Energy release rate approximation for small surface-breaking cracks using the topological derivative

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ABSTRACT

The topological derivative provides the variation of a response functional when an infinitesimal hole of a particular shape is introduced at a point of the domain. In this fracture mechanics work we use the topological derivative to approximate the energy release rate field associated with a small crack at any boundary location and at any orientation. Our proposed method offers significant computational advantages over current finite element based methods since it requires a single analysis, whereas the others require a distinct analysis for each crack location–orientation combination. Moreover, the proposed method evaluates the topological derivative in the non-cracked domain which eliminates the need for tailored meshes in the crack region.

1. Introduction

The need to evaluate the high stress and strain gradients present in the vicinity of a crack front and the continuously evolving crack geometry make crack initiation and propagation simulations a major challenge in computational mechanics. And since failure prediction is a vital role in component design, computational fracture mechanics has been and continues to be an active field of research.

Among the key quantities used to predict crack growth is the energy release rate $G$. Defined as the change of potential energy associated with an infinitesimal change of the crack area, $G$ denotes the amount of energy that is available for crack extension (Griffith, 1920). The energy release rate evaluation requires the computation of stress and strain fields in the vicinity of the crack, and hence many energy release computations utilize the finite element method (FEM). For the linear elastic case, this $G$ evaluation is sometimes accomplished via stress intensity factors, scalar quantities that characterize the stress and displacement fields in the crack tip region (Williams, 1957). The energy release rate may also be computed via an energy-based approach based on Rice's $J$-integral (Rice, 1980), which relates far-field loading conditions to the energy flux flowing into the crack tip region.

We propose an accurate and efficient scheme, based on the topological derivative, to compute the energy release rate $G$ associated with a small crack at any boundary location and at any orientation in a linear elastic isotropic two-dimensional (2-D) domain. The topological derivative field indicates the variation of a response functional when an infinitesimal hole is introduced in the body (Sokołowski and Zochowski, 1999). Originally it found applications in the structural optimization community in the so-called bubble method (Eschenauer et al., 1994). In this method, holes are systematically nucleated in strategic locations to both lighten the structure and maintain load integrity. Once the holes are nucleated, traditional
shape optimization methods enlarge and reconfigure them. This concept has more recently been combined with the fictitious domain finite element method to alleviate remeshing tasks that plague traditional shape optimization (Céa et al., 2000; Allaire et al., 2004; Mei and Wang, 2004; Norato et al., 2007).

More recently the topological derivative has been applied to inverse scattering problems. For example, in Feijoo (2004) it is used to locate the boundaries of impenetrable scatters immersed in an otherwise homogeneous medium. Guzina and Bonnet (2004) similarly solve an inverse problem using the topological derivative to identify the locations of cavities embedded in an elastic solid. Likewise, the topological derivative is applied to detect and locate cracks in an inverse heat conduction problem (Amstutz et al., 2005). The topological derivative is also used to resolve inpainting problems, i.e., to identify the edges of a partially hidden image (Auroux and Masmoudi, 2006).

As demonstrated in Garreau et al. (2001), the topological derivative field for a given response function can be efficiently evaluated via the adjoint sensitivity analysis method. Indeed, as with the usual adjoint sensitivity technique (Haug et al., 1986), only the primal analysis and one adjoint analysis are required to evaluate the response variation for any shape, material and/or load variation.

In this 2-D linear elastic fracture mechanics study, we utilize the topological derivative to approximate the energy release rate \( G \) for any small crack located at any boundary location and any orientation. This contrasts current methods which require a distinct finite element analysis to evaluate \( G \) for each crack size–location–direction combination. Moreover, our energy release rate computation uses the stress field of the non-cracked domain; and hence we eliminate the need for refined meshes in the crack regions.

This paper is organized as follows. In Section 2, we summarize the topological derivative and its application for fracture mechanics. In Section 3, we describe our asymptotic analysis to approximate the energy release rate. Section 4 presents examples to verify the method. Conclusions are drawn in Section 5.

2. Topological derivative for cracked bodies

It is known that the shape sensitivity of the total potential energy \( \psi \) with respect to crack length \( \varepsilon \) is given by the energy release rate \( G \) (Feijoo et al., 2000; Taroco, 2000; Griffith, 1920), i.e.,

\[
G(\Omega, \varepsilon) = -\frac{d}{d\varepsilon} \psi(\Omega, \varepsilon),
\]

where \( \frac{d}{d\varepsilon} \psi(\Omega, \varepsilon) \) is the shape derivative and \( \Omega, \varepsilon \) is the domain with a small crack which has the boundary \( \partial \Omega, \varepsilon = \partial \Omega \cup \gamma, \varepsilon \) with \( \gamma, \varepsilon \) being the crack boundary (Fig. 1) and the total potential energy is given by

\[
\psi(\Omega, \varepsilon) = \frac{1}{2} \int_{\Omega, \varepsilon} \nabla^s \mathbf{u}, \mathbf{v} \, dV - \int_{\gamma, \varepsilon} \mathbf{t}^p \cdot \mathbf{n} \, dS.
\]

In the above the sub-index \( s \) denotes the response quantities evaluated on the cracked domain \( \Omega, \varepsilon \); \( \mathbf{u} \) the displacement vector, \( \nabla^s \mathbf{u} = \mathbf{u}_u + \nabla \mathbf{u}^T \), \( \mathbf{T} = \mathbf{C} \nabla^s \mathbf{u} \) the symmetric Cauchy stress tensor, \( \mathbf{C} \) the elasticity tensor for a linear elastic isotropic material and \( \mathbf{t}^p \) the applied boundary traction on \( \partial \Omega \) satisfy the governing equations of linear elasticity on the domain \( \Omega, \varepsilon \), i.e.,

\[
\begin{align*}
\text{div} \mathbf{T} &= 0 \quad \text{in} \ \Omega, \varepsilon, \\
\mathbf{T}, \mathbf{m} &= 0 \quad \text{on} \ \gamma, \varepsilon, \\
\mathbf{T}, \mathbf{n} &= \mathbf{t}^p \quad \text{on} \ \partial \Omega,
\end{align*}
\]

where \( \mathbf{m} \) and \( \mathbf{n} \) are the outward unit normal vectors to \( \gamma, \varepsilon \) and \( \partial \Omega \) and without loss of generality, body forces are neglected and the crack faces are assumed to be traction free.

Fig. 1. Non-cracked domain \( \Omega \) and cracked domain \( \Omega, \varepsilon \).
Our goal is to evaluate efficiently $G$ of Eq. (1) and moreover to evaluate $G$ for any crack size $\varepsilon$, any orientation $\alpha$ and at any boundary location $\mathbf{x}$. To these ends we express the total potential energy by the following topological asymptotic expansion:

$$
\psi(\Omega) = \psi(\Omega) + \sum_{j=1}^{n} f_j(\varepsilon) D^j_T \psi(\mathbf{\hat{x}}, \mathbf{x}) + \mathcal{R}(f_n(\varepsilon)),
$$

(4)

where $D^j_T \psi$ is the $j$th order topological derivative of $\psi$ (Rocha de Faria, 2007). The gauge functions $f_j$ depend on the crack face boundary conditions; here we consider negative valued gauge functions that monotonically tend to zero as $\varepsilon$ tends to zero, cf. footnotes 1 and 2. These functions also satisfy

$$
\lim_{\varepsilon \to 0} \frac{f_j(\varepsilon)}{f_j(\varepsilon)} = 0, \quad k > j \quad \text{and} \quad \lim_{\varepsilon \to 0} \frac{\mathcal{R}(f_n(\varepsilon))}{f_n(\varepsilon)} = 0,
$$

(5)

where $\mathcal{R}$ is the remainder function.

Differentiating Eq. (4) gives the shape sensitivity of the total potential energy as a function of the topological derivatives, i.e.,

$$
\frac{d}{d\varepsilon} \psi(\Omega) = \sum_{j=1}^{n} f_j(\varepsilon) D^j_T \psi(\mathbf{\hat{x}}, \mathbf{x}) + \mathcal{R}(f_n(\varepsilon)) f'_n(\varepsilon),
$$

(6)

which upon combining with Eq. (1) gives our expression for the energy release rate

$$
G(\varepsilon, \mathbf{\hat{x}}, \mathbf{x}) = - \sum_{j=1}^{n} f_j(\varepsilon) D^j_T \psi(\mathbf{\hat{x}}, \mathbf{x}) + \mathcal{R}(f_n(\varepsilon)) f'_n(\varepsilon).
$$

(7)

Notable in the above expression is the fact that the energy release rate $G$ for a crack of length $\varepsilon$, location $\mathbf{\hat{x}}$ and orientation $\alpha$ is evaluated using the response on the uncracked domain $\Omega$.

One way to evaluate the topological derivatives is the so-called topological-shape sensitivity method (Novotny et al., 2003). In this approach, a crack of length $\varepsilon$ and orientation $\alpha$ is presumed to exist at the location $\mathbf{\hat{x}}$. A shape sensitivity analysis is then performed with respect to the crack length $\varepsilon$ and the limit is taken as $\varepsilon$ goes to zero, i.e.,

$$
D^j_T \psi(\mathbf{\hat{x}}, \mathbf{x}) = \lim_{\varepsilon \to 0} \left\{ \frac{1}{f_j(\varepsilon)} \left( \frac{d}{d\varepsilon} \psi(\Omega) - \sum_{i=1}^{j-1} f_i(\varepsilon) D^i_T \psi(\mathbf{\hat{x}}, \mathbf{x}) \right) \right\}.
$$

(8)

In this work, we limit ourselves to first-order analysis and define the $j=1$ approximations

$$
\psi^{1D}(\varepsilon, \mathbf{\hat{x}}, \mathbf{x}) = \psi(\Omega) + f_1(\varepsilon) D^1_T \psi(\mathbf{\hat{x}}, \mathbf{x}),
$$

$$
G^{1D}(\varepsilon, \mathbf{\hat{x}}, \mathbf{x}) = -f_1(\varepsilon) D^1_T \psi(\mathbf{\hat{x}}, \mathbf{x}),
$$

(9)

which follow from Eqs. (4) and (7). For this $j=1$ value we use the topological derivative equation of Novotny (2004), i.e.,

$$
D_T \psi(\mathbf{\hat{x}}, \mathbf{x}) = \lim_{\varepsilon \to 0} \left\{ \frac{1}{f_1(\varepsilon)} \frac{d}{d\varepsilon} \psi(\Omega) \right\},
$$

(10)

where here and henceforth we eliminate the $j=1$ indices for conciseness. Our challenge now is to evaluate the above expression in which

$$
\frac{d}{d\varepsilon} \psi(\Omega) = - \int_{\gamma} \Sigma_{c} \mathbf{n} \cdot \mathbf{e}, \ dS
$$

(11)

(Taroco, 2000), where $\gamma$ is the crack contour, $\mathbf{e}$, is a unit vector aligned with the crack and oriented in the crack growth direction (cf. Fig. 1) and $\Sigma$ is the energy momentum tensor

$$
\Sigma_{c} = \frac{1}{2} \nabla \mathbf{u}_{c} \cdot \mathbf{T} + \mathbf{T} \nabla \mathbf{u}_{c} - \nabla \mathbf{u}_{c} \mathbf{T}.
$$

(12)

Of course Eq. (11) defines the $J$-integral which is known to be path independent. So upon defining $\gamma$ as $B_r$, i.e., the boundary of a ball of radius $r$ centered at the crack tip, and taking the limit as $r$ tends to zero we obtain

$$
J(\Sigma_{c}) = - \frac{d}{d\varepsilon} \psi(\Omega) = \lim_{r \to 0 / B_{r}} \int_{\gamma} \Sigma_{c} \mathbf{n} \cdot \mathbf{e}, \ dS.
$$

(13)

And hence our challenge is to evaluate $\Sigma_{c}$ in the crack tip region $B_{r}$.

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1. If $f_j$ is a suitable function for Eq. (4), then $\beta f_j$ is also suitable for any scalar $\beta > 0$. Furthermore, from Eq. (8) we see that Eq. (4) is unaffected by the choice of $\beta$.

2. In Eq. (8) we further see that $f_j$ must be defined to make the limit evaluate to a non-zero finite number. As a matter of preference we also define a negative valued function $f_j$ so that the topological derivative of the total potential energy defined in Eq. (2) is positive.
3. Asymptotic analysis

To evaluate the energy momentum tensor $\Sigma_e$ of Eq. (12) we use the following stress composite expansion (Kozlov et al., 1999)

$$T_e(x) = T(x) + \bar{T}(y) + \bar{T}_e(x),$$  \hspace{1cm} (14)

where $T(x)$ is the outer stress, $\bar{T}(y)$ is the inner stress and $\bar{T}_e(x)$ is the remainder stress (Fig. 2). Note that the inner stress is evaluated at the scaled position vector $y = x/\varepsilon$.

The composite expansion of Eq. (14) satisfies the boundary conditions of Eq. (3), i.e.,

$$T_e n = T n + \bar{T}_e y = x \varepsilon n + \bar{T}_e n = t^0, \quad x \in \partial \Omega$$  \hspace{1cm} (15)

and

$$T_e e_\theta = T e_\theta + \bar{T}_e y = x \varepsilon e_\theta + \bar{T}_e e_\theta = 0, \quad x \in \gamma_e,$$  \hspace{1cm} (16)

where we use $m = e_\phi$.

The outer stress $T$ is defined on the domain without a crack, i.e., we find $T$ such that

$$\text{div}T = 0 \quad \text{in} \quad \Omega,$$

$$T n = t^0 \quad \text{on} \quad \partial \Omega.$$  \hspace{1cm} (17)

In general, the field $T$ does not satisfy the traction free boundary condition on the crack face $\gamma_e$, cf. Eq. (16). And since $\gamma_e$ is a small crack, we expand $T(x)$ about $\hat{x} \in \partial \Omega$, i.e., the crack initiation site and use $x - \hat{x} = \delta e_\theta$, to obtain

$$T(x) = T(\hat{x}) + \delta D T(\hat{x})|e_\theta| + \varepsilon^2 \frac{\delta^2}{2!} D^2 T(\hat{x})|e_\theta| e_\theta + \cdots, \quad x \in \gamma_e.$$  \hspace{1cm} (18)

Finally we express $\delta$ in terms of the scaled parameter $\xi = \delta/\varepsilon$, cf. Fig. 2, rendering

$$T(x) = T(\hat{x}) + \varepsilon^2 \frac{\delta^2}{2!} D^2 T(\hat{x})|e_\theta| + \cdots = T(\hat{x}) + O(\varepsilon), \quad x \in \gamma_e.$$  \hspace{1cm} (19)

We define the inner stress $\bar{T}$ to annihilate the leading order term of the traction $T e_\theta$ on the crack face, i.e., $T(\hat{x}) e_\theta$. And because the inner stress is expressed in terms of the stretched position vector $y$, points $y$ far away from the crack correspond to points $x$ only a small distance $O(\varepsilon)$ from $\hat{x}$. Hence the inner boundary value problem is that of a half-space $\mathcal{H}$ with a unit length edge crack (with surface $\gamma_1$) subject to a non-zero crack face traction and zero far-field traction, i.e.,

$$\text{div} \bar{T} = 0 \quad \text{in} \quad \mathcal{H},$$

$$\bar{T} e_\theta = \hat{t} \quad \text{on} \quad \gamma_1,$$

$$\bar{T} \rightarrow 0 \quad \text{at} \quad |y| \rightarrow \infty.$$  \hspace{1cm} (20)

where the boundary traction $\hat{t}$ in cylindrical coordinates is given by

$$\hat{t} = -T(\hat{x}) e_\theta = -(T_{ey}(\hat{x}) e_r + T_{r\theta}(\hat{x}) e_\theta).$$  \hspace{1cm} (21)

Note that using the scaled position vector $y$ the boundary value problem of Eq. (20) is independent of the crack size $\varepsilon$.

Using Muskhelishvili’s complex variable method (Muskheilishvili, 1953) and the distributed dislocation technique

![Fig. 2. Depiction of Eq. (14) shows responses on a domain without the crack, scaled half-space domain with a crack and cracked original domain subject to remainder tractions.](image-url)
(Hills et al., 1996; Rubinstein, 1986), the inner stress components \( \hat{T}_{ij} \) are given by

\[
\hat{T}_{ij}(y) = \int_0^1 \left( b_0(t)K_{ij}(x,y,t) + b_t(t)K_{ij}(x,y,t) \right) dt,
\]

where \( x \) is the crack orientation, cf. Fig. 2. \( K_{ij} \) are known kernels (Hills et al., 1996) and \( b_0 \) and \( b_t \) are the unknown dislocation densities that are obtained by solving the following system of integral equations:

\[
\begin{align*}
\int_0^1 \left( b_0(t)K_{i0}(x,y,t) + b_t(t)K_{i0}(x,y,t) \right) dt &= -T_{i0}(\hat{x}), \quad y \in \gamma_1, \\
\int_0^1 \left( b_0(t)K_{i0}(x,y,t) + b_t(t)K_{i0}(x,y,t) \right) dt &= -T_{i0}(\hat{x}), \quad y \in \gamma_1.
\end{align*}
\]

We emphasize that \( b_0 \) and \( b_t \) are independent of \( \varepsilon \). However, we note that for \( y = x/\varepsilon \) we have \( K_{ij}(x,x/\varepsilon, t) = O(\varepsilon) \) and \( K_{ij}(x,x/\varepsilon, t) = O(\varepsilon) \), cf. Hills et al. (1996). But in the vicinity of the crack where \( y = x/\varepsilon - (\delta/\varepsilon)e_2 = \xi e_2 \), these kernels are \( O(1) \). Hence \( \hat{T}(\xi e_2) = O(1) \) near the crack tip, whereas \( \hat{T}(x/\varepsilon) = O(\varepsilon) \) away from the crack tip, notably for \( x \in \partial \Omega \).

The remainder problem for \( \hat{T} \) is defined in the cracked domain and satisfies the following boundary value problem:

\[
\begin{align*}
\text{div} \hat{T} &= 0 \quad \text{in} \ \Omega_\varepsilon, \\
\hat{T} e_\theta &= t^R e_\theta \quad \text{on} \ \gamma_\varepsilon, \\
\hat{T} n &= t^R \quad \text{on} \ \partial \Omega,
\end{align*}
\]

where the boundary tractions \( t^R e_\theta \) and \( t^R \) are defined such that Eqs. (15) and (16) are satisfied, i.e.,

\[
\begin{align*}
t^R e_\theta(x) &= -(T(x) - T(\hat{x})) e_\theta, \quad x \in \gamma_\varepsilon, \\
t^R(x) &= -\hat{T}(x/\varepsilon) n, \quad x \in \partial \Omega.
\end{align*}
\]

We note that

\[
T(x) - T(\hat{x}) = \varepsilon \partial \eta \partial T(\hat{x})|e_2| + \cdots = O(\varepsilon),
\]

and as previously mentioned \( \hat{T}(x/\varepsilon) = O(\varepsilon) \) for \( x \in \partial \Omega \) which are distant from the crack tip. Therefore, \( \hat{T} = O(\varepsilon) \). Hence we rewrite Eq. (14) as

\[
T(x) = T(\hat{x}) + \hat{T}(y) + O(\varepsilon).
\]

Using the polar coordinate system \((\rho, \theta)\), cf. Fig. 2, and the change of variables \( \rho = r/\varepsilon \) we can also express the inner stress field near the crack tip in terms of an asymptotic series (Williams, 1957), i.e.,

\[
\hat{T}(r/\varepsilon, \theta) = \frac{\sqrt{E}}{\sqrt{r}} A_1 F_1(\theta) + A_2 F_2(\theta) + \frac{\sqrt{F}}{\sqrt{E}} A_3 F_3(\theta) + O(r),
\]

cf. Eq. (22). In this way, we can combine Eqs. (12), (27) and (28) to obtain the following expression for the energy momentum tensor

\[
\Sigma_e = -\frac{E}{r} A_1 F_1(\theta) + \frac{\sqrt{E}}{\sqrt{r}} A_2 F_2(\theta) + \frac{\sqrt{F}}{\sqrt{E}} A_3 F_3(\theta) + O(r).
\]

We emphasize that \( A_1 T_1 \) is only function of \( A_1 F_1 \) since \( T(\hat{x}) \) is uniform. As such, only the leading term of \( \Sigma_e \) contributes to Eq. (13) due to the limit, and we are left with

\[
J(\Sigma_e) = \lim_{r \to 0} \int_{-\pi}^{\pi} \Sigma_e n \cdot e_\theta r \, d\theta = \frac{K_I^2(\hat{x}, x)}{E} \varepsilon, \quad (30)
\]

where we again emphasize that the mode I and II stress intensity factors \( K_I \) and \( K_{II} \) are obtained from the leading term of \( \hat{T} \) in Eq. (28) and therefore they correspond to those associated with the inclined unit length edge crack problem in the half-space.

To compute \( K_I \) and \( K_{II} \) we solve the integral equations (23) and (24). Upon combining Gauss–Chebyshev quadrature for integration and superposition, the stress intensity factors are ultimately given by (see Silva Sohn, 2009 for details)

\[
\begin{pmatrix}
K_I(\hat{x}, x) \\
K_{II}(\hat{x}, x)
\end{pmatrix} = \sqrt{\varepsilon} \begin{pmatrix}
h_{11}(\hat{x}) & h_{12}(\hat{x}) \\
h_{21}(\hat{x}) & h_{22}(\hat{x})
\end{pmatrix} \begin{pmatrix}
T_{i0}(\hat{x}) \\
T_{i\theta}(\hat{x})
\end{pmatrix},
\]

where

\[
\begin{pmatrix}
h_{11}(\hat{x}) & h_{12}(\hat{x}) \\
h_{21}(\hat{x}) & h_{22}(\hat{x})
\end{pmatrix} = \begin{pmatrix}
\frac{1}{K_I(\hat{x}, x)} & \frac{h_{12}(\hat{x})}{K_I(\hat{x}, x)} \\
\frac{h_{21}(\hat{x})}{K_I(\hat{x}, x)} & \frac{1}{K_{II}(\hat{x}, x)}
\end{pmatrix},
\]

\[
\begin{pmatrix}
T_{i0}(\hat{x}) \\
T_{i\theta}(\hat{x})
\end{pmatrix} = \begin{pmatrix}
K_I(\hat{x}, x) \\
K_{II}(\hat{x}, x)
\end{pmatrix}.
\]

We define \( E = E/(1 - \nu^2) \) for plane strain and \( F = E \) for plane stress, in which \( E \) is the Young modulus and \( \nu \) is Poisson’s ratio.

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3 We define \( T = E/(1 - \nu^2) \) for plane strain and \( T = E \) for plane stress, in which \( E \) is the Young modulus and \( \nu \) is Poisson’s ratio.

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yield similar results. The analysis to evaluate their corresponding energy release rates compares them with values computed via finite element method by Beghini et al. (1999). Note that the two computations given parameter values, the total potential energy of the non-cracked domain is size is uniform we obtain a uniform topological derivative field (Eq. (32)). Fig. 4b shows the topological derivative value as a function of the crack orientation \(\alpha\). The parameter values for this analysis are tension (Fig. 4a). The parameter values for this analysis are

4. Examples

Presently we investigate several numerical examples in which we perform one finite element analysis on the non-cracked domain \(\Omega\) and use finite element analysis to evaluate their corresponding energy release rates \(G^{\text{FE}}\). We then show that the topological derivative values \(G^{\text{TD}}\) are in good agreement with the finite element values \(G^{\text{FE}}\). Further verification is performed on a crack emanating from a hole in an infinite space for which analytical analyses as opposed to finite element analyses are performed.

4.1. Plate loaded in uniaxial tension

In this example we study a small crack breaking on the left free edge of a square plate loaded in plane strain uniaxial tension (Fig. 4a). The parameter values for this analysis are \(E=207 \text{ GPa}, \nu=0.3, L=100 \text{ mm}\) and \(t^0 = 100 \text{ MPa}\). For the given parameter values, the total potential energy of the non-cracked domain is \(\psi = -219.807 \text{ N mm}\). Since the stress field is uniform we obtain a uniform topological derivative field (Eq. (32)). Fig. 4b shows the topological derivative value as a function of the crack orientation \(\alpha\). As expected, the maximum topological derivative value occurs at the angle \(\alpha = 0^\circ\), for which \(D_T\psi(\hat{x},0^\circ) = 0.0867 \text{ N/mm} \) and \(G^{\text{TD}}(\epsilon,\hat{x},0^\circ) = 0.1734\).

In order to verify the topological derivative, we use the finite element method to calculate the total potential energy \(\psi^{\text{FE}}\) and energy release rates \(G^{\text{FE}}\) on domains with cracks of different sizes and orientations inserted at \(\hat{x}\).

where \(h_{ij}\) are dimensionless valued functions of the crack orientation \(\alpha\). Fig. 3 shows the function values \(h_{ij}(\alpha)\) and compares them with values computed via finite element method by Beghini et al. (1999). Note that the two computations yield similar results.

We are finally in position to approximate the energy release rate \(G\). Combining Eqs. (10), (13) and (30) gives us

\[
D_T\psi(\hat{x},\alpha) = \lim_{\epsilon \to 0} \left\{ \frac{1}{f(\epsilon)} \left( -\epsilon K_I^2(\hat{x},\alpha) + K_T^2(\hat{x},\alpha) \right) \right\} = \frac{1}{2E} (K_I^2(\hat{x},\alpha) + K_T^2(\hat{x},\alpha)),
\]

with \(f(\epsilon) = -\epsilon^2\), cf. footnote 2. From Eq. (9) and the above we obtain the approximation

\[
G^{\text{TD}}(\epsilon,\hat{x},\alpha) = \frac{E}{2}(K_I^2(\hat{x},\alpha) + K_T^2(\hat{x},\alpha)).
\]

To summarize the energy release rate computation using the topological derivative, i.e., \(G^{\text{TD}}\), we perform the following steps:

1. Perform a finite element analysis on the non-cracked domain \(\Omega\) with boundary traction \(t^0\) to evaluate the stress field \(T\).
2. Evaluate \(K_I(\hat{x},\alpha)\) and \(K_T(\hat{x},\alpha)\) via Eq. (31).
3. Evaluate \(G^{\text{TD}}(\epsilon,\hat{x},\alpha)\) for any crack size \(\epsilon\) via Eq. (33).

It is again emphasized that we know, from the single analysis on the non-cracked domain \(\Omega\), the value of \(G^{\text{TD}}\) for any crack size \(\epsilon\) at any location \(\hat{x}\) on \(\partial\Omega\) and for any angle \(\alpha\) from this one analysis.

Fig. 5 summarizes the finite element results for the total potential energy $\psi_{\text{FE}}$ obtained for cracks initiating at $\alpha = 0^\circ, 30^\circ, 45^\circ$ and compares them with the results obtained via topological derivative $\psi_{\text{TD}}$. One can see that the total potential energy computed using the topological derivative $\psi_{\text{TD}}$ is very close to that computed with the FEM $\psi_{\text{FE}}$ when the crack size is smaller than 5% of the specimen size $L$, i.e., $\epsilon/L < 0.05$. As expected, for larger cracks, the discrepancy between $\psi_{\text{TD}}$ and $\psi_{\text{FE}}$ grows, since the topological derivative is derived from a first-order asymptotic expansion. Fig. 6 compares the finite element results for the energy release rate $G_{\text{FE}}$ with the results obtained via topological derivative $G_{\text{TD}}$ for different crack sizes and orientations. Again one can see that $G_{\text{TD}}$ is very close to $G_{\text{FE}}$ when the crack size is smaller than 5% of the specimen size $L$, i.e., $\epsilon/L < 0.05$.

4.2. Simply supported beam with uniformly distributed bending load

Here we investigate a small crack on the bottom edge of a simply supported beam subject to a distributed uniform top load (Fig. 7). The parameter values for this plane strain analysis are $E = 207$ GPa, $v = 0.3$, $L = 100$ mm, $h = 200$ mm, $b = 25$ mm and $t^0 = -100e_1$, MPa.

Due to the symmetry of the problem, we considered only half of the beam in our model. For the domain with no cracks the total potential energy is $\psi = -30.3746$ kN mm. In this symmetric test, it is known that the crack nucleates at the
Fig. 8 depicts the total potential energy computations $c_{TD}$ and $c_{FE}$ and the energy release rate computations $G_{TD}$ and $G_{FE}$ for a crack of size $e$ and orientation $\alpha = 0^\circ$ at $x$. Again as expected, for larger values of $e$, the discrepancy between $c_{TD}$ and $c_{FE}$ and between $G_{TD}$ and $G_{FE}$ grows.

4.3. Simply supported beam with axial and bending loads

Here we investigate the presence of a small crack on the top and bottom edges of a simply supported beam under axial and bending loads (Fig. 9). The parameter values for this plane strain analysis are $E=207$ GPa, $v=0.3$, $L=20$ mm, $h=50$ mm, $a=5$ mm and $b=1$ mm.

First we impose the loading $t_a^P = -100e_1$ MPa and $t_b^P = 200e_1$ MPa. For the domain with no cracks the total potential energy is $\psi = -46.8356$ N mm. Fig. 10 shows the topological derivative distribution along the bottom and top edges for the
When the crack size is smaller than 5% of the specimen dimension, the total potential energy compares the total potential energy derivative as a function of location. Topological derivative as a function of crack location appears in Fig. 12.

Fig. 10. Topological derivative as a function of crack location $x$ for a simply supported beam under axial and bending loads for a crack perpendicular to the edge, i.e., $x = 0$: (a) top edge and (b) bottom edge.

Fig. 11. Total potential energy and energy release rate vs. normalized crack size for a simply supported beam with axial and bending loads for cracks at the bottom midpoint $x = (0,0)$ perpendicular to the free edge, i.e., $x = 0$. The solid lines represent the topological derivative computations and the symbols represent the finite element computations.

When the crack size is smaller than 5% of the specimen dimension, the total potential energy obtains its highest value $D_T\psi = 0.585376 \text{ N/mm}$ on the bottom edge at the midpoint $x = (0,0)$, indicating the crack location associated with the maximum energy release rate.

Fig. 11 compares the total potential energy values $\psi_{TD}$ and $\psi_{FE}$ and the energy release rates $G_{TD}$ and $G_{FE}$ at $x = (0,0)$. When the crack size is smaller than 5% of the specimen dimension $L$, the values are in close agreement.

We now impose the loading $t_a = -100 e_1 \text{ MPa}$ and $t_b = 400 e_1 \text{ MPa}$. Fig. 12 shows the energy release rate $G_{TD}$ for cracks of various sizes and locations $x$ that are perpendicular to the free top and bottom edges, i.e., $x = 0^\circ$. Note that for this increased loading, the energy release rate is maximal on the top edge at $x = (47.0122, 20)$ mm. The results obtained via the topological derivative and finite element analysis for cracks of size $\varepsilon$ at locations $x = (0,0) \text{ mm}$ and $x = (47.0122, 20)$ mm appear in Fig. 12.

4.4. Crack emanating from a hole on a finite plate

This example considers a crack emanating from a hole on a finite plate. As seen in Fig. 13b, the crack location is defined via cylindrical coordinates as $x = (R, \gamma)$, where $R$ is the hole radius. The parameter values for this plane strain analysis are $E = 207 \text{ GPa}$, $v = 0.3$, $L = 10 \text{ mm}$, $h = 20 \text{ mm}$, $R = 2.5 \text{ mm}$ and $t = 100 e_2 \text{ MPa}$. Fig. 14a shows the topological derivative contour plot as a function of crack location along the hole, i.e., $x = (R, \gamma)$, and orientation $\alpha$. We note that the topological derivative is maximal at $\alpha = 0^\circ$, $\gamma = 0^\circ$ and $x = (R, \gamma) = 180^\circ$. This result is intuitive since these are the locations of maximum stress concentration for a plate subject to uniaxial load. Fig. 14b shows the topological derivative as a function of location $\gamma$ along the hole for a radial crack emanating from the hole, i.e., at orientation $\alpha = 0^\circ$.

We now verify the accuracy of the topological derivative computation by considering a radial crack at $x = (R, 0^\circ)$. For this mode I problem, we evaluate the stress intensity factor $K_{TD}$ from the energy release rate $G_{TD}$ via $K_{TD} = \sqrt{G_{TD}}$. Fig. 15 compares the total potential energy $\psi_{TD}$ and the stress intensity factor $K_{TD}$ obtained via topological derivative method with the $\psi_{FE}$ and $K_{FE}$ obtained with the FEM on the cracked domain. We obtain a good agreement for the stress intensity factor when the crack size is less than 2% of the specimen dimension $(L - R)$. The discrepancy can potentially be explained by the radius of curvature $R$ of the free edge, since our fundamental solution is based on a crack emanating from the free edge of a half-space. However, the proposed method still gives reasonable results for small cracks.

4.5. Crack emanating from a hole on an infinite plate

Here we consider a crack emanating from a hole of radius $R$ on an infinite plate, as shown in Fig. 13a. The plate is subject to a remote uniaxial tension $t_1$ and the crack originates on the hole at $\hat{x}=(R,\gamma)$.

Rubinstein and Sadegh (1986) obtained the stress intensity factors for this problem using the distributed dislocation technique (Hills et al., 1996). We reproduced the results obtained by Rubinstein and Sadegh (1986) to evaluate the energy release rate $G$ as a function of crack location $\hat{x}$ when $\alpha=0$ for the normalized crack sizes $\epsilon/L=(0.005,0.01,0.025,0.05)$. The solid lines represent the topological derivative computations $G^{TD}$ and the symbols represent the finite element computations $G^{FE}$. (a) bottom edge and (b) top edge.

**Fig. 12.** Energy release rate $G$ as a function of crack location $\hat{x}$ when $\alpha=0$ for the normalized crack sizes $\epsilon/L=(0.005,0.01,0.025,0.05)$. The solid lines represent the topological derivative computations $G^{TD}$ and the symbols represent the finite element computations $G^{FE}$. (a) bottom edge and (b) top edge.

**Fig. 13.** Problem geometry for a crack emanating from a hole: (a) hole in an infinite plate and (b) hole in a finite plate.

**Fig. 14.** Topological derivative as a function of crack location $\hat{x}=(R,\gamma)$ and orientation (left) $\alpha \in [-90,90]$ and (right) $\alpha=0$ for a crack emanating from a hole in a finite plate.

4.5. Crack emanating from a hole on an infinite plate

Here we consider a crack emanating from a hole of radius $R$ on an infinite plate, as shown in Fig. 13a. The plate is subject to a remote uniaxial tension $t_1$ and the crack originates on the hole at $\hat{x}=(R,\gamma)$.

Rubinstein and Sadegh (1986) obtained the stress intensity factors for this problem using the distributed dislocation technique (Hills et al., 1996). We reproduced the results obtained by Rubinstein and Sadegh (1986) to evaluate the energy release rate $G$ as a function of crack location $\hat{x}$ when $\alpha=0$ for the normalized crack sizes $\epsilon/L=(0.005,0.01,0.025,0.05)$. The solid lines represent the topological derivative computations $G^{TD}$ and the symbols represent the finite element computations $G^{FE}$. (a) bottom edge and (b) top edge.

**Fig. 12.** Energy release rate $G$ as a function of crack location $\hat{x}$ when $\alpha=0$ for the normalized crack sizes $\epsilon/L=(0.005,0.01,0.025,0.05)$. The solid lines represent the topological derivative computations $G^{TD}$ and the symbols represent the finite element computations $G^{FE}$. (a) bottom edge and (b) top edge.

**Fig. 13.** Problem geometry for a crack emanating from a hole: (a) hole in an infinite plate and (b) hole in a finite plate.

**Fig. 14.** Topological derivative as a function of crack location $\hat{x}=(R,\gamma)$ and orientation (left) $\alpha \in [-90,90]$ and (right) $\alpha=0$ for a crack emanating from a hole in a finite plate.

4.5. Crack emanating from a hole on an infinite plate

Here we consider a crack emanating from a hole of radius $R$ on an infinite plate, as shown in Fig. 13a. The plate is subject to a remote uniaxial tension $t_1$ and the crack originates on the hole at $\hat{x}=(R,\gamma)$.

Rubinstein and Sadegh (1986) obtained the stress intensity factors for this problem using the distributed dislocation technique (Hills et al., 1996). We reproduced the results obtained by Rubinstein and Sadegh (1986) to evaluate the energy release rate $G$ as a function of crack location $\hat{x}$ when $\alpha=0$ for the normalized crack sizes $\epsilon/L=(0.005,0.01,0.025,0.05)$. The solid lines represent the topological derivative computations $G^{TD}$ and the symbols represent the finite element computations $G^{FE}$. (a) bottom edge and (b) top edge.

**Fig. 12.** Energy release rate $G$ as a function of crack location $\hat{x}$ when $\alpha=0$ for the normalized crack sizes $\epsilon/L=(0.005,0.01,0.025,0.05)$. The solid lines represent the topological derivative computations $G^{TD}$ and the symbols represent the finite element computations $G^{FE}$. (a) bottom edge and (b) top edge.

**Fig. 13.** Problem geometry for a crack emanating from a hole: (a) hole in an infinite plate and (b) hole in a finite plate.

**Fig. 14.** Topological derivative as a function of crack location $\hat{x}=(R,\gamma)$ and orientation (left) $\alpha \in [-90,90]$ and (right) $\alpha=0$ for a crack emanating from a hole in a finite plate.
energy release rate as a function of the crack orientation

release rate for cracks of size

the energy release rate computations method.

Simply supported beam with shear load

Fig. 16. Energy release rate for a radial crack (\(\alpha = 0^\circ\)) emanating from a hole at location \(\mathbf{x} = (R,0)\) in an infinite plate with different crack sizes; the solid line represents the energy release rate obtained via topological derivative and the symbols represent the results obtained by Rubinstein and Sadegh (1986) \(G^{\text{TD}}\): (a) \(\varepsilon/R = 0.005\), (b) \(\varepsilon/R = 0.01\) and (c) \(\varepsilon/R = 0.05\).

release rate \(G^{\text{RS}}\) for cracks emanating at different locations \(\mathbf{x}\) and with different orientations \(\alpha\) and compare them to computations obtained via topological derivative, i.e., \(G^{\text{TD}}\). No finite element analysis is performed in this example.

Fig. 16 shows the energy release rate for radial crack, i.e., \(\alpha = 0^\circ\), of sizes \(\varepsilon/R = \{0.005, 0.01, 0.05\}\) as a function of location \(\mathbf{x} = (R,\gamma)\). The solid line represents the energy release rate \(G^{\text{TD}}\) and the symbols represent \(G^{\text{RS}}\). We note that \(G^{\text{TD}} \approx G^{\text{RS}}\) for crack sizes smaller than 1% of the hole radius, i.e., for \(\varepsilon/R < 0.01\). We also note that for any crack size, the energy release rate is higher at \(\gamma = 0^\circ\), which indicates the most critical flaw orientation.

Fig. 17 shows the energy release rate for crack of sizes \(\varepsilon/R = \{0.005, 0.01, 0.05\}\) starting at locations \(\gamma = \{10^\circ, 30^\circ, 45^\circ, 70^\circ\}\) as a function of the crack orientation \(\alpha\). We see that \(G^{\text{TD}}\) is again in good agreement with \(G^{\text{RS}}\) when \(\varepsilon/R < 0.01\). When the crack is very small the energy release rate \(G^{\text{TD}} \approx G^{\text{RS}}\) is higher at \(\alpha = 0^\circ\), i.e., if a very small crack exists it is likely to propagate in the radial direction, characterizing a mode I problem. However, for larger crack sizes for which \(G^{\text{TD}} \approx G^{\text{RS}}\), the energy release rate \(G^{\text{RS}}\) is higher for an angle \(\alpha \neq 0^\circ\), i.e., if a larger crack exists it is likely to propagate with an orientation \(\alpha \neq 0^\circ\) creating a mixed-mode problem. Since our topological derivative approximation is only valid for small crack sizes, it does not capture this effect.

According to Eq. (9), we see that the energy release rate is a scaled function of the topological derivative, more precisely \(G^{\text{TD}} = 2\varepsilon D_T \psi(\mathbf{x},\alpha)\). Therefore, the curves on Fig. 17 consist of scaled versions of the topological derivative curve, which depends on the position \(\mathbf{x}\) and crack orientation \(\alpha\).

4.6. Simply supported beam with shear load

Here we investigate the presence of a small crack on the top edge of a simply supported beam under shear loads, cf. Fig. 18. The parameter values for this plane strain analysis are \(E = 207\) GPa, \(v = 0.3, L = 20\) mm, \(h = 50\) mm and \(b = 1\) mm. Due to the symmetry we only model half of the beam.

In the first analysis we apply the load \(P^p = 50\mathbf{e}_1 + 100\mathbf{e}_2\) MPa over the top edge region \(x_1 \in [25,50]\) mm. Fig. 19 shows the energy release rate computations \(G^{\text{TD}}\) for a crack of size \(\varepsilon = 0.1\) mm and orientations \(\alpha = 0^\circ, 30^\circ, 45^\circ, 60^\circ\) as a function of location \(\mathbf{x}\). To verify our topological derivative calculations, we use the finite element method to evaluate the energy release rate for cracks of size \(\varepsilon = 0.1\) mm, orientations \(\alpha = 0^\circ, 30^\circ, 45^\circ, 60^\circ\) and locations \(\mathbf{x} = (35,20)\) mm and \(\mathbf{x} = (45,20)\) mm. We again emphasize that the finite element energy release rate computations require the generation of a mesh for each crack size–location–orientation combination, eight such combinations in this case. The finite element results, demarcated with the stars, appear in Fig. 19; they deviate from the topological derivative results by at most 1.8%.

This is a mixed-mode example since the normal stress $T_{xx}$ and shear stress $T_{xy}$ are non-zero over the top edge. However, $T_{xx} \gg T_{xy}$, therefore this example can be approximated as a mode I situation. And not surprisingly the maximum energy release rate approximately occurs for normal cracks near the site of maximal hoop stress. In general, however, this

approximation will not be valid. Indeed, according to Eq. (31) both tangential and normal traction components contribute to the energy release rate.

To further illustrate the versatility of our method we now repeat the above example, however, we apply horizontal quadratic varying load

$$t_P(x) = \left(0.5 \cdot 25x^2 - 25x + 0.5 \cdot x_1^2\right) \text{MPa}$$

over the top edge region $x_1 \in [25, 50]$ mm. Fig. 20 shows the energy release rate computations $G^{TD}$ for a crack of size $e = 0.1$ mm and orientations $\alpha = 0^\circ, 30^\circ, 45^\circ, 60^\circ$ as a function of location $\hat{x}$ on the top edge. The four verification finite element energy release rate computations $G^{FE}$ are demarcated with the stars; they deviate from the topological derivative results by at most 2.2%.

In this last example, the crack locations are only subject to tangential traction. And as seen in Figs. 20 and 21, the energy release rate associated with an existing crack of size $e = 0.1$ mm reaches its maximum value at $\hat{x} = (49, 20)$ mm, which does not correspond to the point of maximum normal stress $T_{xx}$ which is at $\hat{x} = (35, 20)$ mm. Rather the maximum site occurs where the shear stress $T_{xy}$ is maximal, i.e., at $\hat{x} = (49, 20)$ mm. Moreover, the energy release rates associated with inclined cracks is far greater than that of a perpendicular crack.

5. Conclusions

In this 2-D linear elastic fracture mechanics work, we use the topological derivative field to approximate the energy release rate for a small crack initiating at any boundary location and at any orientation. And thereby we can readily determine possible fracture locations. Moreover, our method requires a single finite element analysis on the non-cracked domain, as opposed to the multiple finite element analyzes with highly refined crack tip region meshes required for each crack size, orientation and initiation site combination used in traditional methods.

In the numerical examples, we compare our topological derivative energy release rate computations $G^{FE}$ with the finite element energy release rate computations $G^{FE}$. It is important to note once again that the evaluation of $G^{FE}$ requires the
construction of a mesh on the cracked domain for each size–location–orientation combination while the evaluation of $G^{TD}$ requires a single analysis on the non-cracked domain. In all examples, $G^{TD}$ and $G^{FE}$ computations are in close agreement, especially when the crack size is small compared to the geometry features.

Multiple extensions of the method are possible, including the introduction of higher order topological derivatives to obtain more accurate approximations of the energy release rate (Silva et al., 2010), and the application of the method to interfacial and 3-D problems.

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Appendix A. Crack emanating from a circular hole on an infinite space

The problem of a crack emanating from a circular hole on an infinite space was analyzed by Rubinstein and Sadegh (1986), using complex potentials and dislocations. This excellent, but seldom cited work, was used here to verify our topological derivative results, with the following corrections for the typographical errors:

- Eq. (12) should read
  \[
  \psi_{21}(b,z) = -A \frac{b}{2\pi i(z-\zeta)} + \frac{Ab\overline{z}}{2\pi i(z-\zeta)^2}.
  \]

- Eq. (14) should read
  \[
  \psi_3'B(z) = -\frac{AB}{2\pi i z} + \frac{AR^2 B}{\pi i z^3}.
  \]

- Eq. (16) should read
  \[
  P_1(z) = \phi_1(z) + \overline{\phi_1(z)} + e^{2iz}(\overline{z}\phi_1(z) + \psi_1(z)).
  \]

References


