# THE COMPUTATION OF BOUNDS FOR THE EXACT ENERGY RELEASE RATES IN LINEAR FRACTURE MECHANICS

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#### Abstract

We present an *a-posteriori* method for computing rigorous upper and lower bounds of the J-integral in two dimensional linear elasticity. The J-integral, which is typically expressed as a contour integral, is recast as a surface integral which yields a quadratic continuous functional of the displacement. By expanding the quadratic output about an approximate finite element solution, the output is expressed as a known computable quantity plus linear and quadratic functionals of the solution error. The quadratic component is bounded by the energy norm of the error scaled by a continuity constant, which is determined explicitly. The linear component is expressed as an inner product of the errors in the displacement and in a computed adjoint solution, and bounded using standard a-posteriori error estimation techniques. The method is illustrated with two fracture problems in plane strain elasticity. An important feature of the method presented is that the computed bounds are rigorous with respect to the weak solution of the elasticity equation.

### Introduction

The accurate prediction of stress intensity factors in crack tips is essential for assessing the strength and life of structures using linear fracture mechanics theories. A crack is assumed to be stable when the magnitude of the stress concentration at its tip is below a critical material dependent value. Stress intensity factors derived from linearly elastic solutions are widely used in the study of brittle fracture, fatigue, stress corrosion cracking, and to some extend for creep crack growth. Since the analytical methods for solving the equations of elasticity are limited to very simple cases, the finite element method is commonly used as the alternative to treat the more complicated cases. The methods for extracting stress intensity factors from computed displacement solutions fall into two categories: displacement matching methods, and the energy based methods. In the first case, the form of the local solution is assumed, and the value of the displacement near crack tip is used to determine the magnitude of the coefficients in the asymptotic expansion. In the second case, the strength of the singular stress field is related to the energy released rate, i.e. the sensitivity of the total potential energy to the crack position. An expression for calculating the energy release rate in two dimensional cracks was given in (Rice, 1968) and is known as the J-integral. The J-integral is a path independent contour integral involving the projection of the material force derived from Eshelby's (Eshelby, 1970) energy

momentum tensor along the direction of the possible crack extension. An alternative form of the J-integral in which the contour integral is transformed into a domain integral involving a suitably defined weighting function is given in (Li *et al.*, 1985). This alternative expression for the energy release rate appears to be very versatile and has an easier and more convenient generalization to three dimensions than the original form (Rice, 1968).

Regardless of the method chosen to evaluate the stress intensity factor, a good approximation to the solution of the linear elasticity equations is required. Unfortunately, the problems of interest involve singularities and this makes the task of computing accurate solutions much harder. For instance, it is well known (Szabo, 1986) that the convergence rate of energy norm of a standard finite element solution for a linear elasticity problem involving a 180° reentrant corner is no higher than  $O(H^{\frac{1}{2}})$ , where H is the mesh size. This problem was soon realized and as a consequence a number of mesh adaptive algorithms have been proposed which, in general, improve the situation considerably. In some cases (Lo and Lee, 1992; Murthy and Mukhopadhyay, 2001), the adaptivity is driven by errors in the energy norm of the solution, whereas in some others (Heintz *et al.*, 2002; Heintz and Samuelsson, 2002; Ruter and Stein, 2002), a more sophisticated goal-oriented approach based on a linearized form of the output is used.

In this paper we present a method for computing strict upper and lower bounds for the value of the J-integral in two dimensional linear fracture mechanics. The method presented involves no unknown constants or uncertain parameters and therefore the computed bounds we are strict with respect to the exact solution of the underlying partial differential equation. The J-integral is written as a bounded quadratic functional of the displacement and expanded into computable quantities plus additional linear and quadratic terms in the error. The linear terms are bounded using our previous work for linear functional outputs (Paraschivoiu *et al.*, 1997; Patera and Peraire, 2002; Peraire and Patera, 1998) and the quadratic term is bounded with the energy norm of the error scaled by a suitably chosen continuity constant, which can be determined a priori. Moreover, the bound gap can be decomposed into a sum of positive elemental contributions thus naturally leading to an adaptive mesh adaptive approach (Peraire and Patera, 1998). We think that the algorithm presented is an attractive alternative to the existing methods as it guarantees the certainty of the computed bounds. This is particularly important in critical problems relating to structural failure. The method is illustrated for an open mode and a mixed mode crack examples.

## **Problem Formulation**

We consider a linear elastic body occupying a polygonal region  $\Omega \subset \mathbb{R}^2$  where the boundary  $\partial \Omega$  is composed of a Dirichlet portion  $\Gamma_D$ , and a Neumann portion  $\Gamma_N$ , i.e.  $\partial \Omega = \Gamma_D \cup \Gamma_N$ . For simplicity of presentation the Dirichlet boundary conditions are assumed to be homogeneous. The displacement field  $\boldsymbol{u} = (u_1, u_2) \in X \equiv \{\boldsymbol{v} =$   $(v_1, v_2) \in (H^1(\Omega))^2 \mid \boldsymbol{v} = \boldsymbol{0}$  on  $\Gamma_D$  satisfies the weak form of the elasticity equations

$$a(\boldsymbol{u}, \boldsymbol{v}) = (\boldsymbol{f}, \boldsymbol{v}) + \langle \boldsymbol{g}, \boldsymbol{v} \rangle, \quad \forall \boldsymbol{v} \in X,$$
 (1)

in which

$$(\boldsymbol{f}, \boldsymbol{v}) = \int_{\Omega} \boldsymbol{f} \cdot \boldsymbol{v} \, \mathrm{d}\Omega \;, \quad \langle \boldsymbol{g}, \boldsymbol{v} \rangle = \int_{\Gamma_N} \boldsymbol{g} \cdot \boldsymbol{v} \, \mathrm{d}\Gamma \;,$$

where  $\boldsymbol{f} \in (H^{-1}(\Omega))^2$  is the body force and  $\boldsymbol{g} \in (H^{-1/2}(\Gamma_N))^2$  is the traction applied on the Neumann boundary. The bi-linear form  $a(\boldsymbol{w}, \boldsymbol{v}) : X \times X \to \mathbb{R}$  is given by,

$$a(\boldsymbol{w}, \boldsymbol{v}) = \int_{\Omega} \boldsymbol{\sigma}(\boldsymbol{w}) : \boldsymbol{\varepsilon}(\boldsymbol{v}) \ \mathrm{d}\Omega$$

Here,  $\boldsymbol{\varepsilon}(\boldsymbol{v})$  denotes the second order deformation tensor which is defined as the symmetric part of the gradient tensor  $\nabla \boldsymbol{v}$ . That is,  $\boldsymbol{\varepsilon}(\boldsymbol{v}) = (\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T)/2$ . The stress  $\boldsymbol{\sigma}(\boldsymbol{v})$  is related to the deformation tensor through a linear constitutive relation of the form  $\boldsymbol{\sigma}(\boldsymbol{v}) = \boldsymbol{C} : \boldsymbol{\varepsilon}(\boldsymbol{v})$ , where  $\boldsymbol{C}$  is the constant fourth-order elasticity tensor.

It is well known that the solution,  $\boldsymbol{u}$ , to the problem (1) minimizes the total potential energy functional  $\Pi(\boldsymbol{v}): X \to \mathbb{R}$ ,

$$\Pi(oldsymbol{v}) = rac{1}{2}a(oldsymbol{v},oldsymbol{v}) - \langleoldsymbol{f},oldsymbol{v}) - \langleoldsymbol{g},oldsymbol{v}
angle$$

and that  $\Pi(\boldsymbol{u}) = -\frac{1}{2} |||\boldsymbol{u}|||^2$ , where  $||| \cdot ||| = a(\cdot, \cdot)^{1/2}$  denotes energy norm associated with the coercive bilinear form  $a(\cdot, \cdot)$ .

In fracture mechanics we are often interested in determining the strength of the crack tip stress fields. A common way to do that is to relate the so called stress intensity factors to the energy released per unit length of crack advancement (see figure 1). If the total potential energy  $\Pi(u)$  decreases by an amount  $\delta \Pi(u)$  when the crack advances by a distance  $\delta \ell$  in its plane, we are interested in determining the energy release rate, J(u), such that,

$$\delta \Pi(\boldsymbol{u}) = -J(\boldsymbol{u})\delta \ell$$
.

For a two-dimensional linear elastic body the energy release rate,  $J(\boldsymbol{u})$ , can be calculated as a path independent line integral known as the *J*-integral (Rice, 1968). If we consider the geometry shown in figure 1, the *J*-integral has the following expression,

$$J(\boldsymbol{u}) = \int_{\Gamma} \left( W^e n_1 - \boldsymbol{T} \cdot \frac{\partial \boldsymbol{u}}{\partial x_1} \right) \, \mathrm{d}\Gamma \; ,$$

where  $\Gamma$  is any path beginning at the bottom crack face and ending at the top crack face,  $W^e = (\boldsymbol{\sigma} : \boldsymbol{\varepsilon})/2$  is the strain energy density,  $\boldsymbol{T}$  is the traction given as  $\boldsymbol{T} = \boldsymbol{\sigma} \boldsymbol{n}$ , and  $\boldsymbol{n} = (n_1, n_2)$  is the outward unit normal to  $\Gamma$ . An alternative expression for  $J(\boldsymbol{u})$ was proposed in (Li *et al.*, 1985), where the contour integral is transformed to the following area integral expression,

$$J(\boldsymbol{u}) = \int_{\Omega_{\chi}} \left( (\boldsymbol{\nabla}\chi)^T \cdot \boldsymbol{\sigma} \frac{\partial \boldsymbol{u}}{\partial x_1} - W^e \frac{\partial \chi}{\partial x_1} \right) \,\mathrm{d}\Omega.$$
(2)



Figure 1: Crack geometry showing coordinate axes and the J-integral contour and domain of integration.

Here, the weighting function  $\chi$  is any function in  $H^1(\Omega_{\chi})$  that is equal to one at the crack tip and vanishes on  $\Gamma$ .

For a given  $\chi$ ,  $J(\boldsymbol{u})$  is a bounded quadratic functional of  $\boldsymbol{u}$ . For our bounding procedure it is convenient to make the quadratic dependence of  $J(\boldsymbol{u})$  more explicit. To this end, we define the bilinear form  $\bar{q}(\boldsymbol{w}, \boldsymbol{v}) : X \times X \to \mathbb{R}$  as,

$$\bar{q}(\boldsymbol{w},\boldsymbol{v}) = \int_{\Omega_{\chi}} (\boldsymbol{\nabla}\chi)^T \cdot \boldsymbol{\sigma}(\boldsymbol{w}) \frac{\partial \boldsymbol{v}}{\partial x_1} \,\mathrm{d}\Omega - \int_{\Omega_{\chi}} \frac{1}{2} \boldsymbol{\sigma}(\boldsymbol{w}) : \boldsymbol{\varepsilon}(\boldsymbol{v}) \frac{\partial \chi}{\partial x_1} \,\mathrm{d}\Omega,$$

and its symmetric part  $q(\boldsymbol{w}, \boldsymbol{v}) : X \times X \to \mathbb{R}$ ,  $q(\boldsymbol{w}, \boldsymbol{v}) = \frac{1}{2}(\bar{q}(\boldsymbol{w}, \boldsymbol{v}) + \bar{q}(\boldsymbol{v}, \boldsymbol{w}))$ . It is clear from these definitions that,  $J(\boldsymbol{u}) = q(\boldsymbol{u}, \boldsymbol{u})$ , and that there exists  $\eta < \infty$  such that,

$$q(\boldsymbol{v}, \boldsymbol{v}) \le \eta |||\boldsymbol{v}|||^2 , \qquad \forall \boldsymbol{v} \in X.$$
(3)

#### **Bounding Procedure**

Our objective is to compute upper and lower bounds, for  $J(\boldsymbol{u})$ , where  $\boldsymbol{u}$  satisfies problem (1). Let us consider a finite element approximation  $\boldsymbol{u}_H \in X_H$  satisfying

$$a(\boldsymbol{u}_H, \boldsymbol{v}) = (\boldsymbol{f}, \boldsymbol{v}) + \langle \boldsymbol{g}, \boldsymbol{v} \rangle , \quad \forall \boldsymbol{v} \in X_H .$$
 (4)

Here,  $X_H \subset X$  is a finite dimensional subspace of X. For simplicity, we shall assume that  $X_H$  is the space of piecewise linear continuous functions defined over a triangulation,  $\mathcal{T}_H$ , of  $\Omega$  which satisfies the Dirichlet boundary conditions. An approximation to  $J(\boldsymbol{u})$ ,  $J_H$ , can be obtained as  $J_H = q(\boldsymbol{u}_H, \boldsymbol{u}_H)$ , where, for convenience,  $\chi$  in (2) is chosen to be piecewise linear over the elements  $T_H \in \mathcal{T}_H$ . Exploiting the bi-linearity of  $q(\boldsymbol{w}, \boldsymbol{v})$ , we can write

$$J(\boldsymbol{u}) - J_H = q(\boldsymbol{u}, \boldsymbol{u}) - q(\boldsymbol{u}_H, \boldsymbol{u}_H) = q(\boldsymbol{u} - \boldsymbol{u}_H, \boldsymbol{u} - \boldsymbol{u}_H) + 2q(\boldsymbol{u}, \boldsymbol{u}_H) - 2q(\boldsymbol{u}_H, \boldsymbol{u}_H)$$
$$= q(\boldsymbol{e}, \boldsymbol{e}) + 2q(\boldsymbol{e}, \boldsymbol{u}_H) ,$$

where  $\boldsymbol{e} = \boldsymbol{u} - \boldsymbol{u}_H$  is the error in the approximation  $\boldsymbol{u}_H$ . It is clear that if we are able to compute bounds Q and  $L^{\pm}$  for the quadratic and linear error terms,

$$|q(oldsymbol{e},oldsymbol{e})|\leq Q \quad ext{ and } \quad L^-\leq q(oldsymbol{e},oldsymbol{u}_H)\leq L^+,$$

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then, the bounds for  $J(\boldsymbol{u}), J^{\pm}$ , follow as,

$$J^{-} \equiv J_{H} - Q + 2L^{-} \leq J(\boldsymbol{u}) \leq J_{H} + Q + 2L^{+} \equiv J^{+}$$
.

Linear term

In order to derive upper an lower bounds for the linear term  $q(\boldsymbol{e}, \boldsymbol{u}_H)$ , we introduce the following adjoint problem: find  $\boldsymbol{\psi} \in X$  such that

$$a(\boldsymbol{v}, \boldsymbol{\psi}) = q(\boldsymbol{v}, \boldsymbol{u}_H) , \quad \forall \boldsymbol{v} \in X ,$$
 (5)

and the corresponding finite element approximation,  $\psi_H \in X_H \subset X$ , such that

$$a(\boldsymbol{v}, \boldsymbol{\psi}_H) = q(\boldsymbol{v}, \boldsymbol{u}_H) , \quad \forall \boldsymbol{v} \in X_H .$$
 (6)

From (1) and (4), it follows that  $a(\boldsymbol{e}, \boldsymbol{v}) = 0$  for all  $\boldsymbol{v} \in X_H$ . In particular,  $a(\boldsymbol{e}, \boldsymbol{\psi}_H) = 0$ . This, combined with the above equations (5) and (6) gives the following representation for the linear error term,

$$q(\boldsymbol{e}, \boldsymbol{u}_H) = a(\boldsymbol{e}, \boldsymbol{\epsilon}) \; ,$$

where  $\boldsymbol{\epsilon} = \boldsymbol{\psi} - \boldsymbol{\psi}_H$  is the error in the adjoint solution. Now, using the parallelogram identity, we have that for all  $\alpha \in \mathbb{R}$ ,

$$a(\boldsymbol{e},\boldsymbol{\epsilon}) = \frac{1}{4} |||\alpha \, \boldsymbol{e} + \frac{1}{\alpha} \boldsymbol{\epsilon}|||^2 - \frac{1}{4} |||\alpha \, \boldsymbol{e} - \frac{1}{\alpha} \boldsymbol{\epsilon}|||^2 ,$$

and therefore, bounds for  $q(\boldsymbol{e}, \boldsymbol{u}_H)$  can be recovered as

$$\frac{1}{4} |||\alpha \, \boldsymbol{e} + \frac{1}{\alpha} \boldsymbol{\epsilon} |||_{\text{LB}}^2 - \frac{1}{4} |||\alpha \, \boldsymbol{e} - \frac{1}{\alpha} \boldsymbol{\epsilon} |||_{\text{UB}}^2 \le q(\boldsymbol{e}, \boldsymbol{u}_H) \le \frac{1}{4} |||\alpha \, \boldsymbol{e} + \frac{1}{\alpha} \boldsymbol{\epsilon} |||_{\text{UB}}^2 - \frac{1}{4} |||\alpha \, \boldsymbol{e} - \frac{1}{\alpha} \boldsymbol{\epsilon} |||_{\text{LB}}^2 - \frac{1}{\alpha} |||\alpha \, \boldsymbol{e} - \frac{1}{\alpha} \boldsymbol{\epsilon} |||_{\text{LB}}^2 - \frac{1}{\alpha} |||\alpha \, \boldsymbol{e} - \frac{1}{\alpha} \boldsymbol{\epsilon} |||_{\text{LB}}^2 - \frac{1}{\alpha} |||\alpha \, \boldsymbol{e} - \frac{1}{\alpha} \boldsymbol{\epsilon} ||\alpha \, \boldsymbol{e$$

Strict upper bounds for  $|||\alpha e \pm \frac{1}{\alpha} \epsilon |||^2$  are found using the technique presented in (Pares *et al.*, 2003) based on the use of the complementary energy principle, while the lower bounds are found using the dual definition of the energy norm which lead to the reconstruction of continuous approximations of the error (Díez *et al.*, 2003).

#### Quadratic term

In (Xuan *et al.*, 2004) it is shown that for two dimensional linear elasticity, a suitable value for the continuity constant in expression (3) is given by

$$\eta_{\chi} = \max_{T_H \in \mathcal{T}_H} \frac{(3\kappa + 4\mu) |\boldsymbol{\nabla}\chi|^2}{4\sqrt{(3\kappa + \mu) \left(3\mu \left(\frac{\partial\chi}{\partial x_1}\right)^2 + (3\kappa + 4\mu) \left(\frac{\partial\chi}{\partial x_2}\right)^2\right)}},$$
(7)

where  $\mu = E/(2(1 + \nu))$  is the elastic shear modulus,  $\kappa$  is the elastic bulk modulus which is given by  $\kappa = E/(1 + 2\nu)/(3(1 - \nu^2))$  for plane stress, and  $\kappa = E/(3(1 - 2\nu))$ for plain strain. In these expressions, E is Young's elastic modulus and  $\nu$  is the Poisson's ratio. Therefore, we write

$$q(\boldsymbol{e}, \boldsymbol{e}) \leq \eta_{\chi} |||\boldsymbol{e}|||^2$$
.

The computation of a bound for q(e, e) is straightforward once a bound for the error in the energy norm |||e||| has been obtained.

## Example

We consider a plate with two edge cracks subjected to a uniformly distributed tensile stress as shown in figure 2. The plate is assumed to be in plane strain. The value of the tensile force acting on the two ends of the plate is p = 1 and the dimension of the crack is a = 5. The non-dimensionalized Young's modulus is 1.0 and the Poisson's ratio is 0.3. The analytical value of the mode-I normalized stress intensity factor  $\mathcal{K}_{\rm I}$  for the problem has been determined in (Lo and Lee, 1992) to be  $\mathcal{K}_{\rm I}/(p\sqrt{\pi a}) = 1.16279$ . Therefore, the exact value of the J-integral is obtained as  $J_{exact} = (1 - \nu^2)\mathcal{K}_{\rm I}^2/E =$ 19.3270.



Figure 2: Geometry of a double edge-cracked plate subjected to a uniform tensile stress (left) and Support of weighting function  $\chi$  for the evaluation of the J-integral (right).

Due to the symmetry of the problem, we only use one quarter of the plate for the finite element analysis. We use a 5 by 5 square area surrounding the crack tip as the support,  $\Omega_{\chi}$ , of the weighting function  $\chi$  (see figure 2).

An adaptive procedure has been used to reach a relative bound gap  $\frac{J^+ - J^-}{2J_{exact}}$  of 5% and 2%. Table 1 shows the results for the output  $J_H$ , the computed upper and lower bounds,  $J^{\pm}$ , for J, and the relative bound gap for some of the steps of the adaptive procedure. Also the first three meshes of the adaptive procedure and the final mesh for the 5% relative bound gap are shown in figure 3. It is worth noting that due to the slow convergence of the finite element solution for the problem at hand it is crucial to use adaptive strategies to yield accurate bounds for the output of interest J(u).

Table 1: Bound results

416	525	759	1368	2962	10622	43733
17.4156	18.5208	19.1307	19.3498	19.4601	19.5196	19.5369
-27.7619	-2.7875	10.1176	15.1668	17.3981	18.6596	19.1712
86.0779	49.2769	31.5315	24.9273	22.0868	20.5178	19.9343
2.9451	1.3469	0.5540	0.2525	0.1213	0.0481	0.0197
	(b)		$(\mathcal{C})$		(u)	
	416 17.4156 -27.7619 86.0779 2.9451	416 525 17.4156 18.5208 -27.7619 -2.7875 86.0779 49.2769 2.9451 1.3469	416 525 759 17.4156 18.5208 19.1307 -27.7619 -2.7875 10.1176 86.0779 49.2769 31.5315 2.9451 1.3469 0.5540	416       525       759       1368         17.4156       18.5208       19.1307       19.3498         -27.7619       -2.7875       10.1176       15.1668         86.0779       49.2769       31.5315       24.9273         2.9451       1.3469       0.5540       0.2525	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$

Figure 3: Finite element meshes: (a) coarse mesh  $n_{el} = 416$ , (b)  $n_{el} = 525$ , (c)  $n_{el} = 759$  and (f) final mesh for a relative bound gap of 5%,  $n_{el} = 10622$ .

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