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A Priori Error Estimates for Energy-Based Quasicontinuum Approximations of a Periodic Chain

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We derive a priori error estimates for three prototypical energy-based quasicontinuum (QC) methods: the local QC method, the energy-based QC method, and the quasi-nonlocal QC method.

Our analysis decomposes the consistency error into modelling and coarsening errors. While previous results on estimating the modelling error exist, we present a new and simpler proof based on negative-norm estimates. Our stability analysis extends previous results on sharp stability estimates under homogeneous strain to the nonlinear setting. Finally, we present numerical experiments to illustrate the results of our analysis.

Keywords: quasicontinuum method; atomistic/continuum coupling; coarse-graining; a priori error analysis.

AMS Subject Classification: 65N12, 65N15, 70C20

1. Introduction

Quasicontinuum (QC) methods are a class of multiscale methods for coupling an atomistic description of a solid to a matching continuum elasticity description. If performed with care, such a process considerably reduces the computational cost without sacrificing much of the accuracy of atomistic models. A prototypical application is the modelling of localized defects (vacancies, dislocations, etc.) in an elastic far field.

One can broadly distinguish two groups of quasicontinuum methods: energy-based coupling methods,[19,26,8] and force-based coupling methods.[25,3,15] A third group, which avoids the coupling problem and instead uses Galerkin projection and quadrature ideas to coarse-grain the atomistic system, has so far not yielded promising results.[17,13] We refer to the recent review papers Refs. 16 and 17 for a detailed description and history of QC methods.

The error analysis of quasicontinuum methods has received considerable attention in recent years (see Lin,[11,9,12] Ming et al.,[18] Ortner et al.,[23,21,14] Dobson et al.[5,7,6]). The purpose of the present paper is to refine and extend previous analyses of energy-based quasicontinuum approximations,[4,18,9,6,21] in a unified framework in one dimension. We will use the negative-norm techniques developed in Ref. 21 for the quasinonlocal QC method, and extend it to an analysis of the local and original energy-based QC method, obtaining new and sharper estimates on the modelling and coupling errors. In addition, we will for the first time include coarse-graining in the error analysis of these energy-based QC methods. (We note, however, that E and Ming[9] analyze a 1D local QC method within the framework of the *heterogeneous multiscale method* and Lin[12] analyzes a different 2D coarse-graining scheme in the framework of non-conforming finite element methods.) We will obtain the same superconvergence result as obtained for the force-based QC method in Ref. 14. In Section 3.5 we will comment on the differences and similarities of our analysis with previous efforts.

Our analysis is restricted to a second-neighbour pair interaction model in one dimension, since this simple model problem contains much of the structure of more complicated situations. Indeed, our analysis[22] of a recently proposed QC method for 2D problems with finite range interaction[24] largely follows the framework put forward in the present paper.

1.1. *Outline of the analysis*

In Section 2 we formulate the atomistic model and the three different QC methods that we will analyze. We will also introduce some notation that will be used throughout the paper.

We will split the error analysis essentially into three parts: the consistency error analysis (coupling and model error), the coarse-graining error analysis (approximation error), and the stability analysis. Since the most natural norms in which to measure the error are discrete Sobolev norms, the consistency and coarse-graining errors will be measured in corresponding negative Sobolev norms.

In Section 3, we derive the consistency error estimates for the three different QC methods in negative Sobolev norms, using similar techniques as in Refs. 18 and 20. Our estimates will clearly show the error sources for each method.

In Section 4, we combine the consistency error estimates with a coarse-graining error analysis that includes a superconvergence proof, and a stability analysis extending the sharp results in Ref. 6 to nonlinear deformations, to derive error estimates for the QC methods.

In Section 5, we present numerical experiments to complement our analysis.

2. The Atomistic Model and its QC Approximations

2.1. *The atomistic model*

To avoid technical difficulties with boundaries we follow previous analyses of QC methods and formulate a model problem with periodic boundary conditions. To this end, let $N \in \mathbb{N}$ and $\varepsilon = 1/N$, and define the space of N-periodic zero mean displacements as

$$\mathcal{U} = \big\{ \boldsymbol{u} \in \mathbb{R}^{\mathbb{Z}} : u_{\ell+N} = u_\ell, \textstyle\sum_{\ell=1}^N u_\ell = 0 \big\}. \tag{2.1}$$

The set of admissible deformations is given by

$$\mathcal{Y} = \big\{ \boldsymbol{y} \in \mathbb{R}^{\mathbb{Z}} : y_\ell = \varepsilon F \ell + u_\ell,\ \boldsymbol{u} \in \mathcal{U} \big\}, \tag{2.2}$$

where $\varepsilon = 1/N$ is chosen to rescale the computational domain to unit length, and $F > 0$ is a macroscopic deformation gradient.

For simplicity of the presentation and analysis, we adopt a pair interaction model and assume that only nearest neighbours and the next-nearest neighbours interact. The *stored atomistic energy* (per period) of an admissible deformation is then given by

$$\begin{aligned} \mathcal{E}_{\rm a}(\boldsymbol{y}) :=&\ \varepsilon \sum_{\ell=1}^N \phi\Big(\frac{y_\ell - y_{\ell-1}}{\varepsilon}\Big) + \varepsilon \sum_{\ell=1}^N \phi\Big(\frac{y_\ell - y_{\ell-2}}{\varepsilon}\Big) \\ =&\ \varepsilon \sum_{\ell=1}^N \phi(y_\ell') + \varepsilon \sum_{\ell=1}^N \phi(y_\ell' + y_{\ell-1}'), \end{aligned} \tag{2.3}$$

where $y_\ell' = \frac{y_\ell - y_{\ell-1}}{\varepsilon}$, and where $\phi \in C^3((0,+\infty))$ is a Lennard-Jones type interaction potential: We assume that there exists $r_* > 0$ such that ϕ is convex in $(0, r_*)$ and concave in $(r_*, +\infty)$.

Given a dead load $\boldsymbol{f} \in \mathcal{U}$ the *total energy* (per period) of a deformation $y \in \mathcal{Y}$ is given by

$$E_{\rm a}(\boldsymbol{y}) = \mathcal{E}_{\rm a}(\boldsymbol{y}) - \langle \boldsymbol{f}, \boldsymbol{y} \rangle_\varepsilon,$$

where, for $\boldsymbol{v}, \boldsymbol{w} \in \mathbb{R}^{\mathbb{Z}}$,

$$\langle \boldsymbol{v}, \boldsymbol{w} \rangle_\varepsilon = \varepsilon \sum_{\ell=1}^N v_\ell w_\ell.$$

The problem we wish to solve is to find

$$\boldsymbol{y}^a \in \operatorname{argmin} E_{\rm a}(\mathcal{Y}), \tag{2.4}$$

where argmin denotes the set of local minimizers.

2.2. *The local QC method (QCL)*

For 1-periodic functions $u, f \in C^\infty(\mathbb{R})$ we define $\boldsymbol{y}^{(\varepsilon)} \in \mathcal{Y}$ as $y_\ell^{(\varepsilon)} = \varepsilon F \ell + u(\varepsilon \ell)$. It is then easy to see (e.g., see Ref. 2) that, as $N \to \infty$,

$$E_{\rm a}(\boldsymbol{y}^{(\varepsilon)}) \to \int_0^1 \big(\phi(y'(x)) + \phi(2y'(x)) - f(x)y(x)\big)\,{\rm d}x, \tag{2.5}$$

the so-called *Cauchy–Born approximation* of $E_{\rm a}$. The stored energy density $W(r) = \phi(r) + \phi(2r)$ is called the *Cauchy–Born stored energy function.*

The local QC (QCL) energy functional on the atomistic grid is obtained by applying a P1 finite element discretization to (2.5) with ε being the size of the finite element mesh and the reference atom positions being the nodes. The total QCL energy (per period) is given by

$$E_{\rm qcl}(\boldsymbol{y}) = \mathcal{E}_{\rm qcl}(\boldsymbol{y}) - \langle \boldsymbol{f}, \boldsymbol{y} \rangle_\varepsilon, \tag{2.6}$$

where

$$\mathcal{E}_{\rm qcl}(\boldsymbol{y}) = \varepsilon \sum_{\ell=1}^N W(y_\ell') = \varepsilon \sum_{\ell=1}^N \phi(y_\ell') + \varepsilon \sum_{\ell=1}^N \phi(2y_\ell'). \tag{2.7}$$

An alternative argument to derive (2.7) from (2.3) is to assume that $y_\ell' \approx y_{\ell-1}'$ for all ℓ, that is, the local deformation gradients vary slowly everywhere.

In the QCL model, we wish to compute

$$\boldsymbol{y}^{\rm qcl} \in \operatorname{argmin} E_{\rm qcl}(\mathcal{Y}). \tag{2.8}$$

2.3. *The original energy-based QC method (QCE)*

When a material contains a defect, i.e., when the deformation y is not globally smooth, then the Cauchy–Born / local QC approximation is inaccurate. The full atomistic model should be used at the defect while the simpler local QC model (which allows for coarse graining) may be used to describe the far field.

The original energy-based QC method (QCE), introduced by Tadmor et al.[19], is a particularly simple example of a method coupling an atomistic model to its Cauchy–Born approximation. To motivate it, we note that the atomistic and the QCL stored energies may be written in terms of contributions to each atom,

$$\mathcal{E}_{\rm a}(\boldsymbol{y}) = \varepsilon \sum_{\ell=1}^N \mathcal{E}_\ell^{\rm a}(\boldsymbol{y}), \quad \text{and} \quad \mathcal{E}_{\rm qcl}(u) = \varepsilon \sum_{\ell=1}^N \mathcal{E}_\ell^{\rm c}(\boldsymbol{y}),$$

where

$$\mathcal{E}_\ell^{\rm a}(\boldsymbol{y}) = \tfrac12\big\{\phi(y_\ell') + \phi(y_{\ell+1}') + \phi(y_{\ell-1}' + y_\ell') + \phi(y_{\ell+1}' + y_{\ell+2}')\big\}, \quad \text{and} \tag{2.9}$$

$$\mathcal{E}_\ell^{\rm c}(\boldsymbol{y}) = \tfrac12\big\{\phi(y_\ell') + \phi(y_{\ell+1}') + \phi(2y_\ell') + \phi(2y_{\ell+1}')\big\} = \tfrac12\big\{W(y_\ell') + W(y_{\ell+1}')\big\}. \tag{2.10}$$

Next, we decompose the reference lattice into an atomistic region $\mathcal{A}$, which should contain any "defects", and a continuum region $\mathcal{C}$ where the solution is expected to be a "smooth" deformation from the reference lattice. For the sake of simplicity, we assume that

$$\mathcal{A} := \{\ell_1, \dots, \ell_2\}, \quad \text{and} \quad \mathcal{C} := \{1, ..., N\} \backslash \mathcal{A}, \tag{2.11}$$

where $3 < \ell_1 < \ell_1 + 2 < \ell_2 < N - 2$ in order to avoid unnecessary notational complication. The stored energy functional for the *energy-based QC (QCE) method*[19] is then defined as

$$\mathcal{E}_{\rm qce}(\boldsymbol{y}) = \varepsilon \sum_{\ell \in \mathcal{A}} \mathcal{E}^{\rm a}_\ell(\boldsymbol{y}) + \varepsilon \sum_{\ell \in \mathcal{C}} \mathcal{E}^{\rm c}_\ell(\boldsymbol{y}), \tag{2.12}$$

and the corresponding total energy (per period) as $E_{\rm qce}(\boldsymbol{y}) = \mathcal{E}_{\rm qce}(\boldsymbol{y}) - \langle \boldsymbol{f}, \boldsymbol{y} \rangle_\varepsilon$. In the QCE method, we aim to compute

$$\boldsymbol{y}^{\rm qce} \in \operatorname{argmin} E_{\rm qce}(\mathcal{Y}). \tag{2.13}$$

The original motivation behind the QCE method was that it exactly reproduces the energy under uniform strain (Cauchy–Born rule), however, it was later discovered[25,4] that the QCE forces are inaccurate in the interface region. Consequently, new coupling mechanisms were sought that would give better approximations to both energy and forces.

2.4. *The quasinonlocal QC method (QNL)*

An alternative approach to couple the atomistic and continuum energy is to associate the energy with interaction bonds. In our model, the interaction bonds are the nearest neighbour bonds and the next-nearest neighbour bonds. The energy of the nearest neighbour bonds need not be modified, as they are already sufficiently localized. The atomistic energy of the next-nearest neighbour bonds built by atom $\ell - 1$ and $\ell + 1$ is

$$\phi(y'_\ell + y'_{\ell+1}).$$

In the region where the deformation gradients varies slowly, this energy can be approximated by

$$\tfrac{1}{2}\big\{\phi(2y'_\ell) + \phi(2y'_{\ell+1})\big\}.$$

If we perform the same decomposition to the whole domain as before, this leads to an approximation of (2.3) by

$$\mathcal{E}_{\rm qnl}(\boldsymbol{y}) = \varepsilon \sum_{\ell \in \mathcal{A} \cup \mathcal{C}} \phi(y'_\ell) + \varepsilon \sum_{\ell \in \mathcal{A}} \phi(y'_\ell + y'_{\ell+1}) + \varepsilon \sum_{\ell \in \mathcal{C}} \tfrac{1}{2}\big\{\phi(2y'_\ell) + \phi(2y'_{\ell+1})\big\}. \tag{2.14}$$

It is fairly easy to see that in the 'interior' of the continuum region, $\mathcal{E}_{\rm qnl}$ reduces to the local QC method while in the 'interior' of the atomistic region, it reduces to the atomistic model. To be more precise, if we define an *interface region* $\mathcal{I}$ as

$$\mathcal{I} = \big\{\ell_1 - 1, \ell_1, \ell_2, \ell_2 + 1\big\},$$

then this stored energy can be written as

$$\mathcal{E}_{\rm qnl}(\boldsymbol{y}) = \varepsilon \sum_{\ell\in\mathcal{A}\setminus\mathcal{I}} \mathcal{E}^{\rm a}_\ell(\boldsymbol{y}) + \varepsilon \sum_{\ell\in\mathcal{C}\setminus\mathcal{I}} \mathcal{E}^{\rm c}_\ell(\boldsymbol{y}) + \varepsilon \sum_{\ell\in\mathcal{I}} \mathcal{E}^{\rm i}_\ell(\boldsymbol{y}),$$

where $\mathcal{E}^{\rm a}_\ell(\boldsymbol{u})$ and $\mathcal{E}^{\rm c}_\ell(\boldsymbol{u})$ are defined in (2.9) and (2.10) and $\mathcal{E}^{i}_\ell(\boldsymbol{u})$ is appropriately defined.[5] This is the special treatment of the interface in the one dimensional case.[26,8] The above coupling method is conventionally named the *quasinonlocal QC (QNL) method.*

The total QNL energy functional is then given by

$$E_{\rm qnl}(\boldsymbol{y}) = \mathcal{E}_{\rm qnl}(\boldsymbol{y}) - \langle \boldsymbol{f}, \boldsymbol{y}\rangle_\varepsilon. \tag{2.15}$$

In the QNL method, we aim to find

$$\boldsymbol{y}^{\rm qnl} \in \operatorname{argmin} E_{\rm qnl}(\mathcal{Y}). \tag{2.16}$$

2.5. *Notation*

Before we begin the detailed analysis in the next section, we define some notation that will be used throughout.

For $\boldsymbol{v} \in \mathbb{R}^{\mathbb{Z}}$, besides the first order finite difference $v'_\ell := \varepsilon^{-1}(v_\ell - v_{\ell-1})$, we define the second and third order finite differences by

$$v''_\ell = \frac{v'_{\ell+1} - v'_\ell}{\varepsilon} = \frac{v_{\ell+1} - 2v_\ell + v_{\ell-1}}{\varepsilon^2}, \qquad \text{and}$$
$$v'''_\ell = \frac{v''_\ell - v''_{\ell-1}}{\varepsilon} = \frac{v_{\ell+1} - 3v_\ell + 3v_{\ell-1} - v_{\ell-2}}{\varepsilon^3}.$$

In general, the odd differences are associated with bonds, while even differences are associated with nodes. It should be noted that, for $v \in \mathcal{U}$, higher order differences, for example $\boldsymbol{v}'$, $\boldsymbol{v}''$ and $\boldsymbol{v}'''$, are all N-periodic and with mean zero in each period. Thus, all these higher order differences belong to $\mathcal{U}$. It can be checked that, for $\boldsymbol{y} \in \mathcal{Y}$, finite differences of order higher than one, for example $\boldsymbol{y}''$ and $\boldsymbol{y}'''$, also belong to $\mathcal{U}$.

For $\boldsymbol{v} \in \mathcal{U}$, we define the weighted ℓ^p_ε-norms by

$$\|\boldsymbol{v}\|_{\ell^p_\varepsilon} = \begin{cases} \left(\varepsilon \sum_{\ell=1}^N |v_\ell|^p\right)^{1/p}, & 1 \le p < \infty, \\ \max_{\ell=1,\dots,N} |v_\ell|, & p = \infty. \end{cases}$$

The space $\mathcal{U}$ is usually equipped with the discrete Sobolev norms

$$\|\boldsymbol{u}\|_{\mathcal{U}^{1,p}} = \|\boldsymbol{u}'\|_{\ell^p_\varepsilon}, \quad \text{for } u \in \mathcal{U} \text{ and } p \in [1, \infty].$$

When $\mathcal{U}$ is equipped with the $\mathcal{U}^{1,p}$-norm, it is denoted by $\mathcal{U}^{1,p}$. For $p' = p/(p-1)$, with the convention $1' = \infty$ and $\infty' = 1$ being used through out the paper, the norm on the dual $\mathcal{U}^{-1,p} := (\mathcal{U}^{1,p})^*$ is defined by

$$\|T\|_{\mathcal{U}^{-1,p}} := \sup_{\substack{\boldsymbol{v}\in\mathcal{U} \\ \|\boldsymbol{v}\|_{\mathcal{U}^{1,p'}}=1}} T[\boldsymbol{v}], \quad \text{for } T \in \mathcal{U}^{-1,p}.$$

If $\mathcal{D}$ is a subset of $\mathbb{Z}$, for $\boldsymbol{v} \in \mathbb{R}^{\mathbb{Z}}$, we also define the (semi-)norms

$$\|\boldsymbol{v}\|_{\ell^p_\varepsilon(\mathcal{D})} := \Big(\varepsilon \sum_{\ell \in \mathcal{D}} |v_\ell|^p\Big)^{1/p}.$$

Finally, we introduce a function we will use in our analysis to bound derivatives of the interaction potential ϕ. For any $\mathcal{S} \subset \mathbb{R}$, we define

$$M_i(\mathcal{S}) := \sup_{s \in \mathcal{S}} |\phi^{(i)}(s)|, \tag{2.17}$$

where $\phi^{(i)}$ denotes the ith derivative of ϕ.

3. Consistency Error Analysis

3.1. *The variational formulation and the consistency error*

Let $\boldsymbol{y}^{\rm a}$ be a solution of the atomistic model problem (2.4). If $\min_\ell (y^{\rm a})'_\ell > 0$, then E is differentiable at $\boldsymbol{y}^{\rm a}$, and the first-order necessary optimality condition for (2.4), in variational form, is

$$\mathcal{E}'_{\rm a}(\boldsymbol{y}^{\rm a})[\boldsymbol{v}] = \langle \boldsymbol{f}, \boldsymbol{v} \rangle_\varepsilon \qquad \forall \boldsymbol{v} \in \mathcal{U}, \tag{3.1}$$

where

$$\mathcal{E}'_{\rm a}(\boldsymbol{y})[\boldsymbol{v}] = \varepsilon \sum_{\ell=1}^{N} \phi'(y'_\ell) v'_\ell + \varepsilon \sum_{\ell=1}^{N} \big\{\phi'(y'_{\ell-1} + y'_\ell) + \phi'(y'_\ell + y'_{\ell+1})\big\} v'_\ell. \tag{3.2}$$

When using a QC method we are looking for

$$\boldsymbol{y}^{\rm qc} \in \operatorname{argmin} E_{\rm qc}(\mathcal{Y}), \tag{3.3}$$

where $\mathrm{qc} \in \{\mathrm{qcl}, \mathrm{qce}, \mathrm{qnl}\}$. As above, if $\min_\ell (y^{\rm qc})'_\ell > 0$, then $E_{\rm qc}$ is differentiable at $\boldsymbol{y}^{\rm qc}$, and the first order necessary optimality condition for (3.3) in variational form is

$$\mathcal{E}'_{\rm qc}(\boldsymbol{y})[\boldsymbol{v}] = \langle \boldsymbol{f}, \boldsymbol{v} \rangle_\varepsilon \qquad \forall \boldsymbol{v} \in \mathcal{U}.$$

The *consistency error* (for the solution $\boldsymbol{y}^{\rm a}$) of the QC method is

$$\begin{aligned} T_{\rm qc}(\boldsymbol{y}^{\rm a}) &:= E'_{\rm qc}(\boldsymbol{y}^{\rm a}) \\ &= E'_{\rm qc}(\boldsymbol{y}^{\rm a}) - E'_{\rm a}(\boldsymbol{y}^{\rm a}) \\ &= \mathcal{E}'_{\rm qc}(\boldsymbol{y}^{\rm a}) - \mathcal{E}'_{\rm a}(\boldsymbol{y}^{\rm a}), \end{aligned}$$

understood as a functional $T_{\rm qc}(\boldsymbol{y}^{\rm a}) \in \mathcal{U}^*$.

In our error analysis in Section 4 we will need estimates on the consistency error $T_{\rm qc}$ in the negative Sobolev norm $\|\cdot\|_{\mathcal{U}^{-1,2}}$. Since it requires no modifications of our analysis we will in fact produce estimates in all $\mathcal{U}^{-1,p}$-norms, $1 \le p \le \infty$.

3.2. *The consistency error of the QCL method*

For $\boldsymbol{y} \in \mathcal{Y}$ with $\min_\ell y'_\ell > 0$, the first variation of $\mathcal{E}_{\rm qcl}$ at $\boldsymbol{y}$ reads

$$\mathcal{E}'_{\rm qcl}(\boldsymbol{y})[\boldsymbol{v}] = \varepsilon \sum_{\ell=1}^{N} \phi'(y'_\ell) v'_\ell + \varepsilon \sum_{\ell=1}^{N} \phi'(2y'_\ell)\,(2v'_\ell). \tag{3.4}$$

Theorem 3.1. *For $\boldsymbol{y} \in \mathcal{Y}$ with $\min_\ell y'_\ell > 0$, and for $1 \le p \le \infty$, we have*

$$\big\|\mathcal{E}'_{\rm qcl}(\boldsymbol{y}) - \mathcal{E}'_{\rm a}(\boldsymbol{y})\big\|_{\mathcal{U}^{-1,p}} \le \varepsilon^2 \big\{ M_2(\mathcal{S}_1) \|\boldsymbol{y}'''\|_{\ell^p_\varepsilon} + M_3(\mathcal{S}_2) \|\boldsymbol{y}''\|^2_{\ell^{2p}_\varepsilon} \big\} =: \mathscr{E}^{\rm qcl}_{\rm model}(\boldsymbol{y}), \tag{3.5}$$

where $\mathcal{S}_1 := \{2y'_1, \dots, 2y'_N\}$, $\mathcal{S}_2 := [\min_\ell 2y'_\ell, \max_\ell 2y'_\ell]$, and where $M_i(\mathcal{S})$ is defined in (2.17).

Proof. Since $\min_\ell y'_\ell > 0$, $\mathcal{E}_{\rm a}$ and $\mathcal{E}_{\rm qcl}$ are differentiable at $\boldsymbol{y}$. The difference between $\mathcal{E}'_{\rm a}(\boldsymbol{y})[v]$ and $\mathcal{E}'_{\rm qcl}(\boldsymbol{y})[v]$, which are written out in (3.2) and (3.4), respectively, can be written in the form

$$\mathcal{E}'_{\rm qcl}(\boldsymbol{y})[\boldsymbol{v}] - \mathcal{E}'_{\rm a}(\boldsymbol{y})[\boldsymbol{v}] = \varepsilon \sum_{\ell=1}^{N} \big\{ 2\phi'(2y'_\ell) - \phi'(y'_{\ell-1} + y'_\ell) - \phi'(y'_\ell + y'_{\ell+1}) \big\} v'_\ell.$$

From this second difference structure, we can already expect a second-order consistency error. To make this precise, we first note that the second neighbour interactions can be rewritten in terms of nearest neighbour interactions and a strain gradient correction,

$$\begin{aligned} y'_{\ell-1} + y'_\ell =&\ 2y'_\ell - \varepsilon \frac{y'_\ell - y'_{\ell-1}}{\varepsilon} = 2y'_\ell - \varepsilon y''_{\ell-1}, \quad \text{and} \\ y'_{\ell+1} + y'_\ell =&\ 2y'_\ell + \varepsilon \frac{y'_{\ell+1} - y'_\ell}{\varepsilon} = 2y'_\ell + \varepsilon y''_\ell. \end{aligned}$$

Hence, expanding $\phi'(y'_{\ell-1} + y'_\ell)$ and $\phi'(y'_\ell + y'_{\ell+1})$ at $2y'_\ell$ we obtain

$$\phi'(y'_{\ell-1} + y'_\ell) = \phi'(2y'_\ell) - \varepsilon y''_{\ell-1} \phi''(2y'_\ell) + \tfrac{1}{2}(\varepsilon y''_{\ell-1})^2 \phi'''(\eta_1^\ell), \quad \text{and} \tag{3.6}$$

$$\phi'(y'_\ell + y'_{\ell+1}) = \phi'(2y'_\ell) + \varepsilon y''_\ell \phi''(2y'_\ell) + \tfrac{1}{2}(\varepsilon y''_\ell)^2 \phi'''(\eta_2^\ell), \tag{3.7}$$

where $\eta_1^\ell \in {\rm conv}\{2y'_\ell, y'_\ell + y'_{\ell-1}\}$ and $\eta_2^\ell \in {\rm conv}\{2y'_\ell, y'_\ell + y'_{\ell+1}\}$. We note that $\eta_k^\ell \in \mathcal{S}_2$ for $k = 1, 2$ and $\ell = 1, \dots, N$.

Adding these expansions together gives

$$\begin{aligned} &2\phi'(2y'_\ell) - \phi'(y'_{\ell-1} + y'_\ell) - \phi'(y'_\ell + y'_{\ell+1}) \\ =&\ -\big\{ -\varepsilon y''_{\ell-1} \phi''(2y'_\ell) + \tfrac{1}{2}(\varepsilon y''_{\ell-1})^2 \phi'''(\eta_1^\ell) \big\} - \big\{ \varepsilon y''_\ell \phi''(2y'_\ell) + \tfrac{1}{2}(\varepsilon y''_\ell)^2 \phi'''(\eta_2^\ell) \big\} \\ =&\ -\varepsilon^2 y'''_\ell \phi''(2y'_\ell) - \tfrac{1}{2}\varepsilon^2 \big\{ y''^2_{\ell-1} \phi'''(\eta_1^\ell) + y''^2_\ell \phi'''(\eta_2^\ell) \big\}. \end{aligned} \tag{3.8}$$

Thus, we can bound $\mathcal{E}'_{\rm qcl}(\boldsymbol{y})[\boldsymbol{v}] - \mathcal{E}'_{\rm a}(\boldsymbol{y})[\boldsymbol{v}]$ by

$$\begin{aligned} &\big|\mathcal{E}'_{\rm qcl}(\boldsymbol{y})[\boldsymbol{v}] - \mathcal{E}'_{\rm a}(\boldsymbol{y})[\boldsymbol{v}]\big| \\ &\qquad \le \varepsilon^3 \sum_{\ell=1}^{N} \big\{ |\phi''(2y'_\ell)||y'''_\ell| + \tfrac{1}{2}|\phi'''(\eta_1^\ell)||y''_{\ell-1}|^2 + \tfrac{1}{2}|\phi'''(\eta_2^\ell)||y''_\ell|^2 \big\} |v'_\ell|. \end{aligned}$$

Using the fact that $\boldsymbol{y}'', \boldsymbol{v}' \in \mathcal{U}$, and the bounds

$$|\phi''(2y'_\ell)| \le M_2(\mathcal{S}_1), \quad \text{and} \quad |\phi'''(\eta_k^\ell)| \le M_3(\mathcal{S}_2),$$

and applying a weighted Hölder's inequality, we further estimate

$$\begin{aligned}
&\big|\mathcal{E}'_{\rm qcl}(\boldsymbol{y})[\boldsymbol{v}] - \mathcal{E}'_{\rm a}(\boldsymbol{y})[\boldsymbol{v}]\big| \\
&\quad \le \varepsilon^2 \Big\{ M_2(\mathcal{S}_1)\varepsilon \sum_{\ell=1}^N |y'''_\ell||v'_\ell| + M_3(\mathcal{S}_2)\tfrac{1}{2}\varepsilon \sum_{\ell=1}^N |y''_\ell|^2 \big(|v'_\ell| + |v'_{\ell+1}|\big)\Big\} \\
&\quad \le \varepsilon^2 \big\{ M_2(\mathcal{S}_1)\|\boldsymbol{y}'''\|_{\ell^p_\varepsilon}\|\boldsymbol{v}'\|_{\ell^{p'}_\varepsilon} + M_3(\mathcal{S}_2)\|\boldsymbol{y}''\|^2_{\ell^{2p}_\varepsilon}\|\boldsymbol{v}'\|_{\ell^{p'}_\varepsilon}\big\}.
\end{aligned}$$

In view of the definition of the negative norm $\|\cdot\|_{\mathcal{U}^{-1,p}}$, this last estimate establishes the stated result. □

Remark 3.1. It is well-known (see Ref. 10 for instance) that the Cauchy–Born approximation is second-order accurate for simple lattices. This can also be seen in the above result. We note that our estimate is slightly sharper in that we require lower differentiability than the pointwise estimates in Ref. 10 (see also Lemma 6.1 in Ref. 7 for a similar result in a linear setting).

3.3. *The consistency error of the QCE method*

The algebraic expressions for the QCE method can become relatively complex, and hence, in some parts of our following analysis, we will only write out the right half of the atomistic chain in detail, namely, from $\ell = \ell_0$ to $\ell = N$ where $\ell_1+1 < \ell_0 < \ell_2-1$, and indicate the remaining terms by dots.

From (2.12), for $\boldsymbol{y} \in \mathcal{Y}$ with $\min_\ell y'_\ell > 0$, we can compute the first variation of $\mathcal{E}_{\rm qce}$ at $\boldsymbol{y}$ as follows:

$$\begin{aligned}
\mathcal{E}'_{\rm qce}(\boldsymbol{y})\,[\boldsymbol{v}] = \varepsilon\Big\{ &\sum_{\ell=\ell_0}^N \phi'(y'_\ell)v'_\ell + \sum_{\ell=\ell_0}^{\ell_2-1}\big[\phi'(y'_{\ell-1}+y'_\ell) + \phi'(y'_\ell + y'_{\ell+1})\big]v'_\ell \\
&+ \big[\tfrac{1}{2}\phi'(y'_{\ell_2}+y'_{\ell_2+1}) + \phi'(y'_{\ell_2-1}+y'_{\ell_2})\big]v'_{\ell_2} \\
&+ \big[\phi'(2y'_{\ell_2+1}) + \tfrac{1}{2}\phi'(y'_{\ell_2}+y'_{\ell_2+1}) + \tfrac{1}{2}\phi'(y'_{\ell_2+1}+y'_{\ell_2+2})\big]v'_{\ell_2+1} \\
&+ \big[2\phi'(2y'_{\ell_2+2}) + \tfrac{1}{2}\phi'(y'_{\ell_2+1}+y'_{\ell_2+2})\big]v'_{\ell_2+2} \\
&+ \sum_{\ell=\ell_2+3}^N 2\phi'(2y'_\ell)v'_\ell + \dots\Big\}.
\end{aligned} \tag{3.9}$$

In the following theorem we estimate the consistency error for the QCE method in the $\mathcal{U}^{-1,p}$-norm. In its formulation we use the following notation:

$$\mathcal{C}_{K_1,K_2} := \{1, \dots, K_1, K_2, \dots, N\}, \tag{3.10}$$

for any $1 < K_1 < K_2 < N$.

Theorem 3.2. *For $\boldsymbol{y} \in \mathcal{Y}$ with $\min_\ell y'_\ell > 0$, and for $1 \le p \le \infty$, we have*

$$\begin{aligned} \|\mathcal{E}'_{\rm qce}(\boldsymbol{y}) - \mathcal{E}'_{\rm a}(\boldsymbol{y})\|_{\mathcal{U}^{-1,p}} \le\ & 2\varepsilon^{1/p} M_1(\mathcal{S}_1) + \tfrac{1}{2}\varepsilon M_2(\mathcal{S}_1)\|\boldsymbol{y}''\|_{\ell^p_\varepsilon(\mathcal{I}_{\rm qce})} \\ & + \varepsilon^2 M_2(\mathcal{S}_2)\|\boldsymbol{y}'''\|_{\ell^p_\varepsilon(\mathcal{C}_{\ell_1,\ell_2+1})} + \varepsilon^2 M_3(\mathcal{S}_3)\|\boldsymbol{y}''\|^2_{\ell^{2p}_\varepsilon(\mathcal{C}_{\ell_1,\ell_2})} =: \mathscr{E}^{\rm qce}_{\rm model}(\boldsymbol{y}), \end{aligned} \tag{3.11}$$

where

$$\begin{aligned} \mathcal{S}_1 =\ & \{2y'_{\ell_1-1}, 2y'_{\ell_1+1}, 2y'_{\ell_2}, 2y'_{\ell_2+2}\} \\ \mathcal{S}_2 =\ & \{2y'_1, \dots, 2y'_{\ell_1}, 2y'_{\ell_2+1}, \dots, 2y'_N\}, \\ \mathcal{S}_3 =\ & [\min_{\ell \in \mathcal{C}_{\ell_1+1,\ell_2}} 2y'_\ell, \max_{\ell \in \mathcal{C}_{\ell_1+1,\ell_2}} 2y'_\ell], \quad \textit{and} \\ \mathcal{I}_{\rm qce} =\ & \{\ell_1 - 1, \ell_1, \ell_2, \ell_2 + 1\}. \end{aligned}$$

Proof. Using (3.9) and (3.2) we write the consistency error $\mathcal{E}'_{\rm qce}(\boldsymbol{y})[\boldsymbol{v}] - \mathcal{E}'_{\rm a}(\boldsymbol{y})[\boldsymbol{v}]$ as

$$\mathcal{E}'_{\rm qce}(\boldsymbol{y})[\boldsymbol{v}] - \mathcal{E}'_{\rm a}(\boldsymbol{y})[\boldsymbol{v}] =: \varepsilon \sum_{\ell=1}^{N} Q_\ell v'_\ell,$$

where

$$\begin{aligned} Q_\ell &= 0, \quad \text{for } \ell = \ell_0, \dots, \ell_2 - 1, \\ Q_{\ell_2} &= -\tfrac{1}{2}\phi'(y'_{\ell_2} + y'_{\ell_2+1}), \\ Q_{\ell_2+1} &= \phi'(2y'_{\ell_2+1}) - \tfrac{1}{2}\phi'(y'_{\ell_2} + y'_{\ell_2+1}) - \tfrac{1}{2}\phi'(y'_{\ell_2+1} + y'_{\ell_2+2}), \\ Q_{\ell_2+2} &= 2\phi'(2y'_{\ell_2+2}) - \tfrac{1}{2}\phi'(y'_{\ell_2+1} + y'_{\ell_2+2}) - \phi'(y'_{\ell_2+2} + y'_{\ell_2+3}), \quad \text{and} \\ Q_\ell &= 2\phi'(2y'_\ell) - \phi'(y'_{\ell-1} + y'_\ell) - \phi'(y_\ell + y'_{\ell+1}) \quad \text{for } \ell = \ell_2 + 3, \dots, N. \end{aligned}$$

The estimate of Q_ℓ for $\ell \ge \ell_2 + 3$ is already contained in the proof of Theorem 3.1.

Using the expansions (3.6) and (3.7), we can rewrite Q_{ℓ_2}, Q_{ℓ_2+1} and Q_{ℓ_2+2} in the form

$$\begin{aligned} Q_{\ell_2} &= -\tfrac{1}{2}\phi'_2(2y'_{\ell_2}) - \tfrac{1}{2}\varepsilon y''_{\ell_2}\phi''(2y'_{\ell_2}) - \tfrac{1}{4}\varepsilon^2 y''^2_{\ell_2}\phi'''(\eta^{\ell_2}), \\ Q_{\ell_2+1} &= -\tfrac{1}{2}\varepsilon^2 y'''_{\ell_2+1}\phi''(2y'_{\ell_2+1}) - \tfrac{1}{4}\varepsilon^2\left[y''^2_{\ell_2}\phi'''(\eta_1^{\ell_2+1}) + y''^2_{\ell_2+1}\phi'''(\eta_2^{\ell_2+1})\right], \quad \text{and} \\ Q_{\ell_2+2} &= \tfrac{1}{2}\phi'(2y'_{\ell_2+2}) - \tfrac{1}{2}\varepsilon y''_{\ell_2+1}\phi''(2y'_{\ell_2+2}) - \varepsilon^2 y'''_{\ell_2+2}\phi''_2(2y'_{\ell_2+2}) \\ &\quad - \tfrac{1}{4}\varepsilon^2 y''^2_{\ell_2+1}\phi'''(\eta_1^{\ell_2+2}) - \tfrac{1}{2}\varepsilon^2 y''^2_{\ell_2+2}\phi'''(\eta_2^{\ell_2+2}), \end{aligned}$$

where

$$\begin{aligned} &\eta^{\ell_2} \in \mathrm{conv}\{2y'_{\ell_2}, y'_{\ell_2} + y'_{\ell_2+1}\}, \qquad &&\eta_1^{\ell_2+1} \in \mathrm{conv}\{2y'_{\ell_2+1}, y'_{\ell_2} + y'_{\ell_2+1}\}, \\ &\eta_2^{\ell_2+1} \in \mathrm{conv}\{2y'_{\ell_2+1}, y'_{\ell_2+1} + y'_{\ell_2+2}\}, &&\eta_1^{\ell_2+2} \in \mathrm{conv}\{2y'_{\ell_2+2}, y'_{\ell_2+1} + y'_{\ell_2+2}\}, \\ \text{and} \quad &\eta_2^{\ell_2+2} \in \mathrm{conv}\{2y'_{\ell_2+2}, y'_{\ell_2+2} + y'_{\ell_2+3}\}. \end{aligned}$$

After regrouping the terms, using corresponding estimates in the left half of the domain, and using the constants we defined in the statement of the theorem, we get the following estimate:

$$
\begin{aligned}
|\mathcal{E}'_{\rm qce}(\boldsymbol{y})[\boldsymbol{v}] - \mathcal{E}'_{\rm a}(\boldsymbol{y})[\boldsymbol{v}]| \le\ & M_1(\mathcal{S}_1)\Big\{ \tfrac12 \varepsilon |v'_{\ell_1-1}| + \tfrac12 \varepsilon |v'_{\ell_1+1}| + \tfrac12 \varepsilon |v'_{\ell_2}| + \tfrac12 \varepsilon |v'_{\ell_2+2}| \Big\} \\
& + M_2(\mathcal{S}_1)\Big\{ \tfrac12 \varepsilon^2 |y''_{\ell_1-1}||v'_{\ell_1-1}| + \tfrac12 \varepsilon^2 |y''_{\ell_1}||v'_{\ell_1+1}| \\
& \qquad + \tfrac12 \varepsilon^2 |y''_{\ell_2}||v'_{\ell_2}| + \tfrac12 \varepsilon^2 |y''_{\ell_2+1}||v'_{\ell_2+2}| \Big\} \\
& + M_2(\mathcal{S}_2)\Big\{ \varepsilon^3 \sum_{\ell=1}^{\ell_1} |y'''_\ell||v'_\ell| + \varepsilon^3 \sum_{\ell=\ell_2+1}^{N} |y'''_\ell||v'_\ell| \Big\} \\
& + M_3(\mathcal{S}_3)\Big\{ \tfrac12 \varepsilon^3 \sum_{\ell=1}^{\ell_1} |y''_\ell|^2 \big(|v'_\ell| + |v'_{\ell+1}|\big) \\
& \qquad + \tfrac12 \varepsilon^3 \sum_{\ell=\ell_2}^{N} |y''_\ell|^2 \big(|v'_\ell| + |v'_{\ell+1}|\big) \Big\}.
\end{aligned}
$$

The stated consistency result can now be quickly deduced after an application of several weighted Hölder's inequalities. □

3.4. *The consistency error of the QNL method*

From (2.15), we obtain, for $\boldsymbol{y} \in \mathcal{Y}$ with $\min_\ell y'_\ell > 0$, and for $\boldsymbol{v} \in \mathcal{U}$,

$$
\begin{aligned}
\mathcal{E}'_{\rm qnl}(\boldsymbol{y})\,[\boldsymbol{v}] = \dots + \varepsilon \Big\{ & \sum_{\ell=\ell_0}^{N} \phi'(y'_\ell) v'_\ell + \sum_{\ell=\ell_0}^{\ell_2} \big[\phi'(y'_{\ell-1} + y'_\ell) + \phi'(y'_\ell + y'_{\ell+1})\big] v'_\ell \\
& + \big[\phi'(2y'_{\ell_2+1}) + \phi'(y'_{\ell_2} + y'_{\ell_2+1})\big] v'_{\ell_2+1} \\
& + \sum_{\ell=\ell_2+2}^{N} 2\phi'(2y'_\ell) v'_\ell \Big\}.
\end{aligned}
$$

Using this representation, it is easy to establish a consistency error estimate for the QNL method in the $\mathcal{U}^{-1,p}$-norm. A similar estimate was given in Theorem 3.1 of Ref. 21; for the sake of completeness we nevertheless include a proof here as well.

Theorem 3.3. *For any $\boldsymbol{y} \in \mathcal{Y}$ with $\min_\ell y'_\ell > 0$, and for $1 \le p \le \infty$, we have*

$$
\begin{aligned}
\|\mathcal{E}'_{\rm qnl}(\boldsymbol{y}) - \mathcal{E}'_{\rm a}(\boldsymbol{y})\|_{\mathcal{U}^{-1,p}} \le\ & \varepsilon M_2\big(\mathcal{S}_1\big) \|\boldsymbol{y}''\|_{\ell^p_\varepsilon(\mathcal{I}_{\rm qnl})} + \varepsilon^2 M_2(\mathcal{S}_2) \|\boldsymbol{y}'''\|_{\ell^p_\varepsilon(\mathcal{C}_{\ell_1-1,\ell_2+2})} \\
& + \varepsilon^2 M_3(\mathcal{S}_3) \|\boldsymbol{y}''\|^2_{\ell^{2p}_\varepsilon(\mathcal{C}_{\ell_1-1,\ell_2+1})} =: \mathscr{E}^{\rm qnl}_{\rm model}(\boldsymbol{y}), \qquad (3.12)
\end{aligned}
$$

where

$$
\begin{aligned}
\mathcal{S}_1 &= {\rm conv}\{2y'_{\ell_1}, y'_{\ell_1-1} + y'_{\ell_1}\} \cup {\rm conv}\{2y'_{\ell_2+1}, y'_{\ell_2+1} + y'_{\ell_2+2}\}, \\
\mathcal{S}_2 &= \{2y'_1, \dots, 2y'_{\ell_1-1}, 2y'_{\ell_2+2}, \dots, 2y'_N\}, \\
\mathcal{S}_3 &= \big[\min_{\ell \in \mathcal{C}_{\ell_1,\ell_2+1}} 2y'_\ell, \max_{\ell \in \mathcal{C}_{\ell_1,\ell_2+1}} 2y'_\ell\big], \\
\mathcal{I}_{\rm qnl} &= \{\ell_1 - 1, \ell_2 + 1\},
\end{aligned}
$$

and where the sets $\mathcal{C}_{K_1,K_2}$ *are defined in* (3.10).

Proof. As in the proof of Theorem 3.2 we write the consistency error as

$$\mathcal{E}'_{\rm qnl}(\boldsymbol{y})[\boldsymbol{v}] - \mathcal{E}'_{\rm a}(\boldsymbol{y})[\boldsymbol{v}] =: \varepsilon \sum_{\ell=1}^{N} Q_\ell v'_\ell,$$

where

$$\begin{aligned} Q_\ell &= 0, \qquad \text{for } \ell = \ell_0, \dots, \ell_2, \\ Q_{\ell_2+1} &= \phi'(2y'_{\ell_2+1}) - \phi'(y'_{\ell_2+1} + y'_{\ell_2+2}), \\ Q_\ell &= 2\phi'(2y'_\ell) - \phi'(y'_{\ell-1} + y'_\ell) - \phi'(y'_\ell + y'_{\ell+1}), \quad \text{for } \ell > \ell_2 + 1. \end{aligned}$$

Using the expansions (3.6) and (3.7), we can write Q_{ℓ_2+1} as

$$\begin{aligned} \phi'(2y'_{\ell_2+1}) - \phi'(y'_{\ell_2+1} + y'_{\ell_2+2}) &= \phi'(2y'_{\ell_2+1}) - \phi'(2y'_{\ell_2+1} + \varepsilon y''_{\ell_2+1}) \\ &= -\varepsilon y''_{\ell_2+1}\phi''(\eta), \end{aligned}$$

where $\eta \in \operatorname{conv}\{2y'_{\ell_2+1}, y'_{\ell_2+1} + y'_{\ell_2+2}\}$. To estimate Q_ℓ for $\ell \geq \ell_2 + 1$ we use the estimates in the proof of Theorem 3.1.

After some algebraic computations, we get the bound

$$\begin{aligned} |\mathcal{E}'_{\rm qnl}(\boldsymbol{y})[\boldsymbol{v}] - \mathcal{E}'_{\rm a}(\boldsymbol{y})[\boldsymbol{v}]| \leq M_2(\mathcal{S}_1)\Big\{\varepsilon^2 |y''_{\ell_1-1}||v'_{\ell_1}| + \varepsilon^2 |y''_{\ell_2+1}||v'_{\ell_2+1}|\Big\} \\ + M_2(\mathcal{S}_2)\Big\{\varepsilon^3 \sum_{\ell=1}^{\ell_1-1} |y'''_\ell||v'_\ell| + \varepsilon^3 \sum_{\ell=\ell_2+2}^{N} |y'''_\ell||v'_\ell|\Big\} \\ + M_3(\mathcal{S}_3)\Big\{\tfrac{1}{2}\varepsilon^3 \sum_{\ell=1}^{\ell_1-1} |y''_\ell|^2\big(|v'_\ell| + |v'_{\ell+1}|\big) \\ + \tfrac{1}{2}\varepsilon^3 \sum_{\ell=\ell_2+1}^{N} |y''_\ell|^2\big(|v'_\ell| + |v'_{\ell+1}|\big)\Big\}. \end{aligned}$$

The result is obtained after several applications of weighted Hölder inequalities. □

3.5. *Discussion and comparison*

In the analysis of this section we have estimated the consistency errors of three different QC methods in negative Soblev norms. We see that the leading order terms in the upper bounds are $O(\varepsilon^2)$, $O(\varepsilon^{1/p})$ and $O(\varepsilon)$ for the QCL, QCE, and QNL methods, respectively. However, a much finer distinction can and should be made.

First of all, we note that since all three methods reduce to the Cauchy–Born approximation in the continuum region (in the case of the QCL method the entire domain is understood as the continuum region), the corresponding contributions are all of second order.

Second, we see that the QCE method (and only the QCE method) has a zeroth-order term (in a sense that will be made clear in the next paragraph) $2M_1\varepsilon^{1/p}$ in the interface region. The origin of this term is the occurence of "ghost forces", that is, the fact that homogeneous deformations are not equilibria of the QCE model:

$$E'_{\rm qce}(F\boldsymbol{x}) \neq 0.$$

The origin and effect of the ghost forces are discussed in more detail in Refs. 25, 16, 4, 5 and 18.

We call this term zeroth order for several reasons: (i) From any possible perspective, this term is of zeroth order if $p = \infty$, in which case the consistency error is related to the error in the $\mathcal{U}^{1,\infty}$-norm. (ii) The parameter ε is a constant of the problem and does *not* tend to zero. (iii) Indeed, our understanding of the order of consistency is related more closely to the dependence of the error on the smoothness of the solution, and the term $2C_1\varepsilon^{1/p}$ is independent of the magnitude of $\boldsymbol{y}''$ in the interface region. The scaling $\varepsilon^{1/p}$ relates only to the *width* of the interface region.

Finally, we point out the first-order consistency term in the interface region for the QNL method. The origin of this term is, in essence, the loss of symmetry that is introduced by changing the interaction law at the interface between the atomistic and continuum regions. The analysis of Dobson and Luskin[5], and our numerical experiments in the present paper, also show that this asymmetry creates effectively a higher order ghost force.

We also briefly compare our results to similar results in the literature. A detailed discussion of the consistency error estimate for the QNL method can be found in Ref. 21, hence we focus on our analysis of the QCE method. The first detailed analysis of the effect of the ghost force on the quasicontinuum error was given by Dobson and Luskin[4]. In that paper, the authors formulated a linearized model problem, which allowed an explicit calculation of the effect of the ghost force on the quasicontinuum solution. While our analysis is more straightforward, is easily applied in the nonlinear setting, and possibly gives even sharper consistency error estimates, the analysis in Ref. 4 reveals much finer qualitative details such as the decay of the effect of the ghost force in the QCE solution.

4. A Priori Error Analysis

4.1. *Coarse-graining*

The transition from an atomistic to a continuum model is only the first step in the construction of a practical QC method. In the second step, one coarse-grains the continuum region using, e.g., a P1 finite element method in order to reduce the number of degrees of freedom. The following construction of the coarse-grained spaces of displacements and deformations follows largely the convention in Refs. 14 and 15.

We partition the domain by choosing a set of representative atoms (or, *repatoms*)

$$\mathcal{L}_{\rm rep} = \{t_1, t_2, \dots, t_{N_{\rm rep}}\} \subseteq \{1, 2, \dots, N\},$$

such that $N_{\rm rep} \ll N$ and $t_1 < t_2 < \cdots < t_{N_{\rm rep}}$. For simplicity of the implementation and analysis of the QCE and QNL methods we assume that

$$\begin{aligned} &\{\ell_1 - 2, \dots, \ell_2 + 2\} \subset \mathcal{L}_{\rm rep} \text{ for the QCE method, and} \\ &\{\ell_1 - 1, \dots, \ell_2 + 1\} \subset \mathcal{L}_{\rm rep} \text{ for the QNL method.} \end{aligned} \tag{4.1}$$

For the analysis of the QCL method, no restriction of this kind is required.

The grid is extended periodically, that is, we define $t_{i+N_{\rm rep}} = t_i + N$. For simplicity, we also assume that $t_0 = 0$ and $t_{N_{\rm rep}} = N$. The positions of the repatoms in the reference lattice are $x_{t_i} = \varepsilon t_i$. The mesh size functions for the elements and for the nodes are

$$h_i = \varepsilon(t_i - t_{i-1}) \quad \text{and} \quad H_i = \tfrac{1}{2}\varepsilon(t_{i+1} - t_{i-1}), \qquad \text{for } i \in \mathbb{Z}.$$

We then define the mesh-dependent inner product

$$\langle \boldsymbol{v}, \boldsymbol{w} \rangle_h = \sum_{i=1}^{N_{\rm rep}} H_i v_{t_i} w_{t_i} \qquad \forall \boldsymbol{v}, \boldsymbol{w} \in \mathbb{R}^{\mathbb{Z}},$$

which is a trapezoidal rule approximation of $\langle \cdot, \cdot \rangle_\varepsilon$.

Finally, we define the coarse-grained displacement space as

$$\mathcal{U}_{\rm qc} = \big\{ \boldsymbol{u} \in \mathbb{R}^{\mathbb{Z}} : \boldsymbol{u} \text{ is } N\text{-periodic, p.w. affine w.r.t. } \mathcal{L}_{\rm rep}, \text{ and } \langle \boldsymbol{u}, 1 \rangle_h = 0 \big\}, \tag{4.2}$$

and the corresponding space of admissible deformations as

$$\mathcal{Y}_{\rm qc} = \big\{ \boldsymbol{y} \in \mathbb{R}^{\mathbb{Z}} : y_\ell = \varepsilon F \ell + u_\ell, \ \boldsymbol{u} \in \mathcal{U}_{\rm qc} \big\}. \tag{4.3}$$

We remark that if $\boldsymbol{u}$ is a piecewise affine grid function then $\langle \boldsymbol{u}, 1 \rangle_h = \langle \boldsymbol{u}, 1 \rangle_\varepsilon$, and hence $\mathcal{U}_{\rm qc} \subset \mathcal{U}$ and $\mathcal{Y}_{\rm qc} \subset \mathcal{Y}$.

Next, we redefine the total QC energy, by approximating the external forces via the mesh-dependent inner product, as

$$E_{\rm qc}(\boldsymbol{y}) = \mathcal{E}_{\rm qc}(\boldsymbol{y}) - \langle \boldsymbol{f}, \boldsymbol{y} \rangle_h, \tag{4.4}$$

where $\text{qc} \in \{\text{qcl}, \text{qce}, \text{qnl}\}$. We are now seeking a solution to

$$\boldsymbol{y}^{\rm qc} \in \operatorname{argmin} E_{\rm qc}(\mathcal{Y}_{\rm qc}). \tag{4.5}$$

If $\min_\ell (y^{\rm qc})'_\ell > 0$, then $E_{\rm qc}$ is differentiable at $\boldsymbol{y}^{\rm qc}$ and the first-order necessary optimality condition for (4.5), in variational form, reads

$$\mathcal{E}'_{\rm qc}(\boldsymbol{y})[\boldsymbol{v}] = \langle \boldsymbol{f}, \boldsymbol{v} \rangle_h \qquad \forall \boldsymbol{v} \in \mathcal{U}_{\rm qc}. \tag{4.6}$$

After having estimated the consistency error for (4.6) in Section 3, we now need estimates for the coarse-graining error, and stability results. These are established, respectively, in Sections 4.2 and 4.3.

4.2. *A superconvergence estimate*

We define a modified nodal interpolation operator $I_h : \mathcal{U} \to \mathcal{U}_{\rm qc}$ by $(I_h \boldsymbol{u})_{t_i} = u_{t_i} + C$ where the constant C is chosen so that $\langle I_h \boldsymbol{u}, 1 \rangle_h = 0$. With slight abuse of notation, we also define the interpolation operator $I_h : \mathcal{Y} \to \mathcal{Y}_{\rm qc}$ by

$$(I_h \boldsymbol{y})_{t_i} = \varepsilon F t_i + (I_h \boldsymbol{u})_{t_i}. \tag{4.7}$$

As in a typical finite element error analysis, we split the error $\boldsymbol{e} = \boldsymbol{y}^{\rm a} - \boldsymbol{y}^{\rm qc}$ into

$$\|\boldsymbol{e}\|_{\mathcal{U}^{1,2}} \le \|I_h \boldsymbol{e}\|_{\mathcal{U}^{1,2}} + \|\boldsymbol{e} - I_h \boldsymbol{e}\|_{\mathcal{U}^{1,2}} = \|I_h \boldsymbol{y}^{\rm a} - \boldsymbol{y}^{\rm qc}\|_{\mathcal{U}^{1,2}} + \|\boldsymbol{y}^{\rm a} - I_h \boldsymbol{y}^{\rm a}\|_{\mathcal{U}^{1,2}},$$

and we will estimate $\|I_h \boldsymbol{e}\|_{\mathcal{U}^{1,2}}$ and $\|\boldsymbol{e} - I_h \boldsymbol{e}\|_{\mathcal{U}^{1,2}}$ separately to obtain the total error estimate. We will use the fact that, for $\boldsymbol{y}_1, \boldsymbol{y}_2 \in \mathcal{Y}$, $\boldsymbol{y}_1 - \boldsymbol{y}_2 \in \mathcal{U}$, and as a result $\boldsymbol{e}, I_h \boldsymbol{e}, \boldsymbol{y}^{\rm a} - I_h \boldsymbol{y}^{\rm a} \in \mathcal{U}$.

To estimate the interpolation error $\|\boldsymbol{y}^{\rm a} - I_h \boldsymbol{y}^{\rm a}\|_{\mathcal{U}^{1,2}}$ we can use the following result.

Lemma 4.1. *Let $\boldsymbol{y} \in \mathcal{Y}$, and $p \in [1, \infty]$, then*

$$\|\boldsymbol{y}' - I_h \boldsymbol{y}'\|_{\ell^p_\varepsilon} \le \frac{1}{2} \Big(\sum_{i \in \mathcal{C}_c} h_i^2 \|\boldsymbol{y}''\|^p_{\ell^p_\varepsilon(\mathcal{K}_i^2)} \Big)^{\frac{1}{2}},$$

where

$$\mathcal{C}_c = \{ i \in \mathbb{Z} : t_i - t_{i-1} \ge 2 \}, \quad \textit{and} \quad \mathcal{K}_i^2 = \{ t_{i-1} + 1, \dots, t_i - 1 \}.$$

Proof. If the ℓ^p_ε-norm is replaced by the ℓ^q_ε-norm, $q \in \{1, \infty\}$, then the result follows immediately from Theorem A.4 of Ref. 23. For $p \in (1, \infty)$ it is obtained using Riesz' interpolation theorem. □

We will give a complete estimate for $\|I_h \boldsymbol{e}\|_{\mathcal{U}^{1,2}}$ in Section 4.5. In the remainder of the present section, we derive a superconvergence result, which is a crucial ingredient for the error analysis in Section 4.5.

Lemma 4.2. *Let $\boldsymbol{y} \in \mathcal{Y}$ such that $\min_\ell y'_\ell > 0$, then*

$$\sup_{\substack{\boldsymbol{w} \in \mathcal{U}_{\rm qc} \\ \|\boldsymbol{w}'\|_{\ell^2_\varepsilon} = 1}} \big| \{ \mathcal{E}'_{\rm qc}(\boldsymbol{y}) - \mathcal{E}'_{\rm qc}(I_h \boldsymbol{y}) \} [\boldsymbol{w}] \big| \le C_1 \Big(\sum_{i \in \mathcal{C}_c} h_i^4 \|\boldsymbol{y}''\|^4_{\ell^4_\varepsilon(\mathcal{K}_i^2)} \Big)^{\frac{1}{2}} =: \mathscr{E}_{\rm fem}(\boldsymbol{y}) \tag{4.8}$$

for some constant

$$C_1 = \tfrac{1}{8} M_3(\mathcal{S}_1) + M_3(2\mathcal{S}_1), \quad \textit{where } \mathcal{S}_1 = \Big[\min_{\ell \in \mathcal{C}_{\ell_1 - 1, \ell_2 + 2}} y'_\ell, \max_{\ell \in \mathcal{C}_{\ell_1 - 1, \ell_2 + 2}} y'_\ell \Big],$$

and where $M_i(\mathcal{S}_1)$ is defined in (2.17). *(For* qc = qcl *we set $\ell_1 = \ell_2 + 2$ in the definition of $\mathcal{S}_1$.)*

Proof. We begin by noting that the values of $I_h y'_\ell$ in the continuum region are convex combinations of the values of y'_ℓ in the continuum region, and hence $I_h y'_\ell \in \mathcal{S}_1$ for all occurances below.

Whenever $t_i - t_{i-1} = 1$ (i.e., $h_i = \varepsilon$), we have $y'_{t_i} = I_h y'_{t_i}$, and hence it is easy to see, using assumption (4.1), that

$$\big\{\mathcal{E}'_{\rm qc}(\boldsymbol{y}) - \mathcal{E}'_{\rm qc}(I_h\boldsymbol{y})\big\}[\boldsymbol{w}] = \varepsilon \sum_{i\in\mathcal{C}_c} \sum_{\ell=t_{i-1}+1}^{t_i} \big\{W'(y'_\ell) - W'(I_h y'_\ell)\big\} w'_\ell,$$

where we recall that $W'(r) = \phi'(r) + 2\phi'(2r)$. Note also that this formula is independent of the choice of QC method.

A Taylor expansion yields

$$W'(y'_\ell) - W'(I_h y'_\ell) = W''(I_h y'_\ell)(y'_\ell - I_h y'_\ell) + \tfrac{1}{2} W'''(\theta_\ell)(y'_\ell - I_h y'_\ell)^2,$$

for some $\theta_\ell \in \mathcal{S}_1$. Using the property that $\sum_{\ell=t_{i-1}+1}^{t_i}(y'_\ell - I_h y'_\ell) = 0$ and the values of w'_ℓ, $\phi''(I_h y'_\ell)$ and $\phi''(2 I_h y'_\ell)$ do not change inside an element (i.e., they take the same value for $\ell = t_{i-1}+1, \dots, t_i$), we arrive at

$$\big|\{E'_{\rm qc}(\boldsymbol{y}) - E'_{\rm qc}(I_h\boldsymbol{y})\}[\boldsymbol{w}]\big| \le \varepsilon \sum_{i\in\mathcal{C}_c} \sum_{\ell=t_{i-1}+1}^{t_i} \tfrac{1}{2}|W'''(\theta_\ell)||y'_\ell - I_h y'_\ell|^2 |w'_\ell|.$$

Since $W'''(r) = \phi'''(r) + 8\phi'''(2r)$ and $\theta_\ell \in \mathcal{S}_1$, we have

$$\max_\ell |W'''(\theta_\ell)| \le M_3(\mathcal{S}_1) + 8M_3(2\mathcal{S}_1) =: 8C_1.$$

Therefore, we get the following estimate

$$\begin{aligned}
\big|\{E'_{\rm qc}(\boldsymbol{y}) - E'_{\rm qc}(I_h\boldsymbol{y})\}[\boldsymbol{w}]\big| &\le 4C_1\varepsilon \sum_{i\in\mathcal{C}_c} \sum_{\ell=t_{i-1}+1}^{t_i} |y'_\ell - I_h y'_\ell|^2 |w'_\ell| \\
&\le 4C_1 \sum_{i\in\mathcal{C}_c} \tfrac{1}{4} h_i^2\, \varepsilon \sum_{\ell=t_{i-1}+1}^{t_i-1} |y''_\ell|^2 |w'_\ell| \\
&\le C_1 \Big(\sum_{i\in\mathcal{C}_c} h_i^4 \|\boldsymbol{y}''\|^4_{\ell^4_\varepsilon(\mathcal{K}_i^2)}\Big)^{\frac{1}{2}} \|\boldsymbol{w}\|_{\mathcal{U}^{1,2}}.
\end{aligned}$$

The last two steps follow from Lemma 4.1 and a weighted Hölder's inequality. □

4.3. *Stability of QC methods*

Aside from consistency estimates for the QC approximations, which was analyzed in the previous section, their stability is the second key ingredient for deriving error bounds. Since we are in a one-dimensional situation it would not be too difficult to derive stability results in the spaces $\mathcal{U}^{1,p}$, $p \in [1,\infty]$ (see, e.g., Ortner and Süli,[23] Dobson et al.,[3,7] Ming and Yang,[18] Makridakis et al.[14]). However, such stability results would be difficult to obtain in more than one dimension, and therefore, we will only use stability in the space $\mathcal{U}^{1,2}$ in our subsequent error analysis.

For an a priori error analysis, the natural notion of stability for energy minimization problems is coercivity (or, positivity) of the approximate Hessian at the atomistic solution $\boldsymbol{y}^{\rm a}$:

$$E''_{\rm qc}(\boldsymbol{y}^{\rm a})[\boldsymbol{v},\boldsymbol{v}] \ge c_{\rm qc}(\boldsymbol{y}^{\rm a})\|\boldsymbol{v}'\|^2_{\ell^2_\varepsilon} \qquad \forall \boldsymbol{v} \in \mathcal{U}, \tag{4.9}$$

for some constant $c_{\rm qc}(\boldsymbol{y}^{\rm a}) > 0$. In the remainder of this section we derive explicit conditions on the deformations $\boldsymbol{y}^{\rm a}$ such that (4.9) holds.

The simplest of the three Hessian operators is the QCL Hessian, which is given by

$$E''_{\rm qcl}(\boldsymbol{y})[\boldsymbol{v},\boldsymbol{v}] = \varepsilon \sum_{\ell=1}^{N} A_\ell^{\rm qcl} |v'_\ell|^2,$$

where

$$A_\ell^{\rm qcl} = \phi''(y'_\ell) + 4\phi''(2y'_\ell), \qquad \text{for } \ell = \{1,\dots,N\}. \tag{4.10}$$

Hence we immediately see that we can choose $c_{\rm qcl}(\boldsymbol{y}) = \min_\ell A_\ell^{\rm qcl}$.

To obtain similar results for the QCE and QNL energies we need to overcome some difficulties due to the nonlocal interactions, following the ideas developed in Refs. 21 and 6.

The Hessian of the QNL energy functional at $\boldsymbol{y}$ is given by,

$$\begin{aligned} E''_{\rm qnl}(\boldsymbol{y})[\boldsymbol{v},\boldsymbol{v}] = \varepsilon \sum_{\ell=1}^{N} \phi''(y'_\ell)|v'_\ell|^2 &+ \varepsilon \sum_{\ell=1}^{\ell_1} \left[\frac{1}{2}\phi''(2y'_\ell)|2v'_\ell|^2 + \frac{1}{2}\phi''(2y'_{\ell+1})|2v'_{\ell+1}|^2 \right] \\ &+ \varepsilon \sum_{\ell=\ell_1}^{\ell_2} \phi''(y'_\ell + y'_{\ell+1})|v'_\ell + v'_{\ell+1}|^2 \\ &+ \varepsilon \sum_{\ell=\ell_2+1}^{N} \left[\frac{1}{2}\phi''(2y'_\ell)|2v'_\ell|^2 + \frac{1}{2}\phi''(2y'_{\ell+1})|2v'_{\ell+1}|^2 \right]. \end{aligned}$$

We now note that the 'non-local' Hessian terms $|v'_\ell + v'_{\ell+1}|^2$ can be rewritten in terms of the 'local' terms $|v'_\ell|^2$ and $|v'_{\ell+1}|^2$ and a strain-gradient correction,

$$|v'_\ell + v'_{\ell+1}|^2 = 2|v'_\ell|^2 + 2|v'_{\ell+1}|^2 - \varepsilon^2|v''_\ell|^2.$$

Using this formula, we can rewrite the Hessian in the form

$$E''_{\rm qnl}(\boldsymbol{y})[\boldsymbol{v},\boldsymbol{v}] = \varepsilon \sum_{\ell=1}^{N} A_\ell^{\rm qnl}|v'_\ell|^2 + \varepsilon \sum_{\ell=\ell_1}^{\ell_2} \varepsilon^2 B_\ell^{\rm qnl}|v''_\ell|^2,$$

where

$$\begin{aligned} A_\ell^{\rm qnl} &= \phi''(y'_\ell) + \begin{cases} 2\phi''(y'_{\ell-1}+y'_\ell) + 2\phi''(y'_\ell + y'_{\ell+1}), & \ell \in \{\ell_1+1,\dots,\ell_2\}, \\ 2\phi''(y'_\ell + y'_{\ell+1}) + 2\phi''(2y'_\ell), & \ell = \ell_1, \\ 2\phi''(y'_{\ell-1}+y'_\ell) + 2\phi''(2y'_\ell), & \ell = \ell_2+1, \\ 4\phi''(2y'_\ell), & \ell \in \mathcal{C}_{\ell_1-1,\ell_2+2}, \end{cases} \\ B_\ell^{\rm qnl} &= -\phi''(y'_\ell + y'_{\ell+1}). \end{aligned} \tag{4.11}$$

Using similar algebraic manipulations, we can write the QCE Hessian as (see also Equation (15) of Ref. 6 for the case $\boldsymbol{y} = F\boldsymbol{x}$)

$$E''_{\rm qce}(\boldsymbol{y})[\boldsymbol{v},\boldsymbol{v}] = \varepsilon \sum_{\ell=1}^{N} A_\ell^{\rm qce}|v'_\ell|^2 + \varepsilon \sum_{\ell=\ell_1-1}^{\ell_2+1} \varepsilon^2 B_\ell^{\rm qce}|v''_\ell|^2,$$

where

$$A_\ell^{\rm qce} = \phi''(y'_\ell) + \begin{cases} 2\phi''(y'_{\ell-1}+y'_\ell) + 2\phi''(y'_\ell+y'_{\ell+1}), & \ell \in \{\ell_1+2,\dots,\ell_2-1\}, \\ \phi''(y'_{\ell-1}+y'_\ell) + \phi''(y'_\ell+y'_{\ell+1}) + 2\phi''(2y'_\ell), & \ell \in \{\ell_1,\ell_2+1\} \\ \phi''(y'_\ell+y'_{\ell+1}) + 4\phi''(2y'_\ell), & \ell = \ell_1 - 1, \\ \phi''(y'_{\ell-1}+y'_\ell) + 2\phi''(y'_\ell+y'_{\ell+1}), & \ell = \ell_1+1, \\ \phi''(y'_\ell+y'_{\ell+1}) + 2\phi''(y'_{\ell-1}+y'_\ell), & \ell = \ell_2, \\ \phi''(y'_{\ell-1}+y'_\ell) + 4\phi''(2y'_\ell), & \ell = \ell_2+2, \\ 4\phi''(2y'_\ell), & \ell \in \mathcal{C}_{\ell_1-2,\ell_2+3}, \end{cases}$$

$$B_\ell^{\rm qce} = \begin{cases} -\frac{1}{2}\phi''(y'_\ell+y'_{\ell+1}), & \ell \in \{\ell_1-1,\ell_1,\ell_2,\ell_2+1\}, \\ -\phi''(y'_\ell+y'_{\ell+1}), & \ell \in \{\ell_1+1,\dots,\ell_2-1\}, \end{cases} \tag{4.12}$$

Recall our assumption that ϕ is convex in $(0, r_*)$ and concave in $(r_*, +\infty)$. For typical pair interaction potentials, $y'_\ell < r_*/2$ can only be achieved under extreme compressive forces. Since, under such extreme conditions a pair potential may be an inappropriate model to employ anyhow, it is not too restrictive to assume that the atomistic solution $\boldsymbol{y}$ satisfies

$$y'_\ell \geq r_*/2 \qquad \forall \ell \in \{1,\dots,N\}.$$

As a result of this assumption, and the properties of ϕ, we have

$$-\phi''(y'_\ell + y'_{\ell+1}) \geq 0,$$

for all ℓ and thus

$$-B_\ell^{\rm qc} \geq 0,$$

for all ℓ and for qc $\in \{\rm qce, qnl\}$

As an immediate consequence we obtain the following lemma, which gives sufficient conditions under which stability of QC methods can be guaranteed.

Lemma 4.3. *Let $\boldsymbol{y} \in \mathcal{Y}$ satisfy $\min_\ell y'_\ell \geq r_*/2$; then, for* qc $\in \{\rm qcl, qce, qnl\}$,

$$E''_{\rm qc}(\boldsymbol{y})[\boldsymbol{v},\boldsymbol{v}] \geq A_*^{\rm qc}(\boldsymbol{y}) \|\boldsymbol{v}'\|^2_{\ell^2_\varepsilon} \qquad \forall \boldsymbol{v} \in \mathcal{U}, \quad \textit{where} \quad A_*^{\rm qc}(\boldsymbol{y}) = \min_{\ell=1,\dots,N} A_\ell^{\rm qc}.$$

The coefficients $A_\ell^{\rm qc}$ are defined, respectively, in (4.10), (4.12), *and* (4.11).

Proof. If $\min_\ell y_\ell \geq r_*/2$, then

$$E''_{\rm qc}(\boldsymbol{y})[\boldsymbol{v},\boldsymbol{v}] \geq \varepsilon \sum_{\ell=1}^N A_\ell^{\rm qc} |v'_\ell|^2 \geq A_*^{\rm qc}(\boldsymbol{y}) \varepsilon \sum_{\ell=1}^N |v'_\ell|^2 = A_*^{\rm qc}(\boldsymbol{y}) \|\boldsymbol{v}'\|^2_{\ell^2_\varepsilon}. \qquad \square$$

Remark 4.1. Our stability results are extensions of the sharp stability estimates of Dobson et al.[6] to nonlinear deformations. It is explained in Remark 4.6 of Ref. 21, using results of Ref. 6, that the result for the QCL and QNL methods is "almost" sharp in the following sense: if $\boldsymbol{y}$ is a globally smooth deformation then, in the limit as $N \to \infty$, $E''_{\rm qnl}(\boldsymbol{y})$ is positive if and only if $E''_{\rm a}(\boldsymbol{y})$ is positive.

In the case of the QCE method, such a one-to-one correspondence between stability of the QC method and of the atomistic model is false. Even at a homogeneous deformation $\boldsymbol{y} = F\boldsymbol{x}$, we have (see Section 5 of Ref. 6)

$$A_*^{\rm a} = \phi''(F) + 4\phi''(2F) > \phi''(F) + 4.5\phi''(2F) > \inf_{\|\boldsymbol{u}\|_{\ell^2_\varepsilon}=1} E''_{\rm qce}(F\boldsymbol{x})[\boldsymbol{u},\boldsymbol{u}] > A_*^{\rm qce}.$$

An additional complication is the fact that homogeneous deformations are not, in the absence of external forces, equilibria of the QCE model. The interface ghost forces effect a further loss of stability, which is discussed in detail in Section 5 of Ref. 6. This means that there exist stable atomistic configurations near bifurcation points, which *cannot* be approximated by a QCE method.

Nevertheless, it is easy to check that in "deep" minima where next-nearest neighbour interactions are dominated by nearest-neighbour interactions, our stability constant $A_*^{\rm qce}$ is positive. For deformations of this type our error analysis will be valid.

4.4. *Auxiliary results*

Before we present the main theorem and its proof, we state two useful auxiliary results: a local Lipschitz bound on $\mathcal{E}''_{\rm qc}$, and a consistency estimate for the approximation of the forcing terms.

The proof of the following local Lipschitz bound is straightforward, particularly if no explicit constant is required, and is therefore omitted.

Lemma 4.4. *Let* $\rm qc \in \{qcl, qce, qnl\}$*, and let* $\boldsymbol{y},\boldsymbol{z} \in \mathcal{Y}$ *be such that* $\min_\ell y'_\ell \ge \mu$ *and* $\min_\ell z'_\ell \ge \mu$ *for some constant* $\mu > 0$*; then*

$$\big|\{\mathcal{E}''_{\rm qc}(\boldsymbol{y}) - \mathcal{E}''_{\rm qc}(\boldsymbol{z})\}[\boldsymbol{v},\boldsymbol{w}]\big| \le C_{\rm Lip}\|\boldsymbol{y}'-\boldsymbol{z}'\|_{\ell^\infty_\varepsilon}\|\boldsymbol{v}'\|_{\ell^2_\varepsilon}\|\boldsymbol{w}'\|_{\ell^2_\varepsilon} \qquad \forall \boldsymbol{v},\boldsymbol{w}\in\mathcal{U},$$

where $C_{\rm Lip} = M_3([\mu,+\infty)) + 10M_3([2\mu,+\infty))$.

Our second auxiliary result, the consistency estimate for the approximation of the external forces, is a generalization of a similar result in Ref. 23.

Lemma 4.5. *For* $\boldsymbol{f} \in \mathcal{U}$*, we have*

$$\sup_{\substack{\boldsymbol{v}\in\mathcal{U}_{\rm qc}\\ \|\boldsymbol{v}'\|_{\ell^2_\varepsilon}=1}} \big|\langle \boldsymbol{f},\boldsymbol{v}\rangle_h - \langle \boldsymbol{f},\boldsymbol{v}\rangle_\varepsilon\big| \le \bigg(\sum_{i\in\mathcal{C}_c} h_i^4\big[\tfrac{1}{32}\|\boldsymbol{f}''\|^2_{\ell^2_\varepsilon(\mathcal{K}_i^2)} + \tfrac12\|\boldsymbol{f}'\|^2_{\ell^2_\varepsilon(\mathcal{K}_i^1)},\big]\bigg)^{1/2} =: \mathscr{E}_{\rm ext}(\boldsymbol{f}), \tag{4.13}$$

where $\mathcal{K}_i^1 = \{t_{i-1}+1,\dots,t_i\}$*, and where* $\mathcal{K}_i^2$ *and* $\mathcal{C}_c$ *are defined in Lemma 4.1.*

Proof. The proof of this lemma is a modification of the last part of the proof of Theorem 3.2 of Ref. 23. For $\boldsymbol{v}\in\mathcal{U}_{\rm qc}$, we apply Theorem A.4 of Ref. 23 with $p=1$ to esimate

$$|\langle \boldsymbol{f},\boldsymbol{v}\rangle_h - \langle \boldsymbol{f},\boldsymbol{v}\rangle_\varepsilon| \le \sum_{i\in\mathcal{C}_c} \tfrac14 h_i^2|(\boldsymbol{f}\boldsymbol{v})''|_{\ell^1_\varepsilon(\mathcal{K}_i^2)}.$$

Using the fact that $v''_\ell = 0$ for $\ell \in \mathcal{K}_i^2$, we have

$$(\boldsymbol{f}\boldsymbol{v})''_\ell = \frac{f_{\ell+1}v_{\ell+1} - 2f_\ell v_\ell + f_{\ell-1}v_{\ell-1}}{\varepsilon^2}$$
$$= \frac{f_{\ell+1} - 2f_\ell + f_{\ell-1}}{\varepsilon^2}v_\ell + \frac{f_{\ell+1} - f_\ell}{\varepsilon}\frac{v_{\ell+1} - v_\ell}{\varepsilon} + \frac{f_\ell - f_{\ell-1}}{\varepsilon}\frac{v_\ell - v_{\ell-1}}{\varepsilon}.$$

We then obtain the following estimate:

$$|\langle \boldsymbol{f}, \boldsymbol{v}\rangle_h - \langle \boldsymbol{f}, \boldsymbol{v}\rangle_\varepsilon| \le \frac{1}{4}\sum_{i\in\mathcal{C}_c} h_i^2 \big[\|\boldsymbol{f}''\|_{\ell^2_\varepsilon(\mathcal{K}_i^2)}\|\boldsymbol{v}\|_{\ell^2_\varepsilon(\mathcal{K}_i^2)} + 2\|\boldsymbol{f}'\|_{\ell^2_\varepsilon(\mathcal{K}_i^1)}\|\boldsymbol{v}'\|_{\ell^2_\varepsilon(\mathcal{K}_i^1)}\big]$$
$$\le \frac{1}{4}\Big[\sum_{i\in\mathcal{C}_c} h_i^4\|\boldsymbol{f}''\|^2_{\ell^2_\varepsilon(\mathcal{K}_i^2)}\Big]^{\frac{1}{2}}\|\boldsymbol{v}\|_{\ell^2_\varepsilon} + \frac{1}{2}\Big[\sum_{i\in\mathcal{C}_c} h_i^4\|\boldsymbol{f}'\|^2_{\ell^2_\varepsilon(\mathcal{K}_i^1)}\Big]^{\frac{1}{2}}\|\boldsymbol{v}'\|_{\ell^2_\varepsilon}.$$

Application of a discrete Poincare inequality (see Remark 1 of Ref. 5), $\|\boldsymbol{v}\|_{\ell^2_\varepsilon} \le \frac{1}{2}\|\boldsymbol{v}'\|_{\ell^2_\varepsilon}$, and of the inequality $a^{1/2} + b^{1/2} \le (2a + 2b)^{1/2}$, yield the bound

$$|\langle \boldsymbol{f}, \boldsymbol{v}\rangle_h - \langle \boldsymbol{f}, \boldsymbol{v}\rangle_\varepsilon| \le \Big(\Big[\tfrac{1}{64}\sum_{i\in\mathcal{C}_c} h_i^4\|\boldsymbol{f}''\|^2_{\ell^2_\varepsilon(\mathcal{K}_i^2)}\Big]^{\frac{1}{2}} + \Big[\tfrac{1}{4}\sum_{i\in\mathcal{C}_c} h_i^4\|\boldsymbol{f}'\|^2_{\ell^2_\varepsilon(\mathcal{K}_i^1)}\Big]^{\frac{1}{2}}\Big)\|\boldsymbol{v}'\|_{\ell^2_\varepsilon},$$
$$\le \Big(\sum_{i\in\mathcal{C}_c} h_i^4\big[\tfrac{1}{32}\|\boldsymbol{f}''\|^2_{\ell^2_\varepsilon(\mathcal{K}_i^2)} + \tfrac{1}{2}\|\boldsymbol{f}'\|^2_{\ell^2_\varepsilon(\mathcal{K}_i^1)}\big]\Big)^{\frac{1}{2}}\|\boldsymbol{v}'\|_{\ell^2_\varepsilon}.$$

This estimate establishes the stated result. □

4.5. *Error estimates*

In this section, we will derive the error estimates for $\|\boldsymbol{e}\|_{\mathcal{U}^{1,2}}$ for the QCL, QCE, and QNL methods. The following theorem is obtained as a natural combination of the consistency error estimates and stability analysis of the previous sections. To avoid technicalities associated with the nonlinearity of our models, we make an a priori assumption: we assume the existence of atomistic and QC solutions and make a mild requirement on their smoothness and closeness (cf. (4.14)). We comment further on this assumption in Remark 4.2 below.

Theorem 4.1. *Fix* $\mathrm{qc} \in \{\mathrm{qcl}, \mathrm{qce}, \mathrm{qnl}\}$. *Let* $\boldsymbol{y}^{\mathrm{a}}$ *be a solution of the atomistic problem* (2.4) *whose gradients are such that* $\min_\ell (y^{\mathrm{a}})'_\ell \ge r_*/2$ *and* $A_*^{\mathrm{qc}}(\boldsymbol{y}^{\mathrm{a}}) > 0$, *where* A_*^{qc} *is defined in the statement of Lemma 4.3. Suppose, further, that* $\boldsymbol{y}^{\mathrm{qc}}$ *is a solution of the QC model* (4.5) *such that, for some* $\tau > 0$,

$$\|(\boldsymbol{y}^{\mathrm{a}} - I_h\boldsymbol{y}^{\mathrm{a}})'\|_{\ell^\infty_\varepsilon} \le \tau \quad \text{and} \quad \|(\boldsymbol{y}^{\mathrm{a}} - \boldsymbol{y}^{\mathrm{qc}})'\|_{\ell^\infty_\varepsilon} \le \tau. \tag{4.14}$$

Then, if τ *is sufficiently small, we have the error estimate*

$$\|\boldsymbol{y}^{\mathrm{a}} - \boldsymbol{y}^{\mathrm{qc}}\|_{\mathcal{U}^{1,2}} \le \frac{1}{2}\Big(\sum_{i\in\mathcal{C}_c} h_i^2\|\boldsymbol{y}''\|^2_{\ell^2_\varepsilon(\mathcal{K}_i^2)}\Big)^{\frac{1}{2}} + \tfrac{2}{A_*^{\mathrm{qc}}(\boldsymbol{y}^{\mathrm{a}})}\big(\mathscr{E}^{\mathrm{qc}}_{\mathrm{model}} + \mathscr{E}_{\mathrm{fem}} + \mathscr{E}_{\mathrm{ext}}\big), \tag{4.15}$$

as well as the superconvergence result

$$\|I_h\boldsymbol{y}^{\mathrm{a}} - \boldsymbol{y}^{\mathrm{qc}}\|_{\mathcal{U}^{1,2}} \le \tfrac{2}{A_*^{\mathrm{qc}}(\boldsymbol{y}^{\mathrm{a}})}\big(\mathscr{E}^{\mathrm{qc}}_{\mathrm{model}} + \mathscr{E}_{\mathrm{fem}} + \mathscr{E}_{\mathrm{ext}}\big), \tag{4.16}$$

where the QC consistency error $\mathscr{E}^{\rm qc}_{\rm model} = \mathscr{E}^{\rm qc}_{\rm model}(\boldsymbol{y}^{\rm a})$ *is defined in* (3.5)*,* (3.11)*, or* (3.12)*, the superconvergent finite element coarse-graining error* $\mathscr{E}_{\rm fem} = \mathscr{E}_{\rm fem}(\boldsymbol{y}^{\rm a})$ *is defined in* (4.8)*, and the approximation error for the external forces* $\mathscr{E}_{\rm ext} = \mathscr{E}_{\rm ext}(\boldsymbol{f})$ *is defined in* (4.13)*.*

Proof. From the mean value theorem we deduce that there exists $\theta \in {\rm conv}\{I_h\boldsymbol{y}^{\rm a}, \boldsymbol{y}^{\rm qc}\}$ such that

$$\mathcal{E}''_{\rm qc}(\theta)[I_h\boldsymbol{e}, I_h\boldsymbol{e}] = \mathcal{E}'_{\rm qc}(I_h\boldsymbol{y}^{\rm a})[I_h\boldsymbol{e}] - \mathcal{E}'_{\rm qc}(\boldsymbol{y}^{\rm qc})[I_h\boldsymbol{e}].$$

Using the first-order optimality conditions for $\boldsymbol{y}^{\rm a}$ and $\boldsymbol{y}^{\rm qc}$ we obtain

$$\begin{aligned}\mathcal{E}'_{\rm qc}(I_h\boldsymbol{y}^{\rm a})[I_h\boldsymbol{e}] - \mathcal{E}'_{\rm qc}(\boldsymbol{y}^{\rm qc})[I_h\boldsymbol{e}] = &\ \big\{\mathcal{E}'_{\rm qc}(I_h\boldsymbol{y}^{\rm a})[I_h\boldsymbol{e}] - \mathcal{E}'_{\rm qc}(\boldsymbol{y}^{\rm a})[I_h\boldsymbol{e}]\big\} \\ &+ \big\{\mathcal{E}'_{\rm qc}(\boldsymbol{y}^{\rm a})[I_h\boldsymbol{e}] - \mathcal{E}'_{\rm a}(\boldsymbol{y}^{\rm a})[I_h\boldsymbol{e}]\big\} \\ &+ \big\{\langle \boldsymbol{f}, I_h\boldsymbol{e}\rangle_\varepsilon - \langle \boldsymbol{f}, I_h\boldsymbol{e}\rangle_h\big\}.\end{aligned}$$

The first group is estimated in Lemma 4.2, the second group in Theorem 3.1 (QCL), Theorem 3.2 (QCE), or in Theorem 3.3 (QNL), and the last group in Lemma 4.5. Inserting these estimates we arrive at

$$\mathcal{E}''_{\rm qc}(\theta)[I_h\boldsymbol{e}, I_h\boldsymbol{e}] \le \big(\mathscr{E}^{\rm qc}_{\rm model} + \mathscr{E}_{\rm fem} + \mathscr{E}_{\rm ext}\big)\|I_h\boldsymbol{e}'\|_{\ell^2_\varepsilon}. \tag{4.17}$$

It remains to prove a lower bound on $\mathcal{E}''_{\rm qc}(\theta)[I_h\boldsymbol{e}, I_h\boldsymbol{e}]$. From our assumption that $\min_\ell(\boldsymbol{y}^{\rm a})'_\ell \ge r_*/2$, and from (4.14) it follows that

$$\min_\ell \theta'_\ell \ge r_*/2 - \tau.$$

Assuming that τ is sufficiently small, e.g., $\tau \le \tau_1 := \frac{1}{4}\min_\ell y'_\ell$, we can apply Lemma 4.4 to deduce that

$$\begin{aligned}\mathcal{E}''_{\rm qc}(\theta)[I_h\boldsymbol{e}, I_h\boldsymbol{e}] \ge &\ \mathcal{E}''_{\rm qc}(\boldsymbol{y}^{\rm a})[I_h\boldsymbol{e}, I_h\boldsymbol{e}] - C_{\rm Lip}\|(\theta - \boldsymbol{y}^{\rm a})'\|_{\ell^\infty_\varepsilon}\|I_h\boldsymbol{e}'\|^2_{\ell^2_\varepsilon} \\ \ge &\ \mathcal{E}''_{\rm qc}(\boldsymbol{y}^{\rm a})[I_h\boldsymbol{e}, I_h\boldsymbol{e}] - C_{\rm Lip}\tau\|I_h\boldsymbol{e}'\|^2_{\ell^2_\varepsilon}.\end{aligned} \tag{4.18}$$

where $C_{\rm Lip}$ may depend on τ_1.

We can now apply our stability analysis in Section 4.3. Since $(\boldsymbol{y}^{\rm a})'_\ell \ge r_*/2$ for all ℓ, Lemma 4.3 implies that

$$\mathcal{E}''_{\rm qc}(\boldsymbol{y}^{\rm a})[I_h\boldsymbol{e}, I_h\boldsymbol{e}] \ge A^{\rm qc}_*(\boldsymbol{y}^{\rm a})\|I_h\boldsymbol{e}'\|^2_{\ell^2_\varepsilon},$$

which, combined with (4.17) and (4.18), yields

$$\big(A^{\rm qc}_*(\boldsymbol{y}^{\rm a}) - C_{\rm Lip}\tau\big)\|I_h\boldsymbol{e}'\|^2_{\ell^2_\varepsilon} \le \mathcal{E}''_{\rm qc}(\theta)[I_h\boldsymbol{e}, I_h\boldsymbol{e}] \le \big(\mathscr{E}^{\rm qc}_{\rm model} + \mathscr{E}_{\rm fem} + \mathscr{E}_{\rm ext}\big)\|I_h\boldsymbol{e}'\|_{\ell^2_\varepsilon}.$$

Dividing through by $\|I_h\boldsymbol{e}'\|_{\ell^2_\varepsilon}$, and assuming that $\tau \le \min(\tau_1, \tau_2)$ where $\tau_2 = A^{\rm qc}_*(\boldsymbol{y}^a)/(2C_{\rm Lip})$, we deduce that

$$\tfrac{A^{\rm qc}_*(\boldsymbol{y}^{\rm a})}{2}\|I_h\boldsymbol{e}'\|_{\ell^2_\varepsilon} \le \mathscr{E}^{\rm qc}_{\rm model} + \mathscr{E}_{\rm fem} + \mathscr{E}_{\rm ext},$$

which concludes the proof of the superconvergence error estimate (4.16). The standard error estimate (4.15) follows from (4.16) and the interpolation error estimate given in Lemma 4.1. □

Remark 4.2. The assumption that τ be sufficiently small is fairly strong from an analytical point of view and deserves comments. A brief investigation of the proof of Theorem 4.1 shows that we have assumed $\tau \le \min(\tau_1, \tau_2)$, with constants $\tau_1 = \frac{1}{4}\min_\ell (y^{\rm a})'_\ell$ and $\tau_2 = A_*^{\rm qc}(\boldsymbol{y}^{\rm a})/(2C)$, where C is a local Lipschitz constant.

The first restriction, $\tau \le \tau_1$ is only used to obtain some control on $(\boldsymbol{y}^{\rm qc})'$ from below and could be easily replaced by appropriate a priori estimates on the solutions.

However, the second condition, $\tau \le \tau_2$, is fundamental. It requires, essentially, that $\boldsymbol{y}^{\rm a}, I_h\boldsymbol{y}^{\rm a}$, and $\boldsymbol{y}^{\rm qc}$ all belong to a single convex subregion of $\mathcal{Y}$ in which $\mathcal{E}_{\rm qc}$ is convex. At first glance, this assumption may appear too strong to be satisfied in all situations. Indeed, given any two atomistic and QC solutions it would be difficult to justify it, as $\mathcal{E}_{\rm qc}$ is a highly non-convex functional. However, we are only assuming for the existence of *some* QC solution in a suitable neighbourhood of $\boldsymbol{y}^{\rm a}$. With some additional technical effort, this can be made rigorous using a quantitative inverse function theorem; we refer to Refs. 23, 21, 14, 18 and 10 for examples of this technique applied in a similar context.

5. Numerical Experiments

We conclude the paper with a set of numerical experiments illustrating the results of our analysis. Throughout this section we fix $F = 1$, $N = 400$, and let ϕ be the Morse potential

$$\phi(r) = \exp(-2\alpha(r-1)) - 2\exp(-\alpha(r-1)),$$

with the parameter $\alpha = 5$. We will solve two problems with different body forces.

Although our analysis was carried out in terms of deformations $\boldsymbol{y}$, we will show the relative errors with respect to displacements $\boldsymbol{u} = \boldsymbol{y} - \boldsymbol{x}$. While the absolute errors are of course identical, we feel that the relative errors are best measured in terms of the displacement from the undeformed state $\boldsymbol{x}$. Moreover, we will show errors in the $\mathcal{U}^{1,2}$- as well as the $\mathcal{U}^{1,\infty}$-norm. While the former was the object of our analysis and is also closely related to errors in the energy, it does not always capture localised errors such as the interface oscillation caused by the ghost forces as well. Since we are primarily interested in the errors due to the coupling mechanisms, and in order to avoid cluttered graphs, we do not show numerical experiments for the QCL method; however, see Ref. 14 for an interesting example.

For each numerical experiment we present four figures: 1. the displacement gradients of the exact atomistic solution; 2. the relative errors for the QCE and QNL methods in the displacement gradients $|e'_\ell|/\|\boldsymbol{u}^{\rm a}\|_{\mathcal{U}^{1,\infty}}$ plotted against ℓ; 3. The relative errors for the QCE and QNL methods in the $\mathcal{U}^{1,2}$- and $\mathcal{U}^{1,\infty}$-norms, plotted against the size of the atomistic region; and 4. the same relative errors plotted against the mesh size.

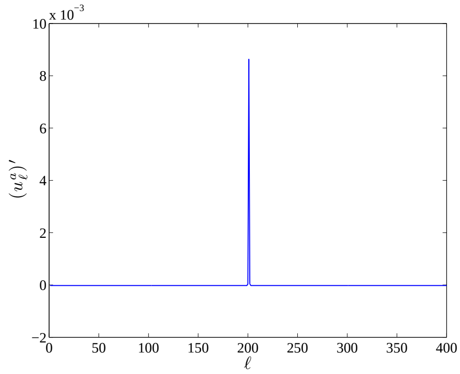


Fig. 1: Plot of $(\boldsymbol{u}^{\mathrm{a}})'$.

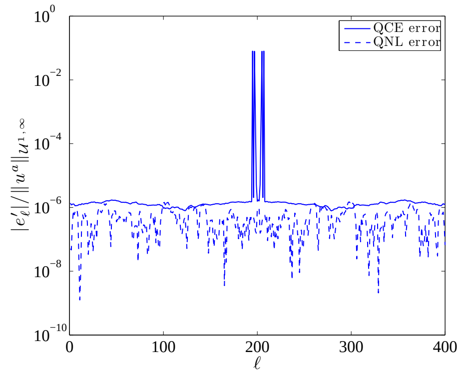


Fig. 2: Plot of $|e'_\ell|/\|\boldsymbol{u}^{\mathrm{a}}\|_{\mathcal{U}^{1,\infty}}$.

5.1. *Construction of $\mathcal{A}$ and $\mathcal{U}_{\mathrm{qc}}$*

We choose the atomistic region symmetrically about the lattice point 200.5, that is, $\ell_1 = 200 - m$ and $\ell_2 = 201 + m$, $m \geq 0$, such that $\#\mathcal{A} = 2m + 2$.

To coarse-grain the continuum region we fix $K \geq 1$ and choose repatoms to create an exponentially graded mesh as follows:

- atom $\ell_2 + 1$ and N are repatoms.
- atom $\ell_2 + 2^{k+1}$ is a repatom when $0 \leq k \leq K$.
- atom $\ell_2 + 2^{K+1} + n2^K$ is a repatom for all $n \geq 1$ such that $\ell_2 + 2^{K+1} + n2^K \leq N$.
- the repatoms in the left-hand half of the domain are chosen symmetrically.

In the figures where we plot errors against mesh size, we understand h to be the maximal mesh size, that is, $h = \varepsilon 2^K$.

5.2. *Numerical experiment I*

For our first numerical experiment, we define the body force $\boldsymbol{f}$ as

$$f_\ell = \begin{cases} -160, & \text{for } \ell = 200, \\ 160, & \text{for } \ell = 201, \\ 0, & \text{otherwise.} \end{cases}$$

This force pulls apart the atoms with indices $\ell = 200, 201$, creating a non-smooth disturbance in the displacement field. The effect on the displacement field is similar, to some extent, to a a very localised defect in a 2D/3D lattice such as a vacancy. We see from Figure 1 that the displacement gradient is large near $\ell = 200, 201$ but decays rapidly to its preferred state.

In Figure 2 we plot the relative errors in the QCE and QNL displacement gradients as functions of ℓ. The size of the atomistic region is fixed to $\#\mathcal{A} = 10$. As

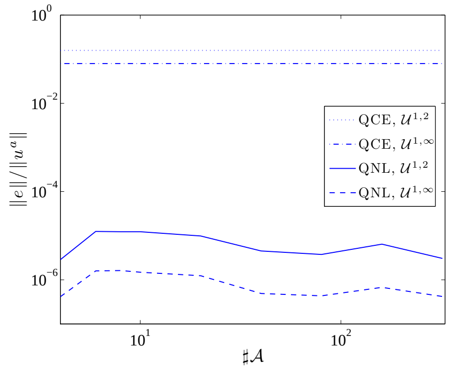


Fig. 3: Plot of $\|\boldsymbol{e}\|_{\mathcal{U}^{1,2}}/\|\boldsymbol{u}^{\rm a}\|_{\mathcal{U}^{1,2}}$ and $\|\boldsymbol{e}\|_{\mathcal{U}^{1,\infty}}/\|\boldsymbol{u}^{\rm a}\|_{\mathcal{U}^{1,\infty}}$ for QCE and QNL, against $\#\mathcal{A}$.

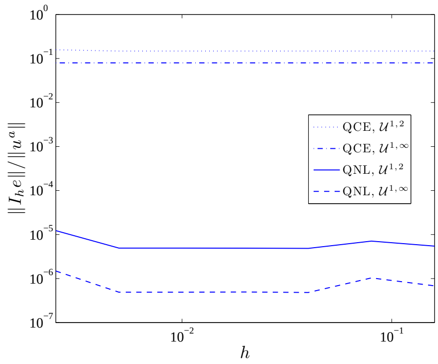


Fig. 4: Plot of $\|I_h\boldsymbol{e}\|_{\mathcal{U}^{1,2}}/\|\boldsymbol{u}^{\rm a}\|_{\mathcal{U}^{1,2}}$ and $\|I_h\boldsymbol{e}\|_{\mathcal{U}^{1,\infty}}/\|\boldsymbol{u}^{\rm a}\|_{\mathcal{U}^{1,\infty}}$ for QCE and QNL, against h.

previously observed and predicted theoretically, we see a large error of the QCE method in the interface, which is due to the presence of ghost forces. In our analysis these oscillations are captured by the zeroth order term $2\varepsilon^{1/p}M_1(\mathcal{S}_1)$ in (3.11). The error plot for the QNL method shows that it has in fact reached the precision of our nonlinear solver; indeed, from Figure 1 we see that the absolute error in the QNL displacement gradient is of the order $O(10^{-9})$.

In Figures 3 and 4 we plot the relative errors of the QCE and the QNL methods as we increase the size of the atomistic region, and as we increase the mesh size in the continuum region. We note that in both graphs, and for both methods, the relative errors remain essentially constant. This is explained by the rapid decay of $(u^{\rm a})'_\ell$ towards a homogeneous state, which implies that $\boldsymbol{u}^{\rm a}$ is essentially constant in continuum region. Thus, the location of the interface or the size of the mesh have only a marginal effect on the accuracy of either method. In the case of the QCE method, the ghost forces dominate all effects, while, in the case of the QNL method we obtain the accuracy of the nonlinear solver.

5.3. *Numerical experiment II*

In the second problem, we assume

$$f_\ell = \begin{cases} -2\frac{\ell-1}{200}, \text{ for } \ell \le 200, \\ 2(1-\frac{\ell-200}{200}), \text{ for } \ell \ge 201. \end{cases}$$

For many real defects in 2D/3D materials, the decay of the displacement due to the presence of the defect is fairly slow, and this body force was chosen to mimic that situation. Indeed, we see from Figure 5 that the displacement gradient of the exact solution is nowhere (locally) uniform, and that the second difference of the

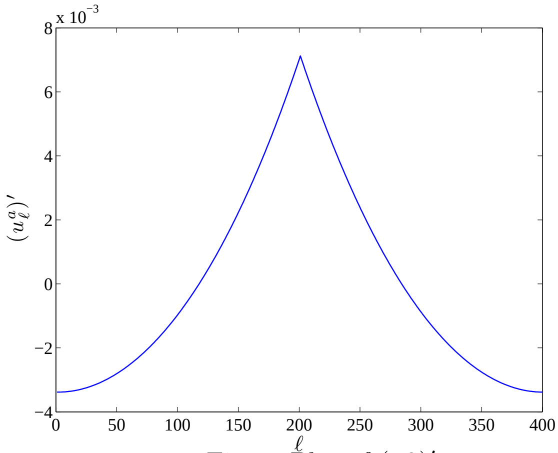
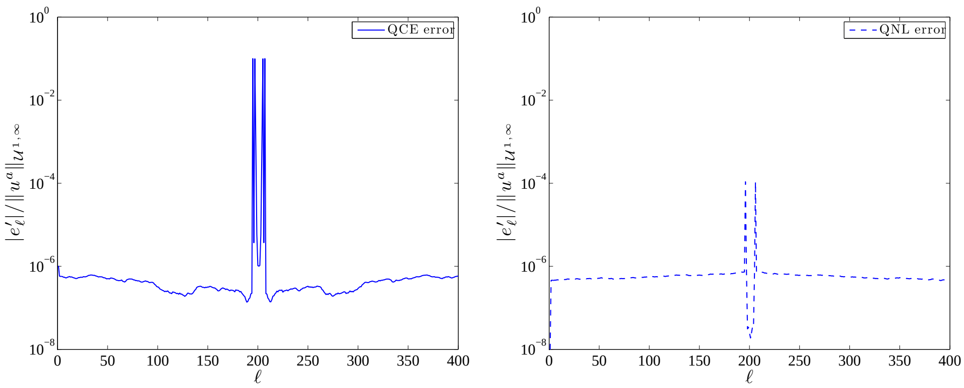


Fig. 5: Plot of $(\boldsymbol{u}^{\mathrm{a}})'$.



(a) QCE

(b) QNL

Fig. 6: Plots of $|e'_\ell|/\|(\boldsymbol{u}^{\mathrm{a}})'\|_{\mathcal{U}^{1,\infty}}$ for QCE and QNL.

atomistic solution decays only slowly away from the centre of the domain.

Figure 6(a) and 6(b) show the relative errors of the QCE and QNL solutions when the size of the atomistic region is fixed to $\#\mathcal{A} = 10$. We now observe a relatively large error in the QNL solution in the interface region, which is still several orders of magnitude smaller than the error in the QCE solution caused by the presence of ghost forces. This error in the QNL solution was predicted in our analysis in (3.12) by the term $\varepsilon M_2(\mathcal{S}_2)\|\boldsymbol{y}''\|_{\ell^p_\varepsilon(\mathcal{I}_{\mathrm{qnl}})}$. This effect will not occur when $\boldsymbol{y}$ is locally homogeneous, as in our first experiment.

Figure 7 shows the relative errors of the QCE and the QNL methods in the $\mathcal{U}^{1,2}$- and $\mathcal{U}^{1,\infty}$-norms as the number of atoms in the atomistic region increases.

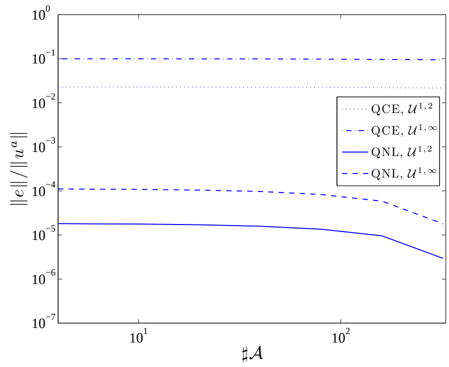


Fig. 7: Plot of $\|\boldsymbol{e}\|_{\mathcal{U}^{1,2}}/\|\boldsymbol{u}^{\mathrm{a}}\|_{\mathcal{U}^{1,2}}$ and $\|\boldsymbol{e}\|_{\mathcal{U}^{1,\infty}}/\|\boldsymbol{u}^{\mathrm{a}}\|_{\mathcal{U}^{1,\infty}}$ for QCE and QNL, against $\#\mathcal{A}$.

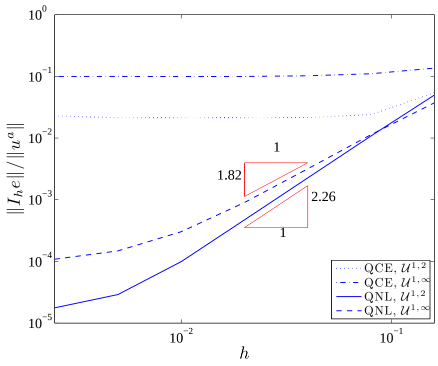


Fig. 8: Plot of $\|I_h\boldsymbol{e}\|_{\mathcal{U}^{1,2}}/\|\boldsymbol{u}^{\mathrm{a}}\|_{\mathcal{U}^{1,2}}$ and $\|I_h\boldsymbol{e}\|_{\mathcal{U}^{1,\infty}}/\|\boldsymbol{u}^{\mathrm{a}}\|_{\mathcal{U}^{1,\infty}}$ for QCE and QNL, against h.

We observe that the relative errors of the QCE method remain in a lower order in both norms while those of the QNL method decreases somewhat for very large atomistic regions when the curvature of $\boldsymbol{y}^{\mathrm{a}}$ at the interface approaches zero. This demonstrates a fundamental difference between the QCE and QNL methods: the leading term of the QCE error bound has no dependance on the smoothness of the atomistic solution and cannot be controlled by adjusting the atomistic regin or the mesh size, whereas that of the QNL error bound does have such a dependence and can therefore be controlled to some extent.

Figure 8 displays the relative errors of the QCE solution and the QNL solution with respect to the displacement gradient in the $\mathcal{U}^{1,2}$- and $\mathcal{U}^{1,\infty}$-norms against the finite element mesh size h. As the result of the non-uniform deformation gradient of the solution, the effect of the mesh size is noticable for both methods. As the mesh size decreases, the error initially decays until it reaches a limit dictated by the modelling error. In the case of the QCE method, this happens very early due to the presence of the ghost forces. In the case of the QNL method, we obtain a satisfactory relative accuracy of the order 10^{-4} to 10^{-5}.

We note that the slopes of the error curves are not precisely 2 as predicted by our analysis. This can be explained by the fact that neither our mesh, nor the second difference $(\boldsymbol{y}^{\mathrm{a}})''$ are uniform.

Conclusion

We have presented a priori error estimates for three different energy-based quasi-continuum methods in one dimension. Using the techniques developed in Ref. 21, we gave optimal order consistency error estimates in the negative Soblev norms and showed the dependence of this error with respect to the smoothness of the solution to the original atomistic model. We also included coarse-graining in the error analysis, giving also a superconvergence result as a consequence of the one dimensional feature of our model problem. The stability results we obtained in this paper are extensions of those given by Dobson et al.[6] to the nonlinear setting. Combining these results we derived quasi-optimal total error estimates. Several features of our analysis were further illuminated in the numerical experiments shown in Section 5.

We conclude by pointing out an interesting issue arising for higher order and *hp*-finite element spaces. It would not be too difficult to extend our analysis to this setting. Note, however, that the Cauchy–Born modelling error is only of second order, while the coupling error is only of first order, which puts a severe lower bound on the accuracy that can be achieved. Thus, if one wants to take full advantage of the high accuracy of higher order finite element spaces, one would also need to construct higher order continuum models such as those of Arndt and Griebel[1] and in particular higher order coupling mechanisms.

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