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Stability, Instability, and Error of the Force-based Quasicontinuum Approximation

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Abstract Due to their algorithmic simplicity and high accuracy, force-based model coupling techniques are popular tools in computational physics. For example, the force-based quasicontinuum (QCF) approximation is the only known pointwise consistent quasicontinuum approximation for coupling a general atomistic model with a finite element continuum model. In this paper, we present a detailed stability and error analysis of this method. Our optimal order error estimates provide a theoretical justification for the high accuracy of the QCF approximation: they clearly demonstrate that the computational efficiency of continuum modeling can be utilized without a significant loss of accuracy if defects are captured in the atomistic region.

The main challenge we need to overcome is the fact that the linearized QCF operator is typically *not* positive definite. Moreover, we prove that no uniform inf-sup stability condition holds for discrete versions of the $W^{1,p}$-$W^{1,q}$ "duality pairing" with $1/p + 1/q = 1$, if $1 \leq p < \infty$. However, we were able to establish an inf-sup stability condition for a discrete version of the

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$W^{1,\infty}$-$W^{1,1}$ "duality pairing" which leads to optimal order error estimates in a discrete $W^{1,\infty}$-norm.

1 Introduction

Localized defects in materials typically interact with elastic fields far beyond the defects' atomic neighborhood. Accurately computing the structure of localized defects requires the use of atomistic models; however, atomistic models are too computationally demanding to be utilized for the entire interacting system. The goal of atomistic to continuum coupling methods such as the quasicontinuum (QC) method is to use the computationally intensive, fully atomistic calculations only in regions with highly non-uniform deformations such as neighborhoods of dislocations, crack tips, and grain boundaries; and to use a (local) continuum model in regions with nearly uniform deformations to reduce the number of degrees of freedom.

The initial computational results obtained with the QC method have excited the materials science community with the promise of the simulation of heretofore inaccessible multiscale materials problems [20, 27, 36]. Variants of the QC method have continued to be developed with the introduction of adaptive methods, improved mesh generation, and faster solvers [1, 2, 8, 16, 25, 31, 33]; yet, in common with many other multiscale methods it lacks the theoretical basis to be considered a predictive computational method.

During the past few years, a mathematical structure has been given to the description and analysis of various flavors of the QC method, clarifying the relation between different approximations and the corresponding sources of error [3,7,9,14,15,17,18,23,24,26,29,30]. In the present paper, we contribute to this effort by providing a detailed stability and error analysis of the force-based quasicontinuum approximation.

Considerable concern has been generated by the discovery that early QC approximations exhibit "ghost" forces in the atomistic to continuum interface when the material is subject to a uniform strain, that is, they do not satisfy the "patch test" criterion of computational mechanics. In the language of numerical analysis, this means that the QC approximation is not consistent with the underlying atomistic model. The first remedy, which is still commonly employed, is known as the ghost force correction. It first applies a dead load that corrects the ghost forces at the current state of a continuation process, then increments the parameter value for the process, then reminimizes the energy at the new parameter value and dead load, and finally recomputes the ghost force corrections for use as a dead load at the next step of the continuation process [27, 33]. In [7, 8] this process was identified as an iterative method to approximate the solution to the equilibrium equations for a purely force-based coupling approach, which we label the *force-based quasicontinuum (QCF) approximation*. This formulation of the QCF method has enabled the development of more efficient iterative and continuation methods for its solution and a more precise understanding of the error [7, 8]. Related force-based modeling approaches, which couple an atomistic region with a continuum region modeled by linear elasticity can be found in [21, 34].

Other research groups have proposed QC approximations that utilize special interfacial atoms at the atomistic to continuum interface in an attempt to develop an energy-based QC method that does not suffer from the ghost force problem mentioned above [14, 35]. The quasi-nonlocal (QNL) approach [35] is easy to implement and removes ghost forces for short range interactions (depending on the lattice structure), but ghost forces remain for longer range interactions. This method was generalized in the reconstruction approach [14] which, in theory, allows for the elimination of all ghost forces; however, explicit methods have only been constructed for planar interfaces so far. Moreover, a computationally efficient implementation of this method has yet to be proposed.

Both of the above methods [14,35] couple the original atomistic model to a new atomistic model with local interactions. To allow for the reduction of degrees of freedom by piecewise linear interpolation in the continuum region as in the finite element method, it is necessary to further couple this local atomistic model to a volume-based local model. However, it is not known how to couple a local atomistic model to a volume-based local model along a nonplanar interface without introducing ghost forces [14]. In contrast, the QCF approximation allows arbitrary atomistic to continuum interfaces and coarsening without ghost forces.

Rather than computing forces from a total energy, the QCF approximation directly assigns forces using a simple rule: *the force on an atom in the atomistic region is computed from the force law of the atomistic model, while the force on a degree of freedom in the continuum region is computed from the force law of the continuum (finite element) approximation* [7, 8]. There is no modification of these equations near the atomistic to continuum interface and it is therefore easy to see (Section 2.3) that the QCF equilibrium equations are consistent with the underlying atomistic model, and in particular, that there are no ghost forces in this approximation. In fact, we will show in Section 2.3 that the QCF approximation has an $\mathrm{O}(\epsilon^2)$ truncation error in the atomistic to continuum interface for all smoothly varying strains. By contrast, it has been shown in [10] that, even when it succeeds in removing ghost forces, the QNL method has an $\mathrm{O}(1)$ truncation error in the atomistic to continuum interfaces for a nonuniform but smooth strain. (This is nevertheless a significant improvement over the $\mathrm{O}(1/\epsilon)$ truncation error in the original QC method.)

With the exception of [30], error analyses of energy-based QC methods have utilized the coercivity (positive-definiteness) of the linearization of the QC equilibrium equations about the energy-minimizing solution [10, 15, 29]. A recent attempt to establish an error analysis for the QCF method has presented an invalid proof of coercivity of the linearized equilibrium equations and an error analysis based on this incorrect coercivity result [28]. In the present paper we prove that, typically, the linearization of the QCF equilibrium equations is *not* coercive (cf. Theorem 1), and consequently, our error analysis will be based on a more general inf-sup stability condition. However, even this more general approach will fail unless the function spaces are chosen with great care. We show in Section 5 that the linearized QCF operator is stable with respect to a discrete version of the $W^{1,\infty}$-$W^{1,1}$ pairing, uni-

formly with respect to the number of atoms, but we show in Section 7 that it is *not* uniformly stable with respect to any other $W^{1,p}$-$W^{1,q}$ pairing where $\frac{1}{p} + \frac{1}{q} = 1$.

Our goal in this paper is to clearly present our techniques in the simplest setting. For this reason, we restrict our presentation to a one-dimensional chain of atoms which interact with nearest and next-nearest neighbors. To further simplify the setting, we consider a linearization of the force-based equilibrium equations about a uniform strain. Although the QCF approximation can be directly formulated and implemented with mesh coarsening in the continuum region, we only consider the modeling error due to the QCF approximation itself and do not consider the coarsening error. Each of these extensions deserve a careful analysis in order to firmly establish the mathematical foundation of the QCF approximation and will be discussed further in the conclusion.

The main result of the present paper is that the strain error for the QCF approximation is $\mathrm{O}(\epsilon^2)$, where ϵ is the lattice spacing scaled by the material dimension. The prefactor for the ϵ^2 error term is a maximum norm of a third divided difference of the displacement restricted to the continuum region only. Thus, our analysis predicts the observed high accuracy of the QCF method when defects are modeled in the atomistic region.

In Section 2, we present a detailed description of the QCF approximation and a first estimate of the truncation error with respect to the fully atomistic model. In Section 3, we show how to formulate the QCF approximation in a "weak form" that allows us to study its stability by considering discrete versions of the $W^{1,p}$-$W^{1,q}$ "duality pairing." This is equivalent to putting the QCF operator into a divergence form, which will indicate an interesting nonlocal effect of the atomistic to continuum interface. This nonlocal effect is the source of the lack of coercivity which we establish in Section 4, based on the explicit construction of an unstable displacement. In Section 5, we derive inf-sup stability results that are then combined, in Section 6, with negative-norm truncation error estimates, to obtain optimal order error estimates for the QCF approximation. We conclude, in Section 7, by showing the lack of a uniform inf-sup constant for many other common choices of duality pairings.

2 The Force-Based Quasicontinuum Approximation

We consider a one-dimensional atomistic chain whose $2M + 1$ atoms occupy the reference positions $x_j = j\epsilon$, where ϵ is the atomic spacing in the reference configuration, and which interact with their nearest and next-nearest neighbors. We denote the deformed positions by y_j for $j = -M, \ldots, M$. The boundary atoms are constrained by

$$y_{-M} = -FM\epsilon \quad \text{and} \quad y_M = FM\epsilon,$$

where $F > 0$ is a macroscopic deformation gradient. The total energy of a deformation $\mathbf{y} \in \mathbb{R}^{2M+1}$ is given by

$$\mathcal{E}^a(\mathbf{y}) - \sum_{j=-M}^{M} \epsilon f_j y_j, \tag{1}$$

where

$$\mathcal{E}^a(\mathbf{y}) = \sum_{j=-M+1}^{M} \epsilon\phi\Big(\frac{y_j - y_{j-1}}{\epsilon}\Big) + \sum_{j=-M+2}^{M} \epsilon\phi\Big(\frac{y_j - y_{j-2}}{\epsilon}\Big), \tag{2}$$

and where ϕ is a scaled two-body interatomic potential (for example, the normalized Lennard-Jones potential $\phi(r) = r^{-12} - 2r^{-6}$) and and f_j, $j = -M, \ldots, M$ are external forces. The equilibrium equations are given by the force balance conditions at the free atoms,

$$\begin{aligned} F_j^a(\mathbf{y}) + f_j &= 0 \qquad \text{for} \quad j = -M+1, \ldots, M-1, \\ y_j &= Fj\epsilon \qquad \text{for} \quad j = -M,\, M, \end{aligned} \tag{3}$$

where the atomistic force (per lattice spacing ϵ) is given by

$$\begin{aligned} F_j^a(\mathbf{y}) &:= -\frac{1}{\epsilon}\frac{\partial \mathcal{E}^a(\mathbf{y})}{\partial y_j} \\ &= \frac{1}{\epsilon}\Bigg\{ \left[\phi'\left(\frac{y_{j+1} - y_j}{\epsilon}\right) + \phi'\left(\frac{y_{j+2} - y_j}{\epsilon}\right)\right] \\ &\qquad - \left[\phi'\left(\frac{y_j - y_{j-1}}{\epsilon}\right) + \phi'\left(\frac{y_j - y_{j-2}}{\epsilon}\right)\right] \Bigg\}. \end{aligned} \tag{4}$$

In (4) the undefined terms $\phi'(\frac{1}{\epsilon}(y_{-M+1} - y_{-M-1}))$ and $\phi'(\frac{1}{\epsilon}(y_{M+1} - y_{M-1}))$ are taken to be zero.

We let u_j be a perturbation from the uniformly deformed state $y_j^F = Fj\epsilon$, that is, we define

$$u_j = y_j - Fj\epsilon \quad \text{for } j = -M, \ldots, M.$$

We linearize the atomistic equilibrium equations (3) about the deformed state $\mathbf{y}^F$, resulting in the linear system

$$\begin{aligned} (L^a\mathbf{u}^a)_j &= f_j \qquad \text{for} \quad j = -M+1, \ldots, M-1, \\ u_j^a &= 0 \qquad \text{for} \quad j = -M,\, M, \end{aligned} \tag{5}$$

where $(L^a\mathbf{v})_j$, for a displacement $\mathbf{v} \in \mathbb{R}^{2M+1}$, is given by

$$(L^a\mathbf{v})_j := \begin{cases} \phi_F''\left[\dfrac{-v_{j+1} + 2v_j - v_{j-1}}{\epsilon^2}\right] + \phi_{2F}''\left[\dfrac{-v_{j+2} + v_j}{\epsilon^2}\right], \\ \qquad\qquad \text{for } j = -M+1, \\ \phi_F''\left[\dfrac{-v_{j+1} + 2v_j - v_{j-1}}{\epsilon^2}\right] + \phi_{2F}''\left[\dfrac{-v_{j+2} + 2v_j - v_{j-2}}{\epsilon^2}\right], \\ \qquad\qquad \text{for } j = -M+2, \ldots, M-2, \\ \phi_F''\left[\dfrac{-v_{j+1} + 2v_j - v_{j-1}}{\epsilon^2}\right] + \phi_{2F}''\left[\dfrac{v_j - v_{j-2}}{\epsilon^2}\right], \\ \qquad\qquad \text{for } j = M-1. \end{cases}$$

Here and throughout we define $\phi''_F := \phi''(F)$ and $\phi''_{2F} := \phi''(2F)$, where ϕ is the interatomic potential in (2). We assume that $\phi''_F > 0$ and $\phi''_{2F} < 0$, which holds for typical pair potentials such as the Lennard-Jones potential under physically relevant deformations. We remark that, for $\phi''_F + 4\phi''_{2F} > 0$, the system (5) has a unique solution. This follows from (14) and from Lemma 4 (see also [10,11] for an analysis of the periodic case which is similar).

The local QC approximation uses the Cauchy-Born extrapolation rule to approximate the nonlocal atomistic model by a local continuum model [7,15, 27,36]. In our context, this corresponds to approximating $y_j - y_{j-2}$ in (2) by $2(y_j - y_{j-1})$ and results in the local QC energy

$$\mathcal{E}^{lqc}(\mathbf{y}) = \sum_{j=-M+1}^{M} \epsilon \left[\phi\left(\frac{y_j - y_{j-1}}{\epsilon} \right) + \phi\left(\frac{2(y_j - y_{j-1})}{\epsilon} \right) \right]. \tag{6}$$

Note that the above expression has one more next-nearest neighbor term than (2). This is because the atoms at $j = -M+1, M-1$ do not "feel" the effect of the boundary in the local approximation. The local QC equilibrium equations are then given by

$$\begin{aligned} F_j^{lqc}(\mathbf{y}) + f_j &= 0 \qquad \text{for} \quad j = -M+1, \ldots, M-1, \\ y_j &= Fj\epsilon \qquad \text{for} \quad j = -M,\, M, \end{aligned}$$

where the local QC force (per lattice spacing ϵ) is given by

$$\begin{aligned} F_j^{lqc}(\mathbf{y}) &:= -\frac{1}{\epsilon} \frac{\partial \mathcal{E}^{lqc}(\mathbf{y})}{\partial y_j} \\ &= \frac{1}{\epsilon} \Bigg\{ \left[\phi'\left(\frac{y_{j+1} - y_j}{\epsilon} \right) + 2\phi'\left(\frac{2(y_{j+1} - y_j)}{\epsilon} \right) \right] \\ &\quad - \left[\phi'\left(\frac{y_j - y_{j-1}}{\epsilon} \right) + 2\phi'\left(\frac{2(y_j - y_{j-1})}{\epsilon} \right) \right] \Bigg\}. \end{aligned} \tag{7}$$

Linearizing the local QC equilibrium equations (7) about the deformed state $\mathbf{y}^F$ results in

$$\begin{aligned} (L^{lqc}\mathbf{u}^{lqc})_j &= f_j \qquad \text{for} \quad j = -M+1, \ldots, M-1, \\ u_j^{lqc} &= 0 \qquad \text{for} \quad j = -M,\, M, \end{aligned}$$

where $(L^{lqc}\mathbf{v})_j$, for a displacement $\mathbf{v} \in \mathbb{R}^{2M+1}$, is given by

$$(L^{lqc}\mathbf{v})_j = (\phi''_F + 4\phi''_{2F}) \left[\frac{-v_{j+1} + 2v_j - v_{j-1}}{\epsilon^2} \right], \quad j = -M+1, \ldots, M-1.$$

The increased efficiency of the local QC approximation is obtained when its equilibrium equations (7) are coarsened by reducing the degrees of freedom using piecewise linear interpolation between a subset of the atoms [7,27]. For the sake of simplicity of exposition, we do not treat coarsening in this paper.

In order to combine the accuracy of the atomistic model with the efficiency of the local QC approximation, the QCF method decomposes the reference lattice into an *atomistic region* $\mathcal{A}$ and a *continuum region* $\mathcal{C}$, and assigns forces to atoms according to the region they are located in. Since the local QC energy (6) approximates $y_j - y_{j-2}$ in (1) by $2(y_j - y_{j-1})$, it is clear that the atomistic model should be retained wherever the strains are varying rapidly. The QCF operator is then given by [7,8]

$$F_j^{qcf}(\mathbf{y}) = \begin{cases} F_j^a(\mathbf{y}) & \text{if } j \in \mathcal{A}, \\ F_j^{lqc}(\mathbf{y}) & \text{if } j \in \mathcal{C}, \end{cases} \tag{8}$$

and the QCF equilibrium equations by

$$\begin{aligned} F_j^{qcf}(\mathbf{y}) + f_j = 0 \qquad & \text{for} \quad j = -M+1, \ldots, M-1, \\ y_j = Fj\epsilon \qquad & \text{for} \quad j = -M,\, M. \end{aligned}$$

The QCF approximation gets its name from the assignment of forces at the atoms in (8). Most other QC approximations build a total energy by summing energy contributions from each region and compute forces on the atoms by differentiating the energy. However, F^{qcf} is a non-conservative force field and cannot be derived from an energy [7].

2.1 Artificial boundary conditions for the computational domain

For large atomistic systems it is necessary to reduce the computational domain, even when a coarse-graining method such as the QC approximation is employed. The reduction of the computational domain requires the use of *artificial boundary conditions* to approximate the effect of the far field. The artificial boundary condition most commonly used in the QC method (and in other atomistic to continuum approximations) sets the displacement to zero at the boundary of the computational domain, for example, at the lateral boundary of the crystal in the nanoindentation problem reported in [19]. More accurate artificial boundary conditions such as those proposed and analyzed in [22] do not seem to have yet been used in QC computations.

We chose to imitate the approach commonly used in the QC method, by choosing $N \ll M$ and $0 < K < N-1$, and letting $\{-N, \ldots, N\}$ be the computational domain. Defining

$$\mathcal{A} = \{-K, \ldots, K\} \quad \text{and} \quad \mathcal{C} = \{-N+1, \ldots, N-1\} \setminus \mathcal{A},$$

to be, respectively, the atomistic and continuum region, the QCF approximation on the computational domain is given by

$$\begin{aligned} F_j^{qcf}(\mathbf{y}) + f_j = 0 \qquad & \text{for} \quad j = -N+1, \ldots, N-1, \\ y_j = Fj\epsilon \qquad & \text{for} \quad j = -N,\, N, \end{aligned} \tag{9}$$

In this paper, we analyze the linearization of (9) about $\mathbf{y}^F$,

$$\begin{aligned} (L^{qcf}\mathbf{u}^{qcf})_j = f_j \qquad & \text{for} \quad j = -N+1, \ldots, N-1, \\ u_j^{qcf} = u_j^a \qquad & \text{for} \quad j = -N,\, N, \end{aligned} \tag{10}$$

where we have taken $u^{qcf}_{-N} = u^a_{-N}$ and $u^{qcf}_N = u^a_N$ so that we may ignore the error induced by the artificial boundary condition and exclusively focus on the error of the QC approximation. Note that, since atoms near the artificial boundary belong to $\mathcal{C}$, only one boundary condition is required at each end.

Setting $\epsilon = 1/N$ throughout, we rescale the problem in the usual way [6], so that the size of the computational domain is of order O(1).

2.2 Notation

We use $D : \mathbb{R}^{2N+1} \to \mathbb{R}^{2N}$ to denote the backward difference operator, defined by

$$(D\mathbf{v})_j = Dv_j = \frac{v_j - v_{j-1}}{\epsilon} \quad \text{for } j = -N+1, \ldots, N.$$

We will frequently employ the weighted ℓ^p-norms,

$$\|\mathbf{v}\|_{\ell^p_\epsilon} := \left(\epsilon \sum_{j=-N}^{N} |v_j|^p \right)^{1/p}, \qquad 1 \le p < \infty,$$
$$\|\mathbf{v}\|_{\ell^\infty_\epsilon} := \max_{-N \le j \le N} |v_j|,$$

and the weighted inner product

$$\langle \mathbf{v}, \mathbf{w} \rangle = \sum_{j=-N}^{N} \epsilon v_j w_j.$$

The definition of the difference operator D, of the norms $\|\mathbf{v}\|_{\ell^p_\epsilon}$ and of the inner product $\langle \mathbf{v}, \mathbf{w} \rangle$ is extended, in an obvious way, for vectors $\mathbf{v}, \mathbf{w} \in \mathbb{R}^K$, where $K \in \mathbb{N}$ is arbitrary. For example, if $\mathbf{v} \in \mathbb{R}^{2M+1}$ then $D\mathbf{v} \in \mathbb{R}^{2M}$. Moreover, in view of this convention, the higher order difference operators D^2, etc., can be defined by successive application of D; for example, $D^2 v_j = \epsilon^{-2}(v_j - 2v_{j-1} + v_{j-2})$.

The subspace of $\mathbb{R}^{2N+1}$ with homogeneous boundary conditions is denoted

$$\mathcal{V}_0 = \big\{ \mathbf{v} \in \mathbb{R}^{2N+1} : v_{-N} = v_N = 0 \big\}.$$

For future reference we note that the following Poincaré inequality holds [30, Lemma A.3]:

$$\|\mathbf{v}\|_{\ell^\infty_\epsilon} \le \tfrac{1}{2} \|D\mathbf{v}\|_{\ell^1_\epsilon} \qquad \text{for all } \mathbf{v} \in \mathcal{V}_0. \tag{11}$$

Furthermore, we note that the linear operator L^{qcf} which has been defined above as a mapping from $\mathbb{R}^{2N+1}$ to $\mathbb{R}^{2N-1}$ will be considered below to be a mapping from $\mathbb{R}^{2N+1}$ to $\mathcal{V}_0$ by the extension

$$(L^{qcf}\mathbf{v})_{-N} = (L^{qcf}\mathbf{v})_N = 0 \qquad \text{for } \mathbf{v} \in \mathbb{R}^{2N+1}.$$

With this in mind, $\langle L^{qcf}\mathbf{v}, \mathbf{w} \rangle$ is well-defined for all $\mathbf{v}, \mathbf{w} \in \mathbb{R}^{2N+1}$.

2.3 Pointwise consistency of the force-based QC approximation

The remarkable simplicity of the formulation of the QCF approximation is mirrored by its equally striaghtforward consistency analysis. Let $\mathbf{u}^a$ be the solution to (5) (assuming $\phi_F'' + 4\phi_{2F}'' > 0$, this system is well-posed), then the truncation error $\mathbf{t} \in \mathbb{R}^{2N+1}$ is defined by $t_{-N} = t_N = 0$ and

$$t_j = (L^{qcf}\mathbf{u}^a - \mathbf{f})_j = (L^{qcf}\mathbf{u}^a - L^a\mathbf{u}^a)_j \qquad \text{for} \quad j = -N+1, \ldots, N-1,$$

where $L^{qcf}\mathbf{u}^a$ is understood by restricting $\mathbf{u}^a$ to the computational domain. Since $(L^{qcf}\mathbf{u}^a)_j = (L^a\mathbf{u}^a)_j$ trivially holds for $j \in \mathcal{A}$ we have $t_j = 0$ for $j \in \mathcal{A}$. For $j \in \mathcal{C}$, on the other hand, we have

$$\begin{aligned}
t_j &= (L^{qcf}\mathbf{u}^a - L^a\mathbf{u}^a)_j \\
&= \phi_{2F}'' \left[4\frac{-u_{j+1}^a + 2u_j^a - u_{j-1}^a}{\epsilon^2} - \frac{-u_{j+2}^a + 2u_j^a - u_{j-2}^a}{\epsilon^2} \right] \\
&= \epsilon^2 \phi_{2F}'' \left[\frac{u_{j+2}^a - 4u_{j+1}^a + 6u_j^a - 4u_{j-1}^a + u_{j-2}^a}{\epsilon^4} \right] \\
&= \epsilon^2 \phi_{2F}'' (\bar{D}^4\mathbf{u}^a)_j,
\end{aligned}$$

where $(\bar{D}^4\mathbf{v})_j = (D^4\mathbf{v})_{j+2}$ is a fourth-order centered finite difference operator. Note also that $\mathbf{u}^a$ is defined outside the computational domain. Thus, for $p \in [1, \infty]$, we obtain an exact truncation error estimate,

$$\|\mathbf{t}\|_{\ell_\epsilon^p} = \epsilon^2 |\phi_{2F}''| \|\bar{D}^4\mathbf{u}^a\|_{\ell_\epsilon^p(\mathcal{C})}, \tag{12}$$

where the label $\mathcal{C}$ indicates that the summation (or maximum) is only taken over atoms in the continuum region.

We have presented the calculations leading up to (12) as a simple argument for the high level of consistency of the QCF method, however, in the error analysis in Section 6 we will use a slightly sharper negative-norm estimate. We also note that, since the computational domain is far from the boundary of the full atomistic domain where boundary layers may occur, it follows from the interior regularity of elliptic finite difference operators [37] that $\|\bar{D}^4\mathbf{u}^a\|_{\ell_\epsilon^p(\mathcal{C})}$ is bounded in the continuum limit $\epsilon \to 0$, provided that $\mathbf{f}$ is the restriction of a smooth function in a neighborhood of the continuum region $\mathcal{C}$ to the lattice points.

To estimate the error between the atomistic and QCF solution, we write

$$L^{qcf}(\mathbf{u}^a - \mathbf{u}^{qcf}) = \mathbf{t} = O(\epsilon^2 |\phi_{2F}''|).$$

Hence, a uniform stability result for the operator L^{qcf} in an appropriate norm would lead to an optimal error estimate. As we have already remarked in the introduction and will make precise in Theorem 1, L^{qcf} is typically *not* coercive and we must therefore prove an inf-sup condition instead. To this end, we will factor the L^{qcf} operator into divergence form, $L^{qcf} = D^T E^{qcf} D$, where D is the discrete difference operator defined above. We will give conditions under which E^{qcf} is row diagonally-dominant and which will lead to an

inf-sup condition for L^{qcf}. Interestingly, however, this approach only leads to uniform stability bounds if the ℓ^∞_ϵ-ℓ^1_ϵ duality pairing is used, while the inf-sup constants for the ℓ^p_ϵ-ℓ^q_ϵ ($1/p + 1/q = 1$, $1 \leq p < \infty$) pairings are not uniform in N (cf. Section 7).

3 Divergence Form of the QCF Operator

We will analyze the QCF equilibrium equations (10) by putting them into a "weak form:" *find* $\mathbf{u}^{qcf} \in \mathbb{R}^{2N+1}$ *such that*

$$\begin{aligned} \langle E^{qcf} D\mathbf{u}^{qcf}, D\mathbf{w}\rangle &= \langle \mathbf{f}, \mathbf{w}\rangle \qquad \text{for all } \mathbf{w} \in \mathcal{V}_0, \\ u^{qcf}_j &= u^a_j \qquad \text{for } j = -N,\, N, \end{aligned}$$

where the linear operator $E^{qcf} : \mathbb{R}^{2N} \to \mathbb{R}^{2N}$ is chosen so that

$$\langle E^{qcf} D\mathbf{v}, D\mathbf{w}\rangle = \langle L^{qcf}\mathbf{v}, \mathbf{w}\rangle \qquad \text{for all } \mathbf{v} \in \mathbb{R}^{2N+1} \text{ and } \mathbf{w} \in \mathcal{V}_0. \tag{13}$$

We call E^{qcf} the conjugate operator. This operator was previously derived for a Neumann problem in [7] and for a problem with mixed boundary conditions in [8].

To motivate the idea we briefly review the conjugate operator for the full atomistic model before deriving E^{qcf}. The atomistic energy (and similarly all QC energies) can be written as functions of the strain $D\mathbf{u}$, $\widehat{\mathcal{E}}^a(D\mathbf{u}) := \mathcal{E}^a(\mathbf{y})$, and its conjugate operator is defined by [7, 8]

$$\left(E^a(\mathbf{r})\right)_j := \frac{1}{\epsilon}\frac{\partial \widehat{\mathcal{E}}^a}{\partial r_j}(\mathbf{r}).$$

Thus, $\left(E^a(\mathbf{r})\right)_j$ is the negative of the force conjugate to the strain $(D\mathbf{u})_j$. It follows from the chain rule that

$$\begin{aligned} F^a_j(\mathbf{y}) := -\frac{1}{\epsilon}\frac{\partial \mathcal{E}^a(\mathbf{y})}{\partial y_j} &= \frac{1}{\epsilon}\left[\frac{\partial \widehat{\mathcal{E}}^a}{\partial r_{j+1}}(\mathbf{r}) - \frac{\partial \widehat{\mathcal{E}}^a}{\partial r_j}(\mathbf{r})\right] \\ &= \left(E^a(\mathbf{r})\right)_{j+1} - \left(E^a(\mathbf{r})\right)_j. \end{aligned}$$

Applying this calculation to the linearized operator L^a, one can easily verify that

$$\langle L^a\mathbf{v}, \mathbf{w}\rangle = \langle E^a D\mathbf{v}, D\mathbf{w}\rangle \quad \text{for all } \mathbf{v}, \mathbf{w} \in \mathbb{R}^{2M+1}, \text{ s.t. } w_{-M} = w_M = 0,$$

where

$$E^a = \phi''_F I + \phi''_{2F} \begin{bmatrix} 1 & 1 & & & \\ 1 & 2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 2 & 1 \\ & & & 1 & 1 \end{bmatrix}. \tag{14}$$

From this representation we obtain immediately that, for $\mathbf{v} \in \mathbb{R}^{2M+1}$ and for $\mathbf{w} \in \mathcal{V}_0$, extended by zero outside the computational domain, the operator L^a can be written in the "weak" form

$$\langle L^a \mathbf{v}, \mathbf{w} \rangle = \sum_{j=-N+1}^{N} \epsilon \big[\phi_F'' Dv_j + \phi_{2F}'' \big(Dv_{j+1} + 2Dv_j + Dv_{j-1} \big) \big] Dw_j. \quad (15)$$

This formula will be used in Section 6 to derive a negative-norm truncation error estimate.

To find a representation for the QCF operator L^{qcf} in terms of a conjugate operator we cannot simply carry out the same computation as above, even in the linearized case, since it is not related to any energy functional. Instead, we will first derive a "weak" form for L^{qcf} from which it will be fairly straightforward to construct the conjugate operator. We begin by writing L^{qcf} in the form $L^{qcf} = \phi_F'' L_1 + \phi_{2F}'' L_2$, where

$$(L_1 \mathbf{v})_j = \epsilon^{-2} \big(-v_{j+1} + 2v_j - v_{j-1} \big), \quad j = -N+1, \ldots, N-1, \quad \text{and}$$

$$(L_2 \mathbf{v})_j = \begin{cases} 4\epsilon^{-2} \big(-v_{j+1} + 2v_j - v_{j-1} \big), & j \in \mathcal{C}, \\ \epsilon^{-2} \big(-v_{j+2} + 2v_j - v_{j-2} \big), & j \in \mathcal{A}, \end{cases}$$

and deriving "weak" representations of the operators L_1 and L_2.

Lemma 1 *For all $\mathbf{v} \in \mathbb{R}^{2N+1}$ and $\mathbf{w} \in \mathcal{V}_0$ the nearest neighbor and next-nearest neighbor interaction operators can be written in the form*

$$\langle L_1 \mathbf{v}, \mathbf{w} \rangle = \sum_{j=-N+1}^{N} \epsilon Dv_j Dw_j, \qquad \textit{and}$$

$$\langle L_2 \mathbf{v}, \mathbf{w} \rangle = \langle L_2^{reg} \mathbf{v}, \mathbf{w} \rangle + \epsilon^2 (D^3 v_{-K+1}) w_{-K} - \epsilon^2 (D^3 v_{K+2}) w_K,$$

where D^3 is the third-order backward finite difference operator,

$$D^3 v_j = \epsilon^{-2} (Dv_j - 2Dv_{j-1} + Dv_{j-2}),$$

and where L_2^{reg} denotes the "regular" component of L_2,

$$\langle L_2^{reg} \mathbf{v}, \mathbf{w} \rangle = \sum_{j=-N+1}^{-K} \epsilon 4 Dv_j Dw_j + \sum_{j=K+1}^{N} \epsilon 4 Dv_j Dw_j + \sum_{j=-K+1}^{K} \epsilon (Dv_{j-1} + 2Dv_j + Dv_{j+1}) Dw_j.$$

Proof We only prove the representation for L_2. To simplify the notation, we will perform all manipulations only in the *right* half of the domain and indicate the remaining terms by dots, for example,

$$\langle L_2 \mathbf{v}, \mathbf{v} \rangle = \cdots + \sum_{j=0}^{K} \epsilon (L_2 \mathbf{v})_j w_j + \sum_{j=K+1}^{N-1} \epsilon (L_2 \mathbf{v})_j w_j.$$

The proof simply requires careful summation by parts, performed separately in the continuum and atomistic region. In the right half of the atomistic region, summation by parts yields

$$\begin{aligned}
\sum_{j=0}^{K} \epsilon (L_2 \mathbf{v})_j w_j = & -\sum_{j=0}^{K} \Big[\Big(\frac{v_{j+2} - v_j}{\epsilon} \Big) - \Big(\frac{v_j - v_{j-2}}{\epsilon} \Big) \Big] w_j \\
= & -\sum_{j=2}^{K+2} \Big(\frac{v_j - v_{j-2}}{\epsilon} \Big) w_{j-2} + \sum_{j=0}^{K} \Big(\frac{v_j - v_{j-2}}{\epsilon} \Big) w_j \\
= & \cdots + \sum_{j=2}^{K} \epsilon \big(Dv_j + Dv_{j-1} \big) \big(Dw_j + Dw_{j-1} \big) \\
& - \big[(Dv_{K+1} + Dv_K) w_{K-1} + (Dv_{K+2} + Dv_{K+1}) w_K \big] \\
= & \cdots + \sum_{j=1}^{K} \epsilon \big(Dv_{j+1} + 2Dv_j + Dv_{j-1} \big) Dw_j \\
& - (Dv_{K+2} + 2Dv_{K+1} + Dv_K) w_K .
\end{aligned}$$

Here, we also used the dots to indicate additional terms which would have canceled had we performed the calculation over the entire domain. A similar computation in the continuum region gives

$$\sum_{j=K+1}^{N-1} \epsilon (L_2 \mathbf{v})_j v_j = \sum_{j=K+1}^{N} \epsilon 4 Dv_j Dw_j + 4 Dv_{K+1} w_K .$$

Considering the symmetry of the problem, or by performing the same calculation in the left half of the domain, we obtain the stated result. □

In order to find the conjugate operator, we only need to write w_K and w_{-K} in terms of the strains Dw_j. This is achieved by connecting these displacements to the boundary, for example, by using the identities

$$w_K = -\sum_{j=K+1}^{N} \epsilon Dw_j \quad \text{and} \quad w_{-K} = \sum_{j=-N+1}^{-K} \epsilon Dw_j .$$

Note, however, that there is no unique way of achieving this. Our choice above simply minimizes the number of non-zero entries for E^{qcf} in each row,

a fact that will become important later on. Thus, we obtain

$$E^{qcf} = \phi_F'' I + \phi_{2F}'' \begin{bmatrix} 4 & & 1 & -2 & 1 & & & & & & \\ & \ddots & \vdots & \vdots & \vdots & & & & & & \\ & & 4 & 1 & -2 & 1 & & & & & \\ & & & 5 & -2 & 1 & & & & & \\ & & & 1 & 2 & 1 & & & & & \\ & & & & 1 & 2 & 1 & & & & \\ & & & & & \ddots & \ddots & \ddots & & & \\ & & & & & & 1 & 2 & 1 & & \\ & & & & & & & 1 & 2 & 1 & \\ & & & & & & & 1 & -2 & 5 & \\ & & & & & & & 1 & -2 & 1 & 4 \\ & & & & & & & \vdots & \vdots & \vdots & & \ddots \\ & & & & & & & 1 & -2 & 1 & & & 4 \end{bmatrix}. \tag{16}$$

With this choice we indeed obtain the identity (13).

4 Lack of Coercivity

Local minimizers of the atomistic energy are characterized, essentially, by the fact that the Hessian is positive definite. It can be shown that the coercivity of the operator L^a in appropriate norms is independent of problem size N, provided that $\phi_F'' + 4\phi_{2F}'' > 0$ (see [10, 11] for a periodic problem; the proof for the Dirichlet boundary value problem is very similar). It can moreover be shown that the *energy-based* quasi-nonlocal approximation always inherits coercivity of the atomistic operator [11].

In Section 5, we will give conditions on ϕ_F'' and ϕ_{2F}'' under which the QCF operator L^{qcf} inherits stability in a more general sense, uniformly in N, even though it does *not* inherit coercivity. In fact, as we show in the following theorem, the L^{qcf} operator is not coercive whenever N is sufficiently large. That is, not only is it lacking uniform coercivity, but it is not even positive definite. This result explains why we need to work with a technically more involved inf-sup stability condition in our error analysis in later sections.

Theorem 1 *Suppose that $\phi_F'' > 0$ and $\phi_{2F}'' \in \mathbb{R} \setminus \{0\}$; then, for sufficiently large N, the operator L^{qcf} is* not *coercive. More precisely, there exist $N_0 \in \mathbb{N}$, $C_1 \geq C_2 > 0$ such that, for all $N \geq N_0$ and $2 \leq K \leq N/2$,*

$$-C_1 N^{1/2} \leq \inf_{\substack{\mathbf{v} \in \mathcal{V}_0 \\ \|D\mathbf{v}\|_{\ell^2_\epsilon} = 1}} \langle L^{qcf}\mathbf{v}, \mathbf{v} \rangle \leq -C_2 N^{1/2}.$$

Proof As in Section 3 we write $L^{qcf} = \phi_F'' L_1 + \phi_{2F}'' L_2$. Since $\langle L_1 \mathbf{v}, \mathbf{v} \rangle = \|D\mathbf{v}\|^2_{\ell^2_\epsilon}$, we need to concentrate on the next-nearest neighbor interaction operator L_2. If we can show that L_2 is neither bounded above nor below, uniformly in N, and with the stated asymptotic behavior, then the upper bound follows. The lower bound follows from the fact that L_1 is bounded while $|\langle L_2 \mathbf{v}, \mathbf{v} \rangle| \leq C_1 N^{1/2} \|D\mathbf{v}\|^2_{\ell^2_\epsilon}$. Both of these facts are established in the following lemma. □

Lemma 2 *Suppose that the conditions of Theorem 1 hold. Then there exist positive constants c_1, c_2, independent of N, and lattice functions $\mathbf{v}^+$, $\mathbf{v}^- \in \mathcal{V}_0$ such that $\|D\mathbf{v}^+\|_{\ell^2_\epsilon} = \|D\mathbf{v}^-\|_{\ell^2_\epsilon} = 1$,*

$$\langle L_2\mathbf{v}^+, \mathbf{v}^+\rangle \geq c_1(N^{1/2} - c_2), \quad \textit{and} \quad \langle L_2\mathbf{v}^-, \mathbf{v}^-\rangle \leq -c_1(N^{1/2} - c_2).$$

Moreover, these bounds are asymptotically optimal in that there exists a constant $c_3 > 0$ such that

$$\big|\langle L_2\mathbf{v}, \mathbf{v}\rangle\big| \leq c_3 N^{1/2} \qquad \textit{for all } \mathbf{v} \in \mathcal{V}_0 \textit{ with } \|D\mathbf{v}\|_{\ell^2_\epsilon} = 1.$$

Proof We write $\langle L_2\mathbf{v}, \mathbf{v}\rangle$ by setting $\mathbf{w} = \mathbf{v}$ in Lemma 1. The crucial observation is that the term $v_K(Dv_{K+2} - 2Dv_{K+1} + Dv_K)$ cannot be expressed as a quadratic form of strains supported at the interface, while all other terms are bounded in terms of (a constant multiple of) $\|D\mathbf{v}\|^2_{\ell^2_\epsilon}$. More precisely, we recall that

$$\begin{aligned}\langle L_2\mathbf{v}, \mathbf{v}\rangle = \langle L_2^{reg}\mathbf{v}, \mathbf{v}\rangle &- v_K(Dv_{K+2} - 2Dv_{K+1} + Dv_K)\\ &+ v_{-K}(Dv_{-K-1} - 2Dv_{-K} + Dv_{-K+1}),\end{aligned}$$

where $|\langle L_2^{reg}\mathbf{v}, \mathbf{v}\rangle| \leq c\|D\mathbf{v}\|^2_{\ell^2_\epsilon}$. Next, we construct the functions $\mathbf{v}^\pm$ by choosing $v_K = 1$ and so that the third difference in the bracket is of order $N^{1/2}$.

To this end, we set $\mathbf{v} = \bar{\mathbf{v}} + \epsilon^{1/2}\boldsymbol{\delta}_{K+1} = \bar{\mathbf{v}} + N^{-1/2}\boldsymbol{\delta}_{K+1}$, where

$$\bar{v}_j = \begin{cases} (N+j)/(N-K-2), & j = -N, \ldots, -K-2\\ 1, & j = -K-2, \ldots, K+2,\\ (N-j)/(N-K-2), & j = K+2, \ldots, N,\end{cases}$$

(that is, $\bar{v}_j = 1$ in the atomistic region and the interface, and interpolates linearly between 1 and 0 in the continuum region) and where $\delta_{K+1,j} = 0$ if $j \neq K+1$ and $\delta_{K+1,\,K+1} = 1$. It is clear that $\|D\mathbf{v}\|_{\ell^2_\epsilon}$ uniformly bounded and isolated from 0, and we obtain

$$\langle L_2\mathbf{v}, \mathbf{v}\rangle = \ \langle L_2^{reg}\mathbf{v}, \mathbf{v}\rangle + 3N^{1/2}.$$

Note that no terms at the left interface occur since $\mathbf{v}$ is a constant there. Upon appropriately rescaling by $\mathbf{v}^+ = \mathbf{v}/\|D\mathbf{v}\|_{\ell^2_\epsilon}$ so that $\|D\mathbf{v}^+\|_{\ell^2_\epsilon} = 1$, we obtain

$$\langle L_2\mathbf{v}^+, \mathbf{v}^+\rangle \geq -c_2 + c_1 N^{1/2}.$$

Setting $\mathbf{v}^- = c(\bar{\mathbf{v}} - \epsilon^{1/2}\boldsymbol{\delta}_{K+1})$ gives the opposite bound.

To prove the final statement, namely that these bounds are asymptotically sharp, we note that all terms of the type $v_K Dv_j$ are of order $N^{1/2}$,

$$\big|v_K Dv_j\big| = \epsilon^{-1/2}|v_K|\epsilon^{1/2}|Dv_j| \leq \epsilon^{-1/2}\|\mathbf{v}\|_{\ell^\infty_\epsilon}\|D\mathbf{v}\|_{\ell^2_\epsilon} \leq (2/\epsilon)^{1/2}\|D\mathbf{v}\|^2_{\ell^2_\epsilon},$$

where we used (11) and a weighted Cauchy–Schwartz inequality to bound $\|\mathbf{v}\|_{\ell^\infty_\epsilon} \leq \sqrt{2}\|D\mathbf{v}\|_{\ell^2_\epsilon}$. □

Remark 1 The proof of Lemma 2 reveals that N needs to be of the order $(1+|\phi_F''/\phi_{2F}''|)^2$ before a loss of coercivity can occur. Although it may seem that this is typically a fairly large number, $(1+|\phi_F''/\phi_{2F}''|)^2$ is not so large for strains F near the edge of a stability region (such as near the critical strain at which the atomistic system "fractures" [5]), or more generally whenever the next-nearest neighbor interaction is not significantly dominated by the nearest neighbor interaction.

5 Stability of the Force-Based Quasicontinuum Solution

We first recall a classical characterization of the norm of the inverse of an operator that we will use to prove the stability of the solution to the QCF approximation. The proof is included for the sake of completeness.

Lemma 3 (Inf-Sup Condition) *Let W and V be finite dimensional normed linear spaces satisfying $\dim W = \dim V$, and let L be a bounded linear operator from V to W' where W' is the dual of W. Suppose that*

$$\inf_{\substack{\mathbf{v}\in V\\ \|\mathbf{v}\|_V=1}} \sup_{\substack{\mathbf{w}\in W\\ \|\mathbf{w}\|_W=1}} \langle L\mathbf{v},\mathbf{w}\rangle = \gamma > 0. \tag{17}$$

Then L is invertible and the solution $\mathbf{u}\in V$ to $L\mathbf{u}=\mathbf{f}$ satisfies the stability bound

$$\|\mathbf{u}\|_V \le \frac{1}{\gamma}\|\mathbf{f}\|_{W'} \quad \text{where} \quad \|\mathbf{f}\|_{W'} := \sup_{\substack{\mathbf{w}\in W\\ \|\mathbf{w}\|_W=1}} \langle \mathbf{f},\mathbf{w}\rangle.$$

Proof The inf-sup condition (17) implies that the nullspace of L must be trivial. Since a finite-dimensional linear operator between two spaces of the same dimension is invertible if and only if it is non-singular, we conclude that there is a unique solution $\mathbf{u}\in V$ to $L\mathbf{u}=\mathbf{f}$ for every $\mathbf{f}\in W'$.

If $\|\mathbf{u}\|_V = 0$, then the stability bound is trivial. Otherwise, we have

$$\|\mathbf{f}\|_{W'} = \sup_{\substack{\mathbf{w}\in W\\ \|\mathbf{w}\|_W=1}} \langle L\mathbf{u},\mathbf{w}\rangle = \|\mathbf{u}\|_V \sup_{\substack{\mathbf{w}\in W\\ \|\mathbf{w}\|_W=1}} \left\langle L\left(\frac{\mathbf{u}}{\|\mathbf{u}\|_V}\right),\mathbf{w}\right\rangle \ge \gamma\|\mathbf{u}\|_V. \quad \square$$

Next, we note that the range of the backward difference operator D is

$$\mathcal{R}(D) = \mathbb{R}^{2N}_* := \left\{\boldsymbol{\xi}\in\mathbb{R}^{2N} : \sum_{j=-N+1}^{N} \xi_j = 0\right\},$$

and therefore

$$\begin{aligned}\inf_{\substack{\mathbf{v}\in\mathcal{V}_0\\ \|D\mathbf{v}\|_{\ell^\infty_\epsilon}=1}} \sup_{\substack{\mathbf{w}\in\mathcal{V}_0\\ \|D\mathbf{w}\|_{\ell^1_\epsilon}=1}} \langle L^{qcf}\mathbf{v},\,\mathbf{w}\rangle &= \inf_{\substack{\mathbf{v}\in\mathcal{V}_0\\ \|D\mathbf{v}\|_{\ell^\infty_\epsilon}=1}} \sup_{\substack{\mathbf{w}\in\mathcal{V}_0\\ \|D\mathbf{w}\|_{\ell^1_\epsilon}=1}} \langle E^{qcf}D\mathbf{v},\,D\mathbf{w}\rangle \\ &= \inf_{\substack{\boldsymbol{\xi}\in\mathbb{R}^{2N}_*\\ \|\boldsymbol{\xi}\|_{\ell^\infty_\epsilon}=1}} \sup_{\substack{\boldsymbol{\eta}\in\mathbb{R}^{2N}_*\\ \|\boldsymbol{\eta}\|_{\ell^1_\epsilon}=1}} \langle E^{qcf}\boldsymbol{\xi},\,\boldsymbol{\eta}\rangle.\end{aligned}$$

The following lemma gives a bound on such an inf-sup constant, for a general matrix A. This result and its proof were inspired by [30, Sec. 3.1].

Lemma 4 *Suppose that $A \in \mathbb{R}^{2N\times 2N}$ satisfies*

$$\min_i \Big(A_{ii} + \sum_{j\neq i} A^-_{ij}\Big) - \max_i \sum_{j\neq i} A^+_{ij} =: \gamma > 0,$$

where $A^-_{ij} = \min(0, A_{ij})$ and $A^+_{ij} = \max(0, A_{ij})$, then

$$\inf_{\substack{\boldsymbol{\xi}\in\mathbb{R}^{2N}_* \\ \|\boldsymbol{\xi}\|_{\ell^\infty_\epsilon}=1}} \sup_{\substack{\boldsymbol{\eta}\in\mathbb{R}^{2N}_* \\ \|\boldsymbol{\eta}\|_{\ell^1_\epsilon}=1}} \langle A\boldsymbol{\xi}, \boldsymbol{\eta}\rangle \geq \gamma/2.$$

Proof Let $\boldsymbol{\xi} \in \mathbb{R}^{2N}_* \setminus \{0\}$ and choose $p, q \in \{-N+1, \ldots, N\}$ such that $\xi_p = \max_j \xi_j$ and $\xi_q = \min_j \xi_j$. Since $\sum_{j=-N+1}^{N} \xi_j = 0$, it follows that $\xi_p > 0$ and $\xi_q < 0$. Moreover, let $P = \{j : \xi_j \geq 0\}$ and $Q = \{j : \xi_j < 0\}$. If we define $\boldsymbol{\eta} \in \mathbb{R}^{2N}_*$ by

$$\eta_i = \begin{cases} \frac{1}{2\epsilon}, & i = p, \\ -\frac{1}{2\epsilon}, & i = q, \\ 0, & \text{otherwise}, \end{cases}$$

then

$$\begin{aligned}
2\langle A\boldsymbol{\xi}, \boldsymbol{\eta}\rangle = &\ \Big\{\sum_j A_{pj}\xi_j\Big\} - \Big\{\sum_j A_{qj}\xi_j\Big\} \\
\geq &\ \Big\{A_{pp}\xi_p + \sum_{j\in Q} A^+_{pj}\xi_j + \sum_{j\in P\setminus\{p\}} A^-_{pj}\xi_j\Big\} \\
&\quad - \Big\{A_{qq}\xi_q + \sum_{j\in P} A^+_{qj}\xi_j + \sum_{j\in Q\setminus\{q\}} A^-_{qj}\xi_j\Big\} \\
\geq &\ \Big\{A_{pp}\xi_p + \sum_{j\in Q} A^+_{pj}\xi_q + \sum_{j\in P\setminus\{p\}} A^-_{pj}\xi_p\Big\} \\
&\quad - \Big\{A_{qq}\xi_q + \sum_{j\in P} A^+_{qj}\xi_p + \sum_{j\in Q\setminus\{q\}} A^-_{qj}\xi_q\Big\} \\
= &\ \Big[A_{pp} - \sum_{j\in P\setminus\{p\}} |A^-_{pj}| - \sum_{j\in P} |A^+_{qj}|\Big]|\xi_p| \\
&\quad + \Big[A_{qq} - \sum_{j\in Q\setminus\{q\}} |A^-_{qj}| - \sum_{j\in Q} |A^+_{pj}|\Big]|\xi_q| \\
\geq &\ \gamma(|\xi_p| + |\xi_q|).
\end{aligned}$$

□

From Lemma 4 and from (16), we can now deduce that

$$\begin{aligned}
&\inf_{\substack{\mathbf{v}\in\mathcal{V}_0 \\ \|D\mathbf{v}\|_{\ell^\infty_\epsilon}=1}} \sup_{\substack{\mathbf{v}\in\mathcal{V}_0 \\ \|D\mathbf{w}\|_{\ell^1_\epsilon}=1}} \langle L^{qcf}\mathbf{v}, \mathbf{w}\rangle \\
&\qquad \geq \frac{1}{2}\Big[\min_i \Big((E^{qcf})_{ii} + \sum_{j\neq i}(E^{qcf})^-_{ij}\Big) - \max_i \sum_{j\neq i}(E^{qcf})^+_{ij}\Big] \qquad (18) \\
&\qquad = \frac{1}{2}\big(\phi''_F + 8\phi''_{2F}\big).
\end{aligned}$$

Combining this estimate with Lemma 3 gives the following stability result.

Theorem 2 *Suppose that $\phi_F'' + 8\phi_{2F}'' > 0$. Then the QCF system (10) has a unique solution $\mathbf{u}^{qcf}$, which satisfies*

$$\left\|D\mathbf{u}^{qcf}\right\|_{\ell^\infty_\epsilon} \leq \frac{2\|\mathbf{f}\|_*}{\phi_F'' + 8\phi_{2F}''} + \left|\frac{u_N^a - u_{-N}^a}{2N}\right|, \tag{19}$$

where

$$\|\mathbf{f}\|_* := \sup_{\substack{\mathbf{w}\in\mathcal{V}_0 \\ \|D\mathbf{w}\|_{\ell^1_\epsilon}=1}} \langle \mathbf{f}, \mathbf{w}\rangle.$$

Proof We write $\mathbf{u}^{qcf} = \mathbf{u} + \mathbf{u}^D$ where $\mathbf{u} \in \mathcal{V}_0$ and where

$$u_j^D = u_{-N}^a + (u_N^a - u_{-N}^a)(N+j)/(2N).$$

Since $\mathbf{u}^D$ is affine, it can be easily seen that $L^{qcf}\mathbf{u}^D = 0$. Hence, the system is equivalent to $L^{qcf}\mathbf{u} = \mathbf{f}$. In view of (18) and Lemma 3 this has a unique solution, and we have the stability bound

$$\|D\mathbf{u}^{qcf}\|_{\ell^\infty_\epsilon} \leq \|D\mathbf{u}\|_{\ell^\infty_\epsilon} + \left\|D\mathbf{u}^D\right\|_{\ell^\infty_\epsilon} \leq \frac{2\|\mathbf{f}\|_*}{\phi_F'' + 8\phi_{2F}''} + \left|\frac{u_N^a - u_{-N}^a}{2N}\right|. \qquad \square$$

6 Convergence

The QCF error $\mathbf{e}^{qcf} = \mathbf{u}^a - \mathbf{u}^{qcf}$, where $\mathbf{u}^a$ is again identified with its restriction to the computational domain whenever necessary, satisfies the equation

$$\begin{aligned} \left(L^{qcf}\mathbf{e}^{qcf}\right)_j &= t_j, \qquad j = -N+1, \ldots, N-1, \\ (\mathbf{e}^{qcf})_j &= 0, \qquad j = -N,\, N. \end{aligned}$$

Using (12) and (11) we see that the truncation error $\mathbf{t} = L^{qcf}\mathbf{u}^a - \mathbf{f}$ (but with $t_N = t_{-N} = 0$) satisfies the negative norm estimate

$$\|\mathbf{t}\|_* = \sup_{\substack{\mathbf{w}\in\mathcal{V}_0 \\ \|D\mathbf{w}\|_{\ell^1_\epsilon}=1}} \langle\, \mathbf{t},\, \mathbf{w}\rangle \leq \sup_{\substack{\mathbf{w}\in\mathcal{V}_0 \\ \|\mathbf{w}\|_{\ell^\infty_\epsilon}=1}} \tfrac{1}{2}\langle\, \mathbf{t},\, \mathbf{w}\rangle = \tfrac{1}{2}\,\|\mathbf{t}\|_{\ell^1_\epsilon} = \tfrac{1}{2}\epsilon^2|\phi_{2F}''|\,\|\bar{D}^4\mathbf{u}^a\|_{\ell^1_\epsilon(\mathcal{C})}.$$

However, we can get a slightly sharper result using the variational representations of the operators L^a and L^{qcf} derived in Section 3.

Lemma 5 *The truncation error satisfies the estimate*

$$\|\mathbf{t}\|_* \leq 2\epsilon^2|\phi_{2F}''|\|D^3\mathbf{u}^a\|_{\ell^\infty_\epsilon(\widetilde{\mathcal{C}})},$$

where $\widetilde{\mathcal{C}} = \{-N+2, \ldots, -K+1\} \cup \{K+2, \ldots, N+1\}$.

Proof Using the "weak" forms of L^a and L^{qcf} derived in (15) and in Lemma 1, we obtain

$$\begin{aligned}\big\langle \mathbf{t}, \mathbf{w}\big\rangle =\ & \big\langle (L^{qcf} - L^a)\mathbf{u}^a, \mathbf{w}\big\rangle \\ =\ & \phi''_{2F}\Bigg\{ \sum_{j=-N+1}^{-K} \epsilon\big(- Du^a_{j-1} + 2Du^a_j - Du^a_{j+1}\big) Dw_j \\ & \quad + \big(Du^a_{-K+1} - 2Du^a_{-K} + Du^a_{-K-1}\big) w_{-K} \\ & \quad + \sum_{j=K+1}^{N} \epsilon\big(- Du^a_{j-1} + 2Du^a_j - Du^a_{j+1}\big) Dw_j \\ & \quad + \big(- Du^a_{K+2} + 2Du^a_{K+1} - Du^a_K\big) w_K \Bigg\} \\ \le\ & \epsilon^2 |\phi''_{2F}| \|D^3\mathbf{u}^a\|_{\ell^\infty_\epsilon(\widetilde{\mathcal{C}})} \big(\|D\mathbf{w}\|_{\ell^1_\epsilon} + 2\|\mathbf{w}\|_{\ell^\infty_\epsilon}\big),\end{aligned}$$

where we used a weighted Hölder inequality in the last step. Using (11) to bound $\|\mathbf{w}\|_{\ell^\infty_\epsilon}$ we obtain the stated bound. □

Combining this negative-norm truncation error estimate with the stability estimate (19), we obtain the following result.

Theorem 3 *Suppose that $\phi''_F + 8\phi''_{2F} > 0$. Then the atomistic problem (5) as well as the QCF approximation (10) have unique solutions, and they satisfy the error estimate*

$$\big\| D(\mathbf{u}^a - \mathbf{u}^{qcf})\big\|_{\ell^\infty_\epsilon} \le 4\epsilon^2 \frac{|\phi''_{2F}| \|D^3\mathbf{u}^a\|_{\ell^\infty_\epsilon(\widetilde{\mathcal{C}})}}{\phi''_F + 8\phi''_{2F}},$$

where the set $\tilde{\mathcal{C}}$ is defined in the statement of Lemma 5.

As in Section 2 we note again that it follows from the interior regularity theory for elliptic finite difference operators [37] that $\|D^3\mathbf{u}^a\|_{\ell^\infty_\epsilon(\tilde{\mathcal{C}})}$ is bounded in the continuum limit $\epsilon \to 0$, provided that $\mathbf{f}$ is the restriction of a smooth function in a neighborhood of the continuum region $\widetilde{\mathcal{C}}$ to the lattice points.

7 Estimates in Other Norms

We conclude this paper by showing that our choice of norms with respect to which we analyzed the stability of the QCF approximation was, in some sense, unique.

Theorem 4 *Suppose that $\phi''_F > 0$, $\phi''_{2F} \in \mathbb{R} \setminus \{0\}$, and that $1 \le p < \infty$, and $1 < q \le \infty$ so that $\frac{1}{p} + \frac{1}{q} = 1$. Then there exists a constant $C > 0$ such that, for $2 \le K \le N/2$,*

$$\inf_{\substack{\mathbf{v}\in\mathcal{V}_0 \\ \|D\mathbf{v}\|_{\ell^p_\epsilon}=1}} \sup_{\substack{\mathbf{w}\in\mathcal{V}_0 \\ \|D\mathbf{w}\|_{\ell^q_\epsilon}=1}} \langle L^{qcf}\mathbf{v},\, \mathbf{w}\rangle \le CN^{-1/p}.$$

Proof We recall from Sections 3 and 5 that

$$\inf_{\substack{\mathbf{v}\in\mathcal{V}_0\\ \|D\mathbf{v}\|_{\ell^p_\epsilon}=1}} \sup_{\substack{\mathbf{w}\in\mathcal{V}_0\\ \|D\mathbf{w}\|_{\ell^q_\epsilon}=1}} \langle L^{qcf}\mathbf{v},\, \mathbf{w}\rangle = \inf_{\substack{\boldsymbol{\xi}\in\mathbb{R}^{2N}_*\\ \|\boldsymbol{\xi}\|_{\ell^p_\epsilon}=1}} \sup_{\substack{\boldsymbol{\eta}\in\mathbb{R}^{2N}_*\\ \|\boldsymbol{\eta}\|_{\ell^q_\epsilon}=1}} \langle E^{qcf}\boldsymbol{\xi},\, \boldsymbol{\eta}\rangle$$
$$\leq \inf_{\substack{\boldsymbol{\xi}\in\mathbb{R}^{2N}_*\\ \|\boldsymbol{\xi}\|_{\ell^p_\epsilon}=1}} \left\|E^{qcf}\boldsymbol{\xi}\right\|_{\ell^p_\epsilon},$$

where the second step follows from Hölder's inequality. Therefore, we obtain the stated result from the following lemma. □

Lemma 6 *Under the conditions of Theorem 4 there exists a constant $C > 0$ such that, for $2 \leq K \leq N/2$,*

$$\inf_{\substack{\boldsymbol{\xi}\in\mathbb{R}^{2N}_*\\ \|\boldsymbol{\xi}\|_{\ell^p_\epsilon}=1}} \left\|E^{qcf}\boldsymbol{\xi}\right\|_{\ell^p_\epsilon} \leq CN^{-1/p}.$$

Proof The terms causing this effect are the nonlocal terms extending from the atomistic to continuum interface to the boundary. It is therefore natural to choose $\boldsymbol{\xi} = \tilde{\boldsymbol{\xi}}/\|\tilde{\boldsymbol{\xi}}\|_{\ell^p_\epsilon}$, and

$$\tilde{\xi}_j = \begin{cases} -1, & j = -N+1, \ldots, -K-1,\\ -\alpha, & j = -K,\\ 0, & j = -K+1, \ldots, K,\\ \alpha, & j = K+1,\\ 1, & j = K+2, \ldots, N, \end{cases}$$

where $\alpha \in \mathbb{R}$ will be specified below. Recalling the matrix representation (16) for E^{qcf}, we see that

$$E^{qcf}\tilde{\boldsymbol{\xi}} = \phi''_F\tilde{\boldsymbol{\xi}} + \phi''_{2F} \begin{cases} -5+2\alpha, & j = -N+1, \ldots, -K-1,\\ -1-2\alpha, & j = -K,\\ -\alpha, & j = -K+1,\\ 0, & j = -K+2, \ldots, K-1,\\ \alpha, & j = K,\\ 1+2\alpha, & j = K+1,\\ 5-2\alpha, & j = K+2, \ldots, N, \end{cases}$$

from which we obtain

$$\left\|E^{qcf}\tilde{\boldsymbol{\xi}}\right\|^p_{\ell^p_\epsilon} = 2\epsilon\Big(\left|\alpha\phi''_{2F}\right|^p + \left|\alpha\phi''_F + (1+2\alpha)\phi''_{2F}\right|^p$$
$$+ (N-K-1)\left|\phi''_F + (5-2\alpha)\phi''_{2F}\right|^p\Big).$$

Choosing $\alpha = (\phi''_F + 5\phi''_{2F})/(2\phi''_{2F})$, and thereby canceling the dominant term $(N-K-1)|\phi''_F + (5-2\alpha)\phi''_{2F}|^p$ in the formula above, gives

$$\left\|E^{qcf}\tilde{\boldsymbol{\xi}}\right\|^p_{\ell^p_\epsilon} = 2\epsilon\Big(\left|\alpha\phi''_{2F}\right|^p + \left|\alpha\phi''_F + (1+2\alpha)\phi''_{2F}\right|^p\Big).$$

Moreover, since

$$\left\|\tilde{\boldsymbol{\xi}}\right\|_{\ell^p_\epsilon}^p = 2\epsilon(N-K-1+|\alpha|^p) \geq 2\epsilon(N/2-1+|\alpha|^p),$$

we conclude that

$$\inf_{\substack{\boldsymbol{\xi}\in\mathbb{R}^{2N}_* \\ \|\boldsymbol{\xi}\|_{\ell^p_\epsilon}=1}} \left\|E^{qcf}\boldsymbol{\xi}\right\|_{\ell^p_\epsilon} \leq \left(\frac{\left|\alpha\phi''_{2F}\right|^p + \left|\alpha\phi''_F + (1+2\alpha)\phi''_{2F}\right|^p}{N/2-1+|\alpha|^p}\right)^{1/p} \leq CN^{-1/p},$$

where C is independent of N. □

Conclusions

We have presented a detailed stability and error analysis of the QCF method in one dimension. Although we were able to establish optimal order error estimates, we have also presented several "negative" results which are, in many respects, even more interesting. The present paper has focused exclusively on the QCF method, but we expect that the lack of coercivity (and more generally lack of stability in most norms) may be present in other force-based coupling methods such as [21, 34] or the QM-MM coupling methods described in [4]. A careful study of these related methods is required to further understand and establish force-based coupling techniques as predictive tools in computational physics.

To conclude, we discuss three important extensions of the analysis presented in this paper, each of which deserves a careful analysis to further establish the mathematical foundations of the quasicontinuum method.

First, we note that we have only proven stability of the QCF method under the condition that $\phi''_F + 8\phi''_{2F} > 0$ (cf. Theorem 2). By contrast, the atomistic model is uniformly stable if *and only if* $\phi''_F + 4\phi''_{2F} + \delta > 0$, where δ is $\mathrm{O}(\epsilon^2)$ [11]. This leads us to expect that our conditions in Theorem 2 are not sharp. In fact, our numerical results, and stability results with respect to different choices of function spaces, reported in [12], indicate that this is indeed the case. In general, we believe that *sharp* stability analyses of quasicontinuum methods are a crucial ingredient to establish their predictive capabilities in the presence of (near-)singularities, and we have initiated a systematic study in [11, 12].

Second, it needs to be investigated whether our results will hold for more general atomistic models. We have no reason to expect the contrary. Nevertheless, care would have to be taken to construct and analyze new test functions in order to establish the counterparts of Theorems 1 and 4. It also seems likely that the stability result of Theorem 2 can be extended to interaction models with an arbitrary *finite* range, although the notational details would be more involved and less control on the deformation range where the result is valid should be expected. Genuine long-range interactions where $\phi(r) \sim 1/r$ as $r \to \infty$ pose additional challenges. Obtaining *sharp* stability estimates such as those we develop in [11, 12] would be more difficult.

Our third remark is on the extension of our results to the two- and three-dimensional setting, which is relevant for applications. Note that, in essence, our proof of Theorem 2 derives an explicit condition on the macroscopic deformation gradient, F, for which the stability of the nearest-neighbor interaction operator dominates all other interaction terms in the $W^{1,\infty}$ norm. As discussed above, even though this stability condition is not sharp, it gives a large stability region for many of the interaction potentials commonly considered, such as the Lennard-Jones potential.

We see no obstacle to extending the argument of Theorem 2 to higher dimensions, although it may be quite technically involved. The most technical component in higher dimensions, namely the stability of the nearest neighbor interaction operator, is close to classical results on the $W^{1,\infty}$-stability of the Ritz projection [32], or extensions and modifications thereof to elliptic systems [13]. However, controlling the stability constants is extremely difficult, and it is conceivable that any stability conditions obtained in this way would give a small or nonexistent stability region for many realistic interaction potentials. Obtaining *sharp* stability results in this setting is a formidable challenge.

Extending our "negative" results, Theorems 1 and 4, to the higher dimensional case may prove to be quite interesting and challenging as well. In the case of sufficiently large flat interfaces, it seems likely that one would be able to extend our one-dimensional arguments, and thereby obtain the loss of coercivity and loss of stability in certain function spaces for such situations. However, we expect that the shape and size of the atomistic region has a much bigger influence in 2D and 3D than it does in 1D. For example, it is unclear to us whether these results remain true if the atomistic region is a small box that is fixed as the number of atoms tends to infinity.

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