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A-Posteriori Analysis and Adaptive Algorithms for the Quasicontinuum Method in One Dimension

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

We prove that, for a stable QC solution with a sufficiently small residual, which is computed in a discrete Sobolev-type norm, there exists an exact solution of the atomistic model problem for which an a-posteriori error estimate holds. We then derive practically computable bounds on the residual and on the inf-sup constants which measure the stability of the QC solution.

Finally, we supplement the QC method with a proximal point optimization method with local error-control. We prove that the parameters can be adjusted so that at each step of the optimization algorithm there exists an exact solution to a related atomistic problem whose distance to the numerical solution is smaller than a pre-set tolerance.

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

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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, Phillips and Tadmor in [15] and subsequently improved by many other authors; see [13] 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 analysed in this paper in §2.1.

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 [11] who considers the QC approximation of the reference state of a one-dimensional Lennard–Jones model. E and Ming [7, 6] analyze the QC method in the context of the heterogeneous multi-scale method [5], which requires the assumption that a nearby smooth, elastic continuum solution is available. In [12], Lin analyzes the QC method for purely elastic deformation in two dimensions without using such an assumption, but making instead a strong hypothesis (Assumptions 1. and 2. in [12]) on the exact solution of the atomistic model as well as on its QC approximation. Essentially, it is assumed that both the exact and the QC solution lie in a region where the atomistic energy is convex. For lattice domains resembling smooth or convex sets this assumption seems intuitively reasonable but would be difficult to verify rigorously. For lattice domains with 'sharp', 're-entrant' boundary sections or defects we should not expect it to hold. Finally, we would like to mention the work of Legoll et al. [2] where a multiscale method similar to the QC method is analyzed, however only nearest-neighbour interactions in one dimension are considered which makes it possible to compute the exact solutions analytically. In our own a-priori analysis [18], while still restricted to one-dimensional problems, we make no additional simplifying assumptions.

To the best of our knowledge no work has been carried out so far on the a-posteriori error analysis of the QC method. The goal of the present work is to fill this gap. Some experimental results, using a gradient-averaging technique for the computation of error indicators, were published in [9].

Probably the most remarkable feature of atomistic models is the multitude of solutions. Already in one dimension, it is fairly straightforward to see for many problems that the number of solutions is at least as large as the number of atoms in the body. Therefore, error estimates must be restricted to local results. Due to the possibility of fracture, stability of solutions can only ever be obtained with respect to a discrete

version of the $\mathrm{W}^{1,\infty}$ Sobolev-norm. Hence our entire analysis will be based on such a topology. As a consequence of this lack of global monotonicity and stability, our a-priori error estimates in [18] are, except possibly in the case of elastic deformation, of purely theoretical value. For example, when an exact solution we wish to approximate is a fractured state then we can prove under come natural conditions that there exists a nearby QC solution, however, we should not expect to find it numerically. If only one atom lies on the wrong side of the crack then the error in the discrete $\mathrm{W}^{1,\infty}$-norm cannot converge to zero, even if we take the full atomistic mesh as our QC mesh.

Our strategy in the present work is to reverse the role of exact and QC solutions. We derive estimates on the residual of the QC solution (cf. Theorem 3 and §3.2) and on an inf-sup constant which measures its stability (cf. Theorem 4 and §3.4) and show in Theorem 2 that, if certain natural conditions are satisfied, there exists an exact solution of the atomistic model for which an a-posteriori error estimate holds. This idea of *a-posteriori existence* is demonstrated in [17] in an abstract setting and for a second-order nonlinear elliptic equation.

We then apply this idea to the development of an adaptive optimization algorithm, loosely based on minimizing movements or proximal point methods. We prove for our algorithm that it is possible to choose the parameters in such a way that at each step of the optimization there exists an exact solution of a related problem whose distance to the numerical solution is less than a given tolerance.

A crucial ingredient in almost all a-posteriori error analysis is a sound knowledge of the (local) stability of the equations. In [18] we have derived a number of such results for one-dimensional atomistic models and we will therefore make heavy use of several intermediate results published therein.

1.1 Discrete function spaces

It will be notationally convenient to define discrete versions of the usual Sobolov 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 of these as follows:

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

Sums or maxima taken over empty sets are understood to be zero. If the label $(\!(i_1, i_2)\!)$ is omitted we mean $i_1 = 0, i_2 = N$. $B(y, R)$ is understood to be the closed ball, centre y, radius R, with respect to the $\mathrm{w}^{1,\infty}_\varepsilon$-semi-norm.

In our analysis of fractured atomistic steady states in [18] we also used the semi-norm

$$|u|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}} = \max_{i\neq\xi} |u_i'|, \tag{1.1}$$

where $\xi \in \{1, \dots, N\}$ is an arbitrary but fixed index denoting the location of the fracture.

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

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

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

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

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

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

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

1.2 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 an energy

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

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

$$E(y) = \sum_{i=1}^{N} \sum_{j=0}^{i-1} \varepsilon J\big(\varepsilon^{-1}(y_i - y_j)\big), \tag{1.2}$$

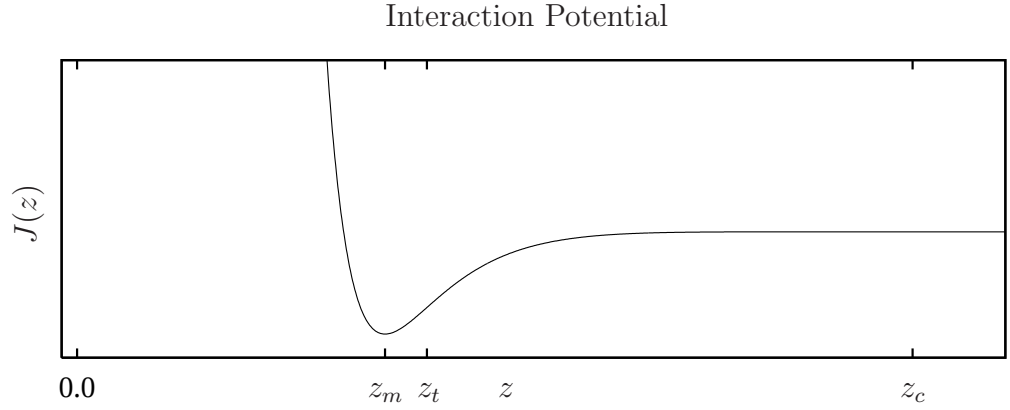

Figure 1: The shape of an atomistic interaction potential J with cut-off radius z_c. For this particular potential (a cut-off Morse potential with $\alpha = 5.0$), we have $z_0 = -\infty, z_m \approx 1, z_t \approx 1.13$ and $z_c = 2.7$. Even though $z_0 = -\infty$, $J(z)$ increases so rapidly as z appraches zero that for practical purposes interpenetration is impossible.

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

Typical examples of atomistic interaction potentials are the Lennard–Jones potential [8],

$$J(z) = Az^{-12} - Bz^{-6}, \tag{1.3}$$

or the Morse potential [14],

$$J(z) = \mathrm{e}^{-2\alpha(z-1)} - 2\mathrm{e}^{-\alpha(z-1)}. \tag{1.4}$$

In practical computations it is furthermore customary to multiply the potential J with a cut-off function, for example,

$$\psi(z) = \begin{cases} (z - z_c)^4/(1 + (z - z_c)^4), & \text{if } z \leq z_c \\ 0, & \text{if } z > z_c. \end{cases}$$

The new potential $\tilde{J}(z) = J(z)\psi(z)$ is then taken as the exact model and its parameters are fitted to the material under consideration. We have analyzed this approximation in detail in the a-priori error analysis in [18], where we showed that the error committed is generally negligible. For the sake of simplicity we shall therefore assume that the exact potential has a cut-off radius z_c beyond which it vanishes. The value of z_c is usually chosen so that next-nearest neighbours are fully resolved but any further interaction is neglected. In our case, this would correspond to taking $z_c \approx 2.5 \times z_m$. The typical shape of an atomistic interaction potential J is shown in Figure 1.

In general, we assume that there exist $z_0 \in [-\infty, +\infty)$, $z_m, z_t, z_c \in \mathbb{R}$ such that

$z_0 < z_m < z_t < z_c$, and

$$\begin{aligned} &J \in \mathrm{C}^3(z_0, \infty), \quad J'(z_m) = 0, \quad J''(z_t) = 0, \quad J(z) = 0 \quad \forall z \geq z_c, \\ &J(z) \to +\infty \text{ as } z \to z_0+, \qquad J(z) = +\infty \quad \forall z \leq z_0, \\ &J''(z) \geq 0 \quad \forall z \in (z_0, z_t] \quad \text{and} \quad J''(z) \leq 0 \quad \forall z \in [z_t, \infty). \end{aligned} \tag{1.5}$$

A simple atomistic model such as (1.2) is not normally used for the simulation of metals, which is the main application of the QC method. However, potentials of the type (1.3) or (1.4) usually form the basis of more sophisticated atomistic models such as the embedded atom method [4] or multi-body interaction models. Thus, we believe that for a theoretical study in one dimension, which is severely restricted in its physical applicability anyhow, we can justify the use of simpler atomistic models, for the sake of a simpler presentation.

Before we define what we mean by an atomistic solution, we need to mention that atomistic deformations are typically only meta-stable states rather than global minimizers (cf. for example [21, 16]). This can be best seen by considering an atomistic body which is clamped at the left-hand end with a small deformation applied to the right-hand end. In that case, the physically observed Cauchy–Born state, the (approximately) affine deformation, is not the energy minimum. Note, however, that the *elastic* state is the correct solution only if we have *started* from an unfractured reference state.

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

$$\mathscr{A} = \{y \in \mathbb{R}^{N+1} : y_0 = 0, y_N = y_N^D\} \quad \text{and} \quad \mathscr{A}_0 = \{y \in \mathbb{R}^{N+1} : y_0 = y_N = 0\}. \tag{1.6}$$

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

$$E'(y; v) = \langle f, v\rangle_\varepsilon \qquad \forall v \in \mathscr{A}_0. \tag{1.7}$$

If y satisfies (1.7), we say that $E'(y) = f$ in $\mathscr{A}$.

The residual of any deformation y is the linear functional $v \mapsto E'(y; v) - \langle f, v\rangle_\varepsilon$. Since we shall analyse the error in the $\mathrm{w}_\varepsilon^{1,\infty}$-norm, we shall measure the residual in the corresponding dual norm defined for each linear functional $\ell\colon \mathscr{A}_0 \to \mathbb{R}$ by

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

The body-force can be understood as the linear functional $\langle f, \cdot\rangle$ and the norm $\|f\|_*$ of f should be interpreted correspondingly.

For future reference, we recall from [18, Section 3.1] that we can write E' and E'' respectively in the form

$$\begin{aligned} E'(y;u) &= \sum_{n=1}^{N-1} E'_n(y)u_n = \sum_{n=1}^{N} \varepsilon F'_n(y)u'_n \qquad \forall u \in \mathscr{A}_0, \text{ where} \\ E'_n(y) &= \tfrac{\partial E}{\partial y_n}(y) = \textstyle\sum_{i=0}^{n-1} J'\big(\varepsilon^{-1}(y_n - y_i)\big) - \sum_{i=n+1}^{N} J'\big(\varepsilon(y_i - y_n)\big), \\ F'_n(y) &= \sum_{i=n}^{N}\sum_{i=1}^{n} J'\big(\varepsilon^{-1}(y_i - y_{j-1})\big), \end{aligned}$$

and

$$\begin{aligned} E''(y;u,v) &= \sum_{n=1}^{N} \varepsilon F'_{nm}(y)u'_n v'_m \qquad \forall u, v \in \mathscr{A}_0, \text{ where} \\ F''_{nm}(y) &= \sum_{i=n\vee m}^{N}\sum_{i=1}^{n\wedge m} J'\big(\varepsilon^{-1}(y_i - y_{j-1})\big). \end{aligned}$$

2 Quasicontinuum approximation and optimization method

2.1 Quasicontinuum approximation

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

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

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

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

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

A straightforward Galerkin approximation to (1.7) would be to *find critical points of* $E(Y) - \langle Y, f\rangle$ *in* $\mathscr{A}(\mathcal{T})$. Any such critical point $Y \in \mathscr{A}$ must satisfy

$$E'(Y;V) = \langle f, V\rangle_\varepsilon \qquad \forall V \in \mathscr{A}_0(\mathcal{T}). \tag{2.1}$$

In the presence of long-range atomistic interactions the computation of the energy and its derivatives would still require the evaluation of very large sums. Due to our assumptions implying finite range interaction only, the sums to compute $E(Y)$ and its derivatives are proportional to K in all practical situations. Prohibitively large sums could only occur under extreme compression which can be ruled out on physical grounds.

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 simple 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 (1.7) is then to *find* $Y \in \mathscr{A}$ *satisfying*

$$E'(Y;V) = \langle f, V\rangle_{\mathcal{T}} \qquad \forall V \in \mathscr{A}_0. \tag{2.2}$$

We conclude this section by stating Poincaré–Friedrichs type inequalities whose proofs have been given in [18]; we also refer to that paper for a discussion of the optimality of the Poincaré–Friedrichs constant 1/2.

Lemma 1 (Discrete Poincaré–Friedrichs 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*

$$\|f\|_{\ell^p_\varepsilon(\!(0,L)\!)} \leq \frac{1}{2}(\epsilon L)|f|_{\mathrm{w}^{1,p}_\varepsilon(\!(0,L)\!)}, \quad \text{and} \tag{2.3}$$

$$\|g\|_{\ell^p_\varepsilon(\!(1,L)\!)} \leq \frac{1}{2}(\epsilon L)|g|_{\mathrm{w}^{1,p}_\varepsilon(\!(1,L)\!)}. \tag{2.4}$$

2.2 Proximal minimization algorithm

As long as the deformation is purely elastic, it is easy to find the critical points of the QC functional, either directly by a Newton method, or, if necessary, using a continuation principle.

However, in order to find critical points with defects, we need to supplement the QC method with an optimization algorithm. Our choice fell on a class of methods called *proximal point algorithms* (PPA). They are important theoretical tools in the analysis of optimization methods and are typically used for the solution of non-smooth problems [19, 20]. Our own intuition regarding these algorithms, however, stems instead from the field of minimizing movements [1] and in particular our previous work on gradient flows of atomistic functionals [16].

Admittedly, our choice is guided to a large extent by mathematical convenience, however, our numerical experiments indicate that the resulting method is quite competitive. Our preferred choice would be to use a trust-region method [3], which seem to be the most efficient local optimization methods available at present. For trust-region methods,

each iteration is a variational inequality rather than an equation which makes their analysis considerably more involved. We believe that if the norm defining the trust-region is chosen to be the $\mathrm{w}^{1,\infty}_\varepsilon$-norm then similar (possibly even stronger) results than the ones presented here can be shown.

Let $Y^{(0)}$ be an *initial guess* for the PPA. This is usually provided from a quasistatic procedure. The ℓth step of the PPA is to *find a critical point* $Y^{(\ell)}$ *of the functional*

$$Y \mapsto \tilde{\Phi}_\ell(Y) = \frac{\gamma_\ell}{2}\|Y - Y^{(\ell-1)}\|^2 + E(Y) - \langle Y, f\rangle_{\mathcal{T}}.$$

The norm $\|\cdot\|$ and the penalty parameters γ_ℓ should be chosen appropriately, to suit the structure of the functional. For example, if E is λ-convex (see §3.3 and [1] for more detail) with respect to the norm $\|\cdot\|$, then, for sufficiently large γ_ℓ the functional $\tilde{\Phi}_\ell$ is strictly convex (in fact, this can be taken as the definition of λ-convexity). In the physically relevant region, atomistic functionals are λ-convex with respect to the $\mathrm{w}^{1,2}_\varepsilon$-semi-norm, uniformly in ε (cf. §3.3).

We supplement the proximal point algorithm with an adaptive procedure. At each step we will, if necessary, adapt the mesh. Therefore, for $\ell = 0, 1, \ldots$, let $\mathcal{T}_\ell$ be QC meshes and let $Y^{(0)} \in \mathscr{A}(\mathcal{T}_0)$ be a starting guess. Recalling that E is differentiable at all deformations which have finite energy, for the ℓth step of the PPA we wish to *find* $Y^{(\ell)} \in \mathscr{A}(\mathcal{T}_\ell)$ *satisfying*

$$\tilde{\Phi}'_\ell(Y^{(\ell)}; V) = 0 \qquad \forall V \in \mathscr{A}_0(\mathcal{T}_\ell), \tag{2.5}$$

where

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

and $\tilde{\Phi}'_\ell$ is given by

$$\tilde{\Phi}'_\ell(Y; V) = \sum_{i=1}^N \varepsilon\big(Y_i - Y_i^{(\ell-1)}\big)' V_i' + E'(Y; V) - \langle f, V\rangle_{\mathcal{T}_\ell}.$$

The PPA (2.5) can be interpreted as the implicit Euler discretization of the gradient flow of $E - \langle f, \cdot\rangle_{\mathcal{T}_\ell}$ with respect to the $\mathrm{w}^{1,2}_\varepsilon$-semi-norm. As such, it is in principle possible to analyze the error of this *discrete evolution*. We could imagine that the PPA is applied first to the full atomistic problem, then to the QC approximation and analyze the error between those two discrete evolutions. However, due to the lack of convexity, the resulting error estimates typically overestimate the actual error by several orders of magnitude. Instead, motivated by standard practice in the field of ODE solvers, we shall analyze the local error instead, i.e., the error committed by replacing the full space $\mathscr{A}$ by the QC space $\mathscr{A}(\mathcal{T}_\ell)$ in the ℓth step of the PPA. In our case, since we are only interested in the efficient computation of a static equilibrium, this is entirely justified. We therefore also define the functional

$$\Phi_\ell(y) = \frac{\gamma_\ell}{2}|y - Y^{(\ell-1)}|^2_{\mathrm{w}^{1,2}_\varepsilon} + E(y) - \langle f, y\rangle_\varepsilon,$$

and the corresponding problem to *find* $y^{(\ell)} \in \mathscr{A}$ *such that*

$$\Phi'_\ell(y^{(\ell)}; v) = 0 \qquad \forall v \in \mathscr{A}_0. \tag{2.6}$$

The embedding of the error analysis and adaptivity into the optimization method achieves a considerable increase in performance. Otherwise the mesh would have to be adapted after the termination of the optimization method and the entire optimization step repeated, which would be particularly cumbersome during the formation of defects when optimization can be a lengthy and tedious process.

3 A-posteriori *existence* and error estimates

In this section, we develop the theory required for an adaptive implementation of the PPA described in Section 2.2. Here, we analyze a single step of the PPA only; thus we omit the sub- and super-scripts ℓ throughout and replace $Y^{(\ell-1)}$ by $Y^{(0)}$. Furthermore, we make the simplifying assumption that, if a mesh is coarsened, then $Y^{(0)}$ is assumed to be a member of the coarse space. We shall approximately enforce this condition by a requirement that an element may be coarsened only if the resulting interpolation error is sufficiently small. This means that we can assume that $Y^{(0)} \in \mathscr{A}(\mathcal{T})$.

In the following theorem, $\|\cdot\|$ is to be taken either as $|\cdot|_{\mathrm{w}^{1,\infty}_\varepsilon}$ or as $|\cdot|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}$. Note that if we set $\gamma = 0$ then Theorem 2 gives an a-posteriori existence result for an atomistic solution. In the residual estimate in Theorem 3, we understand sums over empty sets to be zero.

Theorem 2 (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*

$$0 < \mu(Y) \;\leq\; \min_{\substack{y\in\mathscr{A}\\ \|y-Y\|\le R(Y)}} \; \min_{\substack{u\in\mathscr{A}_0\\ \|u\|=1}} \; \max_{\substack{v\in\mathscr{A}_0\\ |v|_{\mathrm{w}^{1,1}_\varepsilon}=1}} \Phi''(Y;u,v), \quad \text{and} \tag{3.1}$$

$$\|\Phi'(Y)\|_* \;\leq\; \eta(Y). \tag{3.2}$$

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

$$\|y - Y\| \le \frac{\eta(Y)}{\mu(Y)}. \tag{3.3}$$

Theorem 3 (Residual Bound) *Let $Y \in \mathscr{A}(\mathcal{T})$ satisfy $\tilde\Phi'(Y) = 0$ in $\mathscr{A}(\mathcal{T})$. Then,*

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

where

$$\eta_{r,k} \;=\; \max_{i=t_{k-1}+1,\dots,t_k} \left| \sum_{j=t_{k-1}+1}^{i-1} \Phi'_i(Y) - \sum_{j=i}^{t_k-1} \Phi'_i(Y) \right|, \tag{3.4}$$

$$\eta_{s,k} \;=\; \tfrac{3}{2}h_k^2 \max\left(|f|_{\mathrm{w}^{2,\infty}_\varepsilon(\!(t_{k-1},t_k)\!)}, |f|_{\mathrm{w}^{1,\infty}_\varepsilon(\!(t_{k-1}+1,t_k)\!)} + |f|_{\mathrm{w}^{1,\infty}_\varepsilon(\!(t_{k-1},t_k-1)\!)}\right). \tag{3.5}$$

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

A proof of Theorem 3 as well as a detailed discussion about the concrete evaluation of the residual terms and their interpretation and comparison with residual estimates in continuum mechanics is given in §3.2.

Theorem 4 (Stability Estimate) (a) *For each $y \in \mathbb{R}^{N+1}$ with $z' = \min_{i=1,\dots,N} y_i'$, we have*

$$\min_{\substack{u\in\mathscr{A}_0\\ |u|_{\mathrm{w}_\varepsilon^{1,\infty}}=1}} \max_{\substack{v\in\mathscr{A}_0\\ |v|_{\mathrm{w}_\varepsilon^{1,1}}=1}} \Phi''(y;u,v) \;\geq\; \frac{1}{2}\big(\gamma + \min_{i=1,\dots,N} J''(y_i') - \rho_\infty(z')\big), \tag{3.6}$$

$$\text{where} \quad \rho_\infty(z') \;=\; \sum_{r=2}^{\infty} \max_{z\geq rz'} |J''(z)|. \tag{3.7}$$

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

$$\min_{\substack{u\in\mathscr{A}_0\\ |u|_{\mathrm{w}_{\varepsilon,f}^{1,\infty}}=1}} \max_{\substack{v\in\mathscr{A}_0\\ |v|_{\mathrm{w}_\varepsilon^{1,1}}=1}} \Phi''(y;u,v) \geq \frac{1}{2}\big(\gamma + \min_{\substack{i=1,\dots,N\\ i\neq\xi}} J''(y_i') - \rho_\infty(z')\big). \tag{3.8}$$

A proof of Theorem 4 is contained in §3.4. While Theorems 2 and 3 are generic, it must be emphasized that Theorem 4 provides a good estimate only if the deformation y has a generic but nevertheless very specific structure, namely elastic (small) deformation with possibly one single fracture. If $\min_{i=1,\dots,N} y_i' < z_t/2$, then we believe that our 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; cf. §3.4.

3.1 Proof of Theorem 2

Theorem 2 is essentially a specialization of [17, Lemma 2]. However, since it is so central to this paper, we include a proof that is also tailored to the finite-dimensional setting and which gives a slightly sharper result. Lemma 5 is a continuation principle for the Implicit Function Theorem (cf. [22, Section 6.6]) and it implies Theorem 2 by setting $\tilde{y} = Y$, $\tilde{f} = \Phi'(Y)$ and $f = 0$. We formulate this lemma more generally than is necessary for our particular application, in order to emphasize that the technique for proving a-priori and a-posteriori existence results is in fact the same.

Lemma 5 *Let $\|\cdot\|$ be a norm in $\mathscr{A}_0$, let $R > 0$ 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 $\mathscr{A}$; and*

(iii) *there exists $c_0 > 0$ such that for all $y \in \mathscr{Z}$,*

$$c_0 \leq \min_{\substack{u\in\mathscr{A}_0\\ \|u\|=1}} \max_{\substack{v\in\mathscr{A}_0\\ |v|_{\mathrm{w}_\varepsilon^{1,1}}=1}} \Phi''(y;u,v). \tag{3.9}$$

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

$$\|y - \tilde{y}\| \leq c_0^{-1} \|f - \tilde{f}\|_*. \tag{3.10}$$

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

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

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

Upon testing with $v \in \mathscr{A}_0$ and using (3.9), we obtain

$$c_0 \|\tilde{y} - y_t\| \leq \|\tilde{f} - f_t\|_* = t\|\tilde{f} - f\|_* \leq t c_0 R. \tag{3.11}$$

In particular, (3.11) implies that $y_0 = \tilde{y}$.

Since Φ'' satisfies (3.9), it follows that $\Phi''(y_t)$ is non-singular. Furthermore, there exists a neighbourhood of y_t where Φ'' is Lipschitz continuous. Therefore, by the Implicit Function Theorem, there is a $\delta > 0$ such that for all $t \leq s < \delta$ there exists $y_s \in \mathrm{int}(\mathscr{Z})$ satisfying $\Phi'(y_s) = f_s$.

Applying this result to $t = 0$, we find that there is a $T > 0$ such that for $t \in [0, T)$ there exists a solution $y_t \in \mathscr{Z}$ of $\Phi'(y_t) = f_t$. Let T be maximal. Since $\mathscr{A}$ is finite-dimensional, there exists a sequence $t_j \uparrow T$ such that y_{t_j} converges to some $y \in \mathscr{Z}$. Since $f_{t_j} \to f_T$ and Φ' is continuous in $\mathscr{Z}$, it follows that $\Phi'(y) = f_T$. If $T < 1$, then by (3.11) $y \in \mathrm{int}(\mathscr{Z})$. Therefore, there is a $\delta > 0$ such that for $T \leq s < T + \delta$ there exist solutions y_s to $\Phi'(y_s) = f_s$. Since we assumed that T was maximal, it follows that $T = 1$.

Using the same argument as the one leading to (3.11) we find that the solution is unique in $\mathscr{Z}$. ■

3.2 Residual Bounds

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

$$\begin{aligned} \Phi'(Y;u) &= \Phi'(Y; u - \Pi u) + \Phi'(Y; \Pi u) \\ &= \Phi'(Y; u - \Pi u) + \Big(\Phi'(Y;\Pi u) - \tilde{\Phi}'(Y;\Pi u)\Big) \qquad \forall u \in \mathscr{A}_0. \end{aligned} \tag{3.12}$$

The second term in (3.12) was already estimated in [18, Sec. 3.4]; we can mimic the argument therein to obtain

$$\begin{aligned}
&|\Phi'(Y;\Pi u)-\tilde\Phi'(Y;\Pi u)| \le |\langle f,\Pi u\rangle_\varepsilon - \langle f,\Pi u\rangle_{\mathcal T}| \\
&\le \sum_{k=1}^K h_k^2\Big[|f|_{\mathrm{w}_\varepsilon^{2,\infty}(\!(t_{k-1},t_k)\!)}\|\Pi u\|_{\ell^1_\varepsilon(\!(t_{k-1}+1,t_k-1)\!)} \\
&\quad +\big(|f|_{\mathrm{w}_\varepsilon^{1,\infty}(\!(t_{k-1}+1,t_k)\!)}+|f|_{\mathrm{w}_\varepsilon^{1,\infty}(\!(t_{k-1},t_k-1)\!)}\big)\,|\Pi u|_{\mathrm{w}_\varepsilon^{1,1}(\!(t_{k-1},t_k)\!)}\Big] \\
&\le \sum_{k=1}^K h_k^2 \max\big(|f|_{\mathrm{w}_\varepsilon^{2,\infty}(\!(t_{k-1},t_k)\!)}, |f|_{\mathrm{w}_\varepsilon^{1,\infty}(\!(t_{k-1}+1,t_k)\!)}+|f|_{\mathrm{w}_\varepsilon^{1,\infty}(\!(t_{k-1},t_k-1)\!)}\big) \\
&\quad\cdot\big(\|\Pi u\|_{\ell^1_\varepsilon(\!(t_{k-1}+1,t_k-1)\!)}+|\Pi u|_{\mathrm{w}_\varepsilon^{1,1}(\!(t_{k-1},t_k)\!)}\big).
\end{aligned}$$

Using (2.3) 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

$$|\Phi'(Y;\Pi u)-\tilde\Phi'(Y;\Pi u)| \le \sum_{k=1}^K \eta_{s,k}|u|_{\mathrm{w}_\varepsilon^{1,1}(\!(t_{k-1},t_k)\!)}, \tag{3.13}$$

where $\eta_{s,k}$ is defined by (3.5).

For the first term in (3.12), we note that

$$\Phi'(Y;v)=\sum_{i=1}^{N-1}\Phi_i'(Y)v_i, \tag{3.14}$$

where

$$\Phi_i'(Y)=E_i'(Y)-\varepsilon f_i \qquad \forall\, i\in\{0,\dots,N\}\setminus\mathcal T, \tag{3.15}$$

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

$$v_i=\frac12\left(\sum_{j=t_{k-1}+1}^{i}\varepsilon v_j' - \sum_{j=i+1}^{t_k}\varepsilon v_j'\right).$$

Inserting this into (3.14) and rearranging the summation gives

$$\begin{aligned}
\Phi'(Y;v) &= \frac12\sum_{k=1}^K\left[\sum_{i=t_{k-1}+1}^{t_k-1}\Phi_i'(Y)\sum_{j=t_{k-1}+1}^{i}\varepsilon v_j' - \sum_{i=t_{k-1}+1}^{t_k-1}\Phi_i'(Y)\sum_{j=i+1}^{t_k}\varepsilon v_j'\right] \\
&= \frac12\sum_{k=1}^K\left[\sum_{j=t_{k-1}+1}^{t_k-1}\varepsilon v_j'\sum_{i=j}^{t_k-1}\Phi_i'(Y) - \sum_{j=t_{k-1}+2}^{t_k}\varepsilon v_j'\sum_{i=t_{k-1}+1}^{j-1}\Phi_i'(Y)\right] \\
&= \frac12\sum_{k=1}^K\left[\sum_{j=t_{k-1}+1}^{t_k}\varepsilon v_j'\sum_{i=j}^{t_k-1}\Phi_i'(Y) - \sum_{j=t_{k-1}+1}^{t_k}\varepsilon v_j'\sum_{i=t_{k-1}+1}^{j-1}\Phi_i'(Y)\right].
\end{aligned}$$

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

$$\Phi'(Y;v) = \sum_{j=1}^{N} \varepsilon v_j' R_j. \tag{3.16}$$

An application of Hölder's inequality together with

$$|v|_{\mathrm{w}_\varepsilon^{1,1}} = |u - \Pi u|_{\mathrm{w}_\varepsilon^{1,1}} \le |u|_{\mathrm{w}_\varepsilon^{1,1}} + |\Pi u|_{\mathrm{w}_\varepsilon^{1,1}} \le 2|u|_{\mathrm{w}_\varepsilon^{1,1}}$$

gives the bound

$$\begin{aligned} |\Phi'(Y;v)| &\le 2\sum_{k=1}^{K} \Big[\max_{j=t_{k-1}+1,\dots,t_k} |R_j|\Big] \, |u|_{\mathrm{w}_\varepsilon^{1,1}(\!(t_{k-1},t_k)\!)} \\ &\le \sum_{k=1}^{K} \eta_{r,k} \, |u|_{\mathrm{w}_\varepsilon^{1,1}(\!(t_{k-1},t_k)\!)}, \end{aligned} \tag{3.17}$$

where $\eta_{r,k}$ is defined by (3.4). Combining (3.13) with (3.17) we obtain

$$|\Phi'(Y;u)| \le \sum_{k=1}^{K} (\eta_{r,k} + \eta_{s,k}) \, |u|_{\mathrm{w}_\varepsilon^{1,1}(\!(t_{k-1},t_k)\!)} \le \max_{k=1,\dots,K} (\eta_{r,k} + \eta_{s,k}) \, |u|_{\mathrm{w}_\varepsilon^{1,1}}$$

which concludes the proof of Theorem 3.

Formula (3.4) is not necessarily straightforward to implement. We therefore briefly discuss some interesting aspects of the residual estimate and an upper bound which reveals the structure of the residual 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., $\min_i Y_i' \ge z_c/3$. In that case, we can rewrite (3.15) 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 $i \in \{t_{k-1}+1, \dots, t_k - 1\}$, then we always have $J'(Y_i') - J'(Y_{i+1}') = 0$. For $i \in \{t_{k-1}+2, \dots, t_k - 2\}$ 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 $t_k - t_{k-1} \ge 3$, the auxiliary variables R_j can be estimated by

$$\begin{aligned} |R_j| &\le \frac{1}{2}(h_k - \varepsilon)\|f\|_{\ell_\varepsilon^\infty(\!(t_{k-1}+1,t_k-1)\!)} \\ &\quad + \frac{1}{2}\Big(\big|J'(2\overline{Y}_k') - J'(\overline{Y}_k' + \overline{Y}_{k-1}')\big| + \big|J'(2\overline{Y}_k') - J'(\overline{Y}_{k+1}' + \overline{Y}_k')\big|\Big). \end{aligned} \tag{3.18}$$

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

$$|R_j| \le \frac{1}{2}(h_k - \varepsilon)\|f\|_{\ell^\infty_\varepsilon(\!(t_{k-1}+1,t_k-1)\!)} + \frac{1}{2}\big|J'(\overline{Y}'_{k+1} + \overline{Y}'_k) - J'(\overline{Y}'_k + \overline{Y}'_{k-1})\big|. \tag{3.19}$$

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

The first term in (3.18) and (3.19) 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 (3.18) and (3.19) 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 most useful.

Proposition 6 *Suppose that $J(z) = 0$ for $z \ge z_c$. If $\min(i - t_{k-1}, t_k - i) \ge z_c/\overline{Y}'_k$, then $E'_i(Y) = 0$. In particular, we have*

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

Proof Fix $k \in \{1, \dots, K\}$. If $i \in \{t_{k-1} + 1, \dots, t_k - 1\}$, then the derivative with respect to $\langle f, Y\rangle_{\mathcal{T}}$ as well as the penalty term vanish; therefore

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

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

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

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

3.3 The eigenvalues of E''

Having provided a computable estimate on the residual, the crucial missing ingredient for the implementation of an adaptive algorithm is a technique that allows us to determine the inf-sup constant $\mu(Y)$ of Φ''. Instead, in a first step, we analyze the eigenvalues of E''. This analysis will be equally important in the practical implementation of the optimization algorithm and will also show which situations we need to focus on when discussing $\mu(Y)$. Furthermore, in order to justify our formulation of the PPA, we still need to analyse the λ-convexity of E.

For each $y \in \mathbb{R}^{N+1}$ let $\lambda(y)$ be the smallest eigenvalue of $E''(y)$ with respect to the $|\cdot|_{\mathrm{w}_\varepsilon^{1,2}}$-norm,

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

Let $\mathscr{Z}$ be a convex subset of $\mathbb{R}^{N+1}$ over which E is finite, and hence twice differentiable. We say that E is λ-convex in $\mathscr{Z}$ with respect to the $|\cdot|_{\mathrm{w}_\varepsilon^{1,2}}$-norm if there exists a constant $\lambda \in \mathbb{R}$ such that

$$\lambda(y) \geq \lambda \quad \forall y \in \mathscr{Z}, \qquad E(y) < +\infty.$$

As mentioned in the Introduction, this is equivalent to requiring that $E(y) + \frac{\lambda}{2}|y|^2_{\mathrm{w}_\varepsilon^{1,2}}$ is convex in $\mathscr{Z}$.

We analyze the λ-convexity of E in two steps. First, we show that in general E is not uniformly λ-convex in ε. Then we show, however, that the worst-case scenario only occurs under infinite compression. These two results, Propositions 7 and 8, justify our formulation of the PPA.

Proposition 7 *Assume that $z_0 = 0$ and fix y_D. Then, for each $N \in \mathbb{N}$, there exists $y^{(N)} \in \mathscr{A}$ such that $\lambda(y^{(N)}) \to -\infty$ as $N \to \infty$.*

Proof Since the result is a statement about a limit as $N \to \infty$, in the following we can assume without loss of generality that N is arbitrarily large.

Let $z'' > z_t$ be the point where J'' is minimal. Since we assumed that $J''(z_t) = 0$ and $J''(z_m) > 0$ such a point exists and $J''(z'') < 0$. Fix $\delta > 0$ such that $J''(z) \leq J''(z'')/2$ for all $z \in [z'' - \delta, z'' + \delta]$.

Next, we construct a deformation for which most interactions are in the region $[z''-\delta, z''+\delta]$. To this end, let $y'_i = z_m$ for $i = 1, \ldots, i_1$ where i_1 is maximal such that

$$\sum_{i=1}^{i_1} \varepsilon y'_i \leq z'' - \delta.$$

Furthermore, let y'_{i_1+1} be such that

$$\sum_{i=1}^{i_1+1} \varepsilon y'_i = z'' - \delta.$$

Note that the value i_1 is independent of ε. For $i = i_1 + 2, \ldots, N-1$, let $y'_i = 2\delta/N$ so that $\varepsilon^{-1}(y_i - y_0) \in [z'' - \delta, z'' + \delta]$ for $i = i_1 + 1, \ldots, N-1$. Finally let y'_N be an arbitrary value so that a prescribed boundary displacement may be satisfied. Upon choosing N sufficiently large, y'_N may be assumed to be greater than or equal to the cut-off radius z_c.

Next, let the test function u be such that $u'_1 = \frac{1}{\sqrt{2}}\varepsilon^{-1/2}$ and $u'_N = -\frac{1}{\sqrt{2}}\varepsilon^{-1/2}$, then $|u|_{\mathrm{w}_\varepsilon^{1,2}} = 1$ and

$$\begin{aligned} E''(y;u,u) &= \varepsilon F''_{11}(y)(u'_1)^2 + \varepsilon F''_{NN}(y)(u'_N)^2 + 2\varepsilon F''_{1N}(y)u'_1u'_N \\ &= \tfrac{1}{2}\big(F''_{11}(y) + F''_{NN}(y) - 2F''_{1N}(y)\big). \end{aligned}$$

Each of these terms can be easily bounded as follows:

$$\begin{aligned} F''_{11}(y) &= \sum_{i=1}^{N} J''\big(\varepsilon^{-1}(y_i - y_0)\big) \le \text{Const.} + (N - i_1 - 2)J''(z'')/2, \\ F''_{NN}(y) &= \sum_{i=0}^{N-1} J''\big(\varepsilon^{-1}(y_N - y_i)\big) = 0, \quad \text{and} \\ F''_{1N}(y) &= J''\big(\varepsilon^{-1}(y_N - y_0)\big) = 0. \end{aligned}$$

Consequently, $E''(y; u, u) \le c(1 - N)$ when N is sufficiently large. ■

Proposition 8 *For each $z' \in \mathbb{R}$ with $z' > 0$ we have*

$$\sup_{\substack{y \in \mathbb{R}^{N+1} \\ y' \ge z'}} \sup_{\substack{u \in \mathbb{R}^{N+1} \\ |u|_{\mathrm{w}^{1,2}_\varepsilon} = 1}} \big|E''(y; u, u)\big| \le \sum_{r=1}^{\infty} r^2 \max_{z \ge r z'} |J''(z)|.$$

Proof From basic properties of the operator norm of a matrix, it follows that

$$\begin{aligned} |E''(y; u, u)| &\le \sum_{i=1}^{N} \sum_{j=1}^{N} \varepsilon |F''_{ij}(y)| |u'_i| |u'_j| \\ &\le \|F''\| \, |u|^2_{\mathrm{w}^{1,2}_\varepsilon}, \end{aligned}$$

where $\|F''\|$ denotes the ℓ^2-operator norm of the matrix $F'' = (F''_{ij})_{i,j=1}^N$. $\|F''\|$ is the largest eigenvalue (in magnitude) of F'' for which, by Gershgorin's Theorem,

$$\max_{j=1,\ldots,N} \sum_{i=1}^{N} |F''_{ij}|$$

is an upper bound

Using similar computations as for the determination of ρ_2 and ρ_3 in [18, Sec. 3.1], this value can be bounded by

$$\sum_{i=1}^{N} |F''_{ij}| \le \sum_{r=1}^{\infty} r^2 \max_{z \ge r z'} |J''(z)|.$$

■

The knowledge of eigenvalues is only important for the numerical optimization algorithm. Since our analysis is set in the $\mathrm{w}^{1,\infty}_\varepsilon$ topology, they do not enter the error estimate. However, we wish to note one important situation where the discrepancy of the eigenvalues of E'' restricted to $\mathscr{A}_0(\mathcal{T})$ and those of E'' in $\mathscr{A}_0$ is considerable. This is when a deformation gradient in an element $\{t_{k-1}, \ldots, t_k\}$ of length strictly greater than one enters the non-convex region. In this case it is possible that E'' has only positive eigenvalues in $\mathscr{A}_0(\mathcal{T})$ but several negative or zero eigenvalues in $\mathscr{A}_0$. Thus, we may seriously underestimate the possible decrease of energy by local minimization.

Consider for example the case of fracture of a large element. An optimization algorithm would happily accept this state as a local minimum, unless it is somehow able to

recognize along the way that a direction of energy-decay was missed by the QC space. After the fracture has been created, refinement of the element does not help since the gradient may already have entered the cut-off region. These situations need to be detected, either by the adaptive procedure, or through a user-defined mesh.

More generally, we prove that any atomistic state with more than one fracture (for example across one large element, or in two different places) cannot be stable.

Proposition 9 *Let $y \in \mathbb{R}^{N+1}$ with $y'_p \geq z_t$ and $y'_q \geq z_t$, where $p < q \in \{1, \ldots, N\}$. Then, $\lambda(y) \leq 0$. If y'_p or y'_q is strictly greater than but sufficiently close to z_t then $\lambda(y) < 0$.*

Proof We perturb y with the displacement u given by

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

Then, $|u|^2_{\mathrm{w}^{1,2}_\varepsilon} = 2$ and

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

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 not too large then this expression is negative. Hence the result follows. ■

The proof of Proposition 9 reveals, in fact, that negative eigenvalues undetected by the QC method can occur even when $\overline{Y}'_k$ is less than (but sufficiently close to) z_t. Furthermore, it shows that for full-range interactions (without cut-off potential) we always have a negative eigenvalue if two or more fractures are present. Thus, we should rule out such cases from the class of stable configurations.

3.4 Estimation of the inf-sup constant

Our analysis in [18] showed that the inf-sup constants with respect to the $|\cdot|_{\mathrm{w}^{1,p}_\varepsilon}$-norms ($p = 1, \infty$) can be computed using the diagonal dominance of the Hessian matrices (F''_{nm}). Clearly, we do not wish to compute the entire matrix Φ''. In the following discussion we will provide an efficient way to compute the inf-sup constant which is heavily based on our analysis in [18]. While our analysis is not sufficiently general to

cover all possible types of solutions, we believe that it is sufficient for most purposes. We shall demonstrate this in §4.

Recall from [18, Section 3.1] that the inf-sup constant for $E''(Y)$ can be bounded below by

$$\min_{\substack{u\in\mathscr{A}_0\\ |u|_{\mathrm{w}^{1,\infty}_\varepsilon}=1}}\ \max_{\substack{v\in\mathscr{A}_0\\ |v|_{\mathrm{w}^{1,1}_\varepsilon}=1}} E''(Y;u,v) \geq \min_{n=1,\dots,N} \frac{1}{2}\Big(F''_{nn}(Y) - \sum_{n\neq m}|F''_{nm}(Y)|\Big).$$

This was obtained by testing with v given by

$$v'_i = \begin{cases} \frac{1}{2}\varepsilon^{-1}, & \text{if } u'_i = \max_j u'_j \\ -\frac{1}{2}\varepsilon^{-1}, & \text{if } u'_i = \min_j u'_j \\ 0, & \text{otherwise.} \end{cases}$$

Recall also that $u \in \mathscr{A}_0$ and hence u'_j must change sign. This makes it clear that adding $\gamma\mathrm{Id}$ to the matrix $(F''_{nm}(Y))_{n,m=1}^N$ corresponds to simply adding $\frac{1}{2}\gamma$ to the estimate.

We recall from [18, Section 3.1], where the same computation was performed, that we can rewrite the stability factor as

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

Upon setting $z' = \min_{i=1,\dots,N}$ and

$$\overline{J''}(r) = \max_{z\geq rz'}|J''(z)|$$

we obtain the bound

$$\gamma + F''_{nn} - \sum_{m\neq n}|F''_{nm}| \geq \gamma + J''(y'_n) - \sum_{r=2}^{\infty} r^2\overline{J''}(r),$$

which concludes the proof of Theorem 4 (a). Since $J''(z) \leq 0$, this seemingly gross simplification is more-or-less sharp if $z' \geq z_t/2$.

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. Although in our computations it 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 $\min_i y'_i \leq z_m$.

3. We anticipate — and our numerical experiments confirm this — that our estimates are reasonably sharp whenever $\min_i y'_i \geq z_t/2$. The case $\min_i y'_i < z_t/2$ should not occur in practice. To see this, assume that J is the Morse potential with $\alpha = 5.0$. In that case, $J'(z_t/2) \approx -659$ while $J'(z_t) \approx 0.024$, i.e., it requires an amount of force, several orders of magnitude larger to compress the specimen beyond $z_t/2$ than it takes to break it. ◄

Corollary 10 *For every $z' > 0$ there exists $\gamma_0 \geq 0$ such that for all $\gamma \geq \gamma_0$, and for all $y \in \mathbb{R}^{N+1}$ with $y' \geq z'$, $\Phi''(y)$ has a positive inf-sup constant. Furthermore, as γ tends to infinity, so does the inf-sup constant.*

Consider the situation where the solution y has a fracture. In this case, we have no hope of ever obtaining a reasonable bound for the inf-sup constant of $E''(y)$ without regularization. In this case, we may replace the $\mathrm{w}^{1,\infty}_{\varepsilon}$-norm by the $\mathrm{w}^{1,\infty}_{\varepsilon,f}$-norm which we used in the analysis of fracture in [18]. If $\gamma = 0$ then we can obtain (3.8) by the same computations as in [18, Section 4.1]. We only note that for $y'_\xi \geq z_c$ the term $\rho_{2,f}(z_f, z_1)$, defined in [18, Section 4.1], vanishes and thus (3.8) follows immediately from [18, Theorem 4.1]. In general, however, we have to be more careful.

Let $y \in \mathscr{A}$ with $y'_\xi \geq z_c$. Let $u \in \mathscr{A}_0$ and define $P = \{i : u'_i > 0\}$ and $Q = \{i : u'_i < 0\}$. Without loss of generality, we assume that $u'_p = |u|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}$ for some $p \in P$. We distinguish two cases. If $u'_\xi \leq 0$, we proceed as in [18, Section 4.1], setting $v'_p = \frac{1}{2}\varepsilon^{-1}$ and $v'_\xi = -\frac{1}{2}\varepsilon^{-1}$ to obtain

$$\Phi''(y; u, v) \geq \frac{1}{2}\Big(\gamma + F''_{pp}(y) - \sum_{n\in Q} \big|F''_{n\xi}(y)\big|\Big)|u|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}} + \frac{1}{2}\gamma|u'_\xi|,$$

which, using the fact that all interactions across the *crack* vanish, leads to (3.8). The extra term $\frac{1}{2}\gamma|u'_\xi|$ is simply neglected.

On the other hand, if $u'_\xi > 0$ then there exists $q \in Q$ such that y'_q is minimal. In this case, we proceed as in the case without fracture and note that the term u'_ξ appears nowhere in the calculation since $v'_\xi = 0$ and $J''(\varepsilon^{-1}(y_i - y_{j-1})) = 0$ whenever $i \geq \xi$ and $j \leq \xi$. This concludes the proof of Theorem 4.

Finally, we formulate a result that will help us to determine the balls $B_f(Y, R) = \{y \in \mathscr{A} : |y - Y|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}} \leq R\}$. In particular, since we can only compute the inf-sup constant with respect to $|\cdot|_{\mathrm{w}^{1,\infty}_{\varepsilon}}$ if $y'_\xi \geq z_t$, we need to determine under what conditions all elements $y \in B_f(Y, R)$ satisfy this property.

Proposition 11 *Let $Y \in \mathscr{A}$ with $Y'_\xi > z_c$; then,*

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

Proof To see that this is true, note that for $y \in B_f(Y, R)$ we have

$$\begin{aligned} y'_\xi &= \varepsilon^{-1}\big(y^D_N - \sum_{i\neq\xi} \varepsilon y'_i\big) \\ &= \varepsilon^{-1}\big(y^D_N - \sum_{i\neq\xi} \varepsilon Y'_i + \sum_{i\neq\xi}(Y'_i - y'_i)\big) \\ &\geq Y'_\xi - NR. \end{aligned}$$

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

4 Implementation and Numerical Examples

4.1 Implementation of the basic PPA

We begin by describing the implementation of the PPA without an adaptive procedure. Suppose that we are given an initial guess $y^{(0)} \in \mathscr{A}$. Given a penalty parameter γ_ℓ, the ℓth step of the PPA is to find a solution to the problem

$$\gamma_\ell \sum_{i=1}^{N} \varepsilon (y_i - y_i^{(\ell-1)})' u_i' + E'(y;u) - \langle f, u \rangle_\varepsilon = 0 \qquad \forall u \in \mathscr{A}_0. \tag{4.1}$$

We would like to remark at this point that our discussion below applies also if we replace $E - \langle f, \cdot \rangle_\varepsilon$ by a general differentiable functional ϕ and $|\cdot|_{\mathrm{w}_\varepsilon^{1,2}}$ by a general differentiable norm or semi-norm $\|\cdot\|$. The efficiency of the method will depend on how well the norm $\|\cdot\|$ is chosen for the particular functional ϕ.

In order to guarantee that a local solution of the ℓth step (4.1) has lower energy than the previous iterate, we should try to guarantee that (4.1) is a locally convex problem. A necessary condition for this is that the parameter γ_ℓ is at least as large as $-\lambda(y^{(\ell-1)})$, where $\lambda(y)$ is the algebraically smallest generalized eigenvalue of $E''(y)$ with respect to the $|\cdot|_{\mathrm{w}_\varepsilon^{1,2}}$ norm, i.e.,

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

More generally, we define a local curvature estimate λ_ℓ which is initially set to $\lambda(y^{(\ell-1)})$ but may be adjusted during the computation of the ℓth step. In addition, we define a non-negative parameter `POSFAC` which is updated during the computation and can be interpreted as a measure for the change of curvature of the problem. The initial guess and the updating procedure will be discussed in the following paragraphs. We set

$$\gamma_\ell = \max\big(\texttt{POSFAC} - \lambda_\ell, 0\big).$$

This allows the algorithm to reduce to a direct solution (Newton's method) whenever $\lambda_\ell > \texttt{POSFAC}$. If $\lambda(y^{(0)}) > 0$ then we initialize `POSFAC` to $\lambda(y^{(0)})/2$ so that the PPA reduces to Newton's method whenever possible. Otherwise, `POSFAC` is initialized to an arbitrary positive number.

The nonlinear equation (4.1) is solved using Newton's method. If γ_ℓ tends to infinity then the problem becomes essentially quadratic in the limit and hence Newton's method should converge in a single step. We therefore define three further parameters `MAXIT`, `HIGHIT` and `LOWIT`. If the number of Newton iterations required to solve (4.1) is larger than `MAXIT`, we repeat the step with an increased value of γ_ℓ. This is achieved by multiplying `POSFAC` by a constant, the predefined factor `POSFAC_INC`. If Newton's method terminates in at most `MAXIT` iterations then the step is accepted. If the number of iterations is at least `HIGHIT`, we increase `POSFAC` for the next step. If the number of iterations is less than `LOWIT` then the number of iterations is decreased by multiplying `POSFAC` by a constant, the predefined factor `POSFAC_DEC`.

We found that this procedure was reliable in that it quickly finds a value for POSFAC such that Newton's method is successful. In some situations, however, POSFAC was decreased too slowly. We have encountered this eventuality by forcing a decrease of POSFAC whenever λ_ℓ was positive for a certain number (in our specific implementation, ten) of PPA iterations.

Finally, we monitor the local curvature during the Newton iteration. Suppose that $Y^{\langle s \rangle}$ is the sth iteration of Newton's method for solving (4.1). If $\gamma_\ell + \lambda(Y^{\langle s \rangle}) \leq 0$ we interrupt the Newton iteration and repeat the PPA step with an updated curvature value $\lambda_\ell = \lambda(Y^{\langle s \rangle})$.

The PPA terminates if either $\|y^{(\ell)} - y^{(\ell-1)}\| \leq$ STEPTOL or if $\|\phi'(y^{(\ell)})\|_* \leq$ RESTOL, where $\|\cdot\|$ is normally chosen to be the $|\cdot|_{\mathrm{w}_\varepsilon^{1,\infty}}$-norm. Alternatively, one could use the $|\cdot|_{\mathrm{w}_\varepsilon^{1,2}}$-norm for the step-length termination criterion and its dual norm as a residual termination criterion.

The parameter values that we used in all our computations are

$$\begin{aligned} &\texttt{MAXIT} = 6, \quad \texttt{LOWIT} = 2, \quad \texttt{HIGHIT} = 4, \\ &\texttt{POSFAC\_INC} = 4, \quad \texttt{POSFAC\_DEC} = 1/4, \\ &\texttt{STEPTOL} = 0, \quad \texttt{RESTOL} = 10^{-8}. \end{aligned}$$

4.1.1 PPA versus Optimization Toolbox

We have compared our implementation of the PPA to the large-scale trust region method (the command `fminunc` with appropriate set of parameters) of MATLAB's optimization toolbox. Our benchmark is a QC model problem defined as follows.

First we determine a stress-free reference state 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 rather arbitrary. It is sufficiently small so that the body-force does not dominate the equation but 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

$$t = 0.0, 0.025, 0.05, 0.075, 0.1, 0.115, 0.1215, 0.1245, 0.1257, 0.15. \tag{4.2}$$

The initial condition for each step is obtained by adding an affine function to the previously obtained equilibrium and so that it satisfies the boundary condition.

Since the two methods, the PPA and the trust region method, are very different both in terms of their design and implementation it is hard to compare them directly. For

example, our PPA uses a direct method to solve the linear systems while `fminunc` uses a conjugate gradient method. Furthermore, there are no provisions in `fminunc` to take the specific structure of the energy functional into account, which we have done with our choice of penalization norm $|\cdot|_{\mathrm{w}_\varepsilon^{1,2}}$. All we can offer therefore are rough qualitative remarks that are only intended to demonstrate the efficiency of our PPA, specifically for the QC method.

	PPA		Trust Region	
q.s. step	iterations	linear systems	iterations	CG iterations
1	1	1	0	0
2	1	3	2	17
3	1	3	2	19
4	1	3	2	19
5	1	4	3	29
6	1	4	3	31
7	1	4	3	31
8	1	5	3	33
9	89	331	–	–
10	1	5	19	475

Table 1: Iteration count and linear system count for the proximal point algorithm and MATLAB's trust region method `fminunc`.

Table 1 summarizes some results which highlight the performance of the two algorithms. For the first 8 quasistatic steps, the two methods perform very similarly. Essentially, both reduce to a Newton method. Note that while each iteration of the PPA is an application of Newton's method, each iteration (in this case) of the trust region method is only one iteration of Newton's method.

The two methods only start to differ significantly in the presence of defects. In step 9, when the fracture forms, the trust region method `fminunc` failed to converge in 10^4 steps while the PPA converged in under 100 iterations. While we had expected that our PPA would perform much better in the formation of the defect — it is, after all, designed specifically for this purpose — we are somewhat puzzled by the bad performance of `fminunc`. It is perhaps even more surprising that `fminunc` fails to recognise that, for the final step, a simple Newton iteration is again sufficient.

As a final verdict on the performance of our PPA, we would have to test it on a greater variety of benchmark problems and compare it to more advanced optimization packages, such as TRON [10]. In any case, we have some evidence that our optimization method can achieve good performance for the highly non-convex optimization problems occurring in the quasicontinuum method.

4.2 Adaptivity in the PPA

We now add an adaptive procedure into the inner-most loop of the PPA, the solution of the equation (4.1). Suppose that we are given an initial condition $Y^{(0)} \in \mathscr{A}(\mathcal{T}^{(0)})$

and suppose furthermore, that we have already computed the $(\ell-1)$th step $Y^{(\ell-1)} \in \mathscr{A}(\mathcal{T}^{(\ell-1)})$. To compute $Y^{(\ell)}$ we choose a mesh $\mathcal{T}^{(\ell)}$, initially set to $\mathcal{T}^{(\ell)} = \mathcal{T}^{(\ell-1)}$, and solve

$$\tilde{\Phi}'_\ell(Y;U) = 0 \qquad \forall U \in \mathscr{A}_0(\mathcal{T}). \tag{4.3}$$

We solve this equation by the procedure described in §4.1. We also compute the eigenvalues of E'' in $\mathscr{A}_0(\mathcal{T})$ in order to obtain the curvature parameters λ_ℓ. This is motivated by the fact that the solution of (4.3) only depends on the QC eigenvalues but not on the eigenvalues of the full atomistic problem. Our only modification is to define a new non-negative parameter `POSFAC_A`,

$$\texttt{POSFAC\_A} = -\min\big(0, \min_{i=1,\dots,N} J''(y'_i) - \rho_\infty(\min_i y'_i)\big), \tag{4.4}$$

and redefine

$$\gamma_\ell = \max\big(0, \texttt{POSFAC} + \texttt{POSFAC\_A} - \lambda_\ell\big),$$

which allows additional control on the penalization. In particular, it guarantees that the penalization does not tend to zero and we thus avoid an overrefinement of the mesh before the current iterate has entered a region of coercivity. The definition (4.4) is used when the error is measured in the $|\cdot|_{\mathrm{w}^{1,\infty}_\varepsilon}$-semi-norm while we use

$$\texttt{POSFAC\_A} = -\min\big(0, \min_{i\neq\xi} J''(y'_i) - \rho_\infty(\min_i y'_i)\big)$$

instead if the error is measured in the $|\cdot|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}$-semi-norm.

Suppose now that (4.3) has a QC solution $\tilde{Y}$ that was accepted by the PPA. Next, we estimate the error committed and, if necessary, we refine the mesh and repeat the step.

To this end, we compute the residual bound $\eta = \eta(\tilde{Y})$, using Theorem 3 and Proposition 6. These values are 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 inf-sup constants in $B(\tilde{Y}, R)$ and $B_f(\tilde{Y}, R_f)$ with respect to the norms $|\cdot|_{\mathrm{w}^{1,\infty}_\varepsilon}$ and $|\cdot|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}$. These constants can be computed using Theorem 4. In order to determine admissible radii R_f, we use Proposition 11. The following situations can now occur.

1. If no radius R_f exists 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 $\eta/\mu \leq \texttt{TOL}$ set $Y^{(\ell)} = \tilde{Y}$ and increase ℓ by one to continue the PPA. Otherwise, use the refinement criterion to obtain a new mesh $\mathcal{T}_\ell$ 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 $\mathcal{T}_\ell$ with which to repeat the ℓth PPA step.

1.3 There exists no $R > 0$ such that $\mu > 0$: Recompute `POSFAC_A` with the new stability estimate and repeat the ℓth PPA step.

2. If there exists a radius $R_f \le \tilde{Y}'_\xi - z_c$ such that $\eta \le \mu_f R_f$, then we use the $|\cdot|_{\mathrm{w}^{1,\infty}_{\varepsilon,f}}$-norm in the analysis: Take $\eta/\mu_f \le \mathrm{TOL}$ as a refinement criterion. If it is satisfied, set $Y^{(\ell)} = \tilde{Y}$ and increase ℓ by one to continue the PPA. Otherwise, compute a new mesh $\mathcal{T}_\ell$ and repeat the ℓth PPA step.

4.3 Mesh Coarsening

Ideally, an adaptive finite element method should have the capability to refine as well as coarsen a mesh. Translated to our context, a typical criterion to mark an element for coarsening would be

$$\eta_k/\mu \le q \times \min(\mathrm{TOL}, R),$$

where $q \in (0,1)$. This is based on the assumption that, say, doubling the size of an element should increase the residual roughly by a factor of two. However, in our atomistic problems we have no such property. This can best be seen by considering a fractured element which, as we discussed, must have length one and hence the residual in this element vanishes. Such an element would always be marked for coarsening. Because of this (and similar) difficulties we were unable to provide a rigorous analysis of a coarsening strategy. In the following, we shall, however, present a simple idea that seems to work well in practice.

We define a *pseudo-residual* $\tilde{\eta}_k$ which measures the residual in the kth element as if it were a large element. To this end, we recall from the discussion in §3.2 that most of the time only nearest and next-nearest neighbour interactions contribute to the energy. More generally, it is reasonable to assume that the residual contribution from long-range interactions can simply be neglected. Thus, we define

$$\tilde{\eta}_k = h_k \|f\|_{\ell^\infty_\varepsilon(\!(t_{k-1},t_k)\!)} + \left|J'(2\overline{Y}'_k) - J'(\overline{Y}'_k + \overline{Y}'_{k-1})\right| + \left|J'(2\overline{Y}'_k) - J'(\overline{Y}'_{k+1} + \overline{Y}'_k)\right|$$

with a suitable modification for boundary elements, and choose the coarsening criterion

$$\tilde{\eta}_k/\mu \le q \times \min(\mathrm{TOL}, R)$$

in Case 1. of §4.2, and

$$\tilde{\eta}_k/\mu_f \le q \times \min(\mathrm{TOL}, R_f),$$

in the Case 2. of §4.2. In our computations, we chose $q = 1/4$.

As a second criterion, we require that the interpolation error committed during coarsening is less than a specified tolerance, which should be a fraction of the tolerance TOL.

The coarsening is performed at the same time as the error estimation and possible mesh refinement.

4.4 Numerical example

We use the benchmark example from §4.1.1 to test our adaptive implementation. In the very first step of the quasistatic evolution the user has to supply an initial condition in the form of a QC mesh and the nodal values. This initial mesh has to be chosen so that the summation error term η_k^s in the residual can be neglected and does not have to be computed in the adaptive procedure. Consequently, we have also implemented a further safeguard in the coarsening procedure, preventing it to remove any nodes which are present in the original mesh.

For our particular example, it is sufficient to choose $\mathcal{T} = \{0, \xi - 1, \xi, N\}$ as the initial mesh. The benchmark example is run with $N \in \{10^3, 10^4, 10^5, 10^6\}$ and TOL $\in \{10^{-2}, 10^{-3}\}$. The performance of the adaptive PPA is described in Figures 2 – 5 and in the following discussion.

In Figure 2 we notice immediately that that number of iterations of the PPA seems to be roughly independent of both the tolerance level and the number of atoms. Only the case $N = 10^6$, TOL $= 10^{-3}$ seems to stand out. The number of iterations required is considerably larger in this one case because Newton's method often failed to converge and hence the penalty parameter γ_ℓ was set far too high. We believe that this was caused by increased round-off errors (the lengths of the elements range from N^{-1} to 10^{-1}) which begin to influence the computation considerably for such large N and make it more difficult to satisfy the (residual-based) termination criterion of Newton's method. If a lower termination tolerance for Newton's method is used, the problem does not occur.

Similarly, we see in Figure 3 that the number of degrees of freedom (DOF) required to meet the tolerance depends only on TOL but not on N. These results indicate the robustness of the adaptive algorithm.

Next, in Figure 4 we analyze the effectivity of our error estimates. This test was only performed for $N = 10^3$ as it requires the computation of the full atomistic solution. For all tests, the effectivity index, the ratio between the estimated and the true error, lies between 2 and 8. In particular, the effectivity index does not explode as we approach the bifurcation point in step 8 of the quasistatic evolution.

Finally, in Figure 5, we plot the entire history of the adaptive PPA for the 9th quasistatic step which is the most interesting. This is done for $N = 10^3$ and TOL $\in \{10^{-2}, 10^{-3}\}$. We notice that the two *discrete evolutions* behave very similarly. As the local curvature estimate λ_ℓ becomes more and more negative, the penalization parameter increases. As the PPA iterations converge to the equilibrium, the stability (described by the constant μ_f in Theorem 4) increases and hence the number of DOFs required to meet the tolerance decreases as well. Note that between the 20th and 40th PPA iteration the number of DOFs are the same for TOL $= 10^{-2}$ and TOL $= 10^{-3}$. This indicates that the error tolerance was overwritten by the a-posteriori existence condition.

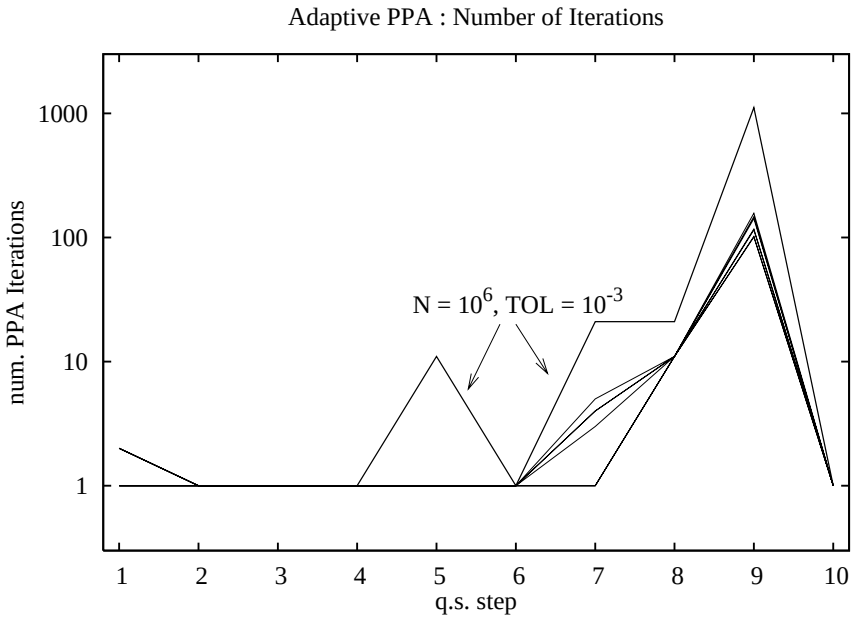

Figure 2: Number of iterations of the adaptive PPA for the benchmark problem described in §4.1.1, for $N \in \{10^3, 10^4, 10^5, 10^6\}$ and TOL $\in \{10^{-2}, 10^{-3}\}$.

5 Conclusion

We have presented an a-posteriori existence and error analysis for the quasicontinuum method in one dimension. We would like to emphasize, in particular, that we consciously avoided assuming the existence of a nearby exact solution to the atomistic model, but have instead developed a technique which allows us to deduce the existence of atomistic solutions from the computation.

We have integrated our a-posteriori error analysis and existence results into an adaptive optimization method based on proximal point algorithms, and our numerical experiments presented in §4 demonstrate the effectiveness of the approach.

While we have seen that the stability-analysis of atomistic equations and the structure of the residual in the quasi-continuum method bear many similarities to the analysis of continuum problems in one dimension, this is no longer true in two or three space dimensions. The abstract a-posteriori existence result, Theorem 2, remains valid of course; however, generalizing the stability estimates to higher dimensions seems a non-trivial challenge. One possibility, that we intend to investigate further, is to numerically solve the min-max problem which supplies the stability constant for the QC space. From this, we hope to be able to estimate the inf-sup constant on the full atomistic test space.

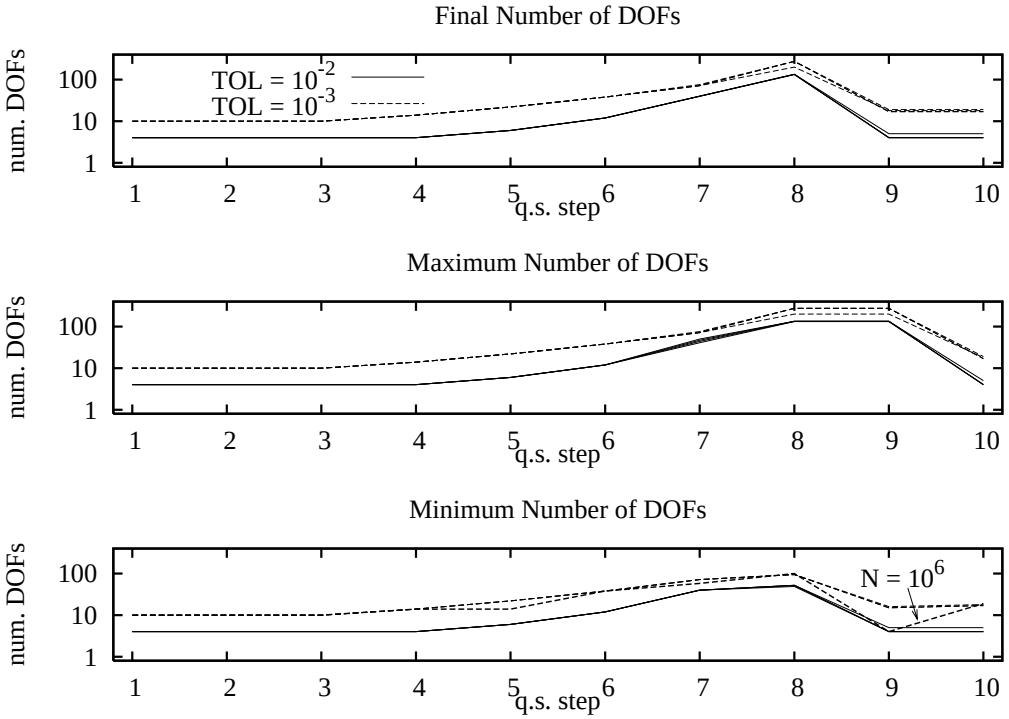

Figure 3: Number of DOFs in the adaptive PPA for the benchmark problem described in §4.1.1. We plot the maximum number of DOFs during each quasistatic iteration, the minimum number of DOFs and also the final number after termination of the PPA.

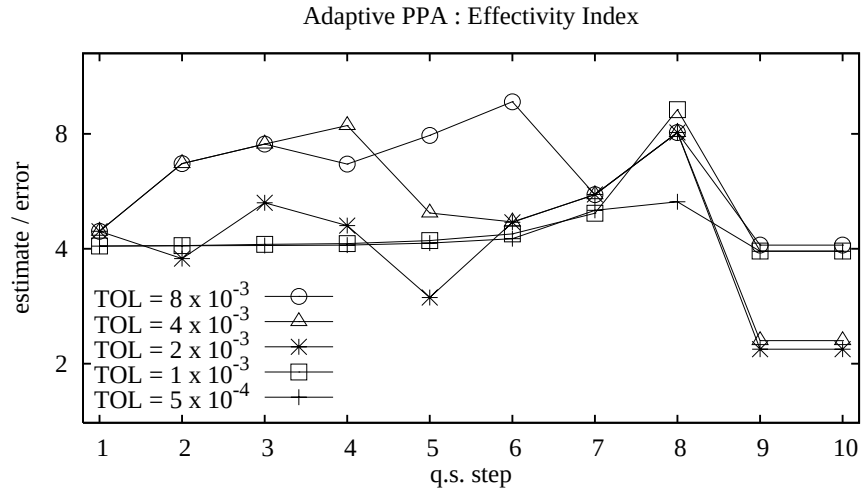

Figure 4: Effectivity index (ratio between estimated and true error) for the final error estimate (after termination of the PPA) for each quasistatic step of the benchmark problem described in §4.1.1. All tests are performed with $N = 10^3$.

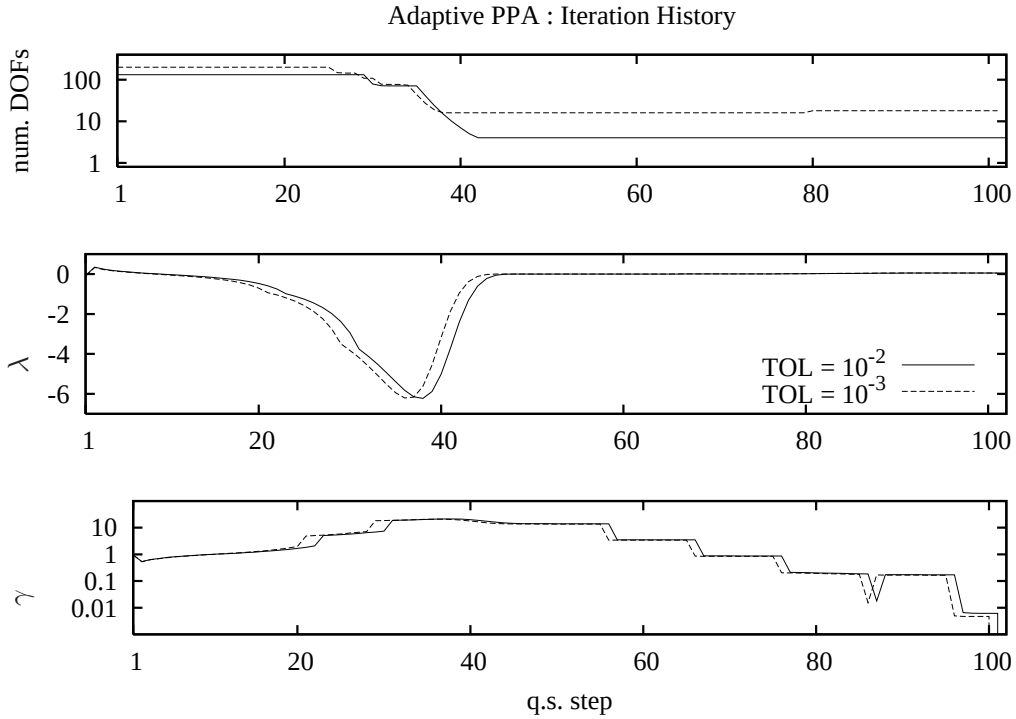

Figure 5: Iteration history of the adaptive proximal point algorithm for the 9th quasistatic step of the benchmark problem described in §4.1.1 where $N = 10^3$ and $\mathrm{TOL} \in \{10^{-2}, 10^{-3}\}$.

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