Using an Augmented Lagrangian Method and block fracturing in the DDA method

C.T. Lin, B. Amadei, S.Sture University of Colorado, Department of Civil Engineering, Boulder Conf-940506--3

J.Jung

Sandia National Laboratories, Yucca Mountain Site Characterization

Project, Albuquerque

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

ABSTRACT: This paper presents two extensions to the Discontinuous Deformation Analysis (DDA) method originally proposed by Shi for modeling the response of blocky rock masses to mechanical loading. The first extension consists of improving the block contact algorithm. An Augmented Lagrangian Method is used to replace the Penalty Method originally proposed. It allows Lagrange multipliers to be introduced without increasing the number of equations that need to be solved and thus, block contact forces can be calculated more accurately. A block fracturing capability based on a three-parameter Mohr-Coulomb criterion represents the second extension. It allows for shear or tensile fracturing of intact blocks and the formation of smaller blocks.

1 INTRODUCTION

Several numerical methods are used in rock mechanics to model the response of rock masses to mechanical loading. These methods include the Finite Element Method (FEM), Boundary Element Methods (BEM), and Discrete Element Methods (DEM). Although rock mass discontinuities can be modeled in a discrete manner using FEM and BEM, the description of discontinuities is usually difficult and there are often restrictions to the degree of deformation permitted. On the other hand, DEM methods are generally more tailored for problems in which there are many material discontinuities, placing special emphasis on how contacts are handled.

The Discontinuous Deformation Analysis (DDA) method is a recently developed technique that falls in the family of DEM methods. It was first proposed by Shi and Goodman for computing the strains and displacements of a blocky system. In 1988, Shi published his PhD thesis entitled "Discontinuous Deformation Analysis: A New Numerical Model for the Statics and Dynamics of Block Systems ". Computer programs based on the method were developed and some applications were presented in the thesis as well as in a recent paper (Shi and Goodman 1989). At the outset, this paper reviews some of the basic concepts of the DDA method.

Then, extensions to the method are discussed in which an Augmented Lagrangian Method is used to improve block contact, and a block fracturing algorithm is proposed.

2 DDA MODELING OF BLOCKY ROCK MASSES

In the DDA method, the formation of blocks is very similar to the definition of a finite element mesh. A finite element type of problem is solved in which all the elements are physically isolated blocks bounded by pre-existing discontinuities. The elements or blocks used by the DDA method can be of any convex or concave shape. When blocks are in contact, Coulomb's law applies to the contact interfaces. and the simultaneous equilibrium equations are selected and solved at each loading or time increment. The large displacements and deformations are the accumulation of small displacements and deformations at each time step. Within each time step, the displacements of all points are small, hence the displacements can be reasonably represented by first order approximations.

adopting first order approximations, the DDA method assumes that each block has constant stresses and strains throughout.

The displacements (u,v) at any point (x,y) in a block i can be represented in two dimensions by six displacement variables:

$$D_{i} = (d_{1i} \ d_{2i} \ d_{3i} \ d_{4i} \ d_{5i} \ d_{6i})^{T} = (u_{o} \ v_{o} \ r_{o} \ \epsilon_{x} \ \epsilon_{y} \ \gamma_{xy})^{T}$$
(1)

where (u_0, v_0) is the rigid body translation at a specific point (x_0, y_0) within the block, r_0 is the rotation angle of the block with rotation center at (x_0, y_0) and ϵ_x, ϵ_y , and γ_{xy} are the normal and shear strains in the block. As shown by Shi (1989), the complete first order approximation of block displacements takes the following form

$$\begin{bmatrix} u \\ v \end{bmatrix} = T_1 D_1 = \begin{bmatrix} 1 & 0 & -(y-y_0) & (x-x_0) & 0 & (y-y_0) / 2 \\ 0 & 1 & (x-x_0) & 0 & (y-y_0) & (x-x_0) / 2 \end{bmatrix} \begin{bmatrix} d_{1i} \\ d_{2i} \\ d_{3i} \\ d_{4i} \\ d_{5i} \\ d_{6i} \end{bmatrix}$$
(2)

where (u,v) are the displacements at any point (x,y) inside block i which are equal to (u_0,v_0) at point (x_0,y_0) .

In the DDA method, individual blocks form a system of blocks through contacts among blocks and displacement constraints on single blocks. Assuming that n blocks are defined in the block system, Shi (1989) showed that the simultaneous equilibrium equations can be written in matrix form as follows

$$\begin{bmatrix} K_{11} & K_{12} & K_{13} & \dots & K_{1n} \\ K_{21} & K_{22} & K_{23} & \dots & K_{2n} \\ K_{31} & K_{32} & K_{33} & \dots & K_{3n} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ K_{n1} & K_{n2} & K_{n3} & \dots & K_{nn} \end{bmatrix} \begin{bmatrix} D_1 \\ D_2 \\ D_3 \\ \vdots \\ D_n \end{bmatrix} = \begin{bmatrix} F_1 \\ F_2 \\ F_3 \\ \vdots \\ \vdots \\ F_n \end{bmatrix}$$
(3)

where each coefficient K_{ij} is defined by the contacts between blocks i and j. Since each block i has six degrees of freedom defined by the components of matrix D_i in equation (1), each K_{ij} in (3) is itself a 6 x 6 sub-matrix. Also, each F_i is a 6 x 1 sub-matrix

that represents the loading on block i. Equation (3) can also be expressed in a more compact form as KD = F where K is a 6n x 6n stiffness matrix and D and F are 6n x 1 displacement and force matrices, respectively.

The simultaneous equations (3) were derived by Shi (1989) by minimizing the total potential energy, Π , of the block system. The i-th row of equation (3) consists of six linear equations

$$\frac{\partial \mathbf{II}}{\partial d_{r,i}} = 0, \qquad r = 1 - 6 \tag{4}$$

where d_{ri} is the deformation variable of block i. The total potential energy is the summation over all the potential energy sources, e.g., individual stresses and forces. The potential energy of each force or stress and their differentiations are computed separately. The differentiations

$$\frac{\partial^2 \mathbf{\Pi}}{\partial d_{ri} \partial d_{sj}}, \qquad r, s=1-6 \tag{5}$$

are the coefficients of unknowns d_{sj} of the equilibrium equation (4) for variable d_{ri} . All terms of equation (5) form a 6 x 6 sub-matrix, which is sub-matrix K_{ij} in (3). Equation (5) implies that matrix K in (3) is symmetric. The differentiations

$$-\frac{\partial \mathbf{\Pi}(0)}{\partial d_{r,i}}, \quad r=1-6 \tag{6}$$

are the free terms of equation (4) after shifting to the right side of equation (3). All terms of equation (6) form a 6 x 1 sub-matrix, which is added to sub-matrix \mathbf{F}_i .

Dr Shi's thesis (1989) covers the details for forming sub-matrices K_{ij} and F_i for elastic stresses, initial stresses, point loads, line loads, volume forces, bolting forces, inertia forces and viscosity forces.

3 AUGMENTED LAGRANGIAN METHOD

The penalty method was originally used in the DDA method to enforce contact constraints at block interfaces. The obvious advantages of such a method are: (1) the number of governing equations is not increased because of contacts and (2) the solution is easily obtained by simply adding contact components

to the stiffness matrix. However, the method has three major disadvantages. First, the accuracy of the contact solution highly depends on the choice of the penalty number and the optimal number cannot be explicitly found beforehand. Secondly, the penalty approach satisfies the contact constraints only approximately. Finally, the contact forces must be calculated using auxiliary calculations. All three limitations can be overcome by using an Augmented Lagrangian Method.

The classical Lagrange Multiplier Method would be one of the best methods to solve block contact problems by explicitly obtaining the contact forces. However, the method increases the number of governing equations and extra computational effort is needed to solve the increased number of equations. A modified Lagrange Multiplier Method (Augmented Lagrangian Method) can be used, instead, to retain the simplicity of the penalty method and minimize the disadvantages of the penalty and classical Lagrange Multiplier Methods.

Consider two blocks 1 and 2 as shown in Figure 1. Let (x_i,y_i) and (u_i,v_i) be, respectively, the coordinates and the displacement increments at point P_i (i=1,2,3). Also let, d, be the distance of penetration of point P_1 (x_1,y_1) into the edge P_2P_3 . When using the penalty method, a spring is applied between point P_1 and the edge P_2P_3 . The strain energy of the contact spring is equal to $pd^2/2$ where p is a large positive penalty number which is also the spring stiffness.

Let λ be the unknown contact force due to the penetration of point P_1 into the edge P_2P_3 . Using the classical Lagrange Multiplier Method, the strain energy of that contact force is equal to λd .

The essential concept behind the Augmented Lagrangian Method is to use both a penalty number p and a Lagrange multiplier $\lambda^* \approx \lambda$ at each block contact (Landers and Taylor 1986). The strain energy of the contact force is equal to λ^*d . To avoid increasing the number of governing equations, an iterative method is used to calculate the Lagrange multiplier λ^* until the distance of penetration d is below a minimum tolerance. A first order updated value for λ^* can be written as

$$\lambda \approx \lambda_{k+1}^* = \lambda_k^* + pd \tag{7}$$

where the penalty number, p, can be variable and does not have to be a very large number as in the penalty method. In equation (7), λ_k^* is the Lagrange multiplier at the k^{th} iteration and λ_{k+1}^* is the updated

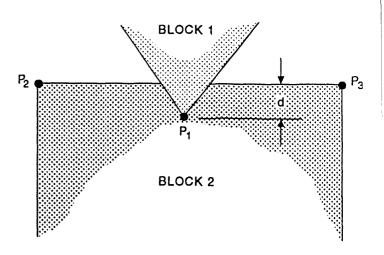


Fig.1 Interaction between two contacting blocks.

Lagrange multiplier. At the k^{th} iteration, the strain energy, Π_s , resulting from the contact force becomes

$$\Pi_s = \lambda_k^* d + \frac{1}{2} p d^2 \qquad (8)$$

Equation (8) consists of two components. The first component is the strain energy created by the iterative Lagrange Multiplier $\lambda^{\circ}_{\mathbf{k}}$, and the penalty constraint creates the second. The contribution of the second component to the 6n x 6n global stiffness matrix \mathbf{K} in equation (3) was already covered by Shi (1989), so only the contribution of the first component of equation (8) is derived below.

After the displacement increments (u_i, v_i) are applied, the distance d between point P_1 (x_1, y_1) and the reference edge P_2P_3 in Figure 1 can be calculated as follows

$$d = \frac{\Delta}{I} = \frac{1}{I} \begin{vmatrix} 1 & x_1 + u_1 & y_1 + v_1 \\ 1 & x_2 + u_2 & y_2 + v_2 \\ 1 & x_3 + u_3 & y_3 + v_3 \end{vmatrix}$$
 (9)

where I is the length of P_2P_3 and Δ is such that

$$\Delta = \begin{vmatrix} 1 & X_1 & Y_1 \\ 1 & X_2 & Y_2 \\ 1 & X_3 & Y_3 \end{vmatrix} + \begin{vmatrix} 1 & u_1 & Y_1 \\ 1 & u_2 & Y_2 \\ 1 & u_3 & Y_3 \end{vmatrix} + \begin{vmatrix} 1 & X_1 & V_1 \\ 1 & X_2 & V_2 \\ 1 & X_3 & V_3 \end{vmatrix} + \begin{vmatrix} 1 & u_1 & V_1 \\ 1 & u_2 & V_2 \\ 1 & u_3 & V_3 \end{vmatrix}$$
(10)

The last term in (10) is negligible since it is a second order infinitesima!. If S_o is the first term in (10), then equation (10) can be approximated as

$$\Delta = S_0 + \begin{vmatrix} 1 & u_1 & y_1 \\ 1 & u_2 & y_2 \\ 1 & u_3 & y_3 \end{vmatrix} + \begin{vmatrix} 1 & x_1 & v_1 \\ 1 & x_2 & v_2 \\ 1 & x_3 & v_3 \end{vmatrix} . \quad (11)$$

Assuming that point P_1 belongs to the i-th block and edge P_2P_3 belongs to the j-th block, combining equations (2), (9) and (11) and after several subsequent derivations, the penetration, d, after the k^{th} iteration can be expressed as follows

$$d = \frac{S_0}{l} + \mathbf{E} \, \mathbf{D_i} + \mathbf{G} \, \mathbf{D_j} \tag{12}$$

where E and G are 1 x 6 matrices with components e_r and g_r (r = 1-6) equal to

$$e_{r} = \frac{1}{2} [(y_{2}-y_{3}) t_{1r}(x_{1}, y_{1}) + (x_{3}-x_{2}) t_{2r}(x_{1}, y_{1})]$$

$$g_{r} = \frac{1}{2} [(y_{3}-y_{1}) t_{1r}(x_{2}, y_{2}) + (13) (x_{1}-x_{3}) t_{2r}(x_{2}, y_{2})] + \frac{1}{2} [(y_{1}-y_{2}) t_{1r}(x_{3}, y_{3}) + (x_{2}-x_{1}) t_{2r}(x_{3}, y_{3})]$$

Multiplying d defined in (12) by λ_k^* , λ_k^* d in (8) takes the form

$$\Pi_{si} = \lambda_k^* \left(\frac{S_0}{l} + E D_i + G D_j \right)$$
 (14)

The derivatives of Π_{s1} with respect to d_{ri} and d_{rj} at 0 are defined as

$$f_{ri} = -\frac{\partial \Pi_{s1}(0)}{\partial d_{ri}} = -\lambda_{k}^{*} e_{r}$$

$$f_{rj} = -\frac{\partial \Pi_{s1}(0)}{\partial d_{rj}} = -\lambda_{k}^{*} g_{r}$$
(15)

(r = 1-6) which form two 6 x 1 matrices $-\lambda_k^* \mathbf{E}^T$ and $-\lambda_k^* \mathbf{G}^T$ that are added to sub-matrices \mathbf{F}_i and \mathbf{F}_j , respectively.

Equations (15) were derived for the first component of the strain energy, Π_s , in (8). The second component in equation (8) is associated with the penalty method and its contribution to the

simultaneous equilibrium conditions (3) was derived by Shi (1989). For the Augmented Lagrangian Method, the combined effect of the first and second components of Π_s to equation (3) can be summarized as follows:

$$\mathcal{D} \mathbf{E}^T \mathbf{E} \to \mathbf{K}_{\bullet,\bullet} \tag{16}$$

is added to sub-matrix K_{ii} in (3),

$$p \mathbf{E}^{\mathrm{T}} \mathbf{G} \to \mathbf{K}_{i,i} \tag{17}$$

is added to sub-matrix K_{ii} in (3),

$$p \mathbf{G}^T \mathbf{E} \to \mathbf{K_{ii}} \tag{18}$$

is added to sub-matrix K_{ii} in (3),

$$p \mathbf{G}^T \mathbf{G} \to \mathbf{K}_{\mathbf{1}\mathbf{1}} \tag{19}$$

is added to sub-matrix K_{ii} in (3),

$$-\left(\lambda_{k}^{*} + \frac{pS_{0}}{l}\right) \mathbf{E}^{T} \rightarrow \mathbf{F}_{i} \tag{20}$$

is added to sub-matrix F_i in (3), and

$$-(\lambda_k^* + \frac{pS_0}{l}) \mathbf{G}^T \rightarrow \mathbf{F_j}$$
 (21)

is added to sub-matrix F_i in (3).

From a physical point of view, the Lagrange multiplier, λ , represents the contact force along a point of contact between two blocks and the penalty number, p, represents the stiffness of the contact spring. According to equations (15), the contact forces calculated at each iteration for all block contact points are added to the external force matrix F on the right hand side of the simultaneous equilibrium equations (3). Using this approach, the final exact contact forces can be obtained by the iterative method even with small initial values of the penalty number. However, if the initial penalty number is too small, many iterations are required, making the method not as efficient. In order to overcome this problem, the penalty number needs to be increased after a certain number of iterations within any time step. The variable penalty number approach represents a major improvement over the penalty method used by Shi (1989). Shi recommended that the penalty number be within 10 to 1000 times the Young's Modulus of the block material in order to prevent the blocks from penetrating one another excessively. This constraint no longer applies when using the variable penalty number approach in the Augmented Lagrangian Method.

The Augmented Lagrangian Method implemented in the original DDA program with a variable penalty number function. Except for substituting the Augmented Lagrangian Method for the penalty method, the basic features of the DDA program developed by Shi (1989) were retained. The most important feature of the new program is that any initial penalty number can now be selected by the user. Then, at each iteration and for each time step within that iteration, the optimal penalty number is found for all contacts by the program itself in order to satisfy the requirements of minimum distance of contact interpenetration.

As an illustrative example, consider the two-block system shown in Figure 2a. The bottom block is fixed and the top block is subject to a vertical load of 1,000 lbs (4.4 kN) and an horizontal load of 2.500 lbs (11.0 kN). The interface between the two blocks has zero cohesion and a friction angle of 30°. The intact material in the blocks has a Young's modulus of 10⁸ psf (4,781 MPa), a Poisson's ratio of 0.25 and a unit weight of 130 pcf (0.02 MN/m^3) . Both the penalty method of Shi (1989) and the Augmented Lagrangian Method with variable penalty number were used to solve the same problem with a low initial value of the penalty number equal to 10⁴ lbs/ft (0.15 MN/m). The deformation of the block system is shown in Figures 2b and 2c after 315 and 90 time steps of 0.01 seconds. Figure 2b shows that when using the Augmented Lagrangian Method no block interpenetration occurs even though the initial penalty number is low. On the other hand, Figure 2c shows that a small penalty number with the classical method is unable penalty to enforce interpenetration constraint.

4 BLOCK FRACTURING

As a second extension of the DDA method, a fracturing capability that allows for shear or tensile fracturing of the intact block material was added to the original DDA program. This capability allows for intact blocks to be broken into smaller blocks.

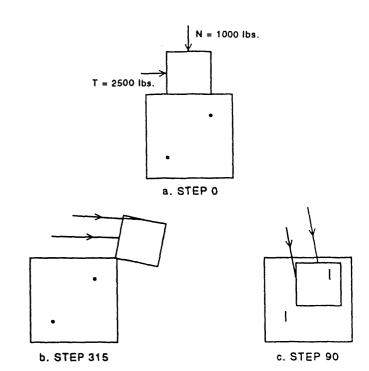


Fig.2 Initial configuration in (a). Deformation of the block system after 315 time steps with the Modified Lagrangian Method in (b) and after 90 time steps with the penalty method in (c).

The criterion selected here for block fracturing is a Mohr-Coulomb criterion with three parameters: s_0 is the cohesion of the block material, ϕ is its friction angle and T_0 represents its tensile strength. Assuming that tensile normal stresses are positive, the three- parameter Mohr-Coulomb criterion is expressed in terms of major and minor principal stresses σ_3 and σ_1 (with $\sigma_3 \geq \sigma_1$) as follows

$$\sigma_1 = -C_0 + \sigma_3 \tan^2\left(\frac{\pi}{4} + \frac{\phi}{2}\right) \qquad (22)$$

when $\sigma_1 < \sigma_{1c}$ and

$$\sigma_3 = T_o \tag{23}$$

when $\sigma_1 \ge \sigma_{1c}$. In equation (22), C_o is the unconfined compressive strength of the block material which is related to the cohesion s_o and friction angle ϕ as follows

$$C_o = 2s_o \tan\left(\frac{\pi}{4} + \frac{\phi}{2}\right) \tag{24}$$

and σ_{1e} is a critical transitional stress between the shear and tensile fracture modes equal to

$$\sigma_{1c} = -C_o + T_o \tan^2(\frac{\pi}{4} + \frac{\phi}{2})$$
 . (25)

The major and minor principal stresses σ_3 and σ_1 are determined at the centroid of each block of the system using the Augmented Lagrangian Method with variable penalty number. If equation (22) is satisfied within a block, shear fracturing is assumed to occur with two fracture planes passing through the block's centroid and inclined at $\pm (\pi/4 - \phi/2)$ with respect to σ_1 . Then, the block is divided into four blocks and the DDA analysis is resumed with a new block configuration. If on the other hand, equation (23) is satisfied, tensile fracturing occurs with a fracture passing through the block's centroid and oriented at right angle to σ_3 . The block is divided into two blocks and the DDA analysis is resumed. This process is repeated for all blocks in the system. Note that no energy dissipation is assumed to occur during shear or tensile fracturing.

As a numerical example, consider the problem shown in Figure 3a, where a block of rock is fractured in uniaxial compression between two rigid platens. The block is 1.6 ft (0.48 m) wide and 4.0 ft (1.22 m) high. Each platen is 2.0 ft (0.61 m) wide and 1.4 ft (0.43 m) high. The top platen drives the rock specimen in the downward direction. The bottom platen is fixed. The contact between the platens and the rock is assumed to be frictional only with a friction angle of 30°. The rock has a Young's modulus of 108 psf (4,781 MPa), a Poisson's ratio of 0.25, a unit weight of 130 pcf (0.020 MN/m^3) , a cohesion s_o of 1.78 x 10⁵ psf (8.55 MPa), a friction angle ϕ of 39.1° and a tensile strength T_o of 0.85 x 10⁵ psf (4.1 MPa). Two symmetric loads of 157.5 klbs (0.702 MN), 0.8 in (0.2 m) apart, are applied in the vertical direction. Figures 3b-3d show the deformation and fracturing of the system after 22, 85 and 120 time steps of 10⁴ seconds. As repeated rock fracturing occurs, the new fractures are assumed to have zero cohesion and a 30° friction angle.

5 CONCLUSIONS

This paper presents two extensions to the DDA method originally proposed by Shi (1989). An Augmented Lagrangian Method is used to model block contacts more accurately than the original penalty method. The method retains the simplicity of the penalty method and reduces the disadvantages of the penalty and classical Lagrange Multiplier

methods. The block fracturing algorithm provides a valuable tool when looking at the mechanical fracturing of already fractured rock masses due to stress concentrations, impact or tool-rock interaction.

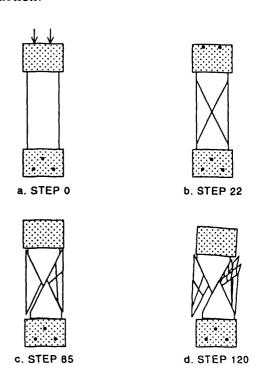


Fig.3. Block of rock under uniaxial compression. Initial geometry in (a). Deformed system after 22,85 and 120 time steps in (b)-(d), respectively.

REFERENCES

Shi, G-H. 1989. Discontinuous deformation analysis. *PhD Thesis*, Univ. of California, Berkeley.

Shi, G-H and Goodman, R.E. 1989. Generalization of two-dimensional continuous deformation analysis for forward modeling. Int. J. Num. & Anal. Methods in Geomech. 13, 359-380. Landers, J.A. and Taylor, R.L. 1986. An augmented Lagrangian formulation for the finite element solution of contact problems. Report No. CR 86.008 to Naval Civil Eng. Lab., Cal.

Acknowledgements: This work was performed under the auspices of the US Department of Energy, Office of Civilian Radioactive Waste Management, Yucca Mountain Site Characterization Project, under contract # DE-AC04-76DP00789. The support of National Science Foundation under grant No. MS 9215397 is also greatly appreciated. The authors are grateful to Dr. Gen-Hua Shi for his comments and suggestions.

4/8 3

