( \frac{1}{2} \phi'_{2F} + \phi''_{2F} u'_{K+1/2} \right) \frac{1}{h} + \frac{1}{2} \phi''_{2F} u''_{K+1/2}, + \frac{5}{24} \phi''_{2F} u'''_{K+1/2} h, & j = K, \\ - \left( \frac{1}{2} \phi'_{2F} + \phi''_{2F} u'_{K+1/2} \right) \frac{1}{h} - \frac{1}{2} \phi''_{2F} u''_{K+1/2}, + \frac{5}{24} \phi''_{2F} u'''_{K+1/2} h, & j = K+1, \\ \left( \frac{1}{2} \phi'_{2F} + \phi''_{2F} u'_{K+1/2} \right) \frac{1}{h} + \frac{1}{2} \phi''_{2F} u''_{K+1/2}, + \frac{7}{24} \phi''_{2F} u'''_{K+1/2} h, & j = K+2, \\ 0, & K+3 \leq j \leq N, \end{cases} \quad (3.5)$$

and  $\rho_j = -\rho_{-j}$ . Although  $\rho_j = O(1/h)$  in the interface  $j = K-1, \dots, K+2$ , we will prove that the effect of  $\boldsymbol{\rho}$  on the error is small away from the interface because it oscillates and the lowest order terms cancel in the sum

$$\Delta \boldsymbol{\rho} := \sum_{j=K-1}^{K+2} \rho_j = h \phi''_{2F} u'''_{K+1/2}. \quad (3.6)$$

The residual term  $\boldsymbol{\rho}$  represents the inconsistency of the operator  $L^{qce,h}$  as a second-order finite difference approximation of the differential equation (3.2). This inconsistency is located only in the interface because the models themselves are second-order approximations.

The residual term  $\boldsymbol{\sigma}$  accounts for the error in approximating the continuum model (2.14) by a second-order finite difference approximation. We can estimate the residual  $\boldsymbol{\sigma}$  from Taylor's Theorem to obtain

$$\|\boldsymbol{\sigma}\|_{\ell_h^2} \leq Ch^2 \left\| u_e^{(4)} \right\|_{L^2}. \quad (3.7)$$

Note that since  $\mathbf{u}_e$ ,  $\mathbf{f}$ , and  $\mathbf{g}$  are odd, and  $\boldsymbol{\rho}$  was constructed to be odd, then  $\boldsymbol{\sigma}$  is odd as well. Therefore, we can split the error  $\mathbf{e}$  as

$$\mathbf{e} = \mathbf{e}_\rho + \mathbf{e}_\sigma$$

such that

$$\begin{aligned} L^{qce,h} \mathbf{e}_\rho &= \boldsymbol{\rho}, & e_{\rho,j} &= -e_{\rho,-j}, \\ L^{qce,h} \mathbf{e}_\sigma &= \boldsymbol{\sigma}, & e_{\sigma,j} &= -e_{\sigma,-j}. \end{aligned} \quad (3.8)$$

**3.1. Global Discretization Error,  $\mathbf{e}_\sigma$ .** We now have by the stability (2.27) of  $L^{qce,h}$  and the estimate of the residual (3.7) that

$$\|D\mathbf{e}_\sigma\|_{\ell_h^2} \leq Ch^2 \left\| u_e^{(4)} \right\|_{L^2}. \quad (3.9)$$

We can extend the bound to

**Lemma 3.1.** For  $\mathbf{e}_\sigma$  defined in (3.8), we have

$$\|\mathbf{e}_\sigma\|_{\ell_h^\infty} \leq \sqrt{2} \|D\mathbf{e}_\sigma\|_{\ell_h^2} \leq Ch^2 \left\| u_e^{(4)} \right\|_{L^2}, \quad (3.10)$$

$$\|D\mathbf{e}_\sigma\|_{\ell_h^p} \leq \begin{cases} Ch^2 \left\| u_e^{(4)} \right\|_{L^2}, & 1 \leq p \leq 2, \\ Ch^{\frac{3}{2} + \frac{1}{p}} \left\| u_e^{(4)} \right\|_{L^2}, & 2 \leq p \leq \infty. \end{cases} \quad (3.11)$$

*Proof.* We obtain the Poincaré inequality [7]

$$\|\mathbf{v}\|_{\ell_h^\infty} \leq \|D\mathbf{v}\|_{\ell_h^1} \leq \sqrt{2} \|D\mathbf{v}\|_{\ell_h^2} \quad (3.12)$$

for all odd periodic  $\mathbf{v}$  from the identity

$$v_j = \begin{cases} \sum_{\ell=1}^j h(Dv_\ell) & \text{if } j > 0, \\ -\sum_{\ell=j-1}^0 h(Dv_\ell) & \text{if } j < 0, \end{cases}$$

which gives the first inequality in (3.12). The second follows from Hölder's inequality. We can then obtain the error estimate (3.10) for  $\|\mathbf{e}_\sigma\|_{\ell_h^\infty}$  from the Poincaré inequality (3.12) and the bound (3.9).

The “inverse” estimate [7]

$$\|D\mathbf{v}\|_{\ell_h^\infty} \leq h^{-1/2} \|D\mathbf{v}\|_{\ell_h^2} \quad (3.13)$$

for all periodic  $\mathbf{v}$ , and the Hölder estimates [26]

$$\|D\mathbf{v}\|_{\ell_h^p} \leq \begin{cases} 2^{\frac{2-p}{2p}} \|D\mathbf{v}\|_{\ell_h^2}, & 1 \leq p \leq 2, \\ \|D\mathbf{v}\|_{\ell_h^2}^{2/p} \|D\mathbf{v}\|_{\ell_h^\infty}^{1-2/p}, & 2 \leq p \leq \infty, \end{cases} \quad (3.14)$$

combine to prove (3.11) by taking  $\mathbf{v} = \mathbf{e}_\sigma$ .  $\square$

**3.2. Interfacial coupling error,  $\mathbf{e}_\rho$ .** In the following, we will bound the error,  $\mathbf{e}_\rho$ , by constructing and estimating an explicit odd solution of

$$L^{qce,h} \mathbf{e}_\rho = \boldsymbol{\rho}. \quad (3.15)$$

Since  $\rho_j$  is zero for all  $j$  except  $j = \pm\{K-1, K, K+1, K+2\}$ ,  $\mathbf{e}_\rho$  satisfies a second-order, homogeneous recurrence relation in the interior of the continuum region and a fourth-order, homogeneous recurrence relation in the interior of the atomistic region. Therefore,  $e_{\rho,j}$  is linear for  $j \geq K+3$  or  $j \leq -K-3$ , and it is the sum of a linear solution and exponential solution for  $-K+2 \leq j \leq K-2$ . The coefficients for these solutions are determined by the equations in the atomistic to continuum interface.

The homogeneous atomistic difference scheme

$$-\phi_{2F}'' u_{j+2} - \phi_F'' u_{j+1} + (2\phi_F'' + 2\phi_{2F}'') u_j - \phi_F'' u_{j-1} - \phi_{2F}'' u_{j-2} = 0 \quad (3.16)$$

has characteristic equation

$$-\phi_{2F}'' \Lambda^2 - \phi_F'' \Lambda + (2\phi_F'' + 2\phi_{2F}'') - \phi_F'' \Lambda^{-1} - \phi_{2F}'' \Lambda^{-2} = 0,$$

with roots

$$1, 1, \lambda, \frac{1}{\lambda}, \quad (3.17)$$

where

$$\lambda = \frac{(\phi_F'' + 2\phi_{2F}'') + \sqrt{(\phi_F'')^2 + 4\phi_F''\phi_{2F}''}}{-2\phi_{2F}''}.$$

Based on the assumptions on  $\phi$  in (2.16) and (2.21) and we have that  $\lambda > 1$ . We note that if  $\phi''_{2F}$  were positive contrary to assumption (2.21), then  $\lambda$  would be negative which would give an oscillatory error in the atomistic region. General solutions of the homogeneous atomistic equations (3.16) have the form  $u_j = C_1 + C_2hj + C_3\lambda^j + C_4\lambda^{-j}$ , but seeking an odd solution reduces this to the form  $u_j = C_2hj + C_3(\lambda^j - \lambda^{-j})$ .

The odd solution of the approximate error equations is thus of the form

$$e_{\rho,j} = \begin{cases} m_1hj + \beta \left( \frac{\lambda^j - \lambda^{-j}}{\lambda^K} \right), & 0 \leq j \leq K, \\ m_2hj - m_2 + \hat{e}_{K+1}, & j = K + 1, \\ m_2hj - m_2, & K + 2 \leq j \leq N, \end{cases} \quad (3.18)$$

where expressing the unknown  $e_{\rho,K+1}$  using a perturbation of the linear solution,  $\hat{e}_{K+1}$ , simplifies the solution of the equilibrium equations. The four coefficients  $m_1$ ,  $m_2$ ,  $\hat{e}_{K+1}$ , and  $\beta$  can be found by satisfying the four equilibrium equations in the interface,  $j = K - 1, \dots, K + 2$ . Summing the equilibrium equations across the interface gives

$$\begin{aligned} \Delta \rho &= \sum_{j=K-1}^{K+2} \rho_j = \sum_{j=K-1}^{K+2} (L^{qce,h} \mathbf{e}_\rho)_j \\ &= \phi''_F \left[ \frac{e_{\rho,K-1} - e_{\rho,K-2}}{h^2} \right] + 4\phi''_{2F} \left[ \frac{e_{\rho,K} + e_{\rho,K-1} - e_{\rho,K-2} - e_{\rho,K-3}}{4h^2} \right] \\ &\quad - (\phi''_F + 4\phi''_{2F}) \left[ \frac{e_{\rho,K+3} - e_{\rho,K+2}}{h^2} \right] \\ &= (\phi''_F + 4\phi''_{2F}) \left( \frac{m_1}{h} - \frac{m_2}{h} \right). \end{aligned}$$

The cancellation of the exponential terms in the final equality holds because

$$\phi''_{2F}(\lambda^K - \lambda^{-K}) + (\phi''_F + \phi''_{2F})(\lambda^{K-1} - \lambda^{-K+1} - \lambda^{K-2} + \lambda^{-K+2}) + \phi''_{2F}(-\lambda^{K-3} + \lambda^{-K+3}) = 0,$$

which can be seen by summing (3.16) with the homogeneous solution  $y_j = -\lambda^j$  for  $j = -K + 2, \dots, K - 2$ . Thus, we have from summing the equilibrium equations (3.15) across the interface that

$$m_1 = m_2 + \frac{h\Delta \rho}{\phi''_F + 4\phi''_{2F}}. \quad (3.19)$$

The equality (3.19) can be interpreted as saying that the interfacial residual  $\rho$  acts as a source  $f = \Delta \rho$  in the continuum equations (3.2) at  $x = x_K$ .

**Lemma 3.2.** *For  $\mathbf{e}_\rho$  defined in (3.8), we have that*

$$\begin{aligned} \|\mathbf{e}_\rho\|_{\ell_h^\infty} &\leq Ch(1 + |u'_{K+1/2}| + h|u''_{K+1/2}| + h|u'''_{K+1/2}|), \\ \|D\mathbf{e}_\rho\|_{\ell_h^p} &\leq Ch^{1/p}(1 + |u'_{K+1/2}| + h|u''_{K+1/2}| + h|u'''_{K+1/2}|), \end{aligned} \quad (3.20)$$

where  $C > 0$  is independent of  $h$ ,  $K$ , and  $p$ ,  $1 \leq p \leq \infty$ .

*Proof.* We will set up the system of equations for the coefficients in (3.18) and bound the decay of the coefficients. We split the interface equations as  $(A + hB)\mathbf{x} = \mathbf{b}$ , where

$$\begin{aligned}
A &= \begin{bmatrix} 0 & \frac{1}{2}\phi''_{2F} & -\frac{1}{2}\phi''_{2F} & \phi''_{2F}\gamma_{K+1} - \frac{1}{2}\phi''_{2F}\gamma_{K-1} \\ 0 & \phi''_F + \frac{5}{2}\phi''_{2F} & -\phi''_F - 2\phi''_{2F} & \phi''_F\gamma_{K+1} + \phi''_{2F}\gamma_{K+2} + \frac{3}{2}\phi''_{2F}\gamma_K \\ 0 & -\phi''_F - \frac{5}{2}\phi''_{2F} & 2\phi''_F + \frac{13}{2}\phi''_{2F} & -\phi''_F\gamma_K - 2\phi''_{2F}\gamma_K - \frac{1}{2}\phi''_{2F}\gamma_{K-1} \\ 0 & -\frac{1}{2}\phi''_{2F} & -\phi''_F - 4\phi''_{2F} & -\frac{1}{2}\phi''_{2F}\gamma_K \end{bmatrix}, \\
B &= \begin{bmatrix} (\frac{1}{2}K + \frac{3}{2})\phi''_{2F} & -(\frac{1}{2}K + \frac{1}{2})\phi''_{2F} & 0 & 0 \\ (K+1)\phi''_F + (\frac{5}{2}K + 2)\phi''_{2F} & -(K+1)\phi''_F - (\frac{5}{2}K + 3)\phi''_{2F} & 0 & 0 \\ -K\phi''_F - (\frac{5}{2}K - \frac{1}{2})\phi''_{2F} & K\phi''_F - (\frac{5}{2}K - \frac{3}{2})\phi''_{2F} & 0 & 0 \\ -\frac{1}{2}K\phi''_{2F} & (\frac{1}{2}K + 1)\phi''_{2F} & 0 & 0 \end{bmatrix}, \\
\mathbf{x} &= \begin{bmatrix} m_1 \\ m_2 \\ \hat{e}_{K+1} \\ \beta \end{bmatrix}, \quad \mathbf{b} = h^2 \begin{bmatrix} \rho_{K-1} \\ \rho_K \\ \rho_{K+1} \\ \rho_{K+2} \end{bmatrix}.
\end{aligned} \tag{3.21}$$

Using the equality (3.19), we rewrite the above as  $(\tilde{A}_K + h\tilde{B})\tilde{\mathbf{x}} = \tilde{\mathbf{b}}$  where

$$\begin{aligned}
\tilde{A}_K &= \begin{bmatrix} \frac{1}{2}\phi''_{2F} & -\frac{1}{2}\phi''_{2F} & \phi''_{2F}\gamma_{K+1} - \frac{1}{2}\phi''_{2F}\gamma_{K-1} \\ -\phi''_F - \frac{5}{2}\phi''_{2F} & 2\phi''_F + \frac{13}{2}\phi''_{2F} & -\phi''_F\gamma_K - 2\phi''_{2F}\gamma_K - \frac{1}{2}\phi''_{2F}\gamma_{K-1} \\ -\frac{1}{2}\phi''_{2F} & -\phi''_F - 4\phi''_{2F} & -\frac{1}{2}\phi''_{2F}\gamma_K \end{bmatrix}, \\
\tilde{B} &= \begin{bmatrix} \phi''_{2F} & 0 & 0 \\ -\phi''_{2F} & 0 & 0 \\ \phi''_{2F} & 0 & 0 \end{bmatrix}, \quad \tilde{\mathbf{x}} = \begin{bmatrix} m_2 \\ \hat{e}_{K+1} \\ \beta \end{bmatrix}, \\
\tilde{\mathbf{b}} &= h^2 \begin{bmatrix} \rho_{K-1} \\ \rho_{K+1} \\ \rho_{K+2} \end{bmatrix} - h^2 \frac{\Delta\rho}{\phi''_F + 4\phi''_{2F}} \begin{bmatrix} (\frac{1}{2}K + \frac{3}{2})\phi''_{2F} \\ -K\phi''_F - (\frac{5}{2}K - \frac{1}{2})\phi''_{2F} \\ -\frac{1}{2}K\phi''_{2F} \end{bmatrix},
\end{aligned} \tag{3.22}$$

and  $\gamma_j = \frac{\lambda^j - \lambda^{-j}}{\lambda^K}$ . We have omitted the second equation, as the full system is linearly dependent after the elimination of  $m_1$  by (3.19).

We note that  $\tilde{A}_K$ ,  $\tilde{B}$ , and  $\tilde{\mathbf{b}}$  do not depend on  $h$  directly, though  $\tilde{A}_K$  may have indirect dependence if  $K$  scales with  $h$ . Therefore, we can neglect  $\tilde{B}$  for sufficiently small  $h$  provided that  $\tilde{A}_K^{-1}$  exists and is bounded uniformly in  $K$ . The following lemma, proven in [11], gives such a bound for  $\tilde{A}_K$ .

**Lemma 3.3.** *For all  $K$  satisfying  $2 \leq K \leq N - 2$ , the matrix  $\tilde{A}_K$  is nonsingular and  $\|\tilde{A}_K^{-1}\| \leq C$  where  $C > 0$  is independent of  $K$  and  $h$ .*

Due to the definition of  $\boldsymbol{\rho}$  (3.5) and  $\Delta\boldsymbol{\rho}$  (3.6), we have that

$$\|\tilde{\mathbf{b}}\|_{\ell^\infty} \leq C(h + h|u'_{K+1/2}| + h^2|u''_{K+1/2}| + h^2|u'''_{K+1/2}|).$$

The  $|u'''_{K+1/2}|$  contribution from  $\Delta\boldsymbol{\rho}$  does not have  $h^3$  as coefficient since  $K$  may scale linearly with  $N = 1/h$ . In general, we only have that  $hK \leq 1$ .

Applying Lemma 3.3, we see that  $\tilde{\mathbf{x}}$  is  $O(h)$ , and by (3.19), so is  $\mathbf{x}$ . From (3.18), we finally conclude (3.20).  $\square$

**3.3. Total error.** Combining the estimates (3.11) and (3.10) given in Lemma 3.1 for  $\mathbf{e}_\sigma$  with the estimate (3.20) in Lemma 3.2 for  $\mathbf{e}_\rho$ , we obtain from the triangle inequality that

**Theorem 3.1.** *Let  $\mathbf{e}$  denote the QCE error. Then for  $1 \leq p \leq \infty$ ,  $2 \leq K \leq N - 2$ , and  $h$  sufficiently small, the error can be bounded by*

$$\begin{aligned} \|\mathbf{e}\|_{\ell_h^\infty} &\leq Ch \left(1 + |u'_{K+1/2}| + h|u''_{K+1/2}| + h|u'''_{K+1/2}| + h \left\| u_e^{(4)} \right\|_{L^2} \right), \\ \|D\mathbf{e}\|_{\ell_h^p} &\leq Ch^{1/p} \left(1 + |u'_{K+1/2}| + h|u''_{K+1/2}| + h|u'''_{K+1/2}| + h \left\| u_e^{(4)} \right\|_{L^2} \right). \end{aligned}$$

We note that the above argument giving optimal order estimates in Theorem 3.1 only utilized the estimate  $\Delta\rho = O(1)$ , rather than the optimal estimate  $\Delta\rho = O(h)$  given in (3.6).

Although our theorems give optimal order rates of convergence, our assumptions on the required regularity on  $u_e$  is not optimal. We have assumed for simplicity of exposition that  $\left\| u_e^{(4)} \right\|_{L^2} < \infty$  and used the estimate (3.7). Lower order estimates for  $\sigma$  such as

$$\|\sigma\|_{\ell_h^2} \leq Ch^{2-s} \left\| u_e^{(4-s)} \right\|_{L^2}, \quad 2 < s < 4,$$

can be used to reduce the regularity assumptions on  $u_e$  and still obtain optimal rates of convergence. Assuming the full regularity on  $u_e$  also makes possible the precise identification and removal of the lower order terms in the error by the modification of the atomistic-to-continuum coupling scheme.

#### 4. CONVERGENCE OF THE QUASI-NONLOCAL QUASICONTINUUM SOLUTION

For the quasi-nonlocal approximation, we split the residual as

$$L^{qnl,h} \mathbf{e} = L^{qnl,h} \mathbf{u}_e - \mathbf{f} = \boldsymbol{\rho} + \boldsymbol{\sigma}, \quad (4.1)$$

where

$$\boldsymbol{\rho} = \begin{cases} 0, & 0 \leq j \leq K-1, \\ -\phi_{2F}'' u_{K+1/2}'' - \frac{1}{2} \phi_{2F}'' u_{K+1/2}''' h, & j = K, \\ \phi_{2F}'' u_{K+1/2}'' - \frac{1}{2} \phi_{2F}'' u_{K+1/2}''' h, & j = K+1, \\ 0, & K+2 \leq j \leq N, \end{cases} \quad (4.2)$$

and where

$$\|\sigma\|_{\ell_h^p} \leq Ch^2 \left\| u_e^{(4)} \right\|_{L^p}.$$

The residual maximum norm  $\|\boldsymbol{\rho}\|_{\ell_h^\infty}$  here is  $O(1)$  as opposed to the energy-based quasicontinuum which has a  $O(1/h)$  residual maximum norm. However, the sum of  $\boldsymbol{\rho}$  is similarly  $O(h)$ , that is,

$$\Delta\rho = -h\phi_{2F}'' u_{K+1/2}'''. \quad (4.3)$$

A similar argument as in the QCE case follows. We split the error as

$$\mathbf{e} = \mathbf{e}_\rho + \mathbf{e}_\sigma,$$

where

$$\begin{aligned} L^{qnl,h} \mathbf{e}_\rho &= \boldsymbol{\rho}, & e_{\rho,j} &= -e_{\rho,-j}, \\ L^{qnl,h} \mathbf{e}_\sigma &= \boldsymbol{\sigma}, & e_{\sigma,j} &= -e_{\sigma,-j}. \end{aligned}$$

The same arguments apply to give the bounds (3.11) and (3.10) on  $\mathbf{e}_\sigma$ . Thus, we need to work through the modified argument to bound  $\mathbf{e}_\rho$ . Since  $\rho$  is non-zero only at  $j = \pm\{K, K+1\}$ , the odd solution  $\mathbf{e}_\rho$  has the form

$$e_{\rho,j} = \begin{cases} m_1 h j + \beta \left( \frac{\lambda^j - \lambda^{-j}}{\lambda^K} \right), & 0 \leq j \leq K, \\ m_2 h j - m_2, & K+1 \leq j \leq N. \end{cases} \quad (4.4)$$

Summing across the interface again gives

$$\begin{aligned} \Delta \rho &:= \sum_{j=K-1}^{K+2} \rho_j = \sum_{j=K-1}^{K+2} (L^{qce,h} \mathbf{e}_\rho)_j \\ &= (\phi_F'' + 4\phi_{2F}'') \left( \frac{m_1}{h} - \frac{m_2}{h} \right). \end{aligned}$$

Thus, we have again that

$$m_1 = m_2 + \frac{h \Delta \rho}{\phi_F'' + 4\phi_{2F}''}. \quad (4.5)$$

We focus on the equations at  $j = K-1, K$ , and  $K+1$  and split the interface equations as  $(A + hB)\mathbf{x} = \mathbf{b}$ , where

$$\begin{aligned} A &= \begin{bmatrix} 0 & \phi_{2F}'' & \phi_{2F}'' \gamma_{K+1} \\ 0 & \phi_F'' + 2\phi_{2F}'' & \phi_F'' \gamma_{K+1} + \phi_{2F}'' \gamma_{K+2} + \phi_{2F}'' \gamma_K \\ 0 & -\phi_F'' - 3\phi_{2F}'' & -\phi_F'' \gamma_K - 2\phi_{2F}'' \gamma_K - \phi_{2F}'' \gamma_{K-1} \end{bmatrix}, \\ B &= \begin{bmatrix} (K+1)\phi_{2F}'' & -(K+1)\phi_{2F}'' & 0 \\ (K+1)(\phi_F'' + \phi_{2F}'') & -(K+1)(\phi_F'' + \phi_{2F}'') & 0 \\ -K(\phi_F'' + 3\phi_{2F}'') + \phi_{2F}'' & K(\phi_F'' + 3\phi_{2F}'') - \phi_{2F}'' & 0 \end{bmatrix}, \\ \mathbf{x} &= \begin{bmatrix} m_1 \\ m_2 \\ \beta \end{bmatrix}, \quad \mathbf{b} = h^2 \begin{bmatrix} \rho_{K-1} \\ \rho_K \\ \rho_{K+1} \end{bmatrix}. \end{aligned} \quad (4.6)$$

Using the equality (4.5), we rewrite the above as  $\tilde{A}_K \tilde{\mathbf{x}} = \tilde{\mathbf{b}}$  where

$$\begin{aligned} \tilde{A}_K &= \begin{bmatrix} \phi_{2F}'' & \phi_{2F}'' \gamma_{K+1} \\ \phi_F'' + 2\phi_{2F}'' & \phi_F'' \gamma_{K+1} + \phi_{2F}'' \gamma_{K+2} + \phi_{2F}'' \gamma_K \end{bmatrix}, \\ \mathbf{x} &= \begin{bmatrix} m_2 \\ \beta \end{bmatrix}, \quad \tilde{\mathbf{b}} = h^2 \begin{bmatrix} \rho_{K-1} \\ \rho_K \end{bmatrix} + h^2 \frac{\Delta \rho}{\phi_F'' + \phi_{2F}''} \begin{bmatrix} (K+1)\phi_{2F}'' \\ (K+1)(\phi_F'' + \phi_{2F}'') \end{bmatrix}. \end{aligned} \quad (4.7)$$

We have omitted the second equation, as the full system is linearly dependent after substitution of  $m_1$ . We have that  $\tilde{A}_K$  has full rank and  $\|\tilde{\mathbf{b}}\|_{\ell^\infty} \leq Ch^2(|u_{K+1/2}''| + |u_{K+1/2}''')|$ , so that we obtain the following error estimate for the quasi-nonlocal approximation.

**Theorem 4.1.** *Let  $\mathbf{e}$  be the solution to the quasi-nonlocal error equation (4.1). Then for  $1 \leq p \leq \infty$ ,  $2 \leq K \leq N-2$ , and  $h$  sufficiently small, the error can be bounded by*

$$\begin{aligned} \|\mathbf{e}\|_{\ell_h^\infty} &\leq Ch^2 \left( |u_{K+1/2}''| + |u_{K+1/2}'''| + \|u_e^{(4)}\|_{L^2} \right), \\ \|D\mathbf{e}\|_{\ell_h^p} &\leq Ch^{1+1/p} \left( |u_{K+1/2}''| + |u_{K+1/2}'''| + \|u_e^{(4)}\|_{L^2} \right), \end{aligned}$$

where  $C > 0$  is independent of  $h, K$ , and  $p$ .

We note that the proof above of the optimal order estimates for the quasi-nonlocal approximation does use the full  $O(h)$  order of the estimate (4.3) for  $\Delta\rho$ .

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