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Bonded Contact Calibration in DEM using Nano Indentation Test

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Abstract

Numerical investigation of crack propagation in rock materials has progressed considerably, with the Discrete Element Method (DEM) providing notable advantages over continuum-based methods in rock mechanics. Particle Flow Code (PFC), an explicit DEM tool, simulates rock behaviour through bonded contact models that describe interactions between rigid particles. Conventionally, calibration of these models relies on a trial-and-error approach, where micro-scale parameters are repeatedly adjusted to reproduce experimentally observed macro-mechanical properties. However, such methods often fail to accurately capture crack initiation from pre-existing flaws and the resulting failure patterns in numerical simulations. The Flat-Jointed Model (FJM) is widely adopted due to its ability to realistically represent the angular and interlocked nature of mineral grains in rock. Nevertheless, calibrating the six required micro-parameters in FJM is complex, time-consuming, and subject to uncertainty. To address this limitation, nano-indentation testing is utilized to directly estimate key micro-mechanical properties, including Young's modulus and stiffness ratio. Using these parameters, crack propagation in flawed synthetic rock specimens under uniaxial loading is simulated in PFC. Validation of the numerical results demonstrates that the proposed calibration approach effectively captures crack growth and reproduces experimentally observed failure patterns with improved accuracy.

Keywords

Particle Flow Code, Rock, Micro-parameters, Nano-indentation, Crack Propagation.

1 Introduction

Numerical modelling of rock using the Distinct Element Method (DEM) has seen significant advancements in recent years. Particle Flow Code 2D (PFC2D) an explicit DEM software has become an important tool for modelling rock. In PFC2D rock is modelled using rigid particles which acts as mineral grains and the bonded contact model (Potyondy 2004) acts as a cementing medium between these mineral grains. By calibrating the bonded contact model, the numerical rock model can replicate the macroscopic mechanical properties of rock.

However, the bonded contact model involves several micro-parameters to be calibrated depending on the type of bonded contact model chosen and the commonly used method of calibration is trial-and-error approach (Itasca 2014). This approach involves matching macro properties (Uniaxial compression strength, Tensile strength, Young's modulus and poisons ratio) of numerical simulated model with laboratory model by varying the micro properties. But the disadvantage of this approach is it is often time-consuming because even though a micro propertycan have a large effect on a specific macro property it can also have a little effect on another macro property. This causes several repeating cycles of varying the micro properties to match the macro properties. To avoid this indirect way of calibrating micro properties a direct way of calibrating micro property involves determining mechanical properties of rock at the micro-scale. Nanoindentation testing enables the measurement of mechanical properties at the Nano-scale.

This paper presents the calibration of micro-parameters using Nano indentation test results. For Validation, crack propagation from a pre-existing flaw is compared between experimental results and numerical models simulated using both the conventional trial-and-error calibration method and the Nano indentation-based calibration approach.

2 Nano indentation test

Nano indentation is an indentation test in which an indent is made on a material to determine its mechanical properties such as hardness and elastic modulus using an indenter with known properties. The applied load is typically in millinewtons, and the displacement is measured in nanometer. A load–indentation depth curve is obtained from the test, from which the elastic modulus (E) and hardness (H) of the material are calculated.

$$E = (1 - \nu^2)(\frac{1}{E_r} - \frac{1-\nu_i{}^2}{E_i})(1)$$

Where E_r Reduced Modulus
E_i Indenter Modulus
ν Poisson's Ratio of Sample
ν_i Poisson's Ratio of indenter

$$H = \frac{P_{max}}{A_c}(2)$$

Where P_{max} Maximum Load Applied
A_c Projected Contact Area

Unlike conventional indentation tests, the contact area (A_c) is calculated depending on the depth of penetration and geometry of the indenter. In our study Berkovich indenter a three-sided pyramidal indenter is used. The projected contact area of Berkovich indenter is given by $24.5\ h_c^2$, where hc is the contact penetration depth.

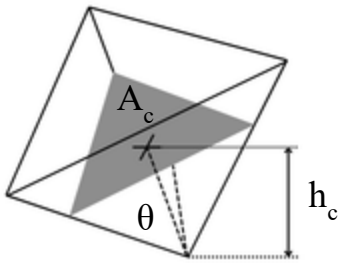
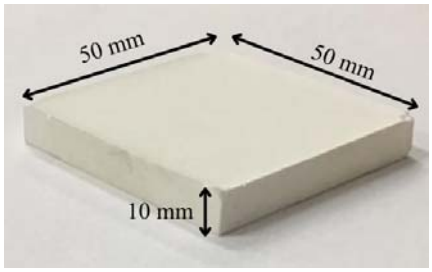


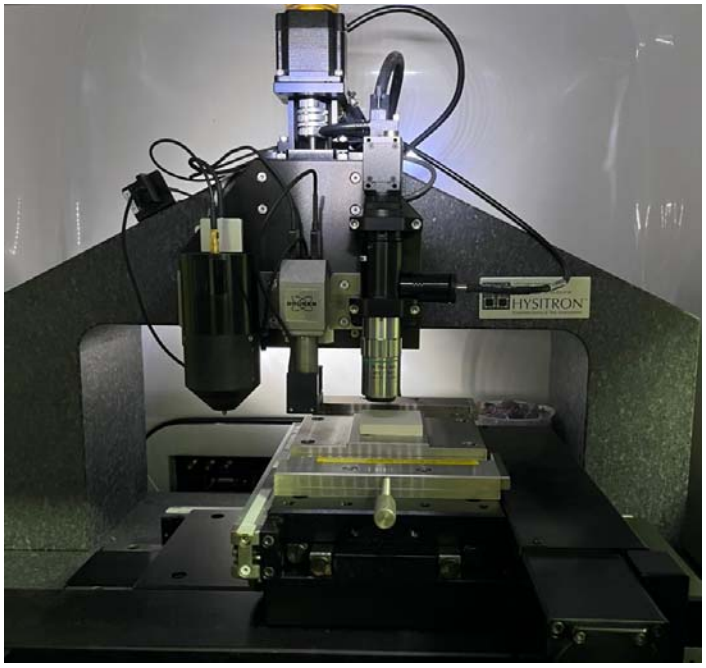
Fig. 1 Berkovich indenter.

2.1 Sample preparation and testing

The present study focuses on homogeneous artificial rock and gypsum was chosen because of its ability to replicate the behaviour of an ideal natural rock (including the presence of secondary crack growth). Additionally, it is easy to prepare in large quantities and specific dimensions.To prepare the gypsum specimen S-35 grade gypsum powder was mixed with 25% water to form a slurry, which was then poured into moulds to produce samples of the required dimensions. A sample of size 50 × 50 × 10 mm was prepared to meet the requirements of the Hysitron TI 950 TriboIndenter as shown in Figure 2. The surface of the specimen is ensured to be smoot has roughness of sample surface can affect the accuracy of results (Yang et al. 2017). Before performing indentation, the indentation locations were selected. The indentation produces a triangular impression on the specimen at the nanoscale, as shown in Figure 3.



(a)



(b)

Fig. 2 a) Sample used for Nano indentation test b) Berkovich indenter c) Hysitron TI 950 Tribo Indenter.

Nano indentation test are performed in three stages. 1) Loading stage - Displacement-controlled mode was selected for testing, and the load was applied until peak load (40,000 µN) is reached. 2) Holding stage - Upon reaching the peak load, a holding stage of 5 seconds was maintained 3) Unloading stage – In this stage the reduced indentation modulus is calculated from the slope of the unloading curve obtained from the load–displacement data, as shown in Figure 4. The Young's modulus of the test sample was then determined using the Young's modulus and Poisson's ratio of the indenter as shown in Eq. 1 and are listed in Table 1.

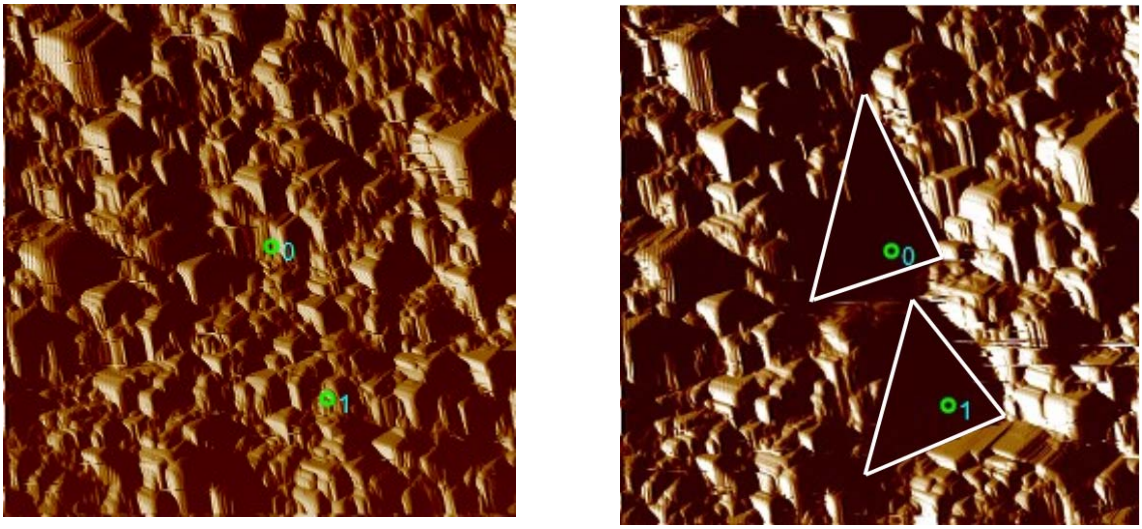


Fig. 3 a) Points marked for Nano indentation (Before Nano indentation) b) After Nano indentation.

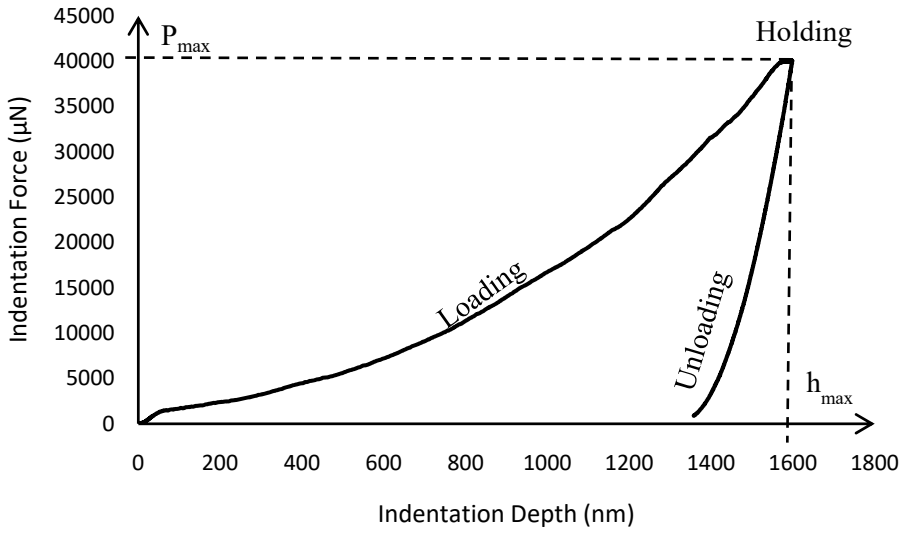


Fig. 4 Load-indentation depth curve of gypsum mineral.

Table 1. Mechanical properties of gypsum determined using Nano indentation.

Nano Indentation Properties	**Value**
Maximum Force, P_{max} (µN)	40031
Maximum Depth, h_{max}(nm)	1598
Reduced Modulus E_r (GPa)	33.97
Young's Modulus E (GPa)	35.72
Hardness (MPa)	733.58

3 Calibration of Micro properties

In Particle Flow Code 2D, Gypsum rock issimulated using 2D rigid particle represents a gypsum mineral grain with voids existing between them and bonded to neighbouring particles using flat-jointed bonded contact model (Potyondy 2012).

To capture the mechanical behaviour of gypsum rock, six microparameters of the flat-jointed model must be calibrated. Previous calibrations proposed by Bahaaddini et al. (2021)were based on a trial-and-error approach in which the microparameters were varied until the macroscopic properties matched the experimental results as shown in Table 2. In the present study, nano indentation testing was used to directly determine two of the six microparameters, while the remaining parameters were calibrated using the trial-and-error method. This approach significantly reduces the complexity of the calibration process.

The Young's modulus of the gypsum mineral obtained from the Nano indentation test was used as input. The stiffness ratio was calculated from Poisson's ratio and is independent of E and G due to the assumed homogeneity of the gypsum material. The particle size distribution was calibrated to match the macroscopic Young's modulus with the known microscopic Young's modulus and stiffness ratio. Finally, the tensile strength, cohesion, and friction angle were calibrated using the trial-and-error method. Table 3 shows the change in micro properties when Nano indentation calibration is adopted. From the micro parameters adopted the calibrated model yields the following macro properties shown in Table 4.

$$k_n = \frac{2E_1E_2}{t(E_1+E_2)} \quad (3)$$

At interior of mineral $E_1 = E_2$

$$k_n = \frac{E}{t} \quad (4)$$

Where E_1,E_2 Young's modulus of mineral on both sides of interface
t Thickness of contact interface
k_nNormal stiffness

$$k_s = \frac{2G_1G_2}{t(G_1+G_2)} \quad (5)$$

At interior of mineral $G_1 = G_2$

$$k_s = \frac{G}{t} \quad (6)$$

Where G_1,G_2 Shear modulus of mineral on both sides of interface
k_s Shear stiffness

Dividing (4) by (5)

$$\frac{k_n}{k_s} = \frac{E}{G} = 2(1+\nu) \quad (7)$$

Where ν Poisson's ratio of the sample

Table 2. Comparison of calibration procedure.

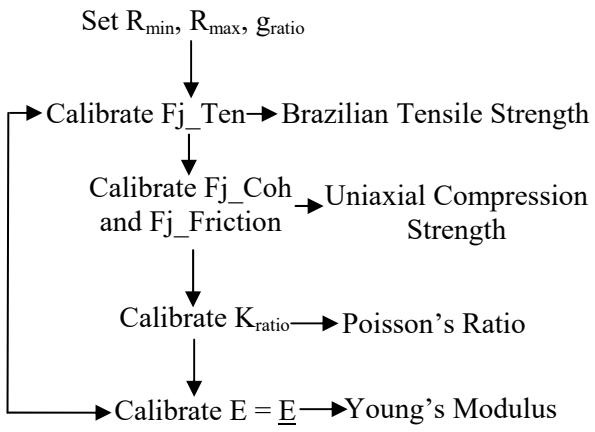
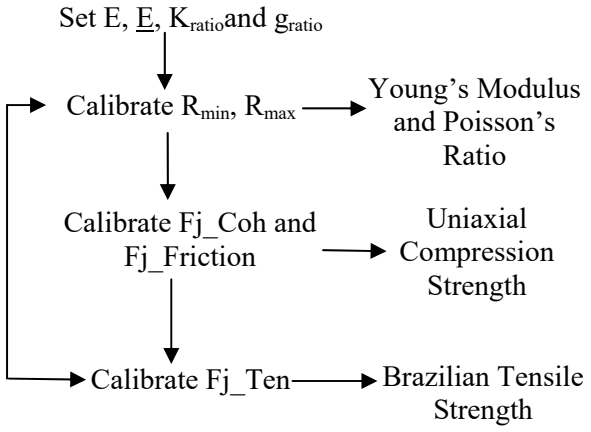
Bahaaddini et al. (2021) Calibration	**Nano Indentation Calibration**
	

Table 3. Comparison of Micro properties.

Micro Properties	**Bahaaddini et al. (2021)**	**Nano indentation**
Elastic modulus, E (GPa)	4.75	32.8
Stiffness ratio, k_n/k_s	1.5	2.7
Tensile Strength (MPa)	12.5	20.25
Cohesion strength (MPa)	22.5	44.5
Friction angle ϕ (°)	10.5	22.0

Table 4. Physico-mechanical properties of experimental and numerical Nano indentation calibrated model.

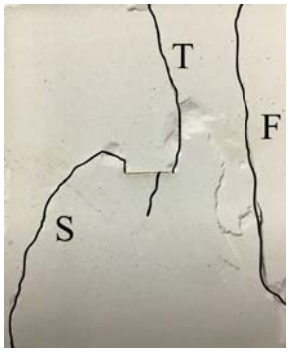
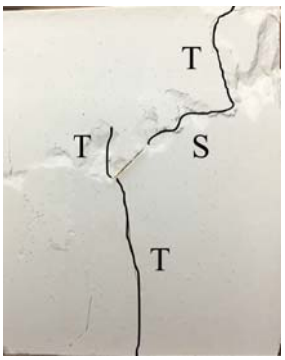
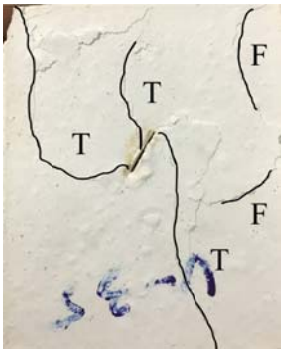
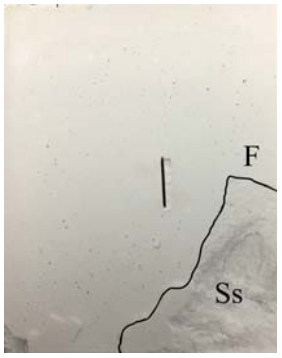
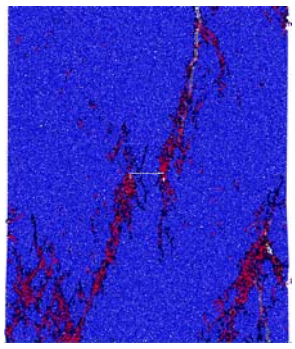
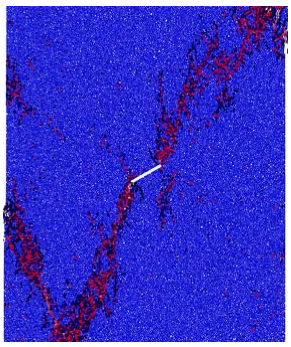
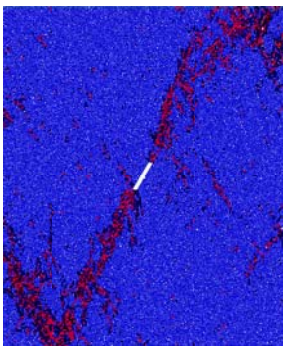
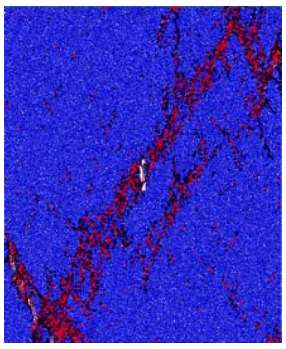
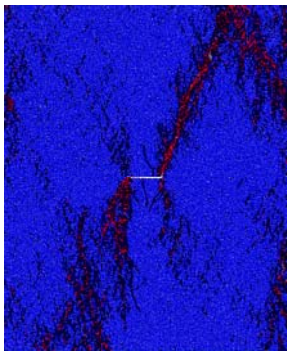
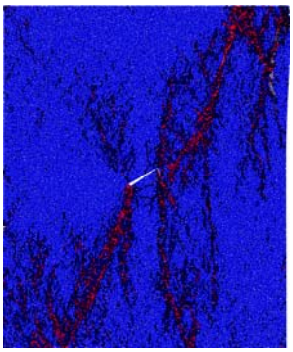
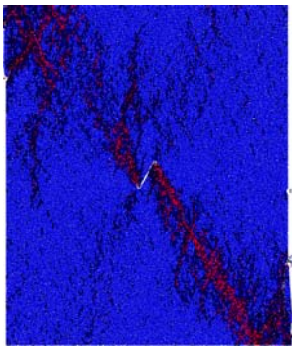
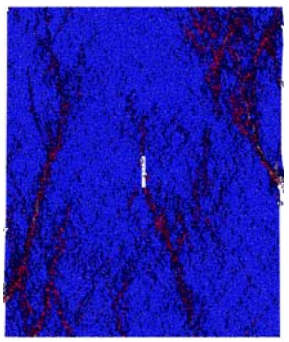
Physico-mechanical properties	**Experimental Results**	**Numerical Results**
Uniaxial Compression Strength (MPa)	42.31	41.71
Young's Modulus (GPa)	2.3385	2.215
Tensile Strength (MPa)	6.25	6.18
Poisson's Ratio	0.35	0.355

Similar calibration approaches have also been applied to multi-mineral rocks such as granite (Liu, Xiu-Yang et al. 2024) and sandstone (Yang et al., 2024), where the particle size in the numerical model is determined based on the mineral grain size (grain-based model). However, this approach is not suitable for the current study. Therefore, an additional calibration step is required to match Young's modulus and Poisson's ratio by employing dual indentation technique namely method developed by Ganneau et al. (2006).

4 Comparison of Results

To evaluate the accuracy of the Nano indentation-calibrated model in capturing crack growth from a pre-existing flaw, a comparison was made between the experimental results and the trial-and-error calibrated model. A specimen of size 52 × 64 × 12 mm was tested under uniaxial loading with a centrally located flaw of length 6mm and thickness 0.6mm inclined at angles ranging from 0° to 90°, in increments of 30°. The differences in the calibrated micro parameters between the two approaches are presented in Table 5.

Table 5. Comparison of crack propagation pattern of experimental and numerical analysis.

0°	30°	60°	90°
Experimental Results			
			
Bahaaddini et al. (2021) Calibration			
			
Nano Indentation Calibration			
			

4.1 0° and 30° flaw orientations

There is no significant difference in the crack propagation patterns between the models, and both agree well with the experimental results. However, the Nano indentation-calibrated model is better able to capture the closure of the pre-existing flaw.

4.2 60° flaw orientation

The final failure pattern shows good agreement with the Nano indentation-calibrated model compared to previous trial and error calibration and a certain degree of flaw closure is observed.

4.3 90° flaw orientation

In the experimental results, the failure pattern is not significantly influenced by the presence of the flaw. This behaviour is not well reflected in the trial and error calibrated model. In contrast the Nano indentation calibrated model limits the influence of the flaw to a greater extent showing better agreement with the experimental observations.

5 Conclusion

In this study, a new calibration method incorporating the Nano indentation technique is proposed. The method is validated by comparing numerical results with experimental observations and it demonstrates improved capability in capturing crack growth from a pre-existing flaw compared to the conventional fully trial-and-error calibration method. The proposed approach also captures the closure of the flaw which subsequently leads to the formation and propagation of tensile anti-wing cracks. The present study focuses on a single homogenous mineral rock (gypsum). Additionally, the current study still involves partial trial-and-error calibration. This limitation can be addressed in future studies by employing the dual-indentation technique, which can help determine the remaining micro-mechanical properties more systematically.

References

Bahaaddini M, Sheikhpourkhani AM, Mansouri H (2021) Flat-joint model to reproduce the mechanical behaviour of intact rocks. European Journal of Environmental and Civil Engineering 25(8): 1427–1448.

Ganneau FP, Constantinides G, Ulm FJ (2006) Dual-indentation technique for the assessment of strength properties of cohesive-frictional materials. International Journal of Solids and Structures 43(6): 1727–1745. DOI.

Itasca Consulting Group Inc (2014) PFC (Particle Flow Code) Version 5.0. Itasca Consulting Group Inc, Minneapolis, United States.

Liu XY, et al. (2024) Study on the micromechanical and crack characteristics of granite based on nano indentation test and discrete element method. Computational Particle Mechanics 11(4): 1547–1563. DOI.

Potyondy DO (2012) A flat-jointed bonded-particle material for hard rock. 46th US Rock Mechanics/Geomechanics Symposium, Chicago, United States, 2012, pp 1510–1519.

Potyondy DO, Cundall PA (2004) A bonded-particle model for rock. International Journal of Rock Mechanics and Mining Sciences 41(8): 1329–1364. DOI.

Yang H, Luo S, Zhang G, Song J (2017) Elasticity of clay shale characterized by nanoindentation. ARMA US Rock Mechanics/Geomechanics Symposium, San Francisco, United States, June 2017.

Yang X, Zhang Y, Li G, Li Z, Feng J, Wang K (2024) Mesoscopic modeling approach and application based on rock thin slices and nanoindentation. Computers and Geotechnics 165: 105875.