An attempt on the application of the gradient particle size discrete element specimen in rock engineering

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Abstract. The discrete element method is widely used in rock mechanics, but its computational efficiency limits its development. To improve the accuracy of a discrete element model, the particle size of the entire model needs to be decreased according to the current theory. However, only the range of interest (ROI) is usually concentrated, and the background (BG) refinement is a waste of computing power. The paper proposes a gradient particle size specimen modeling scheme. The resolution of ROI is increased while the resolution of BG is retained. The probability of particle generation is derived from the statistical point of view that the porosity should be consistent. The computational performance is analyzed from the perspective of time complexity. With the edge particle size being 2.0 times the central particle size, only about 26% of the computing time is required. A series of unconfined compression experiments are subsequently carried out to verify the modeling scheme. The characteristics of the gradient particle specimen modeling scheme and the uniform particle size specimen modeling scheme are highly consistent, including the load-deform curves, crack propagation curves, crack initiation patterns, and failure patterns. Finally, the deficiencies of the modeling scheme are discussed, including the unconfined compressive strength (UCS) reduction, which is probably due to the reduction of the coordination number. Further research will be conducted.

Keywords. discrete element method, computational efficiency, rock mechanics

1. Introduction
The rock mass is a typical heterogeneous material, and its failure progress includes many discontinuous processes[1]. To study its failure process under load, scholars have conducted extensive experiments[2-5]. However, in-situ experiments and laboratory experiments cost much time and money, and some experiments cannot be carried out. Therefore, numerical methods have become an essential method for scholars to study the mechanical response of rock mass[2-5].

There are many discontinuities in the destruction process of the rock mass. The structure of rock mass contains many discontinuities, such as holes, joints, and grains. The destruction process is a discontinuity process in nature. Therefore, computing methods based on continuum mechanics run into challenges when simulating the failure process of rock masses[6, 7]. Computing methods based
on discrete mechanics can effectively solve the problem in which the discrete element method is widely used. However, the discrete element method is an explicit algorithm, so its computational efficiency is one of the leading limitations of its development.

In practice, scholars and engineers mainly concentrate on the ROI of a model, so most numerical algorithms have solutions to only improve the resolution within the ROI. For example, both the finite element method and the finite difference method have mesh refinement algorithms. However, in the discrete element method, to obtain a higher-resolution model, the entire space has to be refined, which causes a huge waste of computing power. Scholars have attempted to solve this problem, such as coupling using the finite element method and the discrete element method[8, 9]. However, most current discrete element refinement schemes have a contact interface, and the mechanical response at the interface is confusing. Therefore, the paper tried a gradient particle size modeling scheme based on probability distribution to make an exploration of the problem. The scheme effectively saves the computing power of the model. The paper first introduces the generation method of the gradient particle size specimen modeling scheme, then introduces the verification results, and finally introduces its shortcomings and future research.

2. Model establishment
This chapter first introduces the algorithm for establishing the gradient particle size specimen and then analyzes the computational power it can save based on algorithm complexity theory.

2.1. Modeling algorithm of gradient particle size specimen
The traditional discrete element method establishes uniform particle size specimens, in which the particle is generated with the same probability distribution at any location in the model. The location coordinates do not affect the particle size, so the particle size only obeys a specified distribution, such as uniform distribution, Gaussian distribution, or other probability distribution. When generating high-resolution specimens, the uniform particle size specimen modeling scheme makes the whole space refined, including the regions at the edges of the specimens that are far away from the ROI and the regions that are not significantly changed. These regions result in a massive waste of computing power. The paper uses a gradient particle size specimen modeling scheme to make a preliminary attempt to solve this problem.

2.1.1. Probability of particle generation considering spatial coordinates. In the uniform particle size specimen modeling scheme, the density at any location in the model keeps constant in the sense of probability. Thus, in the gradient particle size specimen modeling scheme, the paper maintains this characteristic:

\[ \rho_g(x,y,z) = \rho_u(x,y,z) \equiv \rho_0 # (1) \]

where, \( \rho_g \) is the density of gradient particle size specimen, \( \rho_u \) is the density of uniform particle size specimen, \( \rho_0 \) is the density of laboratory specimens. As a preliminary discussion, only the solution to two-dimensional models is derived. In a unit area, the mass of the gradient particle size specimen and the mass of the laboratory specimen should be consistent:

\[ m_0 = m_g = \int_\Omega P(x,y)\rho_p \pi r_p^2(x,y)d\Omega # (2) \]

where, \( m_0 \) and \( m_g \) are the mass in a unit area of laboratory specimen and numerical specimen, \( P(x,y) \) is the probability of particle generation at the location \((x,y)\), \( \rho_p \) is the density of the particle, \( r_p(x,y) \) is the theoretical particle radius of the location \((x,y)\). The particle radius exists objectively in the whole plane, even if there is no particle is generated at the location \((x,y)\) finally. Meanwhile, another relationship exists between particle density and specimen porosity:

\[ \rho_0 = \rho_p (1 - n_0 ) # (3) \]
where, \(n_0\) is the porosity of the specimen, \(\rho_0\) is the density of the specimen, which is a material constant. Thus, the probability of particle generation at the point with plane coordinates \((x, y)\) can be derived:

\[
P(x, y) = \frac{\rho_0}{\rho_p} \frac{1}{\pi r_p^2(x, y)} = (1 - n_0) \frac{1}{\pi r_p^2(x, y)}
\]

As is shown, the particle generation probability at a particular location is a function of the particle radius. Therefore, with the radius distribution specified, based on the assumption that the density of the specimen is constant, the particle generation probability distribution on the plane can be derived.

2.1.2. Particle radius distribution specification. The particle radius distribution is a function of coordinates. Particle generation requires the particle radius distribution. For different experiments and different specimens, the particle radius distributions are different. A recommended particle radius distribution establishment scheme is provided, which requires the coordinate and radius at some key points. In numerical simulations, engineers and scholars usually focus on some points in the ROI and do not focus on the model's edges. Thus, a good practice is to specify the particle radius of focused points as small values and the particle radius at the model's edges as large values. The focused points can be at the flaw tips, at the edge of a hole, on the path of the crack coalescence. Both the points of small values and large values are the key points. In most cases, a two-level particle size scheme is enough. Then, a benchmark particle size and an enlargement factor are required. The particle radius at focused points can be configured as the benchmark particle size, while the points at the edges of the model can be configured as the product of the benchmark particle size and the enlargement factor. The benchmark particle size indicates the resolution of the ROI, and the enlargement factor indicates the gradient of the particle radius. A plane interpolation is then performed to acquire the particle radius distribution on the entire plane, which is used to generate particles. The key point scheme retains flexibility and reduces complexity.

2.1.3. Typical particle size distributions. The paper provides three examples of key points schemes, as shown in figure 1. All the schemes in the figure adopt an enlargement factor of 4. The figure includes three key point schemes: (a) and (b) own a focused point in the specimen center to simulate universal central high-resolution specimens; (c) and (d) own two focused points at both ends of a straight line to simulate a joint in the rock mass; (e) and (f) own series of focused points around a circle to simulate tunnels or holes in a rocky mountain. (a), (c) and (e) adopt the linear interpolation method, while (b), (d), and (f) adopt the natural interpolation method. The distribution obtained by the natural interpolation algorithm is smoother than the linear one. The modeling result of a universal central focused specimen is shown in figure 2.

Figure 1. Three examples of key point schemes with two interpolation algorithms. (a) and (b) represents universal central focused specimens, (c) and (d) represents a flaw, (e), and (f) represents a hole. (a), (c) and (e) adopts the linear interpolation method, (b), (d) and (f) adopts the natural interpolation method. The key points are marked as cyan crosses.
2. Analysis of computing power usage of gradient particle size specimens

2.2.1. Introduction to the time complexity of the discrete element method. The discrete element method is an explicit solution based on Newton’s law to simulate the evolution of the macroscopic world. The simulating circularly repeats the main loop, which mainly includes two processes: according to the geometric relationship between the particles, calculating the resultant force on the particles; according to the resultant force on the particles, calculating the acceleration, velocity, and displacement in a time step. An explicit solution requires a tiny timestep to ensure the convergence, which in the discrete element method can be approximated by the following formula:

\[ \Delta t = \left( \frac{m}{k} \right)^\frac{1}{2} = \left( \frac{4\rho\pi}{3K} \right)^\frac{1}{2} R^{-3/2} = CR^{-3/2} \]  

(5)

where, \( \Delta t \) is the timestep, \( m \) is the mass of the particles, \( K \) is the stiffness of the particles, \( \rho \) is the density of the material, \( R \) is the resolution of the model, \( C \) is a constant. The resolution can be defined as the reciprocal of the particle radius. Generally, with the material determined, the density and stiffness are constant. In the simulation of unit space or area, if using the closest packing, the approximate particles count is:

\[ n = \begin{cases} \sqrt{3}/6r^{-2} = \sqrt{3}/6R^2 & \text{(two dimensions)} \\ \sqrt{2}/8r^{-3} = \sqrt{2}/8R^3 & \text{(three dimensions)} \end{cases} \]  

(6)

where, \( n \) is the particle count. Take a particle calculated in one timestep as a basic operation unit, then, the time complexity to simulate a unit space in a unit time is:

\[ T(R) = \frac{1}{\Delta t} \times n \times O(1) = \begin{cases} O(C_{2D}R^3) & \text{(two dimensions)} \\ O(C_{3D}R^4) & \text{(three dimensions)} \end{cases} \]  

(7)

where, \( T(R) \) is the time complexity of the discrete element method about the resolution, \( O(1) \) is the basic operation unit, \( O(M) \) means to calculate \( M \) times, \( C_{2D} \) and \( C_{3D} \) are constant coefficients in two-dimensional and three-dimensional cases, respectively. The detailed information about the theory of time complexity can be found in the famous books *Introduction to algorithms* [10].

2.2.2. Time-saving ratio of different enlargement factors. The paper generated several gradient particle size specimens with the particle size enlargement factors from 1.0 to 2.0. Based on the time complexity theory, the theoretical computing time is calculated. The computing time of the uniform particle size specimens, generated with a particle size enlargement factor of 1.0, is taken as the benchmark. The computing time ratio of the gradient particle size specimens is calculated. As shown in figure 3, the gradient particle size specimen modeling scheme has a significant effect on the computing efficiency improvement of the discrete element model. When the particle size enlargement factor is 2.0, only 26% calculation time is required.

**Figure 2.** An example of a central high-resolution specimen with the particle size enlargement factor of 2.0.

**Figure 3.** The theoretical computing time of the gradient particle size specimens accounts for the uniform particle size specimen percentage.
3. Numerical simulation verification and analysis

The simulation results of gradient particle size specimens with the uniform particle size specimens are compared to verify the scheme. A series of unconfined compressive experiments on intact rock specimens and prefabricated single-flaw rock specimens were simulated.

3.1. Specimen calibration and generation

3.1.1. Flat-joint contact model calibration. The simulating process of the discrete element model is the alternating calculation of Newton’s law and the contact model response. The mechanical property of a discrete element model highly depends on the contact model. The flat-joint contact model provides the ability to simulating crystalline rock, which requires a calibration process before simulation [11]. The mechanical properties of the granite were tested by our team before [12]. The mechanical properties of the flat-joint model were calibrated and shown in table 1. The uniform particle size specimen is used for calibration to ensure the accuracy of the mechanical properties.

Table 1. Mechanical properties of the flat-joint model.

| Description                  | Symbol | Value |
|------------------------------|--------|-------|
| Effective modulus            | $E/\text{GPa}$ | 80    |
| Normal-to-shear stiffness ratio | $\kappa^*$ | 3.2   |
| Friction coefficient         | $\mu$  | 0.6   |
| Tensile strength             | $\sigma_t/\text{MPa}$ | 25    |
| Cohesion                     | $c/\text{MPa}$  | 60    |
| Friction angle               | $\phi$ | 48.9  |

3.1.2. Specimens preparation for numerical simulation. A series of numerical simulations were conducted with the calibrated parameters. Intact rock specimens and single-flaw rock specimens were simulated. Each kind of specimen was simulated with the particle size enlargement factor from 1.0 to 2.0, with an interval of 0.1. The examples of the modeling result of the uniform particle size specimens and the gradient particle size specimens are shown in figure 4. A preliminary analysis of the experiment results is conducted.

![Specimens used in numerical simulations](image)

Figure 4. Specimens used in numerical simulations. All of the specimens are generated using the same algorithm, in which the gradient particle size specimen adopts the particle size enlargement factor of 1.0.

3.2. Numerical simulation results analysis

3.2.1. Stress-strain curves analysis. The stress-strain curves were analyzed first. As shown in figure 5, the stress-strain curves of uniform particle size specimen and gradient particle size specimen show a high degree of unity. The peak stresses of uniform particle size specimen and gradient particle size specimen are 90.6 MPa and 85.5 MPa, respectively, and the relative error is 5.6%. The strains at peak stress are $1.416 \times 10^{-3}$ and $1.351 \times 10^{-3}$, respectively, and the relative error is 4.6%. The stiffnesses...
are 73.9 GPa and 70.1 GPa, respectively, and the relative error is 5.1%. All the parameters above match well.

3.2.2. Comparison of the fracture process. The number of fracture events can represent the fracture process well. However, for gradient particle size specimens, the number of particles is not constant, so the count of fracture events is also inconsistent. Therefore, the paper defines the fracture process as the number of fracture events divided by the number of particles. The total fracture process, tensile fracture process, and shear fracture process of the two modeling schemes are shown in figure 6. The crack initiation stress can be represented by the stress when the total progress reaches 0.01. It is 40.1 MPa and 37.7 MPa for the uniform particle size specimen and the gradient particle size specimen, respectively, and the relative error is 6.0%. The degree of crack development can be represented by the total process when the stress reaches 80 MPa. It is 0.982 and 0.967, respectively, and the relative error is 1.5%. The tensile process and shear process also supports the rules.

3.2.3. Comparison of crack initiation and failure pattern. The gradient particle size specimen modeling scheme aims to concentrate the computing power in the ROI. Therefore, the paper compares the crack initiation and failure patterns of the gradient particle size specimen and the uniform particle size specimen in the ROI. For the two specimens, the crack initiation patterns are selected at 40 MPa for comparison, and the failure mode is selected at the time of peak load for comparison. As shown in figure 7, the pattern of the gradient particle size specimen is highly consistent with the uniform particle size specimen, and the computing time of the gradient particle size specimen is only about 25% of the computing time of the uniform particle size specimen.
4. Discussion

When comparing the simulation result of the gradient particle size specimens with the uniform particle size specimens, some differences in the UCS were found. Therefore, the trend of UCS and the particle size enlargement factor is analyzed and shown in figure 8. The uniform particle size specimens can be regarded as specimens with particle size enlargement factors of 1.0. As shown in figure 8, with the increase of the particle size enlargement factor, the UCS of the intact specimens and the single-crack specimens show an approximately linear decrease.

![Figure 8](image1.png)

**Figure 8.** UCS both specimens with different particle size enlargement factors.

Many factors are influencing the strength properties of the discrete element model. The gradient particle size specimens change the geometric shape and arrangement of the particles, so the coordination number has a close relationship with the geometric arrangement[13]. Thus, a clear relationship can be obtained that the decrease in strength may be related to the coordination number. The paper then separately calculated the coordination number and the UCS of the intact specimens and the single-flaw specimens, as shown in figure 9. The coordination number and UCS both decrease approximately linearly with the increase of the particle size enlargement factor. This rule is evident in both the intact specimens and the single-flaw specimens.

To solve UCS inconsistency, an obvious solution is to adjust the mechanical parameters of the contact model. However, the modification violated the original intention of the paper that the gradient particle size specimen can replace uniform particle size distribution specimens without adding additional mechanical parameter calibration procedures. Furthermore, the additional parameter calibration procedures make it challenging to use the gradient particle size modeling scheme combined with the GBM or other modeling schemes. Therefore, in the next step of the research, the research team will try to improve the gradient particle size sample modeling scheme by changing the geometric relationship between particles or attempting the enlargement factor of the strength parameter to achieve the matching of UCS.

![Figure 9](image2.png)

**Figure 9.** The coordination number and UCS versus enlargement factors of intact specimens and single-flaw specimens
5. Conclusion
The application scenarios of the discrete element method are limited by its computational efficiency. The paper proposed a gradient particle size specimen modeling scheme to improve calculation efficiency by concentrating computing power in the ROI and reducing resolution in the BG. A series of unconfined compressive experiments were conducted with gradient particle size specimen and uniform particle size specimens to verify the accuracy of the gradient particle size specimen modeling scheme. The main conclusions are as follows:

The gradient particle size specimen modeling scheme is proposed based on the assumption that the specimen's density is consistent in the probabilistic sense. The probability distribution of particle generation is subsequently derived. A typical modeling scheme is recommended that specifying some key points and interpolate them on the whole plane to get radius distribution, which can keep the flexibility and reduce the complexity.

The numerical simulation results of the gradient particle size specimen modeling scheme and uniform particle size specimen modeling scheme are compared, indicating that the stress-strain curves, fracture progress curves, crack initiation, and failure patterns all match nicely. The gradient particle size specimen only requires about 26% computing time.

The gradient particle size specimen modeling scheme still has some problems, including the reduction of the UCS, which is probably caused by the reduction of the coordination number. We will conduct further research on the issues in the future.

6. Acknowledgement
Supported by the National Natural Science Foundation of China (No. U1965108), the Fundamental Research Funds for the Central Universities and the Shanghai Peak Plateau Discipline (Class I).

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