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A-Priori Analysis of the Quasicontinuum Method in One Dimension

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The quasicontinuum method is a coarse-graining technique for reducing the complexity of atomistic simulations in a static and quasistatic setting. In this paper we give an a-priori error analysis for the quasicontinuum method in one dimension. We consider atomistic models with Lennard–Jones type long range interactions and a practical QC formulation.

First, we prove the existence, the local uniqueness and the stability with respect to a discrete $\mathrm{W}^{1,\infty}$–norm of elastic and fractured atomistic solutions. We then use a fixed point technique to prove the existence of a quasicontinuum approximation which satisfies an optimal a-priori error bound.

Key words and phrases: atomistic material models, quasicontinuum method, error analysis, stability

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1 Introduction

For the numerical simulation of microscopic material behaviour like crack-tip studies, nano-indentation, dislocation motion, etc., atomistic models are often employed. However, even on the lattice scale, they are prohibitively expensive and, in fact, inefficient. Even in the presence of defects, the bulk of the material will deform elastically and smoothly. It is therefore advantageous to couple the atomistic simulation of a defect with a continuum or continuum-like model away from it. One of the simplest and most popular examples is the Quasicontinuum (QC) method originally developed by Ortiz, Phillips and Tadmor in [11] and subsequently improved by many other authors; see [9] for a recent survey article. The basic idea of the QC method is to triangulate an atomistic body as in a finite element method and to allow only piecewise affine deformations in the computation, thus considerably reducing the number of degrees of freedom. By taking every atom near a defect to be a node of the triangulation, one obtains a continuum description of the elastic deformation while retaining a full atomstic description of the defect. We give a detailed description of a version of the QC method analyzed in this paper in §2.2.

Despite its growing popularity in the engineering community, the mathematical and numerical analysis of the QC method is still in its infancy. The first noteworthy effort was by Lin [7] who considers the QC approximation of the reference state of a one-dimensional Lennard–Jones model. E and Ming [5, 4] analyze the QC method in the context of the heterogeneous multi-scale method [3], which requires the assumption that a nearby smooth, elastic continuum solution is available. In [8], Lin analyzes the QC method for purely elastic deformation in two dimensions without using such an assumption, but making instead a strong hypothesis (Assumptions 1. and 2. in [8]) on the exact solution of the atomistic model as well as on its QC approximation. Essentially, it is assumed that both the exact and the QC solution lie in a region where the atomistic energy is convex. For lattice domains resembling smooth or convex sets this assumption seems intuitively reasonable but would be difficult to verify rigorously. For lattice domains with sharp reentrant boundary sections or defects we should not expect it to hold. Finally, we would like to mention the work of Legoll et al. [1] where a multi-scale method similar to the QC method is analyzed, however only nearest-neighbour interactions in one dimension are considered which makes it possible to compute the the exact solutions analytically. Except for the work [1], which we believe is in the unrealistic setting of global energy minimization (cf. also [15] and the comments in §2.1), none of the previous attempts were able to consider defects in their analysis of the QC method.

The present work is the first part of an effort to provide a fairly complete approximation theory for the QC method in one dimension. We demonstrate how to derive optimal a-priori error estimates for stable solutions, i.e., solutions which are strict local minimizers of the atomistic energy. While the one-dimensional setting allows us to give complete results with a relatively small effort, we believe that our technique should in principle extend to higher dimensions. The necessary coercivity estimates would, however, be much harder to obtain. It would even be far from straightforward to identify a suitable topology in which to analyze the error. Only for purely elastic deformation of perfect lattices is it clear how to do so (cf. [8]. In order to keep the presentation simple, we also consider only long-range pair-interaction energies with interaction potentials of Lennard–Jones type, but we believe that this is not a true restriction. A detailed description of our model problem is given in §2.1.

While, to some extent, our computations to obtain the coercivity are contained in [7] the novelty of our approach is to look at coercivity and stability with respect to the $\mathrm{w}_\varepsilon^{1,\infty}$–norm, a discrete version of the $\mathrm{W}^{1,\infty}$ Sobolev norm which we define in §1.1. This makes it possible to give precise conditions under which local monotonicity assumptions, such as Assumptions 1. and 2. in [8], are justified. Furthermore, to the best of our knowledge, the case of defects has not so far been analyzed for a realistic QC model with long-range interactions.

Probably the most remarkable feature of atomistic models is the multitude of solutions. Already in one dimension, it is fairly straightforward to see for many problems that the number of solutions is at least as large as the number of atoms in the body. Therefore, error estimates must necessarily be restricted to local results. Due to the possibility of fracture, stability of solutions can only ever be obtained with respect to a discrete version of the $\mathrm{W}^{1,\infty}$ norm (cf. §1.1). Hence our entire analysis will be based on such a topology. The basic idea is to show that if the mesh is able to resolve the exact solution (this can be measured in terms of the interpolation error) then there exists a nearby QC solution for which an error estimate holds.

Ultimately, however, we believe that our results are only realistic in the elastic case, in the sense that we can actually expect to find the QC solution which satisfies the error estimate that we derive. For example, when an exact solution we wish to approximate is a fractured state then we can prove under certain conditions that there exists a nearby QC solution, however, we should not expect to find it numerically. If only one atom lies on the wrong side of the crack then the error in the discrete $\mathrm{W}^{1,\infty}$–norm cannot converge to zero.

The option to analyze the error in a weaker norm is, at least with our technique, unavailable due to the lack of monotonicity and stability. Therefore, in the second part of this work [13], which deals with the a-posteriori error analysis of the QC method in one dimension, we reverse the role of the exact and the QC solution. We derive bounds on the residual of the QC solution and show that, if the QC solution is stable and its residual sufficiently small, there exists an exact solution of the atomistic model for which we give an a-posteriori error bound.

1.1 Discrete function spaces

It will be notationally convenient to define discrete versions of the usual Sobolev norms. First, for $u = (u_i)_{i=0}^N \in \mathbb{R}^{N+1}$, we introduce the discrete derivatives

$$u_i' = \frac{u_i - u_{i-1}}{\varepsilon}, \quad i = 1, \dots, N \quad \text{and} \quad u_i'' = \frac{u_{i+1} - 2u_i + u_{i-1}}{\varepsilon^2}, \quad i = 1, \dots, N-1,$$

where ε is a lattice parameter that can be adjusted to the problem at hand and should roughly be the distance between two neighbouring atoms in an undeformed state. For

$1 \le p < \infty$, $u \in \mathbb{R}^{N+1}$, $0 \le i_1 \le i_2 \le N$, we define the (semi-)norms

$$\begin{aligned} \|u\|_{\ell^p_\varepsilon(\!(i_1,i_2)\!)} &= \left(\sum_{i=i_1}^{i_2} \varepsilon |u_i|^p\right)^{1/p}, \\ |u|_{\mathrm{w}^{1,p}_\varepsilon(\!(i_1,i_2)\!)} &= \left(\sum_{i=i_1+1}^{i_2} \varepsilon |u_i'|^p\right)^{1/p}, \quad \text{and} \\ |u|_{\mathrm{w}^{2,p}_\varepsilon(\!(i_1,i_2)\!)} &= \left(\sum_{i=i_1+1}^{i_2-1} \varepsilon |u_i''|^p\right)^{1/p}. \end{aligned}$$

For $p = \infty$, we define the corresponding versions,

$$\begin{aligned} \|u\|_{\ell^\infty_\varepsilon(\!(i_1,i_2)\!)} &= \max_{i=i_1,\dots,i_2} |u_i|, \\ |u|_{\mathrm{w}^{1,\infty}_\varepsilon(\!(i_1,i_2)\!)} &= \max_{i=i_1+1,\dots,i_2} |u_i'|, \quad \text{and} \\ |u|_{\mathrm{w}^{2,\infty}_\varepsilon(\!(i_1,i_2)\!)} &= \max_{i=i_1+1,\dots,i_2-1} |u_i''|. \end{aligned}$$

Sums or maxima taken over empty sets are understood to be zero. If the label $(\!(i_1, i_2)\!)$ is omitted we mean $i_1 = 0, i_2 = N$. For reasons that will become apparent below, we will only require the $p = 1$ and $p = \infty$ versions of these (semi-)norms in our analysis. $B(y, R)$ is understood to be the closed ball, centre y, radius R, with respect to the $\mathrm{w}^{1,\infty}_\varepsilon$–semi-norm.

For $u, v \in \mathbb{R}^{N+1}$, we define the bilinear form

$$\langle u, v\rangle_\varepsilon = \sum_{i=0}^{N} \varepsilon u_i v_i.$$

Finally, we fix the notation for derivatives of functionals. Let $\phi\colon \mathbb{R}^{N+1} \to \mathbb{R}$ be differentiable at a point $u \in \mathbb{R}^{N+1}$. We understand the derivative of ϕ in u as a linear functional $\phi'(u) = \phi'(u; \cdot)\colon \mathbb{R}^{N+1} \to \mathbb{R}$ defined by

$$\phi(u + v) = \phi(u) + \phi'(u; v) + o(|v|), \quad \text{as } v \to 0,$$

where $|v|$ denotes the Euclidean norm of v. Similarly, if ϕ is twice differentiable at $u \in \mathbb{R}^{N+1}$, the second derivative of ϕ at u is a symmetric bilinear form $\phi''(u) = \phi''(u; \cdot, \cdot)\colon \mathbb{R}^{N+1} \times \mathbb{R}^{N+1} \to \mathbb{R}$ defined by

$$\phi(u + v) = \phi(u) + \phi'(u; v) + \phi''(u; v, v) + o(|v|^2), \quad \text{as } v \to 0.$$

When ϕ' is interpreted as a linear functional we may also write $\phi'(u; v) = \phi'(u)v$. Similarly, we shall write $\phi''(u)v$ for the linear functional defined by $\phi''(u; v, \cdot)$.

Interaction Potential

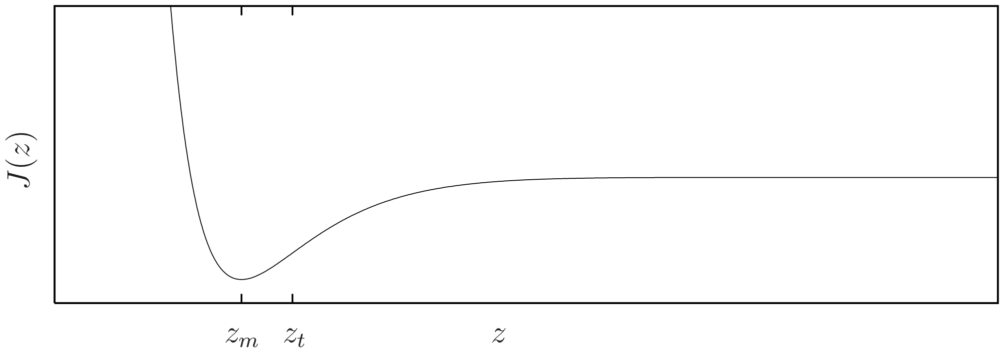

Figure 1: The shape of the atomistic interaction potentials.

2 Model Problem and QC Approximation

2.1 The atomistic model problem

Fix $N \in \mathbb{N}$. Each vector $y = (y_i)_{i=0,\dots,N} \in \mathbb{R}^{N+1}$ represents a state of an atomistic body, consisting of $N+1$ atoms. To each such *deformation* we associate an energy

$$E(y) = \sum_{i=1}^{N} \sum_{j=0}^{i-1} J(y_i - y_j).$$

Upon defining the *lattice parameter* $\varepsilon = 1/N$, and writing y_i instead of εy_i we can rescale the energy to

$$E(y) = \sum_{i=1}^{N} \sum_{j=0}^{i-1} \varepsilon J\big(\varepsilon^{-1}(y_i - y_j)\big), \tag{2.1}$$

without changing the problem. We believe that such a scaling highlights the practically relevant case where ε is small in comparison to the length-scale of the problem.

Typical examples of atomistic interaction potentials are the Lennard–Jones potential [6],

$$J(z) = z^{-12} - z^{-6}, \tag{2.2}$$

and the Morse potential [10],

$$J(z) = \exp\big(-2\alpha(z-1)\big) - 2\exp\big(-\alpha(z-1)\big); \tag{2.3}$$

see also Figure 2.1. More generally, we assume that there exist $z_0 \in [-\infty, +\infty)$, $z_m, z_t \in \mathbb{R}$ such that $z_0 < z_t/2 < z_m < z_t$, and

$$\begin{aligned}
&J \in \mathrm{C}^3(z_0, \infty), \quad J'(z_m) = 0, \quad J''(z_t) = 0, \\
&J(z) \to +\infty \text{ as } z \to z_0+, \quad J(z) = +\infty \quad \forall z \le z_0, \\
&J''(z) \ge 0 \quad \forall z \in (0, z_t] \quad \text{and} \quad J''(z) \le 0 \quad \forall z \in [z_t, \infty).
\end{aligned} \tag{2.4}$$

The condition $z_t/2 < z_m$ considerably simplifies the analysis and is not a true restriction; for example, any realistic potential describing a metal would satisfy it. Having said this, a simple atomistic model such as (2.1) is not normally used for the simulation of metals, which is the main application of the QC method. However, potentials of the type (2.2) or (2.3) usually form the basis of more sophisticated atomistic models such as the embedded atom method [2] or multi-body interaction models. Thus, we believe that for a theoretical study in one dimension, which is severely restricted in its physical applicability anyhow, we can justify the use of simpler atomistic models, for the sake of a simpler presentation.

Before we define what we mean by an atomistic solution, we need to mention that atomistic deformations are typically only meta-stable states rather than global minimizers (cf. for example [15, 12]). This can be best seen by considering an atomistic body which is clamped at the left-hand end with a small deformation applied to the right-hand end. In that case, the physically observed Cauchy–Born state, the (approximately) affine deformation, is not the energy minimum. Note, however, that the *elastic* state is the correct solution only if we have *started* from an unfractured reference state.

We consider only a Dirichlet problem, i.e., where the atomistic deformation is fixed at the endpoints. It would also be possible, and in fact easier, to consider a problem with a Dirichlet condition at one end and a Neumann condition at the other end of the interval. We define the set of admissable deformations as

$$\mathscr{A} = \{y \in \mathbb{R}^{N+1} : y_0 = 0, y_N = y_N^D\} \quad \text{and} \quad \mathscr{A}_0 = \{y \in \mathbb{R}^{N+1} : y_0 = y_N = 0\}. \tag{2.5}$$

Each $f \in \mathbb{R}^{N+1}$ represents a linear body force. The atomistic problem is to *find critical points of the functional* $E(y) - \langle f, y\rangle_\varepsilon$ *in* $\mathscr{A}$. From the assumptions we have made on the interaction potential it follows that E is differentiable at every point which has finite energy. Thus a critical point y of $E(y) - \langle f, y\rangle$ in $\mathscr{A}$ with finite energy must satisfy

$$E'(y; v) = \langle f, v\rangle_\varepsilon \qquad \forall v \in \mathscr{A}_0. \tag{2.6}$$

If y satisfies (2.6), we say that $E'(y) = f$ in $\mathscr{A}$.

Elastic deformations are those whose gradient is sufficiently close to z_m, in a region where the energy E is convex. Such solutions exist whenever f is *sufficiently small.* More precisely, for each $f \in \mathbb{R}^{N+1}$, we define the dual norm

$$\|f\|_* = \max_{\substack{v \in \mathscr{A}_0 \\ |v|_{\mathrm{W}_\varepsilon^{1,1}} = 1}} \langle f, v\rangle_\varepsilon.$$

We use this norm in the following sections to measure the distance of applied body forces. Since we can interpret f as a linear functional, we can extend the definition of the dual norm to linear maps $\ell \colon A_0 \to \mathbb{R}$ by

$$\|\ell\|_* = \max_{\substack{v \in \mathscr{A}_0 \\ |v|_{\mathrm{W}_\varepsilon^{1,1}} = 1}} |\ell(v)|.$$

For future reference, we define the quantities

$$\rho_1(z) = \sum_{r=2}^{\infty} r|J'(rz)|, \quad \text{and} \tag{2.7}$$

$$\rho_2(z_1, z_2) = \sum_{r=1}^{\infty} r^2 \min_{z_1 \le z \le z_2} J''(rz_m), \tag{2.8}$$

which are important in the analysis of existence and stability of elastic deformations. The quantity $\rho_1(z)$ is an estimate for the residual of the affine deformation $y_i = zi/N$ which we use to derive the existence of a reference state. We shall assume throughout that ρ_1 is continuous in a neighbourhood of z_m which, for the Lennard–Jones and the Morse potentials, follows from elementary calculus. The number $\rho_2(z_1, z_2)$ is used to estimate the infsup constant of E'' in the set $\{z_1 \le y_i' \le z_2\}$. For the analysis of the QC approximation, we will also use

$$\rho_3(z_1, z_2) = \sum_{r=1}^{\infty} r^2 \max_{z_1 \le z \le z_2} |J''(rz)|, \tag{2.9}$$

which is a Lipschitz constant of E' in the set $\{z_1 \le y_i' \le z_2\}$.

2.2 Quasicontinuum approximation

A QC mesh $\mathcal{T}$ is defined by choosing indices $0 = t_0 < t_1 < \dots < t_K = N$ and setting $\mathcal{T} = \{t_0, \dots, t_K\}$. For each $k = 1, \dots, K$, we set $h_k = \varepsilon(t_k - t_{k-1})$, the physical length of the kth element. The set of piecewise affine deformations is given by

$$S^1(\mathcal{T}) = \Big\{ V \in \mathbb{R}^{N+1} : V_i = \frac{t_k - i}{t_k - t_{k-1}} V_{t_{k-1}} + \frac{i - t_{k-1}}{t_k - t_{k-1}} V_{t_k}, \text{ if } t_{k-1} \le i \le t_k \Big\}.$$

We define the set of admissable QC deformations and QC test functions respectively as

$$\mathscr{A}(\mathcal{T}) = \mathscr{A} \cap S^1(\mathcal{T}) \quad \text{and} \quad \mathscr{A}_0(\mathcal{T}) = \mathscr{A}_0 \cap S^1(\mathcal{T}).$$

For convenience, we sometimes use the notation $\overline{V}_k = V_{t_k}$ and $\overline{V}'_k = V'_{t_k}$ for the nodal values of an $S^1(\mathcal{T})$ function. For our analysis it is also necessary to define the interpolant $\Pi \colon \mathbb{R}^{N+1} \to S^1(\mathcal{T})$ by $\Pi u = (\Pi u_i)_{i=0}^N$ and

$$\Pi u_{t_k} = u_{t_k}, \qquad k = 0, \dots, K.$$

Note that if $y \in \mathscr{A}$ then $\Pi y \in \mathscr{A}(\mathcal{T})$.

A straightforward Galerkin approximation to (2.6) would be to *find critical points of* $E(Y) - \langle Y, f \rangle$ *in* $\mathscr{A}(\mathcal{T})$. Any such critical point $Y \in \mathscr{A}$ must satisfy

$$E'(Y; V) = \langle f, V \rangle_\varepsilon \qquad \forall V \in \mathscr{A}_0(\mathcal{T}). \tag{2.10}$$

However, in view of the long-range atomistic interaction, which, for the purpose of evaluating the energy and its derivatives still necessitates the computation of very large sums, it is helpful to make some further approximations to the energy functional. First, it is common to replace J by a cut-off potential $\tilde{J}$, which vanishes outside a certain cut-off radius ρ_c. If the deformation gradient is bounded away from zero, then the number of atoms over which one needs to sum is bounded by a small integer. This purely one-dimensional effect means that it is unnecessary to make any further (summation-rule type) approximations to the atomistic energy; thus we define,

$$\tilde{E}(Y) = \sum_{i=1}^{N} \sum_{j=0}^{N-1} \varepsilon \tilde{J}\big(\varepsilon^{-1}(Y_i - Y_j)\big).$$

For the analysis of the coercivity of the QC approximation we will need the quantity

$$\tilde{\rho}_2(z_1, z_2) = \sum_{r=1}^{\infty} r^2 \min_{z_1 \le z \le z_2} \tilde{J}''(rz).$$

To approximate the body force potential, we can use a so-called summation rule, i.e., a discrete version of a quadrature rule. In order to recover the full atomistic problem in the limit, it is reasonable to employ a trapezium rule. Thus, we define the discrete bilinear form

$$\langle f, v \rangle_{\mathcal{T}} = \sum_{i=0}^{N} \varepsilon \Pi(fv)_i.$$

The full QC approximation to (2.6) is then to *find* $Y \in \mathscr{A}(\mathcal{T})$ *satisfying*

$$\tilde{E}'(Y; V) = \langle f, V \rangle_{\mathcal{T}} \qquad \forall V \in \mathscr{A}_0. \tag{2.11}$$

3 Elastic Deformation

In the first part of this paper, we consider elastic deformation only. Recalling the notation of §1.1, we shall prove the following two theorems.

Theorem 1 *Let J satisfy the assumptions of §2.1 and, in addition, assume that there exists an $R \in (0, \min(z_m - z_t/2, z_t - z_m))$ such that $\rho_1(z_m) < R\rho_2(z_m - R, z_m + R)$. Then the following hold:*

(a) *Coercivity: There exist $z_1, z_2 \in \mathbb{R}$, independent of ε, such that $z_1 < z_m < z_2 < z_t$ and*

$$\inf_{y \in \mathscr{Z}_e} \inf_{\substack{u \in \mathscr{A}_0 \\ |u|_{\mathrm{w}_\varepsilon^{1,\infty}} = 1}} \sup_{\substack{v \in \mathscr{A}_0 \\ |v|_{\mathrm{w}_\varepsilon^{1,1}} = 1}} E''(y; u, v) \ge \tfrac{1}{2}\rho_2(z_1, z_2) =: c_0 > 0, \tag{3.1}$$

where $\mathscr{Z}_e = \{y \in \mathbb{R}^{N+1} : z_1 \le y_i' \le z_2, \text{ for } i = 1, \dots, N\}.$

(b) *Existence: There exist $\delta_1, \delta_2 > 0$, independent of ε such that for every $y_N^D \in \mathbb{R}$ with $|y_N^D - z_m| < \delta_1$ and for every $f \in \mathbb{R}^{N+1}$ with $\|f\|_* \le \delta_2$, there exists a solution y_f of (2.6) in $\mathscr{Z}_e$.*

(c) *Stability: Let y_f, y_g be solutions to* (2.6) *in $\mathscr{Z}_e \cap \mathscr{A}$, corresponding respectively to the right-hand sides $f, g \in \mathbb{R}^{N+1}$; then*

$$|y_f - y_g|_{\mathrm{w}_\varepsilon^{1,\infty}} \le c_0^{-1} \|f - g\|_*.$$

Theorem 1 is of theoretical relevance in that it gives a relatively sharp condition under which elastic solutions to (2.6) exist and are stable. It furthermore directly relates the shape of the interaction potential to the coercivity of the energy. In practise, we would numerically determine a region where E'' is coercive and then prove that it contains a reference state, using the condition $\rho_1(z_m) < \min(z_m - z_1, z_2 - z_m)\rho_2(z_1, z_2)$. We demonstrate this in §B.

For the formulation and proof of the a-priori error bound, there are several options. One could simply formulate a QC version of the existence theorem and prove that the elastic QC solution satisfies an error estimate. However, we find it more illuminating to make fewer assumptions on the structure of the problem, and impose stronger assumptions on a particular solution instead. It should be noted, however, that the conditions for a *QC existence theorem for elastic solutions* would be quite similar to the ones we give below.

For any given $f \in \mathbb{R}^{N+1}$ and a solution $y \in \mathscr{A}$ of (2.6), we will identify three error sources: the interpolation error,

$$\mathcal{E}_1 = |y - \Pi y|_{\mathrm{w}_\varepsilon^{1,\infty}}, \tag{3.2}$$

the perturbation of the linear form,

$$\mathcal{E}_2 = \max_{\substack{V \in \mathscr{A}_0(\mathcal{T}) \\ |V|_{\mathrm{w}_\varepsilon^{1,1}} = 1}} \big|\langle f, V\rangle_{\mathcal{T}} - \langle f, V\rangle_\varepsilon\big|, \tag{3.3}$$

and the perturbation of the energy,

$$\mathcal{E}_3 = \max_{Y \in \mathscr{A}(\mathcal{T}) \cap \mathscr{Z}_e} \max_{\substack{V \in \mathscr{A}_0(\mathcal{T}) \\ |V|_{\mathrm{w}_\varepsilon^{1,1}} = 1}} \big|E'(Y; V) - \tilde{E}'(Y; V)\big|. \tag{3.4}$$

Theorem 2

(a) *Let $\mathscr{Z}_e$ be defined as in Theorem 1; then,*

$$\min_{Y \in S^1(\mathcal{T}) \cap \mathscr{Z}_e} \min_{\substack{U \in \mathscr{A}_0(\mathcal{T}) \\ |U|_{\mathrm{w}_\varepsilon^{1,\infty}} = 1}} \max_{\substack{V \in \mathscr{A}_0(\mathcal{T}) \\ |V|_{\mathrm{w}_\varepsilon^{1,1}} = 1}} E''(Y; U, V) \ \ge\ \rho_2(z_1, z_2) = c_0, \text{ and} \tag{3.5}$$

$$\max_{Y \in S^1(\mathcal{T}) \cap \mathscr{Z}_e} \max_{\substack{U \in \mathscr{A}_0(\mathcal{T}) \\ |U|_{\mathrm{w}_\varepsilon^{1,\infty}} = 1}} \max_{\substack{V \in \mathscr{A}_0(\mathcal{T}) \\ |V|_{\mathrm{w}_\varepsilon^{1,1}} = 1}} E''(Y; U, V) \ \le\ \rho_3(z_1, z_2) =: c_1. \tag{3.6}$$

(b) *Let* $y \in \mathscr{Z}_e \cap \mathscr{A}$ *be a solution of* (2.6) *and define* $R = \min_{i=1,\dots,N} \min(z_2 - y_i', y_i' - z_1)$. *Assume, furthermore, that the QC mesh* $\mathcal{T}$ *is sufficiently fine so that*

$$c_1 \mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3 \le c_0 R. \tag{3.7}$$

Then, there exists a solution $Y \in \mathscr{A}(\mathcal{T}) \cap \mathscr{Z}_e$ *of* (2.11) *which satisfies*

$$|y - Y|_{\mathrm{w}_\varepsilon^{1,\infty}} \le c_0^{-1}\Big((c_0 + c_1)\mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3\Big).$$

If $\tilde{\rho}_2(z_1, z_2) > 0$, *then the QC solution is unique in* $\mathscr{A}(\mathcal{T}) \cap \mathscr{Z}_e$.

(c) *The error quantities* $\mathcal{E}_1, \mathcal{E}_2$, *and* $\mathcal{E}_3$ *can be bounded as follows:*

$$\begin{aligned}
\mathcal{E}_1 &\le \max_{k=1,\dots,K} h_k |y|_{\mathrm{w}_\varepsilon^{2,\infty}(\!(t_{k-1},t_k)\!)}, &(3.8)\\
\mathcal{E}_2 &\le \max_{k=1,\dots,K} 2h_k^2 \big(|f|_{\mathrm{w}_\varepsilon^{2,\infty}(\!(t_{k-1},t_k)\!)} + |f|_{\mathrm{w}_\varepsilon^{1,\infty}(\!(t_{k-1}+1,t_k)\!)} &(3.9)\\
&\qquad\qquad + |f|_{\mathrm{w}_\varepsilon^{1,\infty}(\!(t_{k-1},t_k-1)\!)}\big), \text{ and}\\
\mathcal{E}_3 &\le \sum_{r=1}^{\infty} r \max_{z_1 \le z \le z_2} \big|\tilde{J}'(rz) - J'(rz)\big|. &(3.10)
\end{aligned}$$

3.1 Coercivity of the atomistic problem

For this fairly straightforward but tedious analysis it is convenient to rewrite the energy and its derivatives in the following form. First, we rewrite E as

$$E(y) = \sum_{i=1}^{N} \sum_{j=1}^{i} \varepsilon J\left(\sum_{k=j}^{i} y_k'\right). \tag{3.11}$$

For the moment we will only need E'', however, for future reference, we first compute E' which can be written in the form

$$\begin{aligned}
E'(y; w) &= \sum_{i=1}^{N} \sum_{j=1}^{i} \varepsilon J'\left(\sum_{k=j}^{i} y_k'\right)\left(\sum_{n=j}^{i} w_n'\right)\\
&= \sum_{i=1}^{N} \sum_{j=1}^{i} \sum_{n=j}^{i} \varepsilon w_n' J'\big(\varepsilon^{-1}(y_i - y_{j-1})\big)\\
&= \sum_{i=1}^{N} \sum_{n=1}^{i} \varepsilon w_n' \sum_{j=1}^{n} J'\big(\varepsilon^{-1}(y_i - y_{j-1})\big)\\
&= \sum_{n=1}^{N} \varepsilon w_n' \left(\sum_{i=n}^{N} \sum_{j=1}^{n} J'\big(\varepsilon^{-1}(y_i - y_{j-1})\big)\right)\\
&= \sum_{n=1}^{N} \varepsilon F_n'(y) w_n', &(3.12)
\end{aligned}$$

where

$$F_n'(y) = \sum_{i=n}^{N} \sum_{j=1}^{n} J'\big(\varepsilon^{-1}(y_i - y_{j-1})\big) = \sum_{i=n}^{N} \sum_{j=0}^{n-1} J'\big(\varepsilon^{-1}(y_i - y_j)\big).$$

If E is twice differentiable at a point y, then $E''(Y)$ is most conveniently written in the form

$$\begin{aligned} E''(y; v, w) &= \sum_{i=1}^{N} \sum_{j=1}^{i} \varepsilon J''\big(\varepsilon^{-1}(y_i - y_{j-1})\big) \left(\sum_{m=j}^{i} v_m' \right) \left(\sum_{n=j}^{i} w_n' \right) \\ &= \sum_{n=1}^{N} \varepsilon w_n' \sum_{i=n}^{N} \sum_{j=1}^{n} \sum_{m=j}^{i} v_m' J''\big(\varepsilon^{-1}(y_i - y_{j-1})\big) \\ &= \sum_{n=1}^{N} \varepsilon w_n' \sum_{i=n}^{N} \sum_{m=1}^{i} \sum_{j=1}^{n\wedge m} w_m' J''\big(\varepsilon^{-1}(y_i - y_{j-1})\big) \\ &= \sum_{n=1}^{N} \sum_{m=1}^{N} \varepsilon w_n' v_m' \left(\sum_{i=m\vee n}^{N} \sum_{j=1}^{n\wedge m} J''\big(\varepsilon^{-1}(y_i - y_{j-1})\big) \right) \\ &= \sum_{n=1}^{N} \sum_{m=1}^{N} \varepsilon F_{nm}'' v_m' w_n', \end{aligned} \tag{3.13}$$

where

$$F_{nm}''(y) = \sum_{i=m\vee n}^{N} \sum_{j=1}^{n\wedge m} J''\big(\varepsilon^{-1}(y_i - y_{j-1})\big).$$

Our aim in this section is to identify a set of deformations,

$$\mathscr{Z}_e = \{ y \in \mathscr{A} : z_1 \le y_i' \le z_2 \},$$

with $z_1 < z_m < z_2 < z_t$ for which $E''(y)$ satisfies the inf-sup condition

$$\min_{y \in \mathscr{Z}_e} \min_{\substack{u \in \mathscr{A}_0 \\ |u|_{\mathrm{w}_\varepsilon^{1,\infty}} = 1}} \max_{\substack{v \in \mathscr{A}_0 \\ |v|_{\mathrm{w}_\varepsilon^{1,1}} = 1}} E''(y; u, v) \ge c_0 > 0.$$

For convenience, we have assumed in §2.1 that $z_m > z_t/2$, and hence we may assume here that $z_1 \ge z_t/2$ as well. This implies that

$$\begin{cases} J''(z) > 0, & \text{for } z_1 \le z \le z_2, \text{ and} \\ J''(z) \le 0, & \text{for } z \ge 2z_1, \end{cases} \tag{3.14}$$

and consequently $F_{nm}'' \le 0$ whenever $n \ne m$.

The proof of the inf-sup condition is based on an argument related to row diagonally dominant matrices. Fix $u \in \mathscr{A}_0$ and choose $p, q \in \{1, \ldots, N\}$ such that u_p' is maximal and u'_q is minimal. Since $u \in \mathscr{A}_0$ we have $\sum_{i=1}^N u'_i = 0$ and hence $u'_p \geq 0$ and $u'_q \leq 0$. We define the test function v by

$$v'_i = \begin{cases} \frac{1}{2}\varepsilon^{-1}, & \text{if } i = p, \\ -\frac{1}{2}\varepsilon^{-1}, & \text{if } i = q, \text{ and} \\ 0, & \text{otherwise.} \end{cases}$$

It is clear from the definition of v that $v \in \mathscr{A}_0$ and $|v|_{\mathrm{w}^{1,1}_\varepsilon} = 1$. Let $P = \{i : u'_i > 0\}$ and $Q = \{i : u'_i < 0\}$. Using (3.13), we have

$$\begin{aligned} E''(y; u, v) &= \sum_{n=1}^N \sum_{m=1}^N \varepsilon F''_{nm}(y) u'_n v'_m \\ &= \frac{1}{2\varepsilon} \sum_{n=1}^N \varepsilon F''_{np}(y) u'_n - \frac{1}{2\varepsilon} \sum_{n=1}^N \varepsilon F''_{nq}(y) u'_n \\ &= \frac{1}{2} F''_{pp}(y) u'_p + \frac{1}{2} \sum_{n \neq p} F''_{np} u'_n - \frac{1}{2} F''_{qq}(y) - \sum_{n \neq q} F''_{nq}(y) u'_n. \end{aligned}$$

Using (3.14), we see that for $n \neq m$ we have $F''_{nm}(y) \leq 0$. Hence, we obtain

$$\begin{aligned} 2E''(y; u, v) &\geq F''_{pp}(y) u'_p + \sum_{m \in P \setminus \{p\}} F''_{mp}(y) u'_m - F''_{qq}(y) u'_q - \sum_{m \in Q \setminus \{q\}} F''_{mq}(y) u'_m \\ &\geq u'_p \Big[F''_{pp}(y) + \sum_{m \in P \setminus \{p\}} F''_{mp}(y) \Big] + (-u'_q) \Big[F''_{qq}(y) + \sum_{m \in Q \setminus \{q\}} F''_{mq}(y) \Big] \\ &\geq |u|_{\mathrm{w}^{1,\infty}_\varepsilon} \sum_{m=1}^N F''_{mn}(y), \end{aligned} \tag{3.15}$$

where $n \in \{p, q\}$. Thus, to prove the coercivity estimate (3.1), we need to show that the matrix $(F''_{nm})_{n,m=1,\dots,N}$ is strictly row diagonally dominant; more precisely, we need to obtain a lower bound on the sum in the last expression. To do so, we split the sum as follows:

$$\begin{aligned} \sum_{m=1}^N F''_{nm}(y) &= \sum_{m=1}^{n-1} \sum_{i=n}^N \sum_{j=1}^m J''\big(\varepsilon^{-1}(y_i - y_{j-1})\big) + \sum_{m=n+1}^N \sum_{j=1}^n \sum_{i=m}^N J''\big(\varepsilon^{-1}(y_i - y_{j-1})\big) \\ &\quad + \sum_{j=1}^n \sum_{i=n}^N J''\big(\varepsilon^{-1}(y_i - y_{j-1})\big). \end{aligned}$$

For all pairs (i, j) with $i \geq j$ we bound

$$J''(\varepsilon^{-1}(y_i - y_{j-1})) \geq \min_{z_1 \leq z \leq z_2} J''\big((i - j + 1)z\big) =: \underline{J}''(i - j + 1),$$

which we use to estimate

$$\sum_{m=1}^{N} F''_{nm}(y) \geq \sum_{m=1}^{n-1}\sum_{i=n}^{N}\sum_{j=1}^{m} \underline{J}''(i-j+1) + \sum_{m=n+1}^{N}\sum_{j=1}^{n}\sum_{i=m}^{N} \underline{J}''(i-j+1) + \sum_{j=1}^{n}\sum_{i=n}^{N} \underline{J}''(i-j+1). \tag{3.16}$$

In the first triple-sum, we exchange the order of summation three times to obtain

$$\begin{aligned}\sum_{m=1}^{n-1}\sum_{i=n}^{N}\sum_{j=1}^{m} \underline{J}''(i-j+1) &= \sum_{i=n}^{N}\sum_{j=1}^{n-1}\sum_{m=j}^{n-1} \underline{J}''(i-j+1) \\ &= \sum_{j=1}^{n-1}\sum_{i=n}^{N}(n-j)\underline{J}''(i-j+1) \\ &\geq \sum_{j=1}^{n-1}(n-j) \sum_{r=n-j+1}^{\infty} \underline{J}''(r),\end{aligned}$$

where we used the fact that $\underline{J}''(r) \leq 0$ for $r \geq 2$. We change the order of summation again,

$$\begin{aligned}\sum_{j=1}^{n-1}(n-j) \sum_{r=n-j+1}^{\infty} \underline{J}''(r) &= \sum_{r=2}^{\infty} \underline{J}''(r) \sum_{j=n-r+1}^{n-1} (n-j) \\ &= \frac{1}{2}\sum_{r=2}^{\infty} r(r-1)\underline{J}''(r),\end{aligned}$$

where we used $\sum_{j=n-r+1}^{n-1}(n-j) = r(r-1)/2$. Similarly, for the second triple-sum in (3.16), we obtain

$$\sum_{m=n+1}^{N}\sum_{j=1}^{n}\sum_{i=m}^{N} \underline{J}''(i-j+1) \geq \frac{1}{2}\sum_{r=2}^{\infty} r(r-1)\underline{J}''(r).$$

For the third term in (3.16), we have

$$\begin{aligned}\sum_{j=1}^{n}\sum_{i=n}^{N} \underline{J}''(i-j+1) &\geq \sum_{j=1}^{n}\sum_{r=n-j+1}^{\infty} \underline{J}''(r) \\ &= \sum_{r=1}^{\infty}\sum_{j=n-r+1}^{n} \underline{J}''(r) \\ &= \sum_{r=1}^{\infty} r\underline{J}''(r).\end{aligned}$$

On combining this with the previously obtained bounds, and recalling the definition (2.8), we finally arrive at

$$\sum_{m=1}^{N} F''_{nm}(y) \geq \sum_{r=1}^{\infty} r^2 \underline{J}''(r) = \rho_2(z_1, z_2). \tag{3.17}$$

Therefore, returning to (3.15), we obtain

$$\max_{\substack{v\in\mathscr{A}_0\\ |v|_{\mathrm{w}_\varepsilon^{1,1}}=1}} E''(y;u,v) \geq c_0 |u|_{\mathrm{w}_\varepsilon^{1,\infty}}, \tag{3.18}$$

where $c_0 = \frac{1}{2}\rho_2(z_1, z_2)$. We refer to Appendix B for specific values of z_1, z_2 and c_0 for the Lennard–Jones and the Morse potential.

3.2 Proof of Theorem 1

The proof of Theorem 1 as well as the extension to fracture solutions in §4 rely on a local existence result which is essentially a simple corollary of the Implicit Function Theorem (cf. [16, Section 6.6]).

Lemma 3 *Let E be given by* (2.1) *and let $\tilde{y} \in \mathscr{A}$ satisfy $E'(\tilde{y}) = \tilde{f}$ in $\mathscr{A}$. Suppose that there exists a constant $c_0 > 0$ such that, in the set $\mathscr{Z} = B(\tilde{y}, R) \cap \mathscr{A}$, E'' satisfies*

$$0 < c_0 \leq \min_{y\ in \mathscr{Z}} \min_{\substack{u\in\mathscr{A}_0\\ |u|_{\mathrm{w}_\varepsilon^{1,\infty}}=1}} \max_{\substack{v\in\mathscr{A}_0\\ |v|_{\mathrm{w}_\varepsilon^{1,1}}=1}} E''(y;u,v). \tag{3.19}$$

Then, for any $f \in \mathbb{R}^{N+1}$ satisfying $\|f - \tilde{f}\|_* \leq c_0 R$ there exists a unique $y \in \mathscr{Z}$ such that $E'(y) = f$ in $\mathscr{A}$. The solution y satisfies

$$|y - \tilde{y}|_{\mathrm{w}_\varepsilon^{1,\infty}} \leq c_0^{-1} \|f - \tilde{f}\|_*. \tag{3.20}$$

Proof For $t \in [0,1]$ define $f_t = (1-t)\tilde{f} + tf$. We seek $y_t \in \mathscr{Z}$ such that $E'(y_t) = f_t$. To this end, assume that for some $t \in [0,1)$ there exists $y_t \in \mathrm{int}(\mathscr{Z})$ such that $E'(y_t) = f_t$ and let $t < s \leq 1$.

By the Mean Value Theorem, there exists $\theta \in \mathscr{Z}$ such that $E'(\tilde{y}) - E'(y_t) = E''(\theta)(\tilde{y} - y_t)$ and therefore

$$E''(\theta)(\tilde{y} - y_t) = \tilde{f} - f_t.$$

Upon multiplying by $v \in \mathscr{A}_0$ and using (3.19), we obtain

$$c_0 |\tilde{y} - y_t|_{\mathrm{w}_\varepsilon^{1,\infty}} \leq \|\tilde{f} - f_t\|_* = t\|\tilde{f} - f\|_* \leq tc_0 R. \tag{3.21}$$

In particular, (3.21) implies that $y_0 = \tilde{y}$.

Since E'' satisfies (3.19), it follows that $E''(y_t)$ is non-singular. Furthermore, there exists a neighbourhood of y_t where E'' is Lipschitz continuous. Therefore, by the Implicit Function Theorem, there exists $\delta > 0$ such that for all $s \in [t, \delta)$ there is a $y_s \in \mathrm{int}(\mathscr{Z})$ satisfying $E'(y_s) = f_s$.

Applying this result with $t = 0$, we find that there is a $T > 0$ such that for $t \in [0, T)$ there exists a solution $y_t \in \mathscr{Z}$ to $E'(y_t) = f_t$. Let T be maximal. Since $\mathscr{A}$ is finite-dimensional, there exists a sequence $t_j \uparrow T$ such that y_{t_j} converges to some $y \in \mathscr{Z}$. Since $f_{t_j} \to f_T$ and E' is continuous in $\mathscr{Z}$, it follows that $E'(y) = f_T$. If $T < 1$, then by (3.21) $y \in \mathrm{int}(\mathscr{Z})$. Therefore, there exists $\delta > 0$ such that for $T \le s < T + \delta$, there is a solution y_s to $E'(y_s) = f_s$. Since we assumed that T was maximal, it follows that $T = 1$.

Using the same argument as the one leading to (3.21) we find that the solution is unique in $\mathscr{Z}$. ■

Lemma 3 gives a clear path to the proof of Theorem 1. We have already established the necessary conditions for coercivity in the previous section.

To show the existence of a reference state, we define the deformation $y_i^D = \varepsilon i y_N^D$, where we assume that $z_1 < y_N^D < z_2$, and estimate the residual $E'(y^D)$. It is more convenient to do this in the following alternative representation of E':

$$E'(y; v) = \sum_{n=1}^{N-1} E'_n(y) v_i \qquad \forall y \in \mathscr{A}, \forall v \in \mathscr{A}_0, \tag{3.22}$$

where

$$E'_n(y) = \sum_{i=0}^{n-1} J'\big(\varepsilon^{-1}(y_n - y_i)\big) - \sum_{i=n+1}^{N} J'\big((\varepsilon^{-1}(y_i - y_n)\big), \qquad n = 1, \dots, N-1.$$

Using the embedding inequality $\|v\|_{\ell^\infty_\varepsilon} \le \frac{1}{2} |v|_{\mathrm{w}^{1,1}_\varepsilon}$ (cf. Lemma 9) we can estimate

$$|E'(y'; v)| \le \sum_{n=1}^{N-1} |E'_n(y)| \|v\|_{\ell^\infty_\varepsilon} \le \frac{1}{2} \sum_{n=1}^{N-1} |E'_n(y)| |v|_{\mathrm{w}^{1,1}_\varepsilon},$$

which implies that

$$\|E'(y)\|_* \le \frac{1}{2} \sum_{n=1}^{N-1} |E'_n(y)|. \tag{3.23}$$

For $y = y^D$, we have

$$E'_n(y^D) = \sum_{i=0}^{2n-N-1} J'((n-i) y_N^D) - \sum_{i=2n+1}^{N} J'((i-n) y_n^D),$$

and, taking absolute values,

$$|E'_n(y)| \le \sum_{r = n \wedge (N-n)+1}^{\infty} |J'(r y_n^D)|.$$

Thus, we can estimate

$$\begin{aligned} \|E'(y^D)\|_* &\le \frac{1}{2} \sum_{n=1}^{N-1} |E'_n(y^D)| \le \frac{1}{2} \sum_{n=1}^{\infty} \sum_{r=n+1}^{\infty} |J'(r y_N^D)| \\ &\le \frac{1}{2} \sum_{r=2}^{\infty} \sum_{n=1}^{r-1} |J'(r y_N^D)| \le \frac{1}{2} \sum_{r=2}^{\infty} (r-1) |J'(r y_N^D)| = \frac{1}{2} \rho_1(y_N^D). \end{aligned}$$

We now apply Lemma 3 with $\tilde{y} = y^D$ and $f = 0$. Thus, if

$$\tfrac{1}{2}\rho_1(y_N^D) \le \tfrac{1}{2}\rho_2(z_1, z_2) \times \min(z_2 - y_N^D, y_N^D - z_1), \tag{3.24}$$

there exists a reference state $y^* \in \mathscr{A}$ satisfying (2.6) with $f = 0$. From the stability estimate (3.20), we infer that

$$|y^* - y_N^D|_{\mathrm{w}_\varepsilon^{1,\infty}} \le c_0^{-1}\|E'(y^D)\|_* \le \frac{\rho_1(y_N^D)}{\rho_2(z_1, z_2)}.$$

If the inequality in (3.24) is strict, there exists an $R > 0$ such that $\{y \in \mathscr{A} : |y - y^*|_{\mathrm{w}_\varepsilon^{1,\infty}} \le R\} \subset \mathscr{Z}_e$. Thus, for $\|f\|_* \le c_0 R =: \delta$, there exists a unique solution to (2.6) in $\mathscr{Z}_e$.

To complete the proof of Theorem 1 we only need to show that the numbers z_1, z_2 satisfying our assumptions exist. This, however, follows immediately from the assumption that $\rho_1(z_m) < R\rho_2(z_m - R, z_m + R)$ and that ρ_1 is continuous.

3.3 Coercivity of the QC approximation

In order to apply a similar technique as in §3.2 to prove the existence of a QC solution near an exact solution, we need to show that E'' is also coercive in $\mathscr{A}_0(\mathcal{T})$, i.e., that there exists a constant $\tilde{c}_0 > 0$ such that, for all $Y \in \mathscr{Z}_e \cap \mathscr{A}(T)$, we have

$$\inf_{\substack{U \in \mathscr{A}_0(\mathcal{T}) \\ |U|_{\mathrm{w}_\varepsilon^{1,\infty}} = 1}} \sup_{\substack{V \in \mathscr{A}_0(\mathcal{T}) \\ |V|_{\mathrm{w}_\varepsilon^{1,1}} = 1}} E''(Y; U, V) \ge \tilde{c}_0.$$

To this end, fix $U \in \mathscr{A}_0(\mathcal{T})$ and pick $p, q \in \{1, \dots, K\}$ such that $\overline{U}'_p$ is maximal and $\overline{U}'_q$ is minimal. Similarly as before, we also let $P = \{i : \overline{U}'_i > 0\}$ and $Q = \{i : \overline{U}'_i < 0\}$, and we define

$$\overline{V}'_k = \begin{cases} \frac{1}{2}h_p^{-1}, & \text{if } k = p, \\ -\frac{1}{2}h_q^{-1}, & \text{if } k = q, \text{ and} \\ 0, & \text{otherwise.} \end{cases}$$

This gives,

$$\begin{aligned} E''(Y; U, V) &= \sum_{n=1}^{N}\sum_{m=1}^{N} \varepsilon F''_{nm}(Y) U'_n V'_m \\ &= \frac{1}{2h_p}\sum_{n=1}^{N}\sum_{m=t_{p-1}+1}^{t_p} \varepsilon F''_{nm}(Y) U'_n - \frac{1}{2h_q}\sum_{n=1}^{N}\sum_{m=t_{q-1}+1}^{t_q} \varepsilon F''_{nm}(Y) U'_n \\ &\ge \frac{\overline{U}'_p}{2h_p}\sum_{m=t_{p-1}+1}^{t_p} \varepsilon \sum_{n\in P} F''_{nm}(Y) - \frac{\overline{U}'_q}{2h_q}\sum_{m=t_{q-1}+1}^{t_q} \varepsilon \sum_{n\in Q} F''_{nm}(Y). \end{aligned}$$

Using the estimate (3.17), we obtain

$$\begin{aligned} E''(Y; U, V) &\ge \frac{\overline{U}'_p}{2h_p}\sum_{m=t_{p-1}+1}^{t_p} \varepsilon\rho_2(z_1, z_2) - \frac{\overline{U}'_q}{2h_q}\sum_{m=t_{q-1}+1}^{t_q} \varepsilon\rho_2(z_1, z_2) \\ &\ge c_0|U|_{\mathrm{w}_\varepsilon^{1,\infty}}, \end{aligned}$$

where $c_0 = \frac{1}{2}\rho_2(z_1, z_2)$, i.e., we have the same inf-sup constant as in the case of the full test-space $\mathscr{A}_0$.

If we now replace E by $\tilde{E}$ in all the above computations, we obtain instead

$$\min_{Y \in \mathscr{A}(\mathcal{T}) \cap \mathscr{Z}_e} \min_{\substack{U \in \mathscr{A}_0(\mathcal{T}) \\ |U|_{\mathrm{w}_\varepsilon^{1,\infty}} = 1}} \max_{\substack{V \in \mathscr{A}_0(\mathcal{T}) \\ |V|_{\mathrm{w}_\varepsilon^{1,1}} = 1}} \tilde{E}''(Y; U, V) \geq \tfrac{1}{2}\tilde{\rho}_2(z_1, z_2). \tag{3.25}$$

3.4 Proof of Theorem 2

Stimulated by the a-priori error analysis in [14], we begin by rewriting the QC approximation as a fixed-point problem. To this end assume that $Y \in \mathscr{A}(\mathcal{T}) \cap \mathscr{Z}_e$ satisfies (2.11). Let $y \in \mathscr{A} \cap \mathscr{Z}_e$ be an exact solution and let Πy be its interpolant. We then have, for all $V \in \mathscr{A}_0(\mathcal{T})$,

$$\begin{aligned} \int_0^1 E''\big(\Pi y + \tau(Y - \Pi y); Y - \Pi y, V\big)\,\mathrm{d}\tau &= E'(Y; V) - E'(\Pi y; V) \qquad (3.26) \\ &= E'(Y; V) - \tilde{E}'(Y; V) + \langle f, V\rangle_{\mathcal{T}} - \langle f, V\rangle_\varepsilon + E'(y; V) - E'(\Pi y; V) =: \ell_Y(V). \end{aligned}$$

In fact, we see that Y is a solution of (2.11) if, and only if, it solves (3.26) which we rewrite as a fixed point problem. Let $\varphi \in \mathscr{A}(\mathcal{T}) \cap \mathscr{Z}_e$. We define the fixed point map $\mathscr{L} \colon \mathscr{A}(\mathcal{T}) \cap \mathscr{Z}_e \to \mathscr{A}(\mathcal{T})$, $Y_\varphi = \mathscr{L}(\varphi)$ by

$$\int_0^1 E''\big(\Pi y + \tau(\varphi - \Pi y); Y_\varphi - \Pi y, V\big)\,\mathrm{d}\tau = \ell_\varphi(V) \qquad \forall V \in \mathscr{A}_0(\mathcal{T}). \tag{3.27}$$

By the Integral Mean Value Theorem, there exists $\theta \in \operatorname{conv}\{\varphi, \Pi y\} \subset \mathscr{Z}_e$ such that $\int_0^1 E''(\Pi y + \tau(\varphi - \Pi y))\,\mathrm{d}\tau = E''(\theta)$. Hence, if $c_0 > 0$, the map $\mathscr{L}$ is well defined and we can rewrite (3.27) as

$$E''(\theta; Y_\varphi - \Pi y, V) = \ell_\varphi(V) \qquad \forall V \in \mathscr{A}_0(\mathcal{T}).$$

Upon taking the supremum over all $V \in \mathscr{A}_0(\mathcal{T})$ with $|V|_{\mathrm{w}_\varepsilon^{1,1}} = 1$ we obtain

$$c_0 |Y_\varphi - \Pi y|_{\mathrm{w}_\varepsilon^{1,\infty}} \leq \max_{\substack{V \in \mathscr{A}_0(\mathcal{T}) \\ |V|_{\mathrm{w}_\varepsilon^{1,1}} = 1}} |\ell_\varphi(V)| \leq c_1 \mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3,$$

where c_1 is a Lipschitz constant for E' in $\mathscr{Z}_e$ and $\mathcal{E}_i$, $i = 1, 2, 3$, are defined at the beginning of §3. Thus, in order for $\mathscr{L}$ to map $\mathscr{A}(\mathcal{T}) \cap \mathscr{Z}_e$ into itself, it is sufficient that

$$c_1 \mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3 \leq c_0 \min_{i=1,\dots,N} \min(\Pi y_i' - z_1, z_2 - \Pi y_i').$$

Since $\Pi y_{t_k} = y_{t_k}$ for $k = 0, \dots, K$, it follows that

$$\sum_{i=t_{k-1}+1}^{t_k} \varepsilon y_i' - h_k \big(\overline{\Pi y}\big)_k' = 0,$$

and hence $\min(\Pi y_i' - z_1, z_2 - \Pi y_i') \leq R$. We conclude that if (3.7) is satisfied then $\mathscr{L}$ maps $\mathscr{A}(\mathcal{T}) \cap \mathscr{Z}_e$ into itself. The Implicit Function Theorem implies that $\mathscr{L}$ is continuous. Therefore, by Brouwer's fixed point theorem, $\mathscr{L}$ has a fixed point Y in $\mathscr{A}(\mathcal{T}) \cap \mathscr{Z}_e$. From our discussion above it follows that Y is a solution to (2.11). From (3.25) we see that if $\tilde{\rho}_2(z_1, z_2) > 0$ then the QC solution is unique in $\mathscr{A}(\mathcal{T}) \cap \mathscr{Z}_e$. This concludes the proof of part (b) of Theorem 2. We are only left to prove the stated bounds on c_1, and $\mathcal{E}_i$, $i = 1, 2, 3$.

To bound E'' in $\mathscr{Z}_e$, we compute

$$
\begin{aligned}
|E''(\theta; U, V)| &= \sum_{n=1}^{N} \sum_{m=1}^{N} \varepsilon |F''_{nm}(\theta)| |U'_n| |V'_m| \\
&\leq |U|_{\mathrm{w}^{1,\infty}_\varepsilon} \sum_{m=1}^{N} \varepsilon |V'_m| \sum_{n=1}^{N} |F''_{nm}(\theta)| \\
&\leq |U|_{\mathrm{w}^{1,\infty}_\varepsilon} |V|_{\mathrm{w}^{1,1}_\varepsilon} \max_{m=1,\dots,N} \sum_{n=1}^{N} |F''_{nm}(\theta)|.
\end{aligned}
$$

We can bound the sum in the last term by a computation identical to that in (3.17) except that the signs are reversed, and thus we obtain (3.6).

To bound $\mathcal{E}_1$ we simply use Theorem 10 with $p = \infty$. For $\mathcal{E}_2$, we use Theorem 10 with $p = 1$ to estimate

$$
\begin{aligned}
\big|\langle f, V\rangle_{\mathcal{T}} - \langle f, V\rangle_\varepsilon\big| &\leq \sum_{i=1}^{N} \varepsilon \big|\Pi(fV)_i - f_i V_i\big| \\
&\leq \sum_{k=1}^{K} h_k^2 |\Pi(fV)|_{\mathrm{w}^{2,1}_\varepsilon(\!(t_{k-1}, t_k)\!)}.
\end{aligned}
$$

For $i = t_{k-1} + 1, \dots, t_k - 1$, using the fact that $V_i'' = 0$, we have

$$
\begin{aligned}
(fV)_i'' &= \varepsilon^{-2}(f_{i+1}V_{i+1} - 2f_iV_i + f_{i-1}V_{i-1}) \\
&= \frac{f_{i+1} - 2f_i + f_{i-1}}{\varepsilon^2} V_i + \frac{f_{i+1} - f_i}{\varepsilon} \frac{V_{i+1} - V_i}{\varepsilon} + \frac{f_i - f_{i-1}}{\varepsilon} \frac{V_i - V_{i-1}}{\varepsilon}.
\end{aligned}
$$

Thus, using the discrete Friedrichs inequality (A.2), we obtain,

$$
\begin{aligned}
\big|\langle f, V\rangle_{\mathcal{T}} - \langle f, V\rangle_\varepsilon\big| &\leq \sum_{k=1}^{K} h_k^2 \Big[|f|_{\mathrm{w}^{2,\infty}_\varepsilon(\!(t_{k-1}, t_k)\!)} \|V\|_{\ell^1_\varepsilon(\!(t_{k-1}+1, t_k-1)\!)} \\
&\qquad + (|f|_{\mathrm{w}^{1,\infty}_\varepsilon(\!(t_{k-1}+1, t_k)\!)} + |f|_{\mathrm{w}^{1,\infty}_\varepsilon(\!(t_{k-1}, t_k-1)\!)}) |V|_{\mathrm{w}^{1,1}_\varepsilon(\!(t_{k-1}, t_k)\!)} \Big] \\
&\leq \max_{k=1,\dots,K} h_k^2 \big(\tfrac{1}{2} |f|_{\mathrm{w}^{2,\infty}_\varepsilon(\!(t_{k-1}, t_k)\!)} + |f|_{\mathrm{w}^{1,\infty}_\varepsilon(\!(t_{k-1}+1, t_k)\!)} \\
&\qquad + |f|_{\mathrm{w}^{1,\infty}_\varepsilon(\!(t_{k-1}, t_k-1)\!)} \big) \, |V|_{\mathrm{w}^{1,1}_\varepsilon},
\end{aligned}
$$

which proves the bound (3.9).

Finally, using (3.12), the bound (3.10) on $\mathcal{E}_3$ follows from

$$\begin{aligned} |E'(\theta;V) - \tilde{E}'(\theta;V)| &\leq \sum_{n=1}^{N} \varepsilon |F_n'(\theta) - \tilde{F}_n'(\theta)||V_n'| \\ &\leq \max_{n=1,\dots N} |F_n'(\theta) - \tilde{F}_n'(\theta)||V|_{\mathrm{w}_\varepsilon^{1,1}}, \end{aligned}$$

and a computation that is identical to the one leading to (3.24).

4 Fracture

We now look at a class of solutions of the atomistic model (2.6), with a single defect — a fracture. To this end, we fix an index $\xi \in \{1, \dots, N\}$ and consider deformations $y \in \mathscr{A}$ such that $y_\xi' \gg z_t$ while $z_1 \leq y_i' \leq z_2 < z_t$ for $i \neq \xi$. The *fracture* is the broken interaction between the two atoms at y_ξ and $y_{\xi-1}$. Elastic states and fractured states with a single crack are the only stable steady states in one dimension. If at least two gradients y_i', y_j' are greater than or equal to z_t, it can be easilly seen that $E''(y)$ has at least one negative eigenvalue (cf. [13]).

However, even with a single fracture, it should be apparent from the analysis of §3.1 that we cannot expect (3.18) to hold when $|u|_{\mathrm{w}_\varepsilon^{1,\infty}} = |u_\xi'|$, since in that case $J''(u_\xi') \approx 0$. We therefore change the norm in which we analyze the error into the norm $|\cdot|_{\mathrm{w}_{\varepsilon,f}^{1,\infty}}$ defined by

$$|u|_{\mathrm{w}_{\varepsilon,f}^{1,\infty}} = \max_{\substack{i=1,\dots,N \\ i\neq\xi}} |u_i'|.$$

Since we have imposed a Dirichlet condition at both endpoints, $|\cdot|_{\mathrm{w}_{\varepsilon,f}^{1,\infty}}$ is indeed a norm on $\mathscr{A}_0$. As was hinted above, we define

$$\mathscr{Z}_f = \{y \in \mathbb{R}^{N+1} : y_\xi' \geq z_f \text{ and } z_1 \leq y_i' \leq z_2 \text{ for } i = 1, \dots, N, i \neq \xi\},$$

where the constants z_i satisfy $z_1 < z_m < z_2 < z_t$, and z_f is sufficiently large (which we will make precise).

In order to simplify the proofs of coercivity we assume that

$$J'''(z) \geq 0 \qquad \text{for } z \geq z_f. \tag{4.1}$$

This only imposes a typically negligible lower bound on z_f.

We shall also need a further measure of stability,

$$\rho_{2,f}(z_f, z_1) = \sum_{r=0}^{\infty} (r+1) J''(z_f + r z_1).$$

The definition of $\rho_{2,f}$ does not involve z_2 because we have assumed (4.1). The function $\tilde{\rho}_{2,f}$ corresponding to the cut-off potential $\tilde{J}$ is defined analogously. In order to be able to neglect the effect of long-range interactions across the crack, we assume that

$$\forall\, a > 0\ \forall\, z_1 \geq z_t/2\ \exists\, z_D = z_D(a, z_1) :\ N\rho_{2,f}\big(N(z_D - z_t), z_1\big) \geq -a. \tag{4.2}$$

This would typically involve a growth condition for J'', for example, $|J''(z)| \lesssim z^{-k}$, for some $k > 3$ and z sufficiently large.

Theorem 4 *Let J satisfy the assumptions of §2.1 as well as conditions* (4.1) *and* (4.2)*. Assume also that there exists $R \in (0, \min(z_m - z_t/2, z_t - z_m))$ such that $2\rho_1(z_m) < R\rho_2(z_m - R, z_m + R)$. Then the following hold:*

(a) *Coercivity: There exist $z_1 < z_m < z_2 < z_t$ independent of ε, and $z_f = O(\varepsilon^{-1})$ such that*

$$\inf_{y \in \mathscr{Z}_f} \inf_{\substack{u \in \mathscr{A}_0 \\ |u|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}} = 1}} \sup_{\substack{v \in \mathscr{A}_0 \\ |v|_{\mathrm{w}^{1,1}_{\varepsilon}} = 1}} E''(y; u, v) \geq \tfrac{1}{2}\big(\rho_2(z_1, z_2) + 2N\rho_{2,f}(z_f, z_1)\big) =: c_0 > 0, \quad (4.3)$$

where $\mathscr{Z}_f$ is defined as above.

(b) *Existence: There exist $\delta_1, \delta_2 > 0$, independent of ε, such that for every $y_N^D \in \mathbb{R}$ with $y_N^D \geq z_m + \delta_1$ and for every $f \in \mathbb{R}^{N+1}$ with $\|f\|_* \leq \delta_2$, there exists a solution y_f of* (2.6) *in $\mathscr{Z}_f$.*

(c) *Stability: Let y_f, y_g be solutions to* (2.6) *in $\mathscr{Z}_f \cap \mathscr{A}$ with respective right-hand sides f and g; then*

$$|y_f - y_g|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}} \leq c_0^{-1}\|f - g\|_*.$$

For the QC error bounds, let $\mathcal{E}_1 = |y - \Pi y|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}$ and let $\mathcal{E}_2$ and $\mathcal{E}_3$ be defined as in §3.

Theorem 5 *Let J satisfy the conditions of §2.1 as well as* (4.1) *and* (4.2)*, and let $\mathscr{Z}_f$ be defined as above. Furthermore, assume that $\{\xi - 1, \xi\} \subset \mathcal{T}$.*

(a) *We have the coercivity and continuity estimates*

$$\inf_{\theta \in \mathscr{Z}_f} \min_{\substack{U \in \mathscr{A}_0(\mathcal{T}) \\ |U|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}} = 1}} \max_{\substack{V \in \mathscr{A}_0(\mathcal{T}) \\ |V|_{\mathrm{w}^{1,1}_{\varepsilon}} = 1}} E''(\theta; U, V) \geq \tfrac{1}{2}\big(\rho_2(z_1, z_2) + 2N\rho_{2,f}(z_f, z_1)\big) =: c_0, \text{ and} \quad (4.4)$$

$$\max_{Y \in S^1(\mathcal{T}) \cap \mathscr{Z}_f} \max_{\substack{U \in \mathscr{A}_0(\mathcal{T}) \\ |U|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}} = 1}} \max_{\substack{V \in \mathscr{A}_0(\mathcal{T}) \\ |V|_{\mathrm{w}^{1,1}_{\varepsilon}} = 1}} E''(Y; U, V) \leq \rho_3(z_1, z_2) =: c_1. \quad (4.5)$$

(b) *Suppose that $z_f > z_t$ is sufficiently large so that $c_0 > 0$ (cf.* (4.2)*). Let $y \in \mathscr{Z}_f \cap \mathscr{A}$ be a solution of* (2.6) *and define $R = \min_{i \neq \xi} \min(z_2 - y_i', y_i' - z_1)$. Assume furthermore that the QC mesh $\mathcal{T}$ is sufficiently fine so that*

$$c_1\mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3 \leq c_0 \min\big(R, \varepsilon(y_\xi' - z_f)\big). \quad (4.6)$$

Then, there exists a solution $Y \in \mathscr{A}(\mathcal{T}) \cap \mathscr{Z}_f$ of the QC method (2.11) *which satisfies*

$$|y - Y|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}} \leq c_0^{-1}\Big((c_0 + c_1)\mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3\Big).$$

If $\tilde{\rho}_2(z_1, z_2) + 2N\tilde{\rho}_{2,f}(z_f, z_1) > 0$ then the QC solution is unique in $\mathscr{A}(\mathcal{T}) \cap \mathscr{Z}_f$.

(c) *The error quantities $\mathcal{E}_1$ and $\mathcal{E}_2$ satisfy the same bounds as in Theorem 2, while $\mathcal{E}_3$ is now bounded by*

$$\begin{aligned}\mathcal{E}_3 \ \le\ & \sum_{r=1}^{\infty} r \max\Big[\max_{z_1 \le z \le z_2} \big|\tilde{J}'(rz) - J'(rz)\big|, \\ & \max_{z_1 \le z \le z_2} \big|\tilde{J}'(z_f + (r-1)z) - J'(z_f + (r-1)z)\big|\Big].\end{aligned} \tag{4.7}$$

As we remark in §4.4, the condition (4.6) is not overly restrictive. We may think, for example that $z_f = O(\varepsilon^{-1})$ and $y'_\xi \ge 2z_f$. In that case, the upper bound required on the error terms is independent of ε.

4.1 Coercivity of the atomistic problem

For the proof of coercivity in the case of fracture we make use of the fact that the fracture problem can, to some extent, be seen as a combination of two Neumann problems. Fix $y \in \mathscr{Z}_f$ and $u \in \mathscr{A}_0$. Upon multiplying u by (-1), we may assume without loss of generality that $u'_p = |u|_{\mathrm{w}^{1,\infty}_\varepsilon}$. Let $P = \{i : u'_i > 0\}$ and $Q = \{j : u'_j < 0\}$ and define

$$v'_n = \begin{cases} \frac{1}{2}\varepsilon^{-1}, & \text{if } n = p, \\ -\frac{1}{2}\varepsilon^{-1}, & \text{if } n = \xi, \\ 0, & \text{otherwise.} \end{cases}$$

In that case,

$$\begin{aligned} E''(y; u, v) &= \sum_{n=1}^{N}\sum_{m=1}^{N} \varepsilon F''_{nm}(y) u'_n v'_m \\ &= \sum_{n=1}^{N} \varepsilon u'_n \Big[F''_{np}(y)\frac{1}{2\varepsilon} - F''_{n\xi}(y)\frac{1}{2\varepsilon}\Big] \\ &\ge \frac{1}{2}\sum_{n\in P} u'_n F''_{np}(y) - \frac{1}{2}\sum_{n\in Q} u'_n F''_{n\xi}(y). \end{aligned}$$

If we divide the sum over $n \in P$ into those indices which lie on the same side of the fracture as p and the rest, we can estimate $F''_{np} \ge F''_{n\xi}$ for those n which lie on the opposite side of the fracture from p (compare condition (4.1)). If we assume, without loss of generality, that $p < \xi$, we obtain

$$E''(y; u, v) \ge \frac{1}{2}\sum_{n<\xi} |u'_n| F''_{np}(y) + \sum_{n\ne\xi} |u'_n| F''_{n\xi}(y) + |u'_\xi| F''_{\xi\xi}(y).$$

Since $u \in \mathscr{A}_0$, we have $|u'_\xi| \le (N-1)|u|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}$ and hence, we obtain

$$E''(y; u, v) \ge \frac{1}{2}|u|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}\Big[\sum_{n<\xi} F''_{np}(y) + \sum_{n\ne\xi} F''_{n\xi}(y) + (N-1)F''_{\xi\xi}(y)\Big], \tag{4.8}$$

For the first sum in (4.8) we can use the same procedure as in the elastic case, i.e,

$$\sum_{n<\xi} F''_{np}(y) \ge \rho_2(z_1, z_2),$$

while the second sum as well as $F''_{\xi\xi}$ should be practically zero. In this regime the forces should be so weak that we can make fairly crude estimates. Using assumption (4.1) we have $F''_{n\xi} \ge F''_{\xi\xi}$ for all n and hence only need to estimate $F''_{\xi\xi}$,

$$\begin{aligned}
F''_{\xi\xi}(y) &= \sum_{i=\xi}^{N}\sum_{j=1}^{\xi} J''\big(\varepsilon^{-1}(y_i - y_{j-1})\big) \ge \sum_{i=\xi}^{N}\sum_{j=1}^{\xi} J''\big(z_f + (i-j)z_1\big) \\
&\ge \sum_{j=1}^{\xi}\sum_{r=\xi-j}^{\infty} J''(z_f + rz_1) = \sum_{r=0}^{\infty}\sum_{j=\xi-r}^{\xi} J''(z_f + rz_1) \\
&= \sum_{r=0}^{\infty}(r+1)J''(z_f + rz_1) = \rho_{2,f}(z_f, z_1).
\end{aligned}$$

Putting everything together, we obtain

$$E''(y;u,v) \ge \tfrac{1}{2}\big(\rho_2(z_1,z_2) + 2(N-1)\rho_{2,f}(z_f,z_1)\big)|u|_{\mathrm{W}^{1,\infty}_{\varepsilon,f}}. \tag{4.9}$$

4.2 Proof of Theorem 4

Note that we cannot use Lemma 3 directly but need to formulate a version specifically taylored to the set $\mathscr{Z}_f$. First, however, we should finalize the question of coercivity. To this end, let $c_0' = \frac{1}{2}\rho_2(z_1, z_2)$, which we assume to be positive, and choose

$$z_f = N\big(z_D(\alpha c_0', z_1) - z_t\big),$$

where $\alpha \in (0,1)$ is a ratio that we shall determine in a moment. In that case, (4.3) holds with $c_0 = (1-\alpha)c_0'$.

Lemma 6 *Suppose that $y_N^D \ge z_D(\alpha c_0', z_1)$. Let $\tilde{y} \in \mathscr{Z}_f \cap \mathscr{A}$ satisfy $E'(\tilde{y}) = \tilde{f}$ (in the sense of* (2.6)*). Let $R = \min_{n\neq\xi}\min(z_2 - \tilde{y}_n', \tilde{y}_n' - z_1)$ and suppose that $\|f - \tilde{f}\|_* \le c_0 R$. Then, there exists a $y \in \mathscr{Z}_f \cap \mathscr{A}$ such that $E'(y) = f$.*

Proof If we follow the proof of Lemma 3 we obtain, for some t,

$$c_0|\tilde{y} - y_t|_{\mathrm{W}^{1,\infty}_{\varepsilon,f}} \le \|\tilde{f} - f_t\|_*. \tag{4.10}$$

To show that $y_t \in \mathscr{Z}_f$, note that (4.10) implies that $y_t \in \mathscr{A}$ as well as $z_1 \le y_{t,i}' \le z_2$ for $i \ne \xi$, and hence

$$\varepsilon y_\xi' = y_N^D - \sum_{i\neq\xi}\varepsilon y_i' \ge z_D - z_2 \ge z_D - z_t = \varepsilon z_f.$$

This implies that $y_t \in \mathscr{Z}_f$. In fact, if $z_1 < y_{t,i}' < z_2$ it follows that $y_t \in \mathrm{int}(\mathscr{Z}_f \cap \mathscr{A})$ and hence the proof can proceed as in Lemma 3 without further changes. ■

We can now use Lemma 6 to construct a reference state. Let y_N^D be a preliminary reference state defined as follows,

$$(y_i^D)' = \begin{cases} i\varepsilon z_m, & \text{if } i < \xi \\ y_N^D - z_m(1 - i\varepsilon), & \text{if } i \geq \xi. \end{cases}$$

As in the elastic case, we estimate the residual of y^D. Fix $n \in \mathbb{N}$ and assume, without loss of generality, that $n < \xi$. Since $z_f \geq z_t$ and $J''(z) < 0$ for $z > z_t$ it follows that J' is decreasing in that domain. In particular, we have $|J'(z_f + z)| \leq |J'(z_1 + z)|$ whenever $z \geq z_1$. Using this fact, and otherwise closely following the computations in §3.2, we have

$$|E_n'(y^D)| \leq \sum_{r=n\wedge(\xi-n)+1}^{\infty} \big|J'(rz_m)\big|.$$

Summing over $n < \xi$, we obtain

$$\sum_{n<\xi} |E_n'(y^D)| \leq \frac{1}{2}\sum_{r=2}^{\infty}(r-1)|J'(rz_m)|.$$

We now add the terms with $n \geq \xi$ which gives

$$\|E'(y^D)\|_* \leq \rho_1(z_m). \tag{4.11}$$

Setting $\tilde{y} = y^D$, $\tilde{f} = E'(\tilde{y})$, $f = 0$ in Lemma 6 we obtain $y^* \in \mathscr{Z}_f$, satisfying $E'(y^*) = 0$. We note that

$$|y_i^{*\prime} - z_m| \leq c_0^{-1}\|E'(y^D)\|_* \leq 2\frac{\rho_1(z_m)}{(1-\alpha)\rho_2(z_1, z_2)}, \qquad i \neq \xi. \tag{4.12}$$

If the conditions of Theorem 4 are satisfied, then there exists $\alpha > 0$, independent of ε, such that

$$2\frac{\rho_1(z_m)}{(1-\alpha)\rho_2(z_1, z_2)} < R,$$

which implies that $y^* \in \mathrm{int}(\mathscr{Z}_f \cap \mathscr{A})$. All results of Theorem 4 now follow from another application of Lemma 6 setting $\tilde{y} = y^*$ and $\tilde{f} = 0$. In particular, it is sufficient to assume that $y_N^D \geq z_D(\alpha c_0', z_1)$.

4.3 Coercivity of the QC approximation

First of all, we note that the assumption of Theorem 5 allows us to assume that $\{\xi - 1, \xi\} \subset \mathcal{T}$. This is in fact a necessary condition to make an approximation of a fracture in $\mathrm{w}^{1,\infty}_{\varepsilon,f}$ possible.

Let $Y \in \mathscr{Z}_f$ and $U \in \mathscr{A}_0(\mathcal{T})$. Following §4.1 and §3.3 we assume that $\overline{U}_p' = |U|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}$ and define the test function V by

$$\overline{V}_k' = \begin{cases} \frac{1}{2}h_p^{-1}, & \text{if } k = p \\ -\frac{1}{2}\varepsilon^{-1}, & \text{if } k = \xi \\ 0, & \text{otherwise.} \end{cases}$$

Then, assuming again without loss of generality that $t_p < \xi$, and using (4.1), we have

$$\begin{aligned}
E''(Y;U,V) &= \sum_{n=1}^{N}\sum_{m=1}^{N} \varepsilon F''_{nm}(Y)U'_n V'_m \\
&= \frac{\varepsilon}{2h_p}\sum_{n=1}^{N}\sum_{m=t_{p-1}+1}^{t_p} F''_{nm}(Y)U'_n - \frac{1}{2}\sum_{n=1}^{N} F''_{n\xi}(Y)U'_n \\
&\geq \frac{\varepsilon}{2h_p}\sum_{m=t_{p-1}+1}^{t_p}\Big[\sum_{n<\xi} F''_{nm}(Y)U'_n + \sum_{n\geq\xi, n\in P} F''_{n\xi}(Y)U'_n\Big] - \sum_{n\in Q} F''_{n\xi}(Y)U'_n \\
&\geq \frac{\varepsilon}{2h_p}\sum_{m=t_{p-1}+1}^{t_p}\sum_{n<\xi} F''_{nm}(Y)U'_n - \frac{1}{2}\sum_{n\neq\xi} F''_{n\xi}(Y)|U'_n| - \frac{1}{2}|U'_\xi| F''_{\xi\xi}(Y).
\end{aligned}$$

We estimate the first term as in §3.3 and the second and third term as in §4.1 which gives

$$E''(Y;U,V) \geq \frac{1}{2}|U|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}\big(\rho_2(z_1,z_2) + 2N\rho_{2,f}(z_f,z_1)\big),$$

and thus (4.4). If E is replaced by $\tilde{E}$, we have instead

$$\tilde{E}''(Y;U,V) \geq \frac{1}{2}|U|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}\big(\tilde{\rho}_2(z_1,z_2) + 2N\tilde{\rho}_{2,f}(z_f,z_1)\big). \tag{4.13}$$

4.4 Proof of Theorem 5

To prove the QC error estimate we can repeat the fixed point argument of §3.4 almost verbatim. Only two modifications need to be made. First, as in the existence proof of §4.2 we need to show that a solution of the linearized problem appearing in the fixed point argument lies in $\mathscr{Z}_f$. This can be done by the same argument as in the proof of Lemma 6, if we choose y_N^D sufficiently large. This method was suitable for the existence theorem where we needed to contruct a reference solution. Now, however, the reference solution is given by the exact solution y which allows us to follow a more general approach.

As in §3.4 let $Y_\varphi = \mathcal{L}(\varphi)$, then,

$$\begin{aligned}
\varepsilon(Y_\varphi)'_\xi &= y_N^D - \sum_{i\neq\xi}\varepsilon(Y_\varphi)'_i \\
&= \sum_{i=1}^{N}\varepsilon\Pi y'_i - \sum_{i\neq\xi}\varepsilon(Y_\varphi)'_i \\
&= \varepsilon y'_\xi - |\Pi y - Y_\varphi|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}.
\end{aligned}$$

Hence, in order to guarantee $Y_\varphi \in \mathscr{Z}_f$, we require

$$y'_\xi \geq z_f + N|\Pi y - Y_\varphi|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}.$$

This may seem an insurmountable requirement at first but remember that y'_ξ is typically of order N. For $|\Pi y - Y_\varphi|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}$ we have the estimate

$$|Y_\varphi - \Pi y|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}} \le c_0^{-1}\big(c_1\mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3\big).$$

Hence, if (4.6) holds, then we can deduce the existence of a QC solution in the set $\mathscr{Z}_f$.

Our second modification of the proof of §3.4 is to compute a new bound for $\mathcal{E}_3$. To this end, we use (3.12) again to estimate

$$\begin{aligned} |E'(\theta; V) - \tilde{E}'(\theta; V)| &= \sum_{n=1}^{N} \varepsilon |F'_n(\theta) - \tilde{F}'_n(\theta)\Big||V'_n| \\ &\le |V|_{\mathrm{w}^{1,1}_\varepsilon} \max_{n=1,\dots,N} |F'_n(\theta) - \tilde{F}'_n(\theta)\Big|. \end{aligned}$$

For each n, we have

$$|F'_n(\theta) - \tilde{F}'(\theta)| \le \sum_{i=1}^{n}\sum_{j=n}^{N} \big|J'\big(\varepsilon^{-1}(\theta_i - \theta_{j-1})\big) - \tilde{J}'\big(\varepsilon^{-1}(\theta_i - \theta_{j-1})\big)\big|.$$

As in the elastic case, we can estimate and rearrange this sum to obtain (4.7).

5 Concluding Remarks

Clearly, the relative completeness of our results was primarily due to the one-dimensional setting that we have chosen. However, the fundamental approach to error estimation for the QC method, namely a fixed point argument based on the $\mathrm{w}^{1,\infty}_\varepsilon$–norm (or its modifications), can be employed in higher dimensions as well. In fact, it can be seen that, if we assume coercivity directly, rather than proving it as we have done here, then, our result concerning the existence of a QC solution near a stable exact solution carries over immediately. However, the main difference between ellipticity (cf. Lin [8]) and the inf-sup condition which we have employed is that the inf-sup condition does not automatically translate to subspaces. The natural next step therefore has to be a detailed investigation of the inf-sup condition in two and three dimensional atomistic problems, first for regular lattices, and then for several types of defects.

Another fact worth noting is that the $\mathrm{w}^{1,\infty}_\varepsilon$–norm employed in the elastic analysis is actually equivalent (in the sense that the constants are independent of ε) to the *energy norm* $u \mapsto \|E''(\theta)u\|_*$, for any $\theta \in \mathscr{Z}_e$. Similarly, the $\mathrm{w}^{1,\infty}_{\varepsilon,f}$–norm from the analysis in §4 is equivalent to $u \mapsto \|E''(\theta)u\|_*$, for any $\theta \in \mathscr{Z}_f$. This indicates that it may in principle be possible to unify the analysis of stable critical points. For this purpose, one would have to check in each case whether E'' is Lipschitz continuous with respect to this linearized energy norm.

Appendix A Auxiliary Results

In this appendix, we collect some results that are used throughout this paper, and which are closely related to, and whose formulation and proof do not differ much from, their corresponding continuum versions.

Lemma 7 *Let* $(g_i)_{i=1}^L \in \mathbb{R}^L$ *and* $\sum_{i=1}^L g_i = 0$*; then*

$$|g_i| \leq L^{-1} \sum_{k=2}^{L} |g_k - g_{k-1}| \phi_{i,k}, \qquad i = 1, \dots, L, \tag{A.1}$$

where $\phi_{i,k} = k - 1$ *for* $k = 2, \dots, i$ *and* $\phi_{i,k} = L - k + 1$ *for* $k = i + 1, \dots, L$.

Proof Set $\varepsilon = 1$ and let $i \in \{1, \dots, L\}$; then

$$\begin{aligned}
|g_i| &= \left| g_i - L^{-1} \sum_{j=1}^{L} g_j \right| \\
&= L^{-1} \left| \sum_{j=1}^{L} (g_i - g_j) \right| \\
&\leq L^{-1} \sum_{j=1}^{i-1} |g_i - g_j| + L^{-1} \sum_{j=i+1}^{L} |g_i - g_j| \\
&\leq L^{-1} \sum_{j=1}^{i-1} \sum_{k=j+1}^{i} |g_k'| + L^{-1} \sum_{j=i+1}^{L} \sum_{k=i+1}^{j} |g_k'| \\
&= L^{-1} \sum_{k=2}^{i} |g_k'| \sum_{j=1}^{k-1} 1 + L^{-1} \sum_{k=i+1}^{L} |g_k'| \sum_{j=k}^{L} 1 \\
&= L^{-1} \sum_{k=2}^{i} |g_k'|(k-1) + L^{-1} \sum_{k=i+1}^{L} |g_k'|(L-k+1).
\end{aligned}$$

■

Lemma 8 (Discrete Friedrichs and Poincaré Inequalities) *Suppose that* $L \geq 1$, *and that* $(f_i)_{i=0}^L \in \mathbb{R}^{L+1}$ *and* $(g_i)_{i=1}^L \in \mathbb{R}^L$ *such that* $f_0 = f_L = 0$ *and* $\sum_{i=1}^L g_i = 0$. *For* $p \in \{1, \infty\}$ *we have*

$$\begin{aligned}
\|f\|_{\ell^p_\varepsilon(\!(0,L)\!)} &\leq \frac{1}{2}(\epsilon L)|f|_{\mathrm{w}^{1,p}_\varepsilon(\!(0,L)\!)}, \quad \text{and} &\text{(A.2)}\\
\|g\|_{\ell^p_\varepsilon(\!(1,L)\!)} &\leq \frac{1}{2}(\epsilon L)|g|_{\mathrm{w}^{1,p}_\varepsilon(\!(1,L)\!)}. &\text{(A.3)}
\end{aligned}$$

Proof First, we note that all occurances of ε can be removed from the results by simple cancellation. Furthermore, the inequalities are trivial if $L = 1$. Thus, we assume without loss of generality that $\varepsilon = 1$ and $L \geq 2$.

We begin with the case $p = 1$. To obtain (A.2), consider

$$\begin{aligned}
\sum_{i=0}^{L} |f_i| &= \sum_{i=1}^{L-1} |f_i| \\
&= \frac{1}{2} \sum_{i=1}^{L-1} \left[\Big| \sum_{j=1}^{i} (f_j - f_{j-1}) \Big| + \Big| \sum_{j=i+1}^{L} (f_j - f_{j-1}) \Big| \right] \\
&\le \frac{1}{2} \sum_{i=1}^{L-1} \sum_{j=1}^{L} |f_j - f_{j-1}| \\
&= L \frac{1}{2} \Big(1 - \frac{1}{L} \Big) \sum_{j=1}^{L} |f_j - f_{j-1}|.
\end{aligned}$$

To obtain (A.3), we sum inequality (A.1) over $i = 1, \ldots, L$ to obtain

$$\begin{aligned}
\sum_{i=1}^{L} |g_i| &\le L^{-1} \sum_{i=1}^{L} \sum_{k=2}^{i} |g'_k|(k-1) + L^{-1} \sum_{i=1}^{L} \sum_{k=i+1}^{L} |g'_k|(L-k+1) \\
&= L^{-1} \sum_{k=2}^{L} |g'_k| \sum_{i=k}^{L} (k-1) + L^{-1} \sum_{k=2}^{L} |g'_k| \sum_{i=1}^{k-1} (L-k+1) \\
&= \frac{2}{L} \sum_{k=2}^{L} |g'_k|(k-1)(L-k+1) \\
&\le \frac{2}{L} \max_{k=2,\ldots,L} (k-1)(L-k+1) \sum_{k=2}^{L} |g'_k|.
\end{aligned}$$

For $p = \infty$, suppose that $|f_i| = \max_{j=0,\ldots,L} |f_j|$; then

$$\max_{j=0,\ldots,L} |f_j| = |f_i| \le \sum_{j=1}^{i} |f_j - f_{j-1}| \le i \max_{j=1,\ldots,L} |f_j - f_{j-1}|.$$

Similarly, we also have

$$\max_{j=0,\ldots,L} |f_j| = |f_i| \le \sum_{j=i+1}^{L} |f_j - f_{j-1}| \le (L-i) \max_{j=1,\ldots,L} |f_j - f_{j-1}|,$$

and therefore,

$$\max_{j=0,\ldots,L} |f_j| \le \min(i, L-i) \max_{j=1,\ldots,L} |f_j - f_{j-1}|,$$

which gives (A.2) with $p = \infty$.

Using Lemma 7, we have, for each $i = 1, \dots, L$,

$$
\begin{aligned}
|g_i| &\leq L^{-1} \sum_{j=2}^{i} |g'_j|(j-1) + L^{-1} \sum_{j=i+1} |g'_j|(L-j+1) \\
&\leq \frac{1}{L} \max_{j=2,\dots,L} |g'_j| \frac{1}{2}\big[i(i-1) + (L-i)(L-i+1)\big] \\
&= \frac{1}{2L} \max_{j=2,\dots,L} |g'_j| \big[L^2 + L - 2Li + 2i^2 - 2i\big] \\
&= \frac{1}{2L} \max_{j=2,\dots,L} |g'_j| \big[L(L-1) - 2(L-i)(i-1)\big] \\
&\leq L\Big(\frac{1}{2} - \frac{1}{2L}\Big) \max_{j=2,\dots,L} |g'_j|.
\end{aligned}
$$

■

We note that (A.2) and (A.3) are of course valid for any p with constants independend of ε. Furthermore the optimal Friedrichs constants $C_{p,L}$ and Poincaré constants $\bar{C}_{p,L}$ in the cases $p \in \{1, 2, \infty\}$ satisfy

$$
\begin{aligned}
C_{1,L} &= \frac{1}{2} - \frac{1}{2L}, \quad \bar{C}_{1,L} = \begin{cases} 1/2, & \text{if } L \text{ is even,} \\ (1/2) - (1/2L), & \text{if } L \text{ is odd.} \end{cases}, \\
C_{\infty,L} &= \begin{cases} 1/2, & \text{if } L \text{ is even,} \\ (1/2) - (1/2L), & \text{if } L \text{ is odd.} \end{cases}, \text{ and } \bar{C}_{\infty,L} = \frac{1}{2} - \frac{1}{2L}, \text{ and} \\
\frac{1}{\pi} &= \lim_{L\to\infty} C_{2,L} \leq C_{2,L} = \bar{C}_{2,L} = \frac{1}{2L\sin(\pi/(2L))} \leq C_{2,2} = 8^{-1/2}, C_{2,1} = \bar{C}_{2,1} = 0.
\end{aligned}
$$

In one dimension we also have the following imbedding inequality.

Lemma 9 *Let $(f_i)_{i=0,\dots,N} \in \mathbb{R}^{N+1}$ with $f_0 = f_L = 0$. Then,*

$$
\|f\|_{\ell^\infty_\varepsilon} \leq \frac{1}{2}|f|_{\mathrm{w}^{1,\infty}_\varepsilon}.
$$

Proof For each $i \in \{1, \dots, N-1\}$, we have

$$
\begin{aligned}
|f_i| &\leq \sum_{j=1}^{i} \varepsilon |f'_j| \quad \text{as well as} \\
|f_i| &\leq \sum_{j=i+1}^{N} \varepsilon |f'_j|.
\end{aligned}
$$

Adding the two inequalities gives the desired result. ■

Finally, we combine the estimates of Lemma 8 to obtain the following interpolation error estimates.

Theorem 10 (Bounds on the Interpolation Error) *Suppose that $(f_i)_{i=0,\dots,L} \in \mathbb{R}^{L+1}$ and let*

$$
F_i = f_0 + \frac{i}{L}(f_L - f_0)
$$

be the affine interpolant of f. Then, for $p \in \{1, \infty\}$,

$$|f - F|_{\mathrm{w}_\varepsilon^{1,p}(\!(0,L)\!)} \le \frac{1}{2}(\varepsilon L)|f|_{\mathrm{w}_\varepsilon^{2,p}(\!(0,L)\!)}, \quad \text{and} \tag{A.4}$$

$$\|f - F\|_{\ell_\varepsilon^p(\!(0,L)\!)} \le \frac{1}{4}(\varepsilon L)^2|f|_{\mathrm{w}_\varepsilon^{2,p}(\!(0,L)\!)}. \tag{A.5}$$

Proof First note that the grid function $\tilde{f} = f - F$ satisfies $\tilde{f}_0 = \tilde{f}_L = 0$ and therefore $\sum_{i=1}^L \tilde{f}_i' = 0$. Inequality (A.4) therefore follows directly from (A.3).

The estimate (A.5) can be obtained by applying first (A.2) and then (A.3),

$$\begin{aligned}\|f - F\|_{\ell_\varepsilon^p(\!(0,L)\!)} &\le \frac{1}{2}(\epsilon L)|(f-F)'|_{\ell_\varepsilon^p(\!(1,L)\!)} \\ &\le \frac{1}{4}(\epsilon L)^2\|f''\|_{\ell_\varepsilon^p(\!(1,L-1)\!)} \\ &= \frac{1}{4}(\epsilon L)^2|f|_{\mathrm{w}_\varepsilon^{2,p}(\!(0,L)\!)}.\end{aligned}$$

■

Appendix B Computation of Coercivity Regions

In this appendix, we demonstrate that our hypotheses can indeed be satisfied. With the use of simple MATLAB scripts it is straightforward to compute possible values for z_1, z_2 and, in the fracture case, for z_f. We have included only the elastic case here since the additional requirements of the fracture case are very easily met given the fast decay of most interaction potentials.

We slightly rescale the Lennard–Jones potential so that its minimum lies at $z = 1$,

$$J(z) = z^{-12} - 2z^{-6}.$$

Hence, we have $z_m = 1$ and $z_t = (13/7)^{1/6} \approx 1.11$. If we choose $z_1 = 0.88$ and $z_2 = 1.06$, we obtain $\rho_2(z_1, z_2) \approx 12.5$. Furthermore, we have $\rho_1(z_m) \approx 0.2$ which guarantees the existence of a reference state for sufficiently small boundary displacements.

The Morse potential is slightly less forthcoming in this respect. First, we note that $z_m = 1$ and $z_t = 1 + \alpha^{-1}\log(2)$. If we choose $\alpha = 1$ in (2.3) we obtain $\rho_2(z_m, z_m) \approx -3.8$ and we have therefore no hope of constructing an equilibrium with the technique we have used. This does not mean that E has no equilibrium in this case. In fact, the mere existence of a global energy minimum can be easily deduced by a compactness argument. However, numerical experiments indicate that those equilibria are extremely unstable and bear no resemblance to the observed equilibria of metallic materials. Furthermore, there seems to be no convergence of those equilibria to a continuum as $N \to \infty$.

If we make the well steeper, however, we can achieve coercivity. Already for $\alpha = 4$, we can choose $z_1 = 0.9$ and $z_2 = 1.08$ to obtain $\rho_2(z_1, z_2) \approx 5.38$. Since $\rho_1(z_m) \approx 0.3$ is follows that $0.8 \times \rho_2(z_1, z_2) > \rho_1(z_m)$ and hence there exists a reference state for sufficiently small boundary displacements.

Finally, we should note that the steeper the basin of convexity around z_m (the larger α in the Morse potential case) the better the bounds become. The potentials for metals, in particular, have shapes that correspond to a large α.

References

[1] X. Blanc, C. Le Bris, and F. Legoll. Analysis of a prototypical multiscale method coupling atomistic and continuum mechanics. *M2AN Math. Model. Numer. Anal.*, 39(4):797–826, 2005.

[2] M. S. Daw and M. I. Baskes. Embedded-Atom Method: Derivation and Application to Impurities, Surfaces, and other Defects in Metals. *Physical Review B*, 20, 1984.

[3] W. E and B. Engquist. The heterogeneous multiscale methods. *Commun. Math. Sci.*, 1(1):87–132, 2003.

[4] W. E and P. Ming. Analysis of the local quasicontinuum method. Preprint.

[5] W. E and P. Ming. Analysis of multiscale methods. *J. Comput. Math.*, 22(2):210–219, 2004. Special issue dedicated to the 70th birthday of Professor Zhong-Ci Shi.

[6] J.E. Jones. On the Determination of Molecular Fields. III. From Crystal Measurements and Kinetic Theory Data. *Proc. Roy. Soc. London A.*, 106:709–718, 1924.

[7] P. Lin. Theoretical and numerical analysis for the quasi-continuum approximation of a material particle model. *Math. Comp.*, 72(242):657–675 (electronic), 2003.

[8] P. Lin. Convergence analysis of a quasi-continuum approximation for a two-dimensional material without defects. to appear in SIAM J. Num. Ana., 2006.

[9] R.E. Miller and E.B. Tadmor. The Quasicontinuum Method: Overview, Applications and Current Directions. *Journal of Computer-Aided Materials Design*, 9:203–239, 2003.

[10] P.M. Morse. Diatomic Molecules According to the Wave Mechanics. II. Vibrational Levels. *Phys.Rev.*, 34:57–64, 1929.

[11] M. Ortiz, R. Phillips, and E. B. Tadmor. Quasicontinuum Analysis of Defects in Solids. *Philosophical Magazine A*, 73(6):1529–1563, 1996.

[12] C. Ortner. Gradient flows as a selection procedure for equlibria of non–convex energies. To appear in SIAM J. Math. Anal.

[13] C. Ortner and E. Süli. A-posteriori analysis and adaptive algorithms for the quasicontinuum method in one dimension. Technical Report NA06/13, Oxford University Computing Laboratory, 2006.

[14] C. Ortner and E. Süli. Discontinuous Galerkin finite element approximation of nonlinear second-order elliptic and hyperbolic systems. Technical Report NA06/05, Oxford University Computing Laboratory, 2006.

[15] L. Truskinovsky. Fracture as a phase transformation. In R. C. Batra and M. F. Beatty, editors, *Contemporary research in mechanics and mathematics of materials*, pages 322–332. CIMNE, 1996.

[16] E. Zeidler. *Nonlinear functional analysis and its applications. I.* Springer-Verlag, New York, 1986. Fixed-point theorems, Translated from the German by Peter R. Wadsack.