Numerical investigation on determining the optimal heterogeneity index and compressive–tensile ratio of granite using a damage-based numerical manifold method

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Abstract. The heterogeneity of rock at the mesoscopic level and the compressive–tensile ratio affect the macroscopical mechanic behavior and failure mode of rocks. In this study, a damage-based numerical manifold method was used to examine the optimal heterogeneity index and the compressive–tensile ratio of Lac du Bonnet granite. This study examined the numerical manifold method and damage theory, as well as the Weibull distribution. The uniaxial compression test and the Brazilian splitting test on granite were simulated to calibrate the basic input parameters, including the uniaxial compressive strength, Young’s modulus, and Poisson’s ratio. The uniaxial compressive tests on model specimens with different heterogeneity indices and the Brazilian splitting tests on model specimens with different compressive–tensile ratios were conducted using the damage-based numerical manifold method (NMM) program. The simulation of the macroscopic mechanical behavior and the failure mode of model specimens showed good agreement with granite in the laboratory. The relationship among the heterogeneity index, compressive–tensile ratio, macroscopic mechanical behavior, and failure mode were examined. The numerical results indicated that the heterogeneity index had the most significant effect on the crack initiation stress and the peak strength of granite, while the compressive–tensile ratio affects the failure mode the most. Finally, the optimal heterogeneity index and compressive–tensile ratio of Lac du Bonnet granite are proposed. A comparison of the results showed that the optimal heterogeneity index and compressive–tensile ratio could model the cracking behavior of rocks more precisely.

1. Introduction

Rocks are highly heterogeneous in many aspects because of the diversity of their microstructure [1]. Several experimental and numerical studies have been conducted in the past few decades to examine the effects of material heterogeneity on rock strength, deformation, and creep behavior [2-5]. Lan [11] proposed a grain-based model and reported that grain-scale heterogeneities have controlling effects on the distribution of tensile stress and associated extension cracks. Mohsen Nicksiar [7] suggested that the heterogeneity introduced by the grain size distribution has the most significant effect on the peak strength and crack initiation stress. Xu [9] presented a 2-D numerical model accounting for material...
heterogeneity through a stochastic local failure stress field and local material degradation using an 
exponential material softening law. Tang [12] reported that a homogeneous specimen had higher 
strength than a heterogeneous one and more linear deformation behavior before peak stress. Zhou et al. [13] 
examined the dynamic behaviors of granite under combined compression/shear loading by the 
modified split Hopkins on pressure bar device. They reported that the heterogeneity is loading–rate-
dependent and shear–component-dependent. Liu [14] presented a new heterogeneity index to describe 
the micro-geometric heterogeneity induced by grain size variations. Sheorey [15] reported that the 
compressive–tensile ratio of sandstone varies from 7 to 39 by statistical analysis of the experimental 
data. The damage theory has been developed to describe the effects of progressive micro-cracking, 
void nucleation, and micro-crack growth at high-stress levels [16, 17]. Shi [18] invented a numerical 
manifold method (NMM) to simulate the continuities and discontinuities naturally within a uniform 
framework compared to XFEM, GFEM, and DEM. Some researchers applied it to rock mechanics and 
engineering because of its advantages [19, 20]. Fan [21] examined shear band static evolution using 
spatially mobilized plane criterion-based Drucker–Prager model and numerical manifold method. 
Considerable work has been performed to understand the heterogeneity and compressive–tensile ratio 
of rock. On the other hand, determining the optimal heterogeneity index and compressive–tensile ratio 
for a specific rock remains uncertain, making it difficult for simulations and engineering practice. This 
study examined the effects of the material properties heterogeneity, and compressive–tensile ratio on 
the strength and deformation of Lac du Bonnet granite using a damage-based numerical manifold 
method. This paper presents a more straightforward method to determine the optimal heterogeneity 
index and the compressive–tensile ratio of granite.

2. Numerical modeling method
2.1 Numerical Manifold Method
The background of the NMM is reported elsewhere [10, 17-21]. Hence, only the basic concepts of 
NMM are provided. The NMM consists of two important cover systems, i.e., the mathematical cover 
system (MCS) and the physical cover system (PCS).
The union of mathematical patches (MPs) forms the MCS. The mathematical cover can be generated 
by any type of meshes, provided these meshes cover the problem domain. The MCS does not need to 
match the physical meshes determined by the problem domain.
The union of physical patches (PPs) forms the PCS. The physical patches were generated by cutting 
the MPs with physical meshes (PMs), including joints, cracks, material interface, and blocks. For each 
PP, the degrees of freedom (DOFs) were defined on an NMM node.
The communal zone of \( n \) (dependent on the type of mesh used) PPs forms a manifold element (ME) 
after the cutting process. The ME can be in any shape and is adapted to carry out the integration. The 
global displacement function, which is defined over the ME, is expressed as follows:
\[
\mathbf{u}(x) = \sum_{k=1}^{n} w_k(x) \mathbf{u}_k(x),
\]
where \( n \) represents the number of physical patches that the manifold element is covered. The value of 
\( n \) is dependent on the type of mesh utilized; \( w_k \) is the weight function, and it meets the following 
conditions in Eq. (2): \( \mathbf{u}_k(x) \) represents the cover function vector:
\[
\sum_{k=1}^{n} w_k(x) = 1 \quad \text{and} \quad \begin{cases} 0 \leq w_k(x) \leq 1, & \forall x \in P_k, \\ w_k(x) = 0, & \forall x \notin P_k \end{cases}
\]
where \( P_k \) represents the physical cover.
Taking the three-node element as an example, the cover function vector is expressed as follows:
\[
\mathbf{u}_k(x) = \begin{bmatrix} u_k \\ v_k \\ w_k \end{bmatrix},
\]
Substituting Eq. (3) into Eq. (1) yields the following simple form of the global displacement function:
\[
\mathbf{u}(x) = N_j(x) \mathbf{D}_k
\]
where
\[ N_k(x) = \begin{bmatrix} N_1 & 0 & N_2 & 0 & N_3 & 0 \\ 0 & N_1 & 0 & N_2 & 0 & N_3 \end{bmatrix} \] (5)
\[ D_k = [D_1, D_2, D_3]^T, \] (6)
in which \( N_k(x) \) represents the matrix of the shape function, and \( D_k \) represents the degree of freedom (DOF) vector.

2.2 Damage Constitutive Law
In elastic damage mechanics, the stiffness of the elements degrades gradually as damage progresses. The elastic modulus of the damaged material is expressed considering the isotropic continuum damage formulation:
\[ E = (1-D)E_0, \] (7)
where \( D \) represents the damage variable, and \( E \) and \( E_0 \) are the Young’s modulus of the damaged and undamaged material, respectively. \( D \) can be expressed as
\[ D = \begin{cases} 0, & F_1 < 0 \land F_2 < 0 \\ 1 - \frac{\varepsilon_1}{\varepsilon_0}, & F_1 = 0 \land dF_1 > 0 \\ 1 - \frac{\varepsilon_3}{\varepsilon_0}, & F_2 = 0 \land dF_2 > 0 \end{cases} \] (8)
where \( \varepsilon_0 \) and \( \varepsilon_0 \) are the critical strain in tension and the critical strain in compression, respectively; \( \varepsilon_1 \) and \( \varepsilon_3 \) are the major and minor principal strains, respectively. \( F_1 \) and \( F_2 \) are the maximum tensile stress criterion and the Mohr-Coulomb criterion, respectively. The \( F_1 \) and \( F_2 \) are expressed as follows:
\[ F_1 = -\sigma_1 - f_{t0} = 0 \] (9)
\[ F_2 = \sigma_1 - \sigma_3 \frac{1 + \sin \phi}{1 - \sin \phi} - f_{c0} = 0 \] (10)
where \( f_{t0} \) and \( f_{c0} \) can be determined by the mineral composition of rock materials or trial and error, respectively. Figure 1 shows the constitutive damage law of elements under uniaxial tension and compression.

![Figure 1](image)

**Figure 1** Damage constitutive law of elements under uniaxial tension and compression

2.3 Weibull Distribution
A Weibull statistical distribution defined by equation (11) was introduced in the damage-based NMM. A new parameter \( h \) in equation (12) was defined as the heterogeneity index to characterize the heterogeneity of rock material. The equations are as follows:
where \( u \) represents the mechanical property of a single manifold element, i.e., peak strength and Young’s modulus; \( u_0 \) is the mean value of the mechanical properties of the manifold elements; \( m \) represents the homogeneity of the materials. In contrast, \( h \) represents the heterogeneity of the materials. Fig 2 presents the Weibull distribution with different values of \( h \). A lower heterogeneity index \( h \) value indicates a more concentrated distribution of material properties.

3. Simulation

3.1 Geometry of the numerical models

Figure 3 (a) and (b) presents the model geometry and the boundary conditions for the Brazilian splitting test model and the uniaxial compression test model, respectively. The geometry of the Brazilian splitting test model is as follows: \( R = 22.5 \) mm, \( H_1 = 55 \) mm, and \( d = 5 \) mm, and the model was discretized into 4284 triangular manifold elements. The geometry of the uniaxial compression test model was \( W = 50 \) mm, \( H = 125 \) mm, \( H_2 = 135 \) mm, \( d = 5 \) mm, and \( D = 10 \) mm, and the model was discretized into 10064 triangular manifold elements. In both models, the upper platen was subjected to...
a constant loading increment of 0.0024 mm/step. The specimens were assumed to be under plane stress conditions. The properties of the loading platens were $E = 200\text{GPa}$, $\nu = 0.25$, and $\rho = 7.98 \text{g/cm}^3$.

### 3.2 Calibration of the numerical models

Experimental data on Lac du Bonnet granite were used to validate the two numerical models. As shown in Figure 4, the stress–strain curves obtained by the damage-based NMM showed good agreement with the corresponding experimental curves. Tables 1 and 2 list the calibrated parameters and the calibrated results and errors, respectively.

![Figure 4 Stress–strain curves of the experimental result and the damage-based NMM result—(a) Uniaxial compression test and (b) Brazilian splitting test](image)

### Table 1 Calibrated simulation parameters of Lac du Bonnet granite

| Property                        | Units | Value |
|---------------------------------|-------|-------|
| Young’s modulus ($E$)           | GPa   | 66    |
| Uniaxial compressive strength (UCS) | MPa       | 256   |
| Brazilian tensile strength (BTS) | MPa       | 8.8   |
| Heterogeneity index ($h$)       | -     | 1/8   |
| Frictional angle ($\varphi$)    | °      | 59    |
| Density ($\rho$)                | g/cm$^3$  | 2.63  |
| Compressive–tensile ratio ($R_c$) | -      | 10    |
| Poisson’s ratio ($\nu$)         | -     | 0.22  |
| Loading rate                    | mm/step | 0.0024 |

### Table 2 Calibrated results and errors of Lac du Bonnet granite when $h=1/8$, $\varphi=59^\circ$, $\rho=2.63 \text{g/cm}^3$, $R_c=10$ and the loading rate equals 0.0024 mm/step

| Property                        | Units | Laboratory test | Simulation result | Error (%) |
|---------------------------------|-------|-----------------|-------------------|-----------|
| Young’s modulus ($E$)           | GPa   | 70              | 64                | -8.6      |
| Uniaxial compressive strength (UCS) | MPa       | 224             | 227               | 1.3       |
| Brazilian tensile strength (BTS) | MPa       | 8.8             | 9.32              | 5.9       |
| Poisson’s ratio ($\nu$)         | -     | 0.22            | 0.23              | 4.5       |

### 3.3 Numerical applications

After calibrating the numerical models, two sets of numerical applications were conducted. First, the uniaxial compressive simulations were carried out on numerical specimens with different Young’s modulus heterogeneity indices of 2/3, 1/3, 1/6, 1/8, 1/10, and 1/12, respectively. Note that the
compressive–tensile ratio ($R_c$) was maintained at 10 during the uniaxial compressive simulations. Figure 5 compares the numerical specimens with different Young’s modulus heterogeneity indices $h$ of $2/3$, $1/6$, and $1/12$. The colors of the elements highlight the difference in the Young’s moduli among each manifold element. Brazilian splitting tests were conducted under different compressive–tensile ratios of 10, 12, 14, 16, 18, 20, and 22, respectively. The Young’s modulus heterogeneity index $h$ was $1/8$, and the UCS was 256MPa during the Brazilian splitting simulations.

**Figure 5** Numerical specimens with different Young’s modulus heterogeneity indices $h$.

### 4. Results

**Figure 6** Influence of the heterogeneity index ($h$) on the properties of the uniaxial compression test—(a) peak strength; (b) crack initiation stress; (c) stress–strain curves
This section presents the numerical application results. Figure 6 (a) and (b) shows the peak strength and crack initiation stress under different Young’s modulus heterogeneity index $h$, respectively. The peak strength and the crack initiation stress increased with decreasing heterogeneity index $h$. On the other hand, the largest increment occurred in different stages. The peak strength occurred between $h=1/3$ and $h=1/6$. In contrast, the crack initiation stress occurred between $h=2/3$ and $h=1/3$. Furthermore, the value difference between the crack initiation stress and the peak strength of each $h$ decreases, which is in good agreement with the difference in Young’s modulus values in Figure 5. The slope of the stress–strain curve in Figure 6 (c) increased gradually and finally reached a constant with decreasing heterogeneity index $h$. This agrees well with the macroscopic mechanical behavior of the experimental results. Figures 7 (a) and (b) shows the influence of the compressive–tensile ratio ($R_c$) on the peak tensile strength and stress–strain curves as well as the failure modes. The peak tension strength decreased sharply and finally kept constant with increasing $R_c$. A larger $R_c$ means that the simulation result is closer to the theoretical solution. Therefore, $R_c$ affected the failure mode the most. Compared to the results obtained by the simulation, $h = 1/8$ and $R_c = 10$ are the optimal parameters for the simulation of Lac du Bonnet granite because they can characterize the experimental results more precisely.

5. Conclusions
Calibration tests, the uniaxial compressive tests on model specimens with different heterogeneity indices, the Brazilian splitting tests on model specimens with different compressive–tensile ratios were carried out using the damage-based NMM program. The relationship among the heterogeneity index, the compressive–tensile ratio, and the macroscopical mechanical behavior, and the failure mode were then investigated. The calibration results and the simulation results were in good agreement with both the macroscopic mechanical behavior and the failure mode of granite. These results show that the heterogeneity index has the most significant effect on the crack initiation stress and the peak strength of granite, while the compressive–tensile ratio affects the failure mode the most. The optimal heterogeneity index and compressive–tensile ratio of Lac du Bonnet granite were proposed. A comparison of the results showed that the optimal heterogeneity index and compressive–tensile ratio could be used to model the cracking behavior of rocks more precisely.

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