Simulation of the fracturing process in rocks with flaws using a novel continuous-discontinuous technique

Zhaofeng Wang 1,2, Peng-zhi Pan 1,2*, Wenbo Hou 1,2, Zhenhua Wu 1,2, Peiyang Yu 1,2, Shuting Miao 1,2

1 State Key Laboratory of Geomechanics and Geotechnical Engineering, Institute of Rock and Soil Mechanics, Chinese Academy of Sciences, Wuhan, Hubei 430071, China;
2 University of Chinese Academy of Sciences, Beijing 100049, China;
* Corresponding author. E-mail: pzpan@whrsm.ac.cn (P. Z. Pan)
ORCID: https://orcid.org/0000-0002-2833-4964

Abstract. Loading induced cracks can emerge from the tips of pre-existing flaws. The overall process involves the interaction of two contacting surfaces in existing flaws, along with the initiation of wing cracks around the tip presenting the tensile failure, and the continuous crack propagation, and this continues until the final coalescence. The present study focuses on a numerical model to investigate the emergence and propagation of cracks, combined with the interaction behavior of crack internal surfaces. Moreover, a convenient and efficient approach to simulate the fracturing process of rocks from continuity to discontinuity is proposed. The numerical model is an integration of the following basic elements: cellular discretization and cellular automaton updating rule; internal interface formulation for the fracture representation; modified potential function for fracture behavior description; crack propagation algorithm; and re-meshing technique. The proposed numerical model is implemented in Cellular Automata Software for engineering Rockmass fracturing process (CASRock), after which it is verified and validated through a comparison between the simulated results and the analytical solution and experimental results.

1. Introduction
The essence of rock failure is rock fracturing and fragmentation [1]. With the rapid development of computing science, numerical simulation has become an important auxiliary way by which to further understand the failure mechanisms of rock failure. Over the past several decades, numerical methods based on the continuum and discontinuum mechanics have been used to simulate the fracturing process of rocks.
In regard to the numerical analysis methods of rocks, at present there are three main methods used, namely the continuous method, discontinuous (or discrete) method, and continuous-discontinuous coupling method. Continuous methods included the finite element method [2], finite difference method [3], boundary element method [4], meshless method, matter point method, phase-field theory method and peridynamic method. Discontinuous methods include the block-based discrete element method [5], particle flow method [6], discontinuous deformation analysis method, and manifold element method. The continuous-discontinuous coupling method mainly refers to the finite-discrete element method proposed by Munjiza [7]. Moreover, the diffusion crack (weak element) method [8], generalized finite element method (embedded crack) and discrete crack method (Goodman interface element method, etc.) [9] have also been widely applied to analyze the fracturing process of rock.
Most of these methods have inherent advantages. However, the continuous method exhibits inferior performance in reasonably reflecting the fracture, while the discontinuous method possesses some defects in the precise calculation of continuous deformation and stress field. Most of the existing continuous-discontinuous coupling methods adopt the same global updating rules, thus it is quite difficult to reflect the differences between the local brittle fracture and incongruous deformation interaction. Some deficiencies still remain in the localization analysis of discontinuous structure evolution, near-field deformation interaction and co-evolution. In the present study, we proposed a numerical model for quantitatively simulating of the fracturing process in rocks with flaws. After implementing the method in CASRock, the crack behavior and fracture mechanism of the initiated cracks in rocks were studied. Finally, it is verified and validated through a comparison between the simulated results and the analytical solution and experimental results.

2. Theoretical basis

To describe the mechanical behaviour of rocks with flaws, the elastic theory for the entire body and linear elastic fracture mechanics is adopted in this study. Two situations should be considered here, namely the equilibrium state of the initial configuration and the mechanical response of the new configuration with newly formed cracks. The failure criteria of the initial configuration and the crack propagation in the new configuration have also been considered. Next, the equilibrium equation and failure criteria are introduced in the following sections of the paper.

2.1. Equilibrium equation

A domain $\Omega \subset \mathbb{R}^2$ is analyzed here, as shown in Fig. 1(a). The outward unit normal vector of the domain is $\mathbf{n}$, and the body force $\mathbf{b}$ is applied to the whole body. Two kinds of boundary conditions, namely the Dirichlet condition $\mathbf{B}_D$ and Neumann conditions $\mathbf{B}_N$, are also applied to the boundary. In addition, there is also a single flaw in the domain with two internal boundaries $\mathbf{B}_c^+$ and $\mathbf{B}_c^-$. The total equilibrium equation can be written as follows:

$$
\begin{align*}
\nabla \cdot \sigma + b &= 0 \quad \text{in } \Omega \\
\varepsilon &= S : \sigma \quad \text{in } \Omega \\
\varepsilon &= \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^T) \quad \text{in } \Omega \\
\mathbf{u} &= \mathbf{u}_0 \quad \text{on } \mathbf{B}_D \\
f &= \sigma \cdot \mathbf{n} \quad \text{on } \mathbf{B}_N
\end{align*}
$$

where $\sigma$, $\varepsilon$ and $\mathbf{u}$ are the stress, strain tensor and displacement, respectively; $S$ is the fourth-order stiffness tensor, which can be derived from Young’s modulus and Poisson’s ratio using Hooke’s law; and $\mathbf{u}_0$ and $f$ are the corresponding boundary conditions on the Dirichlet and Neumann boundaries, respectively.

For the crack surface as illustrated in Fig. 1(b), a non-penetration, also known as the Karush-Kuhn-Tucker (KKT) condition for the normal displacement and normal surface traction can be expressed as follows [10]:

$$
[u(\mathbf{x})]_N - g(\mathbf{x}) \leq 0, f_N(\mathbf{x}) \leq 0, f_N(\mathbf{x})([u(\mathbf{x})]_N - g(\mathbf{x})), \text{where } \mathbf{x} \in \mathbf{B}_c^+ \quad (2)
$$

where $[u(\mathbf{x})]_N$ is the jump in the normal direction of the flaw and $g(\mathbf{x})$ is the initial gap between two flaw surfaces for point $\mathbf{x}$; and $f_N(\mathbf{x})$ is the surface traction in the normal direction. Here the displacement jump can be calculated as follows:

$$
[u(\mathbf{x})]_N = u(\mathbf{x}) - u(T(\mathbf{x})) \quad (3)
$$

where $T(\mathbf{x})$ is the twin point of point $\mathbf{x}$.

For the tangential force, the relation is similar to the normal case.
The tangential stress on the crack tip is considered here, as follows:

$$
\sigma_{\theta}(r, \theta) = \frac{1}{\sqrt{2\pi}r} \left( K_I \cos^2 \frac{\theta}{2} - \frac{3}{2} K_{II} \cos \frac{\theta}{2} \sin \theta \right)
$$

where $r$ is the distance from the tip and $\theta$ is the inclination angle; and $K_I$ and $K_{II}$ are the stress intensity factors (SIFs). A mixed crack initiation criterion at the crack tip is treated as the failure criterion, i.e. the crack emerges if the tangential stress reaches a critical value. The critical initiation angle $\theta_0$ in respect to the original crack plane can be calculated as follows:

$$
\theta_0 = 2 \tan^{-1} \left( \frac{1}{4} \mu \pm \frac{1}{4} \sqrt{\mu^2 + 8} \right), \mu = \frac{K_I}{K_{II}}
$$

The propagation of the crack in this paper is treated as a constant value, named as $h$. If more than one crack initiates, then Paris’s law is adopted, which reads as follows:

$$
L_{\text{prop}}^i = h \left( \frac{G_i}{G_{\text{max}}(G_i)} \right)^\omega
$$

where $L_{\text{prop}}^i$ is the propagation length of the $i$th crack; $G_i$ is the energy release rate of the crack; $\omega$ is the model parameter, which can be set to 0.35[11]; $G_i$ can be calculated from the SIFs; and the local SIFs can be calculated with the method described in Reference [12].

### 3. Methodology

#### 3.1. Cell space discretization

The rock is treated as an aggregation of cells, and the rock entity can be transformed into the cell space.

For the two-dimensional problems, the cell space includes many types, as shown in Fig. 2. Here, the triangular type is adopted.

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**Figure 1.** Equilibrium equation of an elastic body with a flaw, and (b) the flaw surfaces.

**Figure 2.** The cell space, such as (a) quadrangular type and (b) triangular type.
3.2. **Cellular automaton updating rule**

The updating rules of cellular automata are generally obtained according to the local equilibrium state. When establishing the cellular automata update rule, we only need to consider one cell in the solution domain\[13, 14\]. For example, in the cell, there is the following local equilibrium (Fig. 3):

\[
K_I \Delta u_i = \Delta I_i
\]  

(7)

where \(K_I\) and \(\Delta u_i\) are the stiffness matrix and incremental displacement of the cell node itself, while \(\Delta I_i\) is the incremental unbalanced force caused by the deformation, fracture, contact etc. of the neighbors. As shown in Fig. 3, the types of incremental unbalance force include external force, deformation resistance, intrusive contact resistance, frictional contact resistance, cracking resistance, etc. The term on the right-hand side reflects the influence of the surrounding neighbours on the cell node, while that on the left-hand side reflects the mechanical response of the cell node itself.

The above formula can be used to solve \(\Delta I_i\), and then by calculating the incremental displacement of cell nodes, followed by calculating the cellular state. Each cell in the system is updated according to the same rule, and the force→displacement→force→... updating process continues, until the increment \(\Delta u_i \rightarrow 0\), which indicates that it has reached a self-organizing equilibrium.

![Figure 3. Local equilibrium of the cell](image)

3.3. **Internal interface for the fracture representation**

The internal interface method is applied to represent the fracture, as shown in Fig. 4. This method is straightforward and simple, namely, when the crack initiates, an internal interface is then inserted into the fracturing boundary. If any mechanical responses, such as penetration, tension or friction occur on the boundary, then the corresponding force pairs are added to the right nodes.

![Figure 4. Internal interface fracture representation method](image)

3.4. **Modified potential function for fracture behavior**

A modified potential function method is adopted in this paper to reflect the mechanical behavior on the fracture surface. It follows three steps:

(1) Discretization for the internal interface

The internal interface or the fracture surface can be discretized into many microfacets.

(2) Normal and slipping force calculation
First, we determine the element to which the microfacet belongs, then calculate the distance to the nearest surface as penetration \( u_n \). Next, the normal stress is acquired from the penetration. Finally, the area and normal stress are integrated to calculate the force on the surface, after which the force is equally applied to the nodes of the internal interface. It should be noted that the lipping force is similar to the normal one.

3) CA calculation to acquire the new spatial relation
The new acquired normal and slipping forces are added to the internal interface, and CA calculation is conducted as described in Section 3.2, to acquire the new spatial relation. Steps 1 and 2 are then repeated until the end of the loading.

3.5. Crack propagation
The identification of the crack propagation path follows a maximum tangential stress criterion, and the crack initiation angle around the tip can be calculated according to Eqs. 4 and 5. Moreover, the increment for each tip is defined by the Paris-type law (Eq. 6) for the propagations of more than one crack.

3.6. Re-meshing technique
A local adaptive grid re-meshing technique, based on fast Coulomb force driven Delaunay triangulation[15], is adopted to acquire the higher computational efficiency, and there will be no additional DOFs in this treatment.

4. Numerical investigation

4.1. Numerical implementation
The proposed numerical model is implemented using Cellular Automata Software for the engineering Rockmass fracturing process (CASRock)[16]. The model contains a series of previous developed numerical systems.

In each iteration, the calculation for the rock mass and joint are separated, and the following process in Fig. 5 is conducted.

**Figure 5.** Calculating algorithm in the local cell level

4.2. Application
This numerical method has been applied to simulate the propagation of a planar flaw, and the model configuration is shown in Fig. 6(a). For these cases, the analytical solution of the shear displacement on the fracture surface can be calculated as follows:

\[
u(r) = \frac{2(1-\nu)}{G} \Delta \tau \sqrt{a^2 - r^2}\]

where \( r \) is the distance to the crack tips, \( a \) is the crack half-length; \( \nu \) and \( G \) are the Poisson’s ratio and shearing modulus, respectively; and \( \Delta \tau \) is the shearing stress on the fracture surface. Fig. 6(b) gives the comparison of the analytical solution, our approach, Goodman element [9] and weak element methods [8]. It can be seen that the results achieved using our new method are closer to the analytical solution, thereby indicating that it is more accurate than the other methods.

Fig. 7 illustrates the comparison of the numerical, experimental and theoretical crack propagation paths of beams with different initial flaw positions. It can be observed that the crack propagation angle...
increased as the pre-existing artificial crack shifted away from the mid-point of the beam. The modeling results from the new method in this paper are comparable with the experimental and theoretical results [17].

Figure 6. Simulation of a planar flaw propagation, in which (a) is the model information and (b) is a comparison of the analytical solution, our approach and other methods.

Figure 7. Comparison of the numerical, experimental and theoretical crack propagation paths of beams with different initial flaw positions, where (a) is the experimental and theoretical propagation path of crack propagation in the beam [17], (b) shows simulated results of the beam with a flaw in the middle, and (c) lists simulated results of the beam with a flaw on the left-hand side.
5. Concluding remarks
In this paper, a convenient and efficient technique which can be used to simulate the fracturing process of rocks from continuity to discontinuity is proposed and implemented in cellular automata software for engineering rockmass fracturing process (CASRock). It is verified and validated through a comparison with the analytical solution and experimental results. The main conclusions are drawn as below:
(1) The pre-existing flaw and new fracture surface are considered to be an internal interface, and the contact and friction can be reflected by the equivalent unbalance force applied on cell nodes of the internal interface. The contact and frictional stress of the current loading step are calculated by means of a modified potential function method, and there is no need to conduct contact detection.
(2) The identification of the crack propagation path follows a maximum tangential stress criterion and the crack initiation angle around the tip can be calculated; moreover, the increment for each tip is defined by the Paris-type law for the propagations of more than one crack.
(3) A local adaptive grid re-meshing technique based on fast Coulomb force driven Delaunay triangulation is adopted to acquire the higher computational efficiency, and no additional DOFs are needed in this treatment.

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