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for the Force-based Quasicontinuum Method

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Force-based multi-physics coupling methods are popular techniques to circumvent the difficulties faced in formulating consistent energy-based coupling approaches. Even though the QCF method is possibly the simplest coupling method of this kind, we anticipate that many of our observations apply more generally.

Key words and phrases: atomistic-to-continuum coupling, quasicontinuum method, sharp stability estimates

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ABSTRACT. A sharp stability analysis of atomistic-to-continuum coupling methods is essential for evaluating their capabilities for predicting the formation and motion of lattice defects. We formulate a simple one-dimensional model problem and give a detailed analysis of the stability of the force-based quasicontinuum (QCF) method. The focus of the analysis is the question whether the QCF method is able to predict a critical load at which fracture occurs.

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1. INTRODUCTION

Low energy equilibria for crystalline materials are typically characterized by localized defects that interact with their environment through long-range elastic fields. Atomistic-to-continuum coupling methods seek to make the accurate computation of such problems possible by using the accuracy of atomistic modeling only in the neighborhood of defects where the deformation is highly non-uniform. At some distance from the defects, sufficient accuracy can be obtained by the use of continuum models, which facilitate the reduction of degrees of freedom. The accuracy of the atomistic model at the defect combined with the efficiency of a continuum model for the far field enables, in principle, the reliable simulation of systems that are inaccessible to pure atomistic or pure continuum models.

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Typical test problems for atomistic-to-continuum coupling methods have been dislocation formation under an indenter, crack tip deformation, and deformation and fracture of grain boundaries [18]. In each of these problems, the crystal deforms quasi-statically until the equilibrium equations become singular, for example, when a dislocation is formed or moves or when a crack tip advances. Depending on the nature of the singularity, the crystal will then typically undergo a dynamic process when further loaded.

The quasicontinuum (QC) approximation models the continuum region by using an energy density that exactly reproduces the lattice-based energy density at uniform strain (the Cauchy-Born rule). Several variants of the QC approximation have been proposed that differ in how the atomistic and continuum regions are coupled [3,5,11,13,14,18,20,21]. Analyses of QC approximation have been given in [6,12,16,17,19,21]. We refer to [7] for a detailed review of the formulation and analysis, relevant to the present work, of different QC methods. Other coupling models are analyzed in [1,22,23].

In [7], we have begun to investigate whether the QC method can reliably predict the formation of defects. The main ingredient to establish whether or not this is the case is a sharp analysis to predict under which conditions the QC method is “stable.” More precisely, we ask whether there exist “stable” solutions of the QC method up to a critical load. We have begun to investigate this question in some depth for the most common energy-based QC formulations in [7]. In the present paper, we present a corresponding sharp stability analysis for the force-based quasicontinuum (QCF) method [4,5,24].

We focus on a one dimensional periodic chain with next-nearest neighbour pair interactions, which is introduced in Section 2.1. For this model, the uniform configuration ceases to be stable when the applied tensile strain reaches a critical value (fracture).

For the atomistic model and for energy-based QC formulations, coercivity (positivity) of the second variation evaluated at the equilibrium solution provides the natural notion of stability. However, the QCF method, which we describe in Sections 2.3 and 2.5, leads to non-conservative equilibrium equations, and therefore, positivity of the linearized QCF operator may be an inappropriate notion of stability. Indeed, we prove in Section 4.1 that, generically, the linearized QCF operator is indefinite.

As a consequence, we consider two further notions of stability. First, we investigate for which choices of discrete function spaces (that is, for which choices of topologies) does the linearized QCF operator have an inverse that is bounded uniformly in the size of the atomistic system. In Section 4.2, we present several sharp stability results as well as interesting counterexamples. However, these operator stability results do not necessarily correspond to any physical notion of stability. Hence, in Section 4.4, we propose the notion of dynamical stability, which can be reduced to certain properties of the eigenvalues. A careful numerical study suggests that the spectrum of the linearized QCF operator and that of the linearized quasi-nonlocal QC operator (QNL) (see [26] and Section 4.3) are identical. Combined with our previous results [7], this indicates that the QCF method is dynamically stable up to the critical load for fracture.
2. The force-based quasicontinuum method

2.1. The atomistic model problem. We consider deformations from the reference lattice $\varepsilon \mathbb{Z}$, where $\varepsilon > 0$ is a scaling that we will fix below. For the sake of simplicity, we consider only deformations which are periodic displacements from the uniform state $y_F = F \varepsilon \mathbb{Z} = (F \varepsilon \ell)_{\ell \in \mathbb{Z}}$, that is, we admit deformations from the space

$$\mathcal{Y}_F = y_F + \mathcal{U}$$

where

$$\mathcal{U} = \{ u \in \mathbb{R}^\mathbb{Z} : u_{\ell+2N} = u_\ell \text{ for } \ell \in \mathbb{Z}, \text{ and } \sum_{\ell=-N+1}^N u_\ell = 0 \}.$$

We call $F$ the macroscopic deformation gradient, and we set $\varepsilon = 1/N$ throughout.

Although the energies and forces are defined for general $2N$-periodic displacements, we only admit those with zero mean, as is common for continuum problems with periodic boundary conditions, in order to obtain unique solutions to the equilibrium equations.

We consider only nearest-neighbor and next-nearest neighbor pair interactions so that the potential energy per period of a deformation $y \in \mathcal{Y}_F$ is given by

$$E_a(y) = \varepsilon \sum_{\ell=-N+1}^N \left( \phi'(y'_\ell) + \phi(y'_\ell + y'_{\ell+1}) \right),$$

where

$$y'_\ell = \varepsilon^{-1}(y_\ell - y_{\ell-1}),$$

and where $\phi$ is a Lennard-Jones type interaction potential:

(i) $\phi \in C^3((0, +\infty); \mathbb{R})$,

(ii) there exists $r_* > 0$ such that $\phi$ is convex in $(0, r_*)$ and concave in $(r_*, +\infty)$.

(iii) $\phi^{(k)}(r) \to 0$ rapidly as $r \nearrow \infty$, for $k = 0, \ldots, 3$.

Assumption (iii) is not strictly necessary for our analysis but serves to motivate that next-nearest neighbour interactions are typically dominated by nearest-neighbour terms.

We assume that the atomistic system is subject to $2N$-periodic external forces $(f_\ell)_{\ell \in \mathbb{Z}}$ with zero mean, i.e., $f \in \mathcal{U}$, so that the total energy per period takes the form

$$E_a^{\text{tot}}(y) = E_a(y) - \varepsilon \sum_{\ell=-N+1}^N f_\ell y_\ell.$$

Equilibria $y \in \mathcal{Y}_F$ of the atomistic total energy are solutions to the equilibrium equations

$$\mathcal{F}_{a,\ell}(y) + f_\ell = 0, \quad -\infty < \ell < \infty,$$

where the (scaled) atomistic forces $\mathcal{F}_a : \mathcal{Y}_F \to \mathcal{U}^*$ are defined by

$$\mathcal{F}_{a,\ell}(y) := -\frac{1}{\varepsilon} \frac{\partial E_a(y)}{\partial y_\ell}, \quad -\infty < \ell < \infty,$$

and where $\mathcal{U}^*$ is the space of linear functionals on $\mathcal{U}$. We remark that the translational invariance of the atomistic energy implies that $\mathcal{F}_{a,\ell}(y)$ has zero mean,

$$\sum_{\ell=-N+1}^N \mathcal{F}_{a,\ell}(y) = \frac{d}{ds} E_a \left( y - \frac{s}{\varepsilon} e \right) \bigg|_{s=0} = 0,$$
where \( e = (1)_{\ell \in \mathbb{Z}} \) is the unit translation vector. Thus, we see that, at least heuristically, the external force vector \( f \) lies indeed in the range of the atomistic force operator.

We note, moreover, that \( y_F \) is an equilibrium of the atomistic energy, that is
\[
\mathcal{F}_{a,\ell}(y_F) = 0 \quad -\infty < \ell < \infty, \quad \text{for all } F > 0.
\]
The question which we will investigate in this paper, beginning in Section 3, is for which \( F \) it is a stable equilibrium and whether the force-based QC method is able to predict the stability of \( y_F \).

2.2. The local quasicontinuum approximation. We begin by observing that the atomistic energy can be rewritten as a sum over the contributions from each atom,
\[
\mathcal{E}_a(y) = \varepsilon \sum_{\ell = -N+1}^{N} E^a_\ell(y) \quad \text{where}
\]
\[
E^a_\ell(y) = \frac{1}{2} [\phi(y^\ell_0) + \phi(y^\ell_{\ell+1}) + \phi(y^\ell_{\ell-1} + y^\ell_0) + \phi(y^\ell_{\ell+1} + y^\ell_{\ell+2})].
\]
If \( y \) is “smooth”, that is, if \( y'_\ell \) varies slowly, then the atomistic energy can be accurately approximated by the Cauchy–Born or local quasicontinuum energy
\[
\mathcal{E}_{ql}(y) = \varepsilon \sum_{\ell = -N+1}^{N} E^c_\ell(y), \quad \text{where}
\]
\[
E^c_\ell(y) = \frac{1}{2} [\phi(y'^\ell_0) + \phi(y'^\ell_{\ell+1}) + \phi(2y'_\ell) + \phi(2y'^\ell_{\ell+1})] = \frac{1}{2} [\phi_{cb}(y'_\ell) + \phi_{cb}(y'^\ell_{\ell+1})],
\]
where \( \phi_{cb}(r) = \phi(r) + \phi(2r) \) is the Cauchy–Born stored energy density.

In this approximation we have replaced the next-nearest neighbor interactions by nearest neighbor interactions to obtain a model with stronger locality. This makes it possible to coarsen the model (to remove degrees of freedom), which eventually leads to significant gains in efficiency [5,18]. However, in the present work we will not consider this additional step.

An equilibrium \( y \in \mathcal{Y}_F \) of the local QC energy is a solution to the equilibrium equations
\[
\mathcal{F}_{c,\ell}(y) + f_\ell = 0, \quad -\infty < \ell < \infty,
\]
where the (scaled) local QC forces \( \mathcal{F}_c : \mathcal{Y}_F \rightarrow \mathcal{U}^* \) are defined by
\[
\mathcal{F}_{c,\ell}(y) := -\frac{1}{\varepsilon} \frac{\partial \mathcal{E}_a(y)}{\partial y_\ell}, \quad -\infty < \ell < \infty.
\]
As in (2) it follows that the vector \( \mathcal{F}_c(y) \) has zero mean.

2.3. The force-based quasicontinuum approximation. If a deformation \( y \) is “smooth” except in a small region of the domain, then it is desirable to couple the accurate atomistic description with the efficient continuum description. The force-based quasicontinuum (QCF) approximation achieves this by mixing the equilibrium equations of the atomistic model with those of the continuum model without any interface or transition region.

Suppose that \( y \) is “smooth” except in a region \( A := \{-K, \ldots, K\} \), where \( K > 1 \). We call \( A \) the atomistic region and \( C = \{-N+1, \ldots, N\} \setminus A \) the continuum region. The force-based QC approximation is obtained by evaluating the forces in the atomistic
region by the full atomistic model (1) and the forces in the continuum region by the local QC model (5). This yields the QCF operator for the (scaled) forces $F_{qcf}: Y_F \rightarrow U^*$, defined by
\[
F_{qcf,\ell}(y) := \begin{cases} 
F_{\alpha,\ell}(y), & \text{if } \ell \in A, \\
F_{c,\ell}(y), & \text{if } \ell \in C.
\end{cases}
\]

Force-based coupling methods such as (6) are trivially consistent (provided the continuum model is consistent with the atomistic model) and are therefore a natural remedy for the inconsistencies one observes when formulating simple energy-based coupling methods such as the original QC method [20]. Similar constructions have appeared in the literature under several different names and for various applications (e.g., FeAt [15], CADD [25], or brutal force mixing [2]). In the context of the QC method this method was first described in [5], where it was shown that the force-based QC method is the limit of the so-called ghost-force correction iteration [24]. A basin of attraction and rate for the convergence the ghost-force correction iteration to the force-based QC method was given in [5]. Sharp stability estimates for the ghost-force correction iteration are given in [9].

Unfortunately, the forces generated by the QCF method are non-conservative, and hence cannot be associated with an energy. Moreover, even though both the atomistic forces $F_{\alpha}(y)$ and the local QC forces $F_{C}(y)$ have zero mean, it turns out that this is false for the mixed forces $F_{qcf}(y)$. A straightforward computation shows that
\[
\sum_{\ell = -N+1}^{N} F_{qcf,\ell}(y) = \varepsilon^{-1}[2\phi'(2y'_K') - \phi'(y'_K + y'_{-K-1}) - \phi'(y'_{-K+1} + y'_{-K})]
- \varepsilon^{-1}[2\phi'(2y'_{K+1}) - \phi'(y'_{K+2} + y'_{K+1}) - \phi'(y'_{K+1} + y'_{K})],
\]
which is in general non-zero. After introducing the necessary notation, we will overcome this difficulty by defining a variational form of the QCF method, which effectively projects the QCF forces onto the correct range.

2.4. Norms and variational notation. For future reference, we recall the backward first difference $v'_l = \varepsilon^{-1}(v_l - v_{l-1})$ and also define the centered second difference $v''_l = \varepsilon^{-2}(v_{l+1} - 2v_l + v_{l-1})$.

For displacements $v \in U$ and $1 \leq p \leq \infty$, we define the $\ell^p_p$ norms,
\[
\|v\|_{\ell^p_p} := \begin{cases} 
\left(\varepsilon \sum_{l = -N+1}^{N} |v_l|^p \right)^{1/p}, & 1 \leq p < \infty, \\
\max_{l = -N+1, \ldots, N} |v_l|, & p = \infty,
\end{cases}
\]
and let $U^{0,p}$ denote the space $U$ equipped with the $\ell^p_p$ norm. We further define the $U^{1,p}$ norm
\[
\|v\|_{U^{1,p}} := \|v'\|_{\ell^p_p},
\]
and let $U^{1,p}$ denote the space $U$ equipped with the $U^{1,p}$ norm. Similarly, we define the space $U^{2,p}$ and its associated $U^{2,p}$ norm.

The inner product associated with the $\ell^2_p$ norm is
\[
\langle v, w \rangle := \varepsilon \sum_{l = -N+1}^{N} v_l w_l \quad \text{for } v, w \in U.
\]
We have defined the norms $\| \cdot \|_{L^q}$ and the inner product $\langle \cdot, \cdot \rangle$ on $U$, though we will also apply them for arbitrary vectors from $\mathbb{R}^{2N}$.

The external force $f = (f_t)_{t \in \mathbb{Z}}$ is a $2N$-periodic mean zero vector, and we have seen that the atomistic forces and the forces in the QCL method are also $2N$-periodic mean zero vectors. Using the inner product, we can view $f_t$ as a linear functional on $U$. We recall that the space of linear functionals on $U$ is denoted by $U^*$, and we note that each such $T \in U^*$ has a unique representation as a zero mean $2N$-periodic vector $g_T \in U$,

$$
T[v] = \langle g_T, v \rangle \quad \forall v \in U.
$$

We will normally not make a distinction between these representations. For example, an external force vector $f$ may be equally interpreted as a linear functional (i.e., $f \in U^*$), or identified with its Riesz representation (i.e., $f \in U$).

For $g \in U^*$, $s = 0, 1$, and $1 \leq p \leq \infty$, we define the negative norms $\|g\|_{U^{-s,p}}$ as follows:

$$
\|g\|_{U^{-s,p}} := \sup_{\|v\|_{U^{s,p}} = 1} \langle g, v \rangle,
$$

where $1 \leq q \leq \infty$ satisfies $\frac{1}{p} + \frac{1}{q} = 1$. We let $U^{-s,p}$ denote the space $U^*$ equipped with the $U^{-s,p}$ norm.

Since we can identify elements of $U^*$ with elements of $U$, we can investigate the relationship between the $U^{-0,p}$ and $U^{0,p}$-norms. This will be useful later on in our analysis. It turns out that $\| \cdot \|_{U^{-0,p}} \neq \| \cdot \|_{U^{0,p}}$ in general, but that the following equivalence relation holds:

$$
\|u\|_{U^{-0,p}} \leq \|u\|_{U^{0,p}} \leq 2\|u\|_{U^{-0,p}} \quad \text{for all } u \in U.
$$

To see this, we note that the inequality $\|u\|_{U^{-0,p}} \leq \|u\|_{U^{0,p}}$ follows from (8) and Hölder’s inequality. To prove the second inequality, we use that fact that, for $u \in U$,

$$
\|u\|_{U^{0,p}} = \sup_{v \in \mathbb{R}^{2N}} \langle u, v \rangle = \sup_{\|v\|_q = 1} \sup_{\|v\|_{q'} = 1} \langle u, v - \bar{v} \rangle,
$$

where $\bar{v} = \frac{1}{2N} \sum_{j=-N+1}^{N} v_j$ of $v \in \mathbb{R}^{2N}$. Thus, we can estimate

$$
\|u\|_{U^{0,p}} \leq \|u\|_{U^{-0,p}} \sup_{\|v\|_q = 1} \|v - \bar{v}\|_{q'} \leq 2\|u\|_{U^{-0,p}},
$$

where we also used the fact that, by Hölder’s inequality, $\|\bar{v}\|_{q'} \leq \|v\|_{q'}$ for any $v \in \mathbb{R}^{2N}$.

2.5. **Projection of non-conservative forces.** If we interpret forces as elements of $U^*$, then it is natural to consider the following variational formulation of the QCF method,

$$
\langle \mathcal{F}_{\text{qcf}}(y) + f, u \rangle = 0 \quad \forall u \in U.
$$

In other words, (10) requires that $\mathcal{F}_{\text{qcf}}(y) + f = 0$ as a functional in $U^*$. This formulation guarantees that the QCF operator has the correct range.
To obtain an atom-based description of the equilibrium equations, we explicitly compute the representation of $F_{\text{qcf}}(y) \in \mathcal{U}^*$ as an element of $\mathcal{U}$ (see also (7)), that is as a zero mean 2N-periodic vector $P_{\mathcal{U}}F_{\text{qcf}}(y)$, where $P_{\mathcal{U}}$ is defined by

$$(P_{\mathcal{U}}v)_{\ell} = v_{\ell} - \frac{1}{2N} \sum_{j=-N+1}^{N} v_j.$$ With this notation, the variational equilibrium equations can be understood as projected equilibrium equations in atom-based form,

$$(P_{\mathcal{U}}F_{\text{qcf}}(y))_{\ell} + f_{\ell} = 0, \quad -\infty < \ell < \infty. \quad (11)$$

The equivalent formulations (10) and (11) define the correct force-based QC method for the periodic model problem defined in Section 2.1.

**Remark 1.** The projection of the QCF equilibrium system is an artifact of the periodic boundary conditions. For the displacement boundary conditions that we analyzed in [10], or for the mixed boundary conditions that are considered in [8], this projection is not necessary.

3. **Stability of a Uniform Deformation**

It is easy to see that, in the absence of external forces, the uniformly deformed lattice $y = y_F$ is an equilibrium of the atomistic energy as well as the local QC energy, that is

$$\mathcal{F}_a(y_F) = 0 \quad \text{and} \quad \mathcal{F}_c(y_F) = 0 \quad \text{for all } F > 0.$$ For some values of $F$, the equilibrium will be stable, by which we mean that the second variation

$$\mathcal{E}_a''(y_F)[u, v] = \varepsilon \sum_{\ell=-N+1}^{N} \left\{ \phi_F''u_{\ell}v_{\ell}' + \phi_{2F}''(u_{\ell}' + u_{\ell+1}')(v_{\ell}' + v_{\ell+1}') \right\}, \quad \text{for } u \in \mathcal{U},$$

where

$$\phi_F'' := \phi''(F) \quad \text{and} \quad \phi_{2F}'' := \phi''(2F),$$

is positive definite, that is,

$$\mathcal{E}_a''(y_F)[u, u] > 0 \quad \forall u \in \mathcal{U} \setminus \{0\}.$$ (We note that a second variation, e.g. $\mathcal{E}_a''(y_F)$, may be understood either as a bilinear form on $\mathcal{U}$ or a linear operator from $\mathcal{U}$ to $\mathcal{U}^*$. It can also be expressed as a Hessian matrix with respect to a given basis for the vector space $\mathcal{U}$.)

In order to avoid having to distinguish several cases, we will assume throughout our analysis that $F \geq r_*/2$, which implies by property (ii) of the interaction potential that $\phi_{2F}'' \leq 0$. This assumption holds for most realistic interaction potentials so long as the chain is not under extreme compression.

As above, we can evaluate the second variation of the local QC energy at $y = y_F$,

$$\mathcal{E}_{\text{qcf}}''(y_F)[u, v] = \varepsilon \sum_{\ell=-N+1}^{N} A_Fu_{\ell}'v_{\ell}'$$

where $A_F$ is the interaction potential matrix.
where $A_F$ is the *elastic modulus* of the continuum model,

$$A_F := \phi''_{cb}(F) = \phi''_{c} + 4\phi''_{2F}.$$  

Thus, we say that $y_F$ is stable for the local QC approximation if $E''_a(y_F)[u,u] > 0$ for all $u \in \mathcal{U} \setminus \{0\}$.

In [7], we have given explicit characterizations for which $F$ the equilibrium $y_F$ is stable in the atomistic model and in several energy-based QC models. The results for the atomistic and the local QC models are summarized in the following proposition.

**Proposition 1 (cf. Prop. 1 and 2 in [7]).** Let $F \geq r_*/2$ then the second variations $E''_a(y_F)$, respectively $E''_{qc}(y_F)$, are positive definite if and only if

$$A_F - \lambda_N^2 \varepsilon^2 \phi''_{2F} > 0,$$

where $2 \leq \lambda_N \leq \pi$.

If we denote the critical strains which divide the regions of stability for the atomistic and QCL models, respectively, by $F^*_a$ and $F^*_c$, then a relatively straightforward error analysis [7, Sec. 5] shows that $F^*_a = F^*_c + O(\varepsilon^2)$, that is, the QCL model accurately reproduces the onset of a fracture instability. In the following section, we investigate whether or not the QCF method has a similar property.

### 4. Sharp Stability of the Force-based QC Method

A trivial consequence of the definition of $F_{qcf}$ in (6) is that $y = y_F$ is also a solution of the QCF equilibrium equations (11),

$$F_{qcf}(y_F) = 0 \quad \text{for all } F > 0.$$  

(As a matter of fact, this means that the QCF method is consistent; though this is not the focus of the present work.)

To investigate the stability of the QCF method we define the linearized QCF operator $L_{qcf,F} := -F'_{qcf}(y_F) : \mathcal{U} \to \mathcal{U}^*$ by

$$\langle L_{qcf,F}u, v \rangle := -\langle F'_{qcf}(y_F)[u], v \rangle \quad \text{for all } u, v \in \mathcal{U}.$$  

The equilibrium equations for the linearized force-based approximation are then given by $u \in \mathcal{U}$ satisfying

$$\langle L_{qcf,F}u, v \rangle = \langle f, v \rangle \quad \text{for all } v \in \mathcal{U},$$

or in functional form

$$\mathcal{P}_UL_{qcf,F}u = f.$$  

We remark that, while $L_{qcf,F} \in L(\mathcal{U}, \mathcal{U}^*)$, the projected operator $\mathcal{P}_UL_{qcf,F}$ may be interpreted as a map from $\mathcal{U}$ to $\mathcal{U}$. 
4.1. Lack of coercivity. Since the force field $F_{qcf}(y)$ is non-conservative and the linearized QCF operator $L_{qcf,F}$ is not the second variation of an energy functional, positivity (or coercivity) of $L_{qcf,F}$ may be the incorrect notion of stability for the QCF model. Indeed, it turns out that, if $N$ is large, then $L_{qcf,F}$ cannot be positive definite.

**Theorem 2.** Let $\phi''_F > 0$ and $\phi''_{2F} \neq 0$, then there exist constants $C_1, C_2$ which may depend on $\phi''_F$ and $\phi''_{2F}$, such that, for $N$ sufficiently large and for $2 \leq K \leq N/2$,

$$-C_1 N^{1/2} \leq \inf_{u \in \mathcal{U}} \langle L_{qcf,F} u, u \rangle \leq -C_2 N^{1/2}.$$

In [10], we have shown this result for a Dirichlet boundary value problem. The proof carries over from the Dirichlet case almost verbatim and is therefore omitted. As a matter of fact, the test function which we explicitly constructed in the proof of Lemma 4.1 in [10] is already periodic and, after shifting it to have zero mean, can therefore be used again to prove Theorem 2.

Theorem 2 forces us to consider alternative notions of stability. For example, one could understand $L_{qcf,F}$ as a linear operator between appropriately chosen discrete function spaces, determine for which values of $F$ it is bijective, and estimate the norm of its inverse. Physically, this measures the magnitude of the response of the equilibrium configuration to perturbations in external forces, and in Section 4.2 we attempt to find the largest interval surrounding $F = 1$ and define this region to be stable. However, an operator can be bijective and have bounded norm even when it has negative eigenvalues, so for a general equilibrium state $y_F$, invertibility alone is not a suitable criterion for determining the “physical” stability. To be able to decide whether a stable equilibrium of the QCF equations is also stable in a physical sense, we propose a notion of dynamical stability in Section 4.4.

4.2. Stability as a linear operator. Since $\mathcal{U}$ is a finite-dimensional linear space, the choice of topology with which we equip it is unimportant to the question whether $L_{qcf,F}$ is invertible. However, it has surprising repercussions when we analyze an operator norm of the inverse, that is $\|L_{qcf,F}^{-1}\|$ in the limit as $N \to \infty$.

Our strongest and simplest result is obtained when we view $\mathcal{P}_d L_{qcf,F}$ as a map from $\mathcal{U}^{2,\infty}$ to $\mathcal{U}^{0,\infty}$.

**Theorem 3.** If $|\phi''_F| - (4 + 2\epsilon)|\phi''_{2F}| > 0$, then $\mathcal{P}_d L_{qcf,F} : \mathcal{U} \to \mathcal{U}$ is bijective and

$$\| (\mathcal{P}_d L_{qcf,F})^{-1} \|_{L(\mathcal{U}^{0,\infty}, \mathcal{U}^{2,\infty})} \leq \frac{1}{|\phi''_F| - (4 + 2\epsilon)|\phi''_{2F}|}.$$

**Proof.** Recalling the definition of $L_{qcf,F}$, we can rewrite this operator in the form

$$\mathcal{P}_d L_{qcf,F} = \phi''_F L_1 + \phi''_{2F} \mathcal{P}_d L_2,$$
where \( L_1 \) and \( \tilde{L}_2 \) are given by
\[
(L_1 u)_\ell = -\varepsilon^2 (u_{\ell+1} - 2u_\ell + u_{\ell-1}), \quad \text{and}
\]
\[
(\tilde{L}_2 u)_\ell = \begin{cases} 
-\varepsilon^2 (u_{\ell+2} - 2u_\ell + u_{\ell-2}), & \ell = -K, \ldots, K, \\
-4\varepsilon^2 (u_{\ell+1} - 2u_\ell + u_{\ell-1}), & \text{otherwise}.
\end{cases}
\]

We note that \( \mathcal{P}_u L_1 = L_1 \) which is why we have included the projection only in the second-neighbor operator.

The projection of \( \tilde{L}_2 \) given by \( \mathcal{P}_u \tilde{L}_2 \) is
\[
(\mathcal{P}_u \tilde{L}_2 u)_\ell = (\tilde{L}_2 u)_\ell - \frac{\varepsilon}{2} \sum_{j=-N+1}^{N} (\tilde{L}_2 u)_j.
\]

We will prove below that
\[
\|\mathcal{P}_u \tilde{L}_2\|_{L(\ell^\infty, \ell^0, \infty)} \leq 4 + 2\varepsilon. \tag{12}
\]

Assuming that this bound is established, we obtain
\[
\|\mathcal{P}_u L_{\text{qs}u} R u\|_{\ell^\infty} \geq |\phi''_F|\|L_1 u\|_{\ell^\infty} - |\phi''_F|\|\mathcal{P}_u \tilde{L}_2 u\|_{\ell^\infty} \\
\geq (|\phi''_F| - (4 + 2\varepsilon)|\phi''_F|)\|u''\|_{\ell^\infty},
\]
which is equivalent to the statement of the theorem.

To prove (12), we note that, for \( \ell = -K, \ldots, K \), we have
\[
(\tilde{L}_2 u)_\ell = -(u''_{\ell+1} + 2u'_\ell + u''_{\ell-1}) = -4u'_\ell - (u''_{\ell+1} - 2u''_{\ell-1}).
\]

Using the first representation of \( (\tilde{L}_2 u)_\ell \) above, we immediately see that (for \( \ell \) from the continuum region this statement is trivial)
\[
|(\tilde{L}_2 u)_\ell| \leq 4\|u''\|_{\ell^\infty} \quad \text{for } \ell = -N + 1, \ldots, N.
\]

From the second representation of \( (\tilde{L}_2 u)_\ell \), we obtain
\[
\sum_{\ell=-N+1}^{N} (\tilde{L}_2 u)_\ell = -4 \sum_{\ell=-N+1}^{N} u'_\ell + \sum_{\ell=-K}^{K} (u''_{\ell+1} - 2u''_{\ell} + u''_{\ell-1}) \\
= -u''_{K+1} + u''_{K} + u''_{-K} - u''_{-K-1},
\]
and hence,
\[
|\mathcal{P}_u \tilde{L}_2 u| \leq |(\tilde{L}_2 u)| + \frac{\varepsilon}{2} \sum_{j=-N+1}^{N} (\tilde{L}_2 u)_j \\
\leq 4\|u''\|_{\ell^\infty} + \frac{\varepsilon}{2} (|u''_{K+1}| + |u''_{K}| + |u''_{-K-1}| + |u''_{-K}|) \\
\leq (4 + 2\varepsilon)\|u''\|_{\ell^\infty}.
\]

This establishes (12) and thus concludes the proof of the theorem. \( \Box \)

**Remark 2.** With a small modification, Theorem 3 remains true for an arbitrary choice of the atomistic region \( \mathcal{A} \). The correction \( 2\varepsilon \) then needs to be replaced by \( n_i\varepsilon \) where \( n_i \) is the number of interfaces between the atomistic and the continuum region. \( \Box \)
Remark 3. Theorem 3 also holds in the case of the artificial Dirichlet boundary conditions analyzed in [10]. In that case, the projection $\mathcal{P}_U$ is not required and therefore the correction $2\varepsilon$ does not occur at all. □

Theorem 3 is, in many respects, a very satisfactory result. It shows that, except for a small error, QCF is stable whenever the atomistic model is. However, the choice of function space $U^{2,\infty}$ is somewhat unusual, and it is highly unlikely that such a result would remain true in higher dimensions, as it requires a regularity that is not normally exhibited by linear elliptic systems.

It is therefore also interesting to analyze the QCF operator as a map from $U^{1,p}$ to $U^{-1,p} = (U^{1,p})^*$, where $1 \leq p \leq \infty$. However, we saw in [10, Thm. 7.1] for a Dirichlet problem that, for $1 \leq p < \infty$, the stability of $L_{qcf, F}$ is not uniform in $N$. The following theorem, whose proof is contained in Appendix B, establishes the same result for the periodic model we consider in the present paper.

**Theorem 4.** Suppose that $\phi_F'' > 0$, $\phi_{2F}'' \in \mathbb{R} \setminus \{0\}$, and $1 \leq p < \infty$. Then there exists a constant $C > 0$, depending on $\phi_F''$ and $\phi_{2F}''$, such that, for $2 \leq K < N - 2$,

$$\|L_{qcf, F}^{-1}\|_{L(U^{-1,p}, U^{1,p})} \geq CN^{1/p}.$$ 

It remains to investigate the case $p = \infty$. The following result is an extension of [10, Thm. 5.1] to periodic boundary conditions. Its proof is contained in Appendix A.

**Theorem 5.** If $F \geq r/2$ and $\phi_F'' + 8\phi_{2F}'' > 0$, then

$$\|L_{qcf, F}^{-1}\|_{L(U^{-1,\infty}, U^{1,\infty})} \leq \frac{2}{\phi_F'' + 8\phi_{2F}''}.$$ 

Theorem 5 establishes operator stability of the $L_{qcf, F}$ operator, uniformly in $N$, provided that $\phi_F'' + 8\phi_{2F}'' > 0$. Compared with with Proposition 1 this result predicts a significantly smaller stability region than either the atomistic model or the continuum model. We employ numerical experiments to see whether the condition $\phi_F'' + 8\phi_{2F}'' > 0$ is sharp.

The norm $\|L_{qcf, F}^{-1}\|_{L(U^{-1,\infty}, U^{1,\infty})}$ is difficult to calculate explicitly, so we will estimate it in terms of the $\ell^\infty$-operator norm of a related matrix. To that end, we note that, according to Lemma 11, $L_{qcf, F}$ can be represented in terms of a conjugate operator, $E_{qcf, F}$, by

$$\langle L_{qcf, F} u, v \rangle = \langle E_{qcf, F} u', v' \rangle \quad \forall u, v \in \mathcal{U}.$$ 

An explicit representation of $E_{qcf, F}$ is provided in (17). Formula (17) gives an $\mathbb{R}^{2N \times 2N}$ matrix representation for $E_{qcf, F}$ such that $E_{qcf, F} e = A_F e$ where $e = (1, \ldots, 1)^T$. It thus follows that the projected operator $\mathcal{P}_U E_{qcf, F} : \mathbb{R}^{2N} \to \mathbb{R}^{2N}$ satisfies

$$\mathcal{P}_U E_{qcf, F} : \mathcal{U} \to \mathcal{U}, \quad \text{and} \quad \mathcal{P}_U E_{qcf, F} e = 0.$$ 

Here, and for the remainder of the section, we identify $\mathcal{U}$ with the subspace of $\mathbb{R}^{2N}$ of zero mean vectors. After these preliminary remarks, we establish the following result.
**Proposition 6.** The QCF operator $L_{\text{qcf},F} : U \to U^*$ is invertible if and only if $(\mathcal{P}_u E_{\text{qcf},F} + e \otimes e) \in \mathbb{R}^{2N \times 2N}$ is invertible, and
\[
\frac{1}{2} \|T\|_\infty \leq \|L_{\text{qcf},F}^{-1}\|_{L(\ell^{-1,\infty}, \ell^{1,\infty})} \leq 2 \|T\|_\infty,
\]
where
\[
T = \mathcal{P}_u (\mathcal{P}_u E_{\text{qcf},F} + e \otimes e)^{-1} \mathcal{P}_u,
\]
and where $\|T\|_\infty$ denotes the $\ell^\infty$-operator norm of $T$.

**Proof.** The first statement follows from the discussion above.

To prove the upper bound, we use (7) to estimate
\[
\|T\|_{L(\ell^{-0,\infty}, \ell^{0,\infty})} = \sup_{f \in U, f \neq 0} \frac{\|f\|_{\ell^{-0,\infty}}}{\|f\|_{\ell^{0,\infty}}} \leq \frac{1}{2} \sup_{f \in U, f \neq 0} \frac{\|f\|_{\ell^\infty}}{\|f\|_{\ell^\infty}} = \frac{1}{2} \|T\|_\infty.
\]

To prove the lower bound, we first note that $\mathcal{P}_u f = T$. We will also use the fact that $\|\mathcal{P}_u f\|_{\ell^\infty} \leq 2 \|f\|_{\ell^\infty}$ for all $f \in \mathbb{R}^{2N}$. Employing also (7) again, we can deduce that
\[
\|T\|_{L(\ell^{-0,\infty}, \ell^{0,\infty})} = \sup_{f \in \mathbb{R}^{2N}, f \neq 0} \frac{\|\mathcal{P}_u f\|_{\ell^{0,\infty}}}{\|\mathcal{P}_u f\|_{\ell^{0,\infty}}} \geq \sup_{f \in \mathbb{R}^{2N}, f \neq 0} \frac{\|\mathcal{P}_u f\|_{\ell^{0,\infty}}}{\|\mathcal{P}_u f\|_{\ell^{0,\infty}}} = \sup_{f \in \mathbb{R}^{2N}, f \neq 0} \|f\|_{\ell^\infty} = \frac{1}{2} \|T\|_\infty.
\]

The penultimate equality holds because $\mathcal{P}_u f = 0$ implies $T f = 0$. \qed

In Proposition 6 we have reduced the estimation of the operator norm of $L_{\text{qcf},F}^{-1}$ to the computation of the $\ell^\infty$-operator norm (which is simply the largest row sum) of a matrix $T \in \mathbb{R}^{2N \times 2N}$, which is explicitly available (note that $\mathcal{P}_u = I - \frac{1}{2} e \otimes e \in \mathbb{R}^{2N \times 2N}$).

In Figure 1, we plot the norm of $T$ as a function of $A_F/\phi_F' = 1 + 4\phi_F'/\phi_F$. We clearly observe that $L_{\text{qcf},F}$ is in fact stable for all macroscopic gradients $F$ for which $A_F > 0$, that is, the bound required in Theorem 5 is not sharp. Moreover, the numerical experiments shown in Figure 1 support the following conjecture.
Conjecture 7. If $\phi''_p + 4\phi'_p > 0$, then

$$\|L^{-1}_{qcf,F}\|_{L(U^{-1,\infty}, U^1,\infty)} \leq \frac{1}{\phi''_p} \eta \left(1 + 4 \frac{\phi'_p}{\phi''_p}\right),$$

where $\eta$ does not depend on $N$ or $K$, but $\eta \left(1 + 4 \frac{\phi'_p}{\phi''_p}\right) \to \infty$ as $1 + 4 \frac{\phi'_p}{\phi''_p} \to 0$.

In fact, the numerical experiments suggest that $\|L^{-1}_{qcf,F}\|_{L(U^{-1,\infty}, U^1,\infty)}$ grows faster than $\frac{1}{\phi''_p + 4\phi'_p}$, which would imply that an estimate such as the one in Theorem 5, but with the constant 8 replaced by 4 would be false.

4.3. The quasi-nonlocal coupling method. In preparation for the following section, where we introduce another notion of stability for the QCF method, we review a popular energy-based coupling method. In the next section, we will make numerical comparisons between this method and the QCF method.

The quasi-nonlocal quasicontinuum approximation (QNL) [26] was derived as a modification of the energy-based QC approximation [20] in order to correct the inconsistency at the atomistic-to-continuum interface [5, 24]. In the case of next-nearest neighbour pair interaction, the QNL method can be formulated as follows. Nearest neighbor interaction terms are left unchanged. A next-nearest neighbor interaction term $\phi(\varepsilon^{-1}(y_{\ell+1} - y_{\ell-1}))$ is left unchanged if atom $\ell$ belongs to the atomistic region, but is replaced by a Cauchy–Born approximation

$$\phi(\varepsilon^{-1}(y_{\ell+1} - y_{\ell-1})) \approx \frac{1}{2} [\phi(2y_{\ell}) + \phi(2y_{\ell+1})], \quad \text{if } \ell \in C.$$
This process yields the QNL energy functional

$$\mathcal{E}_{\text{qnl}}(y) = \varepsilon \sum_{\ell=1}^{N} \phi(y_{\ell}) + \varepsilon \sum_{\ell \in A} \phi(y_{\ell} + y_{\ell+1}) + \varepsilon \sum_{\ell \in C} \frac{1}{2} [\phi(2y_{\ell}) + \phi(2y_{\ell+1})].$$

We remark that the QNL method is consistent for our next-nearest neighbour pair interaction model, and in particular, $y_{F}$ is an equilibrium of the QNL energy functional in the absence of external forces. Moreover, in [7] we have established the following sharp stability result for the QNL method, which shows that the QNL method is predictive up to the limit load for fracture.

**Proposition 8 (Proposition 3 in [7]).** Suppose that $F \geq r_{s}/2$ and that $K \leq N-1$, then $\mathcal{E}_{\text{qnl}}''(y_{F})$ is positive definite in $\mathcal{U}$ if and only if $A_{F} > 0$.

4.4. **Dynamical Stability.** We have pointed out in Section 4.1 that operator stability for $L_{\text{qcf},F}$ cannot guarantee that the equilibrium $y_{F}$ is a stable equilibrium of the atomistic model (e.g., a local minimum). To obtain at least a theoretical methodology to determine stability of $y_{F}$ from the QCF operator alone, we propose the notion of dynamical stability. The dynamical system

$$\ddot{u}(t) + \mathcal{P}_{U}L_{\text{qcf},F}u(t) = 0,$$

$$u(0) = u_{0}, \quad u'(0) = 0,$$

has a unique solution $u \in C^\infty([0, +\infty); \mathcal{U})$. We call this dynamical system **stable** if there exists a constant $C$, independent of $N$, such that

$$\|u(t)\|_{\ell_{2}} \leq C\|u_{0}\|_{\ell_{2}}, \quad \forall t > 0, \quad \forall u_{0} \in \mathcal{U}. \quad (13)$$

This condition can be best understood in terms of the spectrum of $\mathcal{P}_{U}L_{\text{qcf},F}$. In numerical experiments, which are shown in Table 1, we have made the surprising observation that $\mathcal{P}_{U}L_{\text{qcf},F}$ and $\mathcal{E}_{\text{qnl}}''(y_{F})$ appear to have the same spectrum. This has led us to make the following conjecture.

**Conjecture 9.** For all $N \geq 4$, $1 \leq K < N$, and $F > 0$, the operator $\mathcal{P}_{U}L_{\text{qcf},F}$ is diagonalizable and its spectrum is identical to the spectrum of $\mathcal{E}_{\text{qnl}}''(y_{F})$.

| $N$ | $\phi_{2F}'$ | -0.1 | -0.15 | -0.2 | -0.25 |
|-----|--------------|------|-------|------|-------|
| 50  | 0            | 1.19e-010 | 9.93e-011 | 7.31e-011 | 6.64e-011 |
| 100 | 0            | 6.97e-010 | 6.19e-010 | 4.71e-010 | 3.16e-010 |
| 150 | 0            | 2.05e-009 | 1.83e-009 | 1.31e-009 | 1.23e-009 |
| 200 | 0            | 4.12e-009 | 3.12e-009 | 2.90e-009 | 2.10e-009 |
| 250 | 0            | 8.25e-009 | 6.38e-009 | 6.38e-009 | 3.96e-009 |
| 300 | 0            | 1.62e-008 | 1.15e-008 | 9.98e-009 | 8.86e-009 |

**Table 1.** The spectra of $\mathcal{P}_{U}L_{\text{qcf},F}$ and $\mathcal{E}_{\text{qnl}}''(y_{F})$ are computed for increasing $N$, for $K = N/2$, for $\phi_{2F}' = 1$, and for different values of $\phi_{2F}''$. The table displays the $\ell_{2}$ norm (not scaled by $\varepsilon$) of the ordered vectors of eigenvalues. The column for $\phi_{2F}'' = 0$ is identically zero since, in this case, the two operators coincide. All other entries are zero to numerical precision of the eigenvalue solver.
we see that subject to the validity of conjecture \( i \) the condition number of \( \phi''_F \) is bounded as

\[
\text{cond}(V) = \|V\|\|V^{-1}\|
\]

where the condition number of \( \phi''_F \) is defined as usual by \( \text{cond}(V) = \|V\|\|V^{-1}\| \). Hence, we see that, subject to the validity of Conjecture 9, the \( L_q\text{-cf},F \) operator satisfies (13) with constant \( C = \text{cond}(V) \). To make this stability independent of \( N \), we require that \( \text{cond}(V) \) is bounded as \( N \to \infty \). This is the subject of further numerical experiments displayed in Table 2. They suggest that this is indeed true if and only if \( A_F > 0 \).

**Conjecture 10.** Let \( V \) denote the matrix of eigenvectors for the force-based QC operator \( P_dL_{q\text{-cf},F} \). If \( A_F > 0 \), then \( \text{cond}(V) \) is uniformly bounded in \( N \).

Conjectures 9 and 10, supported by the results of the numerical experiments that we have presented in Tables 1 and 2, imply that \( P_dL_{q\text{-cf},F} \) is indeed dynamically stable for \( A_F > 0 \), with a stability constant that is uniform in \( N \).

**Conclusion**

We propose that a sharp stability analysis of atomistic-to-continuum coupling methods is an essential ingredient for the evaluation of their predictive capability, as important as a sharp consistency analysis. In the present paper, we have established such a
sharp stability analysis for the force-based QC method, for a simple one-dimensional model problem. We have analyzed three notions of stability:

(i) **Positivity** (coercivity) is generically not satisfied.
(ii) **Operator stability**, uniformly in the size of the atomistic system, holds only with an appropriate choice of function spaces. It does not hold for several natural choices.
(iii) **Dynamical stability** is satisfied up to the critical load. This result is based on the numerical observation that the spectra of the QCF and QNL operators coincide.

Positivity and dynamical stability are equivalent for energy-based methods, and under suitable conditions and choices of function spaces they imply operator stability. However, the fact that the QCF method is non-conservative and gives rise to non-normal operators, leads to a much richer mathematical structure.

Finally, we stress once again that, while the QCF method is possibly the simplest force-based multi-physics coupling scheme, we believe that similar observations can be made for other force-based hybrid methods, such as FeAt [15], CADD [25] or brutal force mixing [2].

**Appendix A. Proof of Theorem 5: Stability of \( L_{\text{qcf,F}} \)**

Theorem 5 states that, if \( \phi^\mu_F + 8\phi''_2F > 0 \), then \( L_{\text{qcf,F}} \) is stable as an operator from \( U^{1,\infty} \) to \( U^{-1,\infty} \), uniformly in \( N \).

The proof of this statement uses a variational representation for the QCF operator, which we derived in [10], and which is also valid for periodic boundary conditions:

\[
L_{\text{qcf,F}} = \phi^\mu_F L_1 + \phi''_2F (L^{\text{reg}}_2 + L^{\text{sng}}_2),
\]

where the three operators \( L_1, L^{\text{reg}}_2, L^{\text{sng}}_2 : U \rightarrow U^* \) are given by

\[
\langle L_1 u, v \rangle = \langle u', v' \rangle,
\]

\[
\langle L^{\text{reg}}_2 u, v \rangle = \varepsilon \sum_{\ell = -N+1}^{-K} 4u'_\ell v'_\ell + \varepsilon \sum_{\ell = -K+1}^{K} (u'_{\ell - 1} + 2u'_\ell + u'_{\ell + 1})v'_\ell + \varepsilon \sum_{\ell = K+1}^{N} 4u'_\ell v'_\ell,
\]

\[
\langle L^{\text{sng}}_2 u, v \rangle = (u'_{-K+1} - 2u'_{-K} + u'_{-K-1})v_{-K} - (u'_{K+2} - 2u'_{K+1} + u'_K)v_K.
\]

We omit the proof of this representation which is a straightforward summation by parts argument and carries over verbatim from [10]. Upon defining

\[
\sigma_\ell(u') = \begin{cases} 
\phi^\mu_F u'_\ell + \phi''_2F (u'_{\ell - 1} + 2u'_\ell + u'_{\ell + 1}), & \ell = -K + 1, \ldots, K, \\
(\phi^\mu_F + 4\phi''_2F)u'_\ell, & \text{otherwise},
\end{cases}
\]

as well as

\[
\alpha_K(u') = \phi''_2F (u'_{K+2} - 2u'_{K+1} + u'_K), \quad \text{and}
\]

\[
\alpha_{-K}(u') = \phi''_2F (u'_{-K+1} - 2u'_{-K} + u'_{-K-1}),
\]

we can rewrite this representation as

\[
\langle L_{\text{qcf,F}} u, v \rangle = \langle \sigma(u'), v' \rangle + \alpha_K(u')v_{-K} - \alpha_K(u')v_K.
\]
Using the periodic heaviside function $h \in U$ given by

$$h_\ell = \begin{cases} \frac{1}{2}(1-\varepsilon\ell) - \frac{\ell}{2}, & \ell \geq 0, \\ \frac{1}{2}(1+\varepsilon\ell) - \frac{\ell}{2}, & \ell < 0, \end{cases}$$

and setting $\tilde{h}_\ell = h_{\ell-1}$, the point evaluation functional $v \mapsto v_0, v \in U$, can be represented by

$$v_0 = \langle h', v \rangle = -\langle \tilde{h}, v' \rangle \quad \text{for all } v \in U.$$ 

Combining these observations, we obtain the following result.

**Lemma 11.** $L_{qcf,F}$ can be written as

$$\langle L_{qcf,F}u, v \rangle = \langle E_{qcf,F}u', v' \rangle \quad \text{for all } u, v \in U,$$

where

$$E_{qcf,F}u' = \sigma\ell(u') - \alpha_K(u')h_{\ell+K-1} + \alpha_K(u')h_{\ell-K-1},$$

for $\sigma, h, \text{ and } \alpha_{K}$ as defined above.

Even though the variational representations of the Dirichlet case and the periodic case are the same, we cannot translate the proof for inf-sup stability that we used in [10], as it required a matrix representation that is unavailable for periodic boundary conditions. Instead, we will compute a fairly explicit characterization of $L_{qcf,F}^{-1}$ to estimate its norm directly. It is most convenient to do so if we define an equivalent norm on $U^{-1,\infty}$. Note that $L_1 : U \rightarrow U^*$ is bijective, and hence we can define

$$\|g\|_{\tilde{U}^{-1,\infty}} = \|L_1^{-1}g\|_{U^{1,\infty}} \quad \text{for } g \in U^*.$$

**Lemma 12.** For all $g \in U^*$, it holds that

$$\frac{1}{2}\|g\|_{\tilde{U}^{-1,\infty}} \leq \|g\|_{U^{-1,\infty}} \leq \|g\|_{\tilde{U}^{-1,\infty}}.$$

**Proof.** Let $z = L_1^{-1}g$, that is,

$$\langle z', v' \rangle = \langle g, v \rangle \quad \forall v \in U.$$

Taking the supremum over $v$ with $\|v'\|_1 = 1$ we obtain the second inequality

$$\|g\|_{U^{-1,\infty}} \leq \|z'\|_{\ell^\infty} = \|g\|_{\tilde{U}^{-1,\infty}}$$

by Hölder’s inequality.

The first inequality follows from the fact, which is proved below, that

$$\frac{1}{2}\|z'\|_{\ell^\infty} \leq \sup_{v' \in \tilde{U}} \langle z', v' \rangle \quad \forall z \in U.$$  

Namely, this implies that

$$\frac{1}{2}\|g\|_{\tilde{U}^{-1,\infty}} = \frac{1}{2}\|z'\|_{\ell^\infty} \leq \sup_{v' \in \tilde{U}} \langle z', v' \rangle = \sup_{v' \in \tilde{U}} \|g\|_{U^{-1,\infty}}.$$
To prove (18), we fix $z \in \mathcal{U}$ and let $\ell_1, \ell_2$ be such that $z'_{\ell_1} = \|z'\|_{L^\infty}^\ell$ and $z'_{\ell_2} < 0$. (A similar argument can be used if $z'_{\ell_2} = \|z'\|_{L^\infty}^\ell$. ) We obtain (18) from the fact that\[ \|z\|^\ell \leq \langle z', v' \rangle \] where $v \in \mathcal{U}$ is defined by\[ v'_\ell = \begin{cases} \frac{1}{2\varepsilon} & \text{if } \ell = \ell_1, \\ -\frac{1}{2\varepsilon} & \text{if } \ell = \ell_2, \\ 0 & \text{otherwise}. \end{cases} \]

**Corollary 13.** Suppose that $F$ is such that $L_{qcf, F} : \mathcal{U} \to \mathcal{U}^*$ is invertible, then\[ \|(L_1^{-1} L_{qcf, F})^{-1}\|_{L(\mathcal{U}^1, \mathcal{U}^1, \mathcal{U}^1)} \leq \|L_{qcf, F}\|_{L(\mathcal{U}^{-1, \infty}, \mathcal{U}^1)} \leq 2\|(L_1^{-1} L_{qcf, F})^{-1}\|_{L(\mathcal{U}^1, \mathcal{U}^1, \mathcal{U}^1)}. \]

**Proof.** Using Lemma 12 twice, we can prove the following bound,\[ \frac{1}{\|(L_1^{-1} L_{qcf, F})^{-1}\|_{L(\mathcal{U}^1, \mathcal{U}^1, \mathcal{U}^1)}} = \inf_{u \in \mathcal{U}} \|L_1^{-1} L_{qcf, F} u\|_{\mathcal{U}^1, \mathcal{U}^1, \mathcal{U}^1} = \inf_{u \in \mathcal{U}} \|L_{qcf, F} u\|_{\mathcal{U}^{-1, \infty}}, \]
which gives the first stated inequality. The second inequality follows from a similar argument. \[ \Box \]

Corollary 13 shows that we can bound the operator norm $\|L_{qcf, F}^{-1}\|_{L(\mathcal{U}^{-1, \infty}, \mathcal{U}^1)}$ in terms of $\|(L_1^{-1} L_{qcf, F})^{-1}\|_{L(\mathcal{U}^1, \mathcal{U}^1, \mathcal{U}^1)}$. The latter operator norm can be computed using the formula\[ \|(L_1^{-1} L_{qcf, F})^{-1}\|_{L(\mathcal{U}^1, \mathcal{U}^1, \mathcal{U}^1)} = \left\{ \inf_{u \in \mathcal{U}} \|(L_1^{-1} L_{qcf, F} u')\|_{L^\infty} \right\}^{-1}. \]

In the next lemma, we establish an explicit representation of $L_1^{-1} L_{qcf, F}$ which will subsequently allow us to construct upper and lower bounds for (19).

**Lemma 14.** Let $z = L_1^{-1} L_{qcf, F} u$, then\[ z'_{\ell} = \sigma(u') - \frac{\varepsilon}{2} \phi_{2F} \{ u'_{-K} - u'_{-K+1} - u'_{K} + u'_{K+1} \} - \alpha_{-K}(u') h_{\ell+K-1} + \alpha_{K}(u') h_{\ell-K-1}, \]
where $\sigma, h, \alpha_K$ are defined above.

**Remark 4.** We note that the term $\frac{\varepsilon}{2} \phi_{2F} \{ u'_{-K} - u'_{-K+1} - u'_{K} + u'_{K+1} \}$ is the average of $\sigma$, and the function $h$ is a periodic heaviside function defined in (15). \[ \Box \]

**Proof of Lemma 14.** The function $z$ is the solution of the variational principle\[ \langle z', v' \rangle = \langle L_{qcf, F} u, v \rangle = \langle E_{qcf, F} u, v' \rangle \]
where $E_{qcf, F}$ is defined in (17), and is given by $E_{qcf, F} u'_\ell = \sigma(u') - \alpha_{-K}(u') h_{\ell+K-1} + \alpha_{K}(u') h_{\ell-K-1}$. 

We note that a function \( w \in \mathbb{R}^{2N} \) is a gradient, that is, \( w = v' \) for some \( v \in \mathcal{U} \), if and only if \( \sum_{\ell=-N+1}^{N} w_\ell = 0 \). Hence, we obtain \( z' = E_{\text{qcf},F}u' - \mathcal{E}_{\text{qcf},F}u' \) where \( \mathcal{E}_{\text{qcf},F}u' := \frac{1}{2} \varepsilon \sum_{\ell=-N+1}^{N} E_{\text{qcf},F}\varepsilon_{\ell} \). Since \( h \) has zero mean, we only need to compute \( \bar{\sigma} \),

\[
\bar{\sigma} := \frac{1}{2N} \sum_{\ell=-N+1}^{N} \sigma_\ell = \frac{A_F}{2N} \sum_{\ell=-N+1}^{N} u'_\ell + \frac{\phi''_{qcf}}{2N} \sum_{\ell=-K+1}^{K} (u'_{\ell-1} - 2u'_\ell + u'_{\ell+1}).
\]

Since \( u \) is periodic, \( u' \) has zero mean, and hence the first sum on the right-hand side vanishes. The second sum has telescope structure, and we obtain

\[
\mathcal{E}_{\text{qcf},F}u' = \bar{\sigma} = \frac{\varepsilon}{2} \phi''_{qcf}(u'_{-K} - u'_{-K+1} - u'_K + u'_{K+1}).
\]

This concludes the proof of the lemma.

We are now ready to conclude the proof of Theorem 5.

**Proof of Theorem 5.** We set \( z = L_{qcf,F}^{-1}L_{qcf,F}u \) and use Lemma 14 to deduce the bound

\[
\|z'\|_{\ell^\infty} \geq \|\sigma(u')\|_{\ell^\infty} - 2\varepsilon|\phi''_{qcf}|\|u'\|_{\ell^\infty}
\]

\[
- \max\{(|\alpha_{-K}(u')|, |\alpha_K(u')|) \max(112 + |h_{\ell+K-1}| + |h_{\ell-K-1}|) \}
\]

To bound the first term on the right-hand side, we note that

\[
|\sigma_\ell(u')| \geq \phi''_{qcf}|u'_\ell| + 4\phi''_{qcf}\|u'\|_{\ell^\infty},
\]

which immediately implies

\[
\|\sigma(u')\|_{\ell^\infty} \geq A_F\|u'\|_{\ell^\infty}.
\]

To bound the third term on the right-hand side of (20), we crudely estimate

\[
\max_{\ell=-N+1,\ldots,N}(112 + 112 + |h_{\ell+K-1}| + |h_{\ell-K-1}|) \leq 1 - \frac{1}{2}\varepsilon,
\]

which is true whenever \( K \geq 1 \), and deduce from (14) that

\[
\max\{(|\alpha_{-K}(u')|, |\alpha_K(u')|) \leq 4|\phi''_{qcf}|.
\]

The additional term \(-\frac{1}{2}\varepsilon\) cancels with the second term on the right-hand side of (20), so that we obtain

\[
\|z'\|_{\ell^\infty} \geq (\phi''_{qcf} + 8\phi''_{qcf})\|u'\|_{\ell^\infty}.
\]

Employing Corollary 13 and Formula (19), we obtain Theorem 5. \( \square \)

**Appendix B. Proof of Theorem 4: Instability of \( L_{qcf,F} \)**

We now prove Theorem 4 on the instability of \( L_{qcf,F} \) as an operator acting between \( \mathcal{U}^{1,p} \) and \( \mathcal{U}^{-1,p} \), \( 1 \leq p < \infty \). The bound \( \|L_{qcf,F}^{-1}\|_{L(\mathcal{U}^{-1,p},L^{1,p})} \geq CN^{1/p} \) follows from the following lemma.

**Lemma 15.** Suppose that \( \phi''_{qcf} > 0 \), \( \phi_{qcf}'' \in \mathbb{R} \setminus \{0\} \), and \( p, q \in \mathbb{R} \) satisfy \( 1 \leq p < \infty \), \( 1 < q \leq \infty \), and \( \frac{1}{p} + \frac{1}{q} = 1 \). Then there exists a constant \( C > 0 \) such that

\[
\inf_{v' \in \mathcal{U}} \sup_{w \in \mathcal{U}} \frac{1}{\|v'\|_{L^{1,p}}^{1/p}} \|w\|_{L^{1,p}} \leq C N^{-1/p}.
\]
Proof. We recall from Lemma 14 that we can represent $L_{qcf,F}v$ in the form

$$
\langle L_{qcf,F}v, w \rangle = \langle E_{qcf,F}v', w' \rangle \quad \forall w \in U,
$$

where

$$
E_{qcf,F}v' = \sigma_t(v') - \alpha_{-K}(v')h_{t+K-1} + \alpha_K(v')h_{t-K-1},
$$

and where

$$
\sigma_t(v') = \begin{cases} 
\phi''_Fv'_t + \phi''_{2F}(v'_{t-1} + 2v'_t + v'_{t+1}), & t = -K + 1, \ldots, K, \\
(\phi''_F + 4\phi''_{2F})v'_t, & \text{otherwise},
\end{cases}
$$

$$
\alpha_K(v') = \phi''_{2F}(v'_{K+2} - 2v'_{K+1} + v'_K),
$$

$$
\alpha_{-K}(v') = \phi''_{2F}(v'_{-K+1} - 2v'_{-K} + v'_{-K-1}),
$$

$$
h_t = \begin{cases} 
\frac{1}{2}(1 - \varepsilon t) - \frac{\varepsilon}{4}, & t \geq 0, \\
-\frac{1}{2}(1 + \varepsilon t) - \frac{\varepsilon}{4}, & t < 0.
\end{cases}
$$

We choose $v \in U$ with derivative given by

$$
v'_t = \begin{cases} 
0, & t = K - 1, \\
-\frac{A_F}{6\phi''_F}, & t = K, \\
\frac{A_F}{3\phi''_{2F}}, & t = K + 1, \\
-\frac{A_F}{6\phi''_{2F}}, & t = K + 2, \\
h_{t-K-1}, & \text{otherwise}.
\end{cases}
$$

Such a representation is possible if and only if the vector $(v'_t)_{t=-N+1}^N$ defined above has zero mean. To see that this holds, we use the symmetry of $h_t$ to calculate

$$
\sum_{t=-N+1}^{N} v'_t = \sum_{t \neq -K-1}^{K+1} h_{t-K-1} = 0.
$$

If we insert $v$ into the equations above, we find that

$$
\alpha_{-K}(v') = 0, \quad \alpha_K(v') = -A_F,
$$

and

$$
\sigma_t(v') = \begin{cases} 
(\phi''_F + 2\phi''_{2F})h_{-3} + \phi''_{2F}h_{-4}, & t = K - 2, \\
\phi''_{2F}h_{-3} - \frac{1}{6}A_F, & t = K - 1, \\
-\frac{\phi''_F A_F}{6\phi''_{2F}}, & t = K, \\
\frac{A_F^2}{3\phi''_{2F}}, & t = K + 1, \\
-\frac{A_F^2}{6\phi''_{2F}}, & t = K + 2, \\
A_F h_{t-K-1}, & \text{otherwise}.
\end{cases}
$$
which implies that

\[
E_{qcf,F}v'_\ell = \begin{cases}
-2\phi''_F h_{-3} + \phi''_F h_{-4}, & \ell = K - 2, \\
\phi''_F h_{-3} - \frac{1}{6}A_F - A_F h_{-2}, & \ell = K - 1, \\
\frac{-\phi''_F A_F}{6\phi''_F} - A_F h_{-1}, & \ell = K, \\
\frac{A_F^2}{3\phi''_F} - A_F h_0, & \ell = K + 1, \\
-\frac{A_F^2}{6\phi''_F} - A_F h_1, & \ell = K + 2, \\
0, & \text{otherwise}
\end{cases}
\]

Note that all the terms above are bounded in absolute value independently of \(N\) and \(K\).

Inserting these formulas into (22), applying Hölder’s inequality, and using the fact that \(E_{qcf,F}v'_\ell\) is nonzero for only five indices, we obtain

\[
\langle L_{qcf,F}v, w \rangle = \langle E_{qcf,F}v', w' \rangle \\
\leq \|E_{qcf,F}v'\|_{\ell^p} \|w'\|_{\ell^q} \\
\leq \varepsilon^{1/p} \left[ 5 \|E_{qcf,F}v'\|_{\ell^\infty}^p \right]^{1/p} \|w'\|_{\ell^q} \\
\leq C\varepsilon^{1/p} \|w'\|_{\ell^q}.
\]

It remains to show that \(\|v'\|_{\ell^p}\) is bounded below as \(N \to \infty\). As a matter of fact, it can be seen from the definition of \(v'_\ell\) that

\[
|v'_\ell| \geq \frac{1}{4} \quad \text{for } j = K + 1 - N/2, \ldots, K - 1,
\]

which gives

\[
\|v'\|_{\ell^p} \geq \left[ \sum_{\ell=K+1-N/2}^{K-1} \varepsilon \left( \frac{1}{4} \right)^p \right]^{1/p} = \frac{4}{1} \left[ (N/2 - 2)\varepsilon \right]^{1/p}.
\]

Thus, replacing \(v\) by \(v/\|v'\|_{\ell^p}\) gives the desired result. \(\square\)

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