DOI: https://doi.org/10.68732/bb74af927b274878

ISBN: 978-9989-2053-7-8

A machine learning-based tool for calibrating UDEC-BBM parameters for modelling intact rocks

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Abstract

Despite the widespread prevalence of the DEM (discrete element method) in rock mechanics and rock engineering, existing trial-and-error and sensitivity analyses for DEM calibration suffer from inefficiency and subjectivity; therefore the calibration of DEM parameters remains a significant challenge.

Given the considerable advantages of the DEM-based UDEC-BBM (universal distinct element code-bonded block model) in modelling intact rocks, we employed machine learning to calibrate the modelling parameters in UDEC-BBM. A comprehensive numerical database with 3,456 UDEC simulations was constructed for training machine learning models to establish the mapping from modelling parameters to modelled properties. Subsequently, the grid search was employed to back-calibrate modelling parameters according to the input target modelled properties (experimental data). This methodology has been implemented by the open-source software UPCal.

To validate the UPCal, we collected experimental data from 99 rock types that served as modelled properties to be input into the UPCal to output the corresponding modelling parameters. The UPCal-calibrated modelling parameters were further imported into UDEC to perform another 1,485 simulations. These UDEC-simulated properties agree well with the experimental values, evidenced by the calibration accuracy as high as overall R^2 = 0.94 for E (Young's modulus), 0.89 for ν (Poisson's ratio), 0.98 for UCS (unconfined compressive strength), 0.90 for BTS (Brazilian tensile strength), 0.76 for c (cohesion), and 0.73 for ϕ (internal friction angle), indicating the reliability and robustness of the UPCal-calibrated modelling parameters.

UPCal achieves the rapid calibration of globally optimal UDEC-BBM modelling parameters using machine learning integrated with grid search, promoting the application of DEM in supporting both scientific research and engineering simulation practice.

Keywords

Machine learning, Universal distinct element code (UDEC), Bonded block model (BBM), Calibration, UPCal.

1 Introduction

Natural rock masses always exhibit discontinuous, inhomogeneous, anisotropic, and non-elastic properties, posing significant challenges to modelling their mechanical behaviours (Hudson and Harrison, 2000). Discrete element method (DEM) has long been recognised as a promising approach to addressing this issue (Cundall, 1971; Potyondy and Cundall, 2004), as it accommodates large displacements, rotations, sliding, and separation of elements, thereby enabling the simulation of complex internal processes, such as crack initiation, propagation, and coalescence (Lisjak and Grasselli, 2014). These processes are executed by iteratively calculating the forces and displacements at bonds to track element motion (Itasca, 2019). Consequently, the DEM simulations depend strictly on the calibration of bond and element parameters.

To calibrate these DEM modelling parameters, trial-and-error method and parametric sensitivity analysis have long been the primary means (Nicksiar and Martin, 2014; Bu et al., 2022a, b), in which modelling parameters are tentatively adjusted, and simulations are repeated numerous times until numerical results closely align with experimental data. Such methods suffer from excessive computational resources and manpower costs (Tawadrous et al., 2009; Bu et al., 2025), high dependence on human subjectivity (Zhai et al., 2019; Shentu and Lin, 2023), and challenge of handling high-dimensional and nonlinear complex mapping from modelling parameters to modelled properties (Bu et al., 2026a, b).

Rapidly advancing artificial intelligence (AI) excels at processing multidimensional data and high-order nonlinear relationships, providing a possible robust framework for DEM parametric calibration. The DEM models an intact rock as an assembly of disc/spherical particles or polygonal/polyhedral blocks, termed bonded particle model (BPM) or bonded block model (BBM), respectively. Early research into AI-driven parametric calibration focused on the BPM, typically implemented within Particle Flow Code (PFC) (Tawadrous et al., 2009; Guo et al., 2013; Boikov et al., 2018; Zhai et al., 2019; Westbrink et al., 2021; Shentu and Lin, 2023). However, the absence of particle interlocking causes PFC-BPM to overpredict tensile strength and fail to capture the failure envelopes of intact rock (Diederichs, 1999; Cho et al., 2007). Although the grain-based model (PFC-GBM) improves this by fusing neighbouring particles into clusters (Cho et al., 2007; Itasca, 2025), it still struggles to accurately reproduce the experimental tensile-to-compressive strength ratio (Fabjan et al., 2015; Turichshev and Hadjigeorgiou, 2017). Consequently, intensive focus on AI-driven optimisation for PFC-BPM may yield diminishing returns when modelling intact rocks.

In contrast to BPM, the BBM employs a highly interlocked structure, enabling it to accurately replicate the experimental failure envelope and tensile-to-compressive strength ratio of intact rock (Turichshev and Hadjigeorgiou, 2017; Sinha and Walton, 2020). Therefore, BBM has become the preferred framework for modelling intact rocks (Lan et al., 2010; Stead and Wolter, 2015; Barton, 2020). BBM can be implemented in both PFC and universal/3D distinct element code (UDEC/3DEC). Rasmussen (2021) introduced the spring network model within the hybrid lattice/discrete element method, which is related to the PFC-BBM. Currently, PFC-BBM utilises rigid blocks that translate and rotate but cannot deform (Itasca, 2025), which may limit its ability to represent the Poisson's ratio effect in confined rock masses or the internal deformation of grains (Lan et al., 2010; Itasca, 2019). Furthermore, PFC-BBM establishes only a single contact point between blocks, where the contact position is either the overlap centroid or a fixed point updated incrementally via bonding (Itasca, 2025). This abstraction may fail to capture the complex force distribution and localised opening-closing mechanics essential for modelling rough-joint interlocking or edge-initiated failure. In contrast, UDEC-BBM supports both rigid and deformable blocks and incorporates a sub-contact framework, offering superior performance for implementing BBM and simulating the mechanical behaviour of intact rocks (Potyondy and Cundall, 2004; Lan et al., 2010; Mayer and Stead, 2017).

Due to fundamental differences in element geometry, deformability, and bond logic, existing AI calibration methods for PFC-BPM, PFC-GBM, and PFC-BBM are largely incompatible with UDEC-BBM. Currently, AI applications in UDEC-BBM calibration remain limited; to the best of our knowledge, Fathipour-Azar (2022) is one of the few to utilise machine learning for UDEC-BBM parametric sensitivity analysis of unconfined compressive strength (UCS). A robust framework for deriving globally optimal UDEC-BBM parameters from experimental targets has yet to be established. Developing such a system requires integrating inversion algorithms with extensive numerical databases to map the relationship between input parameters and mechanical responses, thereby

preventing convergence on local optima. Furthermore, a diverse experimental database is essential to validate the reliability of AI-driven calibration in UDEC-BBM. This study addresses these gaps by developing a machine-learning tool designed to output globally optimal UDEC-BBM modelling parameters directly from experimental data.

2 Methods

2.1 UDEC-BBM algorithm

In this study, UDEC 6.0 is used to model an intact rock as an assembly of deformable blocks, with internal motion resolved at triangular grid points under a finite-strain framework. Contact interactions follow the Coulomb friction law, a configuration proven to reliably simulate rock mechanics tests (Lan et al., 2010; Bu et al., 2025). See Itasca (2019) for more UDEC-BBM details.

2.2 Parametric calibration by machine learning

2.2.1 Numerical database generation

In UDEC, the deformation properties of a rock model (Young's modulus E and Poisson's ratio ν) include contributions from both block properties (block Young's modulus E_b and block Poisson's ratio ν_b) and the stiffness of contacts (normal stiffness k_n, shear stiffness k_s, and k_n/k_s). The strength properties (unconfined compressive strength UCS, Brazilian tensile strength BTS, cohesion c, and internal friction angle ϕ) depend on contact properties (cohesion c_c, friction angle ϕ_c, and tensile strength T_c). To ensure the model encompasses the full spectrum of rock behaviour, broad variation ranges are established for each modelling parameter (E_b, ν_b, k_n, k_n/k_s, c_c, ϕ_c, and T_c). A gradient-based configuration is employed to enhance subsequent training stability (Table 1). Parameter combinations are systematically generated and imported into UDEC to simulate 2,808 unconfined/confined compressive and 648 Brazilian tensile tests. By analysing the resulting stress–strain curves and applying the Mohr–Coulomb failure criterion, modelled properties (E, ν, UCS, BTS, c, and ϕ) for each parameter set are derived.

Table 1. Preset gradient-based modelling parameters.

Type	Minimum	Maximum	Increments
Strength-determining modelling parameters			
Contact cohesion c_c [MPa]	2.5	65	12.5
Contact friction angle ϕ_c [°]	5	50	10
Contact tensile strength T_c [MPa]	6	66	12
Deformation-determining modelling parameters			
Block Young's modulus E_b [GPa]	15	115	20
Block Poisson's ratio ν_b	0.08	0.33	0.05
Contact normal stiffness k_n [$\times 10^4$GPa/m]	1	100	20
Contact stiffness ratio k_n/k_s	1	4	0.6
Shape parameters			
Average edge length of polygons l [mm]	2	4	1

2.2.2 Machine learning

A central component of this framework involves using machine learning to map modelling parameters (E_b, ν_b, k_n, k_n/k_s, c_c, ϕ_c, and T_c) to modelled properties (E, ν, UCS, BTS, c, and ϕ). Utilising the numerical data from the generated numerical database, modelling parameters serve as input variables while modelled properties act as targets, with a 75/25 train-test split. Post-training, the model generates predicted parameters from the test targets, which are then validated against the actual values to ensure dimensional and structural consistency. To maximise predictive accuracy, hyperparameter optimisation is integrated into the machine learning workflow.

2.2.3 Back-calibration

The framework further employs trained machine learning models to back-calibrate modelling parameters (E_b, ν_b, k_n, k_n/k_s, c_c, ϕ_c, and T_c) from experimental data (E, ν, UCS, BTS, c, and ϕ). While a forward mapping uniquely determines modelled properties from modelling parameters, the inverse relationship is inherently one-to-many, where identical properties may arise from distinct parameter sets. Directly training an inverse model under such non-unique mappings often yields unstable or

unphysical results. To address this, a two-stage grid search uses the forward machine learning models as efficient surrogates to comprehensively explore the parameter space. The optimal parameter set is identified by minimising the sum of squared errors between predicted and target properties. By operating within physically meaningful bounds, this approach balances computational efficiency with global optimisation.

2.2.4 Validation

The framework concludes with a validation phase where the machine learning–calibrated parameters are imported back into UDEC for a final round of simulations. The resulting modelled properties are then compared against the experimental data to verify the accuracy and robustness of the calibration.

2.3 Design of the tool

2.3.1 Adaptivity

To ensure adaptivity across varying experimental data completeness, two experimental input schemes are designed based on data availability. Since unconfined compressive tests invariably yield E and v, these are treated as mandatory inputs. In the 6-parameter scheme, where a full dataset is available, the machine learning maps modelling parameters (E_b, v_b, k_n, k_n/k_s, c_c, ϕ_c, and T_c) to six experimental properties (E, v, UCS, BTS, c, and ϕ). If confined compressive tests are missing, c and ϕ are excluded, resulting in a 4-parameter scheme (E, v, UCS, BTS). This framework generalises to any number of experimental inputs, provided the machine learning model is configured with a matching number of input nodes.

2.3.2 Module description

To integrate the proposed calibration framework into a tool, namely UPCal, we designed five modules coordinated by the UPCal Core Controller. The data flow layer handles application startup, user input, and preprocessing tasks like data cleaning. The application logic layer manages the calibration workflow, executing machine learningmodels for inversion and overseeing data export. A Tkinter-based user interface layer provides navigation and progress tracking to facilitate interaction, while the machine learning layer integrates algorithms such as Random Forest (RF), Deep Neural Networks (DNN), Gaussian Process Regression (GPR), and Support Vector Regression (SVR) for model training and evaluation. Finally, the external system layer connects the platform with UDEC, file systems, and visualisation tools, creating a unified environment for automated parameter calibration.

2.3.3 Graphical user interface

Developed with the Python 3.9 Tkinter library, the UPCal graphical user interface (GUI) provides an efficient environment for managing UDEC parameter calibration. The interface features a sidebar navigation panel for accessing data input, parameter definition, and results visualisation, while a central dynamic content area manages active tasks and input forms. To assist users, a contextual help area provides real-time documentation, and a progress tracker monitors ongoing machine learning training or parameter inversion. This structured layout enables seamless navigation between stages without requiring advanced technical expertise. Furthermore, the GUI integrates visualisation tools to display training curves and comparative analyses between simulated and experimental results, ensuring a transparent and user-friendly calibration process.

3 Results

3.1 Experimental database

We take the case with a 6-parameter scheme with the DNN model as an example to illustrate. For validation, we constructed a comprehensive experimental database that contains 99 rock types in previous literature, including 47 igneous, 40 sedimentary, and 12 metamorphic rocks. See Bu et al. (2026a) for more details. Their experimental properties, including E (ranging from 1.15 to 78 GPa), v (0.08 to 0.39), UCS (6.83 to 300.1 MPa), BTS (0.48 to 24.54 MPa), c (1.9–78.13 MPa), and ϕ (10–61.75°) were collected and served as input into the UPCal to output modelling parameters.

3.2 Consistency between experimental and numerical results

Use those UPCal-calibrated parameters to conduct a total of 1,485 UDEC simulations to obtain the modelled properties (E, v, UCS, BTS, c, and ϕ). For igneous rocks (Fig. 1), simulated results align closely with experimental data. Excluding block size effects, UCS yields the highest predictive

accuracy (R^2 = 0.97), followed by E (R^2 = 0.93), while ν and ϕ remain satisfactory at R^2 values of 0.86 and 0.85. Conversely, BTS and c exhibit lower reliability (R^2 of 0.74 and 0.76).

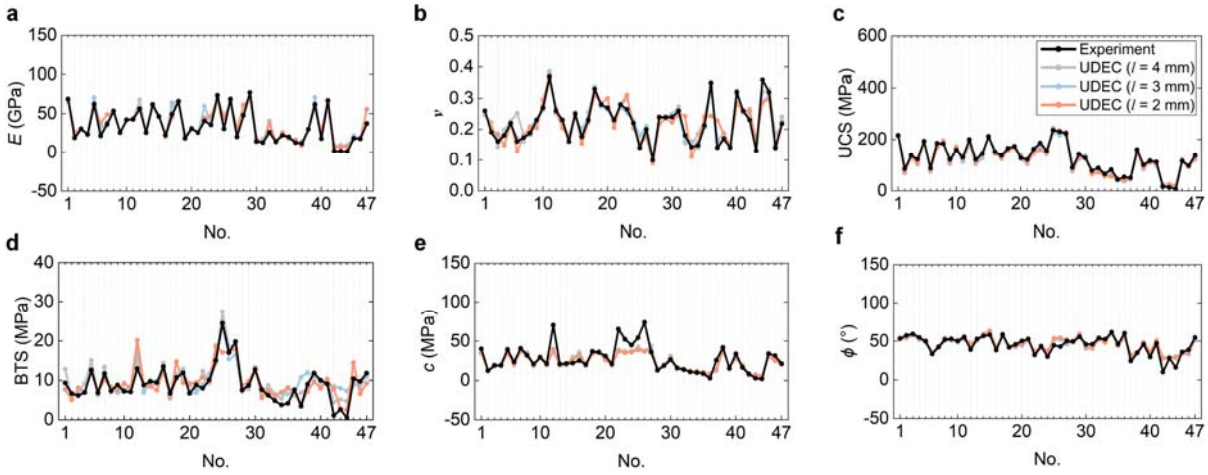


Fig. 1 Comparison of experimental and UDEC-simulated mechanical properties of igneous rocks employing UPCal-calibrated modelling parameters, where the horizontal axis represents the specimen number.

Sedimentary rock calibrations similarly match experimental measurements, where UCS and E achieve primary precision with R^2 values of 0.98 and 0.94. While ν maintains a strong correlation (R^2 = 0.90), predictions for c, ϕ, and BTS are notably less robust, falling to 0.73, 0.51, and 0.68. Metamorphic simulations demonstrate comparable consistency. UCS remains the most accurate parameter (R^2 = 0.98), followed by reliable estimates for deformation properties E (R^2= 0.94), ν (R^2= 0.92), and c (R^2= 0.92). However, the model is less effective for ϕ and BTS, resulting in diminished R^2 values of 0.80 and 0.69.

Despite the general consistency between experimental and numerical results have validated the UPCal-calibrated UDEC-BBM modelling parameters, the block size, lithology, experimental-input schemes, and machine learning models may also have some effects on the calibration accuracy. See Bu et al. (2026a, b) for more details.

4 Conclusion

This study demonstrates that the developed UPCal is a robust tool for machine learning-based UDEC-BBM calibration, which is open-sourced at https://github.com/RuoSL/UPcal. By inputting adaptive experimental data, UPCal automatically outputs optimal UDEC-BBM modelling parameters (E_b, ν_b, k_n, k_n/k_s, c_c, ϕ_c, and T_c). Unlike traditional trial-and-error or sensitivity analyses, UPCal removes manual intervention and repeat simulations, delivering globally optimal parameters that bolster simulation credibility. Distributed as open-source software with an integrated GUI, it facilitates immediate deployment by users regardless of their UDEC-BBM or machine learning expertise, providing a definitive solution for calibrating UDEC-BBM parameters.

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