On an Eigendeformation Approach to Brittle Fracture

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Keywords: Brittle Fracture, eigendeformation, variational element erosion.

SUMMARY. The paper presents a numerical implementation of a novel approximation scheme for Griffith's theory of brittle fracture recently proposed in [1]. The total potential energy of a brittle body (including bulk and surface terms) is variationally approximated by a family of functionals, depending on a small penalty parameter ε. The (two-field) approximating functionals have as arguments the displacement field u and an eigendeformation field γ. The latter describes the regions of the body under high strains, where fracture will occur. Γ-convergence of such a family of functionals to Griffith's energy has been proved in [1]. Here we investigate numerical examples for the quasi-static crack propagation in mixed modes I-II and I-III, through finite element approximation, illustrating the main computational features of the eigenfracture approach.

1 INTRODUCTION

Several free discontinuity models generalizing classical Giffith's theory of brittle fracture have appeared in the literature over the past few years (generalized Griffith's theories, see, e.g., [2, 3]).

The term free discontinuity problems was first introduced by De Giorgi and coworkers [4] to denote problems where the solution can have discontinuity points and, in addition, their jump sets are a priori unknown (see also [5]). As well as from fracture mechanics, examples are derived from image processing, shape optimization and liquid crystals. In fracture mechanics, free discontinuities describe the crack pattern of the body.

With reference to a d-dimensional body, generalized Griffith's models deal with minimization of energy functionals composed of bulk and surface terms, the latter being defined over a $(d-1)$-dimensional set. This jump set forms an argument for the functional to be minimized together with the displacement field of the body. Mathematical research in the field has found sufficient conditions in terms of functional setting (in spaces of special functions of bounded variation), topology of the crack front, shape and growth properties of bulk and surface energies, which ensure existence of solutions.

The original variational model by [2] considers a global minimization problem and only admits displacement-type loads (hard-device conditions). Inclusion of body forces and surface tractions has been carried out in [3] under special assumptions. Existence results for the time-continuous evolution have been obtained in linear and quasiconvex finite elasticity, for quasi-static crack propagation (cf. [3]). Research is ongoing in the direction of generalizing the original time-evolution law by

Francfort and Marigo, to account for local minimality, dynamics and plasticity, cohesive fracture, and damage-fracture transition (cf. e.g. [6, 7, 8, 9, 10, 11, 12]).

The present paper deals with a numerical study of a new weak approximation to generalized Griffith's models of variational fracture [1]. A two-field approach is proposed, with the singular part of the distributional derivative of the displacement field approximated through an eigendeformation field γ (eigenfracture approach) [13]. Such a quantity is defined on d-dimensional sets and localizes over $(d-1)$-dimensional sets as a penalty parameter ε approaches zero. A finite element approximation of the adopted model is given and numerical examples for mixed modes I-II and I-III are presented, illustrating the computational versatility of the eigenfracture approach.

2 THE EIGENFRACTURE MODEL

Let us consider bounded deformations (BD) of a Lipschitz domain $\Omega \subset \mathbb{R}^d$ representing the reference configuration of a d-dimensional elastic body ($d = 1, 2, 3$). We let u denote the displacement field of Ω and recall that $u \in L^1(\Omega, \mathbb{R}^d)$ is of *bounded deformation* if the symmetrized distributional derivative $Eu := \frac{1}{2}((Du)^T + Du)$ is a finite $\mathbb{R}^{d\times d}_{\rm sym}$-valued Radon measure. If the Cantor part of Eu [5] is zero, u is said to be in $SBD(\Omega)$ and Eu can be decomposed as

$$Eu = \mathcal{E}u\mathcal{L}^d + E^s u = \mathcal{E}u\mathcal{L}^d + (u^+ - u^-) \odot n_u \mathcal{H}^{d-1} \lfloor J_u,$$

Here $\mathcal{E}u$ is the absolutely continuous part of Eu with respect to the Lebesgue measure $\mathcal{L}^d$, $\mathcal{H}^{d-1}$ denotes the $(d-1)$-dimensional Hausdorff measure, J_u is an $\mathcal{H}^{d-1}$-rectifiable subset of Ω (the *jump part* of the distributional derivative Du of u), n_u is the normal to J_u, u^+, resp., u^-, are the one-sided limits of u at J_u, and $a \odot b := \frac{1}{2}(a \otimes b + b \otimes a)$. See [14, 5] for an exhaustive treatment of special functions of bounded variation. The function u is said to be an element of $SBD^p(\Omega)$ if in addition $\mathcal{E}u \in L^p$ and $\mathcal{H}^{d-1}(J_u) < \infty$.

Now suppose W is a positive definite quadratic form on $\mathbb{R}^{d\times d}_{\rm sym}$, defining the *strain energy density* of the body and let $\gamma : \Omega \to \mathbb{R}^{d\times d}_{\rm sym}$ be an approximation of the singular part $E^s u$ of Eu, where $\mathbb{R}^{d\times d}_{\rm sym}$ denotes the symmetric $d \times d$ matrices.

Given $u \in L^1(\Omega, \mathbb{R}^d)$ and $\gamma \in \mathcal{M}(\Omega, \mathbb{R}^{d\times d}_{\rm sym})$, we introduce the two-field energy functional

$$E_\varepsilon(u, \gamma) := \begin{cases} \int_\Omega W(\mathcal{E}u - \gamma) + \frac{G}{2\varepsilon}|\{\gamma \neq 0\}_\varepsilon|, & \text{if } u \in W^{1,1}, \|u\|_{L^\infty} \le K, \\ & \gamma \in L^1 \\ \infty, & \text{otherwise,} \end{cases} \tag{1}$$

where ε is a *penalty* parameter, G is the fracture toughness of the material and $\{\gamma \neq 0\}$ is the complement of the zero-set of (the precise representative of) γ. By $\{\gamma \neq 0\}_\varepsilon$ we have denoted the *ε-neighborhood* of $\{\gamma \neq 0\}$.

In [1] it has been proved that E_ε Γ-converges to the following limit functional $E : L^1(\Omega, \mathbb{R}^d) \times \mathcal{M}(\Omega, \mathbb{R}^{d\times d}_{\rm sym}) \to \mathbb{R} \cup \{\infty\}$,

$$E(u, \gamma) := \begin{cases} \int_{\Omega\setminus J_u} W(\mathcal{E}u) + G\mathcal{H}^2(J_u), & \text{if } u \in SBD^2, \|u\|_{L^\infty} \le K \\ & \gamma = E^s u \\ \infty, & \text{otherwise.} \end{cases} \tag{2}$$

as $\varepsilon \to 0$. Here $\mathcal{M}(\Omega, \mathbb{R}^n)$ denote the set of $\mathbb{R}^n$-valued Radon measures on Ω. One can in addition impose the constraint that $\gamma = a \odot n$ be the symmetrization of a rank one function $x \mapsto a(x) \otimes n(x)$, where $a \in L^1(\Omega, \mathbb{R}^d)$ and n is a unit vector field. Functional (2) coincides with the Griffith-type energy functional introduced in [2].

3 FINITE ELEMENT APPROXIMATION

Suppose $\mathcal{T}_h$ is a family of meshes, i.e., each $\mathcal{T}_h$ is a set of simplices with pairwise disjoint interior that cover all of $\mathbb{R}^d$. $\mathcal{T}_h$ could be a family of regular meshes obtained e.g. from a periodic grid in $\mathbb{R}^d$. We will, however, do not make any assumptions on the geometry of the cells, but only suppose that $\sup\{\operatorname{diam} T : T \in \mathcal{T}_h\} \to 0, \quad \text{as} \quad h \to 0$. We denote V_h and W_h the corresponding finite element spaces of piecewise affine functions (which are continuous accross element boundaries) and piecewise constant functions, respectively.

Given a set $A \subset \Omega$ we define the ε-neighborhood $A_{h,\varepsilon}$ with respect to the mesh $\mathcal{T}_h$ as the union of elements $T \in \mathcal{T}_h$ such that $\operatorname{dist}(T, A) := \inf\{|x - y| : x \in T, y \in A\} \leq \varepsilon$.

For $u \in L^1(\Omega, \mathbb{R}^d)$ and $\gamma \in \mathcal{M}(\Omega, \mathbb{R}^{d\times d}_{\mathrm{sym}})$, a finite element approximation of (1) is the following:

$$\tilde{E}_h(u,\gamma) := \begin{cases} \int_\Omega W(\mathcal{E}u - \gamma) + \frac{G}{2\varepsilon}|\{\gamma \neq 0\}_{h,\varepsilon(h)}|, & \text{if } u \in V_h, \|u\|_{L^\infty} \leq K, \\ & \gamma \in W_h, \\ \infty, & \text{otherwise.} \end{cases} \tag{3}$$

As a corollary to the Γ-convergence proof given in [1] , it is not difficult to show that (3) Γ-converges to (2) as $\varepsilon \to 0$.

Next we consider a quasi-static evolution problem governed by a displacement load history $u = \lambda(t)\bar{u}(x)$ on $\partial\Omega_D$, $\lambda(t)$ being a prescribed loading function, and $t \in [0, T]$. Let $0 < t_1 < .... < t_N = T$ be a time discretization of the problem and $V_h^{(j)}$ the finite element set of piecewise linear functions u such that $u = \lambda(t_j)\bar{u}(x)$ on $\partial\Omega_D$. Furthermore, let $\tilde{E}_h^{(j)}$ be the functional defined as $\tilde{E}_h$ in (3) under the replacement of V_h with $V_h^{(j)}$, and $K_h^{(j)}$ the set $\{\gamma_h^{(j)} \neq 0\}$. For the sake of notational simplicity, the superscript (j) is henceforth dropped.

The recovery sequences constructed in the Γ-convergence proof given in [1] satisfy $\gamma = a \odot n$ and $\gamma_h = a_h \odot n_h$, respectively, but nevertheless the above Theorems show that minimizing over arbitrary $\gamma \in \mathcal{M}(\Omega, \mathbb{R}^{d\times d}_{\mathrm{sym}})$ and $\gamma_h \in W_h$ eventually give the same results if h is small. We name *full rank* (FRM) the finite element model that lets γ_h be free in W_h, and *rank one* (ROM) the model instead assuming $\gamma_h = a_h \odot n_h$, for piecewise constant a_h, n_h ($|n_h| = 1$).

Looking at the structure of the above recovery sequences, we adopt a particular choice of γ_h, which proves to be helpful for the numerical implementation of the eigenfracture model, and accordingly reformulate the discrete problem. In detail, we assume $\gamma_h := (\nabla u_h n_h) \odot n_h$ on K_h and zero outside for the ROM, regarding u_h, n_h and K_h as the arguments of the discrete energy functional $\hat{E}_h(u_h, n_h, K_h) := \tilde{E}_h(u_h, \gamma_h(u_h, n_h, K_h))$. Similarly, we assume $\gamma_h := \nabla u_h$ on K_h and zero outside for the FRM, regarding u_h and K_h as the arguments of $\hat{E}_h(u_h, K_h) := \tilde{E}_h(u_h, \gamma_h(u_h, K_h))$. The above assumptions turn out to coincide for the recovery sequences u_h, γ_h constructed in [1] as $h \to 0$, when $\nabla u_h \approx a_h \otimes n_h$, and $(\nabla u_h)^T \nabla u_h \approx |a_h|^2 n_h \odot n_h$ on K_h, for some a_h, n_h. We shortly write $\gamma_h := \hat{\gamma}(u_h, n_h, K_h)$, and $E_h := \hat{E}_h(u_h, n_h, K_h)$, intending that n_h drops for the FRM.

Finite element solutions u_h, n_h, K_h of the discrete problem are determined through an iterative energy-descent procedure, which initially assumes that n_h and K_h remain unchanged with respect to the previous load step. Subsequently, the procedure predicts a number P of virtual extensions ΔK_p of K_h, determining the corresponding displacement fields u_p and and normals n_p through minimization of $\hat{E}_h(\cdot, \cdot, K_h \cup \Delta K_p)$. If the least of the predictor energies $\hat{E}_h(u_p, n_p, K_h \cup \Delta K_p)$ is lower than $\hat{E}_h(u_h, n_h, K_h)$, we assume the corresponding triplet $u_p, n_p, K_h \cup \Delta K_p$ as the new guess of the solution u_h, n_h, K_h for the current load step and re-iterate the virtual crack prediction.

The crack extensions are predicted using an affine d-chain K_h^* (d indicating the dimension of the problem under consideration), composed of S selected mesh elements $\{\Omega^{*1}, ..., \Omega^{*S}\}$ that we name *crack generators*. The predictors ΔK_p are let to coincide with affine d-chains composed of C mesh elements branching off from K_h^* according to a pre-definite pattern (say, e.g., forming a linear collection of mesh simplices). One can think of K_h and K_h^* as the current cracked region and crack front, respectively. However, to be more general, it is useful to distinguish the following two cases: $a)$ K_h is empty at time zero; $b)$ K_h collects a set of *pre-damaged* elements ($\gamma_h \neq 0$) at time zero, simulating a pre-crack in the body (in the first case, a pre-crack might be instead modeled as a portion of the boundary $\partial\Omega$). For the case of $a)$, we identify K_h^* at time zero with the set of the mesh simplices where the S^{th}-largest eigenvalues of $(\nabla u_h)^T \nabla u_h$ are attained. Furthermore, in the same case, we let ΔK_p be either a single simplex or a cluster of simplices belonging to the union of $K_h^* \setminus (K_h^* \cap K_h)$ and the star of ∂K_h^* (with respect to the mesh $\mathcal{T}_h$). For the case of $b)$ we instead identify K_h^* at time zero with the subset of K_h describing the crack front and let ΔK_p be either a single simplex or a cluster of simplices belonging to the star of ∂K_h^*. In each case, a generic virtual crack extension ΔK_p is generated from a simplex $\Omega^{*s} \in K_h^*$, being directly an element of such a set or a d-chain attached to an element of K_h^*. Once a ΔK_p is added to the current crack K_h, the corresponding Ω^{*s} in K_h^* is replaced with the leading element of ΔK_p.

It is worth noting that the proposed solution search strategy allows for modeling an arbitrary crack pattern in any dimension, including e.g. multiple branched cracks, under the condition that the size S of K_h^* is sufficiently large. Due to the recursive exploration of virtual crack extensions, K_h can be augmented with any number of mesh simplices during each time step. Nevertheless, the search of the current crack is obviously influenced by the particular choice made for S, P and C, and thus a convergence study on each of such parameters should be preliminarily performed, searching for sets of parameters that ensure stable predictions. One could assume $P = (d+1)S$, fitting S and C to the problem on hand through numerical experiments. We summarize the main steps of the solution strategy in the Algorithms 1, 2 that follow, observing that it can be read as an energy-descent element erosion technique. Indeed, due to the particular choice made for γ_h, the elements of K_h are either completely inert (FRM), or behave as partially reactive elastic elements, with zero stiffness in the direction of n_h (ROM). The proposed strategy differs from a classical element erosion-type method because it is based on an energy-descent criterion, while standard erosion methods adopt local stress-strain criteria. We enforced the constraint $\nabla u_h \; n_h \cdot n_h \geq 0$ on K_h through a penalty technique. The fracture term of the discrete functional $\hat{E}_h(u_h, n_h, K_h)$ depends on the measure of the ϵ-neighborhood $K_{h,\epsilon(h)}$ of K_h with respect to the mesh $\mathcal{T}_h$. This proves to be useful to avoid mesh anisotropy effects and over-estimation of fracture energy, which are common drawbacks of fixed grid approaches, as demonstrated by the Γ-convergence result of [1]. By way of example, consider a sequence K_h that *"zig-zag"* converges to the jump set J_u of a limit displacement field u, as $h \to 0$. The measure of the middle surface of K_h does not converge to $|J_u|$, while the quantity $\frac{1}{2\varepsilon}|K_{h,\varepsilon(h)}|$ does converge to $|J_u|$ (Fig. 1).

Algorithm 1

Initialize $K_h \leftarrow K_h^{(j-1)};\ n_h \leftarrow n_h^{(j-1)}$
$u_h \leftarrow \text{argmin}_u\ \hat{E}_h(u, n_h, K_h),\ \ \text{s.t. } \nabla u\ n_h \cdot n_h \geq 0 \text{ on } K_h$
propagate $\leftarrow$ true

while propagate **do**

$E_h \leftarrow \hat{E}_h(u_h, n_h, K_h)$
$p \leftarrow 0$

repeat

Predict an extension ΔK_p of K_h
Compute u_p, n_p via Algorithm 2
$E_p \leftarrow \hat{E}_h(u_p, n_p, K_h \cup \Delta K_p)$
$p \leftarrow p + 1$

until $p \leq P$

Let $m \in \{1, ..., P\}$ be such that $E_m = \min\{E_p\}_{p=1,...P}$

if $E_m < E_h$ **then**

Update $u_h \leftarrow u_m$; $n_h \leftarrow n_m$; $K_h \leftarrow K_h \cup \Delta K_m$

else
propagate $\leftarrow$ false

4 NUMERICAL RESULTS

Simulations of brittle crack propagation under combined I-II and I-III modes were conducted with reference to a prismatic plate with a through-the-thickness edge pre-crack. The plate is loaded by uniform distributions of displacements $\bar{u}_1, \bar{u}_2, \bar{u}_3$ on the top and bottom faces, opposite in sign with respect to each other. The examined problems refer to abstract units, assume unit dimensions $H_1 = H_2 = 1$ of the plate in the $x_1 - x_2$ plane, and consider the isotropic strain energy density $W(\mathcal{E}u) = \frac{\hat{\lambda}}{2}|tr(\mathcal{E}u)|^2 + \hat{\mu}|\mathcal{E}u|^2$, where $\hat{\lambda}$ and $\hat{\mu}$ are the Lamé coefficients, set equal to 0.8 and 0.4, respectively.

Crack propagation in brittle solids under mixed mode I-II loading has been investigated by a number of authors on the basis of different energetic and stress-based criteria of linear elasticity (refer e.g. to [15]). Here we apply the eigendeformation fracture model to the prediction of kinking and growth of an edge crack in the $x_1 - x_2$ plane, for $\bar{u}_3 = 0$, an initial crack length of $0.25H_1$, and different loading angles $\alpha = \arctan(\bar{u}_2/\bar{u}_1)$. 2D finite element simulations were conducted employing regular triangulations supported by uniform grids of nodes, for different mesh sizes h and penalty parameters ϵ, assuming either $h = \epsilon/2$ or $h = \epsilon/4$. The plate thickness was set equal to h.

The results corresponding to the rank one model are shown in Figs. 2 and 3, for a variety of loading angles, $G_c = 10^{-6}$, and $h = \epsilon/4 = 0.00625$ (25961 nodes and 51200 elements). Fig. 2 displays the deformed shapes of the cracked plates (displacement magnification factor = 3), while Fig. 3 shows the predicted crack paths in the reference configuration (in red/light) and their epsilon-

Algorithm 2

Initialize $u_p \leftarrow u_h;\ n_p \leftarrow n_h$

repeat

$u_{p'} \leftarrow \text{argmin}_u\ \hat{E}_h(u, n_p, K_h \cup \Delta K_p)$, s.t. $\nabla u\ n_p \cdot n_p \geq 0$ on $K_h \cup \Delta K_p$
Compute $n_{p'}$ on ΔK_p as the eigenvector associated with the largest positive eigenvalue of $(\nabla u_{p'})^T \nabla u_{p'}$
$n_{p'} \leftarrow n_h$ on K_h
$\Delta n \leftarrow \|n_{p'} - n_p\|_{L^\infty}$

until $\Delta n > TOL$

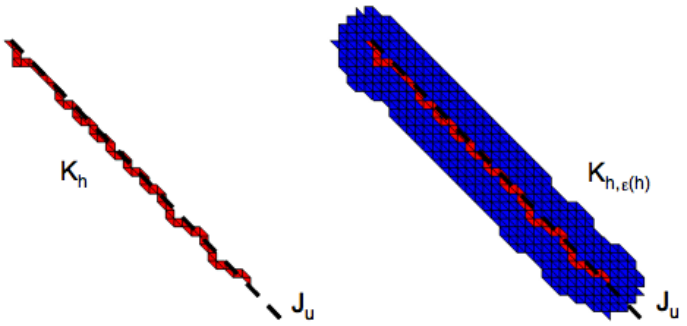


Figure 1: Transverse view of the ϵ-neighborhood $K_{h,\epsilon(h)}$ (right) of a discrete crack set K_h (left) that zig-zag converges to a planar crack surface.

neighborhoods (in blue/dark). A good agreement between the present results and those obtained by [16] through a different variational approach can be observed. For $\alpha = 0$ (mode II), we recorded initial sub-vertical crack kinking, followed by crack growth approximately at -45 deg (Fig. 3, $\alpha = 0$). This outcome is consistent with the predictions of the maximum hoop stress criterion (initial kinking angle $\theta = -70.6$ deg), the maximum energy release rate criterion ($\theta = -75.6$ deg), and the circumstance that in pure mode II the direction of maximum principal stress is 45 deg to the crack line [15]. The results in Fig. 3 show that the ϵ-neighborhood technique is able to correct mesh anisotropy, when 2ϵ is taken about one order greater of h. Oscillations of the crack path, visible in Fig. 3, are expected to smooth out in the limit $h \to 0$.

Crack propagation under in mixed mode I-III loading is a rather complex 3D problem that may exhibit singular features, such as wavy crack paths, riverbed patterns and chaotic surface roughness. In the case of a planar crack, several experimental and theoretical studies have shown that the crack deviates from its initial plane when the ratio between mode III and mode I stress intensity factors exceed a critical value, assuming a wavy profile with progressively increasing wavelength and amplitude [17]. We show hereafter the crack pattern obtained for a 3D plate with an edge pre-crack, for $\bar{u}_3 = 2.0 \times 10^{-4}$, $\bar{u}_1 = 1.0 \times 10^{-4}$, $\bar{u}_2 = 0$, $G_c = 0.025 \times 10^{-6}$, $H_3 = 1$, and pre-crack length equal to $0.15H_1$. A regular triangulation built on a $20 \times 20 \times 20$ uniform grid of nodes was

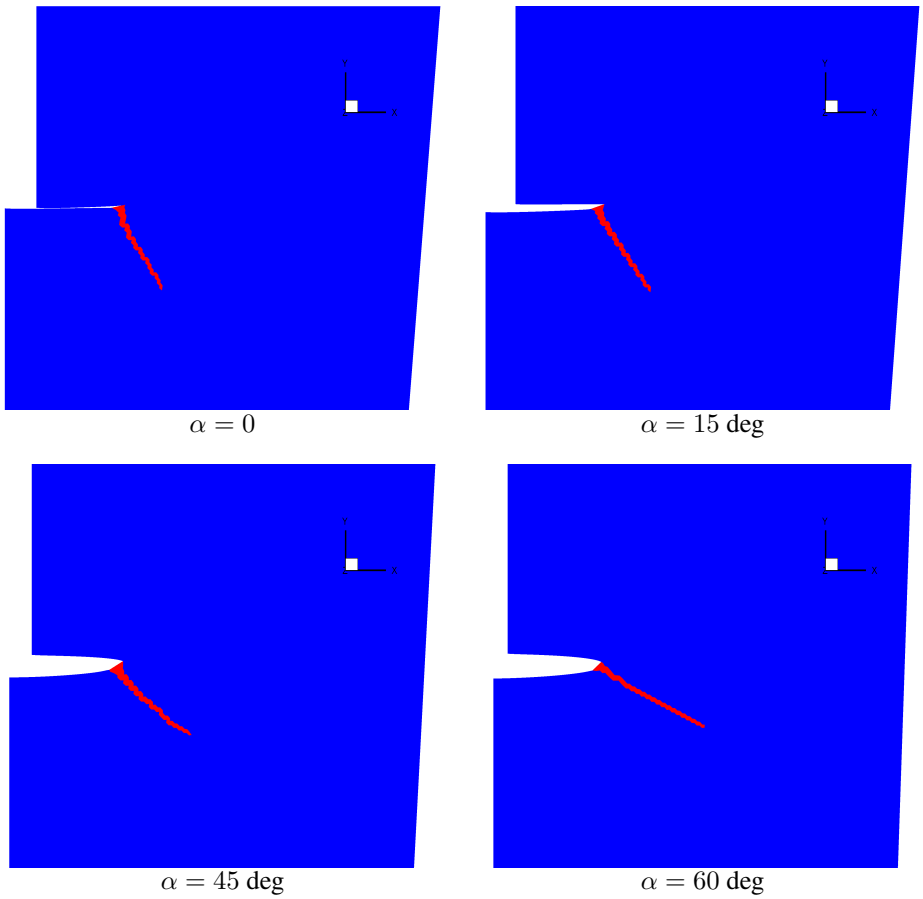
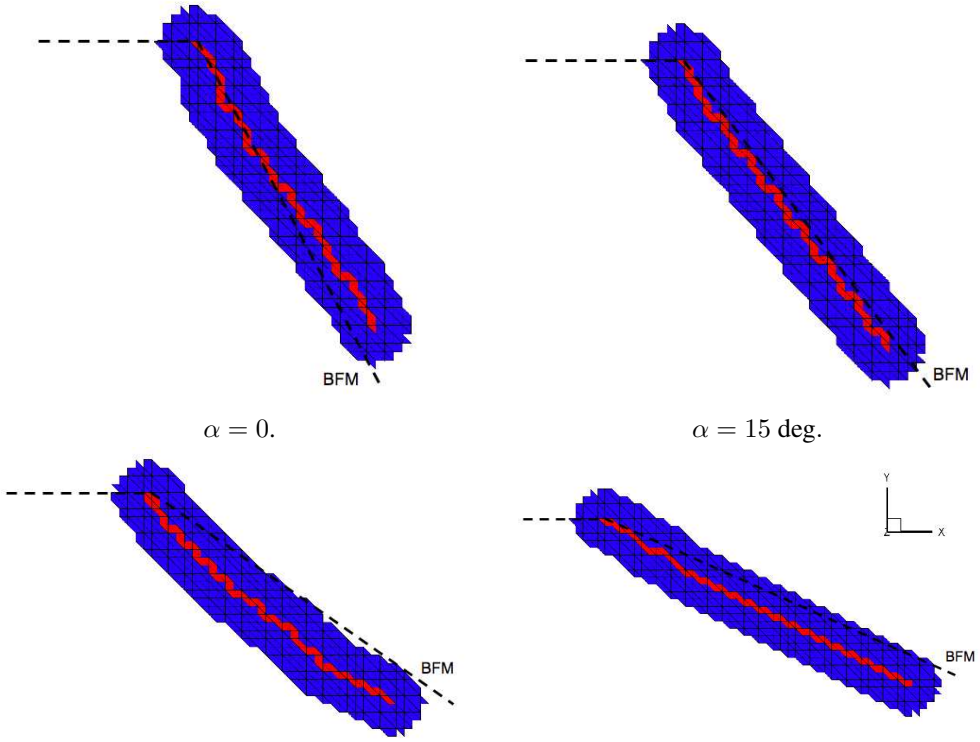


Figure 2: Deformed shapes for $h = \epsilon/4 = 0.00625$ and different loading angles.

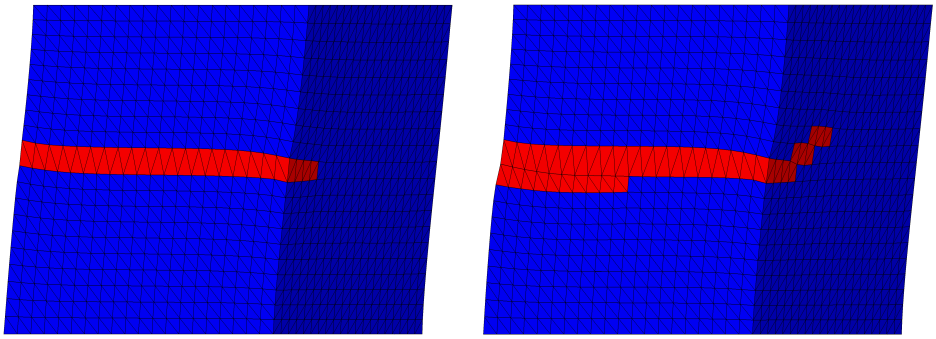


$\alpha = 0$. $\alpha = 15$ deg.

$\alpha = 45$ deg. $\alpha = 60$ deg.

Figure 3: Comparison between current crack path predictions for mixed I-II modes and results by [16] (BFM) for different loading angles.

employed (9282 nodes and 48000 elements). The pre-crack was modeled introducing pre-fractured elements with an S-shaped deviation from the (x_1, x_3) plane. Fig. 4 shows the progression of the crack growth for two different values of the displacement multiplier λ (displacement magnification factor = 25). One can notice that the adopted model is able to average the out-of-plane growth of the crack [17], with a relatively coarse mesh.



Step 1, $\lambda = 12.00$. Step 7, $\lambda = 12.6$.

Figure 4: Crack path and the deformed shape of a pre-cracked plate loaded by combined mode I and mode III loading.

5 CONCLUDING REMARKS

We have presented a new approximation scheme for Griffith's energy functional of brittle fracture by introducing a two-field functional $(u, \gamma) \mapsto E_\varepsilon(u, \gamma)$, thus augmenting the displacement variable u with an *eigendeformation field* γ. The key observation was that by introducing ε-neighborhoods for the damaged region $\{\gamma \neq 0\}$ we obtain an analytically convergent scheme which at the same time is efficient numerically. A numerical implementation based on a direct search method and a graduated-non-convexity strategy has been formulated. It leads to local minima of the discretized two-field functional, through recursive solution of elastic problems with eigenstrains, and can be thought of as a variationally informed element erosion technique. Finite element simulations of crack growth under combined I-II and I-III modes have shown the main computational features of the eigendeformation approach and its capability in technical applications.

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