A method for generating a block system of coarse granular materials that strictly meet gradation requirements

Dongdong Xu, Shaozhong Lin, Bo Lu, Aiqing Wu, Jin Wang, Jiajun Pan and Shuai Wang

Key Laboratory of Geotechnical Mechanics and Engineering of Ministry of Water Resources, Changjiang River Scientific Research Institute, Wuhan, 430010, China

Abstract. The discontinuous deformation analysis (DDA) method provides unique advantages in simulating the mechanical properties of coarse granular materials. However, the DDA method cannot automatically generate numerical samples of coarse granular materials that can strictly meet the gradation requirements. Therefore, to solve this problem, a new generation method is proposed for generating a block system of coarse granular materials. First, a particle is randomly selected from the basic morphology database and randomly scaled and rotated to match the particle size requirements of the current gradation, based on the relevant requirements for laboratory tests of coarse granular materials. The accumulated particle area will enter the next gradation when it meets the area proportion requirements of the gradation, and this step is repeated gradually from the large particle size group to the small particle size group. Second, the random drop area, which has the same diameter as the coarse granular sample but a height several times that of the sample, is defined. The particles are randomly placed in this area in order of large to small particle size groups, and the requirements of nonoverlapping and noncrossing between particles or between particles and boundaries must be met. When the efficiency of random dropping is very low or even fails, it is important to keep increasing the sample height multiplier. Third, a DDA-based compaction operation is performed to obtain a stable block system with close particle contact. Fourth, a coarse granular material sample that fully meets the gradation requirements is obtained by gradually adjusting the height of the prepared sample. Finally, an example is used to demonstrate the feasibility of the proposed algorithm.

1. Introduction

Coarse granular materials are cohesionless mixtures composed of block stone, crushed stone, gravel, sand, and other coarse particles [1-2]. Coarse granular materials are widely used in engineering constructions because of their wide distribution in nature, large reserves, good compactness, strong water permeability, high shear strength, difficulty in producing liquefaction, and other excellent characteristics. Owing to the increase in high earth-rock dams, expressways, and high-speed railways, research into the gradation and mechanical properties of coarse-grained materials has become important in geotechnical engineering [3-5].

Compared to in situ and indoor tests of coarse granular materials, the numerical simulation method offers the following general advantages: no need to consider the scale effect, reduction of labor, saving material resources, and low time and space dependence [6-7]. The most important property is that it is not limited by experimental conditions and scale effects, and it can control the critical state of feature deformation repeatedly and freely [8]. Therefore,
numerical simulation is required to study the gradation and mechanical properties of coarse granular materials. It can be combined with in situ and laboratory tests to provide additional information.

Currently, the numerical simulation method of coarse granular materials is mainly based on the discrete element software, Particle Flow Code (PFC). The PFC software has a rigid and unbreakable disk that cannot naturally simulate the influence of the particle shape of coarse granular materials on their mechanical properties [9-11]. Therefore, PFC uses a basic unit to form a fragmentable particle cluster to represent the polygon block, which is based on cluster technology. However, the cluster is still unable to deform and break after being broken down into basic elements. Thus, the method still requires improvement in terms of the rotation-induced friction problem [12].

The discontinuous deformation analysis (DDA) method, which has perfect theories, rigorous assumptions, and high computational efficiency, uses irregular polygons to characterize the shape of particles. It can rotate and slide the block at the same time, and its open–close iteration algorithm can accurately simulate particle contact [13-14]. Evidently, the DDA method offers some theoretical advantages in the study of coarse granular materials. However, the DDA method does not have the function of automatically generating polygonal particles to meet gradation requirements for coarse granular material simulations, implying that the problem of particle generation and placement in the DDA method must be solved. Currently, most studies on the generation and placement of irregular polygonal particles have mainly focused on concrete aggregates, where the aggregate just serves as a skeleton and does not require mutual contact. Since the coarse granular material particles are in contact with each other, the above methods cannot be directly used for modeling coarse granular materials [15]. A combination of the finite element method and discrete element method provides a generation method for the numerical modeling of coarse granular materials, but the generated samples do not strictly meet the grading requirements of coarse granular materials [16]. Therefore, to use the advanced DDA method to simulate the mechanical properties of coarse granular materials, a method for generating DDA block systems of coarse granular materials that strictly meet gradation requirements must be developed.

2. Generation method of the DDA system

According to the coarse-grained indoor test requirements, polygonal particles that meet the grading requirements are randomly selected based on the basic morphology database and randomly placed in a designated area, which requires that the particles meet the requirements of noncrossing of boundaries and nonoverlapping. Thereafter, a DDA block system with close particle contact and a stable overall structure can be obtained by compaction. The appropriate numerical model for coarse granular materials can be obtained by adjusting the height of the prepared sample. The following is a detailed technical scheme.

Table 1. The gradation of coarse granular materials

| Particle size (mm) | 60  | 40  | 20  | 10  | 5  |
|-------------------|-----|-----|-----|-----|----|
| Percentage of particles less than the particle size (%) | 100 | 89.1| 69.5| 45.1| 0  |

1) First, the basic morphology database of coarse granular material must be established. The particle shape, which can be either triangle, convex polygon, or concave polygon or a collection of real particle shapes obtained via computed tomography section scanning, can be specified in the database. Thereafter, the translation, rotation, and scaling of the particles in the database are used to establish a numerical model for the coarse granular material. This ensures that the particles of the generated sample are diverse and random.

2) Determine the gradation of the coarse granular material sample to be generated, including the particle size corresponding to each gradation and the volume percentage of particles smaller than this particle size, which are recorded as $P_i^s$ and $Q_i^s$, respectively. The following description is based on the gradation distribution listed in Table 1. The percentage of particles smaller than 60 mm is 100%, the percentage of particles smaller than 40 mm is 89.1%, etc.
3) In a two-dimensional case, the coarse granular sample has a rectangle shape, and its length and height are denoted as $L$ and $H$ respectively. Here, $L = 300 \text{ mm}$, and $H = 600 \text{ mm}$. This demonstrates that the coarse granular particles generated according to the gradation will fill a rectangular area of $300 \text{ mm} \times 600 \text{ mm}$ and have a certain porosity because of the randomness of particle contact. Namely, the total area of the coarse granular particles will be less than $300 \text{ mm} \times 600 \text{ mm}$.

4) Set up a preparation sample with a length equal to that of the coarse granular material sample and a height of $H_a$. In the first sample preparation, let $H_a = H$. In the subsequent sample preparation, the updated $H_a$ will be used. The method for updating will be introduced later. A set of coarse granular material particles that meet the gradation requirements can then be generated, and the total area of the particle set must be consistent with the area ($A_z$) of the prepared sample, where $A_z = L \times H_a$. The positions of these particles are temporarily consistent with those in the database. The particle set is generated from large to small particle sizes, which is beneficial for further random particle extraction and can improve delivery efficiency.

5) The total area ($A_i$) of particles with particle sizes ranging from 60 mm to 40 mm can be determined using equation (1).

$$A_i = A_i \times (Q_i - Q_{i+1})$$

Table 1 shows that the total area of the particles with particle sizes ranging from 60 mm to 40 mm is 19620 mm$^2$.

6) Randomly select a particle from the basic morphological database and calculate its minimum circumscribed diameter ($D$) and area ($A_d$). The random scaling factor ($K_R$) of the particle size that is limited to $P_i \sim P_{i+1}$ can be calculated using equations (2)–(4).

$$K_R = K_r + (K_{u} - K_{r}) \times \text{rand}()$$

$$K_k = P_i / D$$

$$K_k = P_i / D$$

Thereafter, the area ($A_i$) of the generated particle can be expressed as

$$A_i = K_R^2 \times A_d$$

7) Accumulate the area of the generated particles and repeat step (6) until the total area ($A_i$) of the generated particles whose size is within $P_i \sim P_{i+1}$ surpasses the total area ($A_i$) calculated according to the gradation for the first time. To make $A_i$ and $A_i$ strictly equal, the overall size scaling ratio ($L_r$) of the generated particles under the gradation can be calculated using equation (6).

$$L_r = \sqrt{A_i / A_i}$$

8) Next, determine the centroid ($O_m = (x_{m0}, y_{m0})^T$) of the particle, $m$, and calculate the direction vector ($D_m$) from the centroid to the vertex ($j$) of the particle. On this basis, the new coordinate ($D_m'$) of the particle vertex can be obtained by scaling the particle size in the same proportion and rotating the particle at the same random angle ($\theta$), as stated in equations (7)–(9).

$$D_m' = O_m + L_r \times K_s T D_m^i$$

$$D_m = (d_m^i, d_m^j)^T - (x_{m0}, y_{m0})^T$$

$$T = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}$$

9) Continue to the next gradation and return to step (6) to generate new particles until all gradation particles have been generated. Thus far, coarse granular material sets that strictly
meet the gradation requirements have been generated. However, their location is still determined by the database. The following random dropping operation is required to drop them evenly and randomly into the designated dropping area.

10) The random placement area is still a rectangle, and its length is consistent with that of the sample, but the height is set at $3H$, which can be increased or decreased depending on the number of particles and placement efficiency. It is still necessary to simulate particle movement under double loads of compaction and free falling from the model created by random dropping to the construction of the final coarse granular material sample model. Therefore, the thickness or length of the bottom restraint plate, the left and right restraint plates, and the top loading plate used in the random dropping model must be clarified further. At the same time, the height from the bottom of the random dropping model to the bottom constraint plate should be indicated. The purpose of setting this height is to provide sufficient space for the random dropping model to adjust and prevent the “stuck” phenomenon during roof loading and free falling. The DDA method is used to simulate the motion of the random dropping model under external load. It is important to note that the friction angle, bond strength, and tensile strength between particles should be set to 0 before the compaction load is applied to the centroid of the top restraint plate. At the same time, a damping coefficient of 0.99 should be set. On the one hand, it is more efficient than pure static calculation. On the other hand, it can activate the energy dissipation mechanism to prevent the particles from rebounding when they touch the bottom.

11) Establish the random dropping model. The principle of random placement is to place the large particle size group first, followed by the small particle size group. For a particle to be placed, the coordinates of its centroid can be calculated using the simplex integral. Thereafter, randomly select a placement point in the placement area. The initial position of the particle can be determined by placing its centroid there.

12) Determine the rectangular box containing the particles, which is composed of their minimum $x$ coordinate, maximum $x$ coordinate, minimum $y$ coordinate, and maximum $y$ coordinate. Analyze the relationship between the rectangular box containing the particles and the random placement area. If both of them overlap, the random placement point must be reselected. At the same time, determine if the rectangular box of the current particles and the rectangular box of the previously placed particles overlap. If they overlap, the random placement point must also be reset.

13) All particles must be randomly placed as in steps (11) and (12). If the speed of random placement is noticeably slowed or fails, the problem can be rectified by increasing the height of the random placement area. Figure 1 depicts a model that has completed the random placement.

![Figure 1. Randomly placed model (after rotating 90° clockwise)](image)

14) It is easy to determine the vertex information based on the thickness or length information of the loading plate, the bottom constraint plate, and the left and right constraint plates set in step (10), and the four blocks are sequentially numbered after the random blocks. Three fixed points are evenly distributed on the bottom constraint plate and the left and right constraint plates, and one loading point is arranged at the centroid of the loading plate. Thus far, all relevant information required by the DDA geometry file have been obtained, including the starting and ending numbers of the vertex characterizing the block, the vertex coordinates, and the numbers of the block and joint materials (all take 1).

15) The DDA geometry information is written into the file using the “fprintf” function, resulting in a DDA calculation file that can be used for further compaction. To meet the requirements of the DDA for expanding the vertex array, add the 0 elements of 3 rows multiplied by 3 columns after the vertex coordinates of each block.
16) After setting the loading steps, loading curve, maximum displacement ratio, time step, damping, and other related information, use the improved DDA program based on the FORTRAN language for particle compaction simulation. After compaction, extract the appropriate compaction model using the DDA post-processing program.

17) Considering the settings in step (2), the height $H_t$ of the coarse granular model must be greater than $H$ because of the presence of porosity. The ratio of the two heights is $H_t = H/H_r$.

It has been discovered that a coarse granular material system that can approximately meet the gradation requirements can be generated under the height $H_g = H_r \cdot H_r$.

18) Based on the estimated height ($H_g$), set $n$ groups of modulated samples with a height of $H_g = H_g \pm n \cdot \delta$, where $\delta$ is the height interval, such as 2 mm. Repeat steps (2) to (16) to form $2n$ groups of new coarse granular models. Analyze all generated samples and select the height closest to $H$ and record it as $H_t$. Using $\delta = 2$ mm as an example, the height error of the coarse granular model can be kept at 1% or lower. The accuracy can be further improved by adjusting the size of $\delta$.

19) If the upper and lower limits of the height of the particles in the $2n$ group do not include $H$, the height nearest to $H$ should be used as the benchmark, the height interval should be increased, and step (18) should be repeated. In this manner, a particle height combination that limits $H$ can always be discovered. Thereafter, reduce the height interval and repeat steps (18) and (19) 2–3 times. Finally, the coarse granular material sample that strictly meets the height and gradation requirements can be achieved. It should be noted that the number of repetitions of model construction is dependent on the rationality of the test height interval selection and the operator's experience. Simultaneously, dichotomy can also be used to aid fine-tuning to improve the efficiency of the trial. Figure 2 depicts the compaction model of the coarse granular material that strictly meets the gradation requirements.

20) Delete the constraint plate and loading plate, retaining only the coarse granular material information. Place a triangular composite latex film on the left and right sides of the coarse granular material sample, and attach a fixed plate and a loading plate to the top and bottom. In this manner, the generation of a DDA block system for coarse granular materials that strictly meet the gradation requirements is completely realized, as shown in Figure 3.
3. Numerical test

A triaxial compression test of rock and soil was carried out for the DDA block system. In the DDA computation, the maximum displacement ratio in each time step was 0.001, the time step was 0.000005 s, and the spring stiffness was 15 GPa. The rock had a friction angle of 50°, cohesive strength of 5 MPa, and tensile strength of 2 MPa. The step-by-step loading method was adopted, and the axial loading curve is shown in Figure 4. \( \Delta t_o \) represents the time taken to jump from one load level to the next. \( \Delta t_s \) represents the time taken for each level of loading to reach convergence, which is determined according to the displacement convergence criterion. The loading duration of confining pressure \( (\sigma_3) \) is represented by \( t_o \). Figures 5–7 depict the displacement distribution, rotation angle distribution, and stress–strain curve. Additional implementation details can be found in the references [17-19].

![Figure 4. Schematic of the axial loading curve](image)

The feasibility and correctness of the proposed algorithm are validated by the good deformation shape, conjugated fracture surface, and expected stress intensity.

![Figure 5. The distribution of the displacements](image)

![Figure 6. Rotation angle](image)

![Figure 7. Deviatoric stress–axial strain curve](image)
4. Conclusions
A method for generating a DDA block system for coarse granular materials that strictly meet the gradation requirements is proposed, and an example is used to verify it. On this basis, a complete calculation system of DDA simulation of the mechanical properties of coarse granular materials, which can meet all engineering calculation requirements in a two-dimensional case, was formed. However, because the problem of coarse granular materials is a three-dimensional one, the development of a three-dimensional DDA method will be a major research focus in the future.

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