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BOUNDARY IDENTIFICATION AND WEAK PERIODIC CONDITION APPLICATION IN DEM METHOD

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Abstract: Meshless character of the DEM method brings forth certain problems that must be solved in a computer implementation, such as the determination of the neighbouring particles, determining the boundaries of the model and the definition of boundary conditions. During large deformations of the model a particular internal particle may become boundary particle and the other way round so it is necessary to re-determine the boundary layer after a given number of steps in the analysis. In this paper, two approaches for defining the boundary layer are shown, whose effectiveness depends on the current positions of the particles, and imperfections in their arrangement. Due to the large computer requirements of the DEM method, only a small part of the real problem is modelled and continuity can be achieved by using periodic boundary conditions. Since the DEM particles have arbitrary radius and the boundary is often irregular, it is not possible to achieve the classic periodic boundary conditions in which the particle that leaves the model on one side enters the model on the other side, but it is possible to apply a soft periodic boundary conditions that transmit only the force from one to another end of the model. Previously mentioned routines are applied to the modelling of shear in the critical layer of granular material.

Key words: DEM method, boundary layer, periodic boundary conditions

1. INTRODUCTION

Granular materials are the second most manipulated material in engineering (water is first), so understanding their behavior is crucial in designing new machines for their transportation, manipulation and processing. Theoretical study of stress and strains in granular material gives great insight into grain interaction [1] while experimental testing shows behavior of whole granular material such as failure of

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overloaded material along narrow shear bands [2]. Within these shear bands vortexes are formed and dissolved and dilatation of material in shear band is observed [2]. To analyze these phenomena a numerical method called Discrete Element Method (DEM) is used [3]. DEM method is based on modeling inter-particle contact forces using non-linear elastic Hertz law which requires very small time step to achieve accurate results [4]. Loads in granular material are not transmitted equally over the whole volume of material, with most of the load transmitted over certain particles that form "force chains", while other particles only have supportive role [5]. During deformations of granular material some chains are broken while new ones are formed [5]. These deformations are sum of all translations and rotations of granular particles, where rotations are more likely to occur due to lower friction coefficient. Rotations also require smaller time step for the calculations [4]. Since this method is very computationally demanding, most of the problems that are analyzed are modeled in 2D using only a section of real-life problems. Determination of the boundary layer is important in the DEM analysis because through the particles of the boundary layer loads are imposed that simulate the interaction of the analyzed part of the granular material with the environment.

2. IDENTIFICATION OF THE BOUNDARY LAYER

In order to include entire model in analysis of boundary layer we must first find the most left particle, then we continued counter-clockwise searching for next boundary particle, until we reach the beginning of the boundary layer (most left particle). We used two methods to search for next boundary particle:

- The most right method
- Smallest deviation angle method

In both methods we have previous particle p_1, current particle p_2 and we search all particles connected to particle p_2 for the best candidate for the next particle p_3. Both methods compare angles in order to find proper next particle.

In the most right method, vector between current and previous particle is defined with $\vec{r}_1 = (x_2 - x_1, y_2 - y_1)$, while $\vec{r}_2 = (x_3 - x_2, y_3 - y_2)$ is calculated for every possible next particle, like it is illustrated in Figure 1.

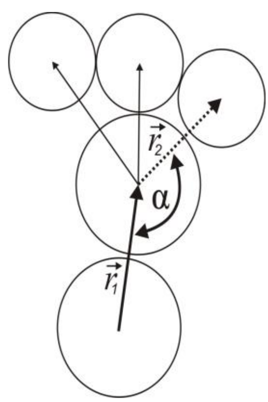


Figure 1. *Identification of the next boundary particle using the most right method*

Using dot product of vectors $\vec{r}_1 \cdot \vec{r}_2 = |\vec{r}_1| \cdot |\vec{r}_2| \cos\alpha$ we can calculate cosine of angle between vectors using equation (1)

$$\cos\alpha = \frac{(x_2 - x_1)(x_3 - x_2) + (y_2 - y_1)(y_3 - y_2)}{\sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2} \cdot \sqrt{(x_3 - x_2)^2 + (y_3 - y_2)^2}} \tag{1}$$

From equation (1) we can obtain angle using arc cosine function and search all contacts for minimum angle (most right particle) but since arc cosine is very expensive mathematical operation, we can avoid using it and search for maximum cosine (which would yield minimum angle). In order to account all possible cases for positions of particles the following if condition is formulated, using equation (2)

$$\begin{aligned} &if\left(\left(\left(x_2 - x_1\right)\left(y_3 - y_2\right) - \left(y_2 - y_1\right)\left(x_3 - x_2\right)\right) > 0\right) then \quad \cos\alpha = \cos\alpha - 2 \\ &\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad else \quad \cos\alpha = -\cos\alpha \end{aligned} \tag{2}$$

The smallest deviation angle method aims to keep boundary as straight as possible which could lead to some particles remain outside of the boundary, but the boundary has more regular particle arrangement. This method is illustrated in Figure 2.

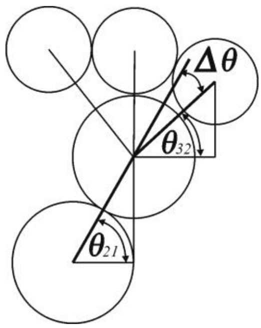


Figure 2. *Identification of the next boundary particle using the smallest deviation method*

Excluded particles can be moved by another routine to more appropriate position and are included in the next boundary search. Angles between vectors and x axis is defined by equations (3) and (4).

$$\theta_{21} = \mathrm{a}\tan\frac{y_1 - y_2}{x_1 - x_2} \tag{3}$$

$$\theta_{32} = \mathrm{a}\tan\frac{y_3 - y_2}{x_3 - x_2} \tag{4}$$

Difference between these angles is the value that we seek to minimize, as given in equation (5)

$$\Delta\theta = \theta_{23} - \theta_{21} \tag{5}$$

Efficiency of both methods depends on several factors such as distance tolerance for determination of neighboring particles. A situation that arises if this parameter is not defined appropriately is shown in Figure 3.

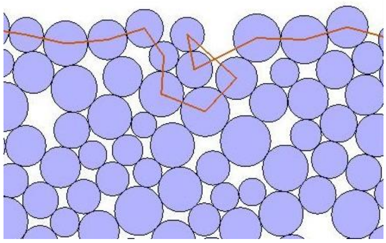


Figure 3. *Selection of wrong boundary particle due to large distance between particles*

Another problem that may occur due to large displacements of particles and that may cause failure of boundary routines is formation of groups of particles that dangle on the sides of the model, Figure 4.

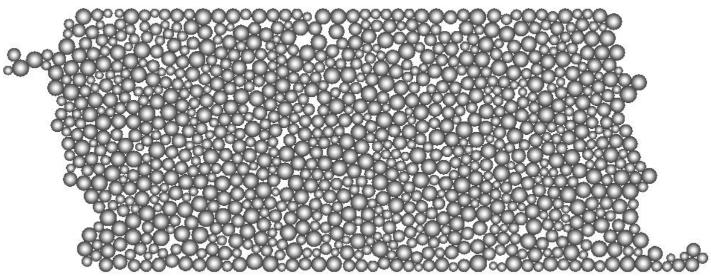


Figure 4. *Formation of groups of dangling particles*

3. APPLICATION OF WEAK PERIODIC CONDITION IN DEM

In order to reduce irregular arrangement of boundary particles which could cause failure of both methods for boundary identification, weak periodic boundary condition is implemented. Classical periodic boundary condition is not applicable to DEM method, because DEM particles have arbitrary radius so that moving certain particle from one side to another could lead to significant overlapping of particles if particular particle has greater radius than there is void space available on the other side. Weak boundary condition only transfers force from one boundary to the other, while particles remain part of their respective boundaries. Force that needs to be transferred to certain particle *k* can be calculated as partial derivate of work given by equation (6)

$$F_k = \frac{\partial W}{\partial v_k} \tag{6}$$

where v_k is horizontal velocity of particle *k.* If we observe certain boundary particle *k* we can see that it is connected to particles *k-1* and *k+1*, while on the other side at the same height there is boundary line that connects particles *m* and *m+1*, as illustrated in Figure 5.

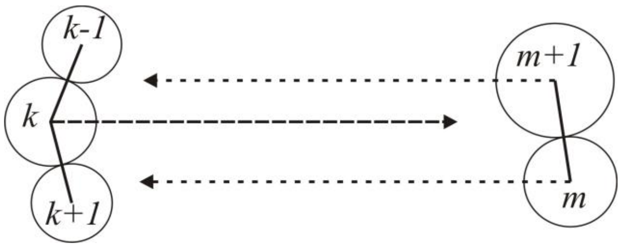


Figure 5. *Particles in boundary layer*

Considering all particles on the left and right side, work on the boundary is given with equation (7)

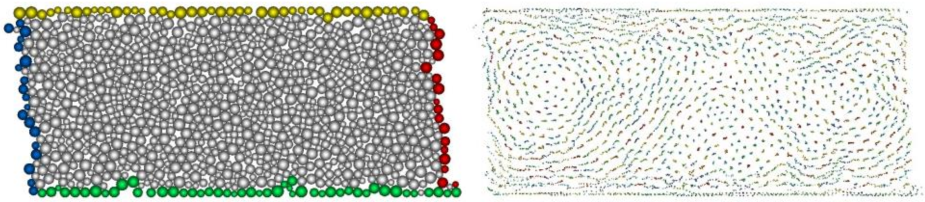
$$W = \sum_L \frac{1}{2} K \left(v^L - \tilde{v}^D \right)^2 + \sum_D \frac{1}{2} K \left(v^D - \tilde{v}^L \right)^2 \tag{7}$$

where *L* is the number of particles on the left side while *D* is the number of particles on the right side. K is the coefficient that depends on average particle mass. Velocity of the real particle on the left side is given with v^L while $\tilde{v}^D$ represents interpolated velocity on the right boundary line. The same notation applies for velocities on the right boundary. Solving partial differential equation (6) for work calculated using equation (7) gives us the force that needs to be applied on particle *k*, which is calculated using equation (8).

$$F_k = \frac{\partial W}{\partial v_k} = K \left[\begin{array}{l} v_k^L - v_{m+1}^D \dfrac{y_k^L - y_m^D}{y_{m+1}^D - y_m^D} + v_m^D \dfrac{y_k^L - y_{m+1}^D}{y_{m+1}^D - y_m^D} - \\ v_m^D \dfrac{y_m^D - y_{k+1}^L}{y_k^L - y_{k+1}^L} + v_k^L \left(\dfrac{y_m^D - y_{k+1}^L}{y_k^L - y_{k+1}^L} \right)^2 - v_{k+1}^L \dfrac{y_m^D - y_{k+1}^L}{y_k^L - y_{k+1}^L} \dfrac{y_m^D - y_k^L}{y_k^L - y_{k+1}^L} + \\ v_{m+1}^D \dfrac{y_{m+1}^D - y_{k-1}^L}{y_{k-1}^L - y_k^L} + v_k^L \left(\dfrac{y_{m+1}^D - y_{k-1}^L}{y_{k-1}^L - y_k^L} \right)^2 - v_{k-1}^L \dfrac{y_{m+1}^D - y_k^L}{y_{k-1}^L - y_k^L} \dfrac{y_{m+1}^D - y_{k-1}^L}{y_{k-1}^L - y_k^L} \end{array} \right] \tag{8}$$

4. RESULTS

Two methods for boundary identification are implemented in DEM code and used in analysis of shear bands in granular material. In order to prevent large deformations of the boundary and irregular arrangement of particles weak periodic boundary condition is implemented. Figure 6a shows the model with boundary layer used to impose velocities on top and bottom particles, with weak periodic condition applied on left and right side. Figure 6b shows the formation of vortexes in modeled problem.



a) b)

Figure 6. *Analysis of granular material shear process a) model with boundary b) vortex formation in model*

5. CONCLUSION

Both analyzed methods are very accurate in identification of boundary particles, but also, they both have limitations which could be exceeded if deformation of model becomes too large and arrangement of particles too irregular. In some distorted particle configurations the first method was able to successfully identify whole boundary while the second method failed, but in some other configurations the first method failed and the second method succeeded. These methods could complement each other, with one method chosen to be primary and used by default, and if it fails to identify the whole boundary the other (secondary) method could be called in to attempt to complete the task. Weak periodic boundary condition virtually connects right and left boundary of the model creating impression of continuity. Using these routines, behavior of granular material in shear band can be successfully modeled and formation of vortexes can be observed.

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