Research on the method of extrapolating 3D particle profile from 2D Fourier spectrum

Zheng Shanxi¹, Zheng Jiagen¹, Guo Xia¹, Sun Bingqi¹,², Shi Chong¹,²,*

¹. Nuclear Industry Huzhou Engineering Survey Institute Co. Ltd., Huzhou 313000, China;
². Research Institute of Geotechnical Engineering, Hohai University, Nanjing, 210024, China)

* Shi Chong: Research Institute of Geotechnical Engineering, Hohai University, Nanjing scvictory@hhu.edu.cn; Tel.: +86-137-7077-3434

Abstract. Based on 2D Fourier analysis, a shape extrapolation method of 3D geotechnical particles with arbitrary roughness is proposed, and the control conditions are discussed. It is realized that the two-dimensional profile is randomly constructed by Fourier description, then the three-dimensional particles are extrapolated using the profiles of multiple sections, lastly the 3D random particles can be generated which are close to the actual particle’s area, volume, roundness and other morphological characterization parameters; and particles with different accuracy can be constructed by controlling the number of sections. This method can provide help for the discrete element numerical calculation of particles.

1. Introduction

Most of the natural geotechnical media are composed of particles with different sizes. The macro deformation and failure law and mechanical properties (such as failure mode, crack propagation, bearing capacity, etc.) are largely dependent on the internal micro structural characteristics (such as particle size composition, particle surface and arrangement, etc.). For example, in the soil rock mixture, the shape and texture of large-size block stone will determine the friction performance of macro medium. In the coarse-grained soil, the profile characteristics of large particles have a great influence on the mechanical parameters. In recent years, more and more attention has been paid to the micro analysis method which links the meso characteristics with the macro characteristics. However, how to describe these mesoscopic characteristics and reconstruct them randomly [1] for mechanical analysis is an important challenge in the study of mesoscopic geotechnical mechanics.

Recently, with the development of research methods for material properties, it has become a hot topic to bring particle characteristics into macro research and analyze mechanical properties with the help of discrete element method (ferrerlec and McDowell, 2010) [2]. For example, when cundall and Strack [3] used the discrete element method to study the mechanical characteristics of sand particles, they found that considering the geometric shape of sand particles can better simulate the mechanical characteristics of sand. Zhou et al. (2013) [4] pointed out that the texture and roughness of the particle surface are the main reasons for the quasi-static shear force such as friction and bite force. Kong and Liang (2011) [5] defined some indexes, such as area, average curvature, roundness, concavity and so on, and studied the microscopic characteristics of particles. Krumbein and Sloss[6] defined the morphological parameters (sphericity and roundness) of particles by combining the microscopic view.
with the standard diagram provided and approximately characterized the mesoscopic characteristics of particles. Bowman et al. (2001) \cite{7} characterized the two-dimensional particle shape based on the Fourier transform descriptors, and its laws were statistically analyzed, and then a relatively fine two-dimensional particle contour reconstruction method was formed by using the inverse Fourier transform \cite{8}.

These studies can better describe the mesoscopic characteristics of materials at the plane level. However, any two-dimensional description is one-sided. In order to study the mechanical behavior of geotechnical media better, a growing number of scholars began to study the three-dimensional characterization methods of particles by means of laser scanning and CT scanning. For example, Mollon and Zhao. (2013) \cite{9} extended the Fourier descriptor from two dimension to three dimension, and constructed three-dimensional particles by using three orthogonal profile, which greatly simplified the difficulty of directly characterizing three-dimensional particles. However, for particles with high degree of irregularity, the reconstructed outer profile of particles is still quite different from the reality. Therefore, it is necessary to introduce more effective methods to achieve quantitative description and accurate construction of particle morphology.

Based on the two-dimensional Fourier analysis method, a simple three-dimensional particle construction method is established by analyzing and reconstructing the multi section profile of a single particle and the accuracy and setting conditions of different particle reconstruction are deeply discussed, which can provide help for the construction and reconstruction of three-dimensional particles with arbitrary roughness and the application to the discrete element calculation.

2. Two dimensional analysis and reconstruction method of micro particle contour

At present, most of the researches on the mesoscopic characteristics of geotechnical medium particles are based on polygon structure and analysis, ignoring the details. However, the real Fourier analysis used in geotechnical engineering can not consider the concave particle profile. Under two-dimensional condition, the shape of rock and soil particles can be represented by closed curve, which can be obtained by means of edge detection and contour recognition of digital image. Suppose that the contour can be expressed as a coordinate sequence: \{(x_m, y_m); m=0, 1, 2, ..., M-1\}, and its complex form is given by formula (1).

\[ z(m) = x_m + iy_m, \quad m=0, 1, 2, ..., M-1 \] (1)

For a closed curve, its complex sequence is periodic and the period is N. For convenience, by normalizing (dividing \(r_0\)) the Fourier spectrum to ensure \(\bar{D}_0\)(average particle radius) is equal to 1, according to the following formula (4), the reconstruction of the given particle is realized.

\[ r_i(\theta) = r_0 + \sum_{n=1}^{N} \left[ A_n \cos(n \theta) + B_n \sin(n \theta) \right] \] (2)

Standardized Fourier spectrum \(\{D_n\}\) is the most commonly used method to analyze particle morphology. However, different Fourier transform calculation methods may lead to different laws of coefficients’ change in different orders. In the random reconstruction, the known amplitude spectrum \(\{D_n\}\) is used, and the phase angle \(\delta_n\) is randomly assigned to each order of Fourier analysis to realize the particle random reconstruction. If these random phases are assumed to be \([0, 2\pi]\) uniformly distributed, the discrete profile information of particles can be obtained.

\[ A_n = D_n \cdot \cos \delta_n \]
\[ B_n = D_n \cdot \sin \delta_n \] (3)

In this paper, N=128 is used for Fourier analysis, as shown in Figure 1, which is a typical two-dimensional particle profile (Fig.1(c)). The spectrum of coefficient modes of each order is shown in Fig.1(a), and the phase spectrum is shown in Fig.1(b).
3. Fourier analysis three-dimensional extrapolation reconstruction method

The outer contour of coarse-grained soil, sand and other micro particles is an important factor to determine the friction performance of medium. Constructing its three-dimensional granular behavior is of great significance to simulate the deformation and strength of real medium. However, there are no two identical particles in nature. Usually, a series of benchmark profiles of typical particles are obtained by laser scanning and other techniques, as shown in Fig.2(a), and then these benchmark templates are used to construct three-dimensional particles. Here, the two-dimensional Fourier continuation structure is used, and the process is as follows:

- For sand, pebble and gravel, a series of reference particles with similar shape are selected by using laser scanning technology as shown in Fig.2(a). Subject to accuracy, the outer contour of each particle may be composed of hundreds of thousands of triangles.
- Taking the centroid of each particle as the reference point, the centroid coordinates of all reference particles are translated to the origin and the radial radius of the particles is scaled in equal proportion to make the particle volume 1.0. This process is called normalization and the longest axis of the particles is pointed to the X axis and the shortest axis to the Y axis.
- Set the number of cut planes and cut all particles by plane in turn to get the set of contour lines. As shown in Fig.2(c), the contour lines of particles are obtained by using three orthogonal cut planes.
- For the contour set of each section, the plane Fourier analysis is carried out by using formulas (1) (2) and (3) and the Fourier coefficients are obtained. Carry out statistical analysis on each Fourier coefficient to get the mean value and variance of each coefficient, as shown in Fig.2(d).
- Using the statistical parameters of each Fourier coefficient, the random contour lines on each section are generated randomly and the outer contour of the whole particle is measured. Fig.2(e) shows the random particle with random structure and its statistical parameters can have good similarity with the original particle.

With this method, random particles can be constructed. The roughness of the outer contour of particles depends on the number of longitudinal control sections and the reference particle profile data. Under the latter condition, the more the number of longitudinal control sections is, the rougher the particles are.
4. Application of particle random construction based on 3D laser scanning data

For any three-dimensional particle, the average radius (the average distance between all contour points and centroid), the maximum polar radius (the maximum distance between contour points and centroid), the minimum polar radius (the minimum distance between contour points and centroid), the outer contour area of particles, the volume of particles, and the sphericity (the proximity between the actual rock particles and the equivalent sphere) are selected as the meso feature characterization data. The sphericity is defined as follows:

\[ \psi = \frac{d_{sv}}{d_{v}} \]  

(6)

Where \( d_{v} \) is the volume diameter, which is the equivalent ball diameter under the same volume for irregular particles. The apparent volume diameter \( d_{sv} \) is the diameter of the ball with the same outer surface volume ratio as the block stone.

Fig. 3 Contour comparison (a) Particle contour with CT scanning (b) Particles contours by provided method

The sand particle size is generally in the millimeter level, so CT scanning is used to scan typical sand particles. As shown in Fig.3(a), there are 25 sand particles with the size of 1 ~ 2mm. After
normalization (the volume of particles is enlarged to 1.0 in equal proportion), the microscopic characteristic information is counted, and the information of 1 particles is shown in Table 1.

| particle number | average radius/m | maximum polar radius/m | minimum polar radius/m | area/m² | volume/m³ | sphericity |
|-----------------|------------------|------------------------|------------------------|---------|-----------|------------|
| 1(CT)           | 0.5922           | 1.0012                 | 0.2327                 | 5.0586  | 0.9999    | 1.0461     |
| 2(CT)           | 0.5995           | 0.815                  | 0.4173                 | 4.9940  | 0.9999    | 1.0327     |
| 3(CT)           | 0.6014           | 1.0573                 | 0.2287                 | 4.9990  | 0.9999    | 1.0338     |
| 4(CT)           | 0.6033           | 1.0458                 | 0.2511                 | 4.9707  | 0.9999    | 1.0279     |
| 5(CT)           | 0.6014           | 1.0350                 | 0.3190                 | 4.9792  | 0.9999    | 1.0297     |
| 1(random generation) | 0.5992 | 0.8532                  | 0.4958                 | 4.8725  | 1.00      | 1.0076     |
| 2(random generation) | 0.5756 | 0.9867                  | 0.4233                 | 4.893   | 1.00      | 1.0118     |
| 3(random generation) | 0.5908 | 0.8761                  | 0.4339                 | 4.9114  | 1.00      | 1.0156     |
| 4(random generation) | 0.5757 | 0.9040                  | 0.3965                 | 4.8955  | 1.00      | 1.0123     |
| 5(random generation) | 0.5975 | 0.7677                  | 0.4810                 | 4.9388  | 1.00      | 1.0213     |

Then a series of particles are randomly constructed, as shown in Fig.3(b), and any 5 micro feature information is shown in Table 1(random generation) . Compared with the results in Table 1, it can be seen that all the micro statistical information is very close, which indicates that the three-dimensional particles constructed by the extension method in this paper can match the apparent contour characteristics of natural sand particles.

5. Discussion

With the increase of the longitudinal control profile, the parameters of the reconstructed particles are closer to the original ones, which makes it easier to approach the real situation of the particles. Generally, for pebble particles with smooth surface, 3-5 control sections are needed to approximate the particles. Cemented particles are rough and uneven and 8-10 longitudinal control sections are suggested.

With the increase of Fourier analysis order, the mesoscopic characteristics of particles will be more clearly. this method is based on the assumption that the effect of the adjustment on the particle profile is at a small level. In addition, the more the number of triangles is, the more realistic the outer profile is. it is recommended to ignore the fine texture features and control it to 2000-4000.

The particle analysis and reconstruction method established in this paper have the following advantages: (1) conventional Fourier random reconstruction requires Fourier analysis and statistics of a large number of particles to obtain the law of Fourier descriptor, while this method directly uses Fourier analysis of corresponding contour lines of particles to construct a large number of random particles based on only one representative particle, which is simpler. (2) If the construction of particles with different sizes, the volume diameter index can be controlled, according to the gradation, then the generated particles can easily achieve the generation of gradation.

6. Conclusion

The main conclusions are as follows:
(1) Through the two-dimensional Fourier spectrum analysis, the arbitrary profile of three-dimensional particles can be described and reconstructed and the outer contour of the same spectrum can be constructed very close to the actual particles.

(2) By describing and reconstructing sand particles, it is shown that the two-dimensional Fourier contour reconstruction can be further extended to three-dimensional particles and random three-dimensional particles with different accuracy can be constructed so as to generate random particles which are close to the original particle area, volume, roundness and other morphological characterization parameters.

Acknowledgements
This work was supported by the National Natural Science Foundation of China (Grants Nos. 51679071).

References
[1] Shi Chong, Zhang Qiang, Wang Shengnian. Numerical Simulation Technology and Application with Particle Flow (PFC5.0) [M]. China Architecture & Building Press, 2018
[2] J. FERELLEC; G. McDOWELL. Modelling realistic shape and particle inertia in DEM[J]. Géotechnique, 2010, 60:227-232.
[3] Cundall P A, Strack O D L, Cundall P A. Discussion: A discrete numerical model for granular assemblies[J]. Géotechnique, 1980, 30.
[4] Zhou, B., et al., DEM investigation of particle anti-rotation effects on the micromechanical response of granular materials. Granular Matter, 2013. 15(3): p. 315-326.
[5] Kong Liang, Peng Ren. Particle flow simulation of influence of particle shape on mechanical properties of quasi-sand [J]. Chinese Journal of Rock Mechanics & engineering, 2011, 30(10):2112-2119.
[6] Krumbein W C, Sloss L L. Stratigraphy and Sedimentation[J]. Soil Science, 1951, 71(5):401.
[7] Bowman E T, Soga K, Mmond W. Particle shape characterisation using Fourier descriptor analysis[J]. Géotechnique, 2001, 51(6):545-554.
[8] Shi Chong, Bai Jinzhou, Yu Shiyuan, et al. Mesostructural characteristic and random reconstruction of soil-rock particles based on plural Fourier analysis [J]. rock and soil mechanics, 2016,37 (10): 2780-2786
[9] Mollon G, Zhao J. Generating realistic 3D sand particles using Fourier descriptors[J]. Granular Matter, 2013, 15(1):95-108.