A simple approach of calibrating input parallel bond model parameters for DEM simulations of rock behaviour

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Abstract. The mineral bonds between grains of rock are usually simulated by parallel bonds in discrete element method (DEM) simulations. The existence of multiple input parameters makes the calibration process tedious and time-consuming. In this paper, a series of parametric studies are firstly conducted by varying the value of each input parameter independently, based on which their distinct influences on the strength and deformation characteristics of simulated specimens are obtained. One-way and multiple-way analysis of variance are conducted to evaluate the sensitivity of macro strength and deformation parameters to the change of input parallel bond model parameters. The order of influence level of these input parameters on the macro behaviour of simulated specimens is obtained and the input parameters with the dominating influences on the macro mechanical properties are identified. Then, empirical correlations between the macro mechanical properties and their dominating input parameters are established separately. These empirical correlations are taken as the basic components in the regression analysis of multiple variables for each macro mechanical property. The regression equations serve as the first estimation of input parameters for the calibration. The adjustment of input parameters is conducted with reference to the partial differentials of the regression equations considering the difference between the simulation results and the experimental data as the increments/decrements. The effectiveness of the proposed calibration approach is validated by simulating a series of triaxial compression tests on mudstone.

1. Introduction

Rock is a typical type of granular medium whose macroscopic responses are governed by microscale interaction and movement of its constituent grains. The discrete element method (DEM) [1] has served as one of the most popular numerical tools which has gained increasing attentions in simulating the rock behaviour in the past decade due to its capacity of measuring both the micro and macro-scale properties during the simulation [2,3]. A key step of applying the DEM model to simulate granular materials is to calibrate the input parameters. The parallel bond model proposed by Potyondy and Cundall [4] has been shown to be able to capture a variety of rock behaviours including the three-dimensional strength-deformation characteristics [5,6] and brittle failure process [7]. However, due to its complex formulation and relatively large number of input parameters, the calibration process is non-trial. Usually, a single-variable approach is adopted by changing a single parameter while retaining the rest input parameters [8,9]. This, however, is inefficient as a number of trial-and-error iterative simulations must be conducted until the differences between the simulation results and experimental/theoretical values are acceptable.
Different calibration approaches have been proposed in the literature. For example, Wang and Tonon [10] used global optimization to minimizing the difference between computed and experimental failure envelopes. Cheng et al. [11] developed an iterative Bayesian filtering framework which can calibrate DEM models in a fast and automatic way. De Simone et al. (2019) proposed using genetic programming (GP) to calibrate input microparameters for uniaxial compression simulation [12]. Although these models are able to calibrate the DEM models more fastly than the original single-variable approach, they did not respect the inherent interrelations between different input parameters. It is also unclear why the input parameters should be varied in the way the calibration program shows.

In this paper, a simple calibration approach is proposed. The dependencies of some key macro mechanical properties on different input parameters of the parallel bond model are firstly examined. The dominating influential factors for each macro mechanical property are identified based on one-way analysis and multi-way analysis of variance. Some empirical correlations between the micro and macro variables are then established, based on which the calibrated input parameters can be readily obtained and then adjusted to yield DEM simulation results that are close to the experimental data.

2. Model setup

Radius expansion method was used to generate the specimen as this method yields homogeneous and isotropic specimens [13]. The particles were initially generated at about $1/m$ of their target sizes within a rigid cylindrical domain of $\Phi 50 \times 100$mm. The radius reduction factor $m$ can be determined by the following formula:

$$m = \left( \frac{1 - n_0}{1 - n} \right)^{\frac{1}{3}}$$  \hspace{1cm} (Eq. 1)

where $n_0$ is the porosity of the generated specimen and $n$ is the target porosity of 0.35. After generation, the particles were expanded until their target sizes were reached. The final particle radiiuses were in a range between 1.0 mm and 1.66 mm. At the sample generation stage, only linear contact model was activated. Once the specimen has been generated, the parallel model was introduced. The generated specimen was isotropically compressed until the prescribed confining pressure has been reached. The specimen was then subjected to triaxial shearing by simultaneously moving the top and bottom loading plates at a constant velocity until failure occurred, while the confining pressure was maintained constant by continuously adjusting the diameter of the cylindrical walls. In order to obtain a complete database for the influence of different input parameters of the parallel bond model on the macro responses of testing specimen, eight key parameters were varied systematically according to Table 1. For these simulations, the confining pressure was fixed at 1.0 MPa and the loading rate was 0.5s$^{-1}$. In total, 60 simulations were conducted.

![Figure 1. DEM specimen](image-url)
Table 1. Variation of the input parameters

| Model parameters                                      | Unit   | Benchmark value | Variation range          |
|-------------------------------------------------------|--------|-----------------|--------------------------|
| Effective modulus, $E_c$                              | MPa    | 100             | 10,30,50,70,500,1000     |
| Normal-to-shear stiffness ratio, $k_n/k_s$            |        | 1               | 2,3,4,5,10,20,50        |
| Effective modulus of parallel bond, $E_{\text{c}}$    | MPa    | 100             | 10,30,50,70,500,1000     |
| Normal-to-shear stiffness ratio of parallel bond, $\tilde{k}_n/\tilde{k}_s$ |        | 1               | 2,3,4,5,10,20,50        |
| Normal strength of parallel bond, $\tilde{\sigma}_c$  | MPa    | 10              | 1.5,10,20,30,40,50      |
| Cohesion of parallel bond, $c$                        | MPa    | 50              | 5,10,20,30,40,50,100,500|
| Friction angle of parallel bond, $\phi$              | °      | 0.5             | 0°,15°,30°,45°,60°,75°,90°|
| Friction coefficient, $\mu$                          |        |                 | 0.0,1,1.2               |

3. Influences of different model parameters on the macro-scale responses

3.1 Representative simulation results

Figure 2 (a) and (b) show the stress-strain curves of DEM specimen with different normal-to-shear stiffnesses ($k_n/k_s$) of parallel bond and different normal strengths of parallel bond ($\tilde{\sigma}_c$), respectively. The peak strength decreases consistently as $k_n/k_s$ increases. The axial strain at which failure occurs also decreases with increasing $k_n/k_s$ and failure becomes more ductile at higher $k_n/k_s$ values. The peak strength and the axial strain at which failure occurs increase as $\tilde{\sigma}_c$ increases. However, the influence of $\tilde{\sigma}_c$ on the stress-strain behaviour becomes saturated when $\tilde{\sigma}_c$ exceeds 20 MPa. Due to the length limit, the influences of other input parameters on the stress-strain responses are not presented.

![Figure 2](image_url)

Figure 2. Influence of (a) normal-to-shear stiffness of parallel bond and (b) normal strength of parallel bond on the stress-strain behaviour

3.2 Influences of different input parameters on the mechanical properties of DEM specimen

Different input parameters could have different degrees of influence on different macro mechanical properties. Therefore, it is important to determine the most influential factors for different mechanical properties so that the calibration process could be more concise. The key mechanical properties of DEM specimen considered in this study include peak strength ($\tilde{\sigma}_p$), the peak axial strain ($\epsilon_p$), Young’s modulus ($E_e$) and Poisson’s ratio ($\nu$). The influences of different input parameters on these variables will be evaluated through both one-way and multi-way analyses of variance. Since different input parameters have different dimensions, for the ease of comparison the Min-Max approach is adopted to normalize the input parameters so that they can all be in the range from 0 to 1. The basic formula of the Min-Max normalization approach is given below:
\[ x^* = \frac{x - x_{\text{min}}}{x_{\text{max}} - x_{\text{min}}} \]  \hspace{1cm} (Eq. 2)

where \( x \) and \( x^* \) are the original and normalized values, \( x_{\text{max}} \) and \( x_{\text{min}} \) are the largest and smallest values of the input parameters, respectively.

3.2.1 One-way analysis of variance

Figure 3 shows the influence of different parameters on \( E_e \). It can be seen that \( E_e \) increases with increasing \( E_c \) and \( \overline{E}_c \), but decreases with increasing \( \overline{k}_n/\overline{k}_s \). The rest parameters have very limiting influences on \( E_e \). Figure 4 shows the variations of \( \sigma_p \) with different input parameters. \( \sigma_p \) increases with increasing \( E_c \), \( \overline{E}_c \), \( \overline{\sigma}_c \) and \( \overline{c} \) but decreases as \( \overline{k}_n/\overline{k}_s \) increases. The influences of these input parameters on are limited and \( \sigma_p \) becomes approximately constant when these input parameters exceed certain values. The dependency of \( \sigma_p \) on the rest parameters is not obvious as these five parameters. Variation of \( \varepsilon_p \) on different input parameters is presented in Figure 5. \( \varepsilon_p \) initially increases with the two strength parameters of parallel bond, \( \overline{\sigma}_c \) and \( \overline{c} \), and becomes approximately constant when these two parameters reach certain values. In contrast, it decreases consistently with increasing \( \overline{E}_c \) and \( \overline{k}_n/\overline{k}_s \). Furthermore, it increases initially with increasing \( E_c \) but then decreases as \( E_c \) is further increased. The influences of the rest parameters on \( \varepsilon_p \) are not obvious in comparison to these five parameters. Figure 6 shows the dependency of \( \nu \) on different input parameters, \( \nu \) increases as \( E_c \) and \( \overline{k}_n/\overline{k}_s \) increase but decreases with increasing \( \overline{E}_c \). However, the influences of \( \overline{k}_n/\overline{k}_s \) and \( \overline{E}_c \) are limited as \( \nu \) remains approximately constant when these two parameters exceed certain values. The influences of other input parameters on \( \nu \) are negligible.

![Figure 3. Influence of different parameters on Young’s modulus](image)

![Figure 4. Influence of different parameters on peak strength](image)
3.2.2 Multi-way analysis of variance

The influences of different input parameters on macro mechanical properties are not isolated but inter-related. In order to gain a comprehensive understanding of the inter-correlations between the influences of different input parameters on the macro mechanical properties, multi-variable analysis of variance is adopted. Each of the mechanical properties is assumed to be linearly correlated with the input parameters; thus, each mechanical property can be expressed in terms of a general linear equation composed of these individual linear correlations. The fitting parameters of this general linear equation can be obtained by regression analysis. Then we can calculate the standard deviations of mechanical properties resulted from varying each input parameter, based on which we can perform F test to get the concomitant probability/significance ‘sig.’ for each input parameter. The calculation procedure was achieved using SPSS software. The significance parameter ‘sig.’ indicates whether the examined parameter has significant influences on the macro mechanical properties. Input parameters with sig. < 0.05 is considered to have significant influences on the macro mechanical variables considered; otherwise, they are considered to have negligible influences on the mechanical variables considered. From Figure 7, it can be inferred that $E_e$ is mainly influenced by $E_c$ and $\bar{E}_c$, $\sigma_p$ can be significantly affected by $E_c$, $\bar{E}_c$, $\bar{\sigma}_c$, $\bar{\varepsilon}$ and $k_n/k_s$, $\epsilon_0$ highly depends on $E_c$, $\bar{E}_c$, $\bar{\sigma}_c$, $\bar{\varepsilon}$ and $k_n/k_s$ as well, while $\nu$ can be influenced by $E_c$, $\bar{E}_c$, $\bar{\sigma}_c$, $k_n/k_s$ and may also be affected by the strength parameter $\mu$ and $\phi$ as well.
4. Macro-micro correlations and calibration procedure

Based on the above analysis, we can establish the correlations between the macro mechanical properties and their key influential factors by multi-variable curve fitting on the 60 simulation datasets, i.e., $E_e$ is correlated with $E_c$, $\bar{E}_c$ and $\bar{k}_n/\bar{k}_s$, $\sigma_p$ is linked to $E_c$, $\bar{E}_c$, $\bar{\sigma}_c$, and $\bar{\varepsilon}_c$, $\varepsilon_p$ is correlated with $E_c$, $\bar{E}_c$, $\bar{\sigma}_c$, $\bar{\varepsilon}_c$, and $\bar{k}_n/\bar{k}_s$, while $\nu$ is linked to $\bar{k}_n/\bar{k}_s$. For simplicity, we take $E_c$ and $\bar{E}_c$ as identical and note that Fig. 3 also shows a high dependency of $E_e$ on $\bar{k}_n/\bar{k}_s$, therefore, we also incorporate $\bar{k}_n/\bar{k}_s$ when establishing the following relationship:

$$E_e = 1.22E_c - 35.62\ln\frac{\bar{k}_n}{\bar{k}_s} + 29.34$$  \hspace{1cm} (Eq. 3)

Similarly, we will have the following correlations of $\sigma_p$, $\varepsilon_p$ and $\nu$ with input parameters:

$$\sigma_p = 0.87\ln E_c - 2.19\ln\frac{\bar{k}_n}{\bar{k}_s} + 1.99\bar{\sigma}_c - 0.01\bar{\varepsilon}_c + 1.92$$  \hspace{1cm} (Eq. 4)

$$\varepsilon_p = -7.18\ln E_c - 0.23\ln\frac{\bar{k}_n}{\bar{k}_s} + 2.28\bar{\sigma}_c + 0.48\bar{\varepsilon}_c + 33.67$$  \hspace{1cm} (Eq. 5)

$$\nu = 0.04\ln\frac{\bar{k}_n}{\bar{k}_s} + 0.15$$  \hspace{1cm} (Eq. 6)

With the above correlations, we can sequentially back calculate the initial input parameters based on the experimental variables using the following equations:

$$\frac{\bar{k}_n}{\bar{k}_s} = e^{0.15\nu - 0.04}$$  \hspace{1cm} (Eq. 7)
$E_c = 0.82E_e + 29.21\ln\frac{\bar{k}_p}{k_s} - 24.06$ (Eq. 8)

$\bar{\sigma}_e = 0.50\sigma_p - 0.43\ln E_e + 1.09\ln\frac{\bar{k}_p}{k_s} - 0.96$ (Eq. 9)

$\bar{\varepsilon} = 2.08\varepsilon_p - 2.38\sigma_p + 17.00\ln E_e - 4.71\ln\frac{\bar{k}_p}{k_s} - 65.58$ (Eq. 10)

Then, the calibration can be conducted by firstly estimate the initial input parameters based on Eqs. 7 to 10 to run the simulation, which is the first time of trial and error. After comparing the simulation results with experimental data, we can get the differences between the two for each mechanical variable, i.e., $\Delta E_e, \Delta \sigma_p, \Delta \varepsilon_p, \Delta \nu$. Substitute these sequentially into the differential equation of Eqs. 7 to 10, we can obtain the adjustment values for each input parameters and the simulation can be run for the second time. This procedure is repeated until the differences between the simulation results and experimental data for all the mechanical variables become acceptable. After matching the stress-strain behaviour, fine adjustment on the friction coefficient can be conducted to obtain a failure mode that is close to the experiment.

5. Calibration example
In this section, we will use a simple example to illustrate how to employ the established macro-micro correlations for calibration based on the experimental data from Jia [14] on a type of mudstone collected from Nanning City, China. We firstly performed calibration based on the triaxial test results under a confining pressure of 1MPa and later the calibrated input parameters are used to perform DEM simulations under the other two confining pressures. We firstly calculate the effective modulus ($E_c$), normal-to-shear stiffness of parallel bond ($\bar{k}_p/\bar{k}_s$), normal strength of parallel bond ($\bar{\sigma}_e$) and cohesion of parallel bond ($\bar{\varepsilon}$) according to Eqs. 7 to 10. These initial values are then input into DEM model, from which we can get the first batch of macro properties: $\nu=0.205$, $E_e=61.61$MPa, $\sigma_p=3.49$MPa and $\varepsilon_p=6.48\%$. Comparing with experimental data, we note that the discrepancies are 2.5%, 4.7%, 7.9% and 1.6% for $\nu$, $E_e$, $\sigma_p$ and $\varepsilon_p$, respectively. The accuracy is acceptable for most of the macro properties, except for $\sigma_p$. Therefore, the input $\bar{\sigma}_e$ must be adjusted according to Eq. 9. Then the simulation is performed for the second time with the new input parameters. The macro properties obtained in the second simulation are $\nu=0.201$, $E_e=58.57$MPa, $\sigma_p=3.85$MPa and $\varepsilon_p=6.91\%$. The discrepancies between DEM simulation results and experimental data are 0.5%, 0.48%, 1.6% and 8.31% for $\nu$, $E_e$, $\sigma_p$ and $\varepsilon_p$, respectively. The discrepancy of $\varepsilon_p$ is obvious; therefore, the input $\bar{\varepsilon}$ needs to be adjusted according to Eq. 10. Then the simulation is rerun and the macro properties become $\nu=0.198$, $E_e=58.03$MPa, $\sigma_p=3.61$MPa and $\varepsilon_p=6.29\%$, which yield discrepancies between numerical and experimental data to be 1.0%, 1.4%, 4.7% and 1.4% for $\nu$, $E_e$, $\sigma_p$ and $\varepsilon_p$, respectively. All these discrepancies are acceptable and the calibration procedure is therefore completed. The calibration procedure is summarized in Table 2. Figure 8 compares the calibrated results with experimental data used the calibrated input parameters listed in Table 3. As can be seen from Figure 8, the pre-peak stress-strain curves obtained in DEM simulations almost coincide with the experimental data for all the three confining stress levels considered. The DEM results deviate slightly from the experimental data, which may be because we did not consider the post-peak response as the essential component in the calibration approach we proposed.

| Table 2. Calibration procedure |
|--------------------------------|
| **Macro properties** | **Model parameters** |
| $E_0$ | $\nu$ | $\sigma_{max}$ | $\varepsilon_{max}$ | $E_c$ | $k_p/k_s$ | $\bar{\sigma}_e$ | $\bar{\varepsilon}$ |
| MPa | — | MPa | % | MPa | — | MPa | MPa |
| Experiment | 58.85 | 0.200 | 3.79 | 6.38 | — | — | — |
Table 3. Calibrated input parameters

| Model parameters                              | Unit | Value  |
|-----------------------------------------------|------|--------|
| Effective modulus, $E_c$                      | MPa  | 60.70  |
| Normal-to-shear stiffness ratio, $k_n/k_s$    |      | 1      |
| Effective modulus of parallel bond, $\overline{E}_c$ | MPa  | 60.70  |
| Normal-to-shear stiffness ratio of parallel bond, $\overline{k}_n/\overline{k}_s$ |      | 3.49   |
| Normal strength of parallel bond, $\sigma_c$  | MPa  | 0.68   |
| Cohesion of parallel bond, $\bar{c}$         | MPa  | 1.00   |
| Friction angle of parallel bond, $\phi$      | °    | 60     |
| Friction coefficient, $\mu$                  |      | 0.1    |

6. Conclusion

This paper proposed a simple method for calibrating input parallel bond parameters for simulating rock behaviour using DEM based on 60 simulations. The one-way and multi-way analysis of variance showed that different input parameters have different degrees of influences on the macro mechanical properties. Specifically, the Young’s modulus $E_c$ is mainly influenced by the effective modulus $E_c$ and effective parallel bond modulus $\overline{E}_c$, the peak strength $\sigma_p$ can be significantly affected by the effective modulus $E_c$, effective parallel bond modulus $\overline{E}_c$, normal strength of parallel bond $\sigma_c$, cohesion of parallel bond $\bar{c}$ and normal-to-shear stiffness ratio of parallel bond $\overline{k}_n/\overline{k}_s$. $\varepsilon_p$ highly depends on $E_c$, $\overline{E}_c$, $\sigma_c$, $\bar{c}$ and $\overline{k}_n/\overline{k}_s$, while $\nu$ can be influenced by $E_c$, $\overline{E}_c$, $\overline{k}_n/\overline{k}_s$ and may also be affected by the strength parameter $\mu$ and $\phi$ as well. Empirical correlations between the micro input parameters and macro mechanical properties were established by multi-variable interpolations, based on which a calibration procedure was developed. Only three trial and error procedures were needed to get close match between the DEM simulation data and the experimental results using the developed calibration approach for the illustration example, indicating the effectiveness of the proposed approach in rapidly calibrating the input parallel bond parameters for simulating rock behaviour using DEM.

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Acknowledgments
The work was supported by the National Natural Science Foundation of China (Grant No. 41672262).