

## Modified Contact Constraints in Sphere-Based 3-D DDA

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### ABSTRACT:

In 2012, a new numerical model, called sphere-based 3-D DDA, for simulation of granular materials consisting of 3-D spheres was presented by the authors (Beyabanaki and Bagtzoglou [1]). In the existing sphere-based 3-D DDA method and in studies performed by other researchers, the penalty method is used to enforce sphere contact constraints. Although this approach is fairly simple to implement, it can lead to inaccuracies that may be large for small values of the penalty number. Moreover, this method creates sphere contact overlap that may violate the physical constraints. In this study, the augmented Lagrangian method is used to overcome these limitations. For this purpose, contact constraints in sphere-based 3-D DDA are modified and the corresponding formulations are presented. The modified contact constraints have been implemented into a sphere-based 3-D DDA numerical code and two test cases are studied in order to verify the formulations. The results show the capability of the modified sphere-based 3-D DDA.

**KEYWORDS:** sphere-based discontinuous deformation analysis, contact constraints, augmented Lagrangian method, Penalty method, numerical method.

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## I. INTRODUCTION

Discontinuous Deformation Analysis (DDA) is a displacement-based method that was originally developed by Shi [2, 3] for modeling large deformation in fractured rock masses. DDA provides a useful tool to analyze the mechanical response of discrete blocks. Several studies have been conducted to validate and develop this numerical approach. Applications of the DDA in rock mechanics and rock engineering are reviewed by Jing and Hudson [4], Jing [5], and Ohnishi and Nishiyama [6]. In a comprehensive study, MacLaughlin and Doolin [7] reviewed more than 100 validation studies on the DDA. Moreover, Shi [8] presented applications of the DDA to rock stability analysis. Applications of the DDA to model slopes and underground openings are also reviewed by Hatzor and Bakon-Mazor [9].

Basic formulations of matrices for different potential terms are presented in detail by Shi [10] and Wu et al. [11]. Applications of 3-D DDA were demonstrated by Liu et al. [12] and Yeung et al. [13, 14]. As the first step in developing 3-D DDA, its contact model was presented and, for this purpose, a point-to-face model for contacts between polyhedral blocks in 3-D DDA was developed by Jiang and Yeung [15]. Also, Wu et al. [16] developed a new contact searching algorithm for frictionless vertex-to-face contact problems. Moreover, Yeung et al. [17] and Wu [18] presented different algorithms for edge-to-edge contacts. Finally, a new algorithm to search and calculate geometrical contacts in 3-D was presented by Beyabanaki et al. [19]. Ahn and Song [20] presented a new contact definition algorithm for 3-D DDA. As the next step, block deformability in 3-D DDA was improved by Beyabanaki et al. [21, 22] who implemented 8-node and 20-node hexahedral isoparametric finite elements into 3-D DDA. Furthermore, as an alternative method to improve block deformability in 3-D DDA, high-order displacement functions were used by Beyabanaki et al. [23, 24]. Finally, validation and application of 3-D DDA with tetrahedron finite element meshed block were presented by Liu et al. [25]. Before using a method for a dynamic problem, it should be demonstrated that the method is able to model dynamic conditions. For this purpose, Beyabanaki et al. [26] compared the 3-D DDA solution for dynamic block displacement with analytical solutions to study the validity of the method in order to show the capability of polyhedral-based 3-D DDA to model dynamic problems. Moreover, Bakun-Mazor et al. [27] validated 3-D DDA by comparing the numerical results obtained for modeling dynamic, single, and double face sliding of a block with their proposed analytical solution. 3-D DDA was coupled with smoothed particle hydrodynamics by

Zhang et al. [28] to study the geological phenomena associated with fluid-solid interaction. Zhu et al. [29] integrated 3-D DDA with binocular photogrammetry and evaluated the stability of tunnels in jointed rock masses. To address rock-cutting and rock-penetration problems, Zhao et al. [30] coupled 3-D DDA with a distinct lattice spring model. Zhang et al. [31] constructed new types of 3-D DDA slope models with GIS techniques and Liu et al. [32] analyzed the velocity distribution and the key point displacements of the brick masonry buildings using 3-D DDA. Recently, Beyabanaki [33] reviewed applications of 3-D DDA.

Relatively little work on the development of the DDA in particulate media has been published. Disk-based DDA in 2-D to model particulate media was presented by Ke and Bray [34]. Rein and Andrés [35] used the method to model granular transport in vibrating feeders. The ability of the DDA to model the response of systems of disks was presented by Thomas and Bray [36], Thomas [37], and Koyama et al. [38]. Beyabanaki and Bagtzoglou [1, 39] presented a new formulation of sphere-based 3-D DDA. The same authors presented a disk-based 2-D DDA with a new contact model (Beyabanaki and Bagtzoglou [40]) and investigated the accuracy of dynamic disk-based DDA (Beyabanaki and Bagtzoglou [41]). Beyabanaki et al. [42] successfully applied disk-based DDA to simulate the Donghekou landslide triggered by the Wenchuan earthquake. A friction contact model in sphere-based 3-D DDA was presented by Huang et al. [43]. Wang et al. [44] presented a new sphere-to-edge contact for sphere-based 3-D DDA. Recently, discontinuous deformation analysis for ellipsoids using cone complementary formulation was presented by Fan et al. [45].

The penalty method was used in the sphere-based 3-D DDA studies to enforce contact constraints at the sphere interface. The accuracy of the contact solution depends highly on the choice of the penalty number, and the optimal number cannot be explicitly found beforehand. A very high penalty number leads to progressive ill-conditioning of the resulting system, and low value leads to overlaps between spheres or spheres and boundaries. Therefore, high-accuracy solutions may not be obtained using this method.

The Augmented Lagrangian Method (ALM) is a well-known method to overcome these problems for equality constrained problems [46]. In this study, contact constraints are enforced in sphere-based 3-D DDA using this method. Two illustrative examples are presented to demonstrate this new approach.

## II. SPHERE-BASED 3-D DDA

Sphere-based 3-D DDA is an implicit technique, and involves formulation and solution of a system of simultaneous equilibrium equations. In this method, the total potential energy is the summation of all potential energy sources for each sphere, which involves the potential energy contributed by the point loads on a sphere, inertia forces, volume forces, fixed points, and potential energy when the spheres contact each other.

Assuming that the spheres are rigid, the relation between them can be presented as below [1]:

$$\begin{Bmatrix} u \\ v \\ w \end{Bmatrix} = [T_i(x, y, z)] \cdot \{D_i\} \quad (1)$$

where

$$[T_i(x, y, z)] = \begin{pmatrix} 1 & 0 & 0 & 0 & (z - z_0) & - (y - y_0) \\ 0 & 1 & 0 & - (z - z_0) & 0 & (x - x_0) \\ 0 & 0 & 1 & (y - y_0) & - (x - x_0) & 0 \end{pmatrix} \quad (2)$$

and

$$\{D_i\}^T = \{u_0 v_0 w_0 r_x r_y r_z\} \quad (3)$$

$(x_0, y_0, z_0)$  are the coordinates of the sphere center, and  $(u_0, v_0, w_0)$  represents rigid body translations;  $(r_x, r_y, r_z)$  indicates the rotation angles in radians of sphere  $i$  with a rotation centre at  $(x_0, y_0, z_0)$ .  $[T_i(x, y, z)]$  is the first order displacement function, and  $\{D_i\}$  is the vector of displacements of sphere  $i$  in three dimensions.

To eliminate the possibility for the error of free expansion under rigid body rotation, the exact solution for the displacements can be used to compute the components of  $(u, v, w)$  due to  $(r_x, r_y, r_z)$  by extending the following rigid body rotation:

$$\begin{cases} u = u_0 + (x - x_0)(\cos r_z - 1) - (y - y_0) \sin r_z \\ + (z - z_0) \sin r_y + (x - x_0)(\cos r_y - 1) \\ v = v_0 + (x - x_0) \sin r_z + (y - y_0)(\cos r_z - 1) \\ + (y - y_0)(\cos r_x - 1) - (z - z_0) \sin r_x \\ w = w_0 + (z - z_0)(\cos r_y - 1) - (x - x_0) \sin r_y \\ + (y - y_0) \sin r_x + (z - z_0)(\cos r_x - 1) \end{cases} \quad (4)$$

The total potential energy for an N spheres system can be expressed in matrix form as follows:

$$\begin{bmatrix} [K_{11}] & [K_{12}] & [K_{13}] & \dots & [K_{1N}] \\ [K_{21}] & [K_{22}] & [K_{23}] & \dots & [K_{2N}] \\ [K_{31}] & [K_{32}] & [K_{33}] & \dots & [K_{3N}] \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ [K_{N1}] & [K_{N2}] & [K_{N3}] & \dots & [K_{NN}] \end{bmatrix} \begin{Bmatrix} \{D_1\} \\ \{D_2\} \\ \{D_3\} \\ \vdots \\ \{D_N\} \end{Bmatrix} = \begin{Bmatrix} \{F_1\} \\ \{F_2\} \\ \{F_3\} \\ \vdots \\ \{F_N\} \end{Bmatrix} \quad (5)$$

where  $\{D_i\}$  and  $\{F_i\}$  indicate displacement variables and loading and moments caused by the stresses and external forces acting on sphere  $i$ , respectively. The stiffness submatrices  $[K_{ij}] \quad |_{i=j}$  depend on the material properties of sphere  $i$ , and  $[K_{ij}] \quad |_{i \neq j}$  is defined by the contacts between spheres  $i$  and  $j$ . The equilibrium equations for each time step are derived by minimizing the total potential energy. The total potential energy  $\Pi$  is the summation over all potential energy forms calculated as below [1]:

$$\Pi = \pi_e + \pi_{is} + \pi_p + \pi_b + \pi_i + \pi_c + \pi_n + \pi_s + \pi_f \quad (6)$$

where  $\pi_e$  = the potential energies due to disk stiffness;  $\pi_{is}$  = the potential energy due to initial stress;  $\pi_p$  = the potential energy due to point loading;  $\pi_b$  = the potential energy due to body force;  $\pi_i$  = the potential energy due to inertia forces;  $\pi_c$  = the potential energy due to constrained spring;  $\pi_n$  = the potential energy due to normal contact;  $\pi_s$  = the potential energy due to shear contact; and  $\pi_f$  = the potential energy due to friction force.

The simultaneous equations are derived by minimizing the total potential energy  $\Pi$  of the disk system:

$$\begin{aligned} [K_{ij}] &= \frac{\partial^2 \Pi}{\partial d_{ir} \partial d_{js}}, r, s = 1, 2, 3 \\ \{F_i\} &= -\frac{\partial \Pi(0)}{\partial d_{ir}}, r = 1, 2, 3 \end{aligned} \quad (7)$$

where 0 refers to the initial state of each time state.

### III. COMPARISON BETWEEN THE PENALTY METHOD AND ALM

The main features of the penalty method are [47]:

- There are no extra equations required by enforcement of constraints.
- The solution can easily be obtained by simply adding contact components to the stiffness matrix.
- The contact solution depends highly on the choice of the penalty number. The constraints are only satisfied in an approximate manner, and the optimal number cannot be explicitly found beforehand.
- If the penalty number is too large, the simultaneous equilibrium matrix becomes difficult to solve. However, the constraints are poorly satisfied if it is too low.

The ALM uses penalty stiffness but iteratively updates the contact traction to impose the contact constraints with a specified precision. The main features of this method are:

- In this method, no additional equations are required.
- In order to avoid the ill conditioning of the stiffness matrices, large penalty values are not required. Nevertheless, if the initial penalty number is too small, a large number of iterations is required.
- The constraints are satisfied within a user-defined required tolerance.

### IV. CONTACT MECHANICS USING ALM

In the penalty method, when a sphere-sphere or sphere-boundary contact occurs, the normal spring with a stiffness of  $P_n$  is introduced into the formulation to return the point to the surface along the shortest distance.

As shown in Figure 1, assume  $P_1(x_1, y_1, z_1)$  indicates the location of the reference point of sphere  $i$  before a displacement increment and  $P_1^*$  represents the location after the displacement increment. The point  $P_0(x_0, y_0, z_0)$  represents the projection of point  $P_1$  on the reference plane  $S$  and  $P_0^*$  indicates this point after the displacement increment. Moreover, assume  $(u_1, v_1, w_1)$  and  $(u_0, v_0, w_0)$  are the displacement increments of points  $P_1$  and  $P_0$ , respectively, and the unit normal vector of the reference plane  $S$  is  $\hat{n}$ .

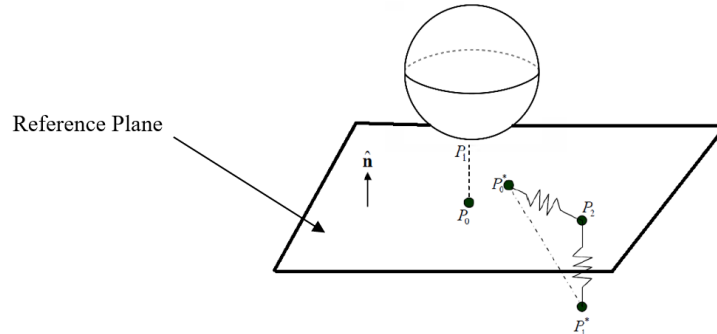


Fig.1. Sphere-sphere and sphere-boundary contacts(adapted from Beyabanaki and Bagtzoglou[1])

When using the ALM, the contact force at the contact point can be accurately approximated by iteratively calculating the Lagrange multiplier  $\lambda^*$ . A first-order updated value for  $\lambda^*$  can be written as follows:

$$\lambda \approx \lambda_{i+1}^* = \lambda_i^* + P_n \cdot d_n \tag{8}$$

where the penalty number,  $P_n$ , can be variable and does not have to be a very large number as in the penalty method. In Equation (8),  $\lambda_i^*$  is the Lagrange multiplier at the  $i$ -th iteration and  $\lambda_{i+1}^*$  is the updated Lagrange multiplier, and the normal distance  $d_n$  of point  $P_1^*$  from the reference plane  $S$  is:

$$d_n = M + [H_i][D_i] - [Q_j][D_j] \tag{9}$$

where

$$M = \hat{n} \cdot \begin{bmatrix} x_1 - x_0 \\ y_1 - y_0 \\ z_1 - z_0 \end{bmatrix} \tag{10}$$

$$[H_i] = \hat{n} \cdot T_i(x_1, y_1, z_1) \tag{11}$$

$$[Q_j] = \hat{n} \cdot T_j(x_0, y_0, z_0) \tag{12}$$

At the  $i$ -th iteration, the potential energy resulting from the contact force is calculated as follows:

$$\pi = \lambda_i^* d_n + \frac{1}{2} P_n d_n^2 \tag{13}$$

Equation (13) consists of two components. The first component is the strain energy resulting from the iterative Lagrange multiplier  $\lambda_i^*$ , and the penalty constraint creates the second. The contribution of the second component to the simultaneous equilibrium equations was already derived by Beyabanaki and Bagtzoglou [1].

The first component of Equation (13) can be written as:

$$\pi^* = \lambda_i^* \left( \frac{M}{l} + [H_i][D_i] - [Q_j][D_j] \right) \tag{14}$$

The derivatives of  $\pi^*$  with respect to  $d_{ki}$  and  $d_{kj}$  at zero are:

$$f_{ki} = - \frac{\partial \pi^*(0)}{\partial d_{ki}} \tag{15}$$

$$f_{kj} = - \frac{\partial \pi^*(0)}{\partial d_{kj}} \tag{16}$$

where 0 refers to the initial state of each time state. They form the following submatrices:

$$f_{ki} = -\lambda_i^* \cdot [H_i] \tag{17}$$

$$f_{kj} = -\lambda_i^* \cdot [Q_j] \tag{18}$$

For the ALM, the combined contribution of the first and second components of Equation (13) to the simultaneous equilibrium equation is summarized below.

The following matrices can be added to submatrices  $[K_{ii}]$ ,  $[K_{ij}]$ ,  $[K_{ji}]$ , and  $[K_{jj}]$  in the global stiffness matrix:

$$[K_{ii}] = P_n [H_i]^T [H] \tag{19}$$

$$[K_{ij}] = P_n [H_i]^T [Q_j] \tag{20}$$

$$[K_{ji}] = P_n [Q_j]^T [H_i] \tag{21}$$

$$[K_{jj}] = P_n [Q_j]^T [Q_j] \tag{22}$$

and the following vectors are calculated and then added to the global force vector:

$$[F_i] = -(\lambda_i^* + P_n \frac{M}{l}) \cdot [H_i]^T \tag{23}$$

$$[F_j] = -(\lambda_i^* + P_n \frac{M}{l}) \cdot [Q_j]^T \tag{24}$$

The final exact contact forces can always be obtained by the iterative method, even with small initial values of the penalty number. The iterative procedure for the ALM is presented in Figure2.

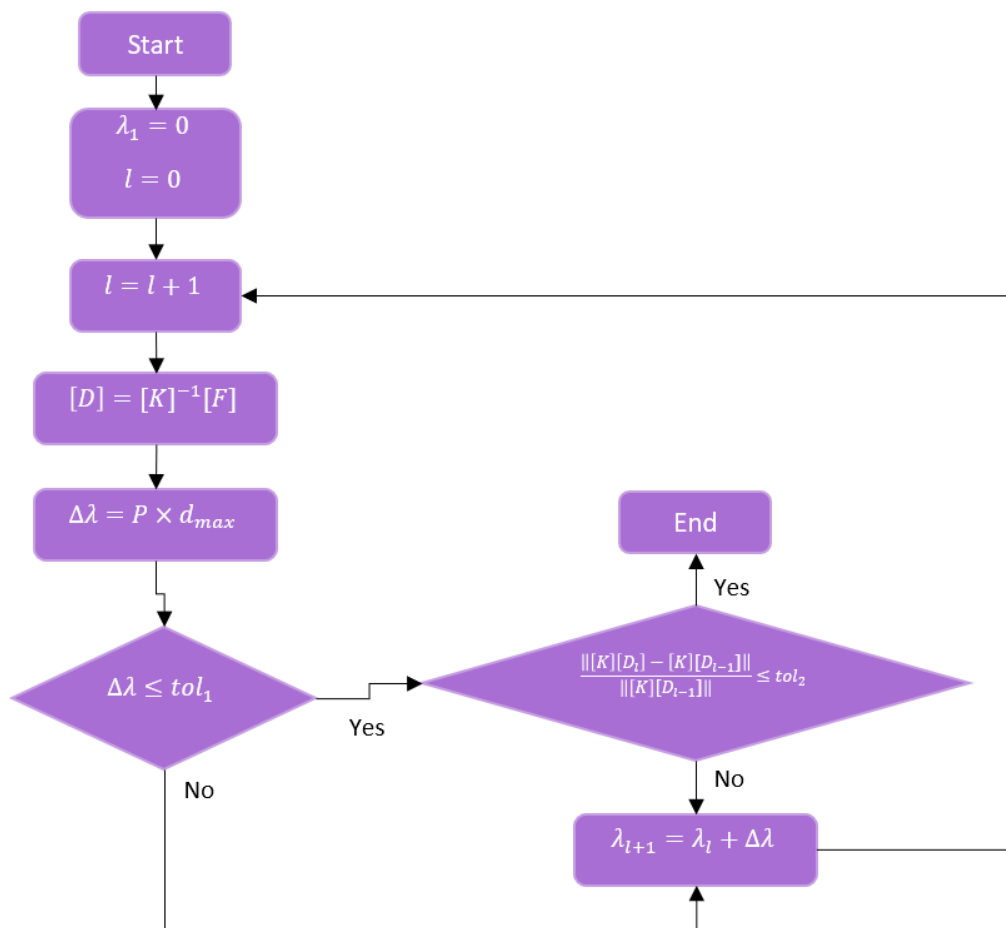


Fig.2. Flowchart of ALM procedure used in sphere-based 3-D DDA

**V. EXAMPLE 1: FUNNEL FLOW**

To investigate the proposed contact mechanics, an example of funnel flow is presented, and the results are compared with the results obtained by using the penalty method in the original formulation.

As shown in Figure 3, there are two layers of spheres with different sizes above a funnel that travel vertically because of gravity. Each disk has a density of  $2500 \text{ kg/m}^3$ ; and the stiffness of the normal contact spring, the time step size, and the friction angle are  $P = 1 \times 10^5 \text{ N/m}$ ,  $0.01\text{s}$  and  $5^\circ$ , respectively. Figures 4 and 5 show the configuration of spheres after 6s and 8.6s using the penalty method and the ALM, respectively. As

can be seen, when using the ALM, no sphere interpenetration occurs, even though the initial penalty number is low. However, without the ALM, there is contact overlap and interpenetration.

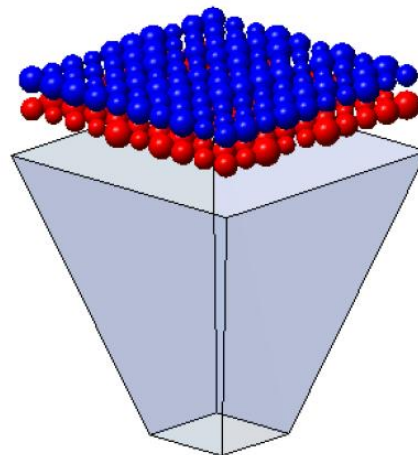


Fig.3. Initial configuration of the funnel system

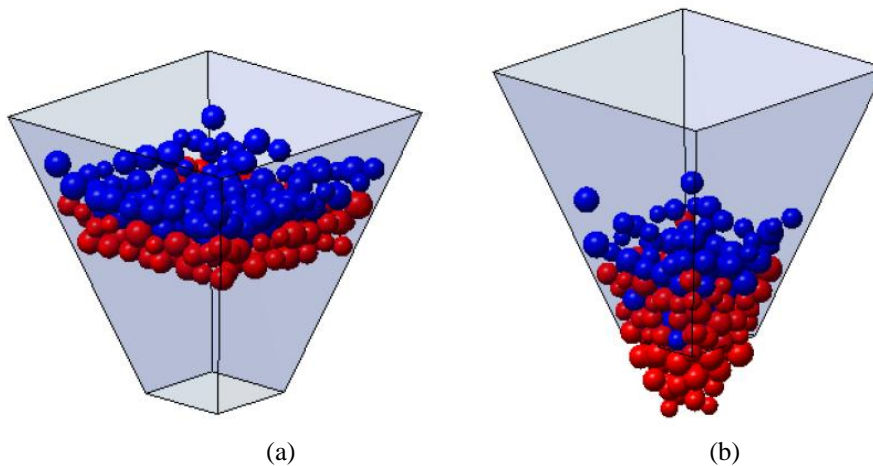


Fig.4. Results of sphere-based 3-D DDA using the ALM: (a) after 6s, (b) after 8.6s

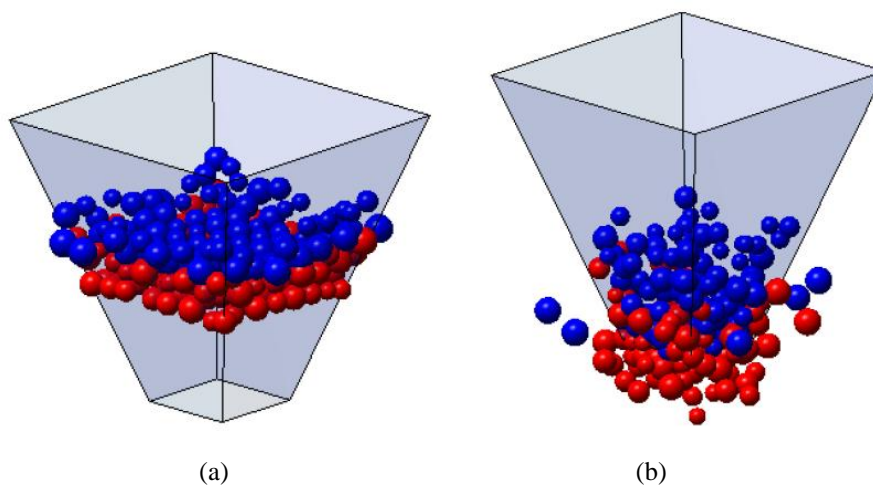
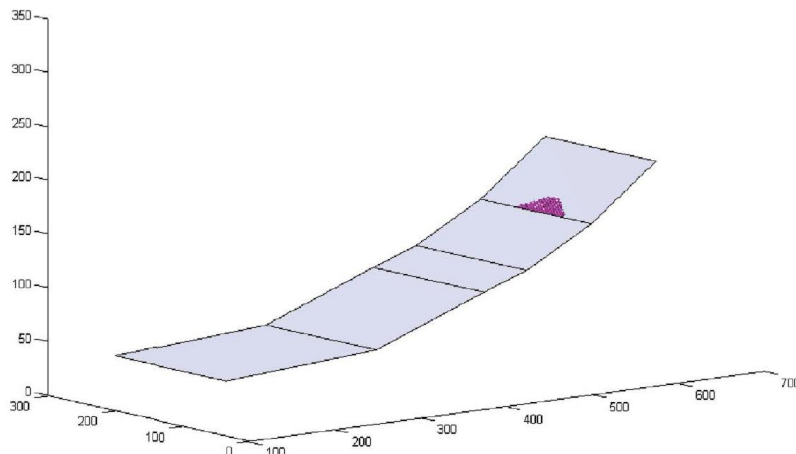


Fig.5. Results of sphere-based 3-D DDA using the penalty method: (a) after 6s, (b) after 8.6s

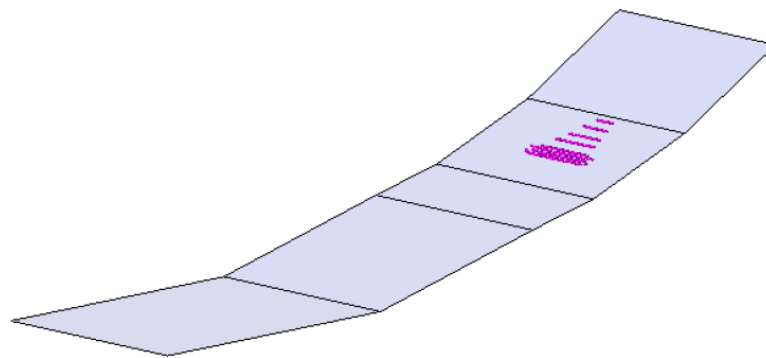
**VI. EXAMPLE 2: MULTIPLE SLOPES**

The example used to test the original developed contact theory for sphere-based 3-D DDA (Beyabanaki and Bagtzoglou [1]) is presented in this section, and the results are compared with the results obtained by using the penalty method in the original formulation.

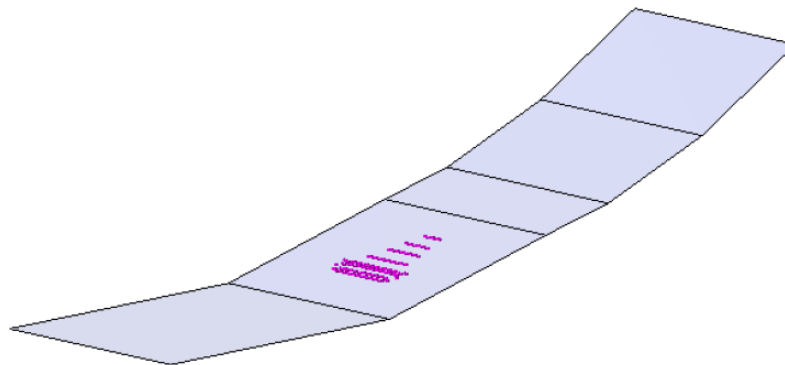
This case is a landslide analogy. In this example, as shown in Figure 6, a slope including five inclined planes is considered. A total of 180 spheres rest on the highest inclined plane. Under the action of gravitational force, the spheres move on the planes. Density of the spheres is  $3500 \text{ kg/m}^3$ , and the stiffness of the normal contact spring and the time interval are assumed to be  $P = 1 \times 10^4 \text{ kN/m}$  and  $0.05\text{s}$ , respectively. Figures 7 and 8 show the configuration of spheres after 20s, 47s, and 63s using the penalty method and the ALM, respectively. As can be seen, the spheres move along the inclined planes without any violation of boundary planes constraints when the ALM is used. However, as shown in Figure 8, a small penalty number with the classical penalty method is unable to enforce the interpenetration constraint.



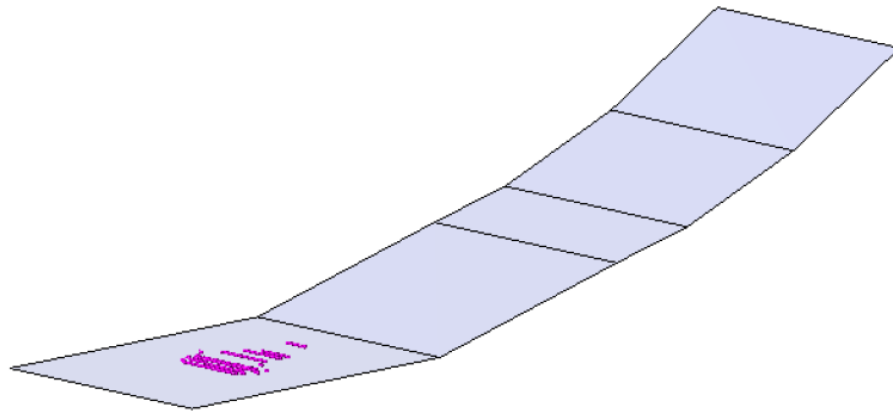
**Fig.6. Initial configuration**



(a)

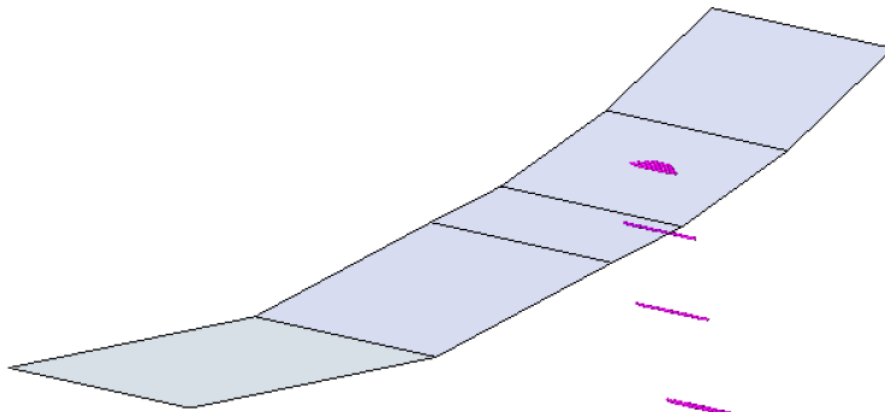


(b)

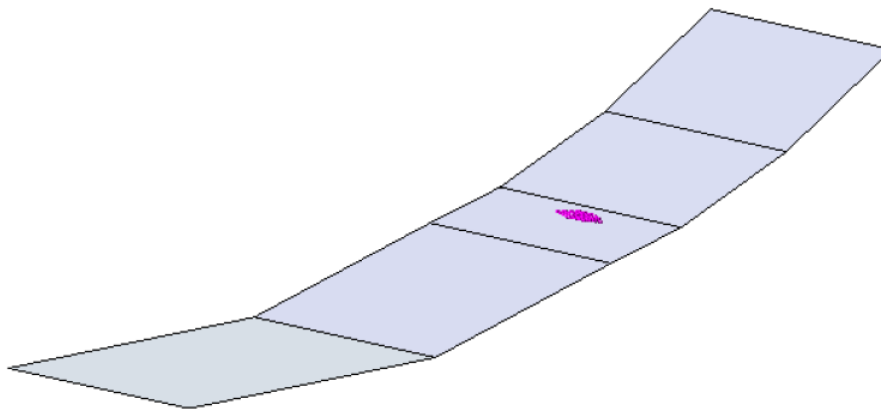


(c)

Fig.7. Results of sphere-based 3-D DDA using ALM: (a) after 20s, (b) after 47s (c) after 63s



(a)



(b)



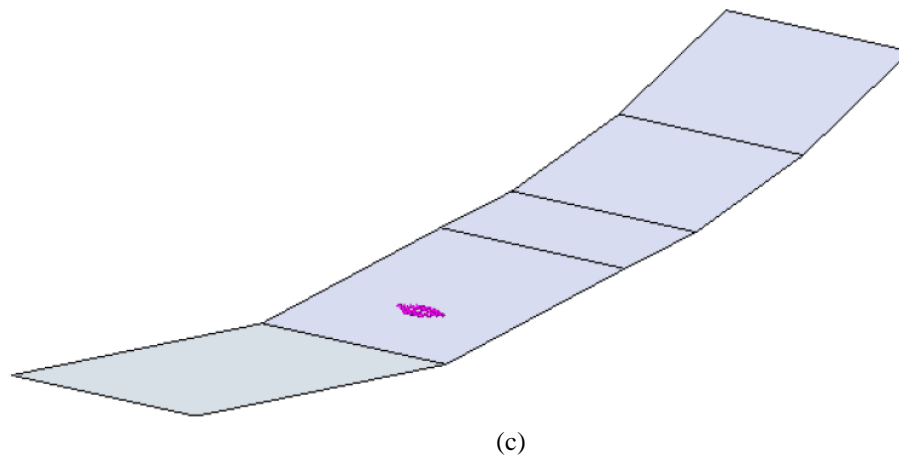


Fig.8. Results of sphere-based 3-D DDA using the Penalty method: (a) after 20s, (b) after 47s (c) after 63s

## VII. CONCLUSIONS

In the existing sphere-based 3-D DDA method, the contact constraints are enforced using the penalty method. The contact solution depends highly on the choice of the penalty number in this approach. Also, the optimal number cannot be explicitly found beforehand. If the penalty number is too low, the constraints are either not met or poorly satisfied. However, if the number is too large, the simultaneous equilibrium equations become difficult to solve. Therefore, it is important to use the ALM approach. In this paper, contact constraints are enforced using the ALM and two illustrative examples are presented to demonstrate the new model. Using the ALM to enforce contact restraints retains the simplicity of the penalty method and reduces its disadvantages.

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