Preliminary study on PFC3D microparameter calibration using optimization of an artificial neural network

J Kim¹, J W Choi¹ and J J Song²

¹ Department of Energy Resources Engineering, Seoul National University, Seoul 08826, Korea
² Department of Energy Resources Engineering, Research Institute of Energy and Resources, Seoul Nation University, Seoul 08826, Korea

songjj@snu.ac.kr

Abstract. Microparameter calibration for matching macroscopic responses of particle flow code 3D (PFC3D) models is generally conducted through trial-and-error which is inefficient and time-consuming. Several automatic calibration methods have been proposed but they are still limitations in the number of calibratable microparameters, range of macroscopic responses and degree of freedom in user-defined constraints. To overcome such limitations, a novel calibration method is proposed utilizing the constrained optimization of an artificial neural network (ANN). The ANN is trained with 600 PFC3D simulations to predict the unconfined compressive strength (UCS), Young’s modulus (E) and Poisson’s ratio (ν) of a PFC3D model for a given set of 15 microparameter values. Unlike other ANN-based DEM calibration methods, the proposed method calibrates microparameters by optimizing the ANN inputs rather than obtaining the calibrated values as the ANN outputs. The integration of a PFC3D-mimicking ANN with constrained optimization enables microparameter calibration for a wider range of microparameters, macroscopic responses and a higher degree of freedom in user-defined constraints.

1. Introduction

For fast DEM microparameter calibration, several automatic calibration methods have been proposed for commercial DEM codes such as particle flow code 2D/3D (PFC2D/3D). Yoon [1] proposed a calibration scheme for PFC2D based on a design of experiment (DOE) approach to derive relations between 7 PFC2D microparameters and its resulting PFC2D UCS, E and ν. Obtained linear and non-linear relations were used to calibrate the microparameters by optimizing the relations with desired UCS, E and ν. Similarly, Simone et al. [2] proposed calibration by applying optimization algorithms to functions explaining the relations between 5 DEM microparameters and the macroscopic responses. In their study, the functions were constructed using genetic programing, a machine learning method based on natural selection. On the other hand, instead of constructing functions between macroscopic responses and microparameters, Wang and Cao [3] employed the improved simulated annealing algorithm to automatically run PFC2D/3D simulations for calibration, automating the trial-and-error procedure.

There also have been efforts to use artificial neural networks (ANN) for DEM microparameter calibration [4], [5]. Tawadrous et al. [4] used a shallow ANN to calibrate 3 PFC3D microparameters for a given UCS, E, ν, model resolution and maximum-to-minimum particle radius ratio. The ANN was
composed of an input layer which received the 5 desired model specifications, a single hidden layer consisted of 9-11 neurons, and an output layer deriving the 3 microparameters. By calibrating microparameters using this network, PFC3D macroscopic responses had an average of 16% deviation from the targeted macroscopic responses. Especially, the derived \( v \) had a high error rate of 27%. Compared with Tawadrous et al. [4], Zhai et al. [5] used a deeper ANN with 16 hidden layers and batch normalization. The ANN was trained to calibrate 5 PFC3D microparameters for 5 macroscopic responses: namely UCS, E, \( v \), cohesion and friction angle. When calibrating laboratory test results for two marble samples from the Jinping hydropower station, the proposed ANN showed error rates of 17% and 4% respectively.

Heretofore various automatic calibration methods have been proposed, but there are some limitations to these methods. First, the number of calibratable micro-parameters is limited under 10 [1] – [5]. Considering that there are over 20 microparameters for the parallel-bonded model in PFC3D (ver6.0) [6], full calibration of microparameters is currently not possible. Secondly, regarding studies which disclose the range of applicable macroscopic responses, the applicable macroscopic responses are limited within 40-170MPa for UCS, 20-50GPa for E and 0.19-0.25 for Poisson’s ratio (\( v \)) [1]. Calibration for macroscopic responses that fall outside or near the range boundaries show poor calibration accuracy [4]. Another limitation, especially regarding microparameter calibration using ANN, is that user-defined microparameter constraints cannot be set in the calibration process [4], [5]. When calibrating microparameters, certain microparameters such as element size or bond stiffness maybe required to be fixed as a specific value but such user-defined constraints are not available during calibration.

In this study, a novel calibration method is proposed and investigated to overcome these limitations. The proposed calibration method calibrates PFC3D microparameters by constrained optimization of an ANN. The ANN, which forms the basis of the proposed calibration method, is trained to predict the UCS, E and \( v \) of a PFC3D model for a given set of 15 microparameters. Unlike other ANN-based DEM calibration methods, the 15 microparameters are calibrated by optimizing the ANN inputs which correspond to the microparameter values. By integrating a PFC3D-mimicking ANN with constrained optimization, the proposed calibration method fully facilitates the high performance of ANNs for mapping complex relations, enabling calibration with a wider selection of microparameters, wider range of macroscopic responses and higher degree of freedom in user-defined constraints.

2. Background

2.1. Microparameters of Particle Flow Code 3D (PFC3D) parallel-bond model

PFC3D is a commercial 3D DEM code from ITASCA which models rock as an assembly of rigid spherical particles. The parallel-bond model is favored for modeling rock since it is able to mimic the cementation of grains within rock [7], [8]. The parallel-bond model simulates rock-like material by assigning bonds between particles that transmit both force and moment before the strength limit is exceeded [6], [9]. If forces exceed the strength limit, bonds are broken and a linear model is applied based on a force-displacement law in which contact forces are calculated from relative displacements and stiffness. The same linear model governs the particle-particle contacts during model generation which is also known as packing. Considering these numerical representations of rock structures, the properties of a PFC3D parallel-bond model are defined by the microparameters in table 1. The scope of the proposed calibration method corresponds to the microparameters and ranges of each microparameter tabulated in table 1. For more details on the role and function of each parameter, refer to Potyondy [6].

In this study, the particle diameter size was distributed uniformly between an upper and lower diameter range which has the ratio of the upper to lower diameter range fixed as 1.66. Also, packing was conducted with the grain-cloud porosity fixed to 0.3. Note that the model’s final porosity and coordination number were not considered as the microparameter inputs of PFC3D in this study.
Table 1. Microparameters of PFC3D parallel-bond model and ranges of each microparameter for the scope of the proposed calibration method.

| Parameter (abbreviation) | Range                              |
|--------------------------|------------------------------------|
| **Parallel-bonded material group** |                                  |
| Linear group:            |                                    |
| Effective modulus (pbm_emod) | 10 ~ 150 (GPa)                    |
| Stiffness ratio (pbm_krat)  | 1 ~ 4                               |
| Friction coefficient (pbm_fric) | 0.2 ~ 2                            |
| Bond effective modulus (pbm_bemod) | 10 ~ 150 (GPa)                  |
| Bond stiffness ratio (pbm_bkrat) | 1 ~ 4                              |
| Tensile strength (mean and std. deviation) | pbm_ten_m × (0 ~ 0.3)  |
| Cohesion (mean and std. deviation) | pbm_coh_m × (0 ~ 0.3)             |
| Friction angle (pbm_fa)  | 15 ~ 75                             |
| **Linear material group** |                                    |
| Effective modulus (lnm_emod) | 10 ~ 100 (GPa)                    |
| Stiffness ratio (lnm_krat)  | 1 ~ 4                               |
| Friction coefficient (lnm_fric) | 0.2 ~ 2                            |
| **Common parameters**    |                                    |
| Density (cm_densityVal) | 1500 ~ 3000 (kg/m$^3$)            |
| Lower diameter range (cm_Dlo) | 2 ~ 4 (mm)                        |

2.2. Constrained optimization of an Artificial neural network (ANN)

ANNs, computational algorithms inspired by biological neural systems, consist of layers of mathematical neurons which deliver and process numerical signals. The first layer of an ANN, the input layer, receives inputs and passes them to the hidden layers which are in between the input layer and output layer. As signals pass multiple hidden layers, weights and biases are applied to the signals and processed by non-linear activation functions. The weights and biases are updated by the backpropagation algorithm during ANN training and, ultimately, the ANN learns high complexity relations within the training dataset.

Owing to its high performance in finding complex relations between multiple variables, ANNs have been used in various rock engineering problems [10] – [12], including DEM microparameter calibration [4], [5], [13]. Similarly, the ANN is adapted in this study for PFC3D microparameter calibration but with modified input-output configuration. As illustrated in figure 1, unlike other ANN-based DEM calibration methods which obtain calibrated microparameter values as the ANN output (figure 1(a)), the proposed method calibrates microparameters by the constrained optimization of the ANN inputs (figure 1(b)). The ANN of the proposed calibration method predicts the macroscopic responses of PFC3D models for a given set of microparameter values, essentially functioning as a computationally cheaper and faster version of PFC3D uniaxial compression simulations. Such ANN configuration benefits from the fact that macroscopic responses of a PFC3D model, namely UCS, E and v, are determined when a set of microparameter values is given; for the other way around, various combinations of
microparameter values can be derived for the same macroscopic responses which makes the training of ANNs with configuration in figure 1(a) difficult. Therefore, with the microparameter-input and macroscopic response-output configuration, the ANN used in this study can be trained for a wider selection of microparameters and wider range of macroscopic responses. The specifications of the ANN used in this study are further explained in Section 3.

![Figure 1](image-url)

**Figure 1.** Configurations of ANN for microparameter calibration; (a) microparameter calibration through the output of ANN, (b) microparameter calibration through optimization of the input of ANN.

The proposed method calibrates PFC3D microparameters by optimizing the ANN inputs to derive desired ANN outputs of UCS, $E$ and $v$. The optimization is conducted by constraint optimization using the trust-region interior point method [15] implemented in the open-source Python library, SciPy. Through constraint optimization, microparameter calibration can be conducted with user-defined constraints for specific microparameters such as particle size, bond strength and bond effective modulus.

3. Prediction of PFC3D macroscopic response using ANN

3.1. Data acquisition

To train an ANN for predicting PFC3D’s macroscopic responses, a large dataset composed of PFC3D microparameters and its corresponding PFC3D simulation results is required. In this study, to effectively obtain PFC3D data, the microparameter sets were sampled using Latin hypercube sampling (LHS) for the sampling ranges listed in table 1. LHS is a statistical sampling method proposed by Mckay et al. [14] as an alternative to simple random sampling in Monte Carlo simulations. From a multidimensional space, samples selected so that only one sample is selected for each axis of the Latin hypercube. Considering that the sampling space is 15-dimensional and that PFC3D uniaxial compression simulations for dataset generation is computationally costly, it is essential to implement efficient sampling schemes such as LHS.

A total of 800 samples consisting of 15 microparameter values were sampled through LHS. For each microparameter set, PFC3D uniaxial simulations were performed to obtain the corresponding macroscopic responses. The results of the PFC3D simulations, which correspond to the stress-strain curves, were interpreted to determine UCS, $E$ and $v$ based on the ISRM suggested methods [16]; the secant method was used for calculating $E$ and $v$. 

4
The obtained dataset for microparameters and corresponding macroscopic responses is visualized in figure 2; note that for simplicity the relation between E and 6 microparameters are plotted only. As depicted in figure 2, the macroscopic responses of PFC3D models are determined by the interaction of various microparameters. Macroscopic response cannot be predicted by individual microparameters, but there were some relatively influential microparameters for each macroscopic response. UCS was strongly correlated with \( pbm\_ten\_m \), the tensile strength of parallel bonds. For models with higher parallel bond tensile strength, the model reached failure at higher uniaxial compression stress. For E and \( v \), \( pbm\_bemod \) and \( pbm\_bkrat \) showed strong positive correlation with E and \( v \), respectively. The obtained dataset shows that macroscopic response of PFC3D models is strongly influenced by the microscopic counterpart of each macroscopic response. However, the wide scatter shown in figure 2 implies that multiple microparameters must be considered comprehensively in order to accurately predict macroscopic responses.

![Figure 2. Scatter plots between E and microparameters (brighter color indicates higher magnitude of pbm\_bemod).](image)

3.2. **ANN training and testing**

Before training the ANN, the dataset was normalized. The microparameters values were normalized to \([-1, 1]\) by linear mapping and the macroscopic response values were normalized by dividing UCS, E and \( v \) values by \( 5 \times 10^7 \), \( 2.5 \times 10^{10} \), and \( 10^{-1} \), respectively. After normalization, the dataset was divided into the training dataset, validation dataset and test dataset of which each dataset has a total of 600, 87 and 50 data, respectively.

In order to predict 3 PFC3D macroscopic responses using 15 microparameter values, an ANN is constructed which has an input layer of 15 neurons and an output layer of 3 neurons with hidden layers placed between. The activation function of the hidden layer neurons is set as the ReLU function and batch normalization layers are placed between the hidden layers. Training is conducted with the mean-squared-error as the loss function and the Adam optimizer as the weight updating algorithm. The maximum number of epochs is set as 1000, while early stopping of training is activated when the error of a sub-validation dataset starts to increase. With the aforementioned specifications, ANNs were constructed and trained using Keras, a Python deep learning API.
The number of hidden layers and neurons within each layer are hyper-parameters which have to be tuned. In this study, the configurations listed in table 2 were considered for tuning. Configurations of 5, 10 and 20 neurons in each hidden layer and 3, 5, and 7 hidden layers were considered. For each configuration, training was conducted and the validation results were compared. The training results show that validation mean absolute error and mean squared error are the smallest for the configuration of 3 hidden layers with 10 neurons each. Therefore, this configuration was ultimately selected for predicting PFC3D macroscopic responses.

Table 2. Hidden layer configurations and their corresponding validation results.

| Hidden layer configurations | Validation results |  |
|----------------------------|-------------------|---|
|                            | Mean absolute error | Mean squared error |
| 5-5-5-5-5                  | 0.298             | 0.179          |
| 10-10-10-10-10            | 0.145             | 0.041          |
| 20-20-20-20-20            | 0.173             | 0.058          |
| 10-10-10                  | 0.125             | 0.031          |
| 10-10-10-10-10-10-10      | 0.159             | 0.046          |

The ANN’s accuracy of predicting PFC3D simulation is evaluated using the test dataset composed of 50 pairs of microparameter-PFC macroscopic response data. The ANN predictions and actual PFC3D simulation results are compared in figure 2 and the corresponding mean absolute error and mean relative error are given in table 3. The ANN shows a mean absolute error of approximately 8MPa, 3GPa and 0.02 for UCS, E and ν, respectively. The overall mean relative error is 8%, which can be considered as accurate when compared to the variation of macroscopic responses for different particle assembly. Simone et al. [2] demonstrated that, even for the same microparameter values, DEM macroscopic responses can vary according to how particles are geometrically assembled. They reported that the coefficient of variation of UCS and E for different particle assemblies is about 8% and 1%, respectively.

Table 3. Mean absolute error and mean relative error of ANN predictions.

| Macroscopic responses | Mean absolute error (units) | Mean relative error (%) |
|-----------------------|-----------------------------|-------------------------|
| UCS                   | 7.7MPa                      | 11%                     |
| E                     | 2.6GPa                      | 6.4%                    |
| ν                     | 0.02                        | 6.0%                    |

Figure 3. Comparisons between ANN predictions of macroscopic response of PFC3D models and actual simulation results.
4. Micro-parameter calibration through ANN optimization

To calibrate microparameters for desired macroscopic responses, the trust-region interior point method [15] is used to optimize the ANN inputs for targeted ANN outputs. The optimized values of the ANN inputs correspond to the calibrated values of the 15 PFC3D microparameters. Note that the trust-region interior point method allows constraints to be applied during optimization, allowing user-defined constraints in microparameter calibration.

The proposed calibration method is tested with two calibration cases. Target macroscopic responses are set as (UCS, E, v) = (70MPa, 40GPa, 0.25) and (UCS, E, v) = (200MPa, 60GPa, 0.2) for each case. For both cases, user-defined constraints are applied for minimum ball size (cm_Dlo) = 3.2mm and density (cm_densityVal) = 2250 kg/m³ during calibration. Calibration of the 15 PFC3D microparameters is performed by optimizing the ANN inputs so that the ANN outputs match the target macroscopic responses for each case. The optimized ANN input values are then converted (or denormalized) to derive the calibrated values for each microparameter.

The microparameters obtained by the proposed method were tested by running PFC3D simulations with the obtained microparameter values. The results of the PFC3D simulations are tabulated in table 4. Comparison with the target macroscopic responses show that the obtained microparameter values result in macroscopic responses that match well with target values, especially for E and v. The mean relative error of the proposed calibration method is 4.8% which is lower than previous ANN-based calibration methods [4], [5].

Table 4. Comparison of target macroscopic responses and macroscopic responses of PFC3D models with microparameters calibrated by proposed method.

|       | Case 1 | Case 2 | Relative error |
|-------|--------|--------|----------------|
|       | Target | Calibrated | Target | Calibrated |          |
| UCS   | 70MPa  | 78.9MPa | 200MPa | 218.5MPa | 11.0%    |
| E     | 40GPa  | 40.5GPa | 60GPa  | 60.6GPa  | 1.1%     |
| v     | 0.25   | 0.244  | 0.2    | 0.204    | 2.2%     |

5. Conclusion

A PFC3D microparameter calibration method is proposed which calibrates microparameters by optimizing the inputs of an ANN. The ANN was trained to predict the macroscopic responses of a PFC3D model, namely UCS, E and v, for a given set of 15 PFC3D microparameters. As a result of training with 600 PFC3D simulations, the ANN was able to predict macroscopic responses within an error rate of 8%. Tests with two calibration cases showed that the proposed method calibrates microparameter values with high accuracy; mean relative error of calibrated UCS, E and v values was 11%, 1.1% and 2.2%, respectively.

Other than its high accuracy, the proposed calibration method overcomes previous limitations regarding the number of microparameters and the range of macroscopic responses. Through the proposed calibration method, 15 microparameters can be calibrated for macroscopic responses within the ranges of UCS - 10MPa~300MPa, E - 5GPa~200GPa and v - 0~0.5. Also, through the optimization process, user-defined constraints can be applied during calibration.

Further work is required for enhancing the calibration accuracy for UCS and more case studies will be required to validate the robustness of the proposed method. Nevertheless, this study can serve as a guideline for expanding ANN-based DEM microparameter calibration to macroscopic responses such as cohesion and friction angle, and to different contact models.
Acknowledgements
This work was supported by a grant from the Human Resources Development program of the Korea Institute of Energy Technology Evaluation and Planning (KETEP), funded by the Ministry of Trade, Industry, and Energy of the Korean Government (No.20204010600250).

References
[1] Yoon J 2007 Application of experimental design and optimization to PFC model calibration in uniaxial compression simulation Int. J. Rock Mech. Min. Sci. 44(6) 871–89
[2] De Simone M, Souza L, and Roehl D 2019 Estimating DEM microparameters for uniaxial compression simulation with genetic programming Int. J. Rock Mech. Min. Sci. 118 33–41
[3] Wang M and Cao P 2017 Calibrating the micromechanical parameters of the PFC2D(3D) models using the improved Simulated annealing algorithm Math. Probl. Eng. 2017
[4] Tawadrous AS, DeGagné D, Pierce M, and Mas Ivars D 2009 Prediction of uniaxial compression PFC3D model micro-properties using artificial neural networks Int. J. Numer. Anal. Methods Geomech. 33(18) 953–62
[5] Zhai S, Zhan J, Ba Y, Chen J, Li Y, and Li Z 2019 PFC model parameter calibration using uniform experimental design and a deep learning network IOP Conf. Ser. Earth Environ. Sci., 304(3)
[6] Potyondy D 2019 ITASCA Consulting Group Memorandum no. ICG7766-L
[7] Park JW and Song JJ 2009 Numerical simulation of a direct shear test on a rock joint using a bonded-particle model Int. J. Rock Mech. Min. Sci. 46(8) 1315–28
[8] Zhang XP and Wong LNY 2013 Crack initiation, propagation and coalescence in rock-like material containing two flaws: A numerical study based on bonded-particle model approach Rock Mech. Rock Eng. 46(5) 1001–21
[9] Potyondy DO and Cundall PA 2004 A bonded-particle model for rock Int. J. Rock Mech. Min. Sci. 41 1329–64
[10] Dantas Neto SA, Indraratna B, Oliveira DAF, and de Assis AP 2017 Modelling the Shear Behaviour of Clean Rock Discontinuities Using Artificial Neural Networks Rock Mech. Rock Eng. 50(7) 1817–31
[11] Lin H, Singh S, Oh J, Canbulat I, Kang WH, Hebblewhite B and Stacey TR 2020 A combined approach for estimating horizontal principal stress magnitudes from borehole breakout data via artificial neural network and rock failure criterion Int. J. Rock Mech. Min. Sci. 136
[12] Miah MI, Ahmed S, Zendehboudi S, and Butt S 2020 Machine learning approach to model rock strength: prediction and variable selection with aid of log data Rock Mech. Rock Eng. 53(10) 4691–4715
[13] Sun MJ, Tang HM, Hu XL, Ge YF and Lu S 2013 Microparameter prediction for a triaxial compression PFC3D model of rock using full factorial designs and artificial neural networks Geotech. Geol. Eng. 31(4) 1249–59
[14] McKay MD, Beckman RJ and Conover WJ 1979 A comparison of three methods for selecting values of input variables in the analysis of output from a computer code Technometrics 21(2) 239–45
[15] Byrd RH, Hribar ME and Nocedal J 1999 An interior point algorithm for large scale nonlinear programming SIAM J. Optim. 9(4) 877–900
[16] Bieniawski ZT and Bernede MJ 1979 Suggested methods for determining the uniaxial compressive strength and deformability of rock materials: Part 1. Suggested method for determining deformability of rock materials in uniaxial compression Int. Soc. Rock Mech. 16(2) 138-140