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Fast and accurate numerical solution to an elastostatic problem involving ten thousand randomly oriented cracks

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Abstract. An algorithm is presented for the multiple crack problem in planar linear elastostatics. The algorithm has three important properties: it is stable, it is adaptive, and its complexity is linear. This means that high accuracy can be achieved and that large-scale problems can be treated. In a numerical example stress fields are accurately computed in a mechanically loaded material containing 10,000 randomly oriented cracks. The computing time is about two and a half hours on a regular workstation.

Keywords: Multiple cracks, random aggregate, integral equation of Fredholm type, effective elastic moduli, large-scale calculation, GMRES, fast multipole method

1. Introduction

The problem of constructing algorithms for computing the stress field in a mechanically loaded, linearly elastic, two-dimensional material with multiple cracks and inclusions has recently attracted much attention in this journal. The typical algorithm presented falls into either of two categories: moderately accurate algorithms based on singular integral equations, and approximate algorithms based on singular integral equations. The moderately accurate algorithms often can not handle more than a few cracks or inclusions, see, for example, Chen (1997), Wang and Chau (1997), Pan (1997), Xueli and Tzuchiang (1996a), and Chang and Mear (1995). Approximate algorithms can handle more cracks, but at the cost of low accuracy, especially when cracks are close to each other, see, for example, Freij-Ayoub, Dyskin, and Galybin (1997), and Brencich and Carpinteri (1996).

There are, in our opinion, three main reasons why many algorithms for multiple crack problems only achieve limited success: The first reason is that they are based on singular integral equations. Singular integral operators often have spectral properties that result in unstable algorithms. The accuracy will eventually decrease due to numerical

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cancellation as the discretization is refined. The second reason is that the algorithms have poor adaptive properties. Uniform discretization is often required. The third reason is that the algorithms are solved with methods which have cubic complexity. As the number of discretization points are doubled the computing cost increases by a factor of eight. Gaussian elimination for solving full systems of linear equations is an example of an algorithm with cubic complexity.

In this paper we present an adaptive algorithm for the multiple crack problem which is stable and which has linear complexity. The algorithm is based on an integral equation of Fredholm's second kind derived in Helsing and Peters (1999). Integral equations of Fredholm's second kind are excellent building blocks in stable numerical algorithms. Upon discretization of the integral equations with a Nyström scheme we get a system of linear equations which is solved iteratively with the GM-RES iterative solver (Saad and Schultz, 1986) and accelerated with the fast multipole method (Rokhlin, 1985; Greengard and Rokhlin, 1987; Carrier, Greengard, and Rokhlin, 1988). The fast multipole method is a "matrix-free" approach to matrix-vector multiplication. It can perform matrix-vector multiplication in O(N) operations, where N is the dimension of the matrix. Adaptivity is incorporated into the algorithm in the manner described in Helsing (1996).

We wish to stress that there is no new theoretical development in this paper per se. The novelty lies in the combination and implementation of algorithms, equations, and ideas that have been presented in the literature on applied mathematics during the last fifteen years. We believe it is of value to unite and incarnate these ideas in an efficient numerical code and to present it to the fracture mechanics community.

2. A Fredholm integral equation

Consider now a material consisting of an infinite medium with twodimensional elastic moduli κ and μ . The material is periodic. In a unit cell there are a number N of cracks. We denote the cracks in the unit cell by Γ^j , $j = 1, \ldots, N$. The union of all cracks in the plane is Γ . The starting point and the endpoint of crack Γ^j , the so-called crack tips, are denoted γ_s^j and γ_e^j . The average strain in the material is denoted $\bar{\epsilon} = (\bar{\epsilon}_{xx}, \bar{\epsilon}_{yy}, \bar{\epsilon}_{xy})$, and the average stress is denoted $\bar{\sigma} = (\bar{\sigma}_{xx}, \bar{\sigma}_{yy}, \bar{\sigma}_{xy})$. We would like to solve the elastostatic equation in the material subject to three different imposed average strains, namely $\bar{\epsilon}_{\rm I} = (1, 0, 0), \ \bar{\epsilon}_{\rm II} = (0, 1, 0), \ {\rm and} \ \bar{\epsilon}_{\rm III} = (0, 0, 1).$

We will start out with a representation of the stress field based on the uppercase potentials Φ and Ψ (Muskhelishvili, 1953; Theocaris and Ioakimidis, 1997) in the following form

$$\Phi(z) = \frac{1}{2\pi i} \int_{\Gamma} \frac{\Omega(\tau)\rho(\tau)\mathrm{d}\tau}{(\tau-z)} + \frac{\alpha}{2},\tag{1}$$

and

$$\Psi(z) = -\frac{1}{2\pi i} \int_{\Gamma} \frac{\overline{\Omega(\tau)\rho(\tau)} d\bar{\tau}}{(\tau-z)} - \frac{1}{2\pi i} \int_{\Gamma} \frac{\bar{\tau}\Omega(\tau)\rho(\tau)d\tau}{(\tau-z)^2} + \beta, \quad (2)$$

where $\Omega(z)$ is an unknown density on Γ and $\rho(z)$ is a weight function which on crack Γ^{j} is given by

$$\rho(z) = ((z - \gamma_{\rm s}^j)(z - \gamma_{\rm e}^j))^{-\frac{1}{2}}.$$
(3)

REMARK 2.1. The uppercase potentials Φ and Ψ of (1,2) of are related to the Airy stress function U via

$$U = \Re e\{\bar{z}\phi + \chi\}, \qquad \Phi = \phi', \qquad \Psi = \chi''.$$

REMARK 2.2. The constants α and β in (1) and (2) represent the forcing terms in our formulation. The two constants take the values κ and $-\mu$ for strain $\bar{\epsilon}_{\rm I}$, the values κ and μ for strain $\bar{\epsilon}_{\rm II}$, and the values 0 and $2i\mu$ for strain $\bar{\epsilon}_{\rm III}$.

It has been proven rigorously by Helsing and Peters (1999) that, using the above representation, the elastostatic partial differential equation can be rewritten as the following integral equation of Fredholm's second kind

$$\left(I + M_4^* (M_1^0 - M_3)\right) \Omega(z) = M_4^* \left(\frac{\bar{n}}{n} \bar{\beta} - \alpha\right), \qquad z \in \Gamma.$$
 (4)

Here I is the identity operator, M_4^* is a singular and bounded integral operator, M_1^0 and M_3 are compact integral operators, and n is the normal unit vector, see Helsing and Peters for details.

3. Effective elastic moduli

The stress- and strain fields in the material and stress intensity factors (SIF) at the crack tips can easily be evaluated once equation (4) is solved for Ω . The so-called "effective elastic moduli" are other quantities that can be easily evaluated as a function of Ω . Effective elastic moduli are particularly simple to define and compute in the setting of a doubly periodic material with a square unit cell of unit area. The

effective moduli of a material can be defined through the following relations between average stress and average strain

$$\begin{pmatrix} \bar{\sigma}_{xx} \\ \bar{\sigma}_{yy} \\ \sqrt{2}\bar{\sigma}_{xy} \end{pmatrix} = \begin{pmatrix} c_{*1} & c_{*2} & c_{*3} \\ c_{*2} & c_{*4} & c_{*5} \\ c_{*3} & c_{*5} & c_{*6} \end{pmatrix} \begin{pmatrix} \bar{\epsilon}_{xx} \\ \bar{\epsilon}_{yy} \\ \sqrt{2}\bar{\epsilon}_{xy} \end{pmatrix}.$$
 (5)

4. A stable and fast algorithm

We have implemented equation (4) as recommended by Helsing and Peters (1999) with two important modifications.

The first modification has to do with the quadrature rule. In Helsing and Peters we used 31st order accurate Gauss-Legendre quadrature on internal quadrature panels and 31st order accurate Gauss-Jacobi quadrature on panels containing crack-tips. In the present implementation we still use 31st order accurate Gauss-Legendre quadrature on internal quadrature panels, but we use 15th order accurate product integration on the panels containing crack-tips. The difference in performance turn out to be minor. The reason for this has to do with a certain interpolation we were forced to do in Helsing and Peters which partially reduced the order of the quadrature. The advantage of product integration is that we can use the same relative spacing between quadrature points on all panels. This simplifies the programming considerably.

The second modification has to do with the iterative solution of the system of linear equations which result after discretizing (4). In Helsing and Peters (1999) we explicitly formed the matrices corresponding to M_1^0 , M_3 , and M_4^* . This procedure resulted in an algorithm with quadratic complexity and we could not handle systems involving more than approximately 20 cracks and inclusions. In this paper we take advantage of the fast multipole method (Rokhlin, 1985; Greengard and Rokhlin, 1987; Carrier, Greengard, and Rokhlin, 1988) which is "matrix free". This gives an algorithm with linear complexity. The fast multipole method was adapted to problems in linear elasticity by Greengard and Helsing (1998).

5. Verification of the algorithm

In the next section we shall solve equation (4) on a geometry involving 10,000 randomly oriented cracks. Upon solving the equation we shall compute effective elastic moduli and present results that we claim are

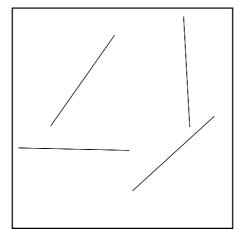


Figure 1. A unit cell of unit side length consisting of 4 cracks of length 0.5.

accurate to nine digits. There is no benchmark result for a geometry of this complexity to compare with. How can we be sure that the results are correct? The question can be split up into three parts.

- 1. Are our equations correct?
- 2. Are the equations implemented correctly in the computer code?
- 3. Is the accuracy claimed for the large-scale computation correct?

One way of answering the first two questions is by comparing results from our code to analytical and numerical solutions to simpler problems made by previous investigators. The problems of a single straight crack and of a circular arc shaped crack in an infinite elastic medium have analytical solutions (Muskhelishvili, 1953). We use computed values for stress intensity factors as a measure of correctness since the concept of effective property does not apply to this type of "free-space" problems. For various lengths, opening angles, and loads on the straight and on the circular arc shaped crack we reproduce the analytically known values for stress intensity factors to at least twelve digits of accuracy.

Two less trivial problems involving two well-separated straight cracks under uniform stress and shear were presented by (Xueli and Tzuchiang, 1996a; Xueli and Tzuchiang, 1996b). These results are also easy to reproduce. We give two examples. For the geometry and load of Xueli and Tzuchiang (1996a) the authors report $K_1 = 0.9751386$ at "crack tip A". We get convergence to $K_1 = 0.9751386767248$. For the geometry and load of Xueli and Tzuchiang (1996b) the authors report $K_2 = 0.1793005$ at "crack tip C". We get convergence to $K_2 =$ 0.179300563605.

We would also like to check that we have implemented the formulas for extracting the effective properties correctly. Unfortunately, we have not been able to find any benchmark results involving cracks on periodic domains. We therefore proceed in the following roundabout way: Four cracks of length 0.5 are placed in a square unit cell of unit side length, see Figure 1. The positions of the centers of the cracks, z_i , are $z_1 = (0.29, 0.21), z_2 = (-0.18, 0.17), z_3 = (0.23, -0.16),$ and $z_4 = (-0.22, -0.14)$. The rotations of the cracks relative to the horizontal axis, α_i , are $\alpha_1 = 1.6$, $\alpha_2 = 0.9$, $\alpha_3 = 0.7$, and $\alpha_4 = 3.1$. The elastic moduli are chosen as $\kappa = 0.5$ and $\mu = 0.5$. Our algorithm gives $c_{*1} = 0.496089506389$, $c_{*2} = -0.020315089385$, $c_{*3} = -0.020315089385$ $0.124564112473, c_{*4} = 0.471847932232, c_{*5} = 0.132897407867, and$ $c_{*6} = 0.482593206859$. The cracked material is now approximated with a two-component composite material where the cracks are replaced by very soft inclusions in the shape of thin ellipses. The effective moduli of the composite is computed with the algorithm of Greengard and Helsing (1998) for ellipses with aspect ratio 16, 32, and 64. The degree of inhomogeneity of the composite is 10^7 . Assuming that the moduli of the composite material approaches that of the cracked material as one over the aspect ratio, three-point Richardson extrapolation gives the effective elastic moduli $c_{*1} = 0.496082, c_{*2} = -0.020313, c_{*3} = 0.124558,$ $c_{*4} = 0.471854, c_{*5} = 0.132894$, and $c_{*6} = 0.482587$. We conclude that the two algorithms give consistent results for effective elastic moduli.

It remains to defend the accuracy claimed. We argue as follows: Integral operators in equations of Fredholm's second kind are of the type "identity plus compact operator". Their spectra are bounded and the singular values of the matrices resulting from their discretization rapidly accumulate at unity. Therefore second kind Fredholm integral equations can be solved iteratively to high accuracy. The number of iterations needed is small. The achievable accuracy, after refinement of the mesh, is limited only by the condition number of the underlying physical problem times the relative error with which the geometry is described in the floating point representation used. In the computations done below we see precisely this: upon mesh refinement the computed values for effective properties converge digit by digit until a certain limit, beyond which nothing more happens. For the 10,000 crack geometry this limit is nine digits. Naturally, when the geometry becomes extremely overresolved it could happen that accumulated roundoff error will propagate into the significant digits or even that certain discretization points no longer are distinct in the floating point representation. Then the algorithm breaks down.

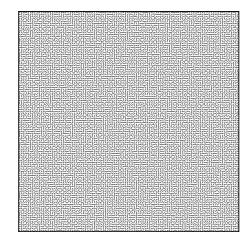


Figure 2. A unit cell consisting of 10,000 randomly oriented cracks centered at evenly spaced gridpoints. The crack length is equal to the distance between nearest-neighbor grid points.

6. A large-scale numerical example

As an example of a large-scale computation we take the square array of 10,000 randomly oriented cracks depicted in Figure 2. The cracks have length 1/100 and their centers are placed on a square grid where the nearest-neighbor gridpoints are separated by a distance of 1/100. Each crack is assigned a random rotation. While most cracks are reasonably well separated, some crack-tips are very close to touching. The twodimensional elastic moduli are chosen as $\kappa = 0.5$ and $\mu = 0.5$. The three average strains $\bar{\epsilon}_{\rm I}$, $\bar{\epsilon}_{\rm II}$, and $\bar{\epsilon}_{\rm III}$ were imposed in three different calculations.

Three quadrature panels were initially placed on each crack, corresponding to 480,000 discretization points. Seven stages of iterative refinement were then used, each adding another 20,000 discretization points. The GMRES iterations were terminated when the residual was less than $10^{-(4+m)}$, where m is the stage of refinement. The convergence typically required 12 + 3m iterations. The three first stages were completed in about 150 minutes per applied load on a SUN Ultra 10 workstation giving about five accurate digits for the effective moduli. After seven stages of refinement the effective elastic moduli had converged to $c_{*1} = 0.447553348$, $c_{*2} = -0.060763888$, $c_{*3} = -0.000803211$, $c_{*4} = 0.449781434$, $c_{*5} = -0.000728138$, and $c_{*6} = 0.448130115$. The memory requirement was about 600 Megabytes for the largest and most accurate calculation.

7. Discussion

We have implemented an algorithm for the multiple crack problem in planar linear elastostatics. We believe that our algorithm, as of today, is the leading algorithm in terms of three basic properties: stability, adaptivity, and complexity. As a numerical piece of evidence we presented a highly accurate solution to a crack problem which is more than a thousand times larger than those typically used as numerical examples in the literature.

One may ask why fast and accurate solvers for linear fracture mechanics problems are needed. After all, most computational problems of engineering importance are nonlinear. High accuracy is seldom required. Our answer to this question is the following: fast linear solvers are needed as fundamental building blocks in more complex solvers which, for example, can simulate micro-crack evolution in composite materials on their way from crack initiation to macroscopic failure, or treat problems involving plasticity. High accuracy may not be required in the final answer, but stability is a crucial property – especially when dealing with nonlinear equations. When we refine the discretization we must be absolutely confident that the error becomes smaller. Otherwise the computation is useless. Demonstrated ability to achieve high accuracy serves as a numerical proof of that an algorithm is stable.

Our algorithm is implemented as a 2400-line FORTRAN program. It is available from the author upon request.

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