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An Efficient Displacement Discontinuity Method Using Fast Multipole Techniques

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An Efficient Displacement Discontinuity Method Using Fast Multipole Techniques

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ABSTRACT: The Displacement Discontinuity method has been widely used in geomechanics because it accurately captures the behavior of fractures within a rock mass by explicitly accounting for discontinuities. Unfortunately, boundary element techniques require the interactions between all pairs of elements to be evaluated and traditional approaches to the Displacement Discontinuity method are computationally expensive for large problem sizes.

Approximate summation techniques, such as the Fast Multipole Method (FMM), calculate the interactions between N entities in time proportional to N. We have implemented a modified Fast Multipole approach which performs the necessary calculations in optimal time and with reduced memory usage. Furthermore, the FMM introduces parameters which can be selected to give the desired trade-off between efficiency and accuracy. The FMM approach permits much larger problems to be solved using desktop computers, opening up a range of applications. We present results demonstrating the speed of the code and several test cases involving rock fracture in compression.

1 INTRODUCTION

The Boundary Element (BE) approach reduces the dimensionality of a problem by considering only the discretization of boundaries. The BE solution requires that the influence of each boundary element upon all others be calculated. Consequently, BE methods are most efficient for problems where the surface to volume ratio is small, such as a simulation of cavities within an infinite medium. However, when crack formation or crack propagation is considered, the region of interest may become densely packed with boundary elements. In these circumstances, traditional approaches to the BE method become less attractive because the computational effort increases dramatically.

Previous authors have taken several approaches to improving the performance of BE methods applied to elasticity. Some methods achieve this by assuming the elements are distributed uniformly in space. For example, "lumping" (Plewman et al. 1969; Ryder & Napier 1985) takes advantage of the rapid far-field decay of the BE kernels to approximate the contribution of distant elements. The spectral BEM(Peirce et al. 1992) exploits the translational invariance of element-to-element interactions assuming the elements are located on a uniform grid. Peirce & Napier (1995) combined these approaches and developed a spectral multipole method where multipole expansions on a regular grid were used to account for distant element-to-element interactions. The Fast Fourier Transform (FFT) was then used to calculate the interactions between the multipole expansions on the regular grid.

The Fast Multipole Method (FMM)(Rokhlin 1985; Greengard & Rokhlin 1987; Greengard 1988; Greengard & Rokhlin 1997) provides an

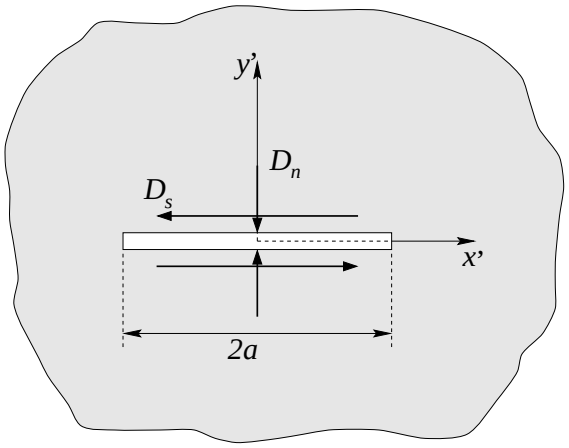


Figure 1: A constant discontinuity in displacement over a finite line segment.

alternative approach for efficiently calculating the interactions between elements. The FMM was originally developed to efficiently solve the many-body problems typical of electrostatics and gravitation. These applications are governed by Laplace's equation, however, it is possible to extend the FMM to boundary element problems, such as elasticity, which involve more complicated partial differential equations. Greenbaum et al. (1992) considered the 2-D biharmonic equation by modifying the integral equations to accommodate the FMM. Peirce & Napier (1995) considered 2-D elasticity and Sangani & Mo (1996) solved the 3-D Stokes' equations by modifying the FMM to accommodate the integral equations.

In this work, we use an approach similar to Fu et al. (1998) and apply the FMM directly to the boundary element equations. In contrast with their work, which considered a boundary element description of particles embedded in an infinite binder, we use boundary elements which represent discontinuities within the elastic solid (the displacement discontinuity method). Following the approach of Fu et al. (1998) we use a complex analytic function to approximate the element-to-element interactions.

2 THEORY

2.1 *The Displacement Discontinuity Method*

The displacement discontinuity method is a boundary element method devised to simulate the effect of thin, slit-like openings and cracks in an elastic solid. The technique is based on the analytical solution to the problem of a constant discontinuity in displacement over a finite line segment in the plane (see Figure 1). Along the length of the discontinuity we define a shear displacement discontinuity

$$D_s = u_{x'}\left(x', 0_-\right) - u_{x'}\left(x', 0_+\right) \tag{1}$$

and a normal displacement discontinuity

$$D_n = u_{y'}\left(x', 0_-\right) - u_{y'}\left(x', 0_+\right) \tag{2}$$

where 0_- and 0_+ denote the limits as 0 is approached from the negative and positive directions respectively. Crouch (1976) derived a solution for the displacements and stresses due to the single crack. For example, the displacements are given by:

$$\begin{aligned} u_{x'}\left(x', y'\right) &= D_s\left[2\left(1-\nu\right) f_{,y'} - y' f_{,x'x'}\right] \\ &\quad + D_n\left[-\left(1-2\nu\right) f_{,x'} - y' f_{,x'y'}\right] \\ u_{y'}\left(x', y'\right) &= D_s\left[\left(1-2\nu\right) f_{,x'} - y' f_{,x'y'}\right] \\ &\quad + D_n\left[2\left(1-\nu\right) f_{,y'} - y' f_{,y'y'}\right] \end{aligned} \tag{3}$$

where f is defined:

$$\begin{aligned} f\left(x', y'\right) = \frac{-1}{4\pi\left(1-\nu\right)} \Bigg[& y'\left(\arctan\frac{y'}{x'-a} - \arctan\frac{y'}{x'+a}\right) \\ & - \left(x'-a\right)\ln\sqrt{\left(x'-a\right)^2 + y'^2} \\ & + \left(x'+a\right)\ln\sqrt{\left(x'+a\right)^2 + y'^2}\Bigg] \end{aligned} \tag{4}$$

The displacement discontinuity method approximates boundaries within the region of interest with a collection of these slit cracks (boundary elements). Boundary conditions are imposed by prescribing displacements or stresses along the length of each element and the method solves

for values of the displacement discontinuities consistent with the prescribed boundary conditions. This necessitates transforming the solutions for local displacement and stress into global co-ordinates x and y to obtain expressions for the contributions to stress and displacement at element i due to element j. For example, the total displacement at element i due to all other elements can be expressed as a sum

$$\begin{aligned} u_s^i &= \sum_j B_{ss}^{ij} D_s^j + \sum_j B_{sn}^{ij} D_n^j \\ u_n^i &= \sum_j B_{ns}^{ij} D_s^j + \sum_j B_{nn}^{ij} D_n^j \end{aligned} \tag{5}$$

The terms A^{ij} and B^{ij} are called influence coefficients and depend upon the relative position of elements i and j and upon the orientation and length of element j. The original formulation of the displacement discontinuity method solved these equations directly using Gaussian elimination. This required the entire matrix of influence coefficients to be kept in memory. Furthermore, the Gaussian elimination algorithm takes order N^3 time (where N is the number of elements). The memory requirements may be reduced by employing an iterative solution. In this work, the system of linear equations was solved using a biconjugate gradient solver(Press et al. 1992) with a preconditioner based upon local clusters of boundary elements. This iterative scheme uses repeated matrix-vector products of the form of equations (5) which each take order N^2 to compute directly. We explain below how the efficiency of this solution is greatly improved by using the Fast Multipole Method to evaluate these products in order N time.

Many applications of the displacement discontinuity method require evaluation of displacement and stress at points distant from the boundary elements. For example, Blair & Cook (1998a, 1998b) simulated fracture propagation using the displacement discontinuity method. Conditions at the rock mass boundaries and on preexisting fractures were approximated using boundary elements. To determine the location of new cracks, stresses due to the boundary elements were calculated at points within the rock and compared with predetermined site strengths. Using straightforward direct summation, the calculations at M points would take order NM time. The FMM performs this work in time proportional to M.

2.2 *The Fast Multipole Method*

The fast multipole method was originally developed to efficiently evaluate an electrostatic potential in two-dimensions.

$$\phi(x,y) = q \log(r) \tag{6}$$

where q is the particle charge and

$$r = \sqrt{x^2 + y^2} \tag{7}$$

It is convenient to use complex numbers to describe the particle positions and the potential. For example, the potential at particle i due to particle j can be written

$$\Phi(z_i) = q_j \log\left(z_i - z_j\right) \tag{8}$$

where

$$z = x + \iota y \tag{9}$$

$$\log z = \ln|z| + \iota\theta \tag{10}$$

Here $\iota^2 = -1$. The total potential at particle i is given by a sum over all other particles:

$$\Phi(z_i) = \sum_{j=1}^{N} q_j log\left(z_i - z_j\right) \tag{11}$$

Evaluating this sum directly for all particles takes time proportional to N^2. The standard FMM algorithm will evaluate these sums for all particles i in order N time.

We will only describe the FMM in brief as the method has been described in detail by other authors(Greengard 1988; Pringle 1994). The computational domain is recursively bisected into smaller cells (see Fig.2). The FMM is a three step procedure which constructs series solutions approximating the combined influence of distant elements upon each of the smallest cells. Interactions between immediate-neighbor elements are evaluated directly.

1. Upward pass - Calculate influence of element clusters on distant elements (see Fig. 2a).

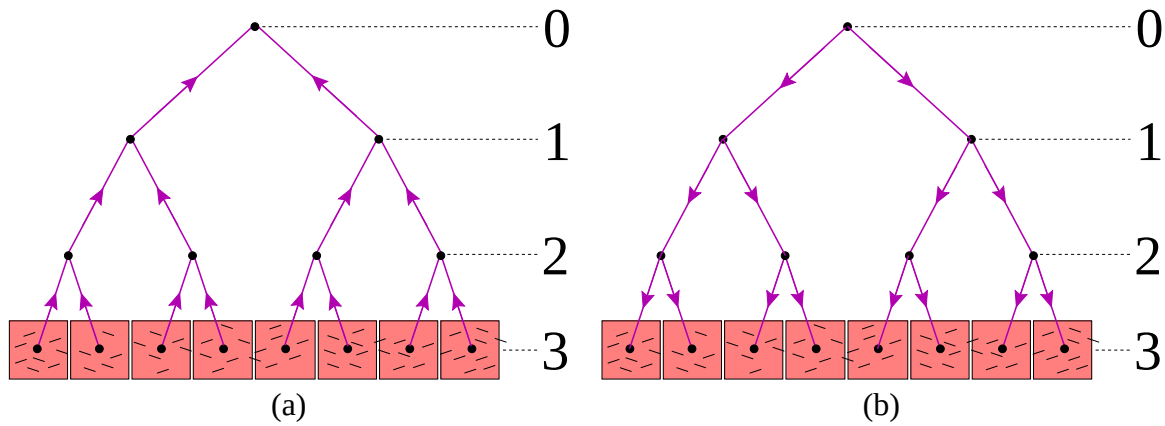


Figure 2: The FMM calculates long range interactions on a recursive grid by using (a) an Upward pass and (b) a Downward pass to construct series expansions to approximate distant elements within each of the smallest cells.

- Calculate contributions of each element to multipole expansions about its cell at the lowest level.
- Combine small cell expansions to give approximations for larger clusters.

2. Downward pass - Calculate influence of distant elements on element clusters (see Fig. 2b).
   - Convert large cell expansions into local expansions.
   - Translate and combine large cell expansions to calculate local expansions for smaller cells.
3. Evaluation step - calculate combined influence of all elements on every other element.
   - Previous steps provide the influence of all elements which are not "nearest neighbors"
   - Calculate element interactions directly within each of the smallest cells and nearest neighbors.

Typically, Step 3 takes the most time to compute. Once the coefficients of the expansion for a cell have been calculated, evaluating the potential at any point takes constant time. Thus, evaluating the potential at all points takes time proportional to the number of points. Furthermore, derivatives of the potential field are obtained analytically by differentiating the series expansions. The size of the smallest cells is determined by the depth of the tree structure. The cells in Fig. 2 have been subdivided 3 times, indicating a depth of 3. The deeper the tree, the smaller the cells and the shorter the distance over which interactions are calculated directly. Consequently, a more shallow tree involves fewer approximations and is typically more accurate. The most efficient tree depth depends upon the number of elements and their spatial distribution.

2.3 *Application of the FMM to the Displacement Discontinuity Method*

It can be shown that the function $f()$ (see equation 4) can be approximated by a log function:

$$\lim_{r\to\infty} f(x,y) = \frac{-a}{2\pi(1-\nu)}(\ln r + 1) \qquad (12)$$

where,

$$r = \sqrt{x^2+y^2} \qquad (13)$$

Figure 3 shows the relative error between (12) and (4) for a element of length $2a = 2$ located at the origin, with $\nu = 0.2$. Beyond a distance of approximately $7a$ the discrepancy between the the approximation and the exact solution is less

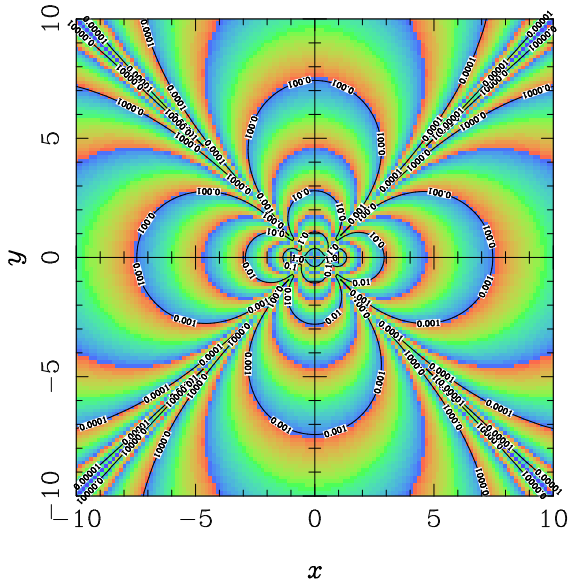


Figure 3: The relative error between the function f (equation 4) and the log approximation (12) for a single element located at the origin.

than 0.1%. This corresponds to a distance of 3.5 element lengths. Beyond this distance, we expect (12) to be a close approximation to (4).

If the constant additive term is neglected, Eq. 12 is of the same form as the electrostatic potential in two-dimensions (6) with

$$q_j = \frac{-a}{2\pi(1-\nu)}. \tag{14}$$

Before the FMM can be used to obtain stresses and displacements at a given location, several enhancements are required.

Since the approximation (12) only applies at separations of several element lengths, the full expression for $f(x,y)$ will be used to calculate the element interactions within neighboring cells (the size of the smallest cells is determined by the depth of the tree structure). Distant contributions will take the form of (12) and can be well approximated using series expansions derived previously for the electrostatic potential (6). We will denote this mixed implementation of the FMM by

$$\mathcal{F}_i(Q) \approx \sum_{j=1}^{N} Q(j)\, f(z_j) \tag{15}$$

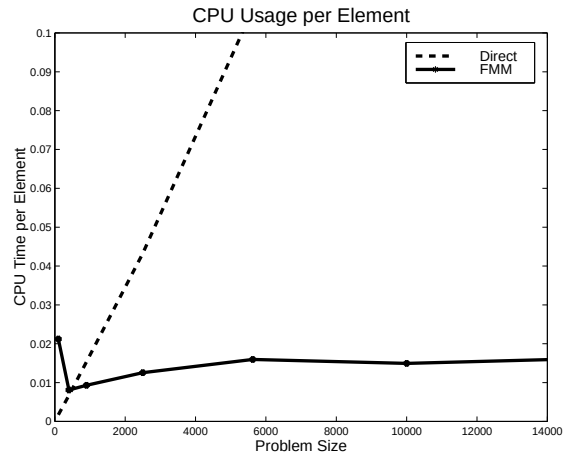


Figure 4: The CPU usage *per element* using the direct method and the FMM with 1% accuracy. The FMM is more efficient for problems involving more than 400 elements.

where Q is a given function which can be evaluated at each particle. For example,

$$\sum_{j=1}^{N} x_j f_{,x}(z_j) \approx \frac{\partial}{\partial x}\mathcal{F}_i(x) \tag{16}$$

It is possible to estimate complicated expressions involving the function $f()$ by combining several instances of the FMM using different functional forms for Q. Fu et al. (1998) used a similar approach to approximate the interactions between particles embedded in an infinite binder.

Equation 3 is in terms of local element coordinates. In order to determine the contribution to displacements and stresses in global coordinates, several transformations must be applied:

$$\begin{aligned} u_x &= u_{x'}\cos\beta - u_{y'}\sin\beta \\ u_y &= u_{x'}\sin\beta + u_{y'}\cos\beta \end{aligned} \tag{17}$$

and

$$\begin{aligned} \frac{\partial}{\partial x'} &= \frac{\partial x}{\partial x'}\frac{\partial}{\partial x} + \frac{\partial y}{\partial x'}\frac{\partial}{\partial y} \\ \frac{\partial}{\partial y'} &= \frac{\partial x}{\partial y'}\frac{\partial}{\partial x} + \frac{\partial y}{\partial y'}\frac{\partial}{\partial y} \end{aligned} \tag{18}$$

where β is the angle of the element to the x-axis. As an example we consider u_x for the case $D_s =$

0.

$$u_{x'}\left(x',y'\right) = D_n\left[-\left(1-2\nu\right) f_{,x'} - y' f_{,x'y'}\right] \quad (19)$$

This represents the contribution to u_x at a point due to a single element located at the origin.

Substituting (3) and (18) into (17), the influence of element j located at x^j, y^j upon element i located at x^i, y^i may be written:

$$\begin{aligned} u_x^{ij}/D_n^j = & \\ & +4\cos^2\beta^j \nu f_{,x}^j - 3\cos^2\beta^j f_{,x}^j \\ & -\cos^2\beta^j f_{,xx}^j x^j + \cos^2\beta^j f_{,xx}^j x^i \\ & +\cos^2\beta^j f_{,xy}^j y^j - \cos^2\beta^j f_{,xy}^j y^i \\ & +4\cos\beta^j \sin\beta^j \nu f_{,y}^j - 3\cos\beta^j \sin\beta^j f_{,y}^j \\ & -\cos\beta^j \sin\beta^j f_{,xx}^j y^j + \cos\beta^j \sin\beta^j f_{,xx}^j y^i \\ & -\cos\beta^j \sin\beta^j f_{,xy}^j x^j + \cos\beta^j \sin\beta^j f_{,xy}^j x^i \\ & -2\nu f_{,x}^j + 2 f_{,x}^j + f_{,xx}^j x^j - f_{,xx}^j x^i \end{aligned} \quad (20)$$

The actual value of of u_x at element i is calculated by summing up contributions from all other elements:

$$u_x{}^i = \sum_j u_x^{ij} \quad (21)$$

The terms appearing in (21) may be evaluated efficiently using the FMM. For example,

$$\sum_j \cos^2\beta^j y^j f_{,xy}^j \approx \frac{\partial^2}{\partial x \partial y} \mathcal{F}_i\left(\cos^2\beta y\right) \quad (22)$$

In addition, once the terms of the expansion for $\mathcal{F}_i\left(\cos^2\beta y\right)$ are calculated little work is required to calculate any derivative. Evaluating all the expressions for u_x^i takes time proportional to the number of elements because the bulk of the work involved in evaluating the $\mathcal{F}_i()$ operators (construction of local expansions within each cell) need only be done once.

The complete calculation of u_x^i requires terms due to D_s, similar to those in (20). The derivations of expressions for u_y^i, σ_{xx}^i, σ_{xy}^i, and σ_{yy}^i proceed in a similar fashion. In all, 27 unique "particle charges" (Q terms) are required. Most of these are used in more than one term to approximate different derivatives.

3 PERFORMANCE

To investigate the performance of the method, a number of random problems were considered. Each case consisted of an N by N square lattice of boundary elements. Simulations were performed with $N = 10, 20, 30, 50, 75$, 100, and 150. These correspond to 100, 400, 900, 2500, 5625, 10000, and 22500 elements, respectively. For each of these cases, simulations were performed using direct summation and with the FMM using tree depths of 2, 3, and 4. For each of the tree depths, simulations were done with different numbers of terms in the FMM expansions (from 0 to 7).

The total CPU time spent evaluating the element influences on displacement and stress at each site were compiled for each simulation. In addition, the relative error between the FMM approximations and the direct summation over the entire lattice was calculated. Finally these results were averaged over 10 random realizations of each choice of N.

Fig. 4 shows the CPU usage *per element* for the direct method and for the FMM using the fastest choice of parameters which provide at least 1% accuracy in the displacement calculation. The cost *per element* of the direct method increases linearly. The time taken per element by the FMM is very nearly independent of the total number of elements, indicating that the method takes $O(N)$ time. The FMM becomes more efficient for approximately 400 boundary elements or more for this level of accuracy.

4 SCALE DEPENDENCE OF BRAZILIAN TESTS

We have performed preliminary simulations of Brazilian tests to investigate the influence of scale upon strength. Experimentally it is observed that compressive strength decreases as sample size increases. Although many applications involve large rock masses, it is usually only practical to test small samples. Numerical simulations can complement laboratory results by providing a means to relate field scale properties to laboratory scale measurements.

Using the method of Blair & Cook (1998a, 1998b), we simulated fracture propagation in rock subjected to Brazilian loading (see Fig.5).

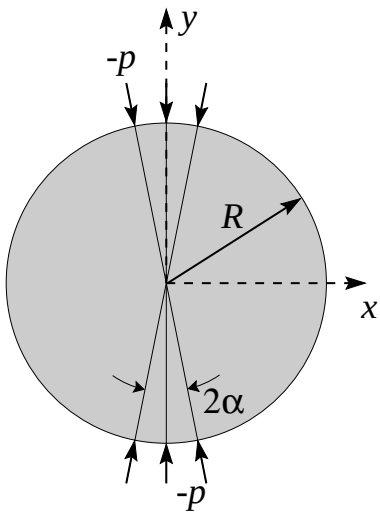


Figure 5: Brazilian loading: A circular disk subjected to diametral compression.

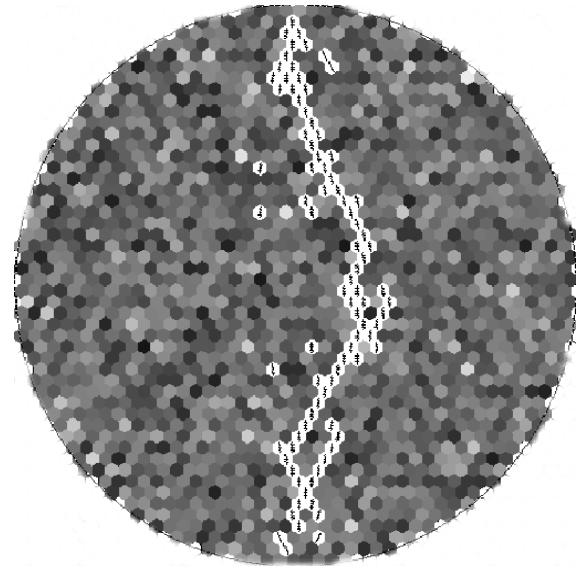


Figure 6: A typical failed disk at the end of one of the simulations. The cracked sites are shown in white with black lines indicating the crack direction. The shades of gray represent local stress heterogeneities.

	case 1	case 2	case 3	case 4
Strength	0.0%	0.25%	0.5%	5%
Stress	0.0%	5%	10%	50%

Table 1: The standard deviations of strength and stress perturbations.

Conditions at the rock boundaries and on cracks which formed were approximated using boundary elements. To determine the location of new cracks, stresses due to the boundary elements were calculated at points within the rock and compared with predetermined site strengths. Heterogeneities in the rock were simulated by introducing spatial variations in strength and local stress concentration. Samples were deemed to fail when a single connected crack spanned more than 40% of the sample diameter. For example, Fig. 6 shows the final state of a typical simulation.

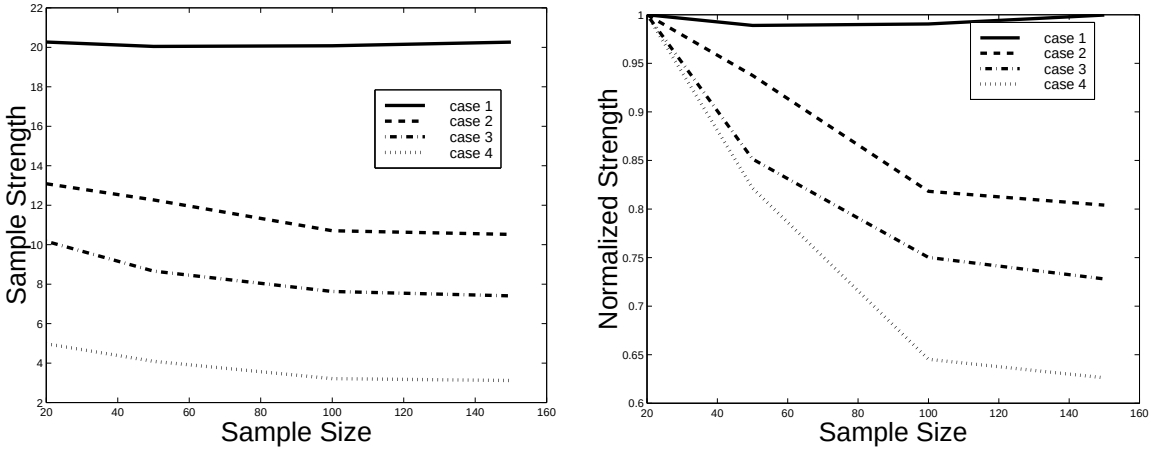
We conducted a series of simulations with diameters of 20, 50, 100, and 150 grains and different stress and strength heterogeneities. The heterogeneities were normally distributed with a mean site strength of 20 and mean stress perturbation of 0. The standard deviations of the heterogeneities for the 4 cases considered are shown in Table 1.

Preliminary results (Fig. 7a) indicate that increased perturbations of site strength and stress led to decreased sample strength. In addition, increased sample size resulted in decreased strength for cases involving non-zero perturbations. Figure 7b shows these same results normalized by the initial strength. These results indicate that larger perturbations of site strength and stress perturbations induce a faster drop in strength with increasing size.

5 SUMMARY

We have demonstrated that the Fast Multipole Method provides an efficient solution for the Displacement Discontinuity method. Our results indicate the ideal $O(N)$ effort for evaluating interactions of N elements can be achieved for certain element arrangements. The accelerated method has been integrated into an existing technique for simulating brittle rock fracture.

Preliminary simulations of Brazilian tests show the expected trends with increasing sample size. Increased perturbations of site strength and stress led to decreased sample strength while increased sample size resulted in decreased strength for cases involving non-zero



(a) (b)

Figure 7: The (a) strength and (b) normalized strength obtained for simulations of cylinders under Brazilian loading. Results indicate that strength decreases with increasing sample size and increasing heterogeneities.

perturbations.

Future work will involve further testing of the fracture algorithm. We plan to use this computational tool to consider more realistic distributions of heterogeneities. In particular, failure in rock with spatial correlations of site strength will be considered.

ACKNOWLEDGMENTS

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