AN ADAPTIVE FINITE ELEMENT APPROXIMATION OF A GENERALISED AMBROSIO–TORTORELLI FUNCTIONAL

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The Francfort–Marigo model of brittle fracture is posed in terms of the minimization of a highly irregular energy functional. A successful method for discretizing the model is to work with an approximation of the energy. In this work a generalized Ambrosio–Tortorelli functional is used. This leads to a bound-constrained minimization problem, which can be posed in terms of a variational inequality. We propose, analyze and implement an adaptive finite element method for computing (local) minimizers of the generalized functional.

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1. Introduction

The Francfort–Marigo model of quasi-static brittle fracture [26] is formulated in terms of a free-discontinuity problem, in which the path of the crack is itself an unknown variable. It is thus free from one of the major constraints for many models from classical fracture mechanics, that of a pre-defined crack path. A brief description of the model is given in Section 1.2.

In practice, the Francfort–Marigo model requires a highly irregular energy functional to be minimized, which poses difficulties for numerical approaches that are based on a direct discretization of the problem. However, there exist a number of numerical schemes in the literature that minimize a regularization of the energy. The Ambrosio–Tortorelli functional is one such regularization, which can be understood as a phase-field model for the crack set. An approximation of the Francfort–Marigo model via the minimization of the *standard* Ambrosio–Tortorelli functional was proposed by Bourdin, Francfort and Marigo [8] and implemented for a range of examples by Bourdin [6, 7]. In addition, an adaptive finite element method for computing numerical solutions of this approximation was proposed and analysed by Burke, Ortner and Süli [14].

Although previous numerical schemes have focused on approximating the Francfort–Marigo energy by the standard Ambrosio–Tortorelli functional, there exists, in fact, an entire family of generalized approximating functionals [10, 24]. In

this paper we consider the minimization of a generalized functional together with a new method for implementing crack irreversibility, which is based on the monotonicity condition proposed by Giacomini [27]. This will be presented in Section 1.3. Our motivation for considering this generalization is to investigate the possibility of selecting a functional so that the resulting minimization problem has certain convenient properties. For example, the profile of a minimizer may allow it to be resolved more easily by a numerical discretization or the minimized energy may be closer to that of the exact solution.

The minimization of the generalized Ambrosio–Tortorelli functional can be posed in terms of a variational equality and inequality (see Section 2), the solutions of which possess an interior layer in the vicinity of the crack. It is therefore necessary to have a sufficiently fine spatial discretization within this layer to resolve the full behaviour of the solution, however, elsewhere a coarser discretization will suffice. Since the location of the crack is unknown a priori we propose using an adaptive finite element method to compute numerical minimizers, in which the mesh-refinement is driven by a pair of residual estimates. These are presented in Section 4.2 and an adaptive algorithm that combines mesh-refinement with an alternating minimization algorithm is given in Section 4.3. The convergence of the algorithm is analyzed in Section 4.5 and we conclude by presenting some computational results in Section 5.

1.1. *Notation*

Throughout the paper, we assume that m, $N \in \mathbb{N}$ with $N \geq 2$. We also assume that Ω is a connected and bounded open domain in $\mathbb{R}^N$. For $p \in [1, \infty]$, we use $\mathrm{L}^p(\Omega)$ to denote the standard Lebesgue spaces on Ω and $\mathrm{H}^1(\Omega)$ to denote the standard Hilbertian Sobolev space on Ω. The N-dimensional Lebesgue and Hausdorff measures are denoted by $\mathcal{L}^N$ and $\mathcal{H}^N$, respectively.

For A, $B \in \mathbb{R}^{N\times N}$ we define, using the summation convention, $A : B := A_{ij}B_{ij}$ and $|A| := (A : A)^{1/2}$. For $a \in \mathbb{R}^N$ we define the standard Euclidean norm $|a| := (a^T a)^{1/2}$.

1.2. *The Francfort–Marigo model of brittle fracture*

In this section we present a short description of the Francfort–Marigo model of brittle fracture [26]. For the sake of brevity we choose not to give a full exposition of the model and its surrounding theory but, instead, direct the reader to appropriate references where further details can be found.

The model will be introduced in the setting of general linearized elasticity, incorporating anti-plane strain, plane strain and three-dimensional elasticity into one unified framework. We consider a linearly elastic body whose crack-free reference configuration is denoted by Ω. In addition to being open, bounded and connected we assume that Ω possesses a Lipschitz boundary $\partial\Omega$ (although we shall later on relax this assumption). We wish to study how the body evolves in time under the

action of a varying load $g(t)$, which is applied on an open subset $\Omega_D \subset \Omega$ of positive N-dimensional Lebesgue measure. The fact that the Dirichlet condition is imposed on a set of positive N-dimensional Lebesgue measure is mostly technical and ensures that the jump set on the *Dirichlet boundary* $\partial\Omega_D \cap \Omega$ is well-defined. We call $\partial\Omega_N := \partial\Omega \backslash \partial\Omega_D$ the *Neumann boundary*. We assume that

$$g \in \mathrm{L}^\infty(0,T;\mathrm{W}^{1,\infty}(\Omega;\mathbb{R}^m)) \cap \mathrm{W}^{1,1}(0,T;\mathrm{H}^1(\Omega;\mathbb{R}^m)).$$

When $N = 2$, we assume that $m = 1$ or $m = 2$ and when $N \geq 3$, we assume that $m = N$. We refer to the case $N = 2, m = 1$ as the *anti-plane strain case*, the case $N = m = 2$ as the *the plane strain case*, and the case $N = m = 3$ as three-dimensional elasticity.

The natural function space setting for the displacement depends on the value of m. When $m = 1$ the displacement is taken from the space of *special functions of bounded variation*, denoted by $\mathrm{SBV}(\Omega;\mathbb{R})$, and when $m \geq 2$ it is taken from the space of *special functions of bounded deformation*, denoted by $\mathrm{SBD}(\Omega;\mathbb{R}^m)$. A full exposition of $\mathrm{SBV}(\Omega;\mathbb{R})$ and $\mathrm{SBD}(\Omega;\mathbb{R}^m)$ is provided in the book by Ambrosio, Fusco and Pallara [3] and the paper by Ambrosio, Coscia and Dal Maso [2], respectively. We note, however, that a function u belonging to $\mathrm{SBV}(\Omega;\mathbb{R})$ or $\mathrm{SBD}(\Omega;\mathbb{R}^m)$ possesses a well-defined jump set, denoted by $J(u)$, and is H^1-regular on $\Omega \setminus J(u)$.

At each time $t \in [0,T]$, the set of admissible displacements of the body is denoted by $\mathcal{A}(t)$, which is defined as follows:

Case 1: When $m = 1$,

$$\mathcal{A}(t) := \big\{u \in \mathrm{SBV}(\Omega;\mathbb{R}) : u|_{\Omega_D} = g(t)|_{\Omega_D}\big\}.$$

Case 2: When $m \geq 2$,

$$\mathcal{A}(t) := \big\{u \in \mathrm{SBD}(\Omega;\mathbb{R}^m) : u|_{\Omega_D} = g(t)|_{\Omega_D},\ \|u\|_{\mathrm{L}^\infty(\Omega)} \leq M\big\},$$

for some constant $M < \infty$, which is independent of t.

The Francfort–Marigo model is formulated in terms of an energy functional, which will now be defined. For each $u \in \mathcal{A}(t)$, $t \in [0,T]$, we define the bulk energy by

$$E_B(u) := \int_\Omega A\nabla u : \nabla u \,\mathrm{d}x \quad \text{for } u \in \mathcal{A}(t),$$

where $A \in \mathbb{R}^{(m\times N)^2}$ is the elasticity tensor. We assume that the tensor A is symmetric (major symmetries) for all $m, N \in \mathbb{N}$ and frame-indifferent (minor symmetries) when $m = N$, and that there exist positive constants C_B and C_K satisfying:

1. $|AP| \leq C_B|P|$ for all $P \in \mathbb{R}^{N\times m}$; (1.1)
2. $AP : P \geq 0$ for all $P \in \mathbb{R}^{N\times m}$; (1.2)
3. $\displaystyle\int_\Omega A\nabla u : \nabla u \,\mathrm{d}x \geq C_K\|\nabla u\|^2_{\mathrm{L}^2(\Omega)}$ for all $u \in \mathrm{H}^1(\Omega;\mathbb{R}^m),\ u|_{\Omega_D} = 0.$ (1.3)

For each Hausdorff measurable set Γ, we define the surface energy by

$$E_S(\Gamma) := \kappa\, \mathcal{H}^{N-1}(\Gamma),$$

where the positive constant κ is known as the *fracture toughness* of the body. This reflects Griffith's principle that, to create a crack one has to *spend* an amount of elastic energy that is proportional to the area of the crack created [28].

For each $u \in \mathcal{A}(t)$, $t \in [0,T]$, and each Hausdorff measurable set Γ, we define the total energy by

$$E(u,\Gamma) := \begin{cases} E_B(u) + E_S(\Gamma), & \text{if } \mathcal{H}^{N-1}(J(u) \setminus \Gamma) = 0, \\ +\infty, & \text{otherwise.} \end{cases}$$

We introduce the Francfort–Marigo model in a time-discrete formulation. Let the time-interval $[0,T]$ be discretized as follows:

$$0 = t_0 < t_1 < \cdots < t_\Lambda = T,$$

where $\Lambda \in \mathbb{N}$, $\Lambda \geq 2$. Define $\Delta t := \max\{t_k - t_{k-1} \,:\, k = 1, \ldots, \Lambda\}$. Given an initial crack $\Gamma(0)$ (which, for technical reasons, should be the jump set of a function $u(0) \in \mathcal{A}(0)$); for $k = 1, \ldots, \Lambda$, we seek $(u(t_k), \Gamma(t_k))$ such that the following two properties hold:

1. *Irreversibility:* $\Gamma(t_k) \supset \Gamma(t_{k-1})$;
2. *Global stability:* $E(u(t_k), \Gamma(t_k)) \leq E(\hat{u}, \hat{\Gamma})$ $\forall \hat{u} \in \mathcal{A}(t_k)$ and $\forall \hat{\Gamma} \supset \Gamma(t_{k-1})$.

In practice, this formulation requires the successive solution of the global minimization problems: find

$$u(t_k) \in \operatorname*{argmin}_{v \in \mathcal{A}(t_k)} \{E_B(v) + E_S(J(v) \cup \Gamma(t_{k-1}))\}, \tag{1.4}$$

followed by an update of the crackset,

$$\Gamma(t_k) := J(u(t_k)) \cup \Gamma(t_{k-1}), \qquad k = 1, \ldots, \Lambda.$$

For further details of the model and the existence of solutions in both the time-discrete form and as $\Delta t \to 0$ we refer to [3, 19, 20, 25, 26]. Finally we note that although the model seeks to globally minimize the energy at each time step, for reasons stated in [14, Section 1.1], we will be satisfied with computing local minimizers in our numerical method. As a matter of fact, we will only be able to prove convergence of our optimization scheme to a critical point. This is a common shortcoming of much of the theory of continuous optimization that does not employ Hessian information. One nevertheless expects that the computed critical points are normally local minimizers.

1.3. *A generalized Ambrosio–Tortorelli approximation*

Finding solutions of the minimization problem (1.4) is a nontrivial task, due to the irregularity of the energy functional and the need to accurately measure the surface area of the crack. There exist a number of numerical methods in the literature that are based on minimizing an approximation of the energy functional $E(u,\Gamma)$, which is able to represent the crack set in a manner more readily tractable by numerical methods. This regularisation is achieved in the sense of Γ-convergence [11], which ensures that minimizers of the approximating functional converge to minimizers of E. A popular choice of regularization is the standard Ambrosio–Tortorelli functional, which will be defined below. This is not, however, the only choice available and in this paper we consider a generalized approximation.

The generalized Ambrosio–Tortorelli functional $J_\varepsilon : \mathrm{H}^1(\Omega;\mathbb{R}^m)\times\mathrm{H}^1(\Omega;[0,1]) \to \mathbb{R}$ is defined, for $0 < \eta \ll \varepsilon \ll 1$, as follows:

$$J_\varepsilon(u,v) := \int_\Omega (F(v)+\eta)\, A\nabla u : \nabla u \,\mathrm{d}x + \kappa \int_\Omega \left(\varepsilon^{-1}G(v) + \varepsilon|\nabla v|^2\right) \mathrm{d}x, \tag{1.5}$$

where $F \in C^3([0,1])$ is an increasing function with $F(0) = 0$ and $F(1) = 1$, and $G \in C^3([0,1])$ is a non-negative function such that $G(z) = 0$ if and only if $z = 1$. We refer to the case $F = v^2$ and $G = \frac{1}{4}(1-v)^2$ as the standard Ambrosio–Tortorelli functional.

Let us define

$$L_\varepsilon(\hat{u},\hat{v}) := \begin{cases} J_\varepsilon(\hat{u},\hat{v}), & \text{if } \hat{u} \in \mathrm{H}^1(\Omega;\mathbb{R}^m),\ \hat{u}|_{\Omega_D} = g(t_k)|_{\Omega_D},\ \hat{v} \in \mathrm{H}^1(\Omega;[0,1]),\\ +\infty, & \text{otherwise,}\end{cases}$$

$$L(\hat{u},\hat{v}) := \begin{cases} E_B(\hat{u}) + C_S E_S(J(\hat{u})), & \text{if } \hat{u} \in \mathcal{A}(t_k),\ \hat{v} = 1 \text{ a.e. on } \Omega,\\ +\infty, & \text{otherwise,}\end{cases}$$

where

$$C_S := 4\int_0^1 \sqrt{G(s)}\,\mathrm{d}s. \tag{1.6}$$

It is reasonable to expect that L_ε Γ-converges to L as $\varepsilon \to 0$, although we do not show the result here. The result was shown by Braides [11, Theorem 4.14] for the anti-plane strain case, while, for the standard Ambrosio–Tortorelli functional, Chambolle [17] has shown the corresponding result for linear elasticity. We therefore believe that it should be possible to combine and extend these results to the generalized functional given above.

Although the Γ-convergence result has not yet been proved we will use J_ε as an approximation of the Francfort–Marigo energy functional. To construct an approximation of the time-discrete Francfort–Marigo model the minimization of J_ε must be supplemented with a criterion for enforcing irreversibility of the crack. We choose to use a modification of the monotonicity condition $v_\varepsilon(t_k) \le v_\varepsilon(t_{k-1})$, $k = 1,\ldots,\Lambda$, specified by Giacomini [27], who showed that this guarantees crack irreversibility in the limit ε, $\Delta t \to 0$. We implement this monotonicity condition at

time t_k, $k = 1, \ldots, \Lambda$, but only on the following subset of Ω:

$$\texttt{MC}(t_{k-1}) := \{x \in \overline{\Omega} : v_\varepsilon(x, t_{k-1}) < \texttt{MCTOL}\},$$

where MCTOL is a user-specified value. Alternative methods for implementing crack irreversibility have been proposed [1,4,21,31]; a nice survey and discussion of these methods is provided in the paper by Amora, Marigo and Maurini [4, p. 1220].

We approximate the time-discrete Francfort–Marigo model as follows. At time $t = t_0$, find

$$(u_\varepsilon(t_0), v_\varepsilon(t_0)) \in \operatorname{argmin}\big\{ J_\varepsilon(\hat{u}, \hat{v}) : \hat{u} \in \mathrm{H}^1(\Omega; \mathbb{R}^N),\ \hat{u}|_{\Omega_D} = g(t_0)|_{\Omega_D};\ \hat{v} \in \mathrm{H}^1(\Omega; [0,1]) \big\}.$$

At subsequent times $t = t_k$, $k = 1, \ldots, \Lambda$, find $(u_\varepsilon(t_k), v_\varepsilon(t_k))$ satisfying

$$(u_\varepsilon(t_k), v_\varepsilon(t_k)) \in \operatorname{argmin}\big\{ J_\varepsilon(\hat{u}, \hat{v}) : \hat{u} \in \mathrm{H}^1(\Omega; \mathbb{R}^N), \hat{u}|_{\Omega_D} = g(t_k)|_{\Omega_D};\ \hat{v} \in \mathrm{H}^1(\Omega; [0,1]), \hat{v} \le v_\varepsilon(t_{k-1}) \text{ on } \texttt{MC}(t_{k-1}) \big\}. \quad (1.7)$$

The Ambrosio–Tortorelli approximation can be thought of as a phase-field model, in which the crack is represented as a diffused interface. At the fixed time $t = t_k$, the function $u_\varepsilon(t_k)$ is an approximation of the displacement of the body $u(t_k)$, with $u_\varepsilon(t_k) \to u(t_k)$ in $\mathrm{L}^1(\Omega)$ as ε, $\Delta t \to 0$. The function $v_\varepsilon(t_k)$, which is constrained to take values in the interval $[0, 1]$, acts as a phase-field variable. The crack is approximated by the subset of the domain on which $v_\varepsilon(t_k)$ takes values close to zero, whilst the unfractured part of the body is represented by the subset of the domain on which $v_\varepsilon(t_k)$ takes values close to one. The transition layer between these two regimes has thickness of order ε.

A fundamental concern for any numerical approximation of the minimization problem (1.7) is that the spatial discretization be sufficiently fine in the vicinity of the crack to resolve the transition layers of the phase-field and displacement variables. Since the location of the crack is unknown a priori it is natural to use an adaptively refined mesh to compute numerical minimizers. Such a method was presented for the standard Ambrosio–Tortorelli approximation by Burke, Ortner and Süli [14], in which an adaptive finite element method is proposed. In this paper we extend this method to the minimization of the generalized Ambrosio–Tortorelli functional, together with a bound-constraint on the phase-field variable for enforcing crack irreversibility.

2. Continuous Minimization Problem and Critical Points

Let us now state the specific minimization problem under consideration. Motivated by our need to partition Ω for the purpose of defining a finite element approximation we shall assume that Ω is an open and bounded polyhedral domain in $\mathbb{R}^N$. By this, we simply mean that Ω possesses a finite partition into nondegenerate N-simplices: *there exist open, disjoint, nondegenerate simplices* $T_1, \ldots, T_K \subset \Omega$ *such*

that $\mathcal{L}^N(\Omega \setminus \cup_k T_k) = 0$ (see also Section 3.1). In that case, it is clear that the usual trace and embedding theorems for Sobolev spaces hold on Ω.

Let ε and η be fixed and set $\kappa = 1$. Fix also the time $t = t_k$ and define the following function spaces:

$$\mathrm{H}^1_g(\Omega) := \{u \in \mathrm{H}^1(\Omega;\mathbb{R}^m) : u = g(t_k) \text{ on } \Omega_D\},$$
$$\mathrm{H}^1_D(\Omega) := \{u \in \mathrm{H}^1(\Omega;\mathbb{R}^m) : u = 0 \text{ on } \Omega_D\}.$$

We wish to incorporate the irreversibility condition into the function space setting for v. We therefore define the following convex subspace of $\mathrm{H}^1(\Omega)$:

$$\mathrm{K} := \{v \in \mathrm{H}^1(\Omega;\mathbb{R}) : 0 \le v(x) \le \chi \ \text{ a.e. } x \in \Omega\},$$

for a given function $\chi \in \mathrm{H}^1(\Omega;[0,1])$. The function χ will be chosen so as to implement the monotonicity condition proposed for imposing irreversibility; the idea being that $\chi(x)$ is equal to $v(x,t_{k-1})$ for $x \in \mathtt{MC}(t_{k-1})$ and then increases continuously to 1 away from $\mathtt{MC}(t_{k-1})$. Since, in practice, we compute a finite element approximation to v at each time, we will restrict χ to lie in the finite element space X_h as soon as it is defined in Section 3.1, at which point we give a precise definition of the function χ to be taken.

To simplify the notation we now relabel the generalized Ambrosio–Tortorelli functional as $J : \mathrm{H}^1_g(\Omega) \times \mathrm{K} \to \mathbb{R}$ where

$$J(u,v) := \int_\Omega (F(v)+\eta)\, A\nabla u : \nabla u \,\mathrm{d}x + \int_\Omega \left(\varepsilon^{-1}G(v) + \varepsilon|\nabla v|^2\right) \mathrm{d}x.$$

The minimization problem can now be stated as follows. Find $(u,v) \in \mathrm{H}^1_g(\Omega)\times\mathrm{K}$ such that

$$(u,v) \in \operatorname{argmin}\{J(\hat u,\hat v) : \hat u \in \mathrm{H}^1_g(\Omega);\ \hat v \in \mathrm{K}\}. \tag{2.1}$$

Proposition 2.1. *The generalized Ambrosio–Tortorelli functional J is Gâteaux differentiable in $(\mathrm{H}^1(\Omega))^m \times \big(\mathrm{H}^1(\Omega)\cap\mathrm{L}^\infty(\Omega)\big)$: Given $(u,v) \in (\mathrm{H}^1(\Omega))^m \times \big(\mathrm{H}^1(\Omega)\cap \mathrm{L}^\infty(\Omega)\big)$, the Gâteaux derivative of J at (u,v) in the direction $(\varphi,\psi) \in (\mathrm{H}^1(\Omega))^m \times \big(\mathrm{H}^1(\Omega)\cap\mathrm{L}^\infty(\Omega)\big)$ is*

$$J'(u,v;\varphi,\psi) = \partial_u J(v;u,\varphi) + \partial_v J(u;v,\psi),$$

where the partial derivatives appearing on the right-hand side are defined by

$$\partial_u J(v;u,\varphi) := 2\int_\Omega (F(v)+\eta) A\nabla u : \nabla\varphi \,\mathrm{d}x, \ \textit{and}$$
$$\partial_v J(u;v,\psi) := \int_\Omega \Big[F'(v)\psi A\nabla u : \nabla u + \varepsilon^{-1}G'(v)\psi + 2\varepsilon\nabla v\cdot\nabla\psi\Big]\,\mathrm{d}x.$$

The proof is omitted since it is a straightforward calculation of the derivative.

A solution $(u,v) \in \mathrm{H}^1_g(\Omega) \times \mathrm{K}$ of the minimization problem (2.1) can be shown to satisfy the following variational equality and inequality [30, Theorem 3.7]:

$$\partial_u J(v;u,\varphi) = 0 \quad \forall\,\varphi \in \mathrm{H}^1_D(\Omega), \tag{2.2}$$
$$\partial_v J(u;v,v-\psi) \le 0 \quad \forall\,\psi \in \mathrm{K}, \tag{2.3}$$

Definition 2.1. We say that $(u, v) \in \mathrm{H}^1_g(\Omega) \times \mathrm{K}$ is a critical point of J if both (2.2) and (2.3) are satisfied.

3. Finite Element Approximation

3.1. *Finite element discretization*

Since we assumed that Ω is a polyhedral domain (see Section 2), we may discretize it as follows. Let $\mathcal{T}_h$ be a subdivision of Ω into N-dimensional open simplices $T \in \mathcal{T}_h$, such that $\overline{\Omega} = \cup_{T\in\mathcal{T}_h} \overline{T}$ and $T_i \cap T_j = \emptyset$ for T_i, $T_j \in \mathcal{T}_h$ with $i \neq j$. The subdivision $\mathcal{T}_h$ is chosen in such a way that the boundary of Ω_D is discretized as the union of faces of simplices from $\mathcal{T}_h$.

We define $h := \max_{T\in\mathcal{T}_h} \mathrm{diam}(T)$ and each simplex $T \in \mathcal{T}_h$ is taken to be an affine image of the open unit simplex

$$\hat{T} := \{\hat{x} = (\hat{x}_1, \ldots, \hat{x}_N) : 0 < \hat{x}_i,\ i = 1, \ldots, N,\ 0 < \hat{x}_1 + \cdots + \hat{x}_N < 1\}.$$

Each simplex $T \in \mathcal{T}_h$ is called an *element*. We assume that the subdivision is conforming, that is, the intersection of the closure of any two elements is either empty or is along an entire k-dimensional face, $0 \leq k \leq N-1$. We also require that the subdivision is shape-regular, i.e.,

$$\sup_{T\in\mathcal{T}_h} \frac{h_T}{d_T} \leq \rho,$$

for some $\rho \in (0, \infty)$, where $h_T := \mathrm{diam}(T)$ and d_T is the diameter of the largest N-dimensional ball contained in T.

Let $N_h \subset \mathbb{N}$ denote an index set for the vertices of $\mathcal{T}_h$. For a vertex with index $i \in N_h$, let x_i denote the position of the vertex and let ζ_i be the continuous piecewise linear basis function such that $\zeta_i(x_j) = \delta_{ij}$. Define $N_h^D := \{i \in N_h : x_i \in \overline{\Omega}_D\}$.

Let $\mathcal{E}_h$ denote the set of $(N-1)$-dimensional open faces in the subdivision with

$$\mathcal{E}_h^D := \{e \in \mathcal{E}_h : e \subseteq \overline{\Omega}_D\},\ \ \mathcal{E}_h^N := \{e \in \mathcal{E}_h : e \subseteq \partial\Omega_N\} \text{ and } \mathcal{E}_h^I := \mathcal{E}_h \backslash (\mathcal{E}_h^D \cup \mathcal{E}_h^N).$$

We define E_h, E_h^D, E_h^N and E_h^I as the union of all faces in $\mathcal{E}_h$, $\mathcal{E}_h^D$, $\mathcal{E}_h^N$ and $\mathcal{E}_h^I$, respectively. For a face $e \in E_h$ we define $h_e := \mathrm{diam}(e)$.

For all $i \in N_h$, let ω_i be the closure of the union of elements $T \in \mathcal{T}_h$ that have x_i as the position of a vertex, that is, $\omega_i := \mathrm{supp}(\zeta_i)$. For a face $e \in \mathcal{E}_h$ and an element $T \in \mathcal{T}_h$ define

$$\omega_e := \bigcup_{i\in N_h : x_i \in \overline{e}} \omega_i \quad \text{and} \quad \omega_T := \bigcup_{i\in N_h : x_i \in \overline{T}} \omega_i.$$

We now define the piecewise linear finite element space

$$\mathrm{X}_h := \Big\{ \sum_{i\in N_h} \lambda_i \zeta_i : \lambda_i \in \mathbb{R} \Big\}.$$

For simplicity we assume that the applied displacement $g \in (\mathrm{X}_h)^m$ and define the following finite element spaces:

$$\mathrm{X}_h^g := (\mathrm{X}_h)^m \cap \mathrm{H}_g^1(\Omega) \quad \text{and} \quad \mathrm{X}_h^D := (\mathrm{X}_h)^m \cap \mathrm{H}_D^1(\Omega).$$

We also assume that $\chi \in \mathrm{X}_h$ and define the finite element space

$$\mathrm{K}_h := \mathrm{X}_h \cap \mathrm{K}.$$

In practice, at time $t = t_k$, we take $\chi = \sum_{i \in N_h} \chi_i \zeta_i(x)$, where

$$\chi_i := \begin{cases} 1, & \text{if } v_h(x_i, t_{k-1}) > \texttt{MCTOL}, \\ v_h(x_i, t_{k-1}), & \text{if } v_h(x_i, t_{k-1}) \leq \texttt{MCTOL}. \end{cases}$$

In the finite element approximation we wish to find $(u_h, v_h) \in \mathrm{X}_h^g \times \mathrm{K}_h$ such that

$$(u_h, v_h) \in \ \text{argmin}\, \{J(\hat{u}_h, \hat{v}_h) : \hat{u}_h \in \mathrm{X}_h^g,\ \hat{v}_h \in \mathrm{K}_h\}. \tag{3.1}$$

Remark 3.1. In practice, for general functions F and G and a given $(u_h, v_h) \in \mathrm{X}_h^g \times \mathrm{K}_h$ it may be difficult to evaluate $J(u_h, v_h)$ exactly. As such it may be necessary to use a numerical quadrature scheme to compute the integral. However, since this is not the main focus of our work and since the algorithm will only be implemented in cases where exact integration is possible, we choose not to consider the effect of quadrature here. We remark, however, that the generalization of Theorem 4.1, the main convergence result, is not entirely straightforward.

3.2. *Discrete variational inequality*

Similarly to the continuous problem, it can be shown that a solution, $(u_h, v_h) \in \mathrm{X}_h^g \times \mathrm{K}_h$, of the discrete minimization problem (3.1) satisfies the following variational equality and inequality:

$$\partial_u J(v_h; u_h, \varphi_h) = 0 \quad \forall \varphi_h \in \mathrm{X}_h^D, \tag{3.2}$$

$$\partial_v J(u_h; v_h, v_h - \psi_h) \leq 0 \quad \forall \psi_h \in \mathrm{K}_h. \tag{3.3}$$

Definition 3.1. We say that $(u_h, v_h) \in \mathrm{X}_h^g \times \mathrm{K}_h$ is a discrete critical point of J if it satisfies both (3.2) and (3.3).

We conclude this section with a proposition showing that the variational inequality (3.3) becomes an equality on a subset of the domain on which the bound constraints are inactive. Before stating the proposition we first define the discrete *contact* and *non-contact* sets.

For all $v_h \in \mathrm{K}_h$ we define the discrete contact set

$$\mathcal{C}_h(v_h) := \bigcup_{i \in N_h^c} \omega_i, \quad \text{where} \quad N_h^c := \{i \in N_h : v_h(x_i) = 0 \text{ or } v_h(x_i) = \chi(x_i)\}.$$

The discrete non-contact set is $\mathcal{N}_h(v_h) := \Omega \setminus \mathcal{C}_h(v_h)$.

Following the work of Chen and Nochetto [18], we also introduce the discrete function $\sigma_h = \sigma_h(u_h, v_h) \in \mathrm{X}_h$, which is defined through the relation

$$\int_\Omega P_h(\sigma_h w_h)\,\mathrm{d}x = \partial_v J(u_h; v_h, w_h) \quad \forall w_h \in \mathrm{X}_h, \tag{3.4}$$

where $P_h : \mathrm{C}(\overline{\Omega}) \to \mathrm{X}_h$ is the standard nodal interpolation operator [12, Section 3.3]. For each fixed $(u_h, v_h) \in \mathrm{X}_h^g \times \mathrm{K}_h$, the existence and uniqueness of the function $\sigma_h(u_h, v_h) \in \mathrm{X}_h$ follows from the Riesz Representation Theorem [23, Appendix D]. For the sake of simplicity, we shall henceforth write σ_h instead of $\sigma_h(u_h, v_h)$ whenever $(u_h, v_h) \in \mathrm{X}_h^g \times \mathrm{K}_h$ is fixed.

Remark 3.2. Given $(u_h, v_h) \in \mathrm{X}_h^g \times \mathrm{K}_h$ we can evaluate $\sigma_h(x_i)$ for all $i \in N_h$ as follows:

$$\partial_v J(u_h; v_h, \zeta_i) = \int_\Omega P_h(\sigma_h \zeta_i)\,\mathrm{d}x = \sigma_h(x_i) \int_{\omega_i} \zeta_i\,\mathrm{d}x.$$

Hence,

$$\sigma_h(x_i) = \frac{1}{(1, \zeta_i)}\,\partial_v J(u_h; v_h, \zeta_i) \quad \forall i \in N_h,$$

where $(\cdot, \cdot)$ denotes the standard L^2 inner product on Ω.

Proposition 3.1. *Let $(u_h, v_h) \in \mathrm{X}_h^g \times \mathrm{K}_h$ satisfy*

$$\partial_v J(u_h; v_h, v_h - \psi_h) \le 0 \quad \forall \psi_h \in \mathrm{K}_h. \tag{3.5}$$

Then, $\sigma_h(x) \equiv 0$ for all $x \in \overline{\mathcal{N}_h}$.

Proof. Suppose that $(u_h, v_h) \in \mathrm{X}_h^g \times \mathrm{K}_h$ satisfies (3.5). Let $i \in N_h$ be such that $0 < v_h(x_i) < \chi(x_i)$. For sufficiently small $t > 0$ we have $v_h - t\,\zeta_i \in \mathrm{K}_h$. Taking $\psi_h = v_h - t\,\zeta_i$ in (3.5) and dividing by t,

$$\partial_v J(u_h; v_h, \zeta_i) \le 0.$$

Similarly, taking $\psi_h = v_h + t\,\zeta_i \in \mathrm{K}_h$ in (3.5) with sufficiently small $t > 0$, we have

$$\partial_v J(u_h; v_h, \zeta_i) \ge 0.$$

This implies, using Remark 3.2, that

$$\sigma_h(x_i) = \frac{1}{(1, \zeta_i)}\,\partial_v J(u_h; v_h, \zeta_i) = 0.$$

It thus follows that $\sigma_h(x_i) = 0$ for all $i \in N_h$ such that $0 < v_h(x_i) < \chi(x_i)$. Therefore, $\sigma_h(x) \equiv 0$ for all $x \in \overline{\mathcal{N}_h}$. □

3.3. *Alternating minimization algorithm*

The following algorithm was originally proposed by Bourdin, Francfort and Marigo [8] for the minimization of the standard Ambrosio–Tortorelli functional. In the following description, `VTOL` is a user-specified termination tolerance.

Alternating Minimization Algorithm

1. Input initial crack field v_h^1.
2. For $n = 1, 2, \ldots$
   (a) $u_h^n = \operatorname{argmin}\{J(z_h, v_h^n) : z_h \in \mathrm{X}_h^g\}$;
   (b) $v_h^{n+1} \in \operatorname{argmin}\{J(u_h^n, z_h) : z_h \in \mathrm{K}_h\}$;
   (c) Repeat until $\|v_h^{n+1} - v_h^n\|_{\mathrm{L}^\infty(\Omega)} < \texttt{VTOL}$.
3. Set $u_h(t_k) = u_h^n$ and $v_h(t_k) = v_h^{n+1}$.

The minimization with respect to v_h takes the form of a bound-constrained minimization problem, which may not possess a unique solution. It is therefore necessary to state a specific minimization algorithm for J with respect to v_h in order for the above algorithm to be well-defined. One such minimization algorithm will be given in Section 5. For the moment, however, we assume that a minimizer of J can be computed on a fixed mesh.

4. Adaptive Finite Element Approximation

Since both the phase-field variable and the displacement variable possess an interior layer in the vicinity of the crack, it is necessary to have a sufficiently fine mesh in this region to resolve the minimizer. However, outside this layer a coarser mesh will suffice. Since we do not know the location of the crack path in advance, it is a natural idea to use an adaptively refined mesh. Following established adaptive finite element theory we use a residual-based *local refinement indicator* to identify those elements where mesh refinement would be most beneficial for improving the accuracy of the solution.

For a discrete critical point $(u_h, v_h) \in \mathrm{X}_h^g \times \mathrm{K}_h$ of J we use a posteriori upper bounds of the residuals

$$\sup_{\varphi \in \mathrm{H}^1_D(\Omega)} \frac{|\partial_u J(v_h; u_h, \varphi)|}{\|\varphi\|_{\mathrm{H}^1(\Omega)}} \quad \text{and} \quad \sup_{\psi \in \mathrm{K}} \frac{\partial_v J(v_h; u_h, v_h - \psi)}{\|\psi\|_{\mathrm{H}^1(\Omega)} + 1} \tag{4.1}$$

as refinement indicator functions for the u and v minimization problems, respectively.

4.1. *Quasi-interpolation operator*

The following interpolation results will be needed for the subsequent residual estimate. Henceforth we use $\lesssim$ to denote $\leq C$ where the positive constant C depends only on the shape-regularity parameter ρ of the mesh but not on the mesh size.

We use the quasi-interpolation operator defined by Carstensen [15]. Its definition requires us to first identify the set of *free* nodes, that is, the set of nodes on which a Dirichlet condition is not enforced. Since, in the estimate of the first residual defined in (4.1) the quasi-interpolation operator will act on functions from $\mathrm{H}^1_D(\Omega)$ on which a homogeneous Dirichlet condition is imposed, whilst, in the estimate of the second residual in (4.1) the quasi-interpolation operator will act on functions from K on which no Dirichlet condition is enforced, we will define two quasi-interpolation operators:

$$\mathcal{I}_h^D : \mathrm{H}^1_D(\Omega) \to \mathrm{X}_h^D \quad \text{and} \quad \mathcal{I}_h : \mathrm{H}^1(\Omega) \to \mathrm{X}_h.$$

We first define $\mathcal{I}_h^D$; let $N_h^F := N_h \setminus N_h^D$ and define a partition of unity, $\{\bar{\zeta}_i : i \in N_h^F\}$, as follows:

$$\bar{\zeta}_i(x) := \frac{\zeta_i(x)}{\zeta(x)} \quad \forall i \in N_h^F, \quad \text{where} \quad \zeta(x) := \sum_{i \in N_h^F} \zeta_i(x).$$

For $\varphi \in \mathrm{H}^1_D(\Omega)$, the quasi-interpolant $\mathcal{I}_h^D \varphi \in \mathrm{X}_h^D$ is defined as follows:

$$\mathcal{I}_h^D \varphi(x) := \sum_{i \in N_h^F} \varphi_i \zeta_i(x), \quad \text{where} \quad \varphi_i := \frac{\int_{\omega_i} \varphi \bar{\zeta}_i \,\mathrm{d}x}{\int_{\omega_i} \zeta_i \,\mathrm{d}x}. \tag{4.2}$$

For $\psi \in \mathrm{H}^1(\Omega)$, the quasi-interpolant $\mathcal{I}_h \psi \in \mathrm{X}_h$ is defined as follows:

$$\mathcal{I}_h \psi(x) := \sum_{i \in N_h} \psi_i \zeta_i(x), \quad \text{where} \quad \psi_i := \frac{\int_{\omega_i} \psi \zeta_i \,\mathrm{d}x}{\int_{\omega_i} \zeta_i \,\mathrm{d}x}. \tag{4.3}$$

Note, however, that $\mathcal{I}_h^D$ reduces to $\mathcal{I}_h$ on taking $N_h^D = \emptyset$, so that $N_h^F = N_h$; hence, all the approximation results for $\mathcal{I}_h$ will follow from those for $\mathcal{I}_h^D$.

Remark 4.1. The quasi-interpolation operators $\mathcal{I}_h^D : \mathrm{H}^1_D(\Omega) \to \mathrm{X}_h^D$ and $\mathcal{I}_h : \mathrm{H}^1(\Omega) \to \mathrm{X}_h$ are positivity preserving; that is, for all $\varphi \in \mathrm{H}^1_D(\Omega)$ and $\psi \in \mathrm{H}^1(\Omega)$ such that $\varphi, \psi \geq 0$ we have $\mathcal{I}_h^D \varphi \geq 0$ and $\mathcal{I}_h \psi \geq 0$.

The following local averaging property is satisfied by the quasi-interpolation operators. Let $\varphi \in \mathrm{H}^1_D(\Omega)$ and $\psi \in \mathrm{H}^1(\Omega)$, then

$$\int_{\omega_i} (\varphi - \varphi_i \zeta) \bar{\zeta}_i \,\mathrm{d}x = 0 \quad \forall i \in N_h^F, \tag{4.4}$$

$$\int_{\omega_i} (\psi - \psi_i) \zeta_i \,\mathrm{d}x = 0 \quad \forall i \in N_h. \tag{4.5}$$

We now state several approximation and stability properties satisfied by the quasi-interpolants, which are modifications of the results presented in [15].

Proposition 4.1.

(a) There exists a constant $\hat{C}_1 > 0$, independent of ω_i, and a patch of elements $\bar{\omega}_i \supseteq \omega_i$, such that,

$$\|(\varphi - \varphi_i\zeta)\bar{\zeta}_i\|_{\mathrm{L}^2(\omega_i)} \leq \hat{C}_1 h_i \|\nabla\varphi\|_{\mathrm{L}^2(\bar{\omega}_i)} \quad \forall\varphi \in \mathrm{H}^1_D(\Omega) \quad \forall i \in N_h^F. \tag{4.6}$$

The patches have uniformly bounded overlap, that is, there exists a universal constant C such that, for all $x \in \Omega$,

$$\#\{i : x \in \bar{\omega}_i\} \leq C. \tag{4.7}$$

(b) There exists a constant $\hat{C}_2 > 0$, independent of e, such that

$$\|\varphi - \mathcal{I}_h^D\,\varphi\|_{\mathrm{L}^2(e)} \leq \hat{C}_2 h_e^{1/2} \|\nabla\varphi\|_{\mathrm{L}^2(\bar{\omega}_e)} \quad \forall\varphi \in \mathrm{H}^1_D(\Omega) \quad \forall e \in E_h, \tag{4.8}$$

where $\bar{\omega}_e := \bigcup_{i:x_i\in\overline{e}} \bar{\omega}_i$.

(c) There exist constants $\hat{C}_3 > 0$ and $\hat{C}_4 > 0$, independent of T, such that

$$\begin{aligned} \|\mathcal{I}_h^D\,\varphi\|_{\mathrm{L}^2(T)} &\leq \hat{C}_3 \|\varphi\|_{\mathrm{L}^2(\omega_T)}, \quad \text{and} \\ \|\nabla(\mathcal{I}_h^D\,\varphi)\|_{\mathrm{L}^2(T)} &\leq \hat{C}_4 \|\nabla\varphi\|_{\mathrm{L}^2(\bar{\omega}_T)}, \quad \forall\varphi \in \mathrm{H}^1_D(\Omega) \quad \forall T \in \mathcal{T}_h, \end{aligned} \tag{4.9}$$

where $\omega_T := \bigcup_{i:x_i\in\overline{T}} \omega_i$ and $\bar{\omega}_T := \bigcup_{i:x_i\in\overline{T}} \bar{\omega}_i$.

Properties (a) to (c) also hold on replacing $\mathcal{I}_h^D$ with $\mathcal{I}_h$ and $\mathrm{H}^1_D(\Omega)$ with $\mathrm{H}^1(\Omega)$.

The proof of Proposition 4.1 is quite technical, and since it is not the main focus of this paper we do not present it here but refer to [13, Appendix A] for the full details.

Remark 4.2. The local averaging properties (4.4) and (4.5) allow us to achieve tighter upper bounds in the estimate of the residuals. For all $f \in \mathrm{L}^2(\Omega)$ and $\varphi \in \mathrm{H}^1_D(\Omega)$, we have

$$\int_\Omega f(\varphi - \mathcal{I}_h^D\,\varphi)\,\mathrm{d}x = \sum_{i\in N_h^F} \int_{\omega_i} f(\varphi - \varphi_i\zeta)\bar{\zeta}_i\,\mathrm{d}x.$$

Therefore, using (4.4), we may subtract any scalars $\alpha_i \in \mathbb{R}$, $i \in N_h^F$, from f as follows:

$$\int_\Omega f(\varphi - \mathcal{I}_h^D\,\varphi)\,\mathrm{d}x = \sum_{i\in N_h^F} \int_{\omega_i} (f - \alpha_i)(\varphi - \varphi_i\zeta)\bar{\zeta}_i\,\mathrm{d}x.$$

Hence, using the approximation property (4.6),

$$\begin{aligned} \int_\Omega f(\varphi - \mathcal{I}_h^D\,\varphi)\,\mathrm{d}x &\leq \sum_{i\in N_h^F} \|f - \alpha_i\|_{\mathrm{L}^2(\omega_i)} \|(\varphi - \varphi_i\zeta_i)\bar{\zeta}_i\|_{\mathrm{L}^2(\omega_i)} \\ &\leq \sum_{i\in N_h^F} \hat{C}_1 h_i \|f - \alpha_i\|_{\mathrm{L}^2(\omega_i)} \|\nabla\varphi\|_{\mathrm{L}^2(\bar{\omega}_i)} \\ &\lesssim \Big[\sum_{i\in N_h^F} h_i^2 \|f - \alpha_i\|^2_{\mathrm{L}^2(\omega_i)}\Big]^{1/2} \|\nabla\varphi\|_{\mathrm{L}^2(\Omega)}, \end{aligned}$$

where, in the last inequality, we have employed the bounded overlap property (4.7).

It can be similarly shown that for all $f \in \mathrm{L}^2(\Omega)$ and $\psi \in \mathrm{H}^1(\Omega)$ we have

$$\int_\Omega f(\psi - \mathcal{I}_h\,\psi)\,\mathrm{d}x \lesssim \Big[\sum_{i\in N_h} h_i^2 \|f-\alpha_i\|^2_{\mathrm{L}^2(\omega_i)}\Big]^{1/2} \|\nabla\psi\|_{\mathrm{L}^2(\Omega)}.$$

In the residual estimates, we will take α_i to be the following average of f in ω_i, for each $i \in N_h^F$:

$$\alpha_i := \bar{f}_i := \frac{1}{|\omega_i|}\int_{\omega_i} f\,\mathrm{d}x. \tag{4.10}$$

4.2. *Residual estimate*

Before stating the main proposition of this section it will be useful to adopt the following definitions.

For all $u_h \in \mathrm{X}_h^g$ and $e \in \mathcal{E}_h$, with unit normal vector n, we define

$$[\![A\nabla u_h]\!]_e := \begin{cases} \big|\big(A\nabla u_h|_{T_1} - A\nabla u_h|_{T_2}\big)n\,\big|, & \text{if } e \subseteq E_h\backslash\partial\Omega, \text{ with } e = \overline{T}_1 \cap \overline{T}_2 \\ & \text{for some } T_1, T_2 \in \mathcal{T}_h, \\ |\big(A\nabla u_h\big)n|_e, & \text{if } e \subseteq \partial\Omega\,. \end{cases}$$

For all $v_h \in \mathrm{K}_h$ and $e \in \mathcal{E}_h$ we define

$$[\![\nabla v_h]\!]_e := \begin{cases} \big|\,\nabla v_h|_{T_1} - \nabla v_h|_{T_2}\,\big|, & \text{if } e \subseteq E_h\backslash\partial\Omega, \text{ with } e = \overline{T}_1 \cap \overline{T}_2 \\ & \text{for some } T_1, T_2 \in \mathcal{T}_h, \\ |\nabla v_h \cdot n|_e, & \text{if } e \subseteq \partial\Omega, \end{cases}$$

where n is the outer unit normal to $\partial\Omega$.

Proposition 4.2. *Let $(u_h, v_h) \in \mathrm{X}_h^g \times \mathrm{K}_h$ be such that*

$$\partial_u J(v_h; u_h, \varphi_h) = 0 \quad \forall \varphi_h \in \mathrm{X}_h^D, \tag{4.11}$$

$$\partial_v J(u_h; v_h, v_h - \psi_h) \le 0 \quad \forall \psi_h \in \mathrm{K}_h. \tag{4.12}$$

Then,

$$|\partial_u J(v_h; u_h, \varphi)| \lesssim \mu_h \|\nabla\varphi\|_{\mathrm{L}^2(\Omega)} \qquad \forall \varphi \in \mathrm{H}^1_D(\Omega),$$

$$\partial_v J(u_h; v_h; v_h - \psi) \lesssim \nu_h\big(\|\psi\|_{\mathrm{H}^1(\Omega)} + 1\big) \quad \forall \psi \in \mathrm{K},$$

where μ_h and ν_h are defined as follows:

$$\mu_h(u_h, v_h) := \Big[\sum_{T\in\mathcal{T}_h} |\mu_T(u_h, v_h)|^2\Big]^{1/2}, \quad \nu_h(u_h, v_h) := \Big[\sum_{T\in\mathcal{T}_h} |\nu_T(u_h, v_h)|^2\Big]^{1/2},$$

where,

$$|\mu_T(u_h,v_h)|^2 := \sum_{\substack{i\in N_h^F:\\ x_i\in\overline{T}}} h_i^2\|p-\bar{p}_i\|^2_{\mathrm{L}^2(\omega_i)} + 4\sum_{e\subseteq\partial T\setminus E_h^D} h_e\|(F(v_h)+\eta)[\![A\nabla u_h]\!]_e\|^2_{\mathrm{L}^2(e)}, \tag{4.13}$$

$$p(u_h,v_h) := 2F'(v_h)(A\nabla u_h)\nabla v_h, \tag{4.14}$$

$$|\nu_T(u_h,v_h)|^2 := \begin{cases} |\nu_T^1(u_h,v_h)|^2 + |\nu_T^2(u_h,v_h)|^2, & \text{if } T\subseteq\mathcal{C}_h(v_h),\\ |\nu_T^1(u_h,v_h)|^2, & \text{if } T\subseteq\mathcal{N}_h(v_h), \end{cases} \tag{4.15}$$

$$|\nu_T^1(u_h,v_h)|^2 := \sum_{i:x_i\in\overline{T}} h_i^2\|q-\bar{q}_i\|^2_{\mathrm{L}^2(\omega_i)} + 4\varepsilon^2\sum_{e\subseteq\partial T} h_e\|[\![\nabla v_h]\!]_e\|^2_{\mathrm{L}^2(e)}, \tag{4.16}$$

$$|\nu_T^2(u_h,v_h)|^2 := \sum_{i:x_i\in\overline{T}}\Big[h_T^{N/2}\|q\|_{\mathrm{L}^2(T)} + \varepsilon\sum_{\substack{e\subseteq\partial T\setminus\partial\mathcal{C}_h(v_h):\\ x_i\in\overline{e}}} h_e^{N-1}[\![\nabla v_h]\!]_e\Big] osc_h(\chi;\omega_i), \tag{4.17}$$

$$q(u_h,v_h) := F'(v_h)A\nabla u_h : \nabla u_h + \varepsilon^{-1}G'(v_h), \tag{4.18}$$

$$osc_h(\chi;\omega_i) := \frac{1}{|(1,\zeta_i)|}\Big|\sum_{j:x_j\in\overline{\omega}_i}\big(\chi(x_i)-\chi(x_j)\big)\int_{\omega_i}\zeta_j\zeta_i\,\mathrm{d}x\Big|. \tag{4.19}$$

Proof.

Part 1. Let us fix $\varphi\in\mathrm{H}^1_D(\Omega)$ and consider first the functional $\varphi\mapsto\partial_u J(v_h;u_h,\varphi)$. The bound for this term is a standard residual estimate with the quasi-interpolant defined in (4.2).

Since (u_h,v_h) satisfies (4.11) it is easily shown (by decomposing the integral as a sum integrals over elements and then applying the divergence theorem) that

$$\begin{aligned}|\partial_u J(v_h;u_h,\varphi)| \le{}& \Big|\int_\Omega p\cdot(\varphi-\varphi_h)\,\mathrm{d}x\Big|\\ &+\Big|\sum_{T\in\mathcal{T}_h} 2\int_{\partial T}\big((F(v_h)+\eta)(A\nabla u_h)n\big)\cdot(\varphi-\varphi_h)\,\mathrm{d}s\Big|,\end{aligned}$$

for all $\varphi_h\in\mathrm{X}_h^D$, where $p=p(u_h,v_h)$ is defined in (4.14).

We choose $\varphi_h=\mathcal{I}_h^D\varphi$; hence, using Remark 4.2 and the approximation prop-

erty (4.8), we have

$$
\begin{aligned}
&|\partial_u J(v_h; u_h, \varphi)| \\
&\lesssim \Big[\sum_{i \in N_h^F} h_i^2 \|p - \bar{p}_i\|^2_{\mathrm{L}^2(\omega_i)} + 4 \sum_{e \subseteq E_h \setminus E_h^D} h_e \| \left(F(v_h) + \eta\right) [\![A \nabla u_h]\!]_e \|^2_{\mathrm{L}^2(e)} \Big]^{1/2} \|\nabla \varphi\|_{\mathrm{L}^2(\Omega)} \\
&\lesssim \Big[\sum_{T \in \mathcal{T}_h} |\mu_T(u_h, v_h)|^2 \Big]^{1/2} \|\nabla \varphi\|_{\mathrm{L}^2(\Omega)},
\end{aligned}
$$

where $\bar{p}_i$ is defined in (4.10) and $\mu_T(u_h, v_h)$ is defined in (4.13).

Part 2 Fix $\psi \in \mathrm{K}$ and consider the functional $\psi \to \partial_v J(u_h; v_h, v_h - \psi)$.

Since we have assumed that (u_h, v_h) satisfies (4.12), we have that

$$
\begin{aligned}
\partial_v J(u_h; v_h, v_h - \psi) &\leq \partial_v J(u_h; v_h, v_h - \psi) + \partial_v J(u_h; v_h, \psi_h - v_h) \\
&= -\partial_v J(u_h; v_h, \psi) + \partial_v J(u_h; v_h, \psi_h),
\end{aligned}
$$

for all $\psi_h \in \mathrm{K}_h$. Hence,

$$
|\partial_v J(u_h; v_h, v_h - \psi)| \leq |\partial_v J(u_h; v_h, \mathcal{I}_h \psi - \psi)| + |\partial_v J(u_h; v_h, \psi_h - \mathcal{I}_h \psi)|, \quad (4.20)
$$

where $\mathcal{I}_h \psi$ is the quasi-interpolant defined in (4.3). We estimate the first and second terms from (4.20) in Part 2(a) and Part 2(b), respectively.

Part 2(a) We estimate the first term in (4.20) in a similar manner to Part 1. We have

$$
\begin{aligned}
\partial_v J(u_h; v_h, \mathcal{I}_h \psi - \psi) &= \int_\Omega q(\mathcal{I}_h \psi - \psi) \, \mathrm{d}x + 2\varepsilon \int_\Omega \nabla v_h \cdot \nabla(\mathcal{I}_h \psi - \psi) \, \mathrm{d}x \\
&= \int_\Omega q(\mathcal{I}_h \psi - \psi) \, \mathrm{d}x + 2\varepsilon \sum_{T \in \mathcal{T}_h} \int_{\partial T} \nabla v_h \cdot n \, (\mathcal{I}_h \psi - \psi) \, \mathrm{d}s,
\end{aligned} \quad (4.21)
$$

where $q = q(u_h, v_h)$ is defined in (4.18).

We estimate the first term in (4.21) using Remark 4.2 and the second term using the approximation property (4.8), giving

$$
\begin{aligned}
&|\partial_v J(u_h; v_h, \mathcal{I}_h \psi - \psi)| \\
&\quad \lesssim \Big[\sum_{i \in N_h} h_i^2 \|q - \bar{q}_i\|^2_{\mathrm{L}^2(\omega_i)} + 4\varepsilon^2 \sum_{e \subseteq E} h_e \| [\![\nabla v_h]\!]_e \|^2_{\mathrm{L}^2(e)} \Big]^{1/2} \|\nabla \psi\|_{\mathrm{L}^2(\Omega)} \\
&\quad \lesssim \Big[\sum_{T \in \mathcal{T}_h} |\nu_T^1(u_h, v_h)|^2 \Big]^{1/2} \|\nabla \psi\|_{\mathrm{L}^2(\Omega)},
\end{aligned}
$$

where $\nu_T^1(u_h, v_h)$ is defined in (4.16).

Part 2(b) We now consider the second term in (4.20), which will be bounded

in terms of the obstacle χ. For all $\psi_h \in \mathrm{K}_h$, it follows from (3.4) and Proposition 3.1 that

$$\begin{aligned}|\partial_v J(u_h; v_h, \psi_h - \mathcal{I}_h\,\psi)| &= \Big| \int_\Omega P_h\big(\sigma_h(\psi_h - \mathcal{I}_h\,\psi)\big)\,\mathrm{d}x\Big| \\ &= \Big| \sum_{i\in N_h} \sigma_h(x_i)(\psi_h(x_i) - \mathcal{I}_h\,\psi(x_i)) \int_{\omega_i} \zeta_i\,\mathrm{d}x\Big| \\ &= \Big| \sum_{i\in N_h^c} \sigma_h(x_i)(\psi_h(x_i) - \mathcal{I}_h\,\psi(x_i)) \int_{\omega_i} \zeta_i\,\mathrm{d}x\Big|.\end{aligned}$$

Thus, using Remark 3.2,

$$|\partial_v J(u_h; v_h, \psi_h - \mathcal{I}_h\,\psi)| \le \sum_{i\in N_h^c} |\partial_v J(u_h; v_h, \zeta_i)|\,|\psi_h(x_i) - \mathcal{I}_h\,\psi(x_i)|.$$

The term $|\partial_v J(u_h; v_h, \zeta_i)|$ is estimated as follows:

$$\begin{aligned}|\partial_v J(u_h; v_h, \zeta_i)| &= \Big| \int_{\omega_i} (q\zeta_i + \varepsilon\nabla v_h\cdot\nabla\zeta_i)\,\mathrm{d}x\,\Big| \\ &\le \sum_{T\subseteq\omega_i} \int_T |q|\,\zeta_i\,\mathrm{d}x + \varepsilon\Big| \sum_{T\subseteq\omega_i} \int_{\partial T} \nabla v_h\cdot n\,\zeta_i\,\mathrm{d}x\,\Big| \\ &\le \sum_{T\subseteq\omega_i} h_T^{N/2}\|q\|_{\mathrm{L}^2(T)} + \varepsilon \sum_{e\subset\omega_i\setminus\partial\omega_i} h_e^{N-1}[\![\nabla v_h]\!]_e.\end{aligned}$$

Therefore,

$$\begin{aligned}&|\partial_v J(u_h; v_h, \psi_h - \mathcal{I}_h\,\psi)| \\ &\quad\le \sum_{i\in N_h^c} \Big[\sum_{T\subseteq\omega_i} h_T^{N/2}\|q\|_{\mathrm{L}^2(T)} + \varepsilon \sum_{e\subset\omega_i\setminus\partial\omega_i} h_e^{N-1}[\![\nabla v_h]\!]_e\Big] |\psi_h(x_i) - \mathcal{I}_h\,\psi(x_i)|.\end{aligned}$$

Clearly, we would like to choose $\psi_h = \mathcal{I}_h\,\psi$; however, $\mathcal{I}_h\,\psi$ may not belong to the finite element space K_h. Following the work of Chen and Nochetto [18], we choose $\psi_h = P_h\big(\min\{\mathcal{I}_h\,\psi, \chi\}\big)$. Hence, $\psi_h \in \mathrm{K}_h$ and

$$\psi_h(x_i) = \min\{\mathcal{I}_h\,\psi(x_i), \chi(x_i)\} \quad \forall i \in N_h. \tag{4.22}$$

The following inequality, derived by Chen and Nochetto [18, Section 5], is key to our analysis. It is seen from Remark 4.1 and (4.22) that

$$0 \le \mathcal{I}_h\,\psi(x_i) - \psi_h(x_i) \le \big(\mathcal{I}_h\,\psi(x_i) - \chi(x_i)\big)_+ \le \big(\mathcal{I}_h\,\chi(x_i) - \chi(x_i)\big)_+;$$

hence,

$$|\psi_h(x_i) - \mathcal{I}_h\,\psi(x_i)| \le |\chi(x_i) - \mathcal{I}_h\,\chi(x_i)|.$$

Since we assumed that $\chi \in \mathrm{X}_h$, we have

$$\begin{aligned}|\chi(x_i) - \mathcal{I}_h\,\chi(x_i)| &= \frac{1}{|(1,\zeta_i)|}\Big|\int_{\omega_i}(\chi(x_i)-\chi)\zeta_i\,\mathrm{d}x\Big| \\ &= \frac{1}{|(1,\zeta_i)|}\Big|\int_{\omega_i}\Big(\chi(x_i) - \sum_{j:x_j\in\overline{\omega}_i}\chi(x_j)\zeta_j\Big)\zeta_i\,\mathrm{d}x\Big| \\ &= \frac{1}{|(1,\zeta_i)|}\Big|\sum_{j:x_j\in\overline{\omega}_i}\big(\chi(x_i)-\chi(x_j)\big)\int_{\omega_i}\zeta_j\zeta_i\,\mathrm{d}x\Big|,\end{aligned}$$

which can be easily computed using the mass matrix. We therefore define

$$osc_h(\chi;\omega_i) := \frac{1}{|(1,\zeta_i)|}\Big|\sum_{j:x_j\in\overline{\omega}_i}\big(\chi(x_i)-\chi(x_j)\big)\int_{\omega_i}\zeta_j\zeta_i\,\mathrm{d}x\Big|,$$

to obtain

$$\begin{aligned}&|\partial_v J(u_h;v_h,\psi_h-\mathcal{I}_h\,\psi)| \\ &\quad\lesssim \sum_{i\in N_h^c}\Big[\sum_{T\subseteq\omega_i}h_T^{N/2}\|q\|_{\mathrm{L}^2(T)} + \varepsilon\sum_{e\subset\omega_i\setminus\partial\omega_i}h_e^{N-1}[\![\nabla v_h]\!]_e\Big]\,osc_h(\chi;\omega_i) \\ &\quad\lesssim \sum_{\substack{T\in\mathcal{T}_h:\\ T\subseteq C_h(v_h)}}|\nu_T^2(u_h,v_h)|^2,\end{aligned}$$

where $\nu_T^2(u_h,v_h)$ is defined in (4.17).

Combining the estimates from Parts 2(a) and 2(b), we have

$$\partial_v J(u_h;v_h;v_h-\psi) \lesssim \Big[\sum_{T\in\mathcal{T}_h}|\nu_T(u_h,v_h)|^2\Big]^{1/2}\big(\|\psi\|_{\mathrm{H}^1(\Omega)}+1\big),$$

where $\nu_T(u_h,v_h)$ is defined in (4.15). □

For all $T\in\mathcal{T}_h$ we use $\mu_T(u_h,v_h)$ and $\nu_T(u_h,v_h)$ as local refinement indicator functions for u_h and v_h, respectively. Note that

$$\begin{aligned}\|\partial_u J(u_h,v_h)\|_{\left(\mathrm{H}^1_D(\Omega)\right)^*} &\lesssim \Big[\sum_{T\in\mathcal{T}_h}|\mu_T(u_h,v_h)|^2\Big]^{1/2}, \quad\text{and} \\ \sup_{\psi\in\mathrm{K}}\frac{\partial_v J(v_h;u_h,v_h-\psi)}{\|\psi\|_{\mathrm{H}^1(\Omega)}+1} &\lesssim \Big[\sum_{T\in\mathcal{T}_h}|\nu_T(u_h,v_h)|^2\Big]^{1/2}.\end{aligned}$$

4.3. *Adaptive algorithm*

We now state the adaptive algorithm. It has a similar structure to the second adaptive algorithm proposed in [14] for the minimization of the standard Ambrosio–Tortorelli functional. The user-specified tolerances `REFTOL_U` and `REFTOL_V` determine when to halt the refinement loops with respect to u and v, respectively. The *marking parameter* θ is a fixed number lying in the interval $(0,1]$. Within each alternating minimization step $n\in\{m/2 : m\in\mathbb{N}\}$ we denote the mesh at the jth

level of refinement by $\mathcal{T}_j^n$ and the associated mesh size $h_j^n := \max_{T\in\mathcal{T}_j^n} \operatorname{diam}(T)$, for all $j \in \mathbb{N}$.

Adaptive Algorithm

1. *Input:* Initial crack field v^1 and initial mesh $\mathcal{T}^{1/2}$.
2. *Alternating minimization loop:* For $n = 1, 2, \ldots$
   (a) Set $\mathcal{T}_1^n = \mathcal{T}^{n-1/2}$
   (b) *Mesh refinement loop:* For $j = 1, 2, \ldots$
   - Compute $u_j^n :=$ argmin $\{J(z, v^n) : z \in \mathrm{X}^g_{h_j^n}\}$;
   - If $\big[\sum_{T\in\mathcal{T}_j^n} |\, \mu_T(u_j^n, v^n)\,|^2\,\big]^{1/2} >$ `REFTOL_U`,
     - Find the smallest set $M_j \subseteq \mathcal{T}_j^n$ such that $\sum_{T\in M_j} |\mu_T(u_j^n, v^n)|^2 \geq \theta \sum_{T\in\mathcal{T}_j^n} |\mu_T(u_j^n, v^n)|^2$;
     - Refine elements in M_j to obtain the new mesh $\mathcal{T}_{j+1}^n$.
   - Repeat until $\big[\sum_{T\in\mathcal{T}_j^n} |\, \mu_T(u_j^n, v^n)\,|^2\,\big]^{1/2} \leq$ `REFTOL_U`.

   (c) Set $u^n = u_j^n$, $\mathcal{T}^n = \mathcal{T}_j^n$ and $\mathcal{T}_1^{n+1/2} = \mathcal{T}^n$.
   (d) *Mesh refinement loop:* For $j = 1, 2, \ldots$
   - Compute $v_j^{n+1} \in$ argmin $\{J(u^n, z) : z \in \mathrm{K}_{h_j^{n+1/2}}\}$;
   - If $\big[\sum_{T\in\mathcal{T}_j^{n+1/2}} |\, \nu_T(u^n, v_j^{n+1})\,|^2\,\big]^{1/2} >$ `REFTOL_V`,
     - Find the smallest set $M_j \subseteq \mathcal{T}_j^{n+1/2}$ such that $\sum_{T\in M_j} |\nu_T(u^n, v_j^{n+1})|^2 \geq \theta \sum_{T\in\mathcal{T}_j^{n+1/2}} |\nu_T(u^n, v_j^{n+1})|^2$;
     - Refine elements in M_j to obtain the new mesh $\mathcal{T}_{j+1}^{n+1/2}$.
   - Repeat until $\big[\sum_{T\in\mathcal{T}_j^{n+1/2}} |\, \nu_T(u^n, v_j^{n+1})\,|^2\,\big]^{1/2} \leq$ `REFTOL_V`.

   (e) Set $v^{n+1} = v_j^{n+1}$ and $\mathcal{T}^{n+1/2} = \mathcal{T}_j^{n+1/2}$;
   (f) Repeat steps (a) to (e) until $\|v^{n+1} - v^n\|_{\mathrm{L}^\infty(\Omega)} <$ `VTOL`.
3. Set $u_h(t_k) = u^n$ and $v_h(t_k) = v^{n+1}$.

We reiterate the comment made in Section 3.3 that, as currently stated, the algorithm is not well-defined since the v-minimization problem in Step 2(d) may not have a unique minimizer. This will not affect the convergence analysis of the algorithm, however, for which it is sufficient to compute any minimizer. We therefore postpone our discussion of a specific minimization algorithm for v until Section 5 and begin with a convergence analysis of the Adaptive Algorithm, for which it is useful to consider the following modification.

Adaptive Iteration:
In step n of the Adaptive Algorithm, we replace `REFTOL_U` and `REFTOL_V` by $\texttt{REFTOL\_U}^n$ and $\texttt{REFTOL\_V}^n$, respectively, and require that $\texttt{REFTOL\_U}^n \to 0$ and $\texttt{REFTOL\_V}^n \to 0$ as $n \to \infty$. Furthermore, we remove the termination condition 2(f) and make the following assumption:

Assumption (B): *Steps (b) and (d) in the Adaptive Algorithm and Adaptive Iteration terminate in a finite number of iterations.*

Assumption (B) is a nowadays well-understood property of adaptive algorithms of the type that we propose [16, 18, 22]. Having said this, our setting is not covered by existing results, and a rigorous justification of termination of the algorithm in a finite number of iterations is beyond the scope of this work.

4.4. *Auxiliary results*

We now state two lemmas that will be useful in the convergence analysis of Section 4.5.

Lemma 4.1. *The sequence* $((u^n, v^n))_{n=1}^\infty \subseteq \mathrm{H}^1_g(\Omega) \times \mathrm{K}$ *generated by the Adaptive Iteration is bounded in* $(\mathrm{H}^1(\Omega))^m \times \mathrm{H}^1(\Omega)$.

Proof. Let $((u^n, v^n))_{n=1}^\infty \subseteq \mathrm{H}^1_g(\Omega) \times \mathrm{K}$ be the sequence generated by the Adaptive Iteration, then $(J(u^n, v^n))_{n=1}^\infty$ is a bounded sequence in $\mathbb{R}$. Since

$$\begin{aligned} J(u^n, v^n) &= \int_\Omega \left[(F(v^n) + \eta) A\nabla u^n : \nabla u^n + \varepsilon^{-1} G(v^n) + \varepsilon |\nabla v^n|^2 \right] \mathrm{d}x \\ &\geq \eta \|A\nabla u^n : \nabla u^n\|_{\mathrm{L}^1(\Omega)} + \varepsilon \|\nabla v^n\|^2_{\mathrm{L}^2(\Omega)}, \end{aligned}$$

it follows that $(\|\nabla v^n\|_{\mathrm{L}^2(\Omega)})_{n=1}^\infty$ and $(\|A\nabla u^n : \nabla u^n\|_{\mathrm{L}^1(\Omega)})_{n=1}^\infty$ are bounded sequences in $\mathbb{R}$. We also have that $0 \leq v^n(x) \leq 1$ for almost every $x \in \Omega$, which implies that $(\|v^n\|_{\mathrm{L}^2(\Omega)})_{n=1}^\infty$ is bounded. Therefore, $(v^n)_{n=1}^\infty$ is bounded in $\mathrm{H}^1(\Omega)$.

Using the coercivity and positivity assumptions on A together with the boundedness of $(\|A\nabla u^n : \nabla u^n\|_{\mathrm{L}^1(\Omega)})_{n=1}^\infty$, it can be shown that $\left(\|\nabla(u^n - g)\|_{\mathrm{L}^2(\Omega)}\right)_{n=1}^\infty$ is bounded. Using a variant of the Friedrichs inequality [9, Chapter 2, Section 1.5] and noting that $(u^n - g) \in \mathrm{H}^1_D(\Omega)$, for all $n \in \mathbb{N}$, we then have

$$\|u^n\|_{\mathrm{H}^1(\Omega)} \leq \|u^n - g\|_{\mathrm{H}^1(\Omega)} + \|g\|_{\mathrm{H}^1(\Omega)} \leq C_F \|\nabla(u^n - g)\|_{\mathrm{L}^2(\Omega)} + \|g\|_{\mathrm{H}^1(\Omega)},$$

where $C_F = C_F(\Omega, N) > 0$ is the Friedrichs constant. Therefore, $(\|u^n\|_{\mathrm{H}^1(\Omega)})_{n=1}^\infty$ is a bounded sequence. Consequently, $((u^n, v^n))_{n=1}^\infty$ is a bounded sequence in $(\mathrm{H}^1(\Omega))^m \times \mathrm{H}^1(\Omega)$. □

Lemma 4.2. *Suppose that the sequences* $(v_j)_{j=1}^\infty \subset \mathrm{K}$ *and* $(w_j)_{j=1}^\infty \subset \mathrm{L}^1(\Omega)$ *are such that* $v_j \to v$ *in* $\mathrm{L}^1(\Omega)$ *and* $w_j \to w$ *in* $\mathrm{L}^1(\Omega)$ *as* $j \to \infty$, *for some* $v \in \mathrm{K}$ *and* $w \in \mathrm{L}^1(\Omega)$. *Let* $s \in \{1, 2\}$; *then,*

$$\lim_{j\to\infty} \int_\Omega |f(v) - f(v_j)|^s \, |w_j| \, \mathrm{d}x = 0 \quad \forall f \in \mathrm{C}([0,1]).$$

Proof. Since $f \in \mathrm{C}([0,1])$,

$$\int_\Omega |f(v) - f(v_j)|^s \, |w_j| \, \mathrm{d}x \leq \int_\Omega |f(v) - f(v_j)|^s \, |w| \, \mathrm{d}x + \|f(v) - f(v_j)\|^s_{\mathrm{L}^\infty(\Omega)} \int_\Omega |w - w_j| \, \mathrm{d}x.$$

Lebesgue's Dominated Convergence Theorem [34, Section 5.2] and the continuity of f imply that the first term converges to zero as $j \to \infty$. The second term converges to zero as a result of the strong convergence $w_j \to w$ in $\mathrm{L}^1(\Omega)$ as $j \to \infty$. □

4.5. *Convergence analysis*

The main result of this section is established in Theorem 4.1; it implies that the sequence $((u^n, v^n))_{n=1}^\infty$ computed by the Adaptive Iteration, under Assumption (B), converges to a critical point of J. Before showing this result we first establish two lemmas concerning the convergence of the partial derivatives of J.

Lemma 4.3. *Suppose that there exists a sequence* $((u_j, v_j))_{j=1}^\infty \subset \mathrm{H}^1_g(\Omega) \times \mathrm{K}$ *and* $(u, v) \in \mathrm{H}^1_g(\Omega) \times \mathrm{K}$ *such that* $(u_j, v_j) \rightharpoonup (u, v)$ *in* $(\mathrm{H}^1(\Omega))^N \times \mathrm{H}^1(\Omega)$. *Suppose also that* $((u_j, v_j))_{j=1}^\infty$ *satisfies*

$$\partial_u J(v_j; u_j, \varphi) \leq \mu_j \|\nabla \varphi\|_{\mathrm{L}^2(\Omega)} \qquad \forall \varphi \in \mathrm{H}^1_D(\Omega), \tag{4.23}$$

for some $\mu_j \in \mathbb{R}_{\geq 0}$ *with* $\mu_j \to 0$ *as* $j \to \infty$.

Then, u *and* v *satisfy*

$$\partial_u J(v; u, \varphi) = 0 \qquad \forall \varphi \in \mathrm{H}^1_D(\Omega),$$

and $u_j \to u$ *strongly in* $(\mathrm{H}^1(\Omega))^N$ *as* $j \to \infty$.

Proof.
Step 1. $\partial_u J(v; u, \varphi) = 0$ for all $\varphi \in \mathrm{H}^1_D(\Omega)$:
Fixing $\varphi \in \mathrm{H}^1_D(\Omega)$ we have

$$\begin{aligned}
\partial_u J(v; u, \varphi) &= 2 \int_\Omega (F(v) + \eta) \, A\nabla u : \nabla \varphi \, \mathrm{d}x \\
&= 2 \int_\Omega (F(v) + \eta) \, A\nabla (u - u_j) : \nabla \varphi \, \mathrm{d}x + 2 \int_\Omega (F(v_j) + \eta) \, A\nabla u_j : \nabla \varphi \, \mathrm{d}x \\
&\quad + 2 \int_\Omega (F(v) - F(v_j)) \, A\nabla u_j : \nabla \varphi \, \mathrm{d}x \\
&=: R_j + S_j + T_j.
\end{aligned}$$

Our aim is to show that R_j, S_j and $T_j \to 0$ as $j \to \infty$.

Using the symmetry of the elasticity tensor,

$$R_j = 2 \int_\Omega (F(v) + \eta) A\nabla \varphi : \nabla (u - u_j) \, \mathrm{d}x.$$

Since $\nabla u_j \rightharpoonup \nabla u$ in $(\mathrm{L}^2(\Omega))^{m\times N}$ and $(F(v)+\eta)A\nabla\varphi \in \mathrm{L}^2(\Omega)$ we have $R_j \to 0$ as $j\to\infty$.

Now let us examine S_j; by (4.23) we have

$$|S_j| \le \mu_j \|\nabla\varphi\|_{\mathrm{L}^2(\Omega)} \to 0 \text{ as } j\to\infty.$$

Finally, we bound T_j as follows

$$\begin{aligned}|T_j| &\le 2\int_\Omega |F(v)-F(v_j)|\,|A\nabla u_j|\,|\nabla\varphi|\,\mathrm{d}x\\ &\le 2C_B\Big(\int_\Omega |F(v)-F(v_j)|^2|\nabla\varphi|^2\,\mathrm{d}x\Big)^{1/2}\|\nabla u_j\|_{\mathrm{L}^2(\Omega)},\end{aligned}$$

where C_B is the boundedness constant from (1.1). As $|\nabla\varphi|^2 \in \mathrm{L}^1(\Omega)$, it follows from Lemma 4.2 that $T_j\to 0$ as $j\to\infty$. Thus we deduce that $\partial_u J(v;u,\varphi)=0$ for all $\varphi\in \mathrm{H}^1_D(\Omega)$.

Step 2. $\nabla u_j \to \nabla u$ strongly in $(\mathrm{L}^2(\Omega))^{m\times N}$:
Using the coercivity assumption (1.3) on A we have

$$\begin{aligned}2C_K\eta\|\nabla u-\nabla u_j\|^2_{\mathrm{L}^2(\Omega)} &\le 2\int_\Omega (F(v_j)+\eta)\,A(\nabla u-\nabla u_j):(\nabla u-\nabla u_j)\,\mathrm{d}x\\ &= -\partial_u J(v_j;u_j,u-u_j)+2\int_\Omega (F(v_j)+\eta)\,A\nabla u:\nabla(u-u_j)\,\mathrm{d}x.\end{aligned}$$

By Step 1 we have $\partial_u J(v;u,u-u_j)=0$; thus

$$\begin{aligned}&2C_K\eta\|\nabla u-\nabla u_j\|^2_{\mathrm{L}^2(\Omega)}\\ &\le -\partial_u J(v_j;u_j,u-u_j)+2\int_\Omega (F(v_j)+\eta)\,A\nabla u:\nabla(u-u_j)\,\mathrm{d}x-\partial_u J(v;u,u-u_j)\\ &= -\partial_u J(v_j;u_j,u-u_j)+2\int_\Omega (F(v_j)-F(v))\,A\nabla u:(\nabla u-\nabla u_j)\,\mathrm{d}x\\ &\le \mu_j\|\nabla u-\nabla u_j\|_{\mathrm{L}^2(\Omega)}+2C_B\|(F(v_j)-F(v))\nabla u\|_{\mathrm{L}^2(\Omega)}\|\nabla(u-u_j)\|_{\mathrm{L}^2(\Omega)}.\end{aligned}$$

In summary,

$$2C_K\eta\|\nabla u-\nabla u_j\|_{\mathrm{L}^2(\Omega)} \le \mu_j + 2C_B\Big(\int_\Omega |F(v_j)-F(v)|^2\,|\nabla u|^2\,\mathrm{d}x\Big)^{1/2},$$

and thus, using Lemma 4.2 and $\mu_j\to 0$ as $j\to\infty$, it follows that $u_j\to u$ strongly in $(\mathrm{H}^1(\Omega))^N$ as $j\to\infty$. □

Lemma 4.4. *Suppose that there exists a sequence $((u_j,v_j))_{j=1}^\infty \subset \mathrm{H}^1_g(\Omega)\times\mathrm{K}$ and $(u,v)\in \mathrm{H}^1_g(\Omega)\times\mathrm{K}$ such that $u_j\to u$ strongly in $\mathrm{H}^1(\Omega)$ and $v_j\rightharpoonup v$ weakly in $\mathrm{H}^1(\Omega)$ as $j\to\infty$. Suppose also that $((u_j,v_j))_{j=1}^\infty$ satisfies*

$$\partial_v J(u_j;v_j,v_j-\psi) \le \nu_j(\|\psi\|_{\mathrm{H}^1(\Omega)}+1) \qquad \forall\psi\in\mathrm{K}, \tag{4.24}$$

for some $\nu_j\in\mathbb{R}_{\ge 0}$ with $\nu_j\to 0$ as $j\to\infty$.

Then, $v_j \to v$ strongly in $\mathrm{H}^1(\Omega)$ as $j \to \infty$. Moreover, u and v satisfy

$$\partial_v J(u; v, v - \psi) \leq 0 \qquad \forall \psi \in \mathrm{K}.$$

Proof.

Step 1. $\nabla v_j \to \nabla v$ strongly in $(\mathrm{L}^2(\Omega))^N$:
Substituting $\psi = v$ into (4.24) gives

$$\int_\Omega \Big[F'(v_j)(v_j - v)\, A\nabla u_j : \nabla u_j + \varepsilon^{-1} G'(v_j)(v_j - v) + 2\varepsilon \nabla v_j \cdot \nabla(v_j - v)\Big]\, \mathrm{d}x \leq \nu_j(\|v\|_{\mathrm{H}^1(\Omega)} + 1),$$

which implies

$$\begin{aligned} 2\varepsilon \int_\Omega |\nabla v_j|^2 \,\mathrm{d}x \leq \nu_j(\|v\|_{\mathrm{H}^1(\Omega)} + 1) + 2\varepsilon \int_\Omega \nabla v_j \cdot \nabla v \,\mathrm{d}x \\ + \varepsilon^{-1} \|G'(v_j)\|_{\mathrm{L}^2(\Omega)}\, \|v - v_j\|_{\mathrm{L}^2(\Omega)} \\ + C_B \|F'(v_j)\|_{\mathrm{L}^\infty(\Omega)} \int_\Omega |v - v_j|\, |\nabla u_j|^2 \,\mathrm{d}x. \end{aligned}$$

Recall that $\nu_j \to 0$, $\nabla v_j \rightharpoonup \nabla v$ in $(\mathrm{L}^2(\Omega))^N$ and $v_j \to v$ in $\mathrm{L}^2(\Omega)$ as $j \to \infty$. Hence, using Lemma 4.2 with $w_j = |\nabla u_j|^2$ and $w = |\nabla u|^2$ it follows that

$$\limsup_{j\to\infty} \|\nabla v_j\|^2_{\mathrm{L}^2(\Omega)} \leq \|\nabla v\|^2_{\mathrm{L}^2(\Omega)}.$$

Hence, using the weak lower semi-continuity of the L^2-norm, we have

$$\|\nabla v\|^2_{\mathrm{L}^2(\Omega)} \leq \liminf_{j\to\infty} \|\nabla v_j\|^2_{\mathrm{L}^2(\Omega)} \leq \limsup_{j\to\infty} \|\nabla v_j\|^2_{\mathrm{L}^2(\Omega)} \leq \|\nabla v\|^2_{\mathrm{L}^2(\Omega)},$$

which implies that $||\nabla v_j||_{\mathrm{L}^2(\Omega)} \to \|\nabla v\|_{\mathrm{L}^2(\Omega)}$ as $j \to \infty$. This result together with the weak convergence of $(\nabla v_j)_{j=1}^\infty$ to ∇v in $(\mathrm{L}^2(\Omega))^N$ implies the strong convergence of $(\nabla v_j)_{j=1}^\infty$ to ∇v in $(\mathrm{L}^2(\Omega))^N$, as $j \to \infty$. Thus, $(v_j)_{j=1}^\infty$ converges strongly to v in $\mathrm{H}^1(\Omega)$ as $j \to \infty$.

Step 2. $\partial_v J(u; v, v - \psi) \leq 0$ for all $\psi \in \mathrm{K}$:
Let $\psi \in \mathrm{K}$; then

$$\begin{aligned} &\partial_v J(v; u, v - \psi) \\ &= \int_\Omega \Big[F'(v_j)(v_j - \psi)\, A\nabla u_j : \nabla u_j + \varepsilon^{-1} G'(v_j)(v_j - \psi) + 2\varepsilon \nabla v_j \cdot \nabla(v_j - \psi)\Big]\, \mathrm{d}x \\ &\quad + \int_\Omega [F'(v)(v - \psi)\, A\nabla u : \nabla u - F'(v_j)(v_j - \psi)\, A\nabla u_j : \nabla u_j]\, \mathrm{d}x \\ &\quad + \varepsilon^{-1} \int_\Omega [G'(v)(v - \psi) - G'(v_j)(v_j - \psi)]\, \mathrm{d}x \\ &\quad + 2\varepsilon \int_\Omega [\nabla v \cdot \nabla(v - \psi) - \nabla v_j \cdot \nabla(v_j - \psi)]\, \mathrm{d}x \\ &=: Q_j + R_j + S_j + T_j, \end{aligned} \tag{4.25}$$

by labelling each of the integrals in turn. We now show that $\limsup_{j\to\infty} Q_j \leq 0$ and $\lim_{j\to\infty} R_j,\, S_j,\, T_j = 0$.

Using (4.24), we have

$$Q_j \leq \nu_j(\|\psi\|_{\mathrm{H}^1(\Omega)} + 1) \to 0 \quad \text{as } j \to \infty.$$

We bound R_j by

$$\begin{aligned}
|R_j| &\leq \int_\Omega |F'(v) - F'(v_j)|\,|v-\psi|\,|A\nabla u : \nabla u|\,\mathrm{d}x + \int_\Omega |F'(v_j)(v-v_j)|\,|A\nabla u : \nabla u|\,\mathrm{d}x \\
&\quad + \int_\Omega |F'(v_j)(v_j-\psi)|\,|A\nabla u : \nabla u - A\nabla u_j : \nabla u_j|\,\mathrm{d}x \\
&\leq \|v-\psi\|_{\mathrm{L}^\infty(\Omega)} \int_\Omega |F'(v) - F'(v_j)||A\nabla u : \nabla u|\,\mathrm{d}x \\
&\quad + \|F'(v_j)\|_{\mathrm{L}^\infty(\Omega)} \int_\Omega |v-v_j|\,|A\nabla u : \nabla u|\,\mathrm{d}x \\
&\quad + C_B\|F'(v_j)\|_{\mathrm{L}^\infty(\Omega)}\|v_j-\psi\|_{\mathrm{L}^\infty(\Omega)}\|\nabla u - \nabla u_j\|_{\mathrm{L}^2(\Omega)}\|\nabla u + \nabla u_j\|_{\mathrm{L}^2(\Omega)}.
\end{aligned}$$

Since v, ψ, $(F'(v_j))_{j=1}^\infty$ and $(v_j)_{j=1}^\infty$ are bounded in $\mathrm{L}^\infty(\Omega)$, it therefore follows from Lemma 4.2 and the strong convergence $\nabla u_j \to \nabla u$ in $(\mathrm{L}^2(\Omega))^{m\times N}$ that $R_j \to 0$ as $j \to \infty$.

Next, let us consider S_j,

$$\begin{aligned}
|S_j| &\leq \varepsilon^{-1} \int_\Omega |G'(v) - G'(v_j)|\,|v-\psi|\,\mathrm{d}x + \varepsilon^{-1}\int_\Omega |G'(v_j)|\,|v-v_j|\,\mathrm{d}x \\
&\leq \varepsilon^{-1} \sup_{0\leq z\leq 1} |G''(z)|\|v-v_j\|_{\mathrm{L}^2(\Omega)}\|v-\psi\|_{\mathrm{L}^2(\Omega)} + \varepsilon^{-1}\|G'(v_j)\|_{\mathrm{L}^2(\Omega)}\,\|v-v_j\|_{\mathrm{L}^2(\Omega)}.
\end{aligned}$$

Since $v_j \to v$ in $(\mathrm{L}^2(\Omega))^N$, it follows that $S_j \to 0$ as $j \to \infty$.

Finally, the strong convergence $\nabla v_j \to \nabla v$ in $(\mathrm{L}^2(\Omega))^N$ implies that $T_j \to 0$ as $j \to \infty$. □

Theorem 4.1. *Let $((u_n, v_n))_{n=1}^\infty \subset \mathrm{H}^1_g(\Omega) \times \mathrm{K}$ be the sequence generated by the Adaptive Iteration under Assumption (B).*

Then, there exists a subsequence $((u_{n_j}, v_{n_j}))_{j=1}^\infty$ of $((u_n, v_n))_{n=1}^\infty$ and $(u, v) \in \mathrm{H}^1_g(\Omega)\times\mathrm{K}$, such that $u_{n_j} \to u$ strongly in $(\mathrm{H}^1(\Omega))^m$ and $v_{n_j} \to v$ strongly in $\mathrm{H}^1(\Omega)$ as $j \to \infty$. In addition, u and v satisfy

$$\partial_u J(v; u, \varphi) = 0 \qquad \forall \varphi \in \mathrm{H}^1_D(\Omega), \tag{4.26}$$

$$\partial_v J(u; v, v-\psi) \leq 0 \qquad \forall \psi \in \mathrm{K}, \tag{4.27}$$

that is, (u, v) is a critical point of J in $\mathrm{H}^1_g(\Omega) \times \mathrm{K}$.

Proof.

Step 1. Existence of convergent subsequences of $((u_n, v_n))_{n=1}^\infty$:
It follows from Lemma 4.1 that the sequence $((u_n, v_n))_{n=1}^\infty$ is bounded in $(\mathrm{H}^1(\Omega))^m \times$

$\mathrm{H}^1(\Omega)$. Since $\mathrm{H}^1(\Omega)$ is a Hilbert space, there exists a subsequence $((u_{n_j}, v_{n_j}))_{j=1}^{\infty}$ such that

$$(u_{n_j}, v_{n_j}) \rightharpoonup (u, v) \qquad \text{in } (\mathrm{H}^1(\Omega))^m \times \mathrm{H}^1(\Omega) \text{ as } j \to \infty,$$

for some $(u, v) \in (\mathrm{H}^1(\Omega))^m \times \mathrm{H}^1(\Omega)$. Since $\mathrm{H}^1_g(\Omega)$ and K are convex closed subsets of $\mathrm{H}^1(\Omega)$ they are both weakly closed [5, Proposition 2.5]. Hence, $(u, v) \in \mathrm{H}^1_g(\Omega) \times \mathrm{K}$.

Upon extracting further subsequences we may assume, without loss of generality, that $u_{n_j-1} \rightharpoonup u'$ and $v_{n_j-1} \rightharpoonup v'$ weakly in $\mathrm{H}^1(\Omega)$ for some $u' \in \mathrm{H}^1_g(\Omega)$ and $v' \in \mathrm{K}$.

Step 2. $\nabla u_{n_j-1} \to \nabla u'$ strongly in $(\mathrm{L}^2(\Omega))^{m\times N}$:
Note that

$$\partial_u J(v_{n_j-1}; u_{n_j-1}, \varphi) \le \mu_{n_j-1} \|\nabla\varphi\|_{\mathrm{L}^2(\Omega)} \quad \forall \varphi \in \mathrm{H}^1_D(\Omega),$$

with $\mu_{n_j-1} \to 0$ as $j \to \infty$. Note also that $(u_{n_j-1}, v_{n_j-1}) \rightharpoonup (u', v')$ in $\mathrm{H}^1(\Omega) \times \mathrm{H}^1(\Omega)$. Therefore, it follows from Lemma 4.3 that $\nabla u_{n_j-1} \to \nabla u'$ in $(\mathrm{L}^2(\Omega))^{m\times N}$ as $j \to \infty$.

Step 3. $\partial_v J(u'; v, v - \psi) \le 0$ for all $\psi \in \mathrm{K}$ and $\nabla v_{n_j} \to \nabla v$ in $(\mathrm{L}^2(\Omega))^N$:
Since

$$\partial_v J(u_{n_j-1}; v_{n_j}, v_{n_j} - \psi) \le \nu_{n_j}(\|\psi\|_{\mathrm{H}^1(\Omega)} + 1),$$

with $\nu_{n_j} \to 0$ as $j \to \infty$ and $\nabla u_{n_j-1} \to \nabla u'$ in $\mathrm{L}^2(\Omega)$, it follows from Lemma 4.4 that

$$\partial_v J(u'; v, v - \psi) \le 0 \quad \forall \psi \in \mathrm{K},$$

and $\nabla v_{n_j} \to \nabla v$ in $(\mathrm{L}^2(\Omega))^N$ as $j \to \infty$.

Step 4. $\partial_u J(v; u, \varphi) = 0$ for all $\varphi \in \mathrm{H}^1_D(\Omega)$ and $\nabla u_{n_j} \to \nabla u$ in $(\mathrm{L}^2(\Omega))^{N\times N}$:
Noting that

$$\partial_u J(v_{n_j}; u_{n_j}, \varphi) \le \mu_{n_j} \|\nabla\varphi\|_{\mathrm{L}^2(\Omega)} \quad \forall \varphi \in \mathrm{H}^1_D(\Omega),$$

with $\mu_{n_j} \to 0$ as $j \to \infty$, it follows from Lemma 4.3 that

$$\partial_u J(v; u, \varphi) = 0 \quad \forall \varphi \in \mathrm{H}^1_D(\Omega),$$

and $\nabla u_{n_j} \to \nabla u$ in $(\mathrm{L}^2(\Omega))^{N\times N}$ as $j \to \infty$.

Step 5. $u' = u$:
Noting that $(J(u_n, v_n))_{n=1}^{\infty}$ is a nonincreasing sequence, we have

$$J(u', v) = \lim_{j\to\infty} J(u_{n_j-1}, v_{n_j}) \le \lim_{j\to\infty} J(u_{n_{j-1}}, v_{n_{j-1}}) = J(u, v).$$

Since u is a critical point of the strictly convex map $\tilde{u} \mapsto J(\tilde{u}, v)$ it is its unique minimizer. Therefore, $J(u', v) = J(u, v)$ and $u' = u$; hence, (u, v) is a critical point of J. □

5. Computational Examples

The computational examples presented in this section aim to address two questions. Firstly, what is the effect of using a monotonicity constraint on the phase-field variable to impose irreversibility of the crack? Secondly, how does the choice of the functions F and G in the generalized Ambrosio–Tortorelli functional affect the evolution of the crack and the profile of the associated minimizers? In order to focus on these two issues we restrict, for simplicity, the computations to the anti-plane setting taking $N = 2$, $m = 1$ and $A\nabla u : \nabla u = |\nabla u|^2$. We state from the outset that while our numerical experiments demonstrate the potential of the approach to irreversibility and the choices of phase field models that we advocate, they also show certain practical difficulties that still need to be overcome.

5.1. *Alternative functionals and cross-sectional profiles*

We shall compute the brittle fracture evolution using four different generalized Ambrosio–Tortorelli functionals. Let J_{ij}, $i, j = 1, 2$, be the functional J with $F(v) = F_i(v)$, $i = 1, 2$ and $G(v) = G_j(v)$, $j = 1, 2$, where

$$F_1(v) = v, \quad F_2(v) = v^2, \quad G_1(v) = \frac{9}{64}(1 - v) \quad \text{and} \quad G_2(v) = \frac{1}{4}(1 - v)^2.$$

The coefficients $\frac{9}{64}$ and $\frac{1}{4}$ in $G_1(v)$ and $G_2(v)$ ensure that the constant C_S, which is the scaling of the surface energy E_S defined in (1.6), is equal to one.

To motivate this choice of functions for F and G we present the results of a simple one-dimensional example, which show the profiles of the displacement and phase-field variables across a crack. We consider the domain $\Omega = (-1, 1)$ with a mesh refined towards the origin. The fixed displacements $u(-1) = -1$ and $u(1) = 1$ are imposed at the two ends of the domain. We only consider the minimization of J_{ij}, $i, j = 1, 2$, at one time and a crack is 'created' at $x = 0$ by starting the minimization algorithm with an initial input close to a local minimizer corresponding to a cracked state. We use the following values for the phase field parameters: $\varepsilon = 10^{-1}$ and $\eta = 10^{-4}$.

Figure 1 shows the profiles of the phase-field and displacement variables across the crack. We first discuss some of the properties exhibited by G. Taking $G = G_1$ results in the constraint $v \leq 1$ being enforced away from the crack, that is, $v = 1$ is an active constraint; hence the transition and cracked regions for v are compactly supported and there is a clear distinction between the 'uncracked' part of the domain and the transition region. Note that this is not true for $G = G_2$ since $v < 1$ throughout the domain. We therefore hypothesize that, in general, a propagating crack will be less affected by the boundary of the domain (or other cracks) with $G = G_1$ than with $G = G_2$. We also note that taking $G = G_1$ produces a transition region for v that is a quadratic function (compared to an exponential function for $G = G_2$); hence, in theory, the phase-field variable can be resolved with fewer elements.

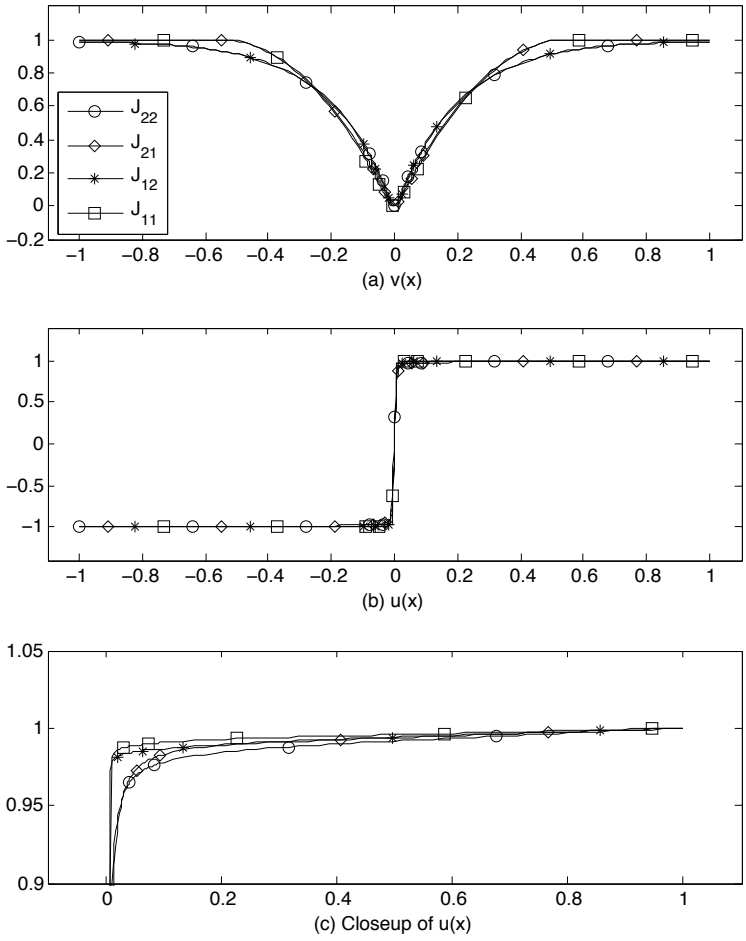


Fig. 1. A comparison of the phase-field and displacement profiles across a one-dimensional crack.

We now discuss some properties exhibited by the function F. Our main observation is that choosing $F = F_1$ ensures more rapid decay of u' towards the constant strain $u' = 0$. Analogous conclusions as for the phase field variable can be drawn from this.

5.2. *Irreversible quasi-static evolutions*

Next, we briefly discuss the implementation of the irreversibility condition in a quasi-static evolution. Given a time-dependent load $g(t)$ we choose a time step $\Delta t = T/\Lambda$ and an initial crack field v_0, and solve, for $k = 1, \dots, \Lambda$,

$$(u_k, v_k) \in \arg\min \big\{ J(u, v) : u \in H^1_{g(k\Delta t)}, v \in K_k \big\}, \tag{5.1}$$

where K_k is the admissible set for the crack field variable:

- *Reversible case:* if we do not implement the irreversibility condition, then we set $K_k = \{v \in H^1 : 0 \leq v \leq 1\}$.
- *Irreversible case:* If we do implement the irreversibility condition, then we set $K_k = \{v \in H^1 : 0 \leq v \leq v_{k-1}\}$.

The minimisation problem (5.1) is solved using the Adaptive Algorithm proposed in Section 4.3, with varying refinement parameters and functionals J_{ij} as discussed in Section 5.1.

The Adaptive Algorithm requires us to find a local minimizer of the generalized Ambrosio–Tortorelli functional with respect to each variable separately. While it is straightforward to minimize J with respect to u (since J is quadratic in u) the minimization with respect to v is more involved due to the bound constraint $v \in K_k$. For general functions F and G satisfying the conditions set out in Section 1.3 it is possible to use a gradient projection method [29, Section 5.2] to solve the v-minimization subproblem. In the following numerical experiments, however, we will restrict our attention to generalized functionals for which F and G are either linear or quadratic. Consequently, the resulting Hessian matrix (for J with respect to v) is strictly positive definite and a projected Newton method may be used. We use the algorithm presented by Kelley [29, Section 5.5.2] but replace the specified line search (Step 1(e)) with the Cauchy point computation given by Nocedal and Wright [33, Section 16.6].

5.3. *Example 1: curved crack*

Our first computational example is chosen to showcase some of the strengths of the modified functionals and adaptive algorithms that we propose. The computational domain, depicted in Figure 2, is a square with a pre-existing crack, from which a section of a circle is removed to break the symmetry of the problem. The applied load is defined by

$$g(x,t) = \begin{cases} t, & \text{for } x_1 > 1, \\ -t, & \text{for } x_1 < 1. \end{cases}$$

The time step is $\Delta t = 0.02$ and the final time is $T = 2$.

We compute the irreversible quasi-static evolution, using the four generalized Ambrosio–Tortorelli functionals J_{ij}, $i, j = 1, 2$, and phase field parameters $\varepsilon = k \times 10^{-2}$, $k = 1, 2, 3, 4$, and $\eta = \varepsilon^2$. The refinement indicator tolerances were chosen (through trial and error) so that the total number of elements would remain around $100,000$ for the case J_{22} and below $500,000$ for J_{12} and J_{11}. In the following table, we display these choices as well as the resulting numbers of elements after the final

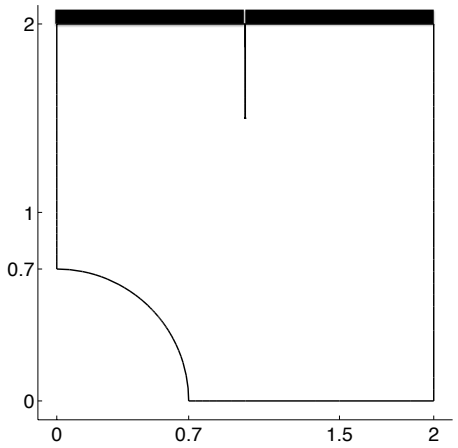


Fig. 2. Computational domain for Example 1, described in Section 5.3. The shaded area denotes the extension of the domain where the Dirichlet condition is applied.

time step (we show only the case $\varepsilon = 10^{-2}$):

	J_{22}	J_{21}	J_{12}	J_{11}
`REFTOL_U`	0.1	0.1	0.2	0.2
`REFTOL_V`	0.08	0.08	1.0	1.0
$\#\mathcal{T}^\Lambda$ for $\varepsilon = 10^{-2}$	101798	176505	529917	504734

The results are shown in Figure 3. We observe that the evolutions with the functionals J_{12} and J_{11} capture the crack path already for a much larger choice of ε, while the evolutions with J_{22} and J_{21} fail to resolve the crack path in that case. Unfortunately, this comes at the cost of a much finer finite element grid. We conjecture that this property of $F = F_1$ is due to the fact that the spurious stress field generated by the phase field variable, which "interacts" with the domain boundary, is much more localized than in the case of the functionals using $F = F_2$.

A second observation that can be drawn from Figure 3 is that the typically observed "widening" of the phase field at the crack tip (in part due to the irreversibility constraint) is less pronounced in the case of the functionals J_{21} and J_{11}, which employ $G = G_1$. In this case, we conjecture that this is due to the compact support of the phase field variable, which prevents it from "interacting" with domain boundaries or other crack fields.

5.4. *Example 2: Straight crack*

We now consider a more demanding test for the generalized Ambrosio–Tortorelli functionals. We consider an example with a straight crack (i.e., the crack path is known a priori) and directly compare the approximate evolutions to the exact Griffith solution. Let Ω be the two-dimensional rectangular domain $(-1, 1)\times(0, 2.2)$,

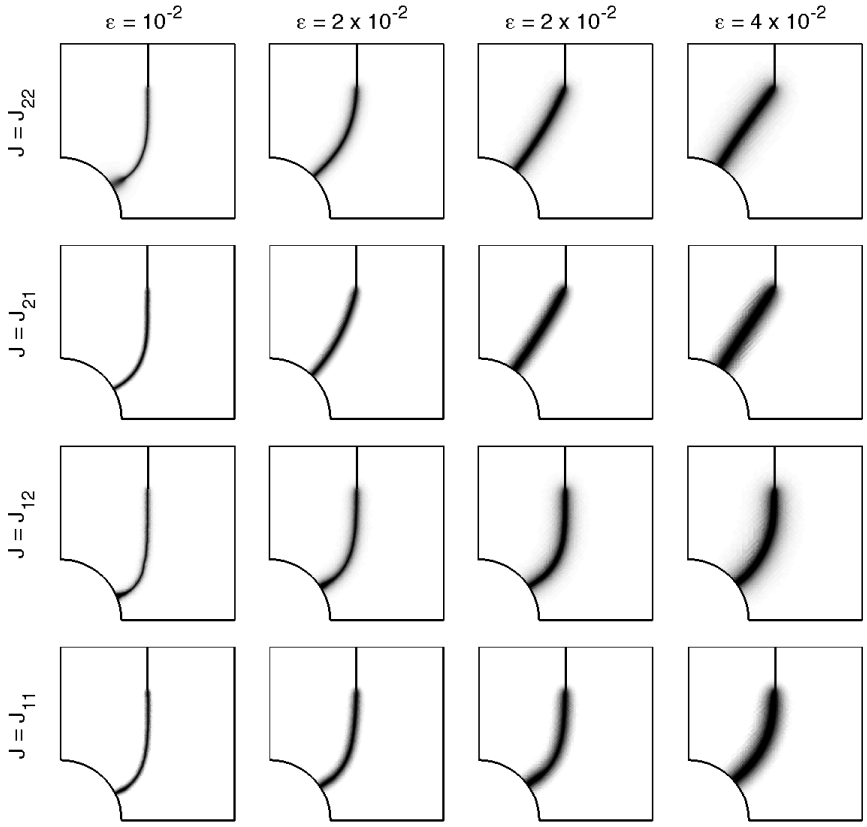


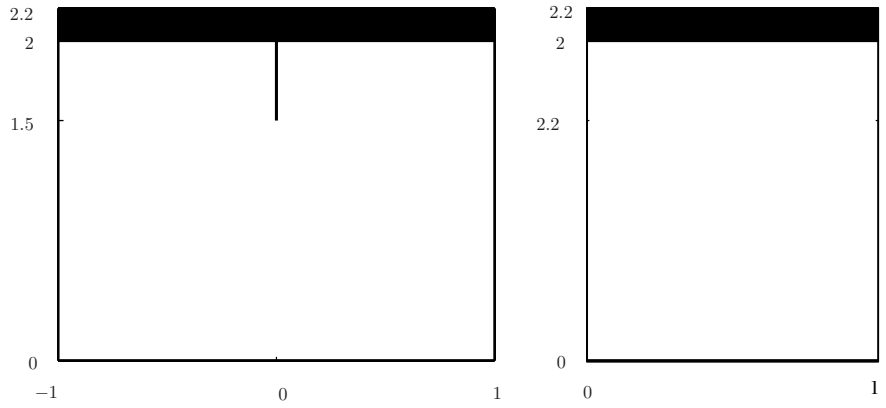
Fig. 3. Result of Example 1, described in Section 5.3. We observe that the functionals J_{12} and J_{11}, using $F = F_1$ are capable of capturing the qualitative behaviour of the crack path for much larger values of ε.

containing a slit along $\{0\}\times[1.5, 2.2]$. This is shown in Figure 4 (a) where the shaded part $\big((-1,0)\cup(0,1)\big)\times(2,2.2)$ is Ω_D. The applied anti-plane displacement $g(x,t)$ is given by

$$g(x,t) = \begin{cases} -t, & \text{on } (-1,0)\times(2,2.2), \\ t, & \text{on } (0,1)\times(2,2.2). \end{cases} \tag{5.2}$$

Rather than computing on the whole domain Ω we exploit the symmetry of the problem to compute on the half-domain $\tilde{\Omega} = (0,1)\times(0,2.2)$, shown in Figure 4 (b). We remark that this considerably simplifies the problem as it forces the crack field v to "move" along the exact crack path. This allows us to focus entirely on the accuracy of the surface energy.

Since we know, a priori, that the crack path lies along the line $x = 0$, Griffith's



(a) The domain Ω. (b) The computational domain $\tilde{\Omega}$.

Fig. 4. The domain used in Example 2, described in § 5.4.

criterion [28] can be used to compute the evolution of the crack together with the associated bulk and surface energies. This will be achieved using Algorithm 1 from [32, p. 1914]. In that algorithm the energy release rate is computed using the formula given on p. 1913 of [32], with the bulk energy (for each fixed crack length) computed using an adaptive finite element method. This method allows the energies to be computed to a high degree of accuracy; we will therefore label them as 'exact' and use them as a basis for comparison with our own computational results.

With this setup, we compute the time-discrete irreversible evolution using the generalized Ambrosio–Tortorelli functionals $J_{ij}, i, j = 1, 2$, as described in Section 5.2. We choose $\varepsilon = 2 \times 10^{-2}$ and $\eta = \varepsilon^2$. Again we had to adjust the refinement tolerance settings for the different functionals. The choices we made and the resulting mesh sizes are given in the following table:

	J_{22}	J_{21}	J_{12}	J_{11}
`REFTOL_U`	0.15	0.15	0.15	0.15
`REFTOL_V`	0.08	0.08	0.2	0.2
$\#\mathcal{T}^\Lambda$	170658	111731	417055	440285

In Figure 5 we show the results of the simulations. We observe that all functionals roughly capture the exact Griffith energy, but none of the functionals provides a quantitative approximation. The closeup around the point of crack initiation shows that using the J_{22} functional results in a smooth profile of the surface energy, which means that the point of crack initiation cannot be predicted. By contrast, the remaining functionals generate an approximate kink in the surface energy. However, we also observe that the crack initiation is delayed when using J_{12} or J_{11}. We conjecture that this is due to an inadequate choice of the refinement tolerance.

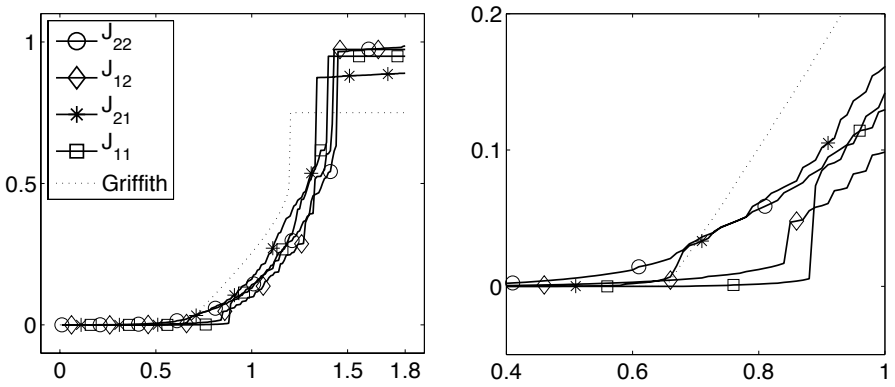


Fig. 5. Surface energies in the straight crack example described in § 5.4.

(This choice was required, however, to ensure that the number of elements remains below 500,000.)

We may deduce from this experiment that in terms of the accuracy of the surface energy, all four functionals are roughly comparable, however our main concern with the functionals J_{11} and J_{12} is that they require very fine meshes to satisfy the tolerance requirements. In order to test whether this is a genuine requirement, or simply due to gross overestimation of a certain component of the residual, we repeat the numerical experiment of this section without mesh adaptivity and without the irreversibility constraint. The mesh is refined a priori towards the crack path at $x_1 = 0$. The total number of finite elements in this simulation is 49345. The resulting surface energies are plotted in Figure 6. Our suspicions are confirmed in that we indeed observe a better accuracy for all four functionals, than we achieved with the adaptive computation, which also required far more elements. Of course such pre-adapted computational meshes can only be constructed in those rare instances when the crack path is known a priori.

6. Conclusion

We have presented an adaptive algorithm for numerically approximating local minimizers of the generalized Ambrosio–Tortorelli functional with a bound constraint on the phase-field variable. We have shown that the algorithm generates a sequence of numerical solutions that converge to a critical point of J as the termination tolerances are driven to zero.

We have tested the algorithm in two simple examples, demonstrating both the potential of our approach as well as certain shortcomings. We can deduce that the generalized Ambrosio–Tortorelli functionals J_{11}, J_{12}, J_{21} have desirable qualitative properties that set them apart from the standard Ambrosio–Tortorelli functional J_{22} (see § 5.1 for the definitions). Unfortunately our numerical experiments also

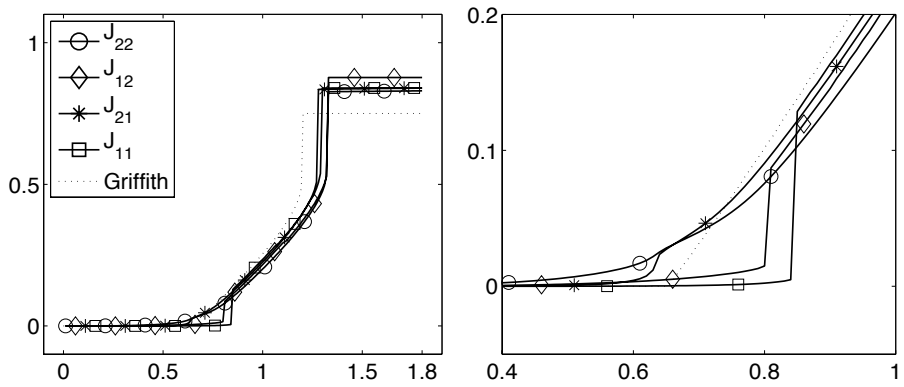


Fig. 6. Surface energies in the straight crack example described in § 5.4, without the irreversibility constraint and without mesh adaptivity.

indicate that our mesh refinement criterion is not efficient in practise. Our adaptive algorithm generates meshes that use far more elements than an a priori refined mesh, which appears to achieve higher accuracy (see § 5.4).

These observations open up a number of possible directions for further research, such as a study of further generalized Ambrosio–Tortorelli functionals, or an in-depth study of the effect of the monotonicity constraint (which we have largely ignored in our numerical experiments). The main challenge, from out perspective, is the derivation of more efficient refinement indicators for the functional J_{11} that would make this a practically viable alternative to the standard Ambrosio–Tortorelli functional.

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