

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 approximation is the only known pointwise consistent quasicontinuum (QC) 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 force-based QC 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 (which we prove) that the linearized QC 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 $1 \leq p < \infty$. We therefore derive an inf-sup stability condition for a discrete version of the $W^{1,\infty}$ - $W^{1,1}$ “duality pairing” which then 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 [19, 26, 33]. 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, 15, 24, 29, 30]; yet, in common with many other multiscale methods it lacks the theoretical basis needed to give predictive computational results.

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, 10, 12–14, 16, 17, 22, 23, 25, 28]. In the present paper,

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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. 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 [26,30]. 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 [20,31].

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 [12,32]. The quasi-nonlocal (QNL) approach [32] 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 [12] 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, that can be used with adaptive atomistic to continuum modeling algorithms, has yet to be proposed.

Both of the above methods [12,32] 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 [12]. In contrast, the force-based quasicontinuum approximation allows arbitrary atomistic to continuum interfaces and coarsening without ghost forces.

Rather than computing forces from a total energy, the force-based quasicontinuum 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 that the QCF equilibrium equations are satisfied exactly by a material under uniform strain, that is, there are no ghost forces in this approximation. Moreover, we will show below that the QCF approximation has an $O(\epsilon^2)$ truncation error in the atomistic to continuum interface for all smoothly varying strains. By contrast, it has been shown in [9] that, even when it succeeds in removing ghost forces, the QNL method has an $O(1)$ truncation error in the atomistic to continuum interfaces for a nonuniform but smooth strain. (This is nevertheless a significant improvement over the $O(1/\epsilon)$ truncation error in the original QC method.)

With the exception of [28], error analyses of energy-based QC methods have utilized the coercivity (positive-definiteness) of the linearization of the quasicontinuum equilibrium equations about the energy-minimizing solution [9,13,14]. 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 [27]. In the present paper we prove that, typically, the linearization of the QCF equilibrium equations is *not* coercive (cf. Theorem 4.1), 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 one chooses the norms particularly carefully. 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, uniformly 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 force-based quasicontinuum approximation.

The main result of the present paper is that the strain error for the QCF approximation is $O(\epsilon^2)$, 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 force-based quasicontinuum 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 force-based quasicontinuum approximation. We conclude, in Section 7, by showing the lack of a uniform inf-sup constant for all 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 $j = -M, \dots, M$. 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 $\mathbf{y} \in \mathbb{R}^{2N+1}$ is given by

$$\mathcal{E}^a(\mathbf{y}) = \sum_{j=-M}^M \epsilon f_j y_j, \tag{2.1}$$

where

$$\mathcal{E}^a(\mathbf{y}) = \sum_{j=-M+1}^M \epsilon \phi\left(\frac{y_j - y_{j-1}}{\epsilon}\right) + \sum_{j=-M+2}^M \epsilon \phi\left(\frac{y_j - y_{j-2}}{\epsilon}\right) \quad (2.2)$$

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

$$\begin{aligned} F_j^a(\mathbf{y}) + f_j &= 0 & \text{for } j = -M+1, \dots, M-1, \\ y_j &= Fj\epsilon & \text{for } j = -M, M, \end{aligned} \quad (2.3)$$

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

$$\begin{aligned} F_j^a(\mathbf{y}) := -\frac{1}{\epsilon} \frac{\partial \mathcal{E}^a(\mathbf{y})}{\partial y_j} &= \frac{1}{\epsilon} \left\{ \left[\phi' \left(\frac{y_{j+1} - y_j}{\epsilon} \right) + \phi' \left(\frac{y_{j+2} - y_j}{\epsilon} \right) \right] \right. \\ &\quad \left. - \left[\phi' \left(\frac{y_j - y_{j-1}}{\epsilon} \right) + \phi' \left(\frac{y_j - y_{j-2}}{\epsilon} \right) \right] \right\}. \end{aligned} \quad (2.4)$$

In (2.4) the undefined terms $\phi'(\epsilon^{-1}(y_{-M+1} - y_{-M-1}))$ and $\phi'(\epsilon^{-1}(y_{M+1} - y_{M-1}))$ 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

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

We linearize the atomistic equilibrium equations (2.3) about the deformed state \mathbf{y}^F , resulting in

$$\begin{aligned} (L^a \mathbf{u}^a)_j &= f_j & \text{for } j = -M+1, \dots, M-1, \\ u_j^a &= 0 & \text{for } j = -M, M, \end{aligned} \quad (2.5)$$

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

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

Here and throughout we define $\phi_F'' := \phi''(F)$ and $\phi_{2F}'' := \phi''(2F)$, where ϕ is the interatomic potential in (2.2). 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 (2.5) has a unique solution. This follows from (3.1) and from Lemma 5.2 (see also [9, 11] for an analysis of the periodic case which is similar).

The local QC approximation uses the Cauchy-Born extrapolation rule to approximate the non-local atomistic model by a local continuum model [7, 13, 26, 33]. In our context, this corresponds to approximating $y_j - y_{j-2}$ in (2.2) by $2(y_j - y_{j-1})$ and results in the local QC energy

$$\mathcal{E}^{lc}(\mathbf{y}) = \sum_{j=-M+1}^M \epsilon \left[\phi \left(\frac{y_j - y_{j-1}}{\epsilon} \right) + \phi \left(\frac{2(y_j - y_{j-1})}{\epsilon} \right) \right]. \quad (2.6)$$

Note that the above expression has one more next-nearest neighbor term than (2.2). 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 quasicontinuum equilibrium equations are then given by

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

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

$$\begin{aligned} F_j^{lqc}(\mathbf{y}) := -\frac{1}{\epsilon} \frac{\partial \mathcal{E}^a(\mathbf{y})}{\partial y_j} &= \frac{1}{\epsilon} \left\{ \left[\phi' \left(\frac{y_{j+1} - y_j}{\epsilon} \right) + 2\phi' \left(\frac{2(y_{j+1} - y_j)}{\epsilon} \right) \right] \right. \\ &\quad \left. - \left[\phi' \left(\frac{y_j - y_{j-1}}{\epsilon} \right) + 2\phi' \left(\frac{2(y_j - y_{j-1})}{\epsilon} \right) \right] \right\}. \end{aligned} \quad (2.7)$$

Linearizing the local quasicontinuum equilibrium equations (2.7) about the deformed state \mathbf{y}^F results in

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

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

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

The increased efficiency of the local QC approximation is obtained when its equilibrium equations (2.7) are coarsened by reducing the degrees of freedom using piecewise linear interpolation between a subset of the atoms [7, 26]. 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 force-based QC 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 (2.6) approximates $y_j - y_{j-2}$ in (2.1) 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]

$$F_j^{qcf}(\mathbf{y}) = \begin{cases} F_j^a(\mathbf{y}) & \text{if } j \in \mathcal{A}, \\ F_j^{lqc}(\mathbf{y}) & \text{if } j \in \mathcal{C}, \end{cases} \quad (2.8)$$

and the QCF equilibrium equations by

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

The force-based quasicontinuum approximation gets its name from the assignment of forces at the atoms in (2.8). Most other quasicontinuum 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 using a coarse-graining method such as the QC approximation. 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 computations using other atomistic to continuum approximations) sets the displacement to zero at the boundary of the computational domain, such as at the lateral boundary of the crystal in the nanoindentation problem reported in [18]. More accurate artificial boundary conditions such as given and analyzed in [21] do not seem to have yet been used in quasicontinuum computations.

We chose to imitate the approach commonly used in the QC method, by choosing $N \ll M$ and $0 < K < N - 1$, letting $\{-N, \dots, N\}$ be the computational domain, $\mathcal{A} = \{-K, \dots, K\}$ the atomistic region, and $\mathcal{C} = \{-N + 1, \dots, N - 1\} \setminus \mathcal{A}$ the continuum region, and defining

$$\begin{aligned} F_j^{qcf}(\mathbf{y}) + f_j &= 0 & \text{for } j = -N + 1, \dots, N - 1, \\ y_j &= Fj\epsilon & \text{for } j = -N, N, \end{aligned} \quad (2.9)$$

to be the QCF approximation on the computational domain. In this paper, we analyze the linearization of (2.9),

$$\begin{aligned} (L^{qcf} \mathbf{u}^{qcf})_j &= f_j & \text{for } j = -N + 1, \dots, N - 1, \\ u_j^{qcf} &= u_j^a & \text{for } j = -N, N, \end{aligned} \quad (2.10)$$

where we have taken $u_{-N}^{qcf} = u_{-N}^a$ and $u_N^{qcf} = u_N^a$ 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 scale the problem [6] so that the size of the computational domain is of order $O(1)$.

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

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

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

$$\begin{aligned} \|\mathbf{v}\|_{\ell_\epsilon^p} &:= \left(\epsilon \sum_{j=-N}^N |v_j|^p \right)^{1/p}, & 1 \leq p < \infty, \\ \|\mathbf{v}\|_{\ell_\epsilon^\infty} &:= \max_{-N \leq j \leq N} |v_j|, \end{aligned}$$

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 $\|\mathbf{v}\|_{\ell_\epsilon^p}$ 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

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

For future reference we note that the following Poincaré inequality holds [28, Lemma A.3]:

$$\|\mathbf{v}\|_{\ell_\infty} \leq \frac{1}{2} \|D\mathbf{v}\|_{\ell_1^1} \quad \text{for all } \mathbf{v} \in \mathcal{V}_0. \quad (2.11)$$

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

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

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 force-based QC approximation is mirrored by its equally simple consistency analysis. Let \mathbf{u}^a be the solution to (2.5) (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

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

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,

$$\|\mathbf{t}\|_{\ell_\epsilon^p} = \epsilon^2 |\phi_{2F}''| \|\bar{D}^4\mathbf{u}^a\|_{\ell_\epsilon^p(\mathcal{C})}, \quad (2.12)$$

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

We have presented (2.12) as a simple argument for the high accuracy 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 it follows from the interior regularity of elliptic finite difference operators [34] that $\|\bar{D}^4\mathbf{u}^a\|_{\ell_\epsilon^p(\mathcal{C})}$ is bounded in the continuum limit $\epsilon \rightarrow 0$ if \mathbf{f} is the restriction of a smooth function in a neighborhood of the continuum region \mathcal{C} to the lattice points since the continuum region \mathcal{C} is far from the boundary of the atomistic problem if $N \ll M$.

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 4.1, 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_ϵ^1 duality pairing is used, while the inf-sup constants for the ℓ_ϵ^p - ℓ_ϵ^q ($1/p + 1/q = 1$, $1 \leq p < \infty$) pairings are not uniform in N (cf. Section 7).

3. DIVERGENCE FORM OF THE QCF OPERATOR

We will analyze the QCF equilibrium equations (2.10) by putting them into a “weak form:” *find* $\mathbf{u}^{qcf} \in \mathbb{R}^{2N+1}$ such that

$$\begin{aligned} \langle E^{qcf} D\mathbf{u}^{qcf}, D\mathbf{w} \rangle &= \langle \mathbf{f}, \mathbf{w} \rangle \quad \forall \mathbf{w} \in \mathcal{V}_0, \\ u_j^{qcf} &= u_j^a \quad \text{for } j = -N, N, \end{aligned}$$

where the linear operator $E^{qcf} : \mathbb{R}^{2N} \rightarrow \mathbb{R}^{2N}$ is chosen so that $\langle E^{qcf} D\mathbf{v}, D\mathbf{w} \rangle = \langle L^{qcf} \mathbf{v}, \mathbf{w} \rangle$ for all $\mathbf{v} \in \mathbb{R}^{2N+1}$ and $\mathbf{w} \in \mathcal{V}_0$. 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]

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

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

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

Applying this calculation to the linearized operator L^a , one can easily verify that $\langle L^a \mathbf{v}, \mathbf{w} \rangle = \langle E^a D\mathbf{v}, D\mathbf{w} \rangle$, for all $\mathbf{v} \in \mathbb{R}^{2M+1}$ and $\mathbf{w} \in \mathbb{R}^{2M+1}$ with $w_{-M} = w_M = 0$, where

$$E^a = \phi_F'' I + \phi_{2F}'' \begin{bmatrix} 1 & 1 & & & \\ 1 & 2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 2 & 1 \\ & & & 1 & 1 \end{bmatrix}. \quad (3.1)$$

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

$$\langle L^a \mathbf{v}, \mathbf{w} \rangle = \sum_{j=-N+1}^N [\phi_F'' Dv_j + \phi_{2F}'' (Dv_{j+1} + 2Dv_j + Dv_{j-1})] Dw_j. \quad (3.2)$$

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

$$\begin{aligned} (L_1 \mathbf{v})_j &= \epsilon^{-2} (-v_{j+1} + 2v_j - v_{j-1}), \quad j = -N+1, \dots, N-1, \quad \text{and} \\ (L_2 \mathbf{v})_j &= \begin{cases} 4\epsilon^{-2} (-v_{j+1} + 2v_j - v_{j-1}), & j \in \mathcal{C}, \\ \epsilon^{-2} (-v_{j+2} + 2v_j - v_{j-2}), & j \in \mathcal{A}, \end{cases} \end{aligned}$$

and deriving “weak” representations of the operators L_1 and L_2 .

Lemma 3.1. *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*

$$\begin{aligned}\langle L_1 \mathbf{v}, \mathbf{w} \rangle &= \sum_{j=-N+1}^N \epsilon Dv_j Dw_j, \quad \text{and} \\ \langle L_2 \mathbf{v}, \mathbf{w} \rangle &= \langle L_2^{reg} \mathbf{v}, \mathbf{w} \rangle + \epsilon^2 (D^3 v_{-K+1}) w_{-K} - \epsilon^2 (D^3 v_{K+2}) w_K,\end{aligned}$$

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 ,

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

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,

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

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

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

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

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

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

Proof. As in Section 3 we write $L^{qc} = \phi_F'' L_1 + \phi_{2F}'' L_2$. Since $\langle L_1 \mathbf{v}, \mathbf{v} \rangle = \|D\mathbf{v}\|_{\ell_\epsilon^2}^2$, 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 $|\langle L_2 \mathbf{v}, \mathbf{v} \rangle| \leq C_1 N^{1/2} \|D\mathbf{v}\|_{\ell_\epsilon^2}^2$. Both of these facts are established in the following lemma. \square

Lemma 4.1. *Under the conditions of Theorem 4.1, there exist positive constants c_1, c_2 , independent of N , and lattice functions $\mathbf{v}^+, \mathbf{v}^- \in \mathcal{V}_0$ such that $\|D\mathbf{v}^+\|_{\ell_\epsilon^2} = \|D\mathbf{v}^-\|_{\ell_\epsilon^2} = 1$,*

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

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

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

Proof. We write $\langle L_2 \mathbf{v}, \mathbf{v} \rangle$ by setting $\mathbf{w} = \mathbf{v}$ in Lemma 3.1. 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) $\|D\mathbf{v}\|_{\ell_\epsilon^2}^2$. More precisely, we recall that

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

where $|\langle L_2^{reg} \mathbf{v}, \mathbf{v} \rangle| \leq c_2 \|D\mathbf{v}\|_{\ell_\epsilon^2}^2$. 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

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

(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 $\delta_{K+1,K+1} = 1$. In that case, $\|D\mathbf{v}\|_{\ell_\epsilon^2}$ is clearly uniformly bounded, 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 $\mathbf{v}^+ = \mathbf{v} / \|D\mathbf{v}\|_{\ell_\epsilon^2}$ so that $\|D\mathbf{v}^+\|_{\ell_\epsilon^2} = 1$, 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 $N^{1/2}$,

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

where we used (2.11) and a weighted Cauchy–Schwartz inequality to bound $\|\mathbf{v}\|_{\ell_\epsilon^\infty} \leq \sqrt{2} \|D\mathbf{v}\|_{\ell_\epsilon^2}$. \square

Remark 4.1. The proof of Lemma 4.1 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 force-based quasicontinuum approximation. The proof is included for the sake of completeness.

Lemma 5.1 (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*

$$\inf_{\substack{\mathbf{v} \in V \\ \|\mathbf{v}\|_V=1}} \sup_{\substack{\mathbf{w} \in W \\ \|\mathbf{w}\|_{W'}=1}} \langle L\mathbf{v}, \mathbf{w} \rangle = \gamma > 0. \quad (5.1)$$

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

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

Proof. The inf-sup condition (5.1) 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

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

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

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

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 [28, Sec. 3.1].

Lemma 5.2. *Suppose that $A \in \mathbb{R}^{2N \times 2N}$ satisfies*

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

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

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

Proof. Let $\boldsymbol{\xi} \in \mathbb{R}_*^{2N} \setminus \{0\}$ and choose $p, q \in \{-N+1, \dots, N\}$ 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

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

From Lemma 5.2 and from (3.3), we can now deduce that

$$\begin{aligned} \inf_{\substack{\mathbf{v} \in \mathcal{V}_0 \\ \|D\mathbf{v}\|_{\ell_\epsilon^\infty} = 1}} \sup_{\substack{\mathbf{w} \in \mathcal{V}_0 \\ \|D\mathbf{w}\|_{\ell_\epsilon^1} = 1}} \langle L^{qcf} \mathbf{v}, \mathbf{w} \rangle &\geq \frac{1}{2} \left[\min_i \left((E^{qcf})_{ii} + \sum_{j \neq i} (E^{qcf})_{ij}^- \right) - \max_i \sum_{j \neq i} (E^{qcf})_{ij}^+ \right] \\ &= \frac{1}{2} (\phi_F'' + 8\phi_{2F}''). \end{aligned} \quad (5.2)$$

Combining this estimate with Lemma 5.1 gives the following stability result.

Theorem 5.1. *Suppose that $\phi_F'' + 8\phi_{2F}'' > 0$. Then the QCF system (2.10) has a unique solution \mathbf{u}^{qcf} , which satisfies*

$$\|D\mathbf{u}^{qcf}\|_{\ell_\epsilon^\infty} \leq \frac{2\|\mathbf{f}\|_*}{\phi_F'' + 8\phi_{2F}''} + \left| \frac{u_N^a - u_{-N}^a}{2N} \right|, \quad (5.3)$$

where

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

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 (5.2) and Lemma 5.1 this has a unique solution, and we have the stability bound

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

6. CONVERGENCE

The quasicontinuum 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

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

Using (2.12) and (2.11) we see that the truncation error $\mathbf{t} = L^{qcf} \mathbf{u}^a - \mathbf{f} = (L^{qcf} - L^a) \mathbf{u}^a$ (but with $t_N = t_{-N} = 0$) satisfies the negative norm estimate

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

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 6.1. *The truncation error satisfies the estimate*

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

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

Proof. Using the “weak” forms of L^a and L^{qcf} derived in (3.2) and in Lemma 3.1, we obtain

$$\begin{aligned} \langle \mathbf{t}, \mathbf{w} \rangle &= \langle (L^{qcf} - L^a) \mathbf{u}^a, \mathbf{w} \rangle \\ &= \phi_{2F}'' \left\{ \sum_{j=-N+1}^{-K} \epsilon (-Du_{j-1}^a + 2Du_j^a - Du_{j+1}^a) Dw_j + (Du_{-K+1}^a - 2Du_{-K}^a + Du_{-K-1}^a) w_{-K} \right. \\ &\quad \left. + \sum_{j=K+1}^N \epsilon (-Du_{j-1}^a + 2Du_j^a - Du_{j+1}^a) Dw_j + (-Du_{K+2}^a + 2Du_{K+1}^a - Du_K^a) w_K \right\} \\ &\leq \epsilon^2 \|D^3 \mathbf{u}^a\|_{\ell_\epsilon^\infty(\tilde{\mathcal{C}})} (\|D\mathbf{w}\|_{\ell_\epsilon^1} + 2\|\mathbf{w}\|_{\ell_\epsilon^\infty}), \end{aligned}$$

where we used a weighted Hölder inequality in the last step. Using (2.11) to bound $\|\mathbf{w}\|_{\ell_\epsilon^\infty}$ we obtain the stated bound. \square

Combining this negative-norm truncation error estimate with the stability estimate (5.3), we obtain the following result.

Theorem 6.1. *Suppose that $\phi_F'' + 8\phi_{2F}'' > 0$. Then the atomistic problem (2.5) as well as the force-based quasicontinuum approximation (2.10) have unique solutions, and they satisfy the error estimate*

$$\|D(\mathbf{u}^a - \mathbf{u}^{qcf})\|_{\ell_\epsilon^\infty} \leq 4\epsilon^2 \frac{|\phi_{2F}''| \|D^3 \mathbf{u}^a\|_{\ell_\epsilon^\infty(\tilde{\mathcal{C}})}}{\phi_F'' + 8\phi_{2F}''}.$$

As in Section 2 we note again that it follows from the interior regularity theory for elliptic finite difference operators [34] that $\|D^3 \mathbf{u}^a\|_{\ell_\epsilon^\infty(\tilde{\mathcal{C}})}$ is bounded in the continuum limit $\epsilon \rightarrow 0$, provided that \mathbf{f} is the restriction of a smooth function in a neighborhood of the continuum region $\tilde{\mathcal{C}}$ 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 force-based QC approximation was, in some sense, unique.

Theorem 7.1. *Suppose that $\phi_F'' > 0$, $\phi_{2F}'' \in \mathbb{R} \setminus \{0\}$, and that $1 \leq p < \infty$, and $1 < q \leq \infty$ so that $\frac{1}{p} + \frac{1}{q} = 1$. Then there exists a constant $C > 0$ such that, for $2 \leq K \leq N/2$,*

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

Proof. We recall from Sections 3 and 5 that

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

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

Lemma 7.1. *Under the conditions of Theorem 7.1 there exists a constant $C > 0$ such that, for $2 \leq K \leq N/2$,*

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

Proof. The terms causing this effect are the nonlocal terms extending from the atomistic to continuum interface to the boundary. Hence, we define

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

where $\alpha \in \mathbb{R}$ will be specified below, and $\boldsymbol{\xi} = \tilde{\boldsymbol{\xi}} / \|\tilde{\boldsymbol{\xi}}\|_{\ell_\epsilon^p}$. Recalling the matrix representation (3.3) for E^{qcf} , we see that

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

from which we obtain

$$\begin{aligned} \|E^{qcf} \tilde{\boldsymbol{\xi}}\|_{\ell_\epsilon^p}^p &= 2\epsilon \left(|\alpha \phi_{2F}''|^p + |\alpha \phi_F'' + (1 + 2\alpha) \phi_{2F}''|^p \right. \\ &\quad \left. + (N - K - 1) |\phi_F'' + (5 - 2\alpha) \phi_{2F}''|^p \right). \end{aligned}$$

Choosing $\alpha = \frac{\phi_F'' + 5\phi_{2F}''}{2\phi_{2F}''}$, and thereby canceling the term $(N - K - 1)|\phi_F'' + (5 - 2\alpha)\phi_{2F}''|^p$ above, gives

$$\|E^{qcf} \tilde{\boldsymbol{\xi}}\|_{\ell_e^p}^p = 2\epsilon \left(|\alpha\phi_{2F}''|^p + |\alpha\phi_F'' + (1 + 2\alpha)\phi_{2F}''|^p \right).$$

Moreover, since

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

we conclude that

$$\inf_{\substack{\boldsymbol{\xi} \in \mathbb{R}_*^{2N} \\ \|\boldsymbol{\xi}\|_{\ell_e^p} = 1}} \|E^{qcf} \boldsymbol{\xi}\|_{\ell_e^p} \leq \left(\frac{|\alpha\phi_{2F}''|^p + |\alpha\phi_F'' + (1 + 2\alpha)\phi_{2F}''|^p}{N/2 - 1 + |\alpha|^p} \right)^{1/p} \leq CN^{-1/p}. \quad \square$$

CONCLUSION

We have presented a detailed stability and error analysis of the force-based QC 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 force-based QC 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 [20, 31] 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.

Finally, let us remark on the fact that we have only proven stability of the QCF method under the condition that $\phi_F'' + 8\phi_{2F}'' > 0$. By contrast, the atomistic model is uniformly stable if, *and only if* $\phi_F'' + 4\phi_{2F}'' > 0$ [11]. Hence, we expect that our above condition is not sharp. Although we have established sharp characterizations of the stability of other QC methods in [11], we were unable to rigorously achieve the same for the force-based QC method as well. While our computational results reported in [11] do indicate that L^{qcf} has only positive eigenvalues if $\phi_F'' + 4\phi_{2F}'' > 0$, this is not enough to ensure stability, uniformly as $N \rightarrow \infty$, in the regime $\phi_F'' + 4\phi_{2F}'' > 0$ for the $W^{1,\infty}$ - $W^{1,1}$ “duality pairing” or for any other norm with a recognizable continuum limit.

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