ANALYSIS OF COHESIVE ZONES IN CRACKS AND SLIP BANDS USING HYPERSINGULAR INTERPOLATIVE QUADRATURES

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Abstract. A numerically efficient and fast method of solution for cracks or slip bands with a crack opening or shearing displacement-dependent cohesive stress can be developed on the basis of a Gauss-Chebyshev quadrature rule for hypersingular integrals. The resulting iterative scheme allows different 'hardening' or 'bridging' laws to be explored in a consistent manner.

1. Introduction. It is well known (Bilby and Eshelby, 1968) that the following integral equation represents the condition of stress equilibrium for a crack in an elastic material

$$\frac{1}{\pi}\int_{-1}^{1}\frac{u'(t)dt}{t-x}=\frac{\sigma(x)}{A}. \tag{1}$$

Here, $u(t)$ denotes the relative displacement of the crack faces, and $u'(t)$ its derivative with respect to the crack length coordinate t chosen so that the tips correspond to $t=\pm 1$. The applied stress is $\sigma(x)$ and the constant $A=\mu/2(1-\nu)$ applies for plain strain deformation, where μ is the shear modulus and ν is Poisson's ratio.

The derivative $u'(t)$ is usually interpreted in terms of a dislocation density function $f(t)$ via the relation $u'(t)=bf(t)$, where b is the magnitude of the Burgers vector. For the purposes of mathematical analysis the dislocations can be 'smeared out', so that the function $f(t)$ (as well as $u(t)$) may be assumed continuous (Hills et al., 1996). Equation (1) also models multiple dislocation pile-up in a slip band (Bilby and Eshelby, 1968), provided that the number of dislocations is large. The effect of stress concentration produced by slip bands is naturally introduced via the concept of *intrinsic friction stress* σ_0, which acts uniformly throughout the slip band to oppose the applied stress. The concept of a friction stress was also extended to model the effect of cohesive, or process zones, near the tips of Mode I (opening mode) cracks. The stress acting on the crack segments adjacent to the crack tip is reduced by the opposing *cohesive stress* σ_0, while the rest of the crack is subjected to σ. In a general formulation of the problem of friction, or cohesive stress, it may be a function of the displacement discontinuity $u(x)$ across the crack line. In this case, $\sigma(x)$ in equation (1) is replaced with $\sigma(x) - C[u(x)]$. Bilby and Swinden (1965) considered a crack tip process zone with linear work hardening. This is equivalent to taking $C[u(x)] = \sigma_0 + \lambda u(x)$ in the cohesive zones, and zero in the remaining segment of the crack. Numerical solutions were obtained for a range of work hardening parameter λ. Evans (1987) considered a crack tip process zone with a non-linear friction stress, taking $C[u(x)] = \lambda[u(x)]^n$. Eq.(1) was converted to homogeneous form by partial inversion following Muskhelishvili's method. A solution was then obtained by numerical quadrature. Eq.(1) can also be considered as a model for fibre bridging in a composite. Willis (1993) converted it to homogeneous form by integration by parts. With the boundary conditions of crack closure at tips $u(\pm 1) = 0$, this gives the hypersingular integral

$$\frac{1}{\pi}\,⨎_{-1}^{1} \frac{u(t)dt}{(t-x)^2} = \frac{\sigma(x) - C[u(x)]}{A}. \tag{2}$$

A solution of (2) can be obtained in series form. Here we consider solutions of Eq(2) based on an efficient hypersingular interpolative quadrature method. Solutions for slip bands with internal work hardening or work softening are obtained. The method is also extended to cracks with non-linear process zones.

2. Quadrature rule. A central part in the present analysis is the use of an efficient interpolatory quadrature rule for hypersingular integrals (Korsunsky 1998). Assume that a solution for $u(t)$ may be represented to a sufficient degree of accuracy by a product of the appropriate weight function $w(t) = \sqrt{1-t^2}$, and a truncated series of Chebyshev polynomials, i.e. $u(t) = \sqrt{1-t^2}g(t)$, $\quad g(t) \simeq \sum_{j=0}^{p} B_j U_j(t)$, where $g(t)$ is bounded for $-1 \le t \le 1$. The following hypersingular integral is considered

$$S(x) = \frac{1}{\pi}\,⨎_{-1}^{1} \frac{g(t)w(t)dt}{(t-x)^2}, \; (-1 < x < 1). \tag{3}$$

The integral must be regularised, e.g. in terms of Hadamard's finite part. An efficient solution can then be developed if the values of the integral $S(x_k)$ at specially chosen *collocation points* x_k are expressed in terms of a linear combination of the unknown values $g(t_i)$ at *nodal points* t_i. The advantages of such approach are (a) that the discretised problem formulation is obtained solely in terms of the function values, not involving any of its derivatives, (b) that the quadrature is expressed by the product of a matrix by the vector of functional values $g(t_i)$, (c) that calculation of the matrix terms is computationally straighforward and fast, and (d) that the procedure lends itself naturally to inversion.

Derivation presented elsewhere (Korsunsky 1998) results in the quadrature

$$S(x_k) \simeq \sum_{i=1}^{n} \left[\frac{(1-t_i^2)}{(n+1)(t_i - x_k)^2} - \frac{(1-t_i^2)}{t_i - x_k} \frac{U_n(x_k)}{T_{n+1}(t_i)} \right] g(t_i). \tag{4}$$

The choice of the nodal and collocation points corresponds to the zeros of the Chebyshev polynomials $T_{n+1}(x_k) = 0$, $U_n(t_i) = 0$. For algorithmic convenience we ascribe specific values to the roots with certain indices,

$$x_k: \quad T_{n+1}(x_k) = 0,\ x_k = \cos\left(\frac{(2k-1)\pi}{2(n+1)}\right),\ k = 1:n+1; \quad U_n(x_k) = \frac{(-1)^{k+1}}{\sqrt{1-x_k^2}},$$

$$t_i: \qquad U_n(t_i) = 0,\ t_i = \cos\left(\frac{i\pi}{(n+1)}\right),\ i = 1:n; \qquad T_{n+1}(t_i) = (-1)^i.$$

These choices lead to the following simplified quadrature rule form:

$$\frac{1}{\pi}\int_{-1}^{1}\frac{\sqrt{1-t^2}\,g(t)\,dt}{(t-x)^2} \simeq \sum_{i=1}^{n}\left\{\frac{(1-t_i^2)}{(n+1)}\frac{1}{(t_i-x_k)^2} + \frac{(1-t_i^2)}{t_i-x_k}\frac{(-1)^{i+k}}{\sqrt{1-x_k^2}}\right\} g(t_i). \tag{5}$$

Without further modification, equation (5) furnishes an efficient method of solution for integral equations of the first kind, i.e. when the unknown function appears only in the integrand of the hypersingular integral. In this case, approximate values of the integral given by the numerical quadrature in Eq. (5) can therefore be directly equated to the applied stress. The discretized version of the integral equation yields a system of $n+1$ algebraic equations for the n unknown values $g(t_i)$. One superfluous equation must be discarded. It is most conveniently chosen to correspond to $x_k = 0$ (when an even value of n used). The stress intensity factors at crack tips are determined from the values $g(\pm 1)$ as follows: $K_i(a) = \sigma\sqrt{\pi a}\,g(1), K_i(-a) = \sigma\sqrt{\pi a}\,g(-1)$, where i is taken to represent I or II, depending on the crack opening mode considered.

3. Analysis procedure. The quadrature formulae presented in the previous section allow the values of the integral to be determined at the collocation points x_k in terms of $g(t_i)$. Note, however, that the right hand side of the governing integral equation also depends explicitly on the values of the unknown crack opening displacement at *collocation* points $u(x_k)$. It is necessary to introduce a further approximation which would to preserve the scheme's efficiency, so that the right hand side must be expressed solely in terms of $g(t_i)$. This is achieved by invoking the Legendre interpolation formula used in the Gaussian quadrature. This choice introduces no additional inaccuracies into the present approach, which remains exact within the class of polynomials of degree not exceeding n for the unknown function $g(t)$ (Szegö 1939)

$$g(x_k) = \sum_{i=1}^{n}\frac{U_n(x_k)}{U_n'(t_i)\,(x_k-t_i)}\,g(t_i) = \sum_{i=1}^{n}\frac{-(-1)^{i+k}(1-t_i^2)}{(n+1)(t_i-x_k)\sqrt{1-x_k^2}}\,g(t_i). \tag{6}$$

The nature of the equation resulting from the discretisation procedure based on the quadrature formulae of the previous section depends on the cohesive stress function $C[u(x)]$. If this function is linear with respect to the crack opening displacement, the discretised system retains its linearity in the form: $\mathbf{L}\underline{g} = \mathbf{b} - \mathbf{M}\underline{g}$, where the vector $\underline{g}$ has components $g(t_i)$, $\mathbf{L}$ is the linear operator proportional to the right hand side of equation (5), and $\mathbf{M}$ is the linear operator derived from the right hand side of the governing equation (2) using (6). This linear system can be readily inverted using one of the standard numerical library routines.

Non-linear dependence of cohesive stress on the crack opening displacement results in the loss of linearity of the integral equation. The discretised problem is now given as a system of non-linear algebraic equations for a finite-dimensional vector $g(t_i)$. A solution of this equation must be sought iteratively. One of the simplest approaches (which does not, however, guarantee convergence) is to consider the non-linear term as a perturbation to the linear problem, with each subsequent approximation obtained from the previous by substitution. A suitable choice of the linear part of the problem can ensure rapid convergence.

4. Slip band with linear hardening. Firstly, Eq.(2) is applied to model a slip band containing an array of edge dislocations with a friction stress that is a linear function of $u(x)$. In this case, the applied stress σ can be interpreted as in-plane shear stress parallel to the slip band. The internal friction stress is represented by $C[u(x)] = \lambda u(x)$, where the parameter λ has units of stress per unit length. To simplify the calculation it is convenient to scale the displacement discontinuity by the dimensionless ratio A/σ. The integral equation for $v(x) = Au(x)/\sigma a$ is given by: $\frac{1}{\pi}\int_{-1}^{1}\frac{v(t)\,dt}{(t-x)^2} = 1 - \left(\frac{\lambda a}{A}\right)v(x)$. Application of the quadrature rule gives rise to a system of linear equations that is easily inverted to give $g(1)$ as a function of the hardening parameter $\lambda a/A$ (Table 1). The results can be curve fitted to give the following relation for the stress intensity factor in the slip band: $K_{II} = \sigma\sqrt{\pi a}[1 + 1.2(\lambda a/A)]^{-0.557}$. The result should be compared with that for a slip band with a constant internal friction stress σ_0, for which the stress intensity factor is $K_{II} = (\sigma - \sigma_0)\sqrt{\pi a}$. The friction stress acts to attenuate the stress intensity factor in both Cases. For a material exhibiting linear work hardening in response to localised slip within a band, the reduction in the stress intensity factor is related to the extent of the band a, which may be assumed to correspond to the grain size. Note that it follows from the above equation that the degree of attenuation is grain size independent for the case of constant friction stress.

5. Linear work softening. Work softening within a slip band can be modelled using a similar approach. In this case, however, a different formulation is required. It is assumed that a limit friction stress σ_0 acts at the edge of the slip zone, and decreases towards the crack tip as a linear function of the relative displacement, $C[u(x)] = \sigma_0 - \lambda u(x)$. For the purpose of calculation it is convenient to introduce a scaling for $u(x)$ as follows: $v(x) = Au(x)/(\sigma - \sigma_0)a$. Eq.(2) becomes: $\frac{1}{\pi}\int_{-1}^{1} \frac{v(t)\,dt}{(t-x)^2} = 1 + \left(\frac{\lambda a}{A}\right) v(x)$. As before, the solution is obtained using the quadrature rule (4). The effect of the hardening parameter λ is also shown in Table 1. Work softening in this case amplifies the stress intensity factor according to the approximate relation: $K_{II} \simeq (\sigma - \sigma_0)\sqrt{\pi a}[1 - 0.821(\lambda a/A)^{1.24}]^{-1}$. As before, amplification is dependent on the slip band length, and can thus be related to the grain size.

6. Non-linear work hardening. To provide examples of non-linear work hardening, we consider two simple approximations of the atomic interaction force. Both cases reflect the well known characteristic behaviour in which initial hardening, i.e. increase in the cohesive stress, is followed by softening, i.e. cohesive stress decreasing to zero at maximum separation. In the first case, a bilinear dependence of stress on separation distance (a triangular pulse) is assumed. In the second case, sinusoidal dependence (half period of a sine wave) is assumed. In both cases we characterise the cohesive stress profile by the maximum separation distance U_m and maximum stress σ_m. Numerical experiments demonstrate that taking account of the initial slope of the stress-separation dependence is critical for ensuring convergence. This initial slope is given by $2\sigma_m/U_m$ for the bilinear case, and by $\pi\sigma_m/U_m$ for the sine.

The non-linear discretised equation can be recast in a form suitable for iterative solution as $(\mathbf{L} + \mathbf{M})\underline{g}_{n+1} = \mathbf{b} - [f(\underline{g}_n) - \mathbf{M}\underline{g}_n]$. Here the operator $\mathbf{M}$ reflects the linear hardening corresponding to the initial slope of the stress-separation dependence. This formulation ensures that the crack tip response at small values of crack opening displacement is captured correctly, and leads to rapid and reliable convergence in the cases considered. We introduce a scaling for $u(x)$ as before, $v(x) = Au(x)/\sigma a$, and use $S_m = \sigma_m/\sigma$ for normalised maximum cohesive stress. Fixing the maximum normalised separation for both hardening laws at 0.1, the normalised stress intensity factor can be computed as a function of the normalised maximum cohesive stress S_m. The results are illustrated in Figure 1. The sinusoidal hardening law induces a stronger attenuation of the stress intensity factor than the bilinear law, since the area under the stress-separation curve is greater for the former if the same maximum stress and maximum separation are used. A prominent feature of the stress intensity factor dependence on the maximum cohesive stress is a discontinuous drop in the SIF value at a certain level of cohesive stress. This transition is accompanied by a change in the crack opening profile and the appearance of a well-defined cohesive zone, illustrated in the insets in Figure 1.

Conclusion. An efficient numerical algorithm for the analysis of crack tip cohesive zones based on the interpolative hypersingular quadrature has been introduced. The advantage of the present approach is its flexibility in dealing with a variety of hardening laws, which is illustrated using simple examples.

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Hardening parameter $\lambda a/A$	SIF $g(1)a\sigma/A$	Softening parameter $\lambda a/A$	SIF $g(1)a(\sigma-\sigma_0)/A$
0	1.000	0	1.000
1	0.646	0.5	1.550
2	0.505	0.8	2.604
4	0.375	0.9	3.490
10	0.240	1.0	5.501
20	0.168	1.1	14.5

Table 1: Normalised SIF's for slip bands with linear hardening and softening.