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# On Cauchy singular integrals and stress intensity factors for 2D mode I cracks in an infinite solid

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**Abstract**

This paper comments on some of the different numerical techniques commonly employed in evaluating Cauchy singular integrals of the first kind; e.g. as pertaining to 2D through cracks in a brittle material undergoing Mode I loading. In addition, a different more direct method is proposed here. Also, two different ways to calculate the stress intensity factor ($K_I$) are contrasted. The accuracy attained by the different methods in calculating $K_I$, and the factors affecting the calculation, are compared. Finally, comments on calculating the stress field of a 2D crack and important considerations are presented.


*Keywords:* Modeling; Crack stresses; Dislocation–crack interaction

## 1. Introduction

Fracture mechanics is an ever-growing science due to its important practical aspects. Not surprisingly therefore, researchers have given a lot of attention to the solution of a variety of cracks problems of different geometry and under a variety of loading modes. One of the earliest and more fundamental problems in fracture mechanics is that of determining the stress field associated with the presence of a 2D through crack in a brittle material subjected to Mode I crack opening. A related problem is that of accurately determining the stress intensity factor ($K_I$) at the tip of the crack. $K_I$ is a fundamental quantity in fracture mechanics as it is characteristic of the stresses of a certain crack (i.e. geometry), in the near tip region, and under certain load distribution (Hills et al., 1996). The value of $K_I$ also governs crack propagation and its accurate determination is strongly desirable.

In dealing with 2D crack problems under Mode I loading (or shearing Mode II for that matter) a Cauchy singular integral of the first kind arises in the formulation whose integrand is not all known (part of it is) but yet its determination is desired. Once the unknown part (called "the regular part of the dislocation density function") of the integrand is determined, $K_I$ can be calculated from it as will be discussed later.

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Also, the crack stresses can be calculated using such solution. The integrand is singular at both crack ends and at interior points along the crack. The evaluation of such integrals has stimulated much good work on devising numerical collocation methods or schemes for this purpose. In subsequent sections, the use of these methods in determining $K_I$ is presented. For example, it will be shown that increasing the number of collocation points is not necessarily always desirable as intuitively might be thought. In addition, a different more direct, and somewhat simpler, method for the evaluation of Cauchy singular integrals is presented.

The factor $K_I$ can be determined via two routes; one involves a numerical limiting procedure and the other relates $K_I$ directly to the crack displacement gradient at the tip (see Eq. (2.22) of Hills et al., 1996). In the latter definition, $K_I$ turns out to be directly calculable if the sought regular part of the dislocation density function (see last paragraph) is known at the tips. Here, we comment on the two routes for finding $K_I$ and how the second routes' accuracy is affected by the peculiarities and special features of the method used in the singular integral evaluation.

Once the regular part of the dislocation density function is determined, it will be possible to calculate the stresses due to the presence of the loaded crack (see below). A knowledge of these stresses is very important, especially for interaction problems where a crack can interact with other defects in the material. For example, multiple cracks interact through their stress fields thus driving or inhibiting the growth of one another or causing the generation of microcracks (see, e.g., Demir and Zbib, 2001). Other possibilities would be the interaction of a crack with a dislocation(s), as the crack stress field will enter into the calculation of the Peach–Koehler force acting on the dislocation, which in turn causes it to glide (Demir and Gulluoglu, 1999). Recently, attention has been given to interaction problems of a dislocation(s) with crystal defects in the context of emerging dislocation dynamics simulations (Khraishi, 2000). The importance here lies in the fact that the dislocation (through its motion) represents the fundamental plastic deformation mechanism in crystalline solids. Hence, it is important to account for its interaction with other defects in the solid (such as cracks), which could affect the dynamics of its motion.

There are a few ways to evaluate Cauchy singular integrals in the literature. The most commonly used method is perhaps the Gauss–Chebyshev (GC) quadrature used by Erdogan and Gupta (1972) and Erdogan et al. (1973). Theocaris and Ioakimidis (1977) considered an alternative method; the Lobatto–Chebyshev (LC) quadrature. Gerasoulis and Srivastav (1981) developed a piece-wise linear polynomial method and Gerasoulis (1982) developed a piece-wise quadratic polynomial method. Results from the above methods are compared below. Demir et al. (1992) applied a collocation method to solve singular integral equations arising in cylindrical crack problems. Their technique has resemblance to a weighted residual method. Kurtz et al. (1994) presented a piece-wise polynomial method for evaluating Cauchy integrals of the first and second kinds. Other notable methods for solving singular integral equations include the Galerkin–Petrov method, which is based on the use of two sets of orthogonal polynomials (Elliott, 1983), the Galerkin–Bubnov method, which was used by Nazarenko (1986) to numerically solve the problem of sub-surface cracks in a half-space subjected to compression. Finally, the works of Rathsfeld (2000), Junghanns and Silbermann (2000) and Monegato and Prössdorf (1993), and their co-workers, among others, provided careful convergence and numerical analysis studies of some previously known methods for solving singular integral equations. It has to be emphasized here that the above list of methods used in solving singular integral equations is not comprehensive and other equally-worthy methods exist in the literature. The current study is a *focus* study on some of the available and common methods that tries to put them in context, with regard to advantages and disadvantages, something that is typically lacking in other works.

In summary therefore, this paper comments on some of the different methods used to evaluate Cauchy singular integrals, and any associated peculiarities, as pertaining to the determination of $K_I$ at the crack tips. It contrasts the results from these method with another more direct method presented here. In addition, the calculation of $K_I$ through numerical limiting is examined. Finally, points pertaining to the calculation of crack stresses are made especially in relation to interaction problems with other defects.

## 2. The Cauchy singular integral

Consider a 2D through crack of length $2a$ lying in a brittle material and to which an $xy$ coordinate system is attached as shown in Fig. 1. The origin of this system is fixed to the crack's midpoint and the crack extends from $x = -a$ to $x = +a$. The $r$ and $\theta$ are polar coordinates centered at the crack tip. The crack is subjected to remotely applied tensile loading, $\sigma_{yy}^{\infty}(x, y = 0)$, normal to its face.

We here briefly review the solution of such a crack problem using the distributed dislocation method (Hills et al., 1996). This problem can be treated as a perturbation problem whereas the stress state at any field point $P$ in the elastic medium is obtained via the linear superposition of the remote stress field and a corrective solution that satisfies the boundary conditions (BCs) of the problem. A self-consistent method to generate the corrective solution is to consider it due to a continuous distribution of dislocations (each with a Burgers vector in the $y$-direction, $\delta b_y$). Fig. 1 shows one such dislocation at a distance $\xi$. Of course the insertion of such fictitious dislocations will provide us with crack opening as expected from the loading. Also, since the stress field of such dislocations decays as $1/d$, where $d$ is the distance from the dislocation core, the stress field at infinity equals only that of the remotely applied stresses as physically conceived. Finally (last BC for the problem), these dislocations provide us with extra or auxiliary stress terms to annul the undesired tractions created on the crack face by the applied stresses.

Since we have a distribution of dislocations, we can define, for the interval between any two consecutive points $\xi$ and $\xi + \delta\xi$ along the crack, a dislocation density function $B_y(\xi)$ such that $B_y(\xi) = \delta b_y/\delta\xi$. Now, the above statements on annulling traction at any point $x$ between the tips can be stated mathematically as follows:

$$-\sigma_{yy}^{\infty}(x, 0) = \int_{-a}^{+a} \frac{2\mu}{\pi(\kappa + 1)} \frac{\mathrm{d}b_y}{x - \xi}, \quad |x| < a. \tag{1}$$

The integrand in the above equation represents the stress in the $y$-direction at a point $x$ along the crack, due to a dislocation situated at point $\xi$ whose Burgers vector is $\delta b_y$ (see Hills et al., 1996). $\mu$ is the shear modulus, and $\kappa$ is Kolosov's constant defined as $(3 - 4v)$ and $(3 - v)/(1 + v)$ for plane strain and plane stress conditions, respectively, where $v$ is Poisson's ratio. In all of the calculations below, a state of plane strain was assumed. Taking the constants out, and replacing $\delta b_y$ by $B_y(\xi)\delta\xi$, the $(x - \xi)^{-1}$ term left in the integrand in (1) is called the "kernel" of the integral. It is obvious that this kernel, and thus the integral, is

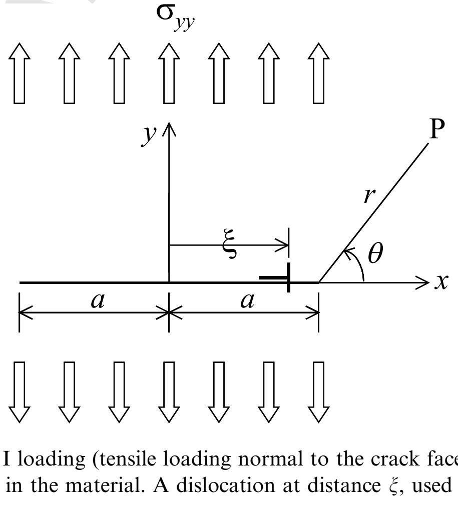


Fig. 1. A 2D through crack under Mode I loading (tensile loading normal to the crack face). The crack's plane is $y = 0$ and extends from $-a < x < a$. Point $P$ is a field point in the material. A dislocation at distance $\xi$, used in the solution, is also shown.

singular when $x = \xi$. Such an integral is called a "Cauchy singular integral" and the whole equation is called a "singular integral equation" that needs to be solved for the unknown function $B_y(\xi)$.

It is easier and more standard to non-dimensionalize the last equation using the substitutions $s = \xi/a$ and $t = x/a$. This allows us to write the last equation as

$$-\frac{\kappa+1}{2\mu}\sigma_{yy}^{\infty}(t,0) = \frac{1}{\pi}\int_{-1}^{+1} B_y(s)\frac{1}{t-s}\,\mathrm{d}s, \quad |t|<1. \tag{2}$$

Furthermore, the dislocation density function can be decomposed into two parts: an unknown function $\phi_y(s)$, called "the regular part of the density function", and a known function $w(s)$, called the "fundamental solution", such that $B_y(s)$ is their product, i.e.,

$$B_y(s) = w(s)\phi_y(s), \tag{3}$$

where $w(s) = 1/\sqrt{1-s^2}$.

The form of the fundamental solution follows from asymptotic analysis (see Hills et al., 1996) and builds into the solution the required singular behavior of a sharp crack at its tips (i.e. $s = \pm 1$). This form of $B_y(s)$ is substituted into Eq. (2) above before any further steps towards a solution are attempted.

There is yet another physical condition imposed on the problem above, and that is of *no net dislocation* as one circles around the crack in a closed loop. Mathematically, this translates to the following so-called side or closure condition:

$$\int_{-a}^{+a} B_y(\xi)\,\mathrm{d}\xi = \int_{-1}^{+1} B_y(s)\,\mathrm{d}s = 0. \tag{4}$$

Now, numerical schemes available for solving the above-listed Cauchy singular equation (2) consist of satisfying it on a set of collocation points $t_k$s (where $k = 1,\ldots,N-1$) along the crack line. The unknown here are the values, or nodal values, of the function $\phi_y(s_i)$ (where $i = 1,\ldots,N$) for a set of $N$ nodal (or integration) points, $s_i$'s, along the crack that are *different* from the collocation points, and to each of which there is assigned a weight, $W_i$. Thus, the Cauchy singular integral on the right-hand side of Eq. (2), *including* the $1/\pi$ factor, is converted to an algebraic summation over the nodal points, and the whole equation is equivalent to a system of equations, each of which corresponding to a collocation point, as follows:

$$\sum_{i=1}^{N} W_i\frac{\phi_y(s_i)}{t_k - s_i} = -\frac{\kappa+1}{2\mu}\sigma_{yy}^{\infty}(t_k,0), \quad k = 1,\ldots,N-1, \tag{5}$$

where the weights, $W_i$'s, are a function of the points, $s_i$'s (or index $i$). For the GC method, $W_i = 1/N$ for $i = 1,\ldots,N$. For the LC method, $W_i = 1/(2N-2)$ for $i = 1$ or $N$, and $W_i = 1/(N-1)$ for any other $i$. The $s_i$'s and $t_k$'s are also a function of position, or their index. For GC, $s_i = \cos(\pi(2i-1)/(2N))$ for $i = 1,\ldots,N$. For LC, $s_i = +1$ for $i = 1$, $-1$ for $i = N$, and $\cos(\pi(i-1)/(N-1))$ for any other $i$. Finally, $t_k = \cos(\pi k/N)$ for GC and $\cos(\pi(2k-1)/(2N-2))$ for LC, for $k = 1,\ldots,N-1$. For the method by Gerasoulis (1982), Gerasoulis (G) method, the ensuing system of equations looks similar to (5) above without the kernel term in the summation or the minus sign on the right-hand side, and with the weights given by lengthier expressions and thus are not provided here. Such an algebraic description of the Cauchy integral (Eq. (2)) is attained by assuming a functional form for $\phi_y$. This form is typically a continuous, or piece-wise continuous, polynomial.

Finally, the side condition (Eq. (5)) also reduces to an algebraic equation of the form:

$$\sum_{i=1}^{N} \lambda_i\phi_y(s_i) = 0, \tag{6}$$

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where $\lambda_i = +1$ for the GC method. For the LC method, $\lambda_i = +1/2$ for $i = 1$ or $N$, and +1 for any other $i$. For the G method, the reader is referred to Gerasoulis (1982) for lengthier $\lambda_i$ expressions.

The set of equations (5) and (6) represent a system of $N$ linear algebraic equations in $N$ unknowns which can be solved, via computer programming, using the solver of choice (e.g. Gauss elimination) for the unknown $\phi_y$ nodal values.

We now present an alternative more direct method for solving the Cauchy integral equation (2). In this method, we divide the crack length into a number of $N$ intervals or elements, and assume that the unknown function $\phi_y$ is piece-wise linear over each element, i.e. it can be represented by a Lagrange linear interpolation polynomial. Hence for any element $i$, $\phi_y$ can be expressed as

$$\phi_y(s) = \left(\frac{s_j - s}{L^i}\right)\mathbf{\Phi}_i + \left(\frac{s - s_i}{L^i}\right)\mathbf{\Phi}_j, \tag{7}$$

where $\mathbf{\Phi}_i$ and $\mathbf{\Phi}_j$ are the two unknown, and yet to be determined, nodal end points of element $i$, and $L^i = s_j - s_i$ is the element length. We will therefore have a total of $N + 1$ unknown nodal values over the crack length.

The integral in (2), call it $I$, after substitution of (3) into it, can be written, *without* approximation, as follows:

$$I = \sum_{i=1}^{N} I^i = \sum_{i=1}^{N} \int_i \phi_y(s)\left(\frac{1}{\sqrt{1-s^2}}\right)\left(\frac{1}{t-s}\right)\mathrm{d}s, \tag{8}$$

where $I^i$ is the elemental integral, or contribution of element $i$.

Furthermore, substituting approximation (7) into the expression for $I^i$, we get an approximate expression for $I^i$ as follows (noting that $\mathbf{\Phi}_i$ and $\mathbf{\Phi}_j$ are constants):

$$I^i = \left[\int_{s_i}^{s_j}\left(\frac{s_j - s}{L^i}\right)\left(\frac{1}{\sqrt{1-s^2}}\right)\left(\frac{1}{t-s}\right)\mathrm{d}s\right]\mathbf{\Phi}_i + \left[\int_{s_i}^{s_j}\left(\frac{s - s_i}{L^i}\right)\left(\frac{1}{\sqrt{1-s^2}}\right)\left(\frac{1}{t-s}\right)\mathrm{d}s\right]\mathbf{\Phi}_j. \tag{9}$$

We will call the first integral in the last equation $I1^i$ and the second integral $I2^i$. Note that the superscript $i$ here still references element $i$'s contribution(s).

Now the problem resides in integrating $I1^i$ and $I2^i$ both of which are singular integrals within their interval or element, due to the kernel term, whenever $t = s$ in the interval. The strategy here is as before, we would like to satisfy the Cauchy integral equation (2) in a point-wise fashion by evaluating the elemental singular integrals at some collocation point, $t_i$, within the element. We can parameterize the location of collocation point $t_i$ within element $i$ using the following relation:

$$t_i = s_i + qL^i, \tag{10}$$

where $i = 1, \ldots, N$, and the parameter $q$ is in the range $0 < q < 1$. For simplicity of the discussion we will pick $q = 0.5$ for now, so that the collocation point is at the center of each element. Once this is decided and in order to evaluate $I1^i$ and $I2^i$ in (9), one simply needs to pick integration points that are *not* coincident with, i.e. *different* from, the element's center or midpoint. This is facilitated, for example, through the use of a Gauss–Legendre integration formula having an *even* number of integration or Gaussian points, $N_g$ (see Chapra and Canale, 1998). The reason for picking formulas with even as opposed to odd number of integration points is that the former points avoid the singularity at the element's center whereas the latter collapse on it by default. It will be shown later that because integrals $I1^i$ and $I2^i$ are highly non-linear, a relatively large number of integration points in the Gauss–Legendre formula will be needed in order to achieve highly accurate estimates of the integrals. As it turns out, this will not have a significant negative impact on the computational effort involved.

We now apply a similar procedure as above to the side or closure condition, Eq. (4). Here, we call the integral in (4) $J$ and immediately write:

$$J = \sum_{i=1}^{N} J^i = \sum_{i=1}^{N} \int_i \phi_y(s)\left(\frac{1}{\sqrt{1-s^2}}\right)\mathrm{d}s, \tag{11}$$

where the $J^i$'s are elemental integrals. Now substituting (7) into $J^i$, we get:

$$J^i = \left[\int_{s_i}^{s_j}\left(\frac{s_j - s}{L^i}\right)\left(\frac{1}{\sqrt{1-s^2}}\right)\mathrm{d}s\right]\mathbf{\Phi}_i + \left[\int_{s_i}^{s_j}\left(\frac{s - s_i}{L^i}\right)\left(\frac{1}{\sqrt{1-s^2}}\right)\mathrm{d}s\right]\mathbf{\Phi}_j. \tag{12}$$

Calling the first integral in (12) $J1^i$ and the second integral $J2^i$, it is possible to evaluate both using a Gauss–Legendre integration formula just as before. And since these integrals do *not* contain a singular kernel, they are well-behaved and either a *small* even or odd number of integration points suffices for accurately estimating them.

Finally, applying Eq. (8), with (9), $N$ times (once for each collocation point $t_k$, $k = 1, \ldots, N$, see (10)) and combining with them Eqs. (11) and (12), one obtains a system of $N+1$ linear algebraic equations in $N+1$ unknowns (the $\mathbf{\Phi}$ nodal values), which can be conveniently solved using the solver of choice on a computer. Note that if one expresses such ensuing system in matrix form as $[A]\{\mathbf{\Phi}\} = \{B\}$, where $[A]$ is a coefficient matrix, $\{B\}$ is a forcing-like vector, and $\{\mathbf{\Phi}\}$ is the solution vector, then the following applies to the $i$th equation, where $i = 1, \ldots, N$:

$$A(i,k) = \begin{cases} I1^k(t_i), & k = 1, \\ I2^{k-1}(t_i) + I1^k(t_i), & k = 2, \ldots, N, \\ I2^k(t_i), & k = N \end{cases} \tag{13}$$

and

$$B(i) = -\pi\frac{(\kappa+1)}{2\mu}\sigma_{yy}^{\infty}(t_i, 0). \tag{14}$$

And for the $(N+1)$th equation, we have

$$A(N+1,k) = \begin{cases} J1^k, & k = 1, \\ J2^{k-1} + J1^k, & k = 2, \ldots, N, \\ J2^k, & k = N \end{cases} \tag{15}$$

and

$$B(N+1) = 0, \tag{16}$$

where in the above the notation $(t_i)$ means evaluated at $t_i$.

It is appropriate here to comment on the error involved in determining the $I$ and $J$ integrals (e.g. Eqs. (9) and (12)) in the method presented here. Since these integrals are evaluated using a Gauss–Legendre formula, the true error, $E_t$, involved in the evaluation is given by (Carnahan et al., 1969) to be

$$E_t = \frac{2^{2n+3}[(n+1)!]^4}{(2n+3)[(2n+2)!]^3} f^{(2n+2)}(\xi), \tag{17}$$

where $n = N_g - 1$, and $f$ is the function in the integrand, and $f^{(2n+2)}(\xi)$ is the $(2n+2)$th derivative of the function after the change of variable with $\xi$ located somewhere on the interval from −1 to 1. Without going into a very rigorous mathematical proof procedure, it will be seen later on (see Table 2), that the error resulting from Eq. (17) is inversely proportional to the number of Gaussian or integration points $N_g$.

## 3. The stress intensity factor $K_I$

The accuracy of the above methods for solving the Cauchy singular equation will now be contrasted based on their estimates of the $K_I$ value for the crack, for loading cases with known analytical solutions. We mentioned earlier that there are two common ways to calculate $K$I for a crack. One of these consists of a numerical limiting procedure where $K_I$ is defined as (see, e.g., Hills et al., 1996):

$$K_I = \lim_{r\to 0} \sqrt{2\pi r}\sigma_{yy}(r, \theta = 0), \tag{18}$$

where the parameters $r$ and $\theta$ are defined in Fig. 1, and the $\sigma_{yy}$ here represents the *combined* stress due to both external loading and the crack field (and is given in Eq. (22) below).

This method, however, of calculating $K_I$, albeit correct, turns out to be a not so accurate method for the calculation and special care should be taken in interpreting the results. More detailed comments on this method will be presented later on. First though, we present a different method that is less prone or sensitive to calculation errors, and which can be used to contrast the methods presented in Section 2 for solving the Cauchy singular equation.

Hills et al. (1996) show that for the Mode I crack, $K_I$ at $s = \pm 1$ can be precisely described using the following formula:

$$K_I(s = \pm 1) = \pm\sqrt{\pi a}\frac{2\mu}{(\kappa + 1)}\phi_y(s = \pm 1). \tag{19}$$

Since the methods above (Section 2) can all provide estimates of the $\phi_y$ $(s = \pm 1)$ values, as part of the solution procedure, one can use these estimates to compare the relative accuracy of the methods and how they perform against benchmark analytical solutions.

To find the value of $\phi_y$ $(s = \pm 1)$ using the GC method, one needs to interpolate via the Krenk's interpolation formula (Krenk, 1975), for example. Note that interpolation potentially adds to the error in the numerical solution of the problem. In the methods of LC, G and the method of this paper, no interpolation is necessary and the values of $\phi_y$ $(s = \pm 1)$ correspond to the nodal value solutions at the crack tips.

The most intuitive and trivial comparison to make between the methods is to test them against the analytical solution for the case when the external stress or loading is uniform across the crack length (i.e. $\sigma_{yy}^{\infty}(x, 0) = p$). Here and in all what follows, $p$ was set arbitrarily to 100 MPa. The exact analytical solution in this case is known to be $K_I(x = +a) = p\sqrt{\pi a}$. For simplicity, the quantity $a$ is taken to be of unit length in all what follows, which basically has the effect of treating $x$ as the non-dimensional variable $s$. We now define our measure of error as $\varepsilon_t$, called the true percent relative error, and given as

$$\varepsilon_t = 100 \times |(K_I^{th} - K_I^{calc})/K_I^{th}|, \tag{20}$$

where $K_I^{th}$ and $K_I^{calc}$ are the theoretical and calculated values of the stress intensity factor, respectively.

In the above simple loading case, the methods of GC, LC, and G all give excellent results even for a very small number of collocation points ($N_c$). For example, using $N_c = 4$, $\varepsilon_t$ for the above methods is 9.92E−6, 2.8E−5, 9.92E−6, respectively. As one can see, all of these methods give essentially the same result for this simple case (basically zero error) and there is no advantage for using one method over the other. In addition, no advantage is gained by increasing $N_c$. On the contrary, relatively large $N_c$ values result in *greater* $\varepsilon_t$'s due to increased round-off errors (i.e. limited computer precision) in solving the system of equations. For example, for $N_c = 200$, the errors are 0.05, 0.054, and 0.33, respectively, and for $N_c = 800$, the errors are 0.3, 1.44, 0.66, respectively.

For the simple case discussed above, the method presented in this paper does not perform as well in determining the $K_I$ value. This is mainly due to the tortuosity and high non-linearity of integrals $I1^i$ and $I2^i$. Here, however, the error can be reduced significantly by using higher order Gauss–Legendre formulas (i.e. a larger number of integration or Gaussian points, $N_g$) in estimating these integrals. Abramowitz and Stegun (1964) list tables of Gaussian integration points for large $N_g$'s. Table 1 shows that, for the current method, $\varepsilon_t$ decreases with increasing $N_g$. However, increasing $N_c$ ($=$N in the current method, see Eqs. (8) and (11)) does not necessarily reduce $\varepsilon_t$ as explained earlier.

The method has one more degree of freedom that allows better estimation of $K_I$. In Eq. (10), if one picks a $q$ value different from 0.5, it is possible to eliminate errors. For example, for $N_c = 30$ and $N_g = 6$, the error $\varepsilon_t$ reduces to 0.032 if one chooses $q$ as 0.505. This extra control provided by the $q$ parameter in this paper is similar to work done by Schmidt (1986) utilizing what is called "ε-collocation".

Now, consider a different loading case from above, where the applied stress can be described as

$$\sigma_{yy}^{\infty}(x, 0) = p(1 - |x|/a). \tag{21}$$

The theoretical $K_I$ value here is given by Tada et al. (2000) as $(1 - 2/\pi)p\sqrt{\pi a}$. For this case where the applied stress gradient is discontinuous at $x = 0$ but the stresses themselves are well-behaved, we plot $\varepsilon_t$ versus $N_c$ in Fig. 2 for the GC, LC, and G methods. We clearly observe violent oscillations in the GC and LC methods. For example, for $N_c = 29$, the error for the GC method is 0.64 (off limits in figure). This error jumps down to 0.044 for $N_c = 34$ and jumps up again to 0.18 for $N_c = 39$. The same applies to the other two methods. For example, for $N_c = 40$, the error for the G method is 0.02 and jumps to 0.153 for $N_c = 50$ and sharply falls again to 0.006 for $N_c = 70$. It is observed however, as supported somewhat in Fig. 2, that the G method, in general, suffers from fewer oscillations. The reason for this is that it assumes a piecewise representation of $\phi_y$ (see Eq. (7) for example) whereas the other two methods use polynomial interpolation over the whole crack length. As generally accepted, piecewise interpolation should induce lesser oscillations in the solution compared to polynomial interpolation (see, e.g., Chapra and Canale, 1998). Based on such an argument, it is expected here that the current method, which is based on piecewise interpolation of $\phi_y$, will also be less susceptible to oscillations, similar to the G method. Indeed, this is what is observed. For example, if $q = 0.5$ and $N_g = 48$, the errors will be 1.45, 1.28, and 1.17 for $N_c$ values of 20, 30, and 50, respectively. Here, the method exhibits stability and decreasing errors with increasing $N_c$. The above comments can be generalized to even more abrupt loading cases than in (21). It is therefore preferable to use a method utilizing piecewise interpolation of $\phi_y$ when estimating $K_I$ via Eq. (19) over one that utilizes polynomial interpolation over the whole crack length. For smooth variations of the applied stresses over the crack face, any of the above-discussed methods would be suitable.

Table 1
The true percent relative error $\varepsilon_t$ in determining $K_I$ value, using the current method, for different $N_g$ (number of Gaussian integration points) and $N_c$ (number of collocation points) values

| $N_g$ | $\varepsilon_t$ | | | |
|---|---|---|---|---|
| | $N_c = 10$ | $N_c = 20$ | $N_c = 30$ | $N_c = 50$ |
| 2 | 27.2007 | 27.3739 | 27.4326 | 27.4773 |
| 4 | 13.7861 | 13.8738 | 13.9042 | 13.9243 |
| 6 | 9.18857 | 9.24521 | 9.26509 | 9.27673 |
| 8 | 6.88741 | 6.92884 | 6.94391 | 6.95015 |
| 10 | 5.50711 | 5.53911 | 5.55166 | 5.55445 |
| 12 | 4.58749 | 4.61369 | 4.62425 | 4.62430 |
| 16 | 3.43856 | 3.45686 | 3.46505 | 3.46108 |
| 20 | 2.74986 | 2.76332 | 2.77000 | 2.76292 |
| 24 | 2.29085 | 2.30092 | 2.30731 | 2.29591 |
| 32 | 1.71753 | 1.72281 | 1.72941 | 1.71421 |
| 40 | 1.37364 | 1.37577 | 1.38165 | 1.36187 |
| 48 | 1.14438 | 1.14302 | 1.15107 | 1.12490 |

Here, $q = 0.5$ in Eq. (10).

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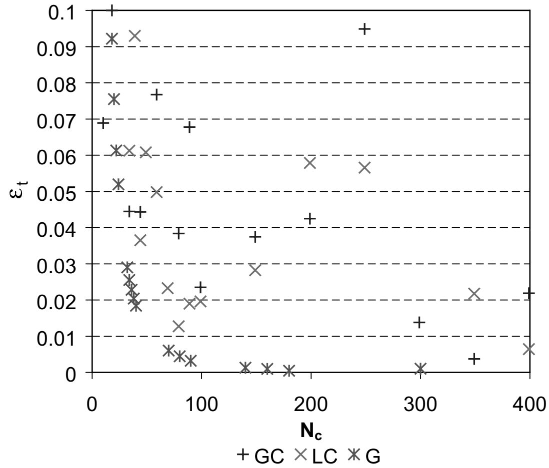


Fig. 2. A plot of the error $\varepsilon_t$ in estimating $K_I$, for a crack subjected to the loading in Eq. (21), versus the number of collocation points $N_c$, used in the Gauss–Chebyshev (GC), Lobatto–Chebyshev (LC), and Gerasoulis (G) methods.

Now regarding the estimation of $K_I$ values via the numerical limiting procedure in (18), we revert back to the example of uniformly applied stress $p$ from before. Here, we limit ourselves to the GC method to illustrate the concepts. If one plots the variation of the ratio $K^{calc}/K^{th}$ versus $r$ for $\theta = 0$ in Fig. 1, we obtain Fig. 3. Here, we dropped the subscript I from $K^{calc}$ and $K^{th}$ since we are only considering Mode I in this paper. In this figure, it is seen that, for any given $N$ in (5), as we approach the crack tip at $r/a = 0$, the ratio of stress intensity factors decreases in value passing through the ideal ratio of unity at some distance ahead of the tip. To approach the tip such that the ratio converges to unity, which is the definition of the limit in (18), one basically needs to indefinitely increase the $N$ value (i.e. solve a much bigger system of equations). Although this result might not come at a great surprise, it illustrates nonetheless the point that Eq. (18) provides us with an inaccurate and expensive way for determining the $K_I$ value at a crack tip. Instead, it is much better as was illustrated earlier to utilize definition (19) for such determination.

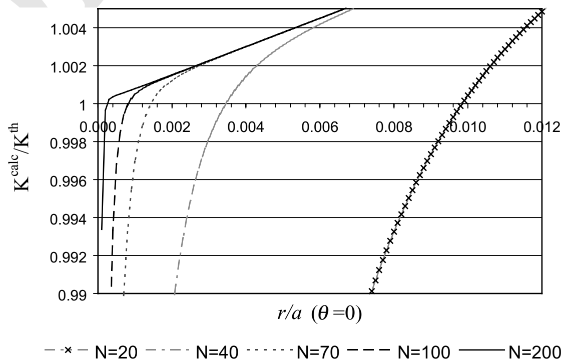


Fig. 3. A plot of $K^{calc}/K^{th}$ versus $r/a$ ratio in Fig. 1 for a Mode I crack (subjected to uniform tensile stress $\sigma_{yy}^{\infty}(x, 0) = p$), for different $N$ values in (5) and (6). Here, $K^{calc}$ is obtained from the GC method and $K^{th} = p\sqrt{\pi a}$.

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## 4. The stress field of 2D cracks

One of the main goals of determining the dislocation density distribution via one of the previously discussed methods, besides the determination of $K_\mathrm{I}$ value, is to use it to determine the crack stress field. To this end, to determine any planar component of stress at a field point, we need to sum up the contributions of the infinitesimal dislocations distributed along the crack. Since our dislocation density function $B_y(s)$ is continuous along the crack face, the summation becomes an integral. The planar crack stresses therefore become

$$\begin{aligned}
\sigma_{xx}(x,y) &= \frac{2\mu}{\pi(\kappa+1)}\int_{-a}^{+a} B_y(\xi)\frac{x-\xi}{r^4}[(x-\xi)^2-y^2]\,\mathrm{d}\xi,\\
\sigma_{yy}(x,y) &= \frac{2\mu}{\pi(\kappa+1)}\int_{-a}^{+a} B_y(\xi)\frac{x-\xi}{r^4}[(x-\xi)^2+3y^2]\,\mathrm{d}\xi+\sigma_{yy}^{\infty}(x),\\
\sigma_{xy}(x,y) &= \frac{2\mu}{\pi(\kappa+1)}\int_{-a}^{+a} B_y(\xi)\frac{y}{r^4}[(x-\xi)^2-y^2]\,\mathrm{d}\xi,
\end{aligned} \tag{22}$$

where $r^2=(x-\xi)^2+y^2$ Note that for any field point $P$ at $(x,y)$, not lying on the crack face, the integrands in (22) are well-behaved and none is singular.

Since the methods of Section 2 rely on discretizing the $B_y(s)$ function, the discretized form of equations (22) is

$$\sigma_{xx}(x=at,y)=\frac{2\mu}{\kappa+1}\frac{1}{N}\sum_{i=1}^{N}\phi_y(s_i)\frac{(t-s_i)[(t-s_i)^2-(y/a)^2]}{[(t-s_i)^2+(y/a)^2]^2}, \tag{23}$$

$$\sigma_{yy}(x=at,y)=\frac{2\mu}{\kappa+1}\frac{1}{N}\sum_{i=1}^{N}\phi_y(s_i)\frac{(t-s_i)[(t-s_i)^2+3(y/a)^2]}{[(t-s_i)^2+(y/a)^2]^2}+\sigma_{yy}^{\infty}(at), \tag{24}$$

$$\sigma_{xy}(x=at,y)=\frac{2\mu}{\kappa+1}\frac{1}{N}\sum_{i=1}^{N}\phi_y(s_i)\frac{(y/a)[(t-s_i)^2-(y/a)^2]}{[(t-s_i)^2+(y/a)^2]^2}. \tag{25}$$

The discretized forms, Eqs. (23)–(25), are provided here for the GC method. For the LC method, similar expressions can be obtained. Finally, for the current method, we can list the following after forgoing some details:

$$\begin{aligned}
\sigma_{yy}(x=at,y) &= \frac{2\mu}{\pi(\kappa+1)}\sum_{i=1}^{N} I_{yy}^{i}+\sigma_{yy}^{\infty}(at),\\
\sigma_{xy}(x=at,y) &= \frac{2\mu}{\pi(\kappa+1)}\sum_{i=1}^{N} I_{xy}^{i},
\end{aligned} \tag{26}$$

where

$$\begin{aligned}
I_{yy}^{i} &= \left[\int_{s_i}^{s_j}\frac{s_j-s}{L^i}\frac{t-s}{\sqrt{1-s^2}}\frac{(t-s)^2+3(y/a)^2}{[(t-s)^2+(y/a)^2]^2}\mathrm{d}s\right]\mathbf{\Phi}_i+\left[\int_{s_i}^{s_j}\frac{s-s_i}{L^i}\frac{t-s}{\sqrt{1-s^2}}\frac{(t-s)^2+3(y/a)^2}{[(t-s)^2+(y/a)^2]^2}\mathrm{d}s\right]\mathbf{\Phi}_j,\\
I_{xy}^{i} &= \left[\int_{s_i}^{s_j}\frac{s_j-s}{L^i}\frac{y/a}{\sqrt{1-s^2}}\frac{(t-s)^2-(y/a)^2}{[(t-s)^2+(y/a)^2]^2}\mathrm{d}s\right]\mathbf{\Phi}_i+\left[\int_{s_i}^{s_j}\frac{s-s_i}{L^i}\frac{y/a}{\sqrt{1-s^2}}\frac{(t-s)^2-(y/a)^2}{[(t-s)^2+(y/a)^2]^2}\mathrm{d}s\right]\mathbf{\Phi}_j.
\end{aligned}$$

Table 2
The error $\varepsilon$ in $\tau^*_{xy}$ calculation in Section 4, for different $N_g$ and $N_c$ values in the current method

| $N_g$ | $\varepsilon$ | | | | |
|---|---|---|---|---|---|
| | $N_c = 20$ | $N_c = 10$ | $N_c = 5$ | $N_c = 4$ | $N_c = 3$ |
| 48 | 0.1458 | 0.3212 | 0.7234 | 0.9225 | 1.2342 |
| 20 | 0.3527 | 0.7712 | 1.7393 | 2.2177 | 2.9651 |
| 6 | 1.1993 | 2.6101 | 5.8586 | 7.4557 | 9.9672 |

The $\sigma_{xx}$ component can be stated in a similar fashion. The integrals in $I^i_{yy}$ and $I^i_{xy}$ above could probably be evaluated analytically. However, preliminary attempts at doing so were not successful as the integrands are very complex. Nonetheless, since these integrals, for a field point not belonging to the crack, are well-behaved and non-singular, they can be accurately estimated using numerical integration techniques (e.g. using a Gauss–Legendre formula).

To demonstrate the use of the stress components equations, lets calculate the Peach–Kohler (PK) force acting on an infinite edge dislocation situated, without loss of generality, at $(x, y) = (a, 0.25a)$ in Fig. 1, and whose line sense is out of the page. For simplicity, $a = 1$ just as before. If the Burgers vector of the edge dislocation, in the coordinates of Fig. 1, is $\mathbf{b} = (b_x, 0, 0)$, then the PK force will be given by $\tau_{xy} b_x$. The calculation of the PK force is important in newly emerging dislocation dynamics codes. For simplicity, we can take $\mathbf{b}$ to be of unit strength or magnitude, i.e. $b_x = 1$. In this case, the value of $\tau_{xy}$ governs the magnitude of the force on the dislocation.

If one uses material constants and uniformly applied tensile loading from above, the GC method gives $\tau^*_{xy} = \tau_{xy}\mu = -1.366\text{E}{-3}$. For this loading condition and $N_c$, the error $\varepsilon_t$ in estimating $K_I$ was essentially zero (or more accurately 2.62E−5). We can therefore assume that this $\tau^*_{xy}$ value is equal to the analytical stress, and we thus denote it as $\tau^{\text{ref}}_{xy}$; the reference $\tau^*_{xy}$ value. Now, if we calculate $\tau^*_{xy}$ using the current method (with $N_c = 20$, $q = 0.5$ and $N_g = 48$), we get $\tau^*_{xy} = -1.364\text{E}{-03}$. The percent relative error $\varepsilon$ here, defined as $\varepsilon = 100 \times |(\tau^*_{xy} - \tau^{\text{ref}}_{xy})/\tau^{\text{ref}}_{xy}|$, is equal to 0.146. We notice that although the current method is less accurate in estimating the $K_I$ value (with an error of 1.14% according to Table 1), it provides an excellent estimate of the PK force on the dislocation. Furthermore, Table 2 shows that even for smaller $N_c$ values, one gets a small $\varepsilon$ error. This is true so long as $N_g$ is high enough (meaning as long as the estimate of the integrals in (9) is accurate enough). For example, even for $N_c$ as small as 3 (which will result in an extremely small system to solve), the error $\varepsilon$ is just 1.23% if $N_g = 48$. Of course, this error can even drop further for higher $N_g$'s. What Table 2 also shows is that for any moderate choices of $N_g$ and $N_c$, the error will be considerably small (less than 10% at the maximum). The reason for this can be explained by Saint Venant's principle. As long as the field point is away from the crack a distance approximately equal to or less than the average spacing between collocation points, then the error is expected to be small. For the current method, one needs to augment the last statement with the condition that $N_g$ also has to be high enough if small errors are desired.

## 5. Conclusions

Above, we presented a comparison between different methods in the literature for calculating $K_I$ value for a 2D through crack. We also presented a different more direct method of solving Cauchy singular equations of the first kind.

An important conclusion here is that the current method performs well over other methods whenever the remote loading has a discontinuity or sharp gradients along the crack length. This is due to the fact that it assumes piecewise element or interval interpolation over the crack length. Other methods that do not utilize piecewise interpolation can suffer oscillations in the solution in the case where the load exhibits sharp gradients along the crack. The current method, however, relies on numerical integration using a relatively large number of Gaussian integration points. This probably can be significantly remedied if one combines Richardson's extrapolation technique (Chapra and Canale, 1998) with the current method. Another important conclusion is that one needs to exercise caution in interpreting results of $K_I$ calculations via the numerical limiting procedure in (18). It was demonstrated here that this procedure is very expensive for accurate results. Finally, it was shown that accurate determination of $K_I$ value is not a necessary condition for accurate stress calculations as long as the field point of interest is at a distance equal to or farther than the average distance between collocation points along the crack length, as determined from the particular solution method. This last conclusion has application to interaction problems of cracks with other defects in an elastic medium. It is worth noting that all of the above discussion applies to Mode II cracks as well.

A last comment regards the applicability of the current method to cracks in *finite* domains and surface-breaking cracks. In these two cases, the resulting Cauchy kernel is no longer of the simple kind found in Eq. (1), rather it is of the "generalized" kind. The current method as presented herein is not formulated to treat such crack problems with generalized Cauchy kernels, although in principle it can be extended to do so owing to its pure numerical nature. However, such crack problems will undoubtedly be more complex with harder to attain convergence (for example at the end point breaking a free surface). The reader is advised to keep these important points in mind.

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