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# Technical note: Evaluation of the mode I stress intensity factor for a square crack in 3D 

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#### Abstract

An algorithm for the computation of mode I stress intensity factors of a square crack together with an error estimate is presented. The algorithm is based on a hypersingular integral equation. The leading singular behavior of the crack opening displacement in the corners is taken into account. The maximum value of the normalized stress intensity factor, $F_{\max }$, is estimated to $F_{\max }=0.7534 \pm 0.0002$. Previous investigators have estimated this quantity in the interval $F_{\max }=0.725$ to $F_{\max }=0.756$.


Key words: square crack, stress intensity factors, hypersingular integral equation, corner singularity

## 1 Introduction

Fracture mechanics has traditionally used two-dimensional models in its theoretical development [1]. Reasons for this are that such models cover the prediction of the general behavior of through-thickness cracks in plates and shells, and that powerful mathematical and numerical tools are available. Often, like when studying part-through cracks or embedded cracks such as delaminations in composites, a full three-dimensional model is required. In three dimensions the analytical and numerical situation is more complicated.

Elliptical cracks, referred to as penny-shaped cracks, have been thoroughly treated. See, for example, $[2,3,4]$. Studies of penny-shaped cracks involve numerical calculations of stress intensity factors $[6,7,8]$ and simulations of crack growth [9]. Studies of other crack shapes are less common. Methods that work well for penny-shaped cracks tend to give poorer results in more general situations. Rectangular cracks are treated in [10, 11, 12, 13].

Here we focus on a square crack. The non-smooth nature of the crack opening displacement is an obstacle which, if not taken into account, destroys accuracy. Our main result is an algorithm for the computation of mode I stress intensity factors. The quantity which is solved for is a reasonably smooth function. Leading singular behavior is captured

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Figure 1: The square crack closed (left) and opened by a uniformly distributed normal stress at infinity (right).
by a weight. Numerical results with unprecedented accuracy and error estimates are presented. The problem of computing stress intensity factors in three dimensions is generically well-conditioned. Very accurate calculations should be possible. At present, however, the analytical difficulties make it hard to obtain as accurate results as in two dimensions.

## 2 Background

### 2.1 Formulation of the general problem

A linearly elastic 3D material with a plane crack in the $x y$-plane is subjected at infinity to a uniformly distributed normal stress, $\sigma_{\infty}$, in the $z$-direction, see Figure 1. The crack surface is denoted $S$ and its boundary is denoted $\partial S$. We want to compute the displacement field inside the material. This problem can be reduced to a hypersingular integral equation which reads [11, 12, 13]

$$
\begin{equation*}
\frac{1}{2 \pi} \int_{S} \frac{u\left(\mathbf{r}^{\prime}\right) \mathrm{d} \sigma^{\prime}}{\left|\mathbf{r}^{\prime}-\mathbf{r}\right|^{3}}=-1, \quad \mathbf{r} \in S \tag{1}
\end{equation*}
$$

where $u$ is proportional to the crack opening displacement and $\mathrm{d} \sigma$ is an infinitesimal area segment. The integral in (1) should be understood in terms of Hadamard finite parts and Cauchy principal values [14]. For a square crack with side length $2 a$ the relation between $u$ and the crack opening displacement $u_{\text {COD }}$ is

$$
\begin{equation*}
u_{\mathrm{COD}}=8 a \frac{\sigma_{\infty}}{E}\left(1-\nu^{2}\right) u, \tag{2}
\end{equation*}
$$

where $E$ is Young's modulus for the material and $\nu$ is Poisson's ratio. The relation (2) also holds for a circle with radius $2 a$.

Equation (1) is equivalent to the pseudo-differential equation

$$
\begin{equation*}
(-\Delta)^{\frac{1}{2}} u(\mathbf{r})=-1, \quad \mathbf{r} \in S, \tag{3}
\end{equation*}
$$

where $\Delta$ is the Laplacian in the plane and $(-\Delta)^{\frac{1}{2}}$ is a non-local pseudo-differential operator [15]. From this we conclude that the integral operator in (1) is unbounded. Upon
uniform discretization the corresponding matrix will have a condition number that grows like $N$, where $1 / N$ is the distance between two discretization points.

Equation (1) must be accompanied by a boundary condition to be uniquely solvable. We use the closure of the crack along the boundary

$$
\begin{equation*}
u(\mathbf{r})=0, \quad \mathbf{r} \in \partial S \tag{4}
\end{equation*}
$$

as a uniqueness condition.
Stress intensity factors can be extracted once the solution to (1) is known. We define the normalized mode I stress intensity factor $F$ as the limit

$$
\begin{equation*}
F(\mathbf{r})=\lim _{\mathbf{d} \rightarrow 0} \frac{u(\mathbf{r}+\mathbf{d})}{|\mathbf{d}|^{\frac{1}{2}}}, \quad \mathbf{r} \in \partial S, \quad \mathbf{r}+\mathbf{d} \in S \tag{5}
\end{equation*}
$$

where $\mathbf{d}$ is a vector perpendicular to $\partial S$ at the point $\mathbf{r}$. The factor $F$ is related to the stress intensity factor $K_{\mathrm{I}}$ by $K_{\mathrm{I}}=F \sigma_{\infty} \sqrt{\pi l}$, where $l$ is a typical length dimension of the crack.

### 2.2 Special cases: ellipse and unit square

Equation (1) accompanied by (4) has an analytical solution for a crack in the shape of an ellipse [2]. For a unit disk the solution simplifies to

$$
\begin{equation*}
u(\mathbf{r})=\frac{2}{\pi}\left(1-|\mathbf{r}|^{2}\right)^{\frac{1}{2}} \tag{6}
\end{equation*}
$$

and $F=2 / \pi$. An ellipse with major axis $a$ and minor axis $b$ has a normalized stress intensity factor that varies along its boundary. The maximum value is given by

$$
\begin{equation*}
F_{\max }=\frac{1}{E\left(\sqrt{1-b^{2} / a^{2}}\right)} \tag{7}
\end{equation*}
$$

where $E(\eta)$ is the complete elliptical integral of the second kind [16].
Interestingly, the integral operator in (1) has an explicit inverse for the ellipse [5]. For the unit disk this inverse, operating on a function $f$, is given by

$$
\begin{equation*}
-\frac{1}{\pi^{2}} \int_{S} \frac{f\left(\mathbf{r}^{\prime}\right)}{\left|\mathbf{r}^{\prime}-\mathbf{r}\right|} \arctan \left(\frac{\left(1-|\mathbf{r}|^{2}\right)^{\frac{1}{2}}\left(1-\left|\mathbf{r}^{\prime}\right|^{2}\right)^{\frac{1}{2}}}{\left|\mathbf{r}^{\prime}-\mathbf{r}\right|}\right) \mathrm{d} \sigma^{\prime}, \quad \mathbf{r} \in S \tag{8}
\end{equation*}
$$

One of the simplest non-trivial plane crack geometries that has been studied is the unit square. Close to a point on the smooth part of the boundary, the crack opening displacement $u$ approaches zero as the square root of the distance to the boundary. In a corner $u$ approaches zero at a rate governed by the leading corner singularity $\lambda$. A weight that is proportional to $u$ close to all parts of the boundary of the unit square, centered at the origin, is

$$
\begin{equation*}
\rho(\mathbf{r})=\frac{\left(1 / 4-x^{2}\right)^{\frac{1}{2}}\left(1 / 4-y^{2}\right)^{\frac{1}{2}}}{\left(1 / 2-x^{2}-y^{2}\right)^{1-\lambda}} \tag{9}
\end{equation*}
$$

A discontinuous and asymptotically incorrect alternative weight is

$$
\rho(\mathbf{r})=\left\{\begin{align*}
(1 / 2-\max \{|x|,|y|\})^{\frac{1}{2}}, & |x| \neq|y|  \tag{10}\\
(1 / 2-|x|)^{\frac{1}{2}}(1 / 2-|y|)^{\frac{1}{2}}, & |x| \approx|y|
\end{align*}\right.
$$

The exponent $\lambda$ has to be calculated numerically. There are different approaches and results. Bažant [17] formulates an eigenvalue problem for Laplace's equation, uses symmetry, partial variable separation, and estimates $\lambda=0.816$. Morrison and Lewis [18] use full variable separation together with a singular perturbation technique and estimate $\lambda=0.8146$. Päivärinta and Rempel [15] use Mellin-operator-calculus and estimate $\lambda=0.7723$. Börje Andersson at The Aeronautical Research Institute of Sweden uses a finite element program [19] and estimates $\lambda=0.81465$ (private communication 1999).

Previous investigators use different weights in their calculations. Weaver [12] uses a weight of the type (10) together with piece-wise quadratic basis functions and reports a value of $F_{\max }=0.736$, see [10]. Murakami and Nemat-Nasser [20] also use a weight of the type (10) together with piece-wise constant basis functions and also report a value of $F_{\max }=0.736$. Isida, Yoshida, and Noguchi [10] use a weight of the type (9) with $\lambda=1$ together with piece-wise constant basis functions and report a value of $F_{\max }=0.756$ based on linear extrapolation. Pihua and Taihua [13] use no weight at all, piece-wise constant basis functions and report a value of $F_{\max }=0.7558$ based on quadratic least-squares interpolation and extrapolation. This value is not computed from (5), but via an integral over $S$.

## 3 Our algorithm

The singular behavior of the solution to (1) will be a source of error in any numerical scheme which does not take it into account. A large number of discretization points, $N^{2}$, will be needed for good resolution. This limits the possibilities of accurate computations since the condition number of the discretized problem increases as $N$.

The leading behavior of the solution $u$ at the boundary is known. We may write

$$
\begin{equation*}
u(\mathbf{r})=\rho(\mathbf{r}) \omega(\mathbf{r}) \tag{11}
\end{equation*}
$$

where $\rho$ is the weight in (9) and $\omega$ is a reasonably smooth function. The quantity $\omega$ can be better approximated, than the quantity $u$, with a given number of polynomial basis functions. The integral equation (1) now reads

$$
\begin{equation*}
\frac{1}{2 \pi} \int_{S} \frac{\omega\left(\mathbf{r}^{\prime}\right) \rho\left(\mathbf{r}^{\prime}\right) \mathrm{d} \sigma^{\prime}}{\left|\mathbf{r}^{\prime}-\mathbf{r}\right|^{3}}=-1, \quad \mathbf{r} \in S \tag{12}
\end{equation*}
$$

Equation (12) will be solved with a collocation scheme. We discretize using piece-wise constant basis functions on a uniform square $N \times N$ mesh. This leads to a system of $N^{2}$ linear equations for $\omega$ which we solve with the GMRES iterative solver [21]. The iterations are terminated when the residual is less than $10^{-11}$. This typically requires $10+\mathrm{N} / 2$ iterations (a little less if point-Jacobi preconditioning is used), which is consistent with our assumption that the condition number grows linearly with $N$.

Equation (12) is singular and the integrand needs to be regularized. We do this as follows. Let $S_{j}$ be a square area segment in the mesh tesselating $S$. Let $\mathbf{r}_{j}$ be the center of that square segment and let $\mathbf{r}_{i}$ be the center of some arbitrary segment. We write the corresponding matrix element as

$$
\int_{S_{j}} \frac{\rho\left(\mathbf{r}^{\prime}\right) \mathrm{d} \sigma^{\prime}}{\left|\mathbf{r}^{\prime}-\mathbf{r}_{i}\right|^{3}}=
$$



Figure 2: Estimates for the normalized stress intensity factor $F_{\max }$ at the midpoint of a side of a square crack with normal load computed with corner singularity $\lambda=0.81465$ (upper curve) and $\lambda=1$ (lower curve). The number of discretization points is $N^{2}$. The symbols ' $*$ ' indicate numerical results. The two curves are seventh order polynomial interpolations.

$$
\begin{gather*}
\int_{S_{j}} \frac{\left(\rho\left(\mathbf{r}_{j}\right)+\left(\left(\mathbf{r}^{\prime}-\mathbf{r}_{j}\right) \cdot \nabla\right) \rho\left(\mathbf{r}_{j}\right)+\left(\left(\mathbf{r}^{\prime}-\mathbf{r}_{j}\right) \cdot \nabla\right)^{2} \rho\left(\mathbf{r}_{j}\right) / 2\right) \mathrm{d} \sigma^{\prime}}{\left|\mathbf{r}^{\prime}-\mathbf{r}_{i}\right|^{3}} \\
+\int_{S_{j}} \frac{\left(\rho\left(\mathbf{r}^{\prime}\right)-\rho\left(\mathbf{r}_{j}\right)-\left(\left(\mathbf{r}^{\prime}-\mathbf{r}_{j}\right) \cdot \nabla\right) \rho\left(\mathbf{r}_{j}\right)-\left(\left(\mathbf{r}^{\prime}-\mathbf{r}_{j}\right) \cdot \nabla\right)^{2} \rho\left(\mathbf{r}_{j}\right) / 2\right) \mathrm{d} \sigma^{\prime}}{\left|\mathbf{r}^{\prime}-\mathbf{r}_{i}\right|^{3}} . \tag{13}
\end{gather*}
$$

The terms in the first integral on the right hand side can be evaluated analytically [13]. The second integral, which does not appear in [13], has a continuous integrand and can be evaluated using a quadrature rule. We use adaptive 16 -point Gauss-Legendre quadrature.

## 4 Results and error estimates

The maximum value of the stress intensity factor will occur at the mid-points of the square sides. We denote by $F_{\max }(1 / N)$ the maximum stress intensity factor computed on an $N \times N$ mesh. Using (5), (9), and (11) we obtain

$$
\begin{equation*}
F_{\max }(1 / N)=(1 / 2)^{(2 \lambda-1)} \omega(x=0.5-0.5 / N, y=0) . \tag{14}
\end{equation*}
$$

Then we compute $F_{\max }$ as the limit

$$
\begin{equation*}
F_{\max }=\lim _{N \rightarrow \infty} F_{\max }(1 / N) . \tag{15}
\end{equation*}
$$

We use eight meshes ranging from $N=29$ to $N=99$, interpolate $F_{\max }(1 / N)$ with a seventh degree polynomial, and estimate $F_{\max }$ by extrapolation.


Figure 3: Estimates for the density $\omega$, related to the crack opening displacement via (2) and (11), for a unit square crack under unit normal load. The left plot refers to corner singularity $\lambda=$ 0.81465 . The density $\omega$ only varies a few per cent over the area of the square. The right plot refers to corner singularity $\lambda=1$. Note that $\omega$ diverges in the corners.

Our estimate of the maximum stress intensity factor is $F_{\max }=0.7534 \pm 0.0002$, see Figure 2. We consider three sources of errors for our computation of $F_{\max }(1 / N)$ in (14): The discretization error, the error in the computation of the matrix elements via (13), and the error in the GMRES solver. In addition, for computing $F_{\max }$ in (15) we need to consider the truncation error and the extrapolation error.

The discretization error for pointwise values of $\omega$ behaves like $1 / N$. This is so since our regularization lowers the order of the composite midpoint rule. The quadrature error of $F_{\max }(1 / N)$ close to the boundary has a better behavior, see Figure 2.

The absolute error in the computation of the individual matrix elements, due to the adaptive quadrature, is estimated to be at most $10^{-7}$. The dominating effect of this error in the values for $F_{\max }(1 / N)$ seems to be a term independent of $N$. The magnitude of this error term in $F_{\max }(1 / N)$ is estimated to $5 \times 10^{-7}$.

The error from the GMRES iterative solver is negligible. This is explained by the low condition number, estimated to be less than 100.

The truncation error in the limiting process of (15) depends on the choice of corner singularity $\lambda$ in the weight function $\rho$. Figure 2 shows that the computations involving the incorrect singularity $\lambda=1$ converge faster than the computations involving the more correct singularity $\lambda=0.81465$. The same behavior for $\lambda=1$ can be discerned in Figure 3 of Isida, Yoshida, and Noguchi [10]. A quadratic, rather than linear, fit to the data of these authors would decrease their extrapolated estimate. That $\lambda=1$ gives a locally better weight function at $\mathbf{r}=(0.5,0)$ than $\lambda=0.81465$ is further illustrated in Figure 3.

The extrapolation error is the dominating error in our calculations. By extrapolation error we mean the aggregate effect of truncating the interpolation at seventh order and the amplification of various errors in $F_{\max }(1 / N)$ due to the extrapolation. By experimental perturbation analysis we estimate the extrapolation error in $F_{\max }$ to be about $10^{-4}$.

The variation of the stress intensity factor along the side of the crack is presented in Figure 4. The results were obtained using the corner singularity $\lambda=0.81465$ and $99 \times 99$


Figure 4: Variation of the normalized stress intensity factor $F$ along the side of a square crack. The results of the previous authors were obtained from graphs in [10, 11, 13]
discretization points. The relative error is estimated to be less than $0.5 \%$. The results presented by previous authors agree in principle with the present, more accurate, results.

## 5 Conclusions

Virtually all attempts to compute $F$ for a planar square crack in the literature are based on hypersingular integral equations. We conclude that previous estimates have been overoptimistic in terms of precision. What has been lacking is chiefly error analysis.

The problem of computing $F$ is well-conditioned. High accuracy could, theoretically, be achieved. Better algorithms could include the use of a non-uniform mesh, higher order basis functions, and preconditioning involving an analytical inverse such as (8).

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