ESAIM: M2AN
Vol. 42, N° 1, 2008, pp. 57–91
DOI: 10.1051/m2an:2007057

ESAIM: Mathematical Modelling and Numerical Analysis
www.esaim-m2an.org

ANALYSIS OF A QUASICONTINUUM METHOD IN ONE DIMENSION*

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Abstract. 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 aim to give a detailed *a priori* and *a posteriori* error analysis for a quasicontinuum method in one dimension. We consider atomistic models with Lennard–Jones type long-range interactions and a QC formulation which incorporates several important aspects of practical QC methods. First, we prove the existence, the local uniqueness and the stability with respect to a discrete $W^{1,\infty}$-norm of elastic and fractured atomistic solutions. We use a fixed point argument to prove the existence of a quasicontinuum approximation which satisfies a quasi-optimal *a priori* error bound. We then reverse the role of exact and approximate solution and prove that, if a computed quasicontinuum solution is stable in a sense that we make precise and has a sufficiently small residual, there exists a 'nearby' exact solution which it approximates, and we give an *a posteriori* error bound. We stress that, despite the fact that we use linearization techniques in the analysis, our results apply to genuinely nonlinear situations.

Mathematics Subject Classification. 70C20, 70-08, 65N15.

Received October 11, 2006. Revised April 17, 2007.

1. Introduction

For the numerical simulation of microscopic material behaviour such as 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 *et al.* [18] and subsequently improved by many other authors; see [16] 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 atomistic description of the defect. We give a detailed description of a version of the QC method analyzed in this paper in Section 2.2.

Keywords and phrases. Atomistic material models, quasicontinuum method, error analysis, stability.

* *The authors acknowledge the financial support received from the European research project HPRN-CT-2002-00284:* New Materials, Adaptive Systems and their Nonlinearities. Modelling, Control and Numerical Simulation*, and the kind hospitality of Carlo Lovadina and Matteo Negri (University of Pavia).*

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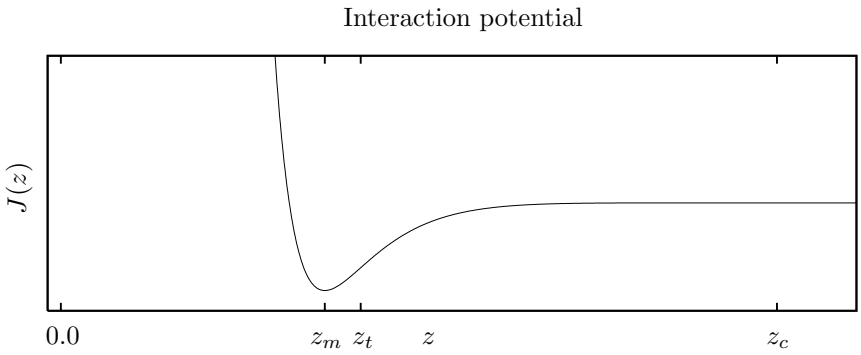

FIGURE 1. The shape of the atomistic interaction potentials with cut-off radius z_c.

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 analytical effort was by Lin [14] who considers the QC approximation of the reference state (without boundary displacements or applied forces) of a one-dimensional Lennard–Jones model. He proves that the global energy minimum of the full atomistic model as well as that of the reduced QC model lie in a region where the interaction potential is uniformly convex and uses these facts to derive an *a priori* error estimate.

E and Ming [9, 10] analyze the local QC method in the context of the heterogeneous multiscale method [8], which requires the assumption that a nearby smooth, elastic continuum solution is available. The error is estimated in terms of the atomic spacing in relation to the domain size as well as the mesh size.

In [15], Lin gives *a priori* error estimates for a modified version of the local 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 [15]) on the exact solution of the atomistic model as well as on its QC approximation. Essentially, he assumed generally what he was able to prove in one dimension, namely 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 still be difficult to verify rigorously. For lattice domains with 'sharp', 're-entrant' boundary sections or defects we should not expect this assumption to hold, at least not in the form used in [15]. Some indication is also given as to how the analysis might be extended to the case of localized defects.

Dobson and Luskin [6] give the first analysis of some important aspects of most practical QC methods, particularly the force-based approximation and the interface between regions where different types of approximation are used (see also Sect. 2.2) which requires a so-called ghost-force correction.

Finally, we mention the work of Blanc *et al.* [1] where a multiscale method similar to the QC method is analyzed. Only nearest-neighbour interactions in one dimension are considered which makes it possible to compute the exact solutions analytically. Nevertheless, it must be emphasized that this is the only analytical work, so far, to consider defects.

To the best of our knowledge, the *a posteriori* error analysis of the QC method has not so far been considered in the literature.

It is not too surprising that so little mathematical analysis is available for atomistic material models. For example, most techniques in continuum finite element analysis apply only if the differential operator appearing in the equation is monotone, *i.e.*, when the associated energy functional is convex, an assumption which is grossly violated for atomistic problems (*cf.* Fig. 1). Furthermore, energy techniques, such as Γ-convergence [2–4], cannot be applied for two reasons: first, atomistic solutions are not, in general, global energy minima (*cf.* [19, 23] for further discussions of this statement), and second, proving convergence alone is meaningless since the function space is finite-dimensional.

The present work is an effort to unify and generalize previous results and 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.*, strict local minimizers of the atomistic energy. In order to keep the presentation simple, we consider only long-range (in the sense that any two atoms interact and that $J'(r)$ is non-zero for all r; *cf.* (1)) 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 Section 2.1.

Under sufficiently strong assumptions on the exact and the QC solution (in essence, one would have to assume a fairly strong *a priori* bound on a discrete $\mathrm{W}^{1,\infty}$-norm of the error) it is always possible to prove quasi-optimal approximation error bounds, for example, with respect to H^1-type norms. Thus, our aim in this paper is to identify situations in which such assumptions are justified. Our primary concern is to be able to answer the following two central questions:

(i) Under what conditions does a QC solution exist which approximates a given exact solution of the atomistic model?

(ii) Given a computed QC solution, does an exact solution of the atomistic model approximated by the QC solution exist?

The answer to both questions is in general negative. However, at least in the one-dimensional setting of this paper we are able to give precise conditions under which they can be answered positively. The *a priori* analysis, related to question (i), is contained in Sections 3 and 4, *cf.* in particular Theorems 3.2 and 4.2. The preliminary results, Theorems 3.1 and 4.1, and the discussion in Appendix B show that the conditions can be satisfied in practise and are reasonably sharp. The *a posteriori* existence condition, raised in question (ii), is analysed in Section 5, in Theorems 5.1–5.3. We conclude in Section 6 with a numerical example which clearly demonstrates that our analysis is both non-trivial and sufficiently sharp that it can be applied to a wide range of genuinely nonlinear situations.

We would like to emphasize the last point further. Our use of the Inverse Function Theorem and similar techniques may give the impression that our analysis is only valid in the linearly elastic regime. This is, however, not the case. Since we linearize around an arbitrary solution, our results apply to genuinely nonlinear situations. Indeed, in the numerical example that we consider, the benchmark problem ranges from the linearly elastic regime to finite elasticity and fracture.

Both question (i) and (ii) are of course fundamental questions which should be raised for any nonlinear problem. We refer to the work of Brezzi *et al.* [5] for an *a priori* analysis of this flavour and to the review article by Plum [22] for a similar *a posteriori* analysis (though with slightly different techniques and different aims).

We conclude the introduction by fixing some notation for discrete function spaces and nonlinear functionals.

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 cases $p = 1, 2, \infty$ 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

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

1.2. **Functionals**

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 at 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 $\phi''(u; v, \cdot)$.

2. Model problem and QC approximation

2.1. The atomistic model problem

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

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

without changing the problem. 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 [12],

$$J(z) = Az^{-12} - Bz^{-6}, \tag{2}$$

and the Morse potential [17],

$$J(z) = \exp\big(-2\alpha(z-1)\big) - 2\exp\big(-\alpha(z-1)\big); \tag{3}$$

see also Figure 1 (the cut-off radius z_c will become important in the QC approximation and should be ignored for the time being). More generally, we assume that there exist $z_0 \in [-\infty, +\infty)$, $z_m, z_t > 0$ such that $z_0 < z_t/2 < z_m < z_t$,

$$\begin{aligned} &J \in \mathrm{C}^3(z_0, \infty), \quad J'(z_m) = 0, \quad J''(z_t) = 0, \\ &J(z) \to +\infty \text{ as } z \to z_0+, \quad J(z) = +\infty \quad \forall z \le z_0, \\ &J''(z) \ge 0 \quad \forall z \in (0, z_t] \quad \text{and} \quad J''(z) \le 0 \quad \forall z \in [z_t, \infty). \end{aligned} \tag{4}$$

The only condition which is not entirely natural is the assumption $z_t/2 < z_m$, which considerably simplifies the analysis and is not a true restriction – any realistic interaction potential should satisfy this. For example, it is satisfied for the Lennard–Jones potential (2) for all positive parameters A, B, and for the Morse potential (3) whenever $\alpha > \ln 2$.

Before we define what we mean by an atomistic solution, we need to mention that atomistic deformations are typically only local minimizers rather than global minimizers (*cf.* for example [19, 23]). 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 a 'Dirichlet' problem where the atomistic deformation is prescribed 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. Given a prescribed boundary deformation $y_N^D > 0$, we define the set of admissible deformations and the set of test functions respectively as

$$\mathscr{A} = \big\{y \in \mathbb{R}^{N+1} : y_0 = 0, y_N = y_N^D\big\} \quad \text{and} \quad \mathscr{A}_0 = \big\{u \in \mathbb{R}^{N+1} : u_0 = u_N = 0\big\}. \tag{5}$$

Each $f \in \mathbb{R}^{N+1}$ represents a linear body force. The atomistic problem is to *find a critical point 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 $E(y) - \langle f, y\rangle_\varepsilon$ in $\mathscr{A}$ with finite energy must satisfy

$$E'(y; v) = \langle f, v\rangle_\varepsilon \qquad \forall v \in \mathscr{A}_0. \tag{6}$$

If y satisfies (6), we say that $E'(y) = f$ in $\mathscr{A}$.

By a *solution* we mean a critical point of $E(y) - \langle f, y\rangle_\varepsilon$, *i.e.*, an atomistic deformation satisfying (6). By a *stable solution* we mean a strict local minimizer of $E(y) - \langle f, y\rangle_\varepsilon$.

Elastic deformations are those whose gradient is sufficiently close to z_m, in a region where the potential J is convex. Such solutions exist whenever f is sufficiently small. This is measured with respect to the *negative norm*

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

Since we can interpret f as a linear functional, we can extend the definition of the negative norm to linear maps $\ell\colon \mathscr{A}_0 \to \mathbb{R}$ by

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

For future reference, we define the quantities

$$\rho_1(z) = \sum_{r=2}^{\infty}(r-1)|J'(rz)|, \quad \text{and} \tag{7}$$

$$\rho_2(z_1, z_2) = \sum_{r=1}^{\infty} r^2 \min_{z_1\le z\le z_2} J''(rz), \tag{8}$$

which are important in the analysis of existence and stability of elastic deformations. For $z \in (0,\infty)$ fixed, 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 inf-sup 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

$$\rho_3(z_1, z_2) = \sum_{r=1}^{\infty} r^2 \max_{z_1\le z\le z_2} |J''(rz)|, \tag{9}$$

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 $0 = t_0 < t_1 < \cdots < t_K = N$ 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 admissible 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 $\overline{V}_k = V_{t_k}$ for the nodal values of an $S^1(\mathcal{T})$ function, and $\overline{V}_k' = V_{t_k}'$ for its derivatives. 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

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

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

The Galerkin approximation of (6) in $\mathscr{A}(\mathcal{T})$ is to *find critical points of* $E(Y) - \langle Y, f\rangle_\varepsilon$ *in* $\mathscr{A}(\mathcal{T})$. Any such critical point $Y \in \mathscr{A}(\mathcal{T})$ must satisfy

$$E'(Y;V) = \langle f, V\rangle_\varepsilon \qquad \forall\, V \in \mathscr{A}_0(\mathcal{T}). \tag{10}$$

However, in view of the long-range atomistic interaction, which, for the purpose of evaluating the energy and its derivatives still requires 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 z_c (*cf.* Fig. 1). In this case, 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

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

For the stability analysis 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 QC approximation to (6) which we analyze in this paper is to *find* $Y \in \mathscr{A}(\mathcal{T})$ *satisfying*

$$\tilde{E}'(Y;V) = \langle f, V\rangle_{\mathcal{T}} \qquad \forall\, V \in \mathscr{A}_0(\mathcal{T}). \tag{11}$$

Several QC methods have been formulated in the past. Our own formulation (11) is such that, in one dimension, it can be implemented requiring only $O(K)$ operations to assemble the energy $\tilde{E}(Y) - \langle f, Y\rangle$, the gradient $\langle \tilde{E}'(Y), V\rangle - \langle f, V\rangle_{\mathcal{T}}$ and the hessian $\tilde{E}''(Y)$. The three main features our QC formulation are: (i) it is an energy-based formulation, *i.e.*, the nonlinear system (11) is the Euler–Lagrange system of an energy; (ii) we have used the usual reduction of degrees of freedom using P1 finite elements; and (iii) on the approximation space the energy is approximated by the energy $\tilde{E}$ in order to render (11) computable. In comparison to most practical QC methods we have not employed any summation rule on the energy itself but only on the forcing term. It should be straightforward to include this in our analysis but, for presentational reasons, we have decided against this option. There are other important aspects of QC method such as force-based formulations where the resulting nonlinear system is not the Euler–Lagrange system of an energy functional, or ghost-force corrections at atomistic-continuum interfaces, which do not feature in our formulation. We refer to [6] for an excellent discussion of these and other aspects of the QC method.

2.3. **Stable equilibria**

In this work, we only analyze 'stable equilibria' of the atomistic energy (1) and the corresponding QC approximation. In principle, we would like to include all critical points y in our definition for which $E''(y;\cdot,\cdot)$ is positive definite. However, we shall be slightly more restrictive. Motivated by Proposition 2.1 below, we shall only analyze purely elastic deformations and deformations which have a single *fracture*, *i.e.*, a deformation gradient $y'_\xi \gg z_t$ for exactly one $\xi \in \{1,\dots,N\}$.

In the following result we state the unsurprising fact that critical points with more than one fracture cannot be uniform local minima of E. For $y \in \mathbb{R}^{N+1}$, we use $\lambda(y)$ to denote the smallest $\mathrm{w}^{1,2}_\varepsilon$-eigenvalue of $E''(y)$, *i.e.*,

$$\lambda(y) = \min_{\substack{u\in\mathscr{A}_0\\ |u|_{\mathrm{w}^{1,2}_\varepsilon}=1}} E''(y;u,u).$$

Proposition 2.1. *If $y \in \mathbb{R}^{N+1}$ with $y'_p \geq z_t$ and $y'_q \geq z_t$, where $1 \leq p < q \leq N$, then $\lambda(y) \leq 0$. If y'_p or y'_q is strictly greater than but sufficiently close to z_t, or if J is strictly increasing in $(z_t,+\infty)$, then $\lambda(y) < 0$.*

The proof of Proposition 2.1 will be given in Section 3.1. The result allows us to divide the stable critical points into two groups: *elastic* deformation (analyzed in Sect. 3) and *fractured* deformation (analyzed in Sect. 4).

3. Elastic deformation

Theorem 3.1. *Let J satisfy the assumptions of Section* 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 $2\rho_1(z_m) < R\,\rho_2(z_m - R, z_m + R)$; then, the following hold:*

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

$$\min_{y\in\mathscr{Z}_e} \min_{\substack{u\in\mathscr{A}_0\\ |u|_{\mathrm{w}^{1,\infty}_\varepsilon}=1}} \max_{\substack{v\in\mathscr{A}_0\\ |v|_{\mathrm{w}^{1,1}_\varepsilon}=1}} E''(y;u,v) \geq \tfrac{1}{2}\rho_2(z_1,z_2) =: c_0 > 0, \tag{12}$$

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

(b) *Existence: Let z_1, z_2 be as in* (a)*. There exist $\delta_1, \delta_2 > 0$, independent of ε, such that for every $y_N^D \in \mathbb{R}$ with $|y_N^D - z_m| < \delta_1$ (see* (5) *for the definition of y_N^D) and for every $f \in \mathbb{R}^{N+1}$ with $\|f\|_* \leq \delta_2$, there exists a solution y_f of* (6) *in $\mathscr{Z}_e$.*

(c) *Stability: Let z_1, z_2 be as in* (a)*. Let y_f, y_g be solutions to* (6) *in $\mathscr{Z}_e \cap \mathscr{A}$, corresponding respectively to the right-hand sides $f, g \in \mathbb{R}^{N+1}$; then*

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

Theorem 3.1 is of theoretical relevance in that it gives a relatively sharp condition under which elastic solutions to (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, *i.e.*, a deformation y^* such that $E'(y^*) = 0$, 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 Appendix 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, it seems more illuminating to make fewer assumptions on the structure of the problem, and impose stronger assumptions on a particular solution instead.

For any given $f \in \mathbb{R}^{N+1}$ and a solution $y \in \mathscr{A}$ of (6), we identify three error sources: the interpolation error,

$$\mathcal{E}_1 = |y - \Pi y|_{\mathrm{w}^{1,\infty}_\varepsilon}, \tag{13}$$

the perturbation of the linear form,

$$\mathcal{E}_2 = \max_{\substack{V\in\mathscr{A}_0(\mathcal{T})\\ |V|_{\mathrm{w}^{1,1}_\varepsilon}=1}} \big|\langle f, V\rangle_{\mathcal{T}} - \langle f, V\rangle_\varepsilon\big|, \tag{14}$$

and the perturbation of the energy,

$$\mathcal{E}_3 = \max_{Y\in\mathscr{A}(\mathcal{T})\cap\mathscr{Z}_e} \max_{\substack{V\in\mathscr{A}_0(\mathcal{T})\\ |V|_{\mathrm{w}^{1,1}_\varepsilon}=1}} \big|E'(Y;V) - \tilde{E}'(Y;V)\big|. \tag{15}$$

Theorem 3.2.

(a) *Let $\mathscr{Z}_e$ be defined as in Theorem* 3.1*; then,*

$$\min_{Y\in S^1(\mathcal{T})\cap\mathscr{Z}_e} \min_{\substack{U\in\mathscr{A}_0(\mathcal{T})\\ |U|_{\mathrm{w}^{1,\infty}_\varepsilon}=1}} \max_{\substack{V\in\mathscr{A}_0(\mathcal{T})\\ |V|_{\mathrm{w}^{1,1}_\varepsilon}=1}} E''(Y;U,V) \;\geq\; \tfrac{1}{2}\rho_2(z_1,z_2) = c_0, \text{ and} \tag{16}$$

$$\max_{Y\in S^1(\mathcal{T})\cap\mathscr{Z}_e} \max_{\substack{U\in\mathscr{A}_0(\mathcal{T})\\ |U|_{\mathrm{w}^{1,\infty}_\varepsilon}=1}} \max_{\substack{V\in\mathscr{A}_0(\mathcal{T})\\ |V|_{\mathrm{w}^{1,1}_\varepsilon}=1}} E''(Y;U,V) \;\leq\; \rho_3(z_1,z_2) =: c_1. \tag{17}$$

(b) *Let $y \in \mathscr{Z}_e \cap \mathscr{A}$ be a solution of* (6) *and define $R = \min_{i=1,\dots,N} \min(z_2 - y_i', y_i' - z_1)$. Assume, furthermore, that the QC mesh $\mathcal{T}$ and the cut-off radius are such that*

$$c_1\mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3 \leq c_0 R. \tag{18}$$

Then, there exists a solution $Y \in \mathscr{A}(\mathcal{T}) \cap \mathscr{Z}_e$ to (11) *which satisfies*

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

If $\tilde{\rho}_2(z_1, z_2) > 0$, 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:*

$$\mathcal{E}_1 \;\leq\; \tfrac{1}{2}\max_{k=1,\dots,K} h_k |y|_{\mathrm{w}^{2,\infty}_\varepsilon(\!(t_{k-1},t_k)\!)}, \tag{19}$$

$$\mathcal{E}_2 \;\leq\; \max_{k=1,\dots,K} h_k^2 \max\big(|f|_{\mathrm{w}^{2,\infty}_\varepsilon(\!(t_{k-1},t_k)\!)}, 2|f|_{\mathrm{w}^{1,\infty}_\varepsilon(\!(t_{k-1}+1,t_k)\!)} + 2|f|_{\mathrm{w}^{1,\infty}_\varepsilon(\!(t_{k-1},t_k-1)\!)}\big), \text{ and} \tag{20}$$

$$\mathcal{E}_3 \;\leq\; \sum_{r=1}^{\infty} r \max_{z_1\leq z\leq z_2} \big|\tilde{J}'(rz) - J'(rz)\big|. \tag{21}$$

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

$$E(y) \;=\; \sum_{i=1}^{N}\sum_{j=1}^{i} \varepsilon J\left(\sum_{k=j}^{i} y_k'\right). \tag{22}$$

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

$$\begin{aligned} E'(y;w) &= \sum_{i=1}^{N}\sum_{j=1}^{i}\varepsilon J'\left(\sum_{k=j}^{i} y'_k\right)\left(\sum_{n=j}^{i} w'_n\right) = \sum_{i=1}^{N}\sum_{j=1}^{i}\sum_{n=j}^{i}\varepsilon w'_n J'\big(\varepsilon^{-1}(y_i - y_{j-1})\big) \\ &= \sum_{i=1}^{N}\sum_{n=1}^{i}\varepsilon w'_n \sum_{j=1}^{n} J'\big(\varepsilon^{-1}(y_i - y_{j-1})\big) = \sum_{n=1}^{N}\varepsilon w'_n\left(\sum_{i=n}^{N}\sum_{j=1}^{n} J'\big(\varepsilon^{-1}(y_i - y_{j-1})\big)\right) \\ &= \sum_{n=1}^{N}\varepsilon F'_n(y) w'_n, \end{aligned} \tag{23}$$

where

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

Here and below we shall use the notation $n\vee m = \min(n,m)$ and $n\wedge m = \max(n,m)$. If E is twice differentiable at a point y, then $E''(y;v,w)$ is more conveniently written in the form

$$\begin{aligned} E''(y;v,w) &= \sum_{i=1}^{N}\sum_{j=1}^{i}\varepsilon J''\big(\varepsilon^{-1}(y_i - y_{j-1})\big)\left(\sum_{m=j}^{i} v'_m\right)\left(\sum_{n=j}^{i} w'_n\right) \\ &= \sum_{n=1}^{N}\varepsilon w'_n \sum_{i=n}^{N}\sum_{j=1}^{n}\sum_{m=j}^{i} v'_m J''\big(\varepsilon^{-1}(y_i - y_{j-1})\big) \\ &= \sum_{n=1}^{N}\varepsilon w'_n \sum_{i=n}^{N}\sum_{m=1}^{i}\sum_{j=1}^{n\wedge m} v'_m J''\big(\varepsilon^{-1}(y_i - y_{j-1})\big) \\ &= \sum_{n=1}^{N}\sum_{m=1}^{N}\varepsilon w'_n v'_m\left(\sum_{i=m\vee n}^{N}\sum_{j=1}^{n\wedge m} J''\big(\varepsilon^{-1}(y_i - y_{j-1})\big)\right) \\ &= \sum_{n=1}^{N}\sum_{m=1}^{N}\varepsilon F''_{nm} v'_m w'_n, \end{aligned} \tag{24}$$

where

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

As a first application of this decomposition, we give the proof of Proposition 2.1.

Proof of Proposition 2.1. We perturb y with a displacement $u \in \mathscr{A}_0$ such that

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

Then, $|u|^2_{\mathrm{w}^{1,2}_\varepsilon} = 2$ and, recalling that $p < q$,

$$\begin{aligned} E''(y;u,u) &= F''_{pp} + F''_{qq} - 2F''_{pq} \\ &= \sum_{i=p}^{N}\sum_{j=1}^{p} J''\big(\varepsilon^{-1}(y_i - y_{j-1})\big) + \sum_{i=q}^{N}\sum_{j=1}^{q} J''\big(\varepsilon^{-1}(y_i - y_{j-1})\big) - 2\sum_{i=q}^{N}\sum_{j=1}^{p} J''\big(\varepsilon^{-1}(y_i - y_{j-1})\big) \\ &= \sum_{i=p}^{q-1}\sum_{j=1}^{p} J''\big(\varepsilon^{-1}(y_i - y_{j-1})\big) + \sum_{i=q}^{N}\sum_{j=p+1}^{q} J''\big(\varepsilon^{-1}(y_i - y_{j-1})\big). \end{aligned}$$

Since $y'_p, y'_q \geq z_t$ it follows that $J''(\varepsilon^{-1}(y_i - y_{j-1})) \leq 0$ for all i and j appearing in the last two sums. If either y'_p or y'_q is strictly greater than but sufficiently close to z_t, or if $J'' < 0$ in $(z_t, +\infty)$, then this expression is negative. Hence the result follows. □

We now continue with the proof of coercivity of the atomistic problem. Our aim in this section is to identify a set of deformations,

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

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

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

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

$$\begin{cases} J''(z) > 0, & \text{for } z_1 \leq z \leq z_2, \text{ and} \\ J''(z) \leq 0, & \text{for } z \geq 2z_1, \end{cases} \tag{25}$$

and consequently $F''_{nm} \leq 0$ whenever $n \neq m$.

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 this definition 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 (24), we have

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

Using (25), we see that for $n \neq m$ we have $F''_{nm}(y) \leq 0$. Hence, we obtain

$$\begin{aligned} 2E''(y;u,v) &\geq F''_{pp}(y)u'_p + \sum_{m\in P\setminus\{p\}} F''_{pm}(y)u'_m - F''_{qq}(y)u'_q - \sum_{m\in Q\setminus\{q\}} F''_{qm}(y)u'_m \\ &\geq u'_p\Big[F''_{pp}(y) + \sum_{m\in P\setminus\{p\}} F''_{pm}(y)\Big] + (-u'_q)\Big[F''_{qq}(y) + \sum_{m\in Q\setminus\{q\}} F''_{qm}(y)\Big] \\ &\geq |u|_{\mathrm{w}^{1,\infty}_\varepsilon} \sum_{m=1}^{N} F''_{nm}(y), \end{aligned} \tag{26}$$

where $n \in \{p,q\}$. Thus, to prove the coercivity estimate (12), we need to show that the matrix $(F''_{nm})_{n,m=1}^N$ 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:

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

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

$$\sum_{m=1}^{N} F''_{nm}(y) \geq \sum_{m=1}^{n-1}\sum_{i=n}^{N}\sum_{j=1}^{m} \underline{J}''(i-j+1) + \sum_{m=n+1}^{N}\sum_{j=1}^{n}\sum_{i=m}^{N} \underline{J}''(i-j+1) + \sum_{j=1}^{n}\sum_{i=n}^{N} \underline{J}''(i-j+1). \tag{27}$$

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 to obtain

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

where we used $\sum_{j=n-r+1}^{n-1}(n-j) = r(r-1)/2$. Similarly, for the second triple-sum in (27), 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 (27), we have

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

On combining this with the previously obtained bounds, and recalling the definition (8), we finally arrive at

$$\sum_{m=1}^{N} F''_{nm}(y) \geq \sum_{r=1}^{\infty} r^2\underline{J}''(r) = \rho_2(z_1, z_2). \tag{28}$$

Therefore, returning to (26), we obtain

$$\max_{\substack{v\in\mathscr{A}_0\\ |v|_{\mathrm{w}_\varepsilon^{1,1}}=1}} E''(y;u,v) \geq c_0|u|_{\mathrm{w}_\varepsilon^{1,\infty}}, \tag{29}$$

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.

Corollary 3.3. *If $y \in \mathscr{Z}_e$ then $E''(y)$ is positive definite in*

$$\mathscr{A}_0' = \{u \in \mathbb{R}^{N+1} : u_0 = 0\}.$$

Proof. From (28) we deduce that the matrix $(F''_{nm})_{n,m=1}^N$ is strictly row diagonally dominant. Using the representation (24), and noting that each $u \in \mathscr{A}_0'$ has a unique representation in terms of u' and *vice versa*, we can immediately deduce that $E''(y)$ is positive definite in $\mathscr{A}_0'$. □

3.2. **Proof of Theorem 3.1**

The proof of Theorem 3.1 as well as its extension to fracture solutions in Section 4 rely on the following local existence result which is, in essence, a continuation principle for the Inverse Function Theorem.

Lemma 3.4. *Let $\|\cdot\|$ be a norm in $\mathscr{A}_0$, $R > 0$ and $\tilde{y} \in \mathscr{A}$, and define $\mathscr{Z} = \{y \in \mathscr{A} : \|y - \tilde{y}\| \leq R\}$. Suppose, further, that:*

(i) $\Phi\colon \mathbb{R}^{N+1} \to (-\infty, +\infty]$ *is three times continuously differentiable in $\mathscr{Z}$;*
(ii) $\Phi'(\tilde{y}) = \tilde{f}$ *in $\mathscr{A}$,* i.e., $\Phi'(\tilde{y}; v) = \langle \tilde{f}, v\rangle_\varepsilon \quad \forall v \in \mathscr{A}_0$;
(iii) *there exists $c_0 > 0$ such that*

$$c_0 \leq \min_{y\in\mathscr{Z}} \min_{\substack{u\in\mathscr{A}_0\\ \|u\|=1}} \max_{\substack{v\in\mathscr{A}_0\\ |v|_{\mathrm{w}_\varepsilon^{1,1}}=1}} \Phi''(y;u,v); \text{ and} \tag{30}$$

(iv) $\Phi''(y)$ *is positive definite for every $y \in \mathscr{Z}$.*

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

$$\|y - \tilde{y}\| \leq c_0^{-1}\|f - \tilde{f}\|_*. \tag{31}$$

Proof. As mentioned above, this result is a standard continuation principle for the Inverse Function Theorem and we therefore omit a complete proof here. We refer to the Zeidler's monograph [25] for an extensive discussion.

Let us simply note that (30) implies that $\Phi''(y)$ is an isomorphism for each $y \in \mathscr{Z}$ and thus, in each point $y \in \mathscr{Z}$ the Inverse Function Theorem can be applied. This fact can be used to successively solve for y_t given by $\Phi'(y_t) = (1-t)\tilde{f} + tf$. Given the condition $\|f - \tilde{f}\|_* \leq c_0 R$, it follows that this process can be continued up to $t = 1$ which yields the desired solution y. The uniqueness, which cannot in general be deduced, is guaranteed by the assumption that Φ'' is positive definite which implies that Φ is strictly convex in $\mathscr{Z}$. □

Lemma 3.4 gives a clear path to the proof of Theorem 3.1. 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 y_N^D will be fixed later, and estimate the residual $E'(y^D;\cdot)$. It is more convenient to do this using the following alternative representation of $E'(y;v)$:

$$E'(y;v) = \sum_{n=1}^{N-1} E_n'(y) v_n \qquad \forall y \in \mathscr{A},\ \forall v \in \mathscr{A}_0, \tag{32}$$

where

$$E_n'(y) = \sum_{i=0}^{n-1} J'\big(\varepsilon^{-1}(y_n - y_i)\big) - \sum_{i=n+1}^{N} J'\big(\varepsilon^{-1}(y_i - y_n)\big), \qquad n = 1, \dots, N-1. \tag{33}$$

Using the embedding inequality $\|v\|_{\ell_\varepsilon^\infty} \le \frac{1}{2}|v|_{\mathrm{w}_\varepsilon^{1,1}}$ (*cf.* Lem. A.3) we can estimate

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

which implies that

$$\|E'(y)\|_* \le \frac{1}{2} \sum_{n=1}^{N-1} |E_n'(y)|. \tag{34}$$

Setting $y = y^D$ in (33), we have

$$E_n'(y^D) = \begin{cases} \sum_{i=0}^{2n-N-1} J'\big((n-i)y_N^D\big), & \text{if } n \ge (N+1)/2, \\ -\sum_{i=2n+1}^{N} J'\big((i-n)y_N^D\big), & \text{if } n \le (N-1)/2, \\ 0, & \text{otherwise,} \end{cases}$$

and, taking absolute values,

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

Thus, we can estimate

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

We now apply Lemma 3.4 with $\Phi = E$, $\|\cdot\| = |\cdot|_{\mathrm{w}_\varepsilon^{1,\infty}}$, $\tilde{y} = y^D$ and $f = 0$. From the assumptions in Theorem 3.1 it follows that there exist z_1, z_2 such that

$$\rho_1(z_m) < \tfrac{1}{2}\rho_2(z_1, z_2) \times \min(z_2 - z_m, z_m - z_1).$$

Since ρ_1 is assumed to be continuous it furthermore follows that there exists $\delta_1 > 0$ such that, for $|y_N^D - z_m| \le \delta_1$,

$$\rho_1(y_N^D) < \tfrac{1}{2}\rho_2(z_1, z_2) \times \min(z_2 - y_N^D, y_N^D - z_1). \tag{35}$$

It therefore follows from Lemma 3.4 that there exists a reference state $y^* \in \mathscr{A}$ satisfying (6) with $f = 0$. From the stability estimate (31), we infer that

$$|y^* - y^D|_{\mathrm{w}^{1,\infty}_\varepsilon} \le c_0^{-1}\|E'(y^D)\|_* \le 2\frac{\rho_1(y^D_N)}{\rho_2(z_1,z_2)} < \min(z_2 - y^D_N, y^D_N - z_1).$$

Hence, there exists $R > 0$ such that $\{y \in \mathscr{A} : |y - y^*|_{\mathrm{w}^{1,\infty}_\varepsilon} \le R\} \subset \mathscr{Z}_e$. Applying Lemma 3.4 again, it follows that, for $\|f\|_* \le c_0 R =: \delta_2$, there exists a unique solution to (6) in $\mathscr{Z}_e$.

3.3. **Coercivity of the QC approximation**

In order to apply a similar technique as in Section 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

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

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

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

Using the estimate (28), we obtain

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

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

$$\min_{Y \in \mathscr{A}(\mathcal{T}) \cap \mathscr{Z}_e} \min_{\substack{U \in \mathscr{A}_0(\mathcal{T}) \\ |U|_{\mathrm{w}^{1,\infty}_\varepsilon} = 1}} \max_{\substack{V \in \mathscr{A}_0(\mathcal{T}) \\ |V|_{\mathrm{w}^{1,1}_\varepsilon} = 1}} \tilde{E}''(Y;U,V) \ge \tfrac{1}{2}\tilde{\rho}_2(z_1,z_2). \tag{36}$$

As in Section 3.1 we can again prove that $\tilde{E}''$ is positive definite.

Corollary 3.5. *Suppose that $\tilde{\rho}_2(z_1, z_2) > 0$. Then, for every $Y \in \mathscr{Z}_e$, $\tilde{E}''(Y)$ is positive definite in*

$$\mathscr{A}_0'(\mathcal{T}) = \{U \in \mathscr{A}(\mathcal{T}) : U_0 = 0\}.$$

3.4. **Proof of Theorem 3.2**

Stimulated by the *a priori* error analysis in [21], 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 (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 $V \in \mathscr{A}_0(\mathcal{T})$,

$$\begin{aligned}\int_0^1 E''\big(\Pi y + \tau(Y - \Pi y); Y - \Pi y, V\big)\,\mathrm{d}\tau &= E'(Y; V) - E'(\Pi y; V) \\ &= E'(Y; V) - \tilde{E}'(Y; V) + \langle f, V\rangle_{\mathcal{T}} - \langle f, V\rangle_{\varepsilon} + E'(y; V) - E'(\Pi y; V) =: \ell_Y(V).\end{aligned} \tag{37}$$

In fact, we see that Y is a solution of (11) if, and only if, it solves (37) 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

$$\int_0^1 E''\big(\Pi y + \tau(\varphi - \Pi y); Y_\varphi - \Pi y, V\big)\,\mathrm{d}\tau = \ell_\varphi(V) \qquad \forall V \in \mathscr{A}_0(\mathcal{T}). \tag{38}$$

Corollary 3.3 implies that there exists a unique Y_φ satisfying (38). Furthermore, we note that the construction of the test function V in Section 3.3 was independent of the base point and can therefore be performed uniformly for all $Y_\tau = \Pi y + \tau(\varphi - \Pi y)$. It therefore follows immediately that

$$\int_0^1 E''(Y_\tau; Y_\varphi - \Pi y, V)\,\mathrm{d}\tau \geq c_0 |Y_\varphi - \Pi y|_{\mathrm{w}^{1,\infty}_\varepsilon},$$

and we obtain

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

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 Section 3. Thus, in order for $\mathscr{L}$ to map $\mathscr{A}(\mathcal{T}) \cap \mathscr{Z}_e$ into itself, it is sufficient that

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

Since $\Pi y_{t_k} = y_{t_k}$ for $k = 0, \ldots, K$, 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 (18) 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 (11). From Corollary 3.5 we see that if $\tilde{\rho}_2(z_1, z_2) > 0$ then $\tilde{E}$ is strictly convex in $\mathscr{A}(\mathcal{T}) \cap \mathscr{Z}_e$ and hence the QC solution is unique in that set. This concludes the proof of part (b) of Theorem 3.2. 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

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

We can bound the sum in the last term by a computation identical to that in (28) except that the signs are reversed, and thus we obtain (17).

To bound $\mathcal{E}_1$ we simply use Theorem A.4 with $p=\infty$. For $\mathcal{E}_2$, we use Theorem A.4 with $p=1$ to estimate

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

For $i=t_{k-1}+1,\ldots,t_k-1$, 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 (69), we obtain

$$\begin{aligned}\big|\langle f,V\rangle_{\mathcal{T}}-\langle f,V\rangle_\varepsilon\big| &\leq \sum_{k=1}^{K}h_k^2\Big[|f|_{\mathrm{w}^{2,\infty}_\varepsilon(\!(t_{k-1},t_k)\!)}\|V\|_{\ell^1_\varepsilon(\!(t_{k-1}+1,t_k-1)\!)} \\ &\qquad +(|f|_{\mathrm{w}^{1,\infty}_\varepsilon(\!(t_{k-1}+1,t_k)\!)}+|f|_{\mathrm{w}^{1,\infty}_\varepsilon(\!(t_{k-1},t_k-1)\!)})|V|_{\mathrm{w}^{1,1}_\varepsilon(\!(t_{k-1},t_k)\!)}\Big] \\ &\leq \max_{k=1,\ldots,K}h_k^2\max\big(|f|_{\mathrm{w}^{2,\infty}_\varepsilon(\!(t_{k-1},t_k)\!)},2|f|_{\mathrm{w}^{1,\infty}_\varepsilon(\!(t_{k-1}+1,t_k)\!)} \\ &\qquad +2|f|_{\mathrm{w}^{1,\infty}_\varepsilon(\!(t_{k-1},t_k-1)\!)}\big)\big(\|V\|_{\ell^1_\varepsilon}+\tfrac12|V|_{\mathrm{w}^{1,1}_\varepsilon}\big).\end{aligned}$$

We apply (69) to estimate $\|V\|_{\ell^1_\varepsilon}\leq\frac12|V|_{\mathrm{w}^{1,1}_\varepsilon}$ and thus prove the bound (20).

Finally, defining $\tilde F'_n$ analogously to F'_n, and using (23), the bound (21) on $\mathcal{E}_3$ follows from

$$|E'(\theta;V)-\tilde E'(\theta;V)|\leq\sum_{n=1}^{N}\varepsilon|F'_n(\theta)-\tilde F'_n(\theta)||V'_n|\leq\max_{n=1,\ldots N}|F'_n(\theta)-\tilde F'_n(\theta)||V|_{\mathrm{w}^{1,1}_\varepsilon},$$

and a computation that is identical to the one leading to (35).

4. Fracture

We now look at a class of solutions of the atomistic model (6) with a single defect — a fracture. We fix an index $\xi\in\{1,\ldots,N\}$ 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 fracture 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 easily seen that $E''(y)$ has at least one negative eigenvalue (*cf.* Sect. 2.3).

However, even with a single fracture, it should be apparent from the analysis of Section 3.1 that we cannot expect (29) to hold when $|u|_{\mathrm{w}^{1,\infty}_\varepsilon} = |u'_\xi|$ since $J''(u'_\xi) \approx 0$. We therefore change the norm in which we analyze the error to the norm $|\cdot|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}$ defined by

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

Since we have imposed a Dirichlet condition at both endpoints, $|\cdot|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}$ is indeed a norm on $\mathscr{A}_0$. We use $B_f(y,R)$ to denote the balls, centre y and radius R, with respect to the $|\cdot|_{\mathrm{w}^{1,\infty}_\varepsilon}$-semi-norm. As was hinted above, we define

$$\mathscr{Z}_f = \big\{ y \in \mathscr{A} : y'_\xi \geq z_f \text{ and } z_1 \leq y'_i \leq z_2 \text{ for } i = 1,\dots,N, i \neq \xi \big\},$$

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

$$J'''(z) \geq 0 \qquad \text{for } z \geq z_f. \tag{39}$$

This typically imposes a negligible lower bound on z_f. We shall also need a further measure of stability,

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

The definition of $\rho_{2,f}$ does not involve z_2 because we have assumed (39). 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

$$\forall a > 0 \quad \forall z_1 \geq z_t/2 \quad \exists\, z_D = z_D(a, z_1) : \; N\rho_{2,f}\big(N(z_D - z_t), z_1\big) \geq -a. \tag{40}$$

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

Theorem 4.1. *Let J satisfy the assumptions of Section 2.1 as well as conditions (39) and (40). Assume also that there exists $R \in (0, \min(z_m - z_t/2, z_t - z_m))$ such that $4\rho_1(z_m) < R\rho_2(z_m - R, z_m + R)$; 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*

$$\min_{y\in\mathscr{Z}_f} \min_{\substack{u\in\mathscr{A}_0 \\ |u|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}=1}} \max_{\substack{v\in\mathscr{A}_0 \\ |v|_{\mathrm{w}^{1,1}_{\varepsilon}}=1}} E''(y;u,v) \geq \tfrac{1}{2}\big(\rho_2(z_1,z_2) + 2N\rho_{2,f}(z_f,z_1)\big) =: c_0 > 0, \tag{41}$$

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 (6) in $\mathscr{Z}_f$.*

(c) *Stability: Let y_f, y_g be solutions to (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 Section 3.

Theorem 4.2. *Let J satisfy the conditions of Section 2.1 as well as (39) and (40), 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*

$$\min_{Y\in\mathscr{Z}_f}\ \min_{\substack{U\in\mathscr{A}_0(\mathcal{T})\\ |U|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}=1}}\ \max_{\substack{V\in\mathscr{A}_0(\mathcal{T})\\ |V|_{\mathrm{w}^{1,1}_{\varepsilon}}=1}} E''(Y;U,V) \geq \tfrac{1}{2}\big(\rho_2(z_1,z_2)+2N\rho_{2,f}(z_f,z_1)\big) =: c_0, \quad \text{and} \tag{42}$$

$$\max_{Y\in S^1(\mathcal{T})\cap\mathscr{Z}_f}\ \max_{\substack{U\in\mathscr{A}_0(\mathcal{T})\\ |U|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}=1}}\ \max_{\substack{V\in\mathscr{A}_0(\mathcal{T})\\ |V|_{\mathrm{w}^{1,1}_{\varepsilon}}=1}} E''(Y;U,V) \leq \rho_3(z_1,z_2) =: c_1. \tag{43}$$

(b) *Suppose that $z_f > z_t$ is sufficiently large so that $c_0 > 0$ (*cf.* (40)). Let $y \in \mathscr{Z}_f \cap \mathscr{A}$ be a solution of* (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*

$$c_1\mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3 \leq c_0 \min\big(R, \varepsilon(y'_\xi - z_f)\big). \tag{44}$$

Then, there exists a solution $Y \in \mathscr{A}(\mathcal{T}) \cap \mathscr{Z}_f$ of the QC method (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* 3.2*, while $\mathcal{E}_3$ is now bounded by*

$$\mathcal{E}_3 \leq \sum_{r=1}^{\infty} r \max\left[\max_{z_1\leq z\leq z_2}\big|\tilde J'(rz) - J'(rz)\big|, \max_{z_1\leq z\leq z_2}\big|\tilde J'(z_f+(r-1)z) - J'(z_f+(r-1)z)\big|\right].$$

As we remark in Section 4.4, the condition (44) is not overly restrictive. We may think, for example that $z_f = O(\varepsilon^{-1})$ and $y'_\xi \geq 2z_f$. 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 mixed Dirichlet–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 $u'_p = |u|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}$ for some $p \in \{1,\dots,N\}\setminus\{\xi\}$. 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,

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

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 $F''_{np} \geq F''_{n\xi}$ for those n which lie on the opposite side of the fracture from p (*cf.* condition (39)).

If we assume, without loss of generality, that $p < \xi$, we obtain

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

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

$$E''(y;u,v) \geq \frac{1}{2}|u|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}} \left[\sum_{n<\xi} F''_{np}(y) + \sum_{n\neq\xi} F''_{n\xi}(y) + (N-1)F''_{\xi\xi}(y)\right]. \tag{45}$$

For the first sum in (45) we can use the same procedure as in the elastic case, *i.e.*,

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

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 (39) we have $F''_{n\xi} \geq F''_{\xi\xi}$ for all n and hence only need to estimate $F''_{\xi\xi}$,

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

Putting everything together, we obtain

$$E''(y;u,v) \geq \tfrac{1}{2}\big(\rho_2(z_1,z_2) + 2(N-1)\rho_{2,f}(z_f,z_1)\big)|u|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}. \tag{46}$$

4.2. **Proof of Theorem 4.1**

First, let us finalize the discussion 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 number that we shall determine in a moment. In that case, (41) holds with $c_0 = (1-\alpha)c'_0$.

In order to use Lemma 3.4 as in Section 3.2, we need to characterize the balls with respect to the $|\cdot|_{\mathrm{w}^{1,\infty}_{\varepsilon}}$-semi-norm. This is achieved in the following lemma.

Lemma 4.3. *Suppose that $y^D_N \geq z_D(\alpha c'_0, z_1)$. Then*

$$\mathscr{A} \cap B_f(\tilde{y}, R) \subset \mathscr{Z}_f \qquad \forall \tilde{y} \in \mathscr{Z}_f, \quad \forall R \leq \min_{n\neq\xi} \min(z_2 - \tilde{y}'_n, \tilde{y}'_n - z_1). \tag{47}$$

Proof. If $\tilde{y} \in \mathscr{Z}_f$ and $y \in \mathscr{A} \cap B_f(\tilde{y}, R)$ then

$$\varepsilon y'_\xi = y^D_N - \sum_{i\neq\xi} \varepsilon y'_i \geq z_D - z_2 \geq z_D - z_t = \varepsilon z_f. \qquad \square$$

Thanks to Lemma 4.3, the coercivity estimate (41) holds for all $y \in B(\tilde{y}, R)$ which makes it possible to use Lemma 3.4.

As in Section 3.2 we use Lemma 3.4 to construct a reference state. Let y^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 $J''(z) \leq 0$ 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 Section 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

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

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

$$\|E'(y^D)\|_* \leq 2\rho_1(z_m). \tag{48}$$

Setting $\Phi = E$, $\|\cdot\| = |\cdot|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}$, $\tilde{y} = y^D$, $\tilde{f} = E'(\tilde{y})$ and $f = 0$ in Lemma 3.4 we can deduce the existence of $y^* \in \mathscr{Z}_f$, satisfying $E'(y^*) = 0$. We note that

$$|y_i^{*\prime} - z_m| \leq c_0^{-1}\|E'(y^D)\|_* \leq \frac{4\rho_1(z_m)}{(1-\alpha)\rho_2(z_1, z_2)}, \qquad i \neq \xi. \tag{49}$$

If the conditions of Theorem 4.1 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 4.1 now follow from another application of Lemma 3.4 setting $\Phi = E$, $\|\cdot\| = |\cdot|_{\mathrm{w}^{1,\infty}_{\varepsilon}}$, $\tilde{y} = y^*$ 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 recall from the assumption of Theorem 4.2 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 Sections 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 (39), we have

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

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

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

and thus (42). If E is replaced by $\tilde{E}$, we have instead

$$\tilde{E}''(Y;U,V) \geq \tfrac{1}{2}|U|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}\big(\tilde{\rho}_2(z_1,z_2) + 2N\tilde{\rho}_{2,f}(z_f,z_1)\big). \tag{50}$$

4.4. **Proof of Theorem 4.2**

To prove the QC error estimate we can repeat the fixed point argument of Section 3.4 almost verbatim. Only two modifications need to be made. First, as in the existence proof of Section 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 4.3, if we choose y_N^D sufficiently large. This method was suitable for the existence theorem where we needed to construct 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 Section 3.4 let $Y_\varphi = \mathcal{L}(\varphi)$; then,

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

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

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

Hence, if (44) holds, then we can deduce the existence of a QC solution in the set $\mathscr{Z}_f$.

Our second modification of the proof of Section 3.4 is to compute a new bound for $\mathcal{E}_3$. We use (23) again to estimate

$$\big|E'(\theta;V) - \tilde{E}'(\theta;V)\big| = \sum_{n=1}^{N}\varepsilon\big|F'_n(\theta) - \tilde{F}'_n(\theta)\big||V'_n| \leq |V|_{\mathrm{w}^{1,1}_{\varepsilon}}\max_{n=1,\dots,N}\big|F'_n(\theta) - \tilde{F}'_n(\theta)\big|.$$

For each n, we have

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

As in the elastic case, we can estimate and rearrange this sum to obtain (45).

5. *A posteriori* existence and error analysis

In Sections 3 and 4 we have analyzed, in the case of elastic deformation and fracture, the conditions under which a QC approximation to an exact atomistic solution to (6) exists, and have estimated its approximation error. In the present section, we turn to the second question which we posed in the Introduction: Given a computed QC solution, is it possible to prove that an exact solution of the atomistic model exists which the QC solution approximates in a sufficiently strong sense?

Let us first discuss this question in a slightly more abstract form. Let $\mathscr{F} : \mathscr{X} \to \mathscr{Y}^*$ be a nonlinear mapping, where $\mathscr{X}$ and $\mathscr{Y}$ are Banach spaces and $\mathscr{Y}^*$ is the topological dual of $\mathscr{Y}$. If $y \in \mathscr{X}$, if $\mathscr{F}'(y)$ is an isomorphism and if $Y \in \mathscr{X}$ lies in a certain neighbourhood of y (determined by a local Lipschitz constant of $\mathscr{F}'$) then

$$\|y - Y\|_{\mathscr{X}} \leq 2\|\mathscr{F}'(y)^{-1}\|_{L(\mathscr{Y}^*,\mathscr{X})}\|\mathscr{F}(Y)\|_{\mathscr{Y}^*}.$$

This estimate was used, for example, by Verfürth [24], Lemma 2.1 for *a posteriori* error estimation for finite element methods for nonlinear equations. However, by reversing the role of y and Y in the above argument, it is not always necessary to assume the existence of a 'nearby' exact solution *a priori*. To see this, set $\mathscr{G}(v) = \mathscr{F}(v) - \mathscr{F}(Y)$. Clearly, Y is a solution of $\mathscr{G}(Y) = 0$. Thus, if $\mathscr{G}'(Y) = \mathscr{F}'(Y)$ is an isomorphism, and if $\|\mathscr{F}(Y)\|_{\mathscr{Y}^*}$ is sufficiently small then, by the Inverse Function Theorem, there exists a solution to $\mathscr{G}(y) = -\mathscr{F}(Y)$, or equivalently to $\mathscr{F}(y) = 0$, in a neighbourhood of Y. After making this argument precise (and sharp), we obtain Theorem 5.1 below. For a recent review article of other applications of this idea we refer to [22].

First, however, we modify our assumptions slightly. We shall assume from now on that J has a finite cut-off radius, *i.e.*, in addition to (4) we assume that there exists $z_c > z_t$ such that $J(z) = 0$ for all $z \geq z_c$ (*cf.* Fig. 1). This allows us to assume that $\tilde{J} = J$. Also, for the sake of a more condensed notation, we define $\Phi(y) = E(y) - \langle f, y\rangle_\varepsilon$, $y \in \mathbb{R}^{N+1}$; and $\tilde{\Phi}(Y) = E(Y) - \langle f, Y\rangle_{\mathcal{T}}$, $Y \in S^1(\mathcal{T})$. We can then rewrite (6) as $\Phi'(y; v) = 0$, $v \in \mathscr{A}_0$; and (11) as $\tilde{\Phi}'(Y; V) = 0$, $V \in \mathscr{A}_0(\mathcal{T})$. We note that $E'' = \Phi'' = \tilde{\Phi}''$.

In the following theorem, $\|\cdot\|$ should be taken either as $|\cdot|_{\mathrm{w}^{1,\infty}_\varepsilon}$ or as $|\cdot|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}$, as defined in Sections 1.1 and 4. See Section 6.2 for an algorithm to compute the radius $R(Y)$ and the stability constant $\mu(Y)$.

Theorem 5.1 (*a posteriori* existence)**.** *Let $\|\cdot\|$ be a norm in $\mathscr{A}_0$. Let $Y \in \mathscr{A}$ and let $R(Y)$, $\mu(Y)$ and $\eta(Y)$ be non-negative numbers satisfying*

$$0 < \mu(Y) \quad \leq \quad \min_{\substack{y \in \mathscr{A} \\ \|y-Y\| \leq R(Y)}} \; \min_{\substack{u \in \mathscr{A}_0 \\ \|u\|=1}} \; \max_{\substack{v \in \mathscr{A}_0 \\ |v|_{\mathrm{w}^{1,1}_\varepsilon}=1}} E''(y; u, v), \quad \text{and} \tag{51}$$

$$\|\Phi'(Y)\|_* \quad \leq \quad \eta(Y). \tag{52}$$

If $\eta(Y) \leq \mu(Y)R(Y)$, then there exists $y \in \mathscr{A}$ satisfying $\Phi'(y) = 0$ in $\mathscr{A}$ and such that

$$\|y - Y\| \leq \frac{\eta(Y)}{\mu(Y)}. \tag{53}$$

Proof. This theorem is an immediate corollary of Lemma 3.4 by setting $\tilde{y} = Y$ and $\tilde{f} = \Phi'(Y)$. □

Theorem 5.2 (residual bound)**.** *Let $Y \in \mathscr{A}(\mathcal{T})$ satisfy $\tilde{\Phi}'(Y) = 0$ in $\mathscr{A}(\mathcal{T})$, then*

$$\|\Phi'(Y)\|_* \leq \max_{k=1,\dots,K} \eta_{r,k} + \max_{k=1,\dots,K} \eta_{s,k} =: \eta(Y),$$

where

$$\eta_{r,k} = \max_{i=t_{k-1}+1,\dots,t_k} \left| \sum_{j=t_{k-1}+1}^{i-1} \Phi_j'(Y) - \sum_{j=i}^{t_k-1} \Phi_j'(Y) \right|, \tag{54}$$

$$\eta_{s,k} = h_k^2 \max\left(|f|_{\mathrm{w}_\varepsilon^{2,\infty}(\!(t_{k-1},t_k)\!)}, 2|f|_{\mathrm{w}_\varepsilon^{1,\infty}(\!(t_{k-1}+1,t_k)\!)} + 2|f|_{\mathrm{w}_\varepsilon^{1,\infty}(\!(t_{k-1},t_k-1)\!)} \right). \tag{55}$$

In particular, if $t_k - t_{k-1} = 1$ then $\eta_{r,k} + \eta_{s,k} = 0$.

A proof of Theorem 5.2 as well as a detailed discussion concerning the concrete evaluation of the residual terms and their interpretation and comparison with residual estimates in continuum mechanics is given in Section 5.1.

Theorem 5.3 (stability estimate)**.**

(a) *For each $y \in \mathbb{R}^{N+1}$ with $z' = \min_{i=1,\dots,N} y_i'$, we have*

$$\min_{\substack{u \in \mathscr{A}_0 \\ |u|_{\mathrm{w}_\varepsilon^{1,\infty},1,\infty} = 1}} \max_{\substack{v \in \mathscr{A}_0 \\ |v|_{\mathrm{w}_\varepsilon^{1,1},1,1} = 1}} \Phi''(y;u,v) \geq \tfrac{1}{2} \left(\min_{i=1,\dots,N} J''(y_i') - \rho_\infty(z') \right), \tag{56}$$

$$\text{where} \quad \rho_\infty(z') = \sum_{r=2}^{\infty} r^2 \max_{z \geq r z'} |J''(z)|. \tag{57}$$

(b) *If, in addition, $y_\xi' \geq z_c$, then*

$$\min_{\substack{u \in \mathscr{A}_0 \\ |u|_{\mathrm{w}_{\varepsilon,f}^{1,\infty},1,\infty} = 1}} \max_{\substack{v \in \mathscr{A}_0 \\ |v|_{\mathrm{w}_\varepsilon^{1,1},1,1} = 1}} \Phi''(y;u,v) \geq \tfrac{1}{2} \left(\min_{\substack{i=1,\dots,N \\ i \neq \xi}} J''(y_i') - \rho_\infty(z') \right). \tag{58}$$

Proof. For $z' \geq z_t/2$, this result follows immediately from Theorem 3.1 (a) and from Theorem 4.1 (a). In the second case, note that $y_\xi' \geq z_c$ and hence the term $\rho_{2,f}(z_f, z_1)$ vanishes. In general, the arguments can be repeated verbatim, given the modified lower bound for the inf-sup constant. □

Remarks.

1. It is important to note that ρ_∞ is in fact very simple to compute efficiently. If z' is not very close to zero then the calculation of ρ_∞ only involves the computation of a relatively small finite sum.

2. While Theorems 5.1 and 5.2 are generic, it must be emphasized that Theorem 5.3 provides a good estimate only if the deformation y has a generic but nevertheless very specific structure, namely elastic deformation with possibly one single fracture. If $\min_{i=1,\dots,N} y_i' < z_t/2$, then the bound is not sharp. On the other hand, if $\max_{i=1,\dots,N} y_i' \geq z_t$ then $\mu(y)$ is zero or negative.

3. For example, although in the computations in Section 6 this was not necessary, it may in general be advantageous not to estimate $\min_i y_i'$ globally but only locally. This could be crucial when $\min_i y_i'$ is significantly smaller than $\max_i y_i'$, for example, if $\max_i y_i'$ is close to z_t but $\min_i y_i' \leq z_m$.

5.1. **Residual bounds**

Let $Y \in \mathscr{A}(\mathcal{T})$ be a QC solution, *i.e.*, suppose that $\tilde{\Phi}'(Y) = 0$ in $\mathscr{A}(\mathcal{T})$. To bound its residual $\|\Phi'(Y)\|_*$, we use the usual Galerkin orthogonality argument to obtain

$$\begin{aligned} \Phi'(Y;u) &= \Phi'(Y;u-\Pi u) + \Phi'(Y;\Pi u) \\ &= \Phi'(Y;u-\Pi u) + \Big(\Phi'(Y;\Pi u) - \tilde{\Phi}'(Y;\Pi u)\Big) \qquad \forall u \in \mathscr{A}_0, \end{aligned} \tag{59}$$

where Πu is the nodal interpolant defined in Section 2.2. The second term in (59) was already estimated in Section 3.4. Using (69) and $|\Pi u|_{\mathrm{w}_\varepsilon^{1,1}} \le |u|_{\mathrm{w}_\varepsilon^{1,1}}$, which can be verified by a straightforward computation, we obtain

$$|\Phi'(Y;\Pi u) - \tilde{\Phi}'(Y;\Pi u)| \le \max_{k=1,\dots,K} \eta_{s,k}\, |u|_{\mathrm{w}_\varepsilon^{1,1}}, \tag{60}$$

where $\eta_{s,k}$ is defined by (55).

For the first term in (59), we note that

$$\Phi'(Y;v) = \sum_{i=1}^{N-1} \Phi_i'(Y) v_i, \tag{61}$$

where

$$\Phi_i'(Y) = E_i'(Y) - \varepsilon f_i \qquad \forall\, i \in \{0,\dots,N\} \setminus \mathcal{T}, \tag{62}$$

and we take $v = u - \Pi u$. For each $i \in \{t_{k-1}+1,\dots,t_k-1\}$, using the fact that v_i vanishes for $i = t_{k-1}$ and for $i = t_k$, we can write v_i as

$$v_i = \frac{1}{2}\left(\sum_{j=t_{k-1}+1}^{i} \varepsilon v_j' - \sum_{j=i+1}^{t_k} \varepsilon v_j' \right).$$

Inserting this into (61) and rearranging the summation gives

$$\begin{aligned} \Phi'(Y;v) &= \frac{1}{2}\sum_{k=1}^{K} \left[\sum_{i=t_{k-1}+1}^{t_k-1} \Phi_i'(Y) \sum_{j=t_{k-1}+1}^{i} \varepsilon v_j' - \sum_{i=t_{k-1}+1}^{t_k-1} \Phi_i'(Y) \sum_{j=i+1}^{t_k} \varepsilon v_j' \right] \\ &= \frac{1}{2}\sum_{k=1}^{K} \left[\sum_{j=t_{k-1}+1}^{t_k-1} \varepsilon v_j' \sum_{i=j}^{t_k-1} \Phi_i'(Y) - \sum_{j=t_{k-1}+2}^{t_k} \varepsilon v_j' \sum_{i=t_{k-1}+1}^{j-1} \Phi_i'(Y) \right] \\ &= \frac{1}{2}\sum_{k=1}^{K} \left[\sum_{j=t_{k-1}+1}^{t_k} \varepsilon v_j' \sum_{i=j}^{t_k-1} \Phi_i'(Y) - \sum_{j=t_{k-1}+1}^{t_k} \varepsilon v_j' \sum_{i=t_{k-1}+1}^{j-1} \Phi_i'(Y) \right]. \end{aligned}$$

Note that, in the last line, sums over empty sets (whenever the lower summation index is larger than the upper summation index) may occur; each such empty sum is considered to be zero. We use this convention in order to avoid complicated formulae. Upon setting

$$R_j = \frac{1}{2}\left[\sum_{i=j}^{t_k-1} \Phi_i'(Y) - \sum_{i=t_{k-1}+1}^{j-1} \Phi_i'(Y) \right] \qquad \text{for } t_{k-1} < j < t_k,$$

using the same summation convention as above, we obtain

$$\Phi'(Y;v) = \sum_{j=1}^{N} \varepsilon v_j' R_j. \tag{63}$$

An application of Hölder's inequality together with

$$|v|_{\mathrm{w}^{1,1}_\varepsilon(\!(t_{k-1},t_k)\!)} \leq |u|_{\mathrm{w}^{1,1}_\varepsilon(\!(t_{k-1},t_k)\!)} + |\Pi u|_{\mathrm{w}^{1,1}_\varepsilon(\!(t_{k-1},t_k)\!)} \leq 2|u|_{\mathrm{w}^{1,1}_\varepsilon(\!(t_{k-1},t_k)\!)}$$

gives the bound

$$\begin{aligned} |\Phi'(Y;v)| &\leq 2\sum_{k=1}^{K} \Big[\max_{j=t_{k-1}+1,\ldots,t_k} |R_j|\Big]\, |u|_{\mathrm{w}^{1,1}_\varepsilon(\!(t_{k-1},t_k)\!)} \\ &\leq \max_{k=1,\ldots,K} \eta_{r,k}\, |u|_{\mathrm{w}^{1,1}_\varepsilon}, \end{aligned} \tag{64}$$

where $\eta_{r,k}$ is defined by (54). Combining (60) with (64) we obtain

$$|\Phi'(Y;u)| \leq \Big(\max_{k=1,\ldots,K} \eta_{r,k} + \max_{k=1,\ldots,K} \eta_{s,k}\Big)\, |u|_{\mathrm{w}^{1,1}_\varepsilon}$$

which concludes the proof of Theorem 5.2.

Formula (54) is not necessarily straightforward to implement. We therefore briefly discuss some interesting aspects of the residual estimate and an upper bound which reveals its structure and gives a form amenable to implementation. To this end, let us first assume that only nearest and next-nearest neighbour interactions occur, *i.e.*, $\min_i Y_i' \geq z_c/3$. In that case, for $i \in \{2,\ldots,N-2\}$, we can rewrite (62) as

$$\Phi_i'(Y) = J'(Y_{i-1}' + Y_i') + J'(Y_i') - J'(Y_{i+1}') - J'(Y_{i+1}' + Y_{i+2}') - \varepsilon f_i.$$

If $i \in \{t_{k-1}+1,\ldots,t_k-1\}$, then we always have $J'(Y_i') - J'(Y_{i+1}') = 0$. For $i \in \{t_{k-1}+2,\ldots,t_k-2\}$ we also have

$$J'(Y_{i-1}' + Y_i') - J'(Y_{i+1}' + Y_{i+2}') = J'(2\overline{Y}_k') - J'(2\overline{Y}_k') = 0.$$

Therefore, if $t_k - t_{k-1} \geq 3$, the auxiliary variables R_j can be estimated by

$$|R_j| \leq \frac{1}{2}(h_k-\varepsilon)\|f\|_{\ell^\infty_\varepsilon(\!(t_{k-1}+1,t_k-1)\!)} + \frac{1}{2}\Big(\big|J'(2\overline{Y}_k') - J'(\overline{Y}_k' + \overline{Y}_{k-1}')\big| + \big|J'(2\overline{Y}_k') - J'(\overline{Y}_{k+1}' + \overline{Y}_k')\big|\Big). \tag{65}$$

Similarly, if $t_k - t_{k-1} = 2$, then

$$|R_j| \leq \frac{1}{2}(h_k-\varepsilon)\|f\|_{\ell^\infty_\varepsilon(\!(t_{k-1}+1,t_k-1)\!)} + \frac{1}{2}\big|J'(\overline{Y}_{k+1}' + \overline{Y}_k') - J'(\overline{Y}_k' + \overline{Y}_{k-1}')\big|. \tag{66}$$

If $t_k - t_{k-1} = 1$, then obviously $\eta_{r,k} = 0$.

The first term in (65) and (66) is the same as the one we would have obtained in the continuum theory, except that the factor $h_k - \varepsilon$ would have been simply h_k. The second term in (65) and (66) is a purely atomistic effect and highlights the non-local interaction of the atoms. It represents a force at the interface between two elements which has not been fully resolved by the QC approximation.

For the practical computation of the indicators $\eta_{r,k}$, the following proposition which is a generalization of the above discussion is useful.

Proposition 5.4. *Suppose that $J(z) = 0$ for $z \geq z_c$. If $\min(i - t_{k-1}, t_k - i) \geq z_c/\overline{Y}_k'$, then $E_i'(Y) = 0$. In particular, we have*

$$\eta_{r,k} \leq (h_k-\varepsilon)\|f\|_{\ell^\infty_\varepsilon(\!(t_{k-1}+1,t_k-1)\!)} + \sum_{\substack{i\in\{t_{k-1}+1,\ldots,t_k-1\} \\ \min(i-t_{k-1},t_k-i)<z_c/\overline{Y}_k'}} |E_i'(Y)|.$$

Proof. Fix $k \in \{1, \dots, K\}$. If $i \in \{t_{k-1}+1, \dots, t_k - 1\}$ then the derivative with respect to the penalty term vanishes and therefore,

$$\Phi_i'(Y) = \sum_{j=0}^{i-1} J'\big(\varepsilon^{-1}(Y_i - Y_j)\big) - \sum_{j=i+1}^{N} J'\big(\varepsilon^{-1}(Y_j - Y_i)\big) - \varepsilon f_i.$$

Since Y is affine in the set $\{t_{k-1}, \dots, t_k\}$, we have $Y_{i+j} - Y_i = Y_i - Y_{i-j}$ for $j = 1, \dots, r$ where $r = \min(i - t_{k-1}, t_k - i)$ and therefore

$$\Phi_i'(Y) = \sum_{j=0}^{i-r-1} J'\big(\varepsilon^{-1}(Y_i - Y_j)\big) - \sum_{j=i+r+1}^{N} J'\big(\varepsilon^{-1}(Y_j - Y_i)\big) - \varepsilon f_i.$$

For the remaining differences, we have $\varepsilon^{-1}|Y_j - Y_i| \geq r\overline{Y}_k'$ and hence $J'(\varepsilon^{-1}|Y_j - Y_i|) = 0$ if $r \geq z_c/\overline{Y}_k'$. □

6. Numerical examples

6.1. **Benchmark problem**

For our QC benchmark problem we compute a time-discrete quasistatic evolution, where the solution ranges through a variety of different states. First, we determine a stress-free reference state $\hat{y}$ by (approximately) solving $E'(\hat{y}) = 0$ with a Dirichlet condition on only the left-hand end of the domain. The atomistic potential is the Morse potential with $\alpha = 5.0$ and cut-off radius $z_c = 2.7$. We define the applied body-force by

$$f_i = \begin{cases} 0.03, & \text{if } i \geq \xi \\ -0.03, & \text{if } i < \xi. \end{cases}$$

This non-smooth body-force creates a stress intensifier between the two atoms at sites $\xi - 1$ and ξ which is where we should physically expect fracture to occur. The constant 0.03 is quite arbitrary. It is sufficiently small so that the body-force does not dominate the equation and also sufficiently large so that the QC method should be able to find the correct fracture.

We then successively solve for $y(t)$ satisfying $E'(y(t)) = f$ subject to the boundary conditions $y_0(t) = 0$ and $y_N(t) = \hat{y}_N + t$, for ten quasistatic steps:

$$t = 0.0, 0.025, 0.05, 0.075, 0.1, 0.115, 0.1215, 0.1245, 0.1257, 0.15. \tag{67}$$

The initial condition for the numerical optimization method, at each step, is obtained by adding an affine function to the previously obtained critical point and so that it satisfies the new boundary condition.

6.2. **Adaptive algorithm**

We shall publish the details of the adaptive algorithm which we have used in the computation of the above benchmark problem elsewhere and will confine ourselves here to a brief outline.

It was recently noted by Higham [11] that there is a close connection between trust region methods and adaptive time-stepping for a discretized gradient flow evolution. In a quite similar spirit, we used an adaptive proximal point algorithm (PPA) (see [13] for an overview), which is essentially a time-discretized version of a gradient flow for E to compute critical points. The novelty of our algorithm is that, motivated by the analysis in [19], we chose the $|\cdot|_{\mathrm{w}^{1,2}_\varepsilon}$-semi-norm as the gradient flow norm. Given an initial condition $Y^{(0)}$, for the ℓth step of the optimization method, we find a critical point (local minimizer) of

$$V \mapsto \frac{\gamma_\ell}{2}|V - Y^{(\ell-1)}|^2_{\mathrm{w}^{1,2}_\varepsilon} + E(V) - \langle f, V\rangle_{\mathcal{T}^{(\ell)}}$$

in $\mathscr{A}(\mathcal{T}^{(\ell)})$. The penalty parameter γ_ℓ, which corresponds to the inverse of the time-step, and the QC mesh $\mathcal{T}^{(\ell)}$ at the ℓth step are chosen adaptively. In particular, it is possible in our formulation that $\gamma_\ell = 0$ and thus the algorithm reduces to Newton's method.

Before we can demonstrate how we compute the *a posteriori* existence condition (*cf.* Thm. 5.1 and the resulting error estimate, we require a final result that allows us to compute balls with respect to the $\mathrm{w}^{1,\infty}_{\varepsilon,f}$-norm, given by $B_f(Y,R) = \{y \in \mathscr{A} : |y-Y|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}} \leq R\}$. In particular, since we can only compute the inf-sup constant with respect to $|\cdot|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}$ if $y'_\xi \geq z_c$, we need to determine under what conditions all elements $y \in B_f(Y,R)$ satisfy this property.

Proposition 6.1. *Let $Y \in \mathscr{A}$ with $Y'_\xi > z_c$; then,*

$$y'_\xi \geq z_c \qquad \forall y \in B_f\big(Y, \varepsilon(Y'_\xi - z_c)\big) \cap \mathscr{A}.$$

Proof. For $y \in B_f(Y,R)$ we have

$$y'_\xi \;=\; \varepsilon^{-1}\left(y^D_N - \sum_{i\neq\xi} \varepsilon y'_i\right) \;=\; \varepsilon^{-1}\left(y^D_N - \sum_{i\neq\xi} \varepsilon Y'_i + \sum_{i\neq\xi}(Y'_i - y'_i)\right) \;\geq\; Y'_\xi - NR.$$

Hence, for $R \leq \varepsilon(Y'_\xi - z_c)$ the required property holds. □

We use the following procedure to determine which norm we use for the *a posteriori* existence condition and the error estimate. Let Y be a QC solution. We compute the residual bound $\eta = \eta(Y)$, using Theorem 5.2 and Proposition 5.4. This value is passed to a search algorithm which tries to find optimal radii (if they exist) R and R_f such that $\eta/\mu \leq R$ and $\eta/\mu_f \leq R_f$ where μ and μ_f are the respective bounds on the inf-sup constants in $B(Y,R)$ and $B_f(Y,R_f)$ with respect to the norms $|\cdot|_{\mathrm{w}^{1,\infty}_\varepsilon}$ and $|\cdot|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}$. In the following description of the search algorithm, we use the symbols $\mu_{(f)}$, $R_{(f)}$, *etc.*, to indicate that each step is performed for both μ, R, *etc.*, as well as for μ_f, R_f, and so forth.

1. We compute $\mu_{(f)}(Y)$ using Theorem 5.3, and possibly Proposition 6.1 for determining the set $B_f(Y,R_f)$.
2. We set $R^0_{(f)} = \eta(Y)\mu_{(f)}(Y)$ and choose $q \in (0,1)$.
3. For $R^j_{(f)} = q^j R_0$, $j = 0,1,2,\ldots,J$, we use Theorem 5.3 and possibly Proposition 6.1 again to compute an upper bound $\mu^j_{(f)}$ on the inf-sup constant in $B_{(f)}(Y,R^j_{(f)})$.
4. If there exists j such that $\eta(Y)\mu^j_{(f)} \leq R^j_{(f)}$ we find j maximizing $\mu^j_{(f)}$, we set $R_{(f)} = R^j_{(f)}$ and $\mu_{(f)} = \mu^j_{(f)}$.

The following situations can now occur.

1. If no radius R_f was found such that $\eta \leq \mu_f R_f$, then we use the $|\cdot|_{\mathrm{w}^{1,\infty}_\varepsilon}$-norm in the analysis:
   - 1.1 There exists R such that $\eta/\mu \leq R$: Find R for which this holds and for which μ is maximal. Use $\eta/\mu \leq \texttt{TOL}$ as a refinement criterion. If $\eta/\mu \leq \texttt{TOL}$ accept the solution. Otherwise, use the refinement criterion to obtain a new QC mesh and repeat the step.
   - 1.2 There exists no R for which $\eta/\mu \leq R$: Find R such that μR is maximal and use $\eta \leq \mu R$ as a refinement criterion to obtain a new mesh with which to repeat the optimization step.
   - 1.3 There exists no $R > 0$ such that $\mu > 0$. In this case it is not clear what to do. The algorithm should terminate if this occurs.
2. If there exists a radius $R_f \leq Y'_\xi - z_c$ such that $\eta \leq \mu_f R_f$, then we use the $|\cdot|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}$-norm in the analysis: Take $\eta/\mu_f \leq \texttt{TOL}$ as a refinement criterion. If it is satisfied, accept the QC solution. Otherwise, we compute a new mesh and repeat the optimization step.

As mentioned above, this procedure is in fact done at each step of the proximal point algorithm. The required error estimates are easily generalized to the time-step functional. For a more detailed description, see [20].

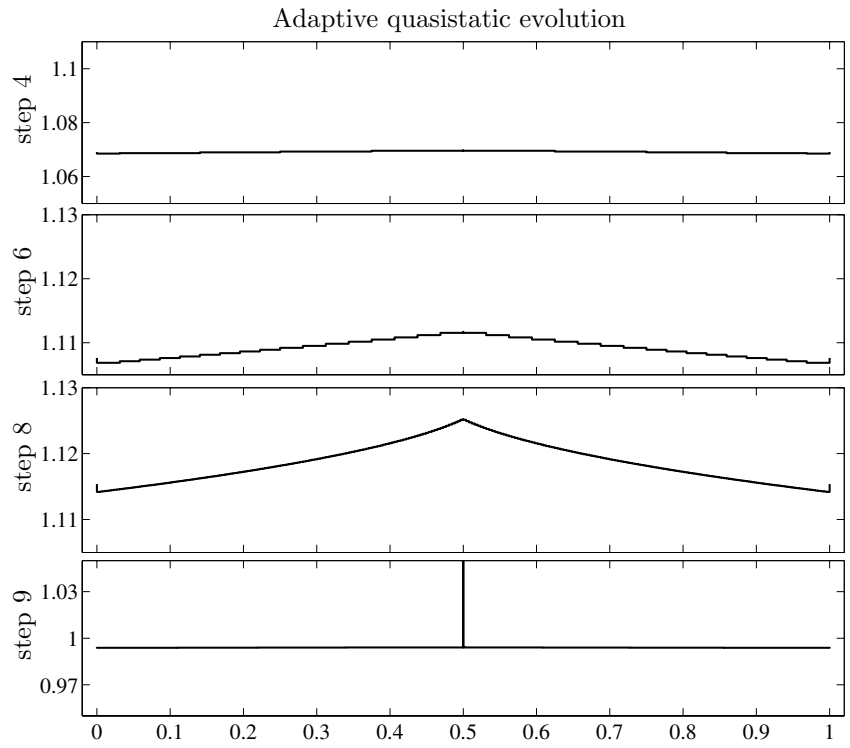

FIGURE 2. The (piecewise constant) gradients of QC solutions in several steps of the quasistatic evolution described in Section 6.1 computed with $N = 10^5$ atoms and with $\texttt{TOL} = 10^{-3}$. Note the different vertical scales in the respective sub-plots.

6.3. **Results**

Using the adaptive optimization algorithm, which was briefly outlined in the previous section, for a given number of atoms $N \in \{10^3, 10^4, 10^5, 10^6\}$ we computed QC solutions $Y(t)$ of the quasistatic benchmark problem described in Section 6.1. For each computed QC solution $Y(t)$, we guarantee the existence of an exact solution $y(t)$ of the atomistic model, such that $|y(t) - Y(t)|_{\mathrm{w}^{1,\infty}_{\varepsilon}} \leq \texttt{TOL}$ where $\texttt{TOL} \in \{10^{-2}, 10^{-3}\}$. Steps 4, 6, 8 and 9 using $N = 10^5$ and $\texttt{TOL} = 10^{-3}$ are shown in Figure 2. We can see the local refinement to resolve the singularity in the center caused by the 'discontinuity' in the forcing term and the refinement due to the surface forces. In step 8 we can clearly see the global refinement which is required to resolve the solution to a sufficient degree near the bifurcation point. These effects become better visible in Figure 3 where we plot the number of degrees of freedom required to meet the *a posteriori* existence condition and the error tolerance, showing that both are roughly independent of N.

For $N = 10^3$ and $\texttt{TOL} = 2^k \times 10^{-3}$, $k = 3, 2, 1, 0, -1$, we plot the efficiency index, *i.e.*, the ratio between estimated and exact error in Figure 4. We note, in particular, that even as the solution approaches the bifurcation point (when the deformation gradient approaches the turning point z_t of J) in step 8 of the quasistatic evolution, the efficiency remains bounded.

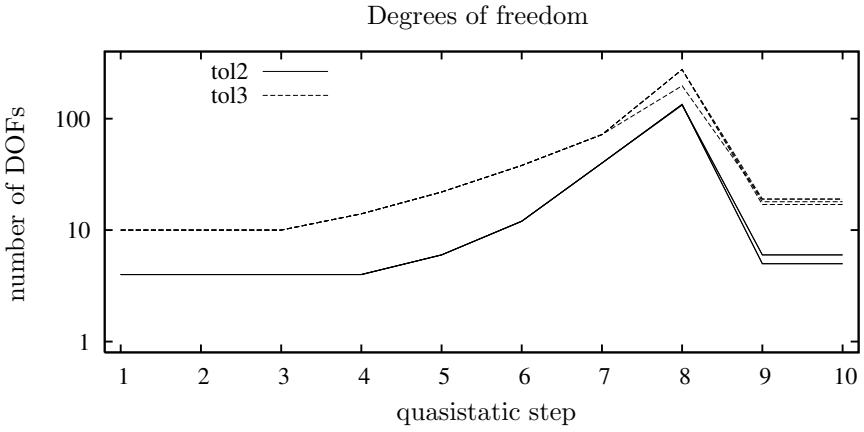

FIGURE 3. Number of degrees of freedom required to meet the *a posteriori* existence criterion and the error tolerance $\texttt{TOL} \in \{10^{-2}, 10^{-3}\}$ with $N \in \{10^3, 10^4, 10^5, 10^6\}$. There are eight curves in this figure, some of which are indistinguishable; four computed with $\texttt{TOL} = 10^{-2}$ (full) and four computed with $\texttt{TOL} = 10^{-3}$ (dashed).

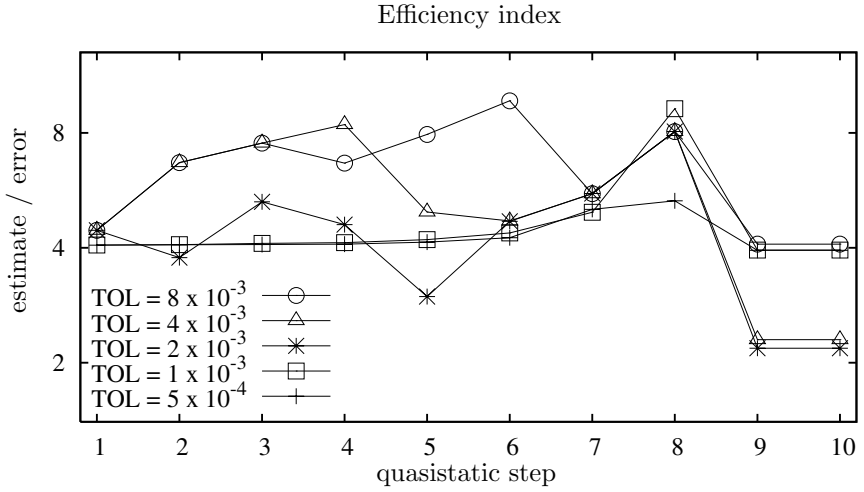

FIGURE 4. Efficiency index (ratio between estimated and true error) for the error estimate for each quasistatic step of the benchmark problem described in Section 6.1. All tests are performed with $N = 10^3$.

7. Concluding remarks

We have presented a fairly complete analysis of the quasicontinuum method in one dimension. Using techniques based on the Inverse Function Theorem we were able to rigorously prove the existence of QC solutions near exact atomistic solutions, as well as the existence of exact atomistic solutions near QC solutions, and to provide quasi-optimal error estimates. All of our estimates were independent of the atomic spacing and the number of atoms in the body.

While the use of the Inverse Function Theorem might suggest that our analysis only applies to the linearly elastic regime, we would like to stress again that this is not the case. Since we linearize around *arbitrary* stable solutions, the results apply to genuinely nonlinear situations.

However, the completeness of our results was primarily due to the one-dimensional setting of this work. While the fundamental approach to the error analysis for the QC method (based on a fixed point argument) is quite attractive, it is not entirely clear whether our results can be generalized to higher dimensions. We note, for example, that it is not possible to prove the inf-sup condition (12) in a two- or three-dimensional setting. We expect (based on BMO-estimates in the work of Dolzmann [7]) that the corresponding inf-sup constant would tend to zero like $|\log(\varepsilon)|^{-1}$ as ε approaches zero. It remains to be seen whether this is sufficient for applications. Other alternatives are to use regularity with respect to even stronger norms, such as discrete $\mathrm{C}^{1,\alpha}$, or $\mathrm{W}^{2,p}$-norms. In this case, however, much stronger bounds on the residual would be necessary and this would, most likely, require a modification of the QC method in order to obtain higher order convergence.

A. Appendix A: Auxiliary results

In this appendix, we collect some useful results that are required throughout this paper, and which are closely related to, and whose formulation and proof do not differ much from, their corresponding continuum versions. The important fact to note is that all bounds are uniform in ε.

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

$$|g_i| \leq L^{-1} \sum_{k=2}^{L} |g_k - g_{k-1}| \phi_{i,k}, \qquad i = 1, \dots, L, \tag{68}$$

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. We set $\varepsilon = 1$ and write $g'_k = g_k - g_{k-1}$ throughout this proof. Let $i \in \{1, \dots, L\}$; then

$$\begin{aligned}
|g_i| &= \Big| g_i - L^{-1} \sum_{j=1}^{L} g_j \Big| \;=\; L^{-1} \Big| \sum_{j=1}^{L} (g_i - g_j) \Big| \\
&\leq L^{-1} \sum_{j=1}^{i-1} |g_i - g_j| + L^{-1} \sum_{j=i+1}^{L} |g_i - g_j| \\
&\leq L^{-1} \sum_{j=1}^{i-1} \sum_{k=j+1}^{i} |g'_k| + L^{-1} \sum_{j=i+1}^{L} \sum_{k=i+1}^{j} |g'_k| \\
&= L^{-1} \sum_{k=2}^{i} |g'_k| \sum_{j=1}^{k-1} 1 + L^{-1} \sum_{k=i+1}^{L} |g'_k| \sum_{j=k}^{L} 1 \\
&= L^{-1} \sum_{k=2}^{i} |g'_k| (k-1) + L^{-1} \sum_{k=i+1}^{L} |g'_k| (L-k+1).
\end{aligned}$$

□

Lemma A.2 (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*

$$\|f\|_{\ell^p_\varepsilon(\langle 0,L \rangle)} \;\leq\; \frac{1}{2}(\epsilon L) |f|_{\mathrm{w}^{1,p}_\varepsilon(\langle 0,L \rangle)}, \quad \text{and} \tag{69}$$

$$\|g\|_{\ell^p_\varepsilon(\langle 1,L \rangle)} \;\leq\; \frac{1}{2}(\epsilon L) |g|_{\mathrm{w}^{1,p}_\varepsilon(\langle 1,L \rangle)}. \tag{70}$$

Proof. First, we note that all occurrences 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 (69), consider

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

To obtain (70), we sum inequality (68) over $i = 1, \ldots, L$ to obtain

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

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

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

Similarly, we also have

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

and therefore,

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

which gives (69) with $p = \infty$.

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

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

□

Note that (69) and (70) are of course valid for any p with constants independent 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

$$C_{1,L} = \bar{C}_{\infty,L} = \frac{1}{2} - \frac{1}{2L}, \quad \bar{C}_{1,L} = C_{\infty,L} = \begin{cases} 1/2, & \text{if } L \text{ is even,} \\ (1/2) - (1/2L), & \text{if } L \text{ is odd,} \end{cases} \quad \text{and}$$

$$\frac{1}{\pi} = \lim_{L\to\infty} C_{2,L} \le C_{2,L} = \bar{C}_{2,L} = \frac{1}{2L\sin(\pi/(2L))} \le C_{2,2} = 8^{-1/2}, C_{2,1} = \bar{C}_{2,1} = 0.$$

In one dimension we also have the following embedding inequality.

Lemma A.3. *Let $(f_i)_{i=0}^L \in \mathbb{R}^{L+1}$ with $f_0 = f_L = 0$. Then,*

$$\|f\|_{\ell^\infty_\varepsilon(\!(0,L)\!)} \le \frac{1}{2} |f|_{\mathrm{w}^{1,1}_\varepsilon(\!(0,L)\!)}.$$

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

$$|f_i| \le \sum_{j=1}^{i} \varepsilon |f_j'| \quad \text{as well as} \quad |f_i| \le \sum_{j=i+1}^{N} \varepsilon |f_j'|.$$

Adding the two inequalities gives the desired result. □

Finally, we combine the estimates of Lemma A.2 to obtain the following interpolation error estimates.

Theorem A.4 (bounds on the interpolation error)**.** *Suppose that $(f_i)_{i=0}^L \in \mathbb{R}^{L+1}$ and let*

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

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

$$|f - F|_{\mathrm{w}^{1,p}_\varepsilon(\!(0,L)\!)} \le \frac{1}{2}(\varepsilon L) |f|_{\mathrm{w}^{2,p}_\varepsilon(\!(0,L)\!)}, \quad \text{and} \tag{71}$$

$$\|f - F\|_{\ell^p_\varepsilon(\!(0,L)\!)} \le \frac{1}{4}(\varepsilon L)^2 |f|_{\mathrm{w}^{2,p}_\varepsilon(\!(0,L)\!)}. \tag{72}$$

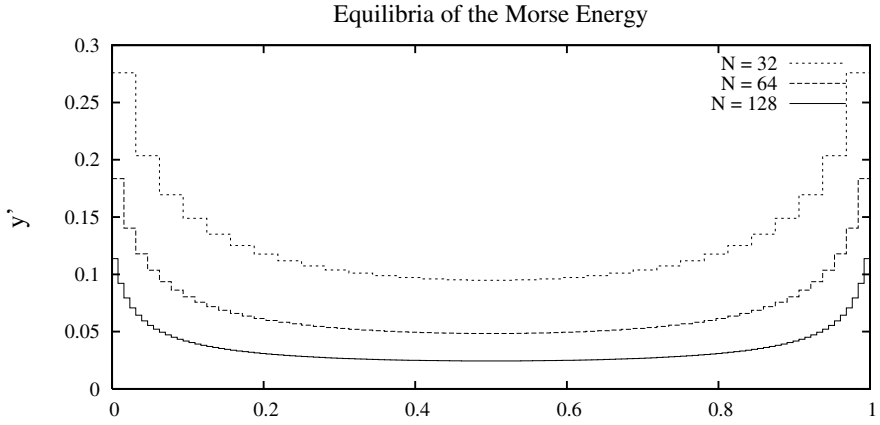

FIGURE 5. Piecewise constant deformation gradient of global minima of the atomistic energy (1), where J is the Morse potential (3) with $\alpha = 1.0$.

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 (71) therefore follows directly from (70).

The estimate (72) can be obtained by applying first (69) and then (70),

$$\|f - F\|_{\ell^p_\varepsilon(\!(0,L)\!)} \leq \frac{1}{2}(\epsilon L)\|(f-F)'\|_{\ell^p_\varepsilon(\!(1,L)\!)} \leq \frac{1}{4}(\epsilon L)^2\|f''\|_{\ell^p_\varepsilon(\!(1,L-1)\!)} = \frac{1}{4}(\epsilon L)^2|f|_{\mathrm{w}^{2,p}_\varepsilon(\!(0,L)\!)}. \qquad \square$$

B. Appendix B: Computation of coercivity regions

In this short appendix, we confirm that the hypotheses made on the interaction potential 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. Only the elastic case is included here since the additional requirements of the fracture case are very easily met given the fast decay of most interaction potentials.

We choose the constants in 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 $z_t = 1 + \alpha^{-1}\ln(2)$. If we choose $\alpha = 1$ in (3) we obtain $\rho_2(z_m, z_m) \approx -3.8$ and we have therefore no hope of constructing a critical point with the technique we have used. This does not mean that E has no critical point in this case. In fact, the mere existence of a global energy minimum can be easily deduced by a compactness argument. However, numerical experiments shown in Figure 5 indicate that those minimizers are extremely unstable and bear no resemblance to the observed steady states of solids. Furthermore, there seems to be no convergence of those minimizers to a continuum as $N \to \infty$.

If we make the well steeper, however, we can achieve coercivity. For example, for $\alpha = 5$, which we have used in our numerical example, we can choose $z_1 = 0.9$ and $z_2 = 1.05$ to obtain $\rho_2(z_1, z_2) \approx 17.4$ and $\rho_1(z_m) \approx 0.15$. The condition $2\rho_1(z_m) \leq R\rho_2(z_m - R, z_m + R)$ becomes $2 \times 0.15 \leq 0.05 \times 17.4$ which is clearly satisfied.

Finally, we should note that, the steeper the basin of convexity around z_m (the larger α in the Morse potential), the better the bounds become.

Acknowledgements. We are grateful to the two anonymous referees for their thoughtful and constructive comments.

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