NUMERICAL SIMULATION OF HETEROGENEOUS MATERIAL FAILURE BY USING THE SMOOTHED PARTICLE HYDRODYNAMICS METHOD

WANG XUEJUN

SCHOOL OF CIVIL AND ENVIRONMENTAL ENGINEERING

2009
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WANG XUEJUN

School of Civil and Environmental Engineering

A thesis submitted to the Nanyang Technological University in fulfillment of the requirement for the degree of Doctor of Philosophy

2009
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Acknowledgements

The thesis is the result of several years of efforts and there are many people to acknowledge and thank. The gratitude cannot be expressed in words.

First, of course, thanks go to my supervisor, Associate Professor Ma Guowei, for his profound vision, invaluable guidance, and much-needed encouragement in conducting this Ph.D work.

Besides, I would like to express my thanks to my fellow graduates worked or studied in the Underground Technology and Rock Engineering (UTRE) group for many fruitful discussions and various supports.

The research scholarship offered by Nanyang Technological University to support this research work is gratefully acknowledged.

And, I am sincerely grateful to my parents, parents-in-law, sister and friends for their continuous concern, encouragement and support.

Finally, I would like to express my deepest appreciation to my wife, Song Wenwen, for her patience, love and the many sacrifices she made during this endeavour.
Summary

Many numerical methods have been proposed in the efforts to reveal the failure mechanism of the brittle materials, such as rock and concrete, under various loading conditions. It is of continuous interests on properly modeling the heterogeneous microstructure and to account for its effects on the macroscopic material failure; and effectively tackling the initial and created discontinuities, such as fractures and fragmentations in the failure process.

In this thesis, a numerical approach based on the mesh-free Smoothed Particle Hydrodynamics (SPH) method is developed that is able to simulate the dynamic failure of brittle materials by capturing the detailed occurring sequence of the microscopic cracks as well as the macro mechanical response. An elasto-plastic damage model based on the extension of the Unified Strength Theory is adopted in order to better reflect the strength behavior of the materials. To model the material heterogeneity, a statistical approach has been utilized. In addition, a polymineral model for the multi-phased materials has been incorporated to simulate heterogeneous materials with different compositions more appropriately.

A series of numerical simulations in 2-D and 3-D on rock-like material failures are performed using the developed program. The influences of material heterogeneity as well as the strain rate on the material fracture process and its dynamic strength are investigated and compared with experimental results. Comparisons show that they agree well qualitatively. Particularly, the results reveal that the strain rate dependency of the dynamic tensile and compressive strength might be ascribed to the apparent confining pressure effects by the rapid loading. It shows that the developed program is very promising in conducting such kind of simulations and deserves further improvements for many other applications.
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c Wave propagation speed

e Energy

\( h, W \) Smoothing length of SPH particle, SPH kernel function

\( \Pi_g, S_{cs} \) Artificial viscous pressure, conservative smoothing function

\( v_\alpha \) Velocity

\( m, \rho \) Mass, density

\( K, G \) Bulk modulus, shear modulus

\( \sigma_{\alpha\beta}, p, S_{\alpha\beta} \) General stress tensor, pressure, deviatoric stress tensor

\( \delta_{\alpha\beta} \) Kronecker delta function

\( \varepsilon, \dot{\varepsilon}, \bar{\varepsilon}_p, \dot{\bar{\varepsilon}}_p, \bar{\varepsilon}'_p \) Strain, strain rate, effective plastic strain, effective plastic strain rate, effective plastic strain to fracture

\( I_1, I_2, I_3 \) The first, second and third stress invariants

\( J_1, J_2, J_3 \) The first, second and third deviatoric stress invariant

\( f, Q, d\lambda \) Yield function, plastic potential, plastic multiplier

\( \sigma_t, \sigma_c \) Uniaxial tensile strength, uniaxial compressive strength

\( \sigma_{\alpha\beta}, \sigma_{\alpha\beta} \) Dynamic uniaxial tensile and compressive strengths

\( D \) Damage

\( [D], [D]_{\alpha\beta} \) Elastic stiffness, elasto-plastic stiffness

\( \sigma_{13}, \sigma_{12}, \sigma_{23} \) Normal stresses corresponding to the three principal shear stresses
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tau_{13}, \tau_{12}, \tau_{23}$</td>
<td>Principal shear stresses</td>
</tr>
<tr>
<td>$\theta_b$</td>
<td>Demarcating angle in deviatoric plane in the strength criterion</td>
</tr>
<tr>
<td>$b$</td>
<td>Weighted coefficient for the second principal shear stress</td>
</tr>
<tr>
<td>$\sigma_1, \sigma_2, \sigma_3$</td>
<td>Principal stresses</td>
</tr>
<tr>
<td>$r_i, r_c, r_{ic}$</td>
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</tr>
<tr>
<td>$\xi, r, \theta$</td>
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</tr>
<tr>
<td>$\sigma^<em>, \sigma^</em>_i, \sigma^<em>_D, \sigma^</em>_f$</td>
<td>Normalized strength; normalized strength for intact, damaged and fractured materials</td>
</tr>
<tr>
<td>$p^*, p_T$</td>
<td>Normalized pressure, hydrostatic tensile pressure limit</td>
</tr>
<tr>
<td>$A$</td>
<td>Normalized strength parameter for compressive meridian for intact material</td>
</tr>
<tr>
<td>$B$</td>
<td>Normalized strength parameter for compressive meridian for fractured material</td>
</tr>
<tr>
<td>$N$</td>
<td>Parameter for strength of intact material</td>
</tr>
<tr>
<td>$M$</td>
<td>Parameter for strength of fractured material</td>
</tr>
<tr>
<td>$D_1$</td>
<td>Parameter in the damage model</td>
</tr>
<tr>
<td>$D_2$</td>
<td>Parameter in the damage model (exponent)</td>
</tr>
<tr>
<td>$\beta, \mu$</td>
<td>Weibull shape parameter (homogeneous index), seed parameter</td>
</tr>
<tr>
<td>$DIF, DIF_p$</td>
<td>Dynamic increment factor for tensile or compressive strength; dynamic increment factor for average pressure</td>
</tr>
</tbody>
</table>
Chapter 1  Introduction

1.1 Background

With the advent of powerful computer hardware and sophisticated numerical codes, numerical simulation has become indispensable in solving engineering problems of large complex systems. It has also been used to replace some costly and time-consuming experiments. With manipulation of the relevant modeling and simulation parameters, numerical simulation can reveal the dominating parameters affecting the targeted specifications for design purposes or scientific investigations. Moreover, it can provide insight understanding of the triggering mechanism behind a phenomenon, which may not be directly measured, or difficult to be acquired by experiments, or other analytical approaches.

As one of the most popular numerical methods, the finite element method (FEM) has been the most sophisticated method and has achieved great success in various areas since its invention in 1950s. Although the FEM is powerful, the fact that its underlying structure relies on the meshes does not work well in discontinuous problems with free surfaces, deformable boundaries and moving interfaces. In such cases, to prevent the severe distortion of meshes and allow mesh lines to remain coincident with the discontinuities, the most viable strategy is to rezone these meshes throughout the evolution of the problem. Although having achieved great success, the meshing and the subsequent adjusting process is absolutely not an easy task. Moreover, additional inaccuracies could incur due to the mesh distortions and the state variables mapping transformations in such processes.

Recently, a new class of numerical methods called mesh-free (or meshless) methods has been developed to overcome the difficulties mentioned above and has drawn considerable attentions. One objective of mesh-free methods is to solve the large deformation problems more effectively by constructing the approxi-
mation entirely on nodes instead of mesh. Thus, it is possible to solve distor-
tional deformation, fracture propagation, fragmentation, etc., which are very computation intensive with mesh-based methods. Many mesh-free methods have been proposed and documented which can be found in Belytschko et al. (1996), Li and Liu (2002), Liu (2003), and Liu and Liu (2003), etc. Their methods may differ from one another in terms of the approximation and implementation processes. However, they all can solve the moving discontinuous problems without using meshes. Thus, simulations will become more adaptive, versatile, and robust.

The earliest mesh-free method is the smoothed particle hydrodynamics (SPH) method. It was first applied to solve astrophysical problems in 3-D open space by Lucy (1977) and Gingold and Monaghan (1977). Since then, the SPH has been extensively applied in various fields, such as fluid dynamics, molecular dynamics and solid mechanics, etc. In the SPH, the system state is represented by a set of particles carrying individual material properties. These particles are able to move under the control of the conservation equations. Its kernel approximation can both smoothly discretize a partial differential equation and provide an interpolant scheme on those moving particles. Due to those features, the SPH can be applied to solve discontinuous problems through continuum mechanics.

Once being coupled with a proper damage model, the SPH can easily be applied on fracture simulations. Libersky and Petschek (1990), Benz and Asphaug (1994), Benz and Asphaug (1995) are among the earliest successful pioneers to show that the SPH was applied to simulate the fracture process for brittle solids. Since it yields much efficient solutions than the FEM did, Monaghan (2005) considered the SPH as a bridge to link the gap between the continuum and fragmentation in a natural way and hence the best current method for the study of brittle fracture and subsequent fragmentation in damaged solids.

Historically most geo-materials, such as rock and concrete, are considered as homogeneous material in computational methods. For most engineering calculations, it is convenient, and often practically necessary. However, these mate-
Materials actually are multi-phased, which is composed of composites or microstructures with varying scales. They may also have preexisting or stress induced defects in the forms of pores, micro cracks, and weak interfaces on grain boundaries. Figure 1-1 shows two samples of cross-sections in the rock and concrete, which are composed of different components.

![Cross-sections of two specimens](image)

**Figure 1-1** Cross-sections of two specimens a) rock b) concrete

The microstructures and defects, their type, shape, orientation, and density are all random and heterogeneous. They will influence the macro behaviors of the material over a wide spectrum of circumstances. For instance, they may cause nonlinear mechanical response of the material. Also, they can ultimately influence the rupture strength and the fracture process especially when subjected to dynamic loadings. However, it is still unclear how such processes are conducted. Further studies are already in progress to gain a better understanding of those behaviors.

The SPH makes it relatively much easier and more effective to perform simulations on the fracture process for brittle materials compared to other traditional continuum or mesh free computational methods. On one hand, its mesh-free advantage makes it feasible to handle large deformations. Dynamic fractures featured by the initiation and propagation of cracks in arbitrary and complex paths could be simulated. On the other hand, microstructure and defects can be represented by different sets of particles with individual material property. Hence it is feasible to be applied to simulate the heterogeneous materials.
Chapter 1 Introduction

1.2 Objective of the research

The purpose of this research is to apply the SPH method to simulate the dynamic failure of brittle materials by considering the material heterogeneity. The specific targets are outlined as follows:

- To develop a computer program using the SPH method and implement a proper elasto-plastic damage constitutive model which can effectively simulate the failure of brittle materials, such as rock and concrete;
- To develop proper microstructure models to reflect material heterogeneity;
- To simulate dynamic failure of brittle rock-like materials and investigate the material microstructure heterogeneity as well as the loading rate effects on the macro mechanical response and fracture process using the developed program.

1.3 Organization of the report

This report is organized into 10 chapters. Chapter 1 introduces the background and the objectives. In Chapter 2, a comprehensive review is given on the SPH method and its applications on the computational solid mechanics. Numerical modeling on brittle material failure is also reviewed. Chapter 3 introduces the methodology of the SPH method, the elasto-plastic damage constitutive model, and the material heterogeneity model. The implementation of the SPH program with the developed models and its calibration is also described in this chapter. In Chapter 4, simulations on the Brazilian splitting test by considering material heterogeneity are performed by using the developed SPH code and the results are discussed. In Chapter 5, dynamic compressive failures of heterogeneous rock-like material are investigated. In Chapter 6, simulations of the unconfined and confined compression test for rock-like material are implemented. In Chapter 7, a new heterogeneous microstructure modeling method for multi-phase materials is presented. Its applications on the polycrystalline granite failure simulations under the low strain rate are presented under 2-D. In Chapter
8, simulations on granite dynamic failure are performed by using the developed heterogeneous microstructure modeling method. In Chapter 9, the proposed heterogeneous microstructure modeling method is extended to 3-D. Its applications on the 3-D granite dynamic failure simulations are presented. Finally, Chapter 10 gives the conclusion and recommendations for future study.
Chapter 2  Literature Review

In this chapter, the mesh-free based computational methods are briefly reviewed firstly. The smoothed particle hydrodynamics (SPH) method, its recent developments and improvements are then presented. Computational methods on simulation of brittle material failure are also introduced. Finally, various applications of the SPH method onto solid mechanics are reviewed and discussed.

2.1 Mesh-free methods

2.1.1 An overview

Many mesh-free methods have been put forward since 1970s. Besides the SPH, a parallel path of constructing mesh-free approximations is the use of moving least square (MLS) approximation. Nayroles et al. (1992) developed a diffuse element method (DEM) that used MLS interpolant in conjunction with Galerkin method to provide a mesh-free computational formulation. Belytschko et al. (1994) refined and modified the DEM and proposed the element-free Galerkin (EFG) method. In the EFG, the derivatives of the interpolants that are omitted in the DEM are included and a more accurate numerical integration method is employed to enhance the solution accuracy. Melenk and Babuska (1996) proposed a partition unity finite element method (PUFEM) subsequently.

Other developments of the mesh-free methods include the generalized finite difference method (GFDM) by Perrone and Kao (1972) and the particle-in-cell (PIC) method by Harlow (1963). The characteristic of GFDM is to handle with the nodes that are arranged arbitrarily in the interest domain, to which Perrone and Kao (1972)made the earliest contributions. Nevertheless, the improvements of GFDM are attributed to Liszka and Orkisz (1979). Sulsky and Schreyer (1996) proposed a material point method (MPM) that is evolved from the PIC method.
Mesh-free methods also include the hp-clouds method proposed by Duarte and Oden (1996), the meshless local Petrov-Galerkin method (MLPG) by Atluri and Zhu (1998).

These mesh-free based computational methods are different from one another in terms of the function approximation and the implementation methods. In summary, there are three kinds of function approximation methods commonly used, i.e., the kernel function method, the moving least-square method (MLS) and the partition of unity method (PUM).

The numerical implementation methods for discretization of these mesh-free methods can be categorized into the collocation method and the Galerkin method, respectively. Table 2-1 gives the typical approximation and implementation methods of several typical mesh-free methods.

<table>
<thead>
<tr>
<th>Mesh-Free Method</th>
<th>Method of Approximation</th>
<th>Method of implementation</th>
</tr>
</thead>
<tbody>
<tr>
<td>SPH</td>
<td>Kernel function</td>
<td>Collocation</td>
</tr>
<tr>
<td>EFG</td>
<td>MLS</td>
<td>Galerkin</td>
</tr>
<tr>
<td>MLPG</td>
<td>MLS</td>
<td>Galerkin</td>
</tr>
<tr>
<td>Hp Clouds</td>
<td>MLS</td>
<td>Galerkin</td>
</tr>
</tbody>
</table>

2.1.2 Smoothed particle hydrodynamics method

The SPH method was invented to solve astrophysical problems in 3D open space and particular polytropes by Lucy (1977), Gingold and Monaghan (1977), because the collective movement of those particles is similar to the movement of a liquid or gas flow, and can be modeled by the governing equations of the classical Newtonian hydrodynamics. The methodology and its applications were expounded in several excellent review papers, including those by Monaghan (1988), Monaghan (1992), Wingate and Miller (1993), Randles and Libersky (1996), Li and Liu (2002), Liu and Liu (2003) and Monaghan (2005) and Liu et al. (2008). Due to several distinct advantages, it has been developed
Numerical Simulation of Heterogeneous Material Failure by using SPH Method

and applied rapidly in various areas especially after 1990s. Initially, the SPH method was based on the Monte Carlo theorem and random sampling for astrophysical applications. Gingold and Monaghan (1982) employed the kernel approximation to give the method a rational explanation, which can also serve as a smoothing interpolation field. Therefore, the foundation of SPH is the interpolation theory. The conservation equations of the continuum dynamics can be transformed into integral equations by using an interpolation function that gives the ‘kernel estimate’ of the field variables at a point. Computationally, information is known only at discrete points, so that the integrals are evaluated as sums over the neighboring particles. The underlying grid is not needed because that functions are evaluated using their values at the discrete neighboring points (particles) and an interpolation kernel.

Generally, a function $f(x)$ can be expressed as

$$f(x) = \int_\Omega f(x') \delta(x-x') dx'$$

(2.1)

where, $f$ is a function of the spatial position $x$, $\Omega$ is the volume of the integral, $\delta(x-x')$ is the Dirac delta function expressed as

$$\delta(x-x') = \begin{cases} +\infty, & x = x' \\ 0, & x \neq x' \end{cases}$$

(2.2)

Obviously, Eq. (2.1) is rigorous and exact. If the Dirac delta function is replaced by a smoothing kernel function $W$, approximation of $f(x)$ on the domain $\Omega$, named $\langle f(x) \rangle$ can be generated

$$\langle f(x) \rangle = \int_\Omega f(x') W(x-x', h) d\Omega,$$

(2.3)

where $\langle f(x) \rangle$ is the approximation of $f(x)$, $h$ is called the smoothing length which defines the support domain of the particle and $W(x-x', h)$ is the smoothing kernel function. The kernel usually should satisfy the following requirements,
• Delta function property when \( h \rightarrow 0, \lim_{h \to 0} W(x - x', h) = \delta(x - x') \)

• Normalized condition, \( \int W(x - x', h) d\Omega = 1 \)

• Compact condition, \( W(x - x', h) > 0 \) when \( x' \) is inside the support domain \( \Omega \), otherwise \( W(x - x', h) = 0 \)

• Monotonically decreasing function property with the distance \( s, s = ||x - x'|| \)

• Smoothing property

The first condition guarantees the convergence. The second condition ensures the consistency in that the integration should produce the unity for the regular arrangement of particles. The third condition enables the approximation to be generated only within a local representation. The fourth one arises from the conception of the physics, which means that the force exerted by one particle on the other decreases with the distance between them. The last property aims to obtain better approximation by requiring that the kernel function must be differentiable at least in its first order. A kernel function with the continuous derivative will prevent large fluctuation in the force felt by the particle providing the particle disorder is not too extreme. This gives the method the name “smoothed” particle hydrodynamics.

Usually any function satisfying the above properties can be employed as the kernel function of the SPH. A typical kernel function named B-spline function in Monaghan and Lattanzio (1985) based on the cubic spline functions is

\[
W(R, h) = \alpha_D \begin{cases} 
\frac{2}{3} - R^2 + \frac{1}{2} R^3, & R \leq 1 \\
\frac{1}{6} (2 - R)^3, & 1 < R \leq 2 \\
0, & R > 2
\end{cases}
\]

where \( \alpha_D = \frac{1}{h}, \frac{15}{7\pi h^2} \) and \( \frac{3}{2\pi h^3} \) in one-, two- and three- dimension, respectively. \( R \) is the relative distance between two points (particles) at point \( x \).
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and \( x', R = \frac{r}{h} = \frac{\|x-x'\|}{h} \), where \( r \) is the distance between the two points and \( h \) is the smoothing length. The B-spline function has been the most widely used smoothing function in the emerged SPH literatures so far. Figure 2-1 gives its plot in three-dimension.

Figure 2-1 Plot of the cubic spline kernel function in three-dimension

Another commonly used kernel function is the Gaussian kernel by Gingold and Monaghan (1977), which can be expressed as,

\[
W(R, h) = \alpha_D \begin{cases} 
  e^{-R^2}, & R \leq 2 \\
  0, & R > 2 
\end{cases} 
\]

(2.5)

where \( \alpha_D \) is \( \frac{1}{\pi^{3/2}h} \), \( \frac{1}{\pi h^2} \) and \( \frac{1}{\pi^{3/2}h^3} \) in one-, two- and three- dimension, respectively.

Fulk and Quinn (1996) divided kernel functions into four categories based on their general shapes: bell shaped, parabolic shaped, hypersonal-bolic shaped and double hump. They analyzed over 20 kinds of kernels commonly used and argued that the bell shaped cubic one usually generate better approximation. Figure 2-2 gives the plot of the four classes of these kernels and their derivatives.
The approximation can be obtained from the discrete form of Eq. (2.3) by numerical quadrature of its right-hand side, which gives

\[
\langle f(x) \rangle = \sum_{i} \Phi_i(x) f_i
\]  

(2.6)

\[
\Phi_i(x) = W(x - x_i, h) \Delta V_i
\]  

(2.7)

\( \Phi_i(x) \) in Eq. (2.7) is also called the shape function by Gingold and Monaghan (1977). By means of the shape function, partial differential equations can be discretized and approximated through a convoluted integration. Details will be given in Chapter 3.

### 2.2 Recent improvements on the SPH method

With the great successful applications of the SPH method to various fields since its invention, some deficiencies of the method has also been noticed. Various improvements on these shortcomings have been carried out. Most of these improvements aimed to overcome the following problems in the numerical simulations,
• Tensile Instability;
• Interpolation Inconsistency;
• Zero Energy Mode;
• Boundary Conditions;

2.2.1 Tensile instability

The phenomena of tensile instability and its causes in SPH simulations are first declared by Swegle et al. (1995). When particles are under certain tensile stress state, motion of these particles becomes unstable or “blows up” as shown in Figure 2-3. The criterion for the instability depends on the sign of the production of the stress and the second derivative of the selected kernel indicated by Figure 2-3. Such instability cannot be smeared by increasing the amount of artificial viscosity. The instability will result in the unphysical constitutive relationship due to the fact that an effective stress amplifies the effective strain, rather than decrease it.

Figure 2-3 Sketch map on particles tensile instability and the mechanic explanation in numerical simulation (after Swegle et al., 1995)

Several kinds of methods have been brought out to remedy the tensile instability. One is to use higher-order kernels, for example, Morris (1996) proposed a new spline interpolants. However, this method cannot guarantee satisfactory results to all cases. Another one is to use the additional dissipative terms, such as the Conservative Smoothing Approach method (CAS) used in Balsara (1995), Randles and Libersky (1996) and Hicks et al. (1997), in which they declared that
CAS can both smooth the oscillation and mitigate the tensile instability. Moreover, the CAS method is quite easy to be implemented. Another method is the stress point method which adds extra stress points as shown in Figure 2-4 in the 2-D space. These stress points act as interpolants for the stress sampling. Other kinematic variables, such as the acceleration, are still evaluated by the SPH points. Dyka et al. (1997) first gave this essential idea and implemented in a one-dimensional analysis. Later on, the stress point method was extended to 2D by Randles and Libersky (2000). Generally, in the SPH method, the stress point plays the role similar to what the “Gauss Quadrature Point” does in the FEM.

![Figure 2-4 2-D distribution of stress points and SPH points (after Randles and Libersky, 2000)](image)

Other relative researches have also been carried out by Chen and Beraun (2000) as well as Monaghan (2000). The former addressed a corrective smoothed particle method (CSPM) and the latter proposed the method by adding an additional artificial force.

### 2.2.2 Interpolation inconsistency

In the SPH method, the kernel function is inconsistent on the boundaries due to the insufficiency of supporting particles. In fact, the inconsistency may lose even for the whole domain in the discrete form due to irregular distribution and large discrepancies caused by the moving particles.

The problem that SPH interpolant cannot represent rigid body motion correctly was first addressed by Liu et al. (1995) and Liu et al. (1995). By the means of multiplying the corrective function with the original kernel, they constructed a corrective kernel to enforce the consistency and named it the reproducing kernel particle method (RKPM). Although the method is very effective, there have some minor drawbacks. One is that the corrective value may become negative.
within the compact domain support. The other one is that the complexity of such methods may destroy the simplicity of the SPH formulation and implementation.

Besides the RKPM, many other corrective methods have also been put forward, such as Monaghan’s symmetrization on the derivative approximation by Monaghan (1988) and Monaghan (1992), the normalized smoothed function method (NFS) by Johnson and Beissel (1996), the Petrov-Galerkin formulation using approximations with corrected derivatives by Belytschko et al. (1998), the corrected smoothed particle method (CSPM) to achieve higher order derivatives by Chen et al. (1999) and Chen et al. (2001), the moving least-square SPH method by Dilts (1999) and Dilts (2000), the kernel integration correction by Bonet and Kulasegaram (2002), stable particle method by Rabczuk et al. (2004) and several other particle consistency restoring methods, such as by Rodriguez-Paz and Bonet (2005), Liu and Liu (2006), Oger et al. (2007) and so on.

2.2.3 Zero energy mode

The so-called zero-energy mode is often referred to the deformation characterized by a pattern of nodal displacement that produces zero strain energy, which has also been found in the finite difference and finite element methods.

Zero energy mode in the SPH method was first noticed by Swegle et al. (1994). The reason is that, in the conventional SPH method, all field variables and their derivatives are calculated at the same locations. In many cases, the kernel function reaches the maximum at its nodal position. Meanwhile, its derivatives become zero. One effective method to remedy such modes is to use stress points as discussed in Section 2.2.1.

The zero-energy mode in the SPH method is not such serious. This is because that the initial uniform particle distribution will become irregular soon due to its Lagrangian nature. Even for the uniformly distributed particles, only very special field variable distributions can trigger spurious energy modes.
2.2.4 Boundary conditions

In the early applications of the SPH method for fluid dynamics, boundary conditions were very simple and most even did not require such conditions. For the free boundaries in the hydrodynamics cases, it is sufficed to give an approximate zero pressure on the boundaries. For the solid material cases, all surface stress components should be zero. Libersky et al. (1993) first introduced ghost particles to reflect symmetrical surface boundary conditions. Similar approach was also addressed by Takeda et al. (1994) for fluid flow boundaries. Later, Randles and Libersky (1996) proposed a more general treatment of the boundary condition by assigning the same boundary value of a field variable to all the ghost particles, and then interpolating smoothly the specified boundary ghost particle value and the calculated values of the interior particles. The method can also heal the well-known kernel sum deficiency at the boundaries.

The approach can be outlined as follows. Providing that particle \( i \) is a boundary particle, its support particles \( N(i) \) can be divided into three subsets: the interior particles \( I(i) \), the boundary particles \( B(i) \) and the exterior (ghost) particles \( G(i) \). Figure 2-5 gives the arrangement of these particles.

![Figure 2-5 “The ghost particle” approach for boundary treatment (after Randles and Libersky, 1996)](image)

For a general scalar field \( f \), the boundary correction formula under the prescribed boundary value \( f_{bc} \) is given as:
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\[ f_{\text{rel}}(i) = f_{bc} + \frac{\sum_{j \in I(i)} \left( f_i - f_{bc} \right) m_j W_{ij}}{1 - \sum_{j \in I(i)} \frac{m_j}{\rho_j} W_{ij}} \]  
(2.8)

2.2.5 Other improvements

Besides the above fundamental issues, there are many other progresses on improving the performance of the SPH method, which have focused on applications as well as algorithmic efficiency. Much effort has been devoted to develop parallelization of the SPH method. Dave et al. (1997) developed a parallelized code based on TreeSPH, which is a unification of the conventional SPH with the hierarchical tree method by Hernquist and Katz (1989). Using message passing interface, it is executed through a domain decomposition procedure and a synchronous hypercube communication paradigm to build self-contained sub-volumes of the simulation on each processor at every time step. Thus, it can greatly enhance the efficiency of the simulations especially for the large 3D problems.

By considering a smoothing operator as a filter, Shapiro et al. (1996) as well as Owen et al. (1998) has developed an adaptive SPH technique (ASPH). It has been found that an adaptive smoothing filter is an efficient tool to resolve both larger-scale and small-scale problems. In the ASPH method, the traditional isotropic (or spherical) kernel function with a scalar smoothing length is replaced by an anisotropic smoothing algorithm using an ellipsoidal kernel function with a tensor smoothing length.

Figure 2-6 shows the scatter and gather approaches of ASPH. The symbols and circles represent the particles and their zones of influence, respectively. Solid and open circles denote the neighbors and non-neighbors of the particle indicated by an asterisk.

The G tensor is used in the ASPH method to take place of the isotropic smoothing length in the SPH method. It has the units of an inverse length-scale, and could be expressed in its primary frame as
where, $h_1$ and $h_2$ represent the smoothing lengths for the semi-major and semi-minor axes, respectively, as shown in Figure 2-7.

In the ASPH, the smoothing length along each axis is evolved so as to follow the variation of the local inter-particle separation surrounding each particle. By deforming and rotating the ellipsoidal smoothing function so as to follow the anisotropic volume changes associated with each particle, the ASPH adapts its spatially resolution scale in time, space and direction. Hence, the ASPH was shown to significantly improve the spatial resolving capability over that of the traditional SPH method for the same number of particles used. The ASPH models are frequently used to treat phenomena with features strongly dependent on directions. One typical example is the gas cloud collapse along a preferential axis in which the initial gas sphere deforms into a flattened disc shape. For such circumstances, an ellipsoidal smoothing function is very suitable for modeling...
the evolution of the system with strong direction-dependent features.

### 2.3 Numerical simulations on brittle material fracture process

Brittle material failure takes place when the stress comes up to the failure stress, which has little or no irreversible deformation in the process. Hallbauer et al. (1973) pointed that the fundamental attribute of brittle failure is the initiation and propagation of cracks and often is caused by tensile stress violation of the failure criteria. Cracks with other defects such as joints and mixtures disturb the continuum and transfer it into a discontinuum. During the fracture process, a fracture appears with the initiation of new surfaces or propagation of preexisting cracks.

#### 2.3.1 Constitutive model

The constitutive model plays an important role in numerical simulations. Most constitutive models are based on the theories of elasticity and plasticity. The linear elastic model based on the generalized Hooke’s law is still widely adopted for the intact materials by far for its simplicity. When the CHILE assumption (Continuous, Homogenous, Isotropic and Linear Elastic) is adopted, the model can be determined by the Young’s modulus ($E$) and the Poisson’s ratio ($\nu$). Based on that, more sophisticated models for isotropic condition can also be easily derived. The plastic and elasto-plastic models have been developed and widely applied to fractured rocks since the 1970s. They are mainly based on the classical theory of plasticity typically with a yield surface, such as Mohr-Coulomb or Drucker-Prager criterion, and the plastic potential. Detailed descriptions and FEM implementation for these classic plastic models can be referred to Owen and Hinton (1980).

Strain-hardening and strain-softening are the two common features of plastic behaviors. For the brittle material without confining pressures, strain-softening is often observed. Relative works have been published by many researchers, such as Read and Hegemier (1984) and Lade and Kim (1995), etc.
Strain rates can greatly affect the material strength especially when subjected to the dynamic loads such as high velocity impact and blast loading. In recent years, rate-dependence studies for different geo-materials have been carried out by many researchers, such as Gary and Bailly (1998), Filler and Wells (1988), Zhao et al. (1999), Zhao and Li (2000), Lok et al. (2002) and Wang and Wu (2004). Results from these studies show that the dynamic strength of the geo-materials will be one or several times of the static strength and will increase with the strain rate. Figure 2-8 shows such effects for tensile and compressive strengths of granite, respectively. Figure 2-9 and Figure 2-10 show the strain rate influences on the tensile and compressive strength of concrete by Eibl and Schmidt-Hurtienne (1999) and Bischoff and Perry (1991), respectively.

![Figure 2-8 Uniaxial tensile (left) and compressive strength (right) with the loading rate effect](image)

Figure 2-8 Strain rate influence on the tensile strength of concrete (after Eibl and Schmidt-Hurtienne, 1999)
2.3.2 Failure criterion

A strength or failure criterion is usually employed to give the yield surface and plastic potential function in a plastic model. Many strength criteria have been proposed since 19th century. They vary from very simple one as one parameter formulations to complex ones involved in multi-parameter forms. In 1864, Tresca proposed a single shear stress strength criterion. In 1876, Rankine developed the maximum tensile stress criterion, which is generally accepted to determine whether a tensile failure has occurred or not. According to this criterion, brittle fracture takes place when the maximum principle stress reaches its tensile strength. Followed by 1913, von Mises suggested the maximum octahedral shear stress strength criterion as shown in Figure 2-11. The criterion implies the yielding begins when the elastic energy of distortion reaches a critical value. It fits the experimental data well for most metals. Its yield surface is sketched in Figure 2-11. Although these criteria have been widely used due to simplicity, the over-simplification often cannot account for the complex strength characteristics of geo-materials. For example, it is well recognized that the failure strength of such materials are related to the hydrostatic stress. This leads to the Mohr-Coulomb criterion (Figure 2-12). The Mohr-Coulomb criterion can explain the shear failure well and match the fact that a hydrostatic stress does influence the yielding in the stress space. The linear approximation of the Mohr-Coulomb model is poor at low confinement, where the experimen-
tal strength curves exhibit greatly non-linearity, but for most materials, it is a reasonable approximation for confinements below the brittle-ductile transition. The model is independent of the intermediate principal stress resulting in the failure plane manifesting itself necessarily parallel to this direction.

Figure 2-11 Geometrical representation of the of von Mises yield surface. The Mohr-Coulomb criterion (Figure 2-12) is used for the failure envelop in the expression of the shear failure stress \( \tau \), the internal friction \( \phi \) and the inherent material cohesion \( c_0 \), it gives

\[
|\tau| = c_0 - \sigma_n \tan \phi
\]  

(2.10)

The normal stress \( \sigma_n \) is defined to be negative in compression here. And its expression in the principal stress space is given by,

\[
\frac{1}{2} (\sigma_{\text{max}} - \sigma_{\text{min}}) + \frac{1}{2} (\sigma_{\text{max}} + \sigma_{\text{min}}) \sin \phi = c \cdot \cos \phi
\]  

(2.11)

where \( \sigma_{\text{max}} \) and \( \sigma_{\text{min}} \) are the maximum and minimum principal stresses respectively.

Figure 2-12 Geometrical representation of the Mohr-Coulomb and Drucker-Prager yield surfaces in principal stress space.
The Drucker-Prager criterion (shown in Figure 2-12) modified the Mohr-Coulomb criterion by using a circle as a shape function in the deviatoric section instead of the hexahedral shape by Drucker et al. (1952). It provides phenomenological explanations for the pressure dependent flow due to the internal friction, which is a typical feature of brittle materials. It can also allow the evolution of the deformation to be tracked through the strain-hardening and the strain-softening within the framework of finite deformation kinematics. The Drucker-Prager criterion has an advantage to represent the strength property of a material since it includes all the six stress components in its expression. Generally speaking, the Mohr-Coulomb and the Drucker-Prager criteria are two of the most commonly used failure criteria for rock and rock-like materials. And many recently developed criteria are their revised versions on different purposes and will not reiterate here.

In 1961, Yu suggested a new criterion called a twin-shear stress criterion based on the two larger principal shear stresses. In the criterion, the tensile and compressive meridians are the same straight lines parallel to the hydrostatic axis. Its shape function in the deviatoric plane is piece-wise linear with one parameter. The mathematical expression is very simple and the parameter has physical meaning. However, it is more suitable to materials with nearly same tensile and compressive strengths, such as metals. In an improved version in 1983, Yu (1983) took into account all stress components in the octahedral shear stress plane. In the mathematical form, the criterion is equal to the sum of the two larger principal shear stresses plus the weighted corresponding normal stresses. The shape function keeps the same with the previous expression. Though the tensile and compressive meridians are still straight lines, they are not the same in this extended version. And this extends its applicability to a wide range of materials with different tensile and compressive strengths. Later on in 1991, Yu and He (1991) introduced a weighting coefficient for the second principal shear stress and its corresponding normal stress and proposed the Unified Twin-shear Strength (UTSS) theory. The shape function of this theory in the deviatoric plane has two parameters. One is the ratio of the tensile radius to compressive radius in the deviatoric plane. The other one is the weighting coefficient for the
second principal shear stress and its corresponding normal stress, namely the parameter $b$. The value of $b$ varies from 0 to 1 which is corresponding to the lower and upper limits of any convex cross-section in the deviatoric plane. In addition, Yu modified the formulation of the meridians by introducing nonlinear terms of hydrostatic stress. As a result, the Yu’s criterion becomes a comprehensive one encompassing almost all established strength criteria. For example, the Mohr-Coulomb criterion is its one specific case of form where the meridian is linear and $b$ is set to zero. The von Mises criterion and Drucker-Prager criterion can be also approximated by the Yu’s Criterion with different values of $b$ (within 0.5 to 0.75) and different formulations of the meridians. In general, Yu’s criterion can be applied to almost all materials including metals, crystals and geo-materials. Figure 2-13 illustrates the principal shear stresses act on four faces of an octahedral stress element in the UTSS theory. Generally, this series of twin-shear strength theories consider the maximum principal shear stress $\tau_{13}$ and intermediate principal shear stress $\tau_{12}$ (or $\tau_{23}$), and the influence of the normal stresses $\sigma_{13}$ and $\sigma_{12}$ (or $\sigma_{23}$) acting on the same section, respectively.

\[ F[\tau_{13}, \tau_{12}; \sigma_{13}, \sigma_{12}] = C, \text{ when } f(\tau_{12}, \sigma_{12}) \geq f(\tau_{23}, \sigma_{23}) \]
\[ F[\tau_{13}, \tau_{23}; \sigma_{13}, \sigma_{23}] = C, \text{ when } f(\tau_{12}, \sigma_{12}) \leq f(\tau_{23}, \sigma_{23}) \]

(2.12)
2.3.3 Damage mechanics model

Continuum damage mechanics principles was proposed first by Kachanov (1958) based on scalar, vector or tensor representations of the void formation, micro-cracking or embedded fracture phenomena in materials under loading. Since this theory is very closely related to both continuum mechanics and fracture mechanics, Oliver (2000) regards that it serves a connecting bridge between these two fields. Comprehensive reviews on continuum damage mechanics including its development, trends, characteristics and weakness can be referred to Krajcinovic (1989), Krajcinovic (2000) and de Borst (2002).

The definition of damage proposed by Rabotnov (1963) is a scalar variable used for the creep rupture. This scalar variable describes the decrease of effective area or the density of micro-void in a representative volume element (see Figure 2-14),

\[
D = \frac{A_v}{A_0} = \frac{A_0 - A_{\text{eff}}}{A_0}
\]  

(2.13)

where, \(A_0\) is the nominal area, \(A_v\) and \(A_{\text{eff}}\) are the void and effective areas, and \(D\) is the damage scalar.

![Figure 2-14 Damage scalar in a uniaxial tension bar](image)

With the definition for the damage variables, one can get the stress-strain relationship for the damage material by using the concept of effective stress. The effective stress \(\sigma_{\text{eff}}\) is the “true stress” in the effective area \(A_{\text{eff}}\) and is defined in one dimension sense as,

\[
\sigma_{\text{eff}} = \frac{\sigma}{1 - D}
\]  

(2.14)
where $\sigma$ is the nominal stress. From the definition of Eq.(2.14), the strain constitutive equation can be written as

$$\varepsilon = \frac{\sigma}{E(1-D)} \quad (2.15)$$

where $E$ is the elastic modulus. Once the damage scalar $D$ is determined, an elastic damage model can be easily constructed, damage evolvement or development can subsequently be given. Various methods have been employed to construct the damage evolution law, such as curve fitting of the experimental data, statistical method and thermodynamics method. For instance, Mazars (1986) proposed a damage evolution law mainly from experimental results and take the thermodynamics into consideration. Wang (1998) adopted the statistical method to construct the damage evolution law. While in Holmquist et al. (2001), the damage is defined in terms of the effective shear plastic strain evolution.

Usually, the continuum damage models can be classified into the elastic damage model and the elastic-plastic damage one. Figure 2-15 by Ma et al. (1998) gives a schematic diagram of brittle material failure and approximations by using different damage models, where (a) denotes the unloading response of elastic damage model and (c) represents the response of a plastic-damage model.

![Figure 2-15 Elastic brittle and elasto-plastic properties of rock (after Ma et al., 1998)](image)

In the elastic-damage models, the material inelastic behavior is reflected only by the stiffness degradation, and there is no permanent deformation in the material after a complete unloading. For example, Zhu and Tang (2004) used an
isotropic tensile strain damage coupled with the elastic brittle model to simulate the rock fracture process. On the contrary, in the elastic-plastic-damage model, a coupling between the plasticity of the material and its stiffness degradation is often used. For instance, Frantziskonis and Desai (1987) developed a strain-softening constitutive model combined with the plasticity theory by considering that the behavior of a material element consists of a topical part and a damaged part. Simo and Ju (1987) proposed a simple strain-based anisotropic plastic damage model that can predict crack development parallel to the axis of loading. Wang (1998) also proposed a plastic damage model by considering the tensile damage in the principal stress direction. Other successful applications of the plastic-damage model includes Lubliner et al. (1989), Jeeho and Gregory (1998), Nechnech et al. (2002), Kojic (2002), Addessi et al. (2002), Jason et al. (2006), Shao et al. (2006), Grassl and Jirásek (2006) and so on.

Generally speaking, the elastic-plastic-damage model is very promising and can reasonably describe the mechanical behavior of materials. It merits further developments and studies.

2.3.4 Material heterogeneity and micromechanical models

Geo-materials, such as rock and concrete, are often considered as homogeneous material in most large-scale engineering calculations for the convenience and practical necessary. However, these materials are inhomogeneous on length scales below the centimeter scale, due to pores, micro-cracks, grains, minerals, etc. Although the fact that such heterogeneity can greatly affect the macroscopic behavior and the failure process has long been noticed, it is still unclear how such processes are conducted.

Since computational methods are obviously well suited for studying the process of rock strength degradation and failure, many micromechanics models have been proposed in order to gain a better understanding on such behaviors and processes. Paterson and Wong (2005), Yuan and Harrison (2006) and Jaeger et al. (2007) have reviewed these numerous stochastic and statistical approaches based on the fracture mechanics and the continuum damage mechanics. Reviews are only given on those based on the damage mechanics.
The first attempt to apply the statistical method to describe the rock failure might be ascribed to Scholz (1968). In his work, a rock sample is assumed to be divided into many small elements. The local stress and local strength within each of these elements were distributed about their mean values. Individual elements were assumed to fail when the local stress reaches the local strength, and this failed region propagates to an adjacent element if that element has the appropriate combination of higher stress and/or lower strength. As the stress is increased incrementally, the entire rock specimen may eventually fail, as the local regions of failed rock percolate throughout the body.

To quantitatively apply this concept to the rock mechanical behavior, Hudson and Fairhurst (1969) emphasized that, as the strength of rock is not an intrinsic property but the result of a stochastic chain reaction, the Weibull distribution by Weibull (1951) is appropriate for describing the mechanical breakdown process. By this concept, a suite of theoretical complete stress-strain curves can be synthesized that reflects different degrees of heterogeneity, as shown in Figure 2-16. This work can be considered as a pioneer for those later methods that adopted the Weibull distribution to develop statistical modeling in terms of both continuum and discrete approaches.

Figure 2-16 Stress-strain curves characterized by different degrees of heterogeneity (after Hudson and Fairhurst, 1969)

Allegre et al. (1982) considered an array of eight cubical elements, each of which is either intact or already “failed,” with two different probabilities. By
considering all possible topological combinations, they calculated the probability of the 8-cube array to be in the failed state, and then grouped this macro cube with seven adjacent macro cubes, continuing the process to find that the entire sample will be in a macroscopic “failed” state. Madden (1983) extended this approach by relating the probability of failure \( p \) to the local crack density. Lockner and Madden (1991) assumed that each failed element contained a micro crack and accounted for possible crack closure and frictional sliding. Hence, their model can predict the development of dilatancy and shear localization.

Blair and Cook (1998) developed a lattice-based model (see Figure 2-17) in which the local elements are allowed to fail by tensile cracking if the local tensile stress exceeds the local tensile strength, which was assumed to be distributed either uniformly over a certain range. They found that the locations of cracked elements are initially random, but eventually these failed elements coalesce to form a macroscopic fracture, which is consistent with experimental observation. Reuschlé (1998) used a similar network model to study the influence of heterogeneity and loading conditions on the fracture process. These types of network models can also be used to study other inelastic deformation processes, such as unstable fault slip by Hazzard et al. (2002).

![Figure 2-17 Lattice model in the analysis of compressive fracture in rock (after Blair and Cook, 1998)](image)

Tang et al. (2000a) developed a finite element code in which elements of rock materials in an experimental specimen are represented by an elastic-brittle constitution. The elastic modulus and strength of the individual elements were assumed to follow a Weibull distribution. It is able to predict many of the features of rock deformation, both pre- and post failures as shown in Figure 2-18.
Fang and Harrison (2002) developed a similar model that also considers the strengthening effect that the confining pressure has on the individual elements. Their model was able to predict the brittle-ductile transition characteristics of the stress-strain curve with the increasing confining pressure, as shown in Figure 2-19.

![Figure 2-18 Simulated rock progressive failure by RFPA code (after Tang et al., 2000a)](image)

![Figure 2-19 Simulated fracture patterns and stress-strain curves on confining pressure obtained using the local degradation approach (after Fang and Harrison, 2002)](image)

Besides these continuum and network based statistical models, a synthetic rock mass model (SRM) is proposed by Potyondy and Cundall (2004) by applying the PFC code (see Figure 2-20). The model is used to create an assembly of bonded particles representing a large intact rock sample. A discrete fracture network is then generated which honors the joint measures derived from drilling and mapping on site (e.g. spacing, trace length, orientation). The entire network is then embedded within the bonded assembly, which is subjected to stress changes expected in the field. Joints are inserted into the PFC particle assembly
using a developed smooth joint model which allows slip and opening on internal planar surfaces.

Figure 2-20 Complex grain-like shapes in PFC 2D (left, after Potyondy and Cundall, 2004); A Synthetic Rock Mass Model (SRM) by Itasca (right)

Chen et al. (2004) and Chen et al. (2007) applied one digital image approach to reconstruct rock microstructures. By feeding the obtained micro structural information into the commercial software FLAC, they simulated the fracture process of the heterogeneous rock sample under static Brazilian tensile test as shown in Figure 2-21. Therefore, the simulation can represent the real cases.

Figure 2-21 Digital image-based numerical modeling method for prediction of inhomogeneous rock failure using FLAC (after Chen et al., 2004)

Based on those studies, the statistical approach seems to be one promising technique to model heterogeneous rock failures.

2.4 SPH applications on solid mechanics

2.4.1 An overview

Historically, the SPH method was developed by astrophysicists and used pri-
marily for hydrodynamic fluid dynamics problems, where only the pressure was of concern. Libersky and Petschek (1990) first cast the SPH method to the solid continuum by adding the deviator stresses to make a full stress tensor and including a simple elasto-perfectly plastic constitutive description into the SPH formulae. In a series of papers, such as Libersky et al. (1993), Benz and Asphaug (1994), and Randles and Libersky (1996), various applications were successfully simulated, such as 3D thick-wall bomb explosion and fragmentation problem, rod impact and penetration problem, etc.

Impact and penetration simulations have also been extensively conducted. Johnson et al. (1993) described how SPH could be incorporated into a standard Lagrangian code such as EPIC for modeling inelastic, damage and large deformation problems when subjected to high velocity impact. In Johnson et al. (1996) and Johnson and Beissel (1996), a new particle method called the normalized smoothing function (NSF) method coupled with FEM method is used. A generalized particle algorithm for high velocity impact computations was put forward by Johnson et al. (2000) and Johnson et al. (2002), which provides stable computations for large tensile strains and enhanced the stability for 2D and 3D axisymmetric geometry.

2.4.2 Coupled with other Lagrangian codes

With special techniques used, SPH can be coupled with other Lagrangian codes to meet various ends. A number of papers and reports have been published on coupled FEM-SPH solvers. The earliest attempts were by Attaway et al. (1994), Johnson (1994) and Johnson and Beissel (1996).

Attaway et al. (1994) used the master-slave algorithm to couple an SPH solver to PRONTO, a hydrocode developed at Sandia National Laboratories. The algorithm for interaction between elements and particles is described for a 2D case and is based on a predictor-corrector method. The authors reported that iteration once was usually sufficient to obtain a satisfactory contact treatment.

Johnson (1994) and Johnson and Beissel (1996) also used a master-slave algorithm. When a slave particle penetrates the master segment the following three
conditions are enforced: conservation of linear momentum, conservation of angular momentum and the normal velocity components of the particle and the master segment are identical. More recently Johnson et al. (2002) introduced a contact and coupling algorithm which is based on a viscous-elastic contact stiffness.

Besides FEM, SPH can also be combined with other numerical methods. For example, Cleary and Prakash (2003) employed a discrete element method model coupled with SPH to model complex three-dimensional environmental particulate flows.

Although these coupled models have obtained successes, some limitations need to be improved. For example, the techniques to better process the boundary linking between the different types of meshes, the corresponding contact model to process the boundary contacts, and so on.

2.4.3 Contact problems

Campbell et al. (2000) described the development and testing of a contact algorithm for SPH. They defined the position of the boundary at \( h \), where \( h \) is the smoothing length. First, the boundary nodes are determined and then a particle to particle contact force is applied between particles in contact. This algorithm was developed and demonstrated for 2D. This approach removes the need to define the material boundary as a line in 2D or a surface in 3D, and has similarities with the pinball contact algorithm by Belytschko and O. Neal (1991). However, due to non-uniqueness of the surface normal at vertices it was necessary to calculate two surface normals for each boundary particle, and detect a corner particle when the angle between the two normals exceeds a specified angle. The penalty formulation was used to enforce the contact condition, and several equations for the penalty force calculation were considered. The contact algorithm was tested for one and two-dimensional problems. Other recent improvements on SPH contact treatment are by Rabczuk and Areias (2006) and Vignjevic et al. (2006).
2.4.4 Fracture and fragmentation

From the point view of solid mechanics, the most appealing attribute of SPH lies in its ability to fracture in a realistic manner without unduly compromising its ability in subsequent computation. Under expansive strain fields, SPH particles can fracture numerically due to loss of communication between neighbors, unless provisions are made for a comparable expansion of the smoothing length. Great efforts have been made to incorporate damage and fracture algorithms into SPH which takes an advantage of its mesh-free attributes while instilling physical realism in the mechanics of progressive damage and ultimate fracture.

Stellingwerf and Wingate (1993) pointed out that the simplest approach in the SPH computation for the fracture was to allow the object to respond naturally to the body stresses at each point by setting the yield stress and the spall strength criterion according to the adopted model for the material. They also used the fragmentation model of Grady and Kipp in Atkinson (1987) to simulate the hypervelocity impact phenomena and have obtained promising results.

Benz and Asphaug (1994) and Benz and Asphaug (1995) were among those first to implement ideas of incorporating damage and fracture algorithms into SPH to study brittle material fracture under impact. Both of these efforts were using a statistically-based fracture theory for brittle materials which was developed by Grady and Kipp (1980). This theory postulates a brittle micro-cracking damage growth equation that makes the damage rate proportional to the current number of flaws per unit volume and the current state of stress. A set of flaws (cracks) is assigned to the SPH particles at random, according to the Weibull distribution. Depending on the flaw, tension may or may not cause it to grow. The growth is associated with the local damage quantified by the damage. When no damage occurs it means that, the material is perfectly elastic and when damage increases to 1.0, the material is completely damaged and the contribution of the deviatoric stress is zero. The precise way in which the flaws are assigned, and the equation for damage evolution, are discussed in detail by Benz and Asphaug (1994) and Benz and Asphaug (1995).

Randles and Libersky (1996) used a heuristic form of continuum tensile damage
that has no direct connection with microscopic material phenomenon. The damage evolution equation has a threshold equal to the static tensile strength and a time parameter to control the rate of damage accumulation. In the article, damage was viewed as an evolving, non-decreasing field variable responding to current states of stress and damage. The damage, in turn, softened some of the material properties. Under the dynamic setting with one or more spatial dimensions, such an interaction could result in the possibility of spatial localization failure. The failure often occurred within these regions having rapidly increasing damage with the accompanying softening. Such a local failure gave stress relief to surrounding material and is interpreted as the onset of cracking.

The advantageous feature of the SPH is that fracture as the end result of damage can be easily accomplished through simple rules of kinematics constraints between neighboring particles. Mesh-based code has the limitation in a large damage extent, especially in simulation of a fragmentation process. Mesh-based codes have to deal with decoupling element nodes, killing elements, rezoning, etc. to allow for the generation of new boundaries resulting from the crack propagation. Since SPH involves only a region of neighboring particles, fracture can be easily handled. SPH, in particular, gives a good description of the fragments and provides a natural transition from the continuum to the fragmented state.
Chapter 3 The SPH Method and Its Program Implementation

The present chapter introduces the fundamentals of the SPH method and its program implementation and calibration. It builds up the foundation of the thesis work to numerically simulate the brittle failure of heterogeneous materials based on the SPH method. The formulation of the SPH method is based on the pioneer work by Monaghan (1992) and Libersky et al. (1993). An elasto-plastic damage constitutive model, which can better describe the brittle material behaviors, is put forward. A statistic model based on the Weibull distribution law, which can reflect the material microstructure heterogeneity, is implemented.

3.1 The smoothed particle hydrodynamics method

3.1.1 Collocation implementation of the SPH method

Although the SPH method can be realized by using the Galerkin method such as by Swegle et al. (1994), in most cases, it is implemented by a collocation method.

Assume $W$ is a kernel function that satisfies the conditions described in section 2.1.2, the integral interpolant of any function $f(x)$ can be expressed by its kernel approximation $\langle f(x) \rangle$

$$\langle f(x) \rangle = \int_{\Omega} f(x') W(x-x', h) dx'$$

(3.1)

Similarly, approximation of the spatial derivatives for $f(x)$ can be expressed as

$$\langle \nabla f(x) \rangle = \int_{\Omega} \left[ \nabla f(x') \right] W_s(x-x', h) dx'$$

(3.2)
Assuming that the kernel function could be differential, the integration by parts of Eq. (3.2) gives,

\[
\langle \nabla f(x) \rangle = \oint_S f(x') W(x-x', h) \hat{n} dS - \int_{\Omega} f(x') \nabla \left[ W_s(x-x', h) \right] dx
\]  

(3.3)

where, \( \hat{n} \) is the unit normal to the surface \( S \). Since \( W \) usually is defined with a compact support, the surface integral contributions in Eq. (3.3) is negligible. Hence, the approximation of the derivative for \( f(x) \) can be written as,

\[
\langle \nabla f(x) \rangle = -\int_{\Omega} f(x') \nabla \left[ W_s(x-x', h) \right] dx'
\]

\[
= \int_{\Omega} f(x') \nabla \left[ W_s(x-x', h) \right] dx'
\]

(3.4)

In the last integral in Eq.(3.4), the symmetric property of the kernel \( W \) has been used, as \( \nabla \left[ W_s(x-x', h) \right] = -\nabla \left[ W_s(x-x', h) \right] \), where the gradient is taken with respect to \( x' \) and \( x \), respectively.

Considering a problem domain, which is discretized by a body of particles as shown in Figure 3-1, the state of the system can be represented by these particles in that each particle is associated with some field properties. These particles can be used not only for integration, interpolation, and differencing, but also for representing the material as mass particles. One may regard these particles as the mass centers of the corresponding sub-domains of the material. The volume of a sub-domain is lumped on the corresponding particle. Therefore, each particle is associated with a fixed lumped volume. If we associate with particle \( j \) a volume to introduce the concept of particle mass \( m_j \),

\[
dx_j = \frac{m_j}{\rho_j}
\]

(3.5)

Assume the kernel function has a compact supporting radius of \( kh \), an approximation form of Eq. (3.1) by the discretized particles becomes

\[
\langle f(x) \rangle_{x=x_i} = \sum_{j=1}^{N} \frac{m_j}{\rho_j} f(x_j) W \left( x_i - x_j, h \right)
\]

(3.6)

where, the summation is over all the particles (with a total number of \( N \), in-
cluding particle \( i \) within the supporting domain \( \Omega \) of the given particle \( i \), the label \( j \) here denotes these influenced particles. Those influenced particles are the neighboring particles of particle \( i \). Obviously, particle \( j \) has mass \( m_j \), position \( x_j \), density \( \rho_j \) and velocity \( v_j \) and other properties.

**Figure 3-1 Illustration of the kernel function and the supporting domain**

Based on Eq. (3.4), further approximation of the differential form of \( f(x) \) at particle \( i \) can be constructed by using its neighboring particles as

\[
\left\langle \nabla f(x) \right\rangle_{x=x_i} = \sum_{j=1}^{N} f(x_j) \frac{m_j}{\rho_j} \cdot \nabla \left[ W_{kh}(x, x_j, h) \right]
\]

(3.7)

where, the gradient \( \nabla W_{kh} \) is taken with respect to particle \( i \).

However, when particles are arbitrarily distributed, this form of gradient will give poor numerical results due to the fact that a constant distribution of \( f(x) \) will result in a non-zero gradient. This is directly related to lack of consistency of the SPH kernel function. An efficient and economic method to minimize the inherent lack of consistency on irregular meshes is called the symmetrized form method by Monaghan (1992), which can develop the differential functions for a higher accuracy by writing the divergence of \( f(x) \) at particle \( i \).
By introducing one differential function $\Phi$, one can write

$$\nabla (\Phi f) = \Phi \nabla f + f \nabla \Phi$$  \hspace{1cm} (3.8)

Eq. (3.8) can be expressed into another form as,

$$\nabla f (x) = \frac{1}{\Phi} \left[ \nabla (\Phi f) (x) - f (x) \nabla \Phi \right]$$ \hspace{1cm} (3.9)

The SPH approximation form of Eq.(3.9) is,

$$\langle \nabla f (x) \rangle_{x=x_i} = \frac{1}{\Phi} \sum_{j=1}^{N} \Phi_j \frac{m_j}{\rho_j} (f (x_j) - f (x_i)) \nabla \left[ W_h (x_i - x_j, h) \right]$$ \hspace{1cm} (3.10)

If we take $\Phi = 1$, then the above equation can be written as,

$$\langle \nabla f (x) \rangle_{x=x_i} = -\sum_{j=1}^{N} \frac{m_j}{\rho_j} (f (x_j) - f (x_i)) \nabla \left[ W_h (x_i - x_j, h) \right]$$ \hspace{1cm} (3.11)

This representation will result in zero gradients for a constant distribution of $f (x)$ even the particles are in disordered.

### 3.1.2 Continuum governing equations and their approximation forms

The conservation equations of continuum mechanics are:

- the continuity equation, \[ \frac{d \rho}{dt} = -\rho \cdot \frac{\partial v_\alpha}{\partial x_\alpha} \] \hspace{1cm} (3.12)
- the momentum equation, \[ \frac{dv_\alpha}{dt} = \frac{1}{\rho} \cdot \frac{\partial \sigma_{\alpha\beta}}{\partial x_\beta} \] \hspace{1cm} (3.13)
- the energy equation, \[ \frac{de}{dt} = \frac{1}{\rho} \cdot \sigma_{\alpha\beta} \cdot \frac{\partial v_\alpha}{\partial x_\beta} \] \hspace{1cm} (3.14)
- the particle moving equation, \[ \frac{dx_\alpha}{dt} = v_\alpha \] \hspace{1cm} (3.15)

In the above equations, dependent variables are the scalar density ($\rho$) and internal energy ($e$), the velocity components ($v_\alpha$), and the stress tensor ($\sigma_{\alpha\beta}$) is
defined as $\sigma_{\alpha\beta} = p\delta_{\alpha\beta} + S_{\alpha\beta}$ in terms of the pressure $p = \frac{Tr(\sigma)}{3}$ and the traceless symmetric deviatoric stress $S_{\alpha\beta}$). The independent variables are the spatial coordinates ($x_\alpha$) and the time ($t$). The total time derivative operator ($\frac{d}{dt}$) is taken in the moving Lagrangian frame. In the above equations, the Greek superscripts $\alpha$ and $\beta$ are used to denote the coordinate directions. The summation is taken over repeated Greek indices in those equations. Stresses are positive in tension and negative in compression.

From now on, for brevity, we take

$$W_{ij} = W(x_i - x_j, h); \quad \frac{\partial W_{ij}}{\partial x_j} = \frac{\partial [W(x_i - x_j, h)]}{\partial x_j}$$ (3.16)

For the mass conservation equations, there are two popular kinds of approximation forms for the density approximation. One is the summation density form based on Eq. (3.6),

$$\rho_i = \sum_{j=1}^{N} m_j W_{ij}$$ (3.17)

With this equation, only particle coordinates and masses are required to compute the density, and the Eq. (3.12) is automatically satisfied. However, the disadvantage appears due to the deficiency of particles, such as situations near boundaries. One simple corrective approach is by using the Shepard interpolation technique by Shepard (1968) to rewrite Eq. (3.17) as,

$$\rho_i = \sum_{j=1}^{N} m_j (W_{ij})_S; \quad (W_{ij})_S = \frac{W_{ij}}{\sum_{j=1}^{N} m_j W_{ij}}$$ (3.18)

This allows reproducing exactly uniform functions.

Another one is the time dependent form based on Eq. (3.11) as

$$\frac{d\rho_i}{dt} = \sum_{j=1}^{N} m_j (v_\alpha)_j \frac{\partial W_{ij}}{\partial (v_\alpha)_i}$$ (3.19)
where, \((v_a)_i = (v_a)_j - (v_a)_j\) in the equation and elsewhere in the report. The benefit of this equation is that, the use of the relative velocities in antisymmetrized form serves an approach to mitigate particle inconsistency. Therefore, it can improve the approximation accuracy. When the calculation involves two or more kind of materials, and their densities differ by more than a factor of 2, according to Gray et al. (2001) the following formula is preferred,

\[
\frac{d\rho_i}{dt} = \rho_i \sum_{j=1}^{N} \frac{m_j}{\rho_j} (v_a)_i \frac{\partial W_{ij}}{\partial (x_a)_j}
\]  

(3.20)

To derive the approximation of the momentum equation, we start from the strain rate equations. The strain rate tensor \(\dot{\varepsilon}_{\alpha\beta}\) can be expressed by the derivatives of the velocity as

\[
\dot{\varepsilon}_{\alpha\beta} = \frac{1}{2} \left( \frac{\partial v_{\alpha}}{\partial x_{\beta}} + \frac{\partial v_{\beta}}{\partial x_{\alpha}} \right)
\]  

(3.21)

Followed by Libersky and Petschek (1990), the SPH approximation for the Eq. (3.21) can be derived based on Eq. (3.11) as

\[
(\dot{\varepsilon}_{\alpha\beta})_i = -\frac{1}{2} \sum_{j=1}^{N} \frac{m_j}{\rho_j} \left( (v_{\alpha})_j \frac{\partial W_{ij}}{\partial (x_{\beta})_j} + (v_{\beta})_j \frac{\partial W_{ij}}{\partial (x_{\alpha})_j} \right)
\]  

(3.22)

Once \(\dot{\varepsilon}_{\alpha\beta}\) is determined, the stress rate \(\dot{\sigma}_{\alpha\beta}\) tensor can be obtained based on the adopted constitutive model. Consequently, the stress tensor \(\sigma_{\alpha\beta}\) can be calculated by an explicit time integration approach.

The derivation of SPH formulations for particle approximation of momentum evolution is somewhat similar to the continuity density approach, and usually involves some transformations. Again, using different transformations can derive different forms of momentum approximation equations. Directly applying the SPH particle approximation concepts to the gradient on the RHS of the momentum equation in Eq. (3.13) yields following equation

\[
\frac{d (v_a)}{dt} = \frac{1}{\rho_i} \sum_{j=1}^{N} \frac{m_j}{\rho_j} (\sigma_{\alpha\beta})_j \frac{\partial W_{ij}}{\partial (x_{\alpha})_j}
\]  

(3.23)
Consider the following identity,
\[
\sum_{j=1}^{N} \frac{m_j}{\rho_i \rho_j} (\sigma_{\alpha \beta})_{ij} \frac{\partial W_{ij}}{\partial (x_i)} = \frac{\sigma_{\alpha \beta}}{\rho_i} \sum_{j=1}^{N} m_j \frac{\partial W_{ij}}{\partial (x_i)} = \frac{(\sigma_{\alpha \beta})_{ij}}{\rho_i} \left[ \nabla (1) \right] = 0 \tag{3.24}
\]

Adding Eq. (3.24) to Eq. (3.23), it will lead to
\[
\frac{d (v_{\alpha})_i}{dt} = \sum_{j=1}^{N} m_j \left( \frac{\sigma_{\alpha \beta}}{\rho_i \rho_j} \right) \frac{\partial W_{ij}}{\partial (x_i)} \tag{3.25}
\]

If we consider the following identity,
\[
\frac{1}{\rho_i} \frac{\partial \sigma_{\alpha \beta}}{\partial x_{\beta}} = \frac{\sigma_{\alpha \beta}}{\rho_i} \frac{\partial \rho}{\partial x_{\beta}} + \sigma_{\alpha \beta} \frac{\partial \rho}{\rho_i^2} \frac{\partial \rho}{\partial x_{\beta}}, \tag{3.26}
\]

by applying the SPH particle approximation to the gradients, one can get,
\[
\frac{d (v_{\alpha})_i}{dt} = \left( \sum_{j=1}^{N} m_j \left( \frac{\sigma_{\alpha \beta}}{\rho_i^2} \right) \frac{\partial W_{ij}}{\partial (x_i)} + \frac{\sigma_{\alpha \beta}}{\rho_i} \sum_{j=1}^{N} m_j \frac{\partial W_{ij}}{\partial (x_i)} \right) \tag{3.27}
\]

Monaghan (1992) pointed that Eq. (3.27) had an advantage over Eq. (3.25) in that linear and angular momentums were conserved for it produced a symmetric central force between pair particles.

Consequently, the energy equation (3.14) has two approximation forms. One is
\[
\frac{de_i}{dt} = -\frac{1}{2} \sum_{j=1}^{N} m_j \left( \frac{\sigma_{\alpha \beta}}{\rho_i \rho_j} \right) (v_{\beta})_j \frac{\partial W_{ij}}{\partial (x_i)} \tag{3.28}
\]

The other one is
\[
\frac{de_i}{dt} = -\frac{1}{2} \sum_{j=1}^{N} m_j \left( \frac{(\sigma_{ij})_i}{\rho_i^2} + \frac{(\sigma_{ij})_j}{\rho_j^2} \right)(v_i)_j \frac{\partial W_{ij}}{\partial (x_i)} 
\]

(3.29)

### 3.1.3 Artificial viscosity

The “artificial viscosity” was introduced by von Neumann and Richtmyer (1950) which aimed to smooth shocks over a few resolution lengths and to stabilize numerical solutions. For the SPH, an additional term is introduced into the Eq. (3.25)~ (3.29) as an artificial viscous pressure \( \Pi \) by Gingold and Monaghan (1977),

\[
\Pi_{ij} = \begin{cases} 
-\alpha c_i \mu_{ij} + \beta \mu_v, & (v_i - v_j) \cdot (x_i - x_j) < 0 \\
0, & (v_i - v_j) \cdot (x_i - x_j) \geq 0 
\end{cases}
\]

(3.30)

where,

\[
\mu_{ij} = h \frac{(v_i - v_j) \cdot (x_i - x_j)}{|x_i - x_j|^2 + \epsilon h^2}
\]

(3.31)

and,

\[
c_{ij} = \frac{c_i + c_j}{2}; \quad \rho_{ij} = \frac{\rho_i + \rho_j}{2}
\]

(3.32)

The parameters \( \alpha \) and \( \beta \) usually take around 1 and 2 respectively. The parameter \( \epsilon \) in Eq. (3.31) is to prevent singularities and takes around 0.1. The parameter \( c_i \) and \( c_j \) in Eq. (3.32) are the stress wave propagation speed.

### 3.1.4 Conservative smoothed solution for the SPH tensile instability

As discussed in section 2.2.1, the SPH may suffer the tensile instability in numerical simulations. The current program takes the conservative smoothing method by Randles and Libersky (1996) as
$$S_{cs}(U_i, \alpha_{cs}) = U_i + \alpha_{cs} \left[ \sum_{j \neq i} \frac{m_j U_j W_{ij}}{\rho_j} - U_i \right]$$  \quad (3.33)$$

In Eq. (3.33), $U_i$ denotes the velocity, density and internal energy respectively; $\alpha_{cs}$ usually takes within a range from 0 to 0.5.

### 3.1.5 Smoothing length evolution

Although the global constant smoothing can be used during the whole simulation, the large deformation will result in severe pack or loose spacing for the particles. In order to maintain a healthy neighborhood as the continuum deforms, the smoothing length $h$ can be evolved during the calculation. The most commonly used one by Benz (1989) can be expressed as

$$\frac{d (h_i)_n}{dt} = - \frac{1}{D (\rho_i)_n} \frac{d (\rho_i)_n}{dt}.$$  \quad (3.34)$$

where $(h_i)_n$ and $(\rho_i)_n$ are the smoothing length and the density of particle $i$ at $n^{th}$ time step, respectively. $D$ is the problem dimension. Eq. (3.34) can be written in the form of particle approximation as,

$$\frac{d (h_i)_n}{dt} = - \frac{1}{D (\rho_i)_n} \sum_{j=1}^{N} m_j \frac{\partial (W_{ij})_n}{\partial (v_{\alpha})_i}$$  \quad (3.35)$$

The smoothing length at the next step becomes,

$$(h_i)_{n+1} = (h_i)_n + \frac{d (h_i)_n}{dt} \delta t.$$  \quad (3.36)$$

### 3.1.6 Nearest neighboring particle searching

An important step in the SPH computation is the neighbor search. This task can be extremely time-consuming. The neighbor search routine lists the particles that are inside the neighborhood of each particle at each time step. The process of finding these particles is commonly referred to as nearest neighboring par-
particle searching (NNPS).

There are three kinds of popular NNPS approach in the current applications, named the direct search, the link-list search and the tree search algorithm. The direct search is performed between every two particles. Thus it is particularly inefficient. The tree search is most efficient. However, it is a little complex to be implemented. The link-list search algorithm takes the advantages of both the efficiency in arithmetic and simplicity in implementation and hence is the mostly preferred one.

![Figure 3-2 Link-list algorithm for searching the nearest neighboring particles in two-dimension](image)

In the link-list method, an underlying grid is generated and the particles are sorted according to the box in which they are located (Figure 3-2). Then for each particle, only those contained in the same box and the surrounding boxes need to be checked to find its neighbors. This allows the computational time to be cut down from a default time proportional to \( N^2 \) for the direct search to \( N \log N \), where \( N \) is the total number of particles.

### 3.1.7 Adopted SPH approximation equations and some numerical aspects

Based on the results in the previous sections, the SPH approximations of the continuum conservation equations adopted in the current research are as follows,

\[
\frac{d \rho_i}{dt} = \rho_i \sum_{j=1}^{N} \frac{m_j}{\rho_j} \left( \frac{v_{ij}}{\sqrt{\sigma}} \right) \frac{\partial W_{ij}}{\partial (x_{ij})} \tag{3.37}
\]
\[
\frac{d (v_i)}{dt} = \sum_{j=1}^{\infty} m_j \left( \frac{(\sigma_{ij})_i}{\rho_i^2} + \frac{(\sigma_{ij})_j}{\rho_j^2} + \Pi_{ij} \delta_{ij} \right) \frac{\partial W_j}{\partial (x_j)_i} \quad (3.38)
\]

\[
\frac{de_i}{dt} = -\frac{1}{2} \sum_{j=1}^{\infty} m_j \left( \frac{(\sigma_{ij})_i}{\rho_i^2} + \frac{(\sigma_{ij})_j}{\rho_j^2} + \Pi_{ij} \delta_{ij} \right) (v_j)_i \frac{\partial W_j}{\partial (x_j)_i} \quad (3.39)
\]

In Eq. (3.38) and Eq. (3.39), \( \Pi_{ij} \) represents the artificial pressure term described in Eq. (3.30).

The interpolation kernel named B-spline, which has been addressed in Eq. (2.4) is adopted as it is the most widely used in the SPH, such as Monaghan and Lattanzio (1985), Libersky et al. (1993) and Randles and Libersky (1996) and so on. This kernel interpolates to second order in smoothing length \( h \) and is always non-negative. The kernel also has a compact support of \( 2h \). This provides a clear limit on the number of neighbor particles. During each time step, the link-list method is employed to search the neighbor particles.

It is noted that the smoothing length \( h \) needs not be constant and can be a function of space and time as discussed in 3.1.5. Some calculations might be difficult to perform with SPH unless a variable smoothing length is used. For instance, in the simulations of explosions and hypervelocity impact of thin plates, \( h \) must increase in order to maintain adequate resolutions. However, it will also incur some inconveniences, for instance, \( W_j \neq W_j \), \( \frac{\partial W_j}{\partial (x_j)_i} \neq \frac{\partial W_j}{\partial (x_j)_j} \)

due to \( h_i \neq h_j \). In the present studies, the smoothing length keeps to be constant during the calculation.

Since each SPH particle carries a fixed mass, and if the number of particles is constant, the mass conservation is intrinsically satisfied. Monaghan (1992) considered that Eq. (3.37) has a minor drawback on not exactly retaining the consistency between mass, density and occupied area of the particle. Therefore, Eq. (3.18) is periodically applied to restore the density field, for instance, every 20 time steps.
To solve the tensile instability, the conservative smoothing method in Eq. (3.33) is adopted to smooth the density, the velocity and the energy fields in the simulations.

Although the particles can be set arbitrarily to represent a physical domain, it is clearly that the SPH interpolation can be more accurate if the particles are evenly distributed. Hence, in the current work, particles are packed in an evenly distributed manner. Firstly, the particle smoothing length is provided. Since the smoothing length can also be interpreted as the effective diameter of each particle, this value also defines the number of particles that can be applied to the physical domain. Next, the physical domain is filled by these evenly distributed particles. Only those particles whose centers are interior the boundaries are selected to represent the domain. The boundary particles are those located on the domain’s outer layer. Figure 3-3 shows the arrangement of the SPH particles in a square domain and a circular domain, respectively.

![Figure 3-3 Illustration of the arrangement of the SPH particles in a square domain (left) and a circular domain (right) in two-dimension.](image)

After these SPH particles are generated and their coordinates are determined, they will be assigned the material and initial conditions accordingly. In this manner, different materials and initial conditions can be applied to different regions of the particles.

As discussed in Chapter 2, the boundary condition in the SPH method has long been neglected. The commonly used approaches are the ghost particles method by Libersky et al. (1993) for the symmetrical surface boundary conditions and the general treatment of the boundary condition method by Randles and Li-
bersky (1996). However, it is still an open issue on how to properly process the boundary conditions in the SPH method. Since the SPH approximations in the current research are derived based on the collocation method, the boundary conditions can be applied directly on those boundary particles. Actually, such a method is also employed by the commercial software in the SPH solver, such as AUTODYN.

The stress-free boundary conditions can be approximately satisfied without special treatments on those boundary particles. This is simply because that, for those boundary particles, the missing neighbor interpolation particles act as if they were zeroed out in momentum kernel sums due to the zero stress or pressure components on those missing particles, which allows for the simple approximation on the stress-free boundaries.

3.1.8 Time integration approach and time step

Once the interaction terms have been computed, the evolution for each particle can be stepped forward in time by using a suitable integrator. Similar to other explicit computational methods, the discrete SPH approximation equations can be integrated with standard methods, such as the second-order accurate Leap-Frog, predictor-corrector, and Runge-Kutta schemes.

The Leap–Frog is the most frequently used algorithm for time integration in SPH, such as in Gingold and Monaghan (1977) and Libersky et al. (1993). The advantage of the Leap-Frog algorithm is its low memory storage required in the computation and the efficiency for one force evaluation each step. The particle velocities and positions are offset by a half time-step when integrating the equations of motion. At the end of the first time-step $t_0$, the change in density, energy, and velocity are used to advance the density, energy, and velocity at half a time step, while the particle positions are advanced in a full time step as
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\[ t = t_0 + \Delta t \]

\[ \rho_i^{(n, \frac{\Delta t}{2})} = \rho_i^{(n)} + \frac{\Delta t}{2} \cdot \dot{\rho}_i \]

\[ e_i^{(n)} = e_i^{(n)} + \frac{\Delta t}{2} \cdot \dot{e}_i \]

\[ \left( v_{\alpha} \right)_i^{(n, \frac{\Delta t}{2})} = \left( v_{\alpha} \right)_i^{(n)} + \frac{\Delta t}{2} \cdot \frac{d \left( v_{\alpha} \right)_i^{(n)}}{dt} \]

\[ \left( x_{\alpha} \right)_i^{(n, \frac{\Delta t}{2})} = \left( x_{\alpha} \right)_i^{(n)} + \Delta t \cdot \left( v_{\alpha} \right)_i^{(n)} \]  

(3.40)

As mentioned earlier, \( \alpha \) is used to denote the coordinate directions. \( \dot{\rho} \) and \( \dot{e} \) represent the density changing rate and the energy changing rate with the time for the particle.

In order to keep the calculations consistent at each subsequent time step, at the start of each subsequent time step, the density, energy, and velocity of each particle needs to be predicted at half a time step to coincide the position.

\[ \rho_i^{\left( \alpha \right)} = \rho_i^{\left( \frac{\Delta t}{2} \right)} + \frac{\Delta t}{2} \cdot \dot{\rho}_i^{\left( \alpha \right)} \]

\[ e_i^{\left( \alpha \right)} = e_i^{\left( \frac{\Delta t}{2} \right)} + \frac{\Delta t}{2} \cdot \dot{e}_i^{\left( \alpha \right)} \]

\[ \left( v_{\alpha} \right)_i^{\left( \alpha \right)} = \left( v_{\alpha} \right)_i^{\left( \frac{\Delta t}{2} \right)} + \frac{\Delta t}{2} \cdot \frac{d \left( v_{\alpha} \right)_i^{\left( \alpha \right)}}{dt} \]

(3.41)

At the end of the subsequent time step, the particle density, internal energy, stress, velocity, and position are advanced in the standard Leap–Frog scheme.

\[ t = t + \Delta t \]

\[ \rho_i^{\left( \frac{\Delta t}{2} \right)} = \rho_i^{\left( \frac{\Delta t}{2} \right)} + \frac{\Delta t}{2} \cdot \dot{\rho}_i^{\left( \alpha \right)} \]

\[ \left( \sigma_{\alpha\beta} \right)_i^{\left( \alpha \right)} = \left( \sigma_{\alpha\beta} \right)_i^{\left( \frac{\Delta t}{2} \right)} + \frac{\Delta t}{2} \cdot \dot{\sigma}_{\alpha\beta} \]

\[ e_i^{\left( \frac{\Delta t}{2} \right)} = e_i^{\left( \frac{\Delta t}{2} \right)} + \frac{\Delta t}{2} \cdot \dot{e}_i^{\left( \alpha \right)} \]

\[ \left( v_{\alpha} \right)_i^{\left( \alpha \right)} = \left( v_{\alpha} \right)_i^{\left( \frac{\Delta t}{2} \right)} + \frac{\Delta t}{2} \cdot \frac{d \left( v_{\alpha} \right)_i^{\left( \alpha \right)}}{dt} \]

\[ \left( x_{\alpha} \right)_i^{\left( \alpha \right)} = \left( x_{\alpha} \right)_i^{\left( \frac{\Delta t}{2} \right)} + \frac{\Delta t}{2} \cdot \left( v_{\alpha} \right)_i^{\left( \frac{\Delta t}{2} \right)} \]

(3.42)
In the above equation, $\dot{\sigma}^{\alpha\beta}$ represent the particle stress-changing rate with time.

The Leap-Frog scheme is conditional stable. As other explicit integral methods, its stability and accuracy can be guaranteed under the Courant-Friedrichs-Lewy (CFL) type condition. The time step adopted here is by Libersky et al. (1993) as,

$$\delta t \leq \text{Min} \left( \frac{\omega h_i}{c_i + v_i} \right)$$

(3.43)

where $c_i$ is the adiabatic sound speed for particle $i$, $v_i$ is the particle speed and $\omega$ is a constant factor around 0.3.

In order to mitigate the tensile instability, the conservative smoothing equation (3.33) will be performed in conjunction with Eq. (3.42) to smooth the density, the velocity and the energy fields once each of these quantities has been updated. The following sequence suggested by Randles and Libersky (1996) is adopted, as $\rho_i \rightarrow S_{sc}(\rho_i, \alpha_{cs}); (v_{\alpha})_i \rightarrow S_{sc}((v_{\alpha})_i, \alpha_{cs}); e_i \rightarrow S_{sc}(e_i, \alpha_{cs})$.

### 3.2 Elasto-plastic damage model for brittle material failure simulations

A non-linear elasto-plastic damage model has been developed. The model includes two surfaces to represent the intact and fractured strengths of the brittle material. It also has a damage model that represents the transitions of the material from an intact state to a fractured state. The strength criterion is based on an extension form of the Unified Twin Shear Strength Theory, including two hydrostatic pressure dependent medians representing the generalized tensile and compressive strength states, respectively.

#### 3.2.1 Generalized form of yield criterion based on the UTSS theory

The Twin Shear Strength (UTSS) theory was proposed by Yu and He (1991).
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The theory considers the maximum principal shear stress $\tau_{13}$ and intermediate principal shear stress $\tau_{12}$ (or $\tau_{23}$), and the influence of the normal stresses $\sigma_{13}$ and $\sigma_{12}$ (or $\sigma_{23}$) acting on the same section, respectively. The stresses acted on four faces of an octahedral stress element are shown in Figure 3-4.

These faces are perpendicular to each other. Among the three principal shear stresses, only two are independent because the maximum principal shear stress is the sum of the other two. The relationship between the principal shear stresses and their corresponding normal stresses in terms of principal stresses $\sigma_1$, $\sigma_2$ and $\sigma_3$ are

$$
\begin{align*}
\tau_{13} &= \frac{\sigma_1 - \sigma_3}{2}; \\
\tau_{12} &= \frac{\sigma_1 - \sigma_2}{2}; \\
\tau_{23} &= \frac{\sigma_2 - \sigma_1}{2} \\
\sigma_{13} &= \frac{\sigma_1 + \sigma_3}{2}; \\
\sigma_{12} &= \frac{\sigma_1 + \sigma_2}{2}; \\
\sigma_{23} &= \frac{\sigma_2 + \sigma_3}{2}
\end{align*}
$$

This theory assumes that the yielding or failure begins when the two larger principal shear stresses and the corresponding normal stresses meets the following formula,

$$
F = \tau_{13} + b\tau_{12} + \beta(\sigma_{13} + b\sigma_{12}) - c = 0 \text{ when } \tau_{12} + \beta\sigma_{12} \geq \tau_{23} + \beta\sigma_{23}
$$

$$
F = \tau_{13} + b\tau_{23} + \beta(\sigma_{13} + b\sigma_{23}) - c = 0 \text{ when } \tau_{12} + \beta\sigma_{12} < \tau_{23} + \beta\sigma_{23}
$$

in which $\beta$ is the coefficient to reflect the effect of the normal stresses which can be determined from experimental results of the uniaxial tensile strength $f_t$ and the uniaxial compressive strength $f_c$ by
\[
\beta = \frac{1 - \alpha}{1 + \alpha} ; \quad c = \frac{1 + b}{1 + \alpha} f_i
\]  

(3.46)

where \( \alpha \) is the ratio of \( f_i \) over \( f_c \). \( b \) is a weighting coefficient reflecting the relative effect of the intermediate principal shear stress and its corresponding normal stress. The value of \( b \) is within the range from 0 to 1 for any convex strength surface. When \( b \) approaches 0, the UTSS theory becomes an approximation of Mohr-Coulomb criterion. When \( b \) is 1, it becomes the Twin Shear Strength theory by Yu (1983). Therefore, a series of yield or failure criteria can be established when this value between 0 and 1.

The trajectories of the UTSS criterion in deviatoric plane with different \( b \) values are shown in Figure 3-5. The tensile and compressive meridians are two different straight lines similar to those of the Mohr-Coulomb criterion. The UTSS theory has a clear physical concept and simple mathematical formulae. In addition, by varying the weighting coefficient \( b \), a series of strength or yield criteria can be obtained which are suitable for different kind of materials.

Figure 3-5 Varieties of the Unified Strength Theory on the deviatoric plane (after Yu et al., 2002)
Reminiscent of the essence of the UTSS theory, its advantage is that it unifies the existing criteria by introducing a weighting coefficient $b$ in the mathematical expressions. It can be further extended to include different tensile and compressive meridians by adopting any form of expression of the hydrostatic stress in its formulae. As a result, it can be applied to various materials, the meridians and the shape functions of the deviatoric plane can be expressed separately. The expressions of tensile and compressive meridians are functions of the hydrostatic stress and can be determined by catering for the experimental results. For the shape function, the piecewise-linear formulation in line with the concept of the UTSS theory can give very successful approximation.

In the UTSS theory, when $b = 1$ it gives the upper limit of the convex shape function; when $b = 0$, it gives the lower limit convex shape function. A generalized multi-parameter unified yield criterion can be developed following the suggestions by Wang (1998) and Fan and Wang (2002).

Figure 3-6(a, b) shows the deviatoric planes when $b = 0$ and $b = 1$ in the UTSS theory. If the vectors of $r_t$ and $r_c$ on the deviatoric plane with respect to a certain hydrostatic pressure $p$ is determined, Figure 3-6 (a) gives the minimum (or inner) convex shape, while Figure 3-6 (b) gives the maximum (or outer) one of the failure surface on the deviatoric plane. Any failure criteria satisfying the convex requirement should lie in between the inner and outer shapes.
Since the triangle $ABD$ is similar to that of $ACE$ in Figure 3-6 (a), we can obtain
\[
\frac{BD}{CE} = \frac{AB}{AC}
\]
and
\[
BD = r \sin \theta \\
CE = r_c \sin 60^\circ \\
AB = r_i - r \cos \theta \\
AC = r_i - r_c \cos 60^\circ
\]

Substitute Eq.(3.48) into Eq.(3.47) and rewrite Eq. (3.47), it can be derived that
\[
r = \frac{rr_c \sin 60^\circ}{r \sin \theta + r_c \sin (60^\circ - \theta)} \quad \text{when } b = 0
\]

Similarly we can derive the formula for \( b = 1 \) as shown in Figure 3-6(b)
\[
r = \begin{cases} 
\frac{r}{\cos \theta} & \text{when } 0^\circ \leq \theta \leq \theta_b \\
\frac{r_c}{\cos (60^\circ - \theta)} & \text{when } \theta_b \leq \theta \leq 60^\circ
\end{cases} \quad \text{when } b = 1
\]

The value of $\theta_b$ which corresponds to the corners of the outer shape in Figure 3-6 (b) can be obtained by equating the two vector lengths of Eq. (3.50) as
\[
\theta_b = \arctan \left[ \frac{1}{\sqrt{3}} \left( \frac{2r_c}{r_i} - 1 \right) \right]
\]

When $0 < b < 1$, the formulae determined by a linear interpolation between those of $b = 0$ and $b = 1$ as follows,
\[
r = \begin{cases} 
\frac{rr_c \sin 60^\circ}{r \sin \theta + r_c \sin (60^\circ - \theta)} \left(1 - b\right) + b \frac{r}{\cos \theta} & \text{when } 0^\circ \leq \theta \leq \theta_b \\
\frac{rr_c \sin 60^\circ}{r \sin \theta + r_c \sin (60^\circ - \theta)} \left(1 - b\right) + b \frac{r_c}{\cos (60^\circ - \theta)} & \text{when } \theta_b \leq \theta \leq 60^\circ
\end{cases}
\]
In the above equations, \( \theta = \frac{1}{3} \arccos \left( \frac{3\sqrt{3}J_3}{2(\sqrt{J_2})^3} \right) \).

The convex shape in the deviatoric plane has the threefold symmetry. If its shape in the range of 60° is given, the full expression can be obtained. The value of \( b \) is a material parameter which can be obtained by fitting experimental results of the material under consideration. Analysis of the static true triaxial test data from Yu et al. (2002) suggest that, for rock materials, such as dolomite, marble, granite and trachyte, \( b \) can take a value between 0.5 and 1.0. In the current model, \( b \) takes 0.6 unless it is specifically stated.

In the following section, the UTSS theory with the above simplification of the deviatoric plane model is adopted to simulate rock failure. The two meridians, for instance, the change of \( r_i \) and \( r_c \) with respect to the hydrostatic pressure are determined by analyzing the uniaxial and triaxial compression test results.

### 3.2.2 Empirical strength meridians for rock material and the damage model

The strength meridians include the intact, the damaged and the fracture surfaces and are schematically presented in Figure 3-7 in the \( p^* - \sigma^* \) plane.

![Figure 3-7](image)

Figure 3-7 Illustration of the strength surfaces for the intact, the damaged and the fractured materials.

The damage strength surfaces comprise a series surfaces varying between those
with respect to the fractured (totally damaged) material and the intact (no damage) material. Inspired by the strength model developed by Holmquist et al. (2001), the normalized intact strength envelope is defined by

$$\sigma_i^* = A \left(1 - p^*\right)^N \quad (3.53)$$

and the normalized fractured strength envelope is given by

$$\sigma_f^* = B \left(-p^*\right)^M \quad (3.54)$$

The material constants are $A$, $N$, $B$, $M$. In the equations, the normalized effective stresses ($\sigma^*$, $\sigma_i^*$, $\sigma_f^*$) have the general form

$$\sigma^* = \frac{\bar{\sigma}}{\sigma_c} \quad (3.55)$$

where $\bar{\sigma}$ is the actual effective stress; $\sigma_c$ is the uniaxial compression strength; $\sigma_i^*$ is the normalized intact strength and $\sigma_f^*$ is the normalized fracture strength. The general form of the effective stress is defined as

$$\bar{\sigma} = \sqrt{\frac{1}{2} \left[ \left(\sigma_x - \sigma_y\right)^2 + \left(\sigma_y - \sigma_z\right)^2 + \left(\sigma_z - \sigma_x\right)^2 + 6 \left(\tau_{xy}^2 + \tau_{xz}^2 + \tau_{yz}^2\right) \right]} = \sqrt{3J_2} \quad (3.56)$$

where $\sigma_x$, $\sigma_y$, and $\sigma_z$ are the three normal stresses, and $\tau_{xy}$, $\tau_{xz}$, and $\tau_{yz}$ are the three shear stresses. The normalized pressure is $p^* = \frac{p}{p_T}$, where $p$ is the actual pressure (positive in tension) and $p_T$ is the maximum tensile hydrostatic pressure the material can withstand. Considering the brittle failure may happen at a lower volumetric tensile pressure such as the uniaxial tensile condition, the value is taken as $p_T = \frac{\sigma_i}{3}$, where $\sigma_i$ is the uniaxial tensile strength. Surely, this value is a cutoff one compared with the maximum hydrostatic strength in the triaxial tensile condition.

The normalize damaged strength $\sigma_D^*$ is defined as
\[
\sigma_D^* = \sigma_i^* - D(\sigma_i^* - \sigma_j^*) \tag{3.57}
\]

where \( D \) is the scalar damage variable \( (0 \leq D \leq 1.0) \) and is defined as

\[
D = \sum \frac{\Delta \varepsilon_p}{\bar{\varepsilon}_p} \tag{3.58}
\]

where \( \Delta \varepsilon_p \) is the effective plastic strain during a cycle of integration and \( \bar{\varepsilon}_p \) is the effective plastic strain to fracture under a constant pressure \( p \). The specific expression is

\[
\bar{\varepsilon}_p = D_1(1 - p^*)^b_1 \tag{3.59}
\]

where \( D_1 \) and \( D_2 \) are two damage constants. The schematic representation of Eq. (3.59) is depicted in Figure 3-8.

Figure 3-8 Illustration of the effective plastic strain to fracture diagram in the damage model with the normalized pressure

The material cannot undertake any plastic strain at \( p^* = 1.0 \). The incremental effective plastic strain is defined as

\[
\Delta \varepsilon_p = \int \sqrt{\frac{2}{3} \left( \varepsilon_{\alpha\beta} : \varepsilon_{\alpha\beta} \right)_p} \tag{3.60}
\]

This model has the advantage to properly account for the material strength degradation from the intact state to the damaged state by employing a scalar damage variable induced by the effective plastic strain. A pressure-cutoff failure criterion is also applied to reflect the volumetric tensile failure. Thus, it exhibits
the capacity to simulate both tension induced brittle cracks and compression-shear dominated crushing zone failure.

### 3.2.3 Determination of the parameters in the two strength meridians and the damage model for the granitic rock

Parameters in the two strength meridians and the damage model can be determined by curve-fitting from experimental results. We adopt data from the static uniaxial and triaxial compressive experiment results by Zhao (1999) on the Singapore granite samples. The axial stress over axial strain curves are shown in Figure 3-9.

![Figure 3-9 Axial stress vs. axial strain under various confining pressure (after Zhao, 1999)](image)

Table 3-1 gives the test data from the uniaxial tensile test, uniaxial compression test and confined triaxial compression test, where the uniaxial compressive strength $\sigma_c$ is 157 MPa, and the tensile strength $\sigma_t$ is 16.1 MPa. These data are used to determine the parameters of the compressive strength meridian and damage model. The normalized pressure, normalized intact stress and effective plastic strain to fracture are calculated using the equations given in the previous section. The mean pressure is given as

$$p = \frac{1}{3} (\sigma_1 + \sigma_2 + \sigma_3)$$  \hspace{1cm} (3.61)
The compressive meridian for the intact material and the damage model can be regressed from the existing scattered experiment data points given in the Table 3-1. Parameters \( A \) and \( N \) are obtained for the regressed compressive meridian curve as 0.1334 and 0.8536, respectively. Similarly, parameters for the damage model can be determined by \( D_1 = 1.748 \times 10^{-4} \) and \( D_2 = 0.9327 \).

For the tensile meridian curve for the intact material, we assume its shape is similar to the compressive one. By determining the ratio of the tensile radius \( r_t \) to the compressive \( r_c \) at the same pressure, the tensile meridian can be obtained from the compressive one as illustrated in Figure 3-10.

According to the UTSS theory, the equal biaxial compression result that represents the generalized tensile stress state can be used to determine the ratio \( r_c \). Take biaxial compression strength as 1.15 times of the uniaxial compressive strength, its coordinate on the tensile meridian curve can be expressed by the normalized mean pressure (\( p^* \)) and normalized effective stress (\( \bar{\sigma}^* \)) as point \( P (-21.0, 1.15) \) shown in the figure. The corresponding location of point \( P \)

<table>
<thead>
<tr>
<th>Experimental test</th>
<th>( p ) (MPa)</th>
<th>( p^* )</th>
<th>( \sigma^* )</th>
<th>( \bar{\sigma}^* ) (1×10^{-3})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Uniaxial tension</td>
<td>5.367</td>
<td>1.00</td>
<td>0.0</td>
<td>0</td>
</tr>
<tr>
<td>Uniaxial compression</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>sample 1</td>
<td>-49.167</td>
<td>-9.16</td>
<td>0.9395</td>
<td>1.1</td>
</tr>
<tr>
<td>sample 2</td>
<td>-55.33</td>
<td>-10.30</td>
<td>1.0573</td>
<td>1.2</td>
</tr>
<tr>
<td>Triaxial compression</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>sample 1</td>
<td>-110.333</td>
<td>-20.56</td>
<td>1.7992</td>
<td>3.01</td>
</tr>
<tr>
<td>sample 2</td>
<td>-120.750</td>
<td>-22.50</td>
<td>2.0191</td>
<td>3.34</td>
</tr>
<tr>
<td>sample 3</td>
<td>-158.167</td>
<td>-29.50</td>
<td>2.4490</td>
<td>4.70</td>
</tr>
<tr>
<td>sample 4</td>
<td>-203.333</td>
<td>-37.90</td>
<td>3.0255</td>
<td>5.03</td>
</tr>
<tr>
<td>sample 5</td>
<td>-247.135</td>
<td>-46.05</td>
<td>3.5732</td>
<td>6.00</td>
</tr>
</tbody>
</table>
on the compressive meridian with the same pressure is \((-21.0, 1.972)\). Therefore, \(r_{tc}\) can be calculated as

\[
r_{tc} = \frac{1.15}{1.972} = 0.5831
\]  

(3.62)

Figure 3-10 Determination of the tensile meridian from the compressive one.

Figure 3-11 The regressed compressive strength curves for intact and fractured materials, tensile strength curves for intact and fractured materials, and experimental data from granite samples compression tests. For the fractured strength curve, it is assumed that the damaged rock has a residual strength of one third of the intact one for both meridians. The regressed
intact compressive strength curve, fractured strength curve, intact tensile strength curve and fractured tensile strength curve are shown in the Figure 3-11. The effective plastic strain to fracture curve for the damage model is plotted in Figure 3-12. The parameters are listed in Table 3-2.

![Figure 3-12 The regressed effective plastic strain to fracture and the experimental data](image-url)
Table 3-2 Parameter values in the compressive and tensile strength meridians and the damage model for the granitic rock

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Symbol</th>
<th>Unit</th>
<th>Granite</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td>( \rho )</td>
<td>( \text{kg/m}^3 )</td>
<td>2670</td>
</tr>
<tr>
<td>Young’s modulus</td>
<td>( E )</td>
<td>( \text{GPa} )</td>
<td>75.20</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>( v )</td>
<td>-</td>
<td>0.2</td>
</tr>
<tr>
<td>Bulk modulus</td>
<td>( K )</td>
<td>( \text{GPa} )</td>
<td>41.78</td>
</tr>
<tr>
<td>Shear modulus</td>
<td>( G )</td>
<td>( \text{GPa} )</td>
<td>31.33</td>
</tr>
<tr>
<td>Tensile strength of intact rock</td>
<td>( \sigma_t )</td>
<td>( \text{MPa} )</td>
<td>16.1</td>
</tr>
<tr>
<td>Uniaxial compressive strength of intact rock</td>
<td>( \sigma_c )</td>
<td>( \text{MPa} )</td>
<td>157.0</td>
</tr>
<tr>
<td>Hydrostatic tensile pressure limit</td>
<td>( p_T )</td>
<td>( \text{MPa} )</td>
<td>5.367</td>
</tr>
<tr>
<td>Normalized strength parameter for compressive</td>
<td>( A )</td>
<td>-</td>
<td>0.1334</td>
</tr>
<tr>
<td>meridian for the intact granite</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Normalized strength parameter for compressive</td>
<td>( B )</td>
<td>-</td>
<td>0.04446</td>
</tr>
<tr>
<td>meridian for the fractured granite</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ratio of the tensile meridian radius to the</td>
<td>( r_w )</td>
<td>-</td>
<td>0.5831</td>
</tr>
<tr>
<td>compressive meridian radius</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Strength parameter for the intact material</td>
<td>( N )</td>
<td>-</td>
<td>0.8536</td>
</tr>
<tr>
<td>(exponent)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Strength parameter for the fractured material</td>
<td>( M )</td>
<td>-</td>
<td>0.8536</td>
</tr>
<tr>
<td>(exponent)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Parameter for damage model</td>
<td>( D_1 )</td>
<td>-</td>
<td>( 1.748 \times 10^{-4} )</td>
</tr>
<tr>
<td>Parameter for damage model (exponent)</td>
<td>( D_2 )</td>
<td>-</td>
<td>0.9326</td>
</tr>
</tbody>
</table>

In the \( p^* - \sigma^* \) plane, the intact and fractured tensile meridians are,
and the intact and fractured compressive meridians are,

\[
\sigma_i^* = 0.07845 \left(1 - p^*\right)^{0.8536}
\]
\[
\sigma_f^* = 0.02615 \left(-p^*\right)^{0.8536}
\]

The effective plastic strain to fracture is

\[
\varepsilon_p^f = 1.748 \times 10^{-4} \left(1 - p^*\right)^{0.9326}
\]

In the following, we derive the expressions of the meridians under the Haigh-Westergaard coordinate system \((\xi, r, \theta)\) in the deviatoric plane to be consistent with the derived yield criterion in section 3.2.1.

Figure 3-13 illustrate a stress point \(P(\sigma_1, \sigma_2, \sigma_3)\) under the Haigh-Westergaard coordinate system \((\xi, r, \theta)\) in the deviatoric plane. Hence, stress point \(P\) can be expressed as,

\[
\xi = \frac{1}{\sqrt{3}} (\sigma_1 + \sigma_2 + \sigma_3) = \sqrt{3} p
\]

\[
r = \sqrt{\frac{1}{3} \left[ (\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2 \right]} = \sqrt{2J_2}
\]

\[
\theta = \arccos \left( \frac{2\sigma_1 - \sigma_2 - \sigma_3}{2\sqrt{3J_2}} \right)
\]

\(\sigma^*\) and \(p^*\) can be expressed as

\[
\sigma^* = \frac{\sqrt{3J_2}}{\sigma_c} = \frac{3}{2} \frac{r}{\sigma_c}
\]
\[
p^* = \frac{3p}{\sigma_i} = \frac{\sqrt{3}}{\sigma_i} \xi
\]
Figure 3-13 Illustration of the stress point \( P(\sigma_1, \sigma_2, \sigma_3) \) under the Haigh-Westergaard coordinate system \( (\zeta, r, \theta) \) in the deviatoric plane.

Then the derived tensile meridian \( (r_t) \) and compressive meridian \( (r_c) \) with a damage value \( D \) can be expressed as

\[
\begin{align*}
    r_t &= \sqrt{\frac{2}{3}} \sigma_c \left( 0.07845 \left( 1 - \frac{\sqrt{3} \zeta}{\sigma_t} \right)^{0.8536} - D \right) \\
    r_c &= \sqrt{\frac{2}{3}} \sigma_c \left( 0.1334 \left( 1 - \frac{\sqrt{3} \zeta}{\sigma_t} \right)^{0.8536} - D \right)
\end{align*}
\]

(3.68)

By combining Eq. (3.68) with Eq. (3.52), one can get explicit expression of the non-linear elasto-plastic damage model in the deviatoric plane.

### 3.2.4 Elasto-plastic strain-stress relationship

The elastic constitutive model based on the Hooke’s Law can be expressed as,

\[
p = K \epsilon_{\gamma \gamma} \delta_{\alpha \beta} \\
S_{\alpha \beta} = 2G \left( \epsilon_{\alpha \beta} - \frac{1}{3} \epsilon_{\gamma \gamma} \delta_{\alpha \beta} \right)
\]

(3.69)

where, \( \delta_{\alpha \beta} = \begin{cases} 1, & \alpha = \beta \\ 0, & \alpha \neq \beta \end{cases} \); \( K \) and \( G \) are the bulk modulus and shear modulus,
respectively.

Since the stress rate is proportional to the strain rate, based on the SPH approximation equations of strain rate, they can be derived as

$$\frac{dp}{dt} = K \dot{\varepsilon}_{\alpha\beta}$$ (3.70)

$$\frac{dS_{ap\beta}}{dt} = 2G \left( \dot{\varepsilon}_{ap\beta} - \frac{1}{3} \delta_{ap\beta} \dot{\varepsilon}_{\gamma\gamma} \right)$$

$$= -G \cdot \sum_{j=1}^{N} \frac{m_j}{\rho_j} \left( (v_\alpha)_j \frac{\partial W_{ij}}{\partial (x_\beta)_j} + (v_\beta)_j \frac{\partial W_{ij}}{\partial (x_\alpha)_j} \right)$$

$$\cdot \frac{2}{3} (v_\gamma)_j \frac{\partial W_{ij}}{\partial (x_\gamma)_j} \delta_{ap\beta}$$ (3.71)

The stress can be obtained by an explicit time integration using the above equations.

The yield criterion determines the stress level at which plastic deformation begins. Based on the derived general form of the UTSS strength criterion in conjunctions with the tensile and compressive meridians, the plastic loading function can be expressed as,

$$f(\sigma_{ap\beta}, \theta) = r - \sqrt{2J_2} = 0$$ (3.72)

where \( r \) is defined in Eq. (3.52). In the elastic region, the stress-strain relation can be determined by Eq. (3.69). After the initial yielding, the material behavior will be partially elastic and be partially plastic. The strain increment are assumed to be composed by elastic and plastic components,

$$d\varepsilon_{ap\beta} = (d\varepsilon_{ap\beta})_e + (d\varepsilon_{ap\beta})_p$$ (3.73)

The method to calculate the plastic strain is based on the classic plastic theory. Assuming that yielding is independent of any hydrostatic stress is valid, \((d\varepsilon_{\gamma\gamma})_p = 0\), the effective deviatoric plastic strain \(\varepsilon_p\) is defined,

$$\varepsilon_p = \int_0^{\varepsilon_p} d\left(\varepsilon_p\right)_p : d\left(\varepsilon_p\right)_p = \sqrt{\frac{2}{3} \left( \varepsilon_{ap\beta} \right)_p : \left( \varepsilon_{ap\beta} \right)_p}$$ (3.74)
where, \( d\left(\tau\right)_p \) denotes the effective deviatoric plastic strain rate. To determine the direction of the plastic strain rate, the non-associated flow rule is adopted. The potential function is defined as

\[
Q(\sigma) = \sqrt{J_2}
\]  
(3.75)

where \( J_2 = \frac{1}{2} \left( S_{\alpha\beta} : S_{\alpha\beta} \right) \) is the second stress invariants in the terms of deviatoric stress. Assume that the plastic strain increment is proportional to the stress gradient of a plastic potential \( Q \),

\[
\left( \varepsilon_{\alpha\beta} \right)_p = d\lambda \frac{\partial Q}{\partial \sigma_{\alpha\beta}}
\]  
(3.76)

d\( \lambda \) is the corresponding plastic multiplier. By using Eq. (3.74), (3.75) and (3.76), we can get

\[
\left( \varepsilon_{\alpha\beta} \right)_p = \frac{d\lambda}{\sqrt{3}}.
\]  
(3.77)

Therefore, the Eq. (3.73) becomes

\[
d\varepsilon_{\alpha\beta} = [D]_e^{-1} d\sigma_{\alpha\beta} + d\lambda \frac{\partial Q}{\partial \sigma_{\alpha\beta}}
\]  
(3.78)

in which \([D]_e\) is the matrix of elastic constants. Based on the general isotropic hardening rule, the plastic multiplier \( d\lambda \) can be derived as

\[
d\lambda = \frac{1}{A + \{a\}^T [D]_e \{a\}} [D]_e d\varepsilon_{\alpha\beta}
\]  
(3.79)

where, \( \{a\}^T = \frac{\partial f}{\partial \sigma_{\alpha\beta}} \), \( \{a\}^* = \frac{\partial Q}{\partial \sigma_{\alpha\beta}} \), and \( A \) is a parameter related to the hardening conditions. For the perfectly plastic situation, \( A = 0 \).

Combining Eq. (3.78) and (3.79), the complete elasto-plastic incremental stress-strain relation can be obtained as,

\[
d\sigma_{\alpha\beta} = [D]_{\alpha\beta} d\varepsilon_{\alpha\beta}
\]  
(3.80)
in which \( [D]_{ap} = [D]_a - \frac{[D]_a \{a^*\} \{a^T\} [D]_a}{A + \{a^T\} [D]_a \{a^*\}} \).

In the following, we will determine the flow vector \( \{a\} \). The component of \( \{a\} \) can be derived by,

\[
\frac{\partial f}{\partial \sigma_{ab}} = \frac{\partial r}{\partial \xi} \frac{\partial \xi}{\partial \sigma_{ab}} + \frac{\partial r}{\partial \theta} \frac{\partial \theta}{\partial \sigma_{ab}} + \frac{\partial f}{\partial \rho} \frac{\partial \rho}{\partial \sigma_{ab}} - \frac{\partial \left( \sqrt{2} J_2 \right)}{\partial \sigma_{ab}} \quad (3.81)
\]

where, \((\xi, \rho, \theta)\) is the Haigh-Westergaard coordinate system. \( \{a\} \) can be expressed as,

\[
\{a\} = \{a_1, a_2, a_3\} = C_1 \{a_1\} + C_2 \{a_2\} + C_3 \{a_3\} \quad (3.82)
\]

where,

\[
\{a_1^T\} = \frac{\partial \xi}{\partial \sigma_{ab}} = \frac{\partial \xi}{\partial \sigma_{ab}} \frac{\partial I_1}{\partial \sigma_{ab}} = \frac{1}{\sqrt{3}} \frac{\partial I_1}{\partial \sigma_{ab}}
\]

\[
\{a_2\} = \frac{\partial \rho}{\partial \sigma_{ab}} = \frac{\partial \rho}{\partial \sqrt{J_2}} \frac{\partial J_2}{\partial \sigma_{ab}} = \sqrt{2} \frac{\partial J_2}{\partial \sigma_{ab}}
\]

\[
\{a_3^T\} = \frac{\partial \theta}{\partial \sigma_{ab}} = \frac{\partial \theta}{\partial J_3} \frac{\partial J_3}{\partial \sigma_{ab}} = -\frac{\sqrt{3}}{2 \sqrt{(J_3)^2 \sin^2 \theta}} \frac{\partial J_3}{\partial \sigma_{ab}} + \frac{3 \sqrt{3}}{2 (J_2)^2 \sin^2 \theta} \frac{\partial \sqrt{J_2}}{\partial \sigma_{ab}}
\]

In Eq. (3.83),

\[
\frac{\partial I_1}{\partial \sigma_{ab}} = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 \end{bmatrix}
\]

\[
\frac{\partial \sqrt{J_2}}{\partial \sigma_{ab}} = \frac{1}{2 \sqrt{J_2}} \begin{bmatrix} (\sigma_{11}) & (\sigma_{22}) & (\sigma_{33}) & 2\sigma_{12} & 2\sigma_{13} & 2\sigma_{23} \end{bmatrix}
\]

\[
\frac{\partial J_3}{\partial \sigma_{ab}} = \frac{1}{2 \sqrt{J_2}} \begin{bmatrix} (\sigma_{22})(\sigma_{33}) - \sigma_{23}\sigma_{32} + \frac{J_3}{3} & (\sigma_{11})(\sigma_{33}) - \sigma_{13}\sigma_{31} + \frac{J_3}{3} & (\sigma_{11})(\sigma_{22}) - \sigma_{12}\sigma_{21} + \frac{J_3}{3} & 2 \left[ \sigma_{13}\sigma_{21} - (\sigma_{11})(\sigma_{23}) \right] & 2 \left[ \sigma_{23}\sigma_{12} - (\sigma_{22})(\sigma_{13}) \right] \end{bmatrix}
\]
The expression for \( C_1 \) can be expressed as

\[
C_1 = \frac{\partial r}{\partial \xi} = \frac{\partial r}{\partial r} \cdot \frac{\partial r}{\partial \xi} + \frac{\partial f}{\partial \xi} \cdot \frac{\partial r}{\partial \xi}
\]  
(3.85)

where

\[
\frac{\partial f}{\partial r} = \frac{\partial r}{\partial r}
\]  
(3.86)

Similarly,

\[
\frac{\partial f}{\partial \theta} = \frac{\partial r}{\partial \theta}
\]  
(3.88)

where,

\[
\frac{\partial r}{\partial r} = \frac{r^2 \sin 60^\circ \sin(60^\circ - \theta)}{\left[ r \sin \theta + r_s \sin(60^\circ - \theta) \right]^2} (1-b) + \frac{b}{\cos \theta} \quad \text{when } 0^\circ \leq \theta \leq \theta_b
\]  
(3.89)

\[
\frac{\partial r}{\partial \theta} = \frac{r^2 \sin 60^\circ \sin \theta}{\left[ r \sin \theta + r_s \sin(60^\circ - \theta) \right]^2} (1-b) + \frac{b}{\cos(60^\circ - \theta)} \quad \text{when } \theta_b \leq \theta \leq 60^\circ
\]  
(3.90)

\[
C_2 = \frac{\partial r}{\partial \rho} = 1
\]  
(3.90)

\[
C_3 = \frac{\partial r}{\partial \theta}
\]  
(3.91)

where,
Based on Eq. (3.68), \( \frac{\partial r}{\partial \xi} \) and \( \frac{\partial r}{\partial \eta} \) can be expressed as

\[
\frac{\partial r}{\partial \xi} = -\frac{2}{3} \frac{\sigma_c}{\sigma_t} \left\{ 0.1334 \left( 1 - \frac{\sqrt{3} \xi}{\sigma_t} \right)^{-0.1464} \right. \\
\left. - D \left[ 0.1334 \left( 1 - \frac{\sqrt{3} \xi}{\sigma_t} \right)^{-0.1464} - 0.04446 \left( -\frac{\sqrt{3} \xi}{\sigma_t} \right)^{-0.1464} \right] \right\}
\]

(3.93)

\[
\frac{\partial r}{\partial \eta} = -\frac{2}{3} \frac{\sigma_c}{\sigma_t} \left\{ 0.07845 \left( 1 - \frac{\sqrt{3} \xi}{\sigma_t} \right)^{-0.1464} \right. \\
\left. - D \left[ 0.07845 \left( 1 - \frac{\sqrt{3} \xi}{\sigma_t} \right)^{-0.1464} - 0.02615 \left( -\frac{\sqrt{3} \xi}{\sigma_t} \right)^{-0.1464} \right] \right\}
\]

(3.94)

Based on the above equations, one can obtain the flow vector \( \{ a \} \). By assuming the perfectly plastic situation where \( A = 0 \), it can be determined the complete expression of \( d\lambda \) and \( [D_{sp}] \). The effective plastic strain can be obtained by Eq. (3.76). It is noted that, the flow vector is not uniquely defined at the demarcation points in the yield surface. It occurs at \( \theta = 0^\circ, \theta = \theta_b \) and \( \theta = 60^\circ \). The corresponding points are \( A \), \( B \) and \( C \) as shown in Figure 3-14. Numerical difficulty will be encountered as the stress state approaches these points.
Figure 3-14 Illustration of the flow vector determination on the singular corner points

In the program, the matter is dealt with by following the approach by Nayak and Zienkiewicz (1972). If the stress state is within those singular points then \( \{ a \} \) is evaluated on either side of the singularity and an average value assumed.

The procedure corresponds to a rounding off the singularity corners.

### 3.2.5 Stress integration

Numerical implementation of the model requires integrating the rate form of the constitutive relations in the finite time step \( \delta t^{(n+1)} = t^{(n+1)} - t^{(n)} \). The procedure can be regarded as strain driven in a sense that the total strain vector \( \varepsilon^{(n)} \), the plastic strain vector \( (\varepsilon_p)^{(n)} \), the damage \( D^{(n)} \) and the internal variables are known at time \( t^{(n)} \), and that the finite incremental strain vector \( \Delta \varepsilon^{(n+1)} \) in the current time \( t^{(n+1)} \). The objective is to determine the unknown internal state variables such as \( \sigma^{(n+1)} \), \( (\varepsilon_p)^{(n+1)} \) and \( D^{(n+1)} \) at time \( t^{(n+1)} \).

To make it more clear, Figure 3-15 and Figure 3-16 give the schematic representations of the initial yield surface \( (D = 0) \), the damaged surface \( (0 < D < 1) \) and the fractured yield surface \( (D = 1) \) in the \( p^* - \sigma^* \) stress plane and the deviatoric stress planes.
Figure 3-15 Illustration of the yield surfaces for initial, damaged and fractured materials, respectively, in the $p^* - \sigma^*$ plane.

Initially, the stress state is under the elastic and governed by the Hooke's law without damage until it meets the initial yield surface. After that, the stress state reaches the plastic region. With the development of the plastic strain, damage occurs. Then the stress state is determined by the corresponding yield surface for damaged material. With the development of the plastic strains, the damage increases and the stresses are subsequently updated. If the accumulated damage equals to one, then the stress state will be finally controlled by the fractured yield surface since the damage is irreversible.
After the initial yield, both plasticity and damage progresses may take place. The damaged trail stress and plastic correction are both determined by solving a simultaneous system of non-linear equations in terms of the plastic multiplier $\Delta \lambda^{(n+1)}$ and the damage increment $\Delta D^{(n+1)}$. Figure 3-17 illustrates such a process under the one dimension.

**Figure 3-17** Schematic representation of stress integral process in one dimension.

At time $t^{(n+1)}$, the strain is updated from $\varepsilon^{(n)}$ to $\varepsilon^{(n+1)}$ with a finite incremental strain $\Delta \varepsilon$. The stress tensor is updated to the trial stress $(\sigma_{(i)})_{\text{trial}}^{(n+1)}$ at $A_{(i)}$ by means of the damaged stiffness, 

$$
(\sigma_{(i)})_{\text{trial}}^{(n+1)} = \sigma^{(n)} + (1 - D^{(n)}) D_{c} \Delta \varepsilon^{(n+1)}
$$

(3.95)

The corresponding trail plastic strain $(\varepsilon_{(i)})_{p}^{(n+1)}$ can be determined by unloading the trial stress from $A_{(i)}$ to $B_{(i)}$ with the initial stiffness matrix $D_{c}$. Then the damage is evaluated with the new plastic strain $(\varepsilon_{(i)})_{p}^{(n+1)}$. Hence the yield sur-
face for the damaged material is updated and the stress is adjusted to $A_{(2)}$ with the new trial stress $(\sigma_{(2)})_{\text{trial}}^{(n+1)}$. Unloading the stress from $A_{(2)}$ to $B_{(2)}$, one can obtain the trail plastic strain $(\varepsilon_{(2)}^p)^{(n+1)}$. If $(\varepsilon_{(2)}^p)^{(n+1)} > (\varepsilon_{(1)}^p)^{(n+1)}$, the damage increases and the new yield surface is determined. So is the new trail stress. Repeat the above steps to $m^{th}$ step until the updated trail plastic strain converges.

Finally, the stress can reach the point $A_{(m)}$ and get the updated state variables such as $(\varepsilon_p)^{(n+1)}$, $D^{(n+1)}$ and $\sigma^{(n+1)}$ at time $t^{(n+1)}$.

A brief summary of the algorithm used in the implementation is provided in Table 3-3.

<table>
<thead>
<tr>
<th>Step</th>
<th>Algorithm</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Calculate the trial elastic stresses by using the Eq. (3.95)</td>
</tr>
<tr>
<td>2</td>
<td>Check for yielding by using the Eq. (3.72).</td>
</tr>
<tr>
<td>3</td>
<td>If yield, determine the $(\varepsilon_p)^{(n+1)}$ and $D^{(n+1)}$ iteratively until convergence.</td>
</tr>
<tr>
<td>4</td>
<td>Return the stress to the current yield surface by using Eq. (3.80)</td>
</tr>
<tr>
<td>5</td>
<td>Go to 1 for the next time step</td>
</tr>
<tr>
<td>6</td>
<td>If not yield, update the stress using the Hooke’s law of Eq. (3.69) and go to 1 for the next time step.</td>
</tr>
</tbody>
</table>

3.3 Statistical material microstructure heterogeneity modeling method

3.3.1 Weibull distribution and material microstructure heterogeneity

The best approach to model the material heterogeneity is to obtain the complete information on its compositions and microstructures. However, it is unrealistic. Based on the literature review, the statistical method is widely applied to model
the material microstructure heterogeneity. Therefore, the Weibull distribution proposed by Weibull (1951) is selected to characterize the material heterogeneity for it can describe the experimental data well for material’s microstructures.

The Weibull distribution can be expressed using two parameters as,

$$ f(T) = \frac{\beta}{\mu} \left( \frac{T}{\mu} \right)^{\beta-1} e^{-\left( \frac{T}{\mu} \right)^{\beta}} $$

where $\mu$ is the scale parameter of the distribution of $T$, $\beta$ is the shape parameter describing the scatter of $T$. The mathematical expectation and dispersion of the two-parameter Weibull distribution are,

$$ E(T) = \mu \cdot \Gamma \left( 1 + \frac{1}{\beta} \right) $$

and,

$$ D(T) = \mu^2 \left[ \Gamma \left( 1 + \frac{2}{\beta} \right) - \Gamma^2 \left( 1 + \frac{1}{\beta} \right) \right] $$

respectively, where $\Gamma$ is the gamma function.

Figure 3-18 shows the relationship between the scaled mathematical expectation and the dispersion in terms of the shape parameter $\beta$. 
Figure 3-18 Scaled mathematical expectation (top) and dispersion (bottom) of the Weibull distribution with shape parameter.

As can be seen from the Figure 3-18, when \( \beta \) increases, the scaled mathematical expectation will gradually approach 1. As \( \beta \) trends to the infinity, the mathematical dispersion will be gradually close to zero. Therefore, \( \beta \) can be considered as the homogeneous index to describe the degree of heterogeneity for materials. The scale parameter \( \mu \) can be regarded as the seed parameter.

Figure 3-19 and Figure 3-20 show the normalized Weibull distributions with the typical homogeneous index \( \beta \) ranging from 1 to 10 for the same seed \( \mu = 1.0 \).

Figure 3-19 Probability density for several typical homogeneous indices of the Weibull distribution.

As can be seen, with the increasing homogeneous index value, the generated Weibull distribution data are more concentrated around the seed value. Hence,
the material is more homogenous. Even for the same $\beta$ and $\mu$, the stochastically generated Weibull distributions may be different from one another. Such spatial variations reflect the disorder of the microstructures with the same degree of heterogeneity.

![Figure 3-20 Cumulative distribution for homogeneous indices of the Weibull distribution](image)

### 3.3.2 Statistical heterogeneity model implementation

Usually the disorder of the probability distribution in physical space can be achieved by the Monte Carlo method. One simple method is to generate a series of random data which have a uniform distribution between 0 and 1. Because the Weibull distribution is non-monotone, the integral distribution function is derived as follows,

$$Q(T) = \int_0^T \varphi(x)dx = 1 - e^{-\left(\frac{T}{\eta}\right)^{\beta}}$$  \hfill (3.99)

The random data between 0 and 1 generated by the Monte Carlo method have certain values of the integral distribution function as shown in Figure 3-19. The corresponding values along the abscissa are the expected values. Therefore, a series of random data map a series of parameters, which can be assigned to the discretized parts of the material, for example, the particles in the SPH method.

Based on the previous discussions, the statistical approach to model the material
heterogeneity characteristics can be constructed by the Weibull distribution in terms of its two characteristic parameters: the homogeneous index $\beta$ and the seed parameter $\mu$. For any specific material, $\beta$ can be determined on the basis of the defect distribution of the microstructure and $\mu$ can be obtained from laboratory tests.

In the current constitutive model, the following parameters which may affect the heterogeneous behaviors can be set to follow the Weibull distributions: the density ($\rho$), the elastic modulus ($E$), the uniaxial compressive stress ($\sigma_c$), the uniaxial tensile strength ($\sigma_t$) and the damage model parameter ($D_{1}$).

Two independent normalized Weibull distributions $A_1$ and $A_2$ are applied in the model to reflect the heterogeneous microstructure of the material as listed in Table 3-4. $A_1$ is used to reflect density ($\rho$) heterogeneity of the specimen. The other distribution $A_2$ represents the heterogeneity of the elastic modulus ($E$), the uniaxial compressive strength ($\sigma_c$), the uniaxial tensile strength ($\sigma_t$) and the damage model parameter ($D_{1}$). Thus, those parameters of each particle in the specimen all have random distributions, as

$$
\begin{align*}
\rho_{(i)} &= \rho A_{1(i)} \\
E_{(i)} &= E A_{2(i)} \\
\sigma_{c(i)} &= \sigma_{c} A_{2(i)} \\
\sigma_{t(i)} &= \sigma_{t} A_{2(i)} \\
D_{1(i)} &= D_{1} A_{2(i)}
\end{align*}
$$

(3.100)

where $i$ denotes the $i_{th}$ SPH particle of the specimen.

Figure 3-21 gives the three different heterogeneous specimens a), b) and c) with homogenous index values of 3, 5 and 10, respectively. The intense of the gray color is proportional to the magnitude of the strength.

By using such an approach, material microstructure heterogeneity can be modeled using the statistical Weibull distribution.

Table 3-4 Material heterogeneity model configurations in the current program
<table>
<thead>
<tr>
<th>Model parameters</th>
<th>Weibull distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Random data space</td>
</tr>
<tr>
<td>$\rho$</td>
<td>$A_1$</td>
</tr>
<tr>
<td>$E, \sigma_e, \sigma_t, D_1$</td>
<td>$A_2$</td>
</tr>
</tbody>
</table>

Figure 3-21 Generated heterogeneous numerical specimens with different homogeneous index values. The intense of the gray color denotes the magnitude of the strength.

Clearly, the strength distribution is more homogeneous in the specimen with a bigger homogeneous index $\beta$.

### 3.4 Program Implementation and Calibration

#### 3.4.1 Program implementation

A SPH program has been developed based on the methodology described in Sections 3.1 to 3.3. To reflect the failure mechanism of brittle materials, an elastoplastic damage constitutive model has been developed and incorporated into the SPH program. Also, a statistical approach based on the Weibull distribution law is utilized to model the material microstructure heterogeneity.

The program is written using mixed C++ and FORTRAN languages. For the conveniences of the maintenance and extension in the future, the object oriented programming (OOP) method and Standard Template Library (STL) are employed in programming. The program is intended to simulate the 2D and 3D
problems for both homogenous and heterogeneous materials.

The program includes three parts. The first part is a pre-processor, which initializes the parameters. It comprises several components for parameters configuring and processing, including those for the global, the heterogeneity model, the SPH method, the constitutive model and the damage model. The second part is the solver which calculates the internal variables at each time step. The third part is the post-processor which processes the numerical results. The detailed flowchart for the program is described in Figure 3-22.

Figure 3-22 Flowchart of the developed 3D SPH code.
3.4.2 Program calibration

Since the constitutive relation and the statistical heterogeneous model implemented in the developed SPH code have unique features that most available commercial software do not have, the calibration example ensures only that the SPH algorithm and the plastic flow rules work properly, which serves as the core of the program. The statistical heterogeneous model and the UTSS theory are extensions of the core program which cannot be compared with other analytical or numerical results due to the unique feature of the developed program.

Since the von Mises criterion has been widely used in the commercial software, the current program also implements this yield criterion in order to calibrate the SPH algorithm and the plastic flow rule. The von Mises criterion can be expressed as

\[
f(\sigma_{op}) = \frac{1}{2 \sqrt{3}} \left[ (\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_1 - \sigma_3)^2 \right] - \sigma_y = 0 \quad (3.101)
\]

where, \( \sigma_y \) denotes the uniaxial yield strength. The potential function \( Q \) is same with the existing one in Eq. (3.75).

The modified code is calibrated by using the commercial software AUTODYN 2D with its finite difference grid solver by performing the uniaxial compression test on a homogeneous aluminum specimen under the plane strain condition. The perfect plastic model without considering the damage is adopted as the constitutive law. The uniaxial yield stress is 50.0 MPa. The aluminum specimen has a cross-section of 50 mm in length and 50 mm in width. It is sandwiched between two rigid walls with the upper wall applied to a constant downward velocity at \(-0.001 \text{ m/s}\). The geometry and the boundary conditions of the specimen are given in Figure 3-23. Four points were selected as the monitoring points as shown in the figure. Their coordinates are listed in Table 3-5.
Figure 3-23 Geometry and the loading conditions of the specimen.

<table>
<thead>
<tr>
<th>Coordinates</th>
<th>#1</th>
<th>#2</th>
<th>#3</th>
<th>#4</th>
</tr>
</thead>
<tbody>
<tr>
<td>X(mm)</td>
<td>26.25</td>
<td>11.25</td>
<td>31.25</td>
<td>26.25</td>
</tr>
<tr>
<td>Y(mm)</td>
<td>11.25</td>
<td>26.25</td>
<td>26.25</td>
<td>41.25</td>
</tr>
</tbody>
</table>

The specimen is discretized into 10000 evenly distributed particles having the same smoothing length of 0.5 mm. The SPH configurations for the calculation are in Table 3-6.

<table>
<thead>
<tr>
<th>Component</th>
<th>Configurations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Global</td>
<td>2-D plane strain</td>
</tr>
<tr>
<td>NNPS</td>
<td>Link-list</td>
</tr>
<tr>
<td>SPH Model</td>
<td></td>
</tr>
<tr>
<td>Kernel function</td>
<td>Cubic spline</td>
</tr>
<tr>
<td>Artificial viscosity force</td>
<td>Selected</td>
</tr>
<tr>
<td>Conservative smoothing</td>
<td>Selected</td>
</tr>
<tr>
<td>Smoothing length evolution</td>
<td>Not used</td>
</tr>
<tr>
<td>Constitutive Model</td>
<td>Elastic and perfectly plastic</td>
</tr>
<tr>
<td>Criterion</td>
<td>von Mises yield criterion</td>
</tr>
</tbody>
</table>
To calibrate the program, the similar simulation is performed using the commercial software AUTODYN 2D with its finite difference grid solver. The specimen is discretized into 40 by 40 regularly arranged grids. Each grid size is 2.5 mm by 2.5 mm.

Two cases are performed for the same duration of 3.05 ms. For each monitoring point, the pressure \( p \), the vertical stress \( \sigma_{yy} \) and the effective plastic strain \( \varepsilon_p \) are recorded. The stress is positive in tension.

The time history of \( p \), \( \sigma_{yy} \) and \( \varepsilon_p \) (calculated using Eq. (3.74)) for point 1, 2, 3 and 4 are plotted in Figure 3-24, Figure 3-25, Figure 3-26 and Figure 3-27, respectively. In these plots, the values of \( p \) and \( \sigma_{yy} \) are normalized by the aluminum’s yield strength \( \sigma_y \). As it can be seen from these figures, the four points enter the plastic stage almost simultaneously at the time of around 2.5 ms. Before that, they kept linear elastic.

At the elastic stage, it can be observed that all variables calculated by the two programs at the four points match excellently well. The developed SPH program demonstrates a very high accuracy in calculation.

At the plastic stage, the vertical stresses calculated by the two programs also match well with each other at the four points. For the pressure and the effective plastic strain, there are some slight discrepancies between the values by the two programs. It may be due to the different approaches in the plastic deformation calculations. However, as it can be seen from these plots, such discrepancies are rather small. Therefore, it can be concluded that the results of the developed SPH code agree very well with the results by the AUTODYN 2D.
Figure 3-24 Variations of a) normalized pressure and normalized $\sigma_{yy}$; b) effective plastic strain with the time of point #1
Figure 3-25 Variations of a) normalized pressure and normalized $\sigma_{yy}$; b) effective plastic strain with the time of point #2
Figure 3-26 Variations of a) normalized pressure and normalized $\sigma_{yy}$; b) effective plastic strain with the time of point #3.
Figure 3-27 Variations of a) normalized pressure and normalized $\sigma_{yy}$; b) effective plastic strain with the time of point #4.
Chapter 4 Numerical Simulations on Brazilian Splitting Tests by Considering Material Heterogeneity

4.1 Introduction

4.1.1 Background

Better understanding of the dynamic fracture behaviors on rock and rock-like materials will benefit us in many areas from mining engineering to rock carven and tunnel constructions. For instance, in order to assess the stability of rock structures and design effective shields under high velocity impacts or explosives, knowledge on how fractures initiate and propagate under different loading conditions will be greatly useful.

The tensile strength of rock and rock-like materials is much lower than the compressive strength; hence, in many cases, material failure is mainly caused by tensile failure. During the past decades, many researches have been conducted on the tensile strength property and its subsequent effects on the fracture process under different loading conditions, such as by Price and Knill (1966), Lindholm et al. (1974), Goldsmith et al. (1976), Grady and Kipp (1979), Ahrens and Rubin (1993), Zhao and Li (2000) and Cho et al. (2003), etc. Their studies showed that the mechanical properties and failure characteristics are sensitive to the loading rate, for instance, its dynamic strength increases with the loading rate.

Experimental work showed that the material heterogeneity also has influence on its mechanical response and the fracture process. Such effects may come from the pre-existing cracks or flaws, such as their activations, growths and coalescences. Several theoretical models have been proposed to explain such effects
by Grady and Kipp (1979), Taylor et al. (1986) and Ravichandran and Subhash (1995), etc. Although they can provide elementary interpretations, the dynamic failure process is too complex to be formulated theoretically. Numerical simulations including FEM, FDM, DEM and BEM methods are also successfully performed using the micromechanical models by many researchers such as Nemati-Nasser and Deng (1994), Podrezov et al. (1997), etc. All those studies considered the heterogeneous effect by using the microstructure models coupled with either fracture mechanics or continuum damage mechanics. However, in the classic fracture mechanics extent, it is difficult to determine micromechanical parameters such as crack density and toughness for different mode cracks. Mesh-based numerical methods also have limitations in processing the large deformations, crack propagations and fragmentations.

4.1.2 Experimental Brazilian splitting tests

The Brazilian splitting test is the most widely adopted method by far to indirectly determine the tensile strength for rock and rock-like brittle materials due to its relative simplicity and the steadiness of the results obtained.

The conventional Brazilian tensile test is performed under the quasi-static load. For dynamic loading condition, it can be carried out by either a hydraulically servo-controlled compression machine or split Hopkinson pressure bar (SHPB) test. The strain rate for a specimen loaded by a hydraulically servo-controlled machine is in the region of $10^{-4} \sim 10^{-2} \, s^{-1}$, while the SHPB test method provides a much higher strain rate region about $10^{0} \sim 10^{2} \, s^{-1}$.

The schematic map of the quasi-static Brazilian test is shown in Figure 4-1, where the load is illustrated with bold arrows. The compressive load produces the tensile stress at the centre of the specimen. When the stress reaches the tensile strength of the specimen, the disc splits along the loading diameter and is divided into two halves ideally. The recommended loading strain rate for the static test is limited within $10^{-6} \sim 10^{-5} \, s^{-1}$. 
Assuming that the material is homogeneous, isotropic and linear elastic, Hondsros (1959) reached a complete analytical solutions (Figure 4-2). The two normal stresses along the vertical loading diameter can be estimated using the following solution,

$$
\sigma_\theta = -\frac{P}{\pi RaL} \left[ \frac{1 - \frac{r^2}{R^2}}{1 - \frac{2r^2}{R^2}} \cos 2\alpha + \frac{r^4}{R^4} \right]
$$

$$
\sigma_r = -\frac{P}{\pi RaL} \left[ \frac{1 - \frac{r^2}{R^2}}{1 - \frac{2r^2}{R^2}} \sin 2\alpha - \frac{r^4}{R^4} \right]
$$

Figure 4-1 Schematic map for the Brazilian tensile test

At the disc center $r$ is zero, it has

$$
\sigma_\theta = -\frac{P}{\pi RL\alpha} (\sin 2\alpha - \alpha) \approx -\frac{P}{\pi RL} \tag{4.3}
$$

$$
\sigma_r = \frac{3P}{\pi RL} \tag{4.4}
$$
Under plane strain state, for instance, when $L$ is commensurable with $2R$, due to stress $\sigma_z$ exists, at the disc center, $\sigma_\theta$ becomes

$$\sigma_\theta = E\varepsilon_\theta = -\frac{P}{\pi RL}(1+\nu)(1+2\nu)$$  \hspace{1cm} (4.5)\\

Figure 4-2 Quantities participating in solutions of Hondros.

The Brazilian test is applicable when the primary fracture initiates from the center of the disc. Its tensile strength can be estimated by calculating the horizontal stress $\sigma_x$ that corresponds to the applied peak load. Eq. (4.3) and Eq. (4.5) can be used to estimate the tensile strength indirectly from the applied peak load, under plane stress and plane strain state, respectively.

Figure 4-3 shows different failure patterns in static Brazilian tensile test on fresh granite. A common problem in the Brazilian test is that failure does not start from the central part of the specimen. As pointed by Fairhurst (1964), “in practice, failure may actually first occur at some other point where, although the calculated stress condition is not the most severe, the material is locally weaker due, for example, to a flaw, inclusion, grain boundary etc.” Mellor and Hawkes (1971) proved quite conclusively that, in a properly conducted test, cracking cannot start at the centre. Andreev (1991a) and Andreev (1991b) analyzed several factors that may induce such a problem, for instance, the contact conditions and the ratio of the compressive strength to the tensile strength. Generally, most researchers agree that this condition can be achieved by applying a distributed load over a short strip of the circumference at both ends of the disc.
Numerical Simulation of Heterogeneous Material Failure by using SPH Method

Figure 4-3 Different failure patterns in static Brazilian tensile test on fresh granite samples.

The split Hopkinson pressure bar (SHPB) has long been employed as an apparatus to carry out the dynamic tests on rock-like materials by many researchers, such as Lindholm et al. (1974), Zhang et al. (1999), and Zhao and Li (2000), etc. Results show that the dynamic tensile strength increases with the increasing loading rate or strain rate.

Figure 4-4 Schematic setup of SHPB

medium strain rate (50 s\(^{-1}\))  higher strain rate (80 s\(^{-1}\))

Figure 4-5 Failure pattern for Brazilian splitting test on fresh granite using SHPB

The typical experimental setup of the SHPB splitting test is illustrated in Figure 4-4. The specimen is held diametrically between the bars using steel bearing bars to avoid local failure due to the point load. During the test, the incident bar is impacted to create a compressive wave traveling down the specimen and then the transmitter bar. The pressure applied on the both ends of the specimen can
be calculated with the help of the electric apparatus. Thus the obtained peak pressure can be used to determine the dynamic tensile strength by Eq. (4.3). Figure 4-5 shows the failure pattern for Brazilian splitting tensile test on fresh granite under the strain rate of 50 and 80 s\(^{-1}\).

### 4.1.3 Numerical simulations on the Brazilian splitting test

The aforementioned experiments are useful tools to study material’s tensile strength properties. However, they are unable to provide sufficient information for the better understanding on the fracture process and failure mechanism in the microscopic views. Hence, many researchers have carried out numerical studies and some are listed below:

Tedesco et al. (1989) and Tedesco et al. (1991) simulated the SHPB splitting tests on concrete using the commercial software ADINA with a tensile strength cut-off damage model. The method is to increase the tensile strength cut-off value to simulate the different failure patterns under different strain rates. They concluded that the tensile strength increased with the increase of the strain rate. Tang et al. (2001) successfully employed the RFPA to simulate the static Brazilian tensile test by considering material heterogeneity using the statistical Weibull distribution model. The simulation can depict the fracture process of the heterogeneous rock. Zhu and Tang (2006) further studied the dynamic failure patterns of the heterogeneous Brazilian disc by using the RFPA code. Their study showed that the failure patterns of the rock disc are different with different amplitudes of the applied incident compressive stress waves. Chen et al. (2004) also simulated the fracture process of the heterogeneous rock sample under static Brazilian tensile test using the commercial software FLAC. By applying the digital image method, the micro-structural information of the rock can be obtained.

Most of the existing studies on the Brazilian splitting tests are carried out under quasi-static cases. Besides, the material heterogeneous effects on the specimen’s dynamic strength and failure patterns are not well investigated. Therefore, the strain rate effect observed from the experiments need to be further examined.
4.1.4 Objectives

The developed SPH code can handle both discontinuities and material heterogeneity. Therefore, it can provide a helpful tool to carry out such simulations especially under dynamic loading conditions. The objective of this chapter is to investigate the effects of the strain rate as well as the material heterogeneity on the fracture processes and the tensile properties for rock-like materials. Besides, influences of the parameter $b$ employed in the yield criterion on the specimen’s tensile strength is also being examined by adopting the different values of 0, 0.6 and 1.

4.2 Numerical model configuration

4.2.1 Specimen geometry and loading conditions

The geometry and loading condition for the rock disc specimen are shown in Figure 4-6. In the simulation, a thin disc is sandwiched between two rigid walls loaded by boundary velocities. Particles within the upper and bottom boundaries were directly given the velocity $v(t)$ defined as,

$$v(t) = \begin{cases} \frac{t}{t_0} v_0, & \text{when } t \leq t_0 \\ v_0, & \text{when } t > t_0 \end{cases}$$

where, $t_0 \geq n \frac{2L}{c}$ is usually adopted in the SHPB test to help to achieve the stress equilibrium and prevent the premature failures due to the stepwise increasing force on the loading boundaries. $L$ is the nominal length of the specimen and $c$ is the stress wave propagation speed in the specimen. $n$ is usually taken 3 or 4. In the current simulation, $t_0 = 5.0 \times 10^{-5} \text{ s}$ is adopted.

After $t_0$, the prescribed velocity on the boundaries is kept at a constant value $v_0$. The nominal strain rate $\dot{\epsilon}$ is constant after the time $t_0$, which is defined as $\dot{\epsilon} = \frac{v_0}{R}$, where $R$ is the disc radius. Loading cases and their corresponding
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strain rates are shown in Table 4-1. Along with the specimen’s deformation, the compressive forces on the two boundaries increase correspondingly. After the specimen fails, they drop down. The average value of the compressive forces on the two boundaries is taken as the loading force of the specimen. The apparent tensile strength can be calculated using Eq.(4.3) under different strain rates.

![Figure 4-6 Geometry and loading conditions for the specimen.](image)

Table 4-1 Loading conditions for numerical Brazilian splitting simulations

<table>
<thead>
<tr>
<th>Loading cases</th>
<th>Quasi</th>
<th>Low</th>
<th>Medium</th>
<th>High</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>$v_0 (m/s)$</td>
<td>0.0025</td>
<td>0.025</td>
<td>0.25</td>
<td>0.75</td>
</tr>
<tr>
<td>$\dot{\varepsilon} (s^{-1})$</td>
<td>0.1</td>
<td>1</td>
<td>10</td>
<td>30</td>
</tr>
</tbody>
</table>

4.2.2 Numerical approach and material parameters

The developed SPH code is applied to simulate the dynamic Brazilian splitting test. The elasto-plastic damage model described in Chapter 3 is employed as the constitutive law. The statistical method based on the Weibull distribution law is adopted to reflect the rock microstructure heterogeneity.

To investigate the effects of material heterogeneity, three specimens are configured to represent different degrees of heterogeneity. The heterogeneous model configurations are listed in Table 4-2. The first sample is homogenous. The second one and the third one are heterogeneous and configured with two normalized Weibull distributions with homogeneous index values of 10 and 5, respectively. The densities in these heterogeneous specimens are assumed rela-
tively homogeneous and assigned with a homogeneous index value 50.

Table 4-2 Specimen’s heterogeneity configuration

<table>
<thead>
<tr>
<th>Specimen</th>
<th>Homogeneous</th>
<th>Homogeneous index 10</th>
<th>Homogeneous index 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1</td>
<td>Not applicable</td>
<td>50</td>
<td>50</td>
</tr>
<tr>
<td>A2</td>
<td>Not applicable</td>
<td>10</td>
<td>5</td>
</tr>
</tbody>
</table>

For the heterogeneous specimen, firstly, each particle in the specimen is assigned with the same model parameter values given in the last chapter. After that, the particle is assigned a random number from the generated Weibull distribution space. The assigned number is further multiplied with its strength related model parameter values, such as the elastic modulus \( E \), the uniaxial compressive stress \( \sigma_c \), the uniaxial tensile strength \( \sigma_t \) and the damage model parameter \( D_1 \) to obtain the heterogeneous strength values of particle \( i \) by

\[
\begin{align*}
E_{(i)} &= EA_{2(i)} \\
\sigma_{c(i)} &= \sigma_c A_{3(i)} \\
\sigma_{t(i)} &= \sigma_t A_{2(i)} \\
D_{1(i)} &= D_1 A_{2(i)}
\end{align*}
\]

(4.7)

The density of particle \( i \) is determined by the Weibull distribution \( A_i \) by

\[
\rho_{(i)} = \rho A_{3(i)}
\]

(4.8)

Figure 4-7 shows the normalized Weibull distributions where \( \beta = 5 \) and \( \beta = 10 \). Hence, those two distributions indicate different degrees of heterogeneous conditions. The case of \( \beta = 10 \) corresponds to the more homogeneous material compared with the one of \( \beta = 5 \).

Each numerical Brazilian specimen is composed by 12281 particles with the same smoothing length of 0.4 mm. These particles are evenly distributed in a lattice manner. Figure 4-8 shows those generated numerical specimens with different levels of heterogeneity. The enlarged upper right part is for a better view of the particle arrangement.
Figure 4-7 Normalized Weibull distribution in two heterogeneous numerical models with $\beta = 5$ and $\beta = 10$ from left to right.

Figure 4-8 Illustration of the numerical specimens with different homogenous index $\beta$, 5 and 10 from left to the right, respectively. Intense of the gray scale indicates the magnitude of the particle strength.

According to results by Zhao (1999), Zhao et al. (1999) and Zhao and Li (2000), the Poisson’s ratios and Young’s modulus of rock vary very small with the variation of the loading rates and confining pressure. However, it is still an open issue on whether those parameters are independent or not. For instance, Chong and Boresi (1990) argued that the Young’s modulus increases with the loading rates. In the current simulations, the strain rate effects on the initial Young’s modulus and the Poisson’s ratio are not considered. The parameter $b$ employed in the simulations takes 0.6 unless it is specifically stated.
4.3 Simulations under quasi-static loading condition

The recommended loading strain rate for the quasi-static test is usually within $10^{-6} \sim 10^{-5} \, s^{-1}$. However, the computational effort is much expensive when applied such a low strain rate analysis using the SPH code. Our simulation results show that, when applied strain rate is below $1.0 \, s^{-1}$, the failure processes and mechanical responses are not much different for the same numerical sample. Therefore, cases of strain rate $0.1 \, s^{-1}$ are chosen to represent the quasi-static cases.

4.3.1 Effect of material heterogeneity on the stress distribution along the loading axis

For quantitative evaluations of the heterogeneous effect, Figure 4-9 shows the distributions of the simulated stresses $\sigma_\theta$, $\sigma_r$ along the loading diameter for these cases under the elastic stage. They are compared with analytical solutions which are also plotted in the graphs based on Eq. (4.1) and Eq. (4.2).

For the homogenous case in Figure 4-9, it demonstrates good agreements. When the specimen becomes heterogeneous, stresses distributions are getting scattered and fluctuate along their analytical results. Such phenomena are due to the fact that the analytical solution is based on the assumption of homogenous condition. The non-uniform distribution of the stresses may cause premature failures on those locations with severe stress. Thus, the splitting crack may not exactly start from the disc center.
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Figure 4-9 Analytical and simulated stress distributions along the loading diameter for homogenous specimen (top), heterogeneous specimens (index 10 and 5, bottom, from left to right, respectively)

The photo-elastic fringes of maximum shear stress for the three cases are also plotted during these simulations as shown in Figure 4-10, Figure 4-11 and Figure 4-12, where tags below each frame indicate the loading steps and the corresponding loading force ratio to the peak value. Result from the homogenous case is in good agreement with the experimental test (Figure 4-18) by Gomez et al. (2001). The heterogeneous cases exhibit the non-uniform stress distributions during the loading process as described previously.

Figure 4-10 Photo elastic fringes of maximum shear stress for homogeneous rock specimen
Figure 4-11 Photo elastic fringes of maximum shear stress of homogeneous index 10 rock specimen

Figure 4-12 Photo elastic fringes of maximum shear stress of homogeneous index 5 rock specimen

Figure 4-13 Static Homalite-100 tensile-splitting fringe pattern (after Gomez et al., 2001)
4.3.2 Analysis on the profiles of loading force with displacement and fracture processes

Figure 4-14 shows profiles of the loading force with the diametric displacement during the fracture process for these three specimens, where marks (a-d) on the homogeneous curve correspond to the different stages in the following specimen failure process in Figure 4-15. As can be seen from these plots, the response loading forces increase almost linearly to their peak values. Then they dropped down substantially after the discs fail. The predicted tensile strengths for the three cases are given in the Table 4-3. It can be concluded that the loading capacity and the tensile strength increases when the material is more homogeneous. In addition, the specimen appears more “brittle” when it is more homogeneous.

![Diagram showing loading force vs. diametrical displacement for three specimens under strain rate 0.1 s⁻¹.]

Table 4-3 predicted tensile strengths under strain rate 0.1 s⁻¹

<table>
<thead>
<tr>
<th>case</th>
<th>Homogeneous</th>
<th>Homogenous index 10</th>
<th>Homogenous index 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\sigma_t) (MPa)</td>
<td>11.87</td>
<td>4.21</td>
<td>2.93</td>
</tr>
</tbody>
</table>

Fracture processes of the three samples are presented by damage distribution at their representative stages in sequence as shown in Figure 4-15. The label under each frame indicates the loading steps and the loading force ratio to the peak.
value. Those frames after the peak load are in post-peak stage.

Figure 4-15 Fracture process of the three specimens as homogeneous, heterogeneous with index 10 and index 5 cases, from top to bottom; Damaged particles are plotted in dark black.

For the homogenous case, the initial crack exactly started from the sample center at the peak load and then propagates along the loading diameter plane as can
be compared with the experimental test on the green polyethylene sample shown in Figure 4-16. Tensile fractures at the disc brims are formed due to the bending moments. Since the disc is homogenous, all the cracks are symmetric along the loading diameter plane.

![Figure 4-16 Initialization and propagation of splitting for a green polyethylene sample under the Brazilian test (after Andreev, 1995)](image)

In the two heterogeneous cases, initial cracks are found around the disc center and then propagated toward both ends. Due to the heterogeneous effect, the crack growing paths are not straight and cracks are no longer symmetrical as that in the homogenous disc. At this strain rate level, the fracture patterns are in good agreement with those shown in Figure 4-3.

### 4.4 Simulation results under dynamic loading conditions

#### 4.4.1 Homogeneous case

Figure 4-17 shows the profile of loading force with the vertical diametric displacement. The curve under strain rate $0.1 \text{ s}^{-1}$ is also plotted to compare the results between the quasi-static and dynamic cases. It can be seen that the disc loading capacity is sensitive to the loading rate. The following phenomena can be concluded:

- When the strain rate is low, the force-displacement curve behaves like ideal brittle failure. The force displacement curves of strain rate $0.1 \text{ s}^{-1}$ and $1.0 \text{ s}^{-1}$ are almost identical. With the increasing strain rates, it ap-
pears strain-softening, especially when the strain rate is above $60 \text{ s}^{-1}$.

- In generally, the disc loading capacity increases when the strain rate is below $120 \text{ s}^{-1}$. Above this level, strain rate effect is not obvious.

Figure 4-17 Loading force vs. displacement for the homogeneous disc under different strain rates

Figure 4-18 presents the fracture process of the rock disc under different strain rates. It can be observed that strain rate $1.0 \text{ s}^{-1}$ case is identical to the $0.1 \text{ s}^{-1}$ case as shown previously.
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strain rate 30 s$^{-1}$

strain rate 60.0 s$^{-1}$

strain rate 80.0 s$^{-1}$

strain rate 120.0 s$^{-1}$
Figure 4-18 Failure process of homogeneous Brazilian disc under strain rate $1.0 \text{ s}^{-1}$ to $200.0 \text{ s}^{-1}$

Failure processes for those cases with strain rate above $1.0 \text{ s}^{-1}$ and below $120.0 \text{ s}^{-1}$ are also similar. A major crack initiates at the center of the rock disc and then propagates toward both ends along the vertical diameter. Eventually this will perpetuate a failure. The major crack kept straight at the tensile region of the horizontal stress. Once it reaches near the bi-compressive stresses regions at both ends, bifurcation will be initialized. Shear cracks and induced conical zones can also be observed near the loading boundaries mainly due to the stress concentration near the loading boundaries.

For the case of strain rate $120 \text{ s}^{-1}$, besides the major crack long the diametric line, two subsidiary cracks also occurred symmetrically and along the major crack. After the peak load, the fracture process is similar to those with cases of lower strain rates. Besides, there are more flexural tensile cracks along the circular boundary.

Failure processes for cases with strain rate $160 \text{ s}^{-1}$ and $200 \text{ s}^{-1}$ are different
from other cases. At the time of peak load in both cases, no major crack occurs. Shear zones can be found near the loading boundaries. For the case of the strain rate 160 $s^{-1}$, major and subsidiary cracks are formed and developed similarly as those in the case with the strain rate of 120 $s^{-1}$. However, for the strain rate of 200 $s^{-1}$ case, primary cracks are initiated near the two loading boundaries and propagates towards the disc center along the vertical diameter. In both cases, flexural tensile cracks are extensively along the sample edges.

It is worth noting that, although the splitting failure is the major mode for all cases, the primary crack initiation and subsequent developments are very sensitive to the loading strain rate.

Figure 4-19 Profiles of stress distributions along the loading diameter for homogenous specimen with strain rate 60 $s^{-1}$.

Figure 4-19 presents profiles of stress distributions along the loading diameter during the specimen failure process with the strain rate 60 $s^{-1}$. The primary crack at the disc center has just been formed when the applied load reached 73% of the peak load as shown in Figure 4-19 a). Both horizontal and vertical
stresses at the disc center drop toward zero. Except for the damage zone, the simulated distributions of the two stresses match still well with the analytical solutions similar with those under the quasi-static loading condition. As the particles in the cracked zone are completely damaged, the stresses in the cracked zone vanish as shown in Figure 4-19 b). As a result, a major crack is developed. The propagation of the diametrical crack results in the stress field redistribution as shown in Figure 4-19 c) and d). Splitting process in such a dynamic case is similar to that in a quasi-static load where stress equilibriums are perfectly achieved.

Under higher strain rate loadings, for instance, above 120 $s^{-1}$, the loading stress increase rapidly and the static equilibrium cannot be achieved before the disc failure. Figure 4-20 gives profiles of the stress distributions along the loading diameter during the rock failure process with a strain rate of 200 $s^{-1}$ to illustrate such non-equilibrium stress fields during the fracture process.

Figure 4-20 Profiles of stress distributions along the loading diameter for homogeneous specimen with strain rate 200 $s^{-1}$ during the failure process, where b)-d) are in the post-peak region.
As can be seen in Figure 4-20 a) at the peak load, the two stresses along the loading diameter do not reach the equilibrium from a quasi-static solution. Due to failure at the loading boundaries, the loading force decreases as shown in Figure 4-20 b). Local failures occurred nearby the loading boundaries as shown in Figure 4-20 c). With the propagations of the developed cracks nearby the loading boundaries and the stress redistributions, the stresses along the loading diameter vanish and the disc is split due to the diametric crack propagation and coalesces. It seems that premature failures nearby the loading boundaries prevent the further increment of the loading force. Obviously, the assumptions on the Brazilian test are not valid in such higher strain rate cases.

4.4.2 Heterogeneous case with homogenous index of 10

Figure 4-21 shows curves of loading force with the vertical diametrical displacement under strain rate ranging from $0.1 \text{ } s^{-1}$ to $200 \text{ } s^{-1}$. Dependence of the disc loading capacity with the strain rate can be observed. The following phenomena can be concluded:

- The force-displacement curve behaves from ideal brittle when strain rate is below $1.0 \text{ } s^{-1}$ to strain-softening post-failure when the strain rate increases.

- Similar to the homogeneous case, the disc loading capacity increases when the strain rate is below $120.0 \text{ } s^{-1}$. Above this level, the strain rate effect is not obvious.

Figure 4-22 presents the fracture processes of the disc under different strain rates. Again, the result obtained from the strain rate of $1.0 \text{ } s^{-1}$ case is identical to that in the strain rate $0.1 \text{ } s^{-1}$. For the strain rate of $10.0 \text{ } s^{-1}$ case, the initial crack bifurcates around the disc center during its propagation and coalesces with other developed crack to split the disc finally.

Failure processes for those cases with strain rate above $10.0 \text{ } s^{-1}$ and below $160.0 \text{ } s^{-1}$ are similar. A cluster of micro cracks initiate at the center of the disc and propagates independently and roughly along the vertical diameter. Eventually these cracks coalesce and form a crack band to perpetuate a failure. In the
cases with a higher loading rate, the cracks coalesce at disc-end boundaries and form wedge-shaped zones. Obviously, the crack band becomes more evidently as the strain rate increases. Flexural tensile cracks can also be clearly observed in the post-peak stage in these cases.

Figure 4-21 Profiles of loading force vs. displacement for the heterogeneous disc with homogeneous index 10 under different strain rates

For cases with strain rates of $160 \; \text{s}^{-1}$ and $200 \; \text{s}^{-1}$, several clusters of micro-cracks can be observed near the two loading boundaries around the vertical diameter plane. At the peak load at strain rate $200 \; \text{s}^{-1}$, only a few cracks can be observed. In post-peak stages of both cases, the crack bands formed by micro-cracks can be observed. In addition, flexural tensile cracks have developed more extensively at the brim of the disc.
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strain rate 60.0 s⁻¹

strain rate 80.0 s⁻¹

strain rate 120.0 s⁻¹
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4.4.3 Heterogeneous case with homogenous index 5

Curves of loading force with the vertical diametric displacement under strain rate ranging from 0.1 s\(^{-1}\) to 200.0 s\(^{-1}\) for this heterogeneous disc are shown in Figure 4-23. Similar to the results of the previous heterogeneous specimen, the force-displacement curves show relatively brittle below strain rate at 1.0 s\(^{-1}\) and a smoother softening post-failure region occurs as the strain rate increases. Also, the maximum loading force increases remarkably with the increase of the strain...
rate.

Figure 4-23 Profiles of loading force vs. displacement for the heterogenous disc with homogeneous index 5 under different strain rates

Fracture processes for different strain rate cases are presented in Figure 4-24. Again, the failure pattern with the strain rate of 1.0 s\(^{-1}\) is identical to that with the strain rate of 0.1 s\(^{-1}\) as shown previously. For the case of strain rate 10.0 s\(^{-1}\), the initial crack bifurcates around the disc center during its propagation and link up with other developed crack. For these two cases, the disc is mainly split by the major cracks.

Failure processes for those cases with strain rate above 10.0 and below 160.0 are similar. Discs are mainly split by crack bands formed by the coalescence of growing micro-cracks. The higher the loading rate, the wider the crack band becomes. Cases with strain rate 160 s\(^{-1}\) and 200 s\(^{-1}\) are also similar to those in the homogenous index 10 specimen case in that crack bands are developed in the post-peak stage, especially for the case of strain rate 200 s\(^{-1}\).
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strain rate 1.0 s\(^{-1}\)

strain rate 10.0 s\(^{-1}\)

strain rate 30.0 s\(^{-1}\)
Numerical Simulation of Heterogeneous Material Failure by using SPH Method

strain rate 60.0 s\(^{-1}\)

strain rate 80.0 s\(^{-1}\)

strain rate 120.0 s\(^{-1}\)
4.5.1 Particle size effect on the loading response force and failure pattern

Since the whole domain is represented by the particles in the SPH method, the particle size will affect the resolution accuracy as well as the fracture patterns.
Three cases are constructed to investigate this effect for the homogenous index 5 case under strain rate 0.1 s\(^{-1}\). The smoothing lengths are 1 mm, 0.5 mm and 0.4 mm, respectively. Accordingly, their total particle numbers are 1976, 7860 and 12281. Simulation results are given in Figure 4-25.

![Figure 4-25](image)

**Figure 4-25** Comparison of numerical results corresponding to different particle size in the same domain. a) Curves of response force with the loading displacement, and b) failure patterns at 69% peak force in post-peak stages.

It can be seen that numerical solutions in the current model are dependent on the particle size. Simulated tensile strengths are 3.39 MPa, 3.32 MPa and 2.93 MPa, from the three cases, respectively. In a word, the predicted disc loading capacity decreases with the particle size. This particle-size-sensitivity can be explained from the statistical theory similarly as addressed by Zhou and Molinari (2004). For the statistical data generated in the Weibull distribution with
the same index, the larger population has more chance of having small values than that in the smaller one. Therefore, the disc with more particles will have a larger possibility to produce a smaller tensile strength.

4.5.2 Spatial variation effect on the loading response force and failure pattern

In laboratory tests, the variation or uncertainty of experimental results can be often observed. For example, in Brazilian splitting tests, specimens’ tensile strengths and failure patterns are different from one to another. Such differences are often induced by the randomly distributed micro-defects in the specimens.

The heterogeneous specimen is constructed statistically, where the mechanical parameters of those particles randomly follow a given Weibull’s distribution. The Weibull distribution data are generated randomly by the program using the Monte Carlo method. Hence, even for the same homogeneous index $\beta$ value, the values and sequences of these Weibull distribution data are different.

Four series of Weibull distribution data with the same homogenous index 10 are generated. Then, each is used to generate one specimen. Hence, these four specimens have different local characteristics for individual particles spatially with the same macro properties. These four Brazilian specimens are performed under the strain rate $20 \text{ s}^{-1}$. Profiles of their response loading forces with the loading displacements as well as their corresponding failure patterns are presented in Figure 4-26.

It can be observed that these curves are very similar. They are consistent during the initial loading period but behave differently when approaching their peak loads. Their failure patterns are also different from one to another. Such differences are due to the stochastic distributions of their mechanical parameters. Results manifest that the model can well represent such uncertainties or variations induced by heterogeneity as can be often observed in experiments.

The predicted tensile strengths for these four specimens are given in Table 4-4. As can be seen, in spite of different failure patterns, their tensile strengths are very close due to having the same degree of heterogeneity.
Numerical Simulation of Heterogeneous Material Failure by using SPH Method

a) Curves of response force with the loading displacement

b) Failure patterns in post-peak stages

Figure 4-26 Effects of spatial variations with the same degree of material heterogeneity illustrated by four different specimens, all with the same homogeneous index 10.

Table 4-4 Predicted tensile strengths of four different specimens with the same homogeneous index 10 under the strain rate 20 s⁻¹

<table>
<thead>
<tr>
<th>Homogenous index 10</th>
<th>case 1</th>
<th>case 2</th>
<th>case 3</th>
<th>case 4</th>
<th>average</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_{10} (MPa)$</td>
<td>7.727</td>
<td>8.383</td>
<td>8.027</td>
<td>7.386</td>
<td>7.881</td>
</tr>
</tbody>
</table>

4.5.3 Heterogeneous effect on fracture process and failure patterns

From predicted sequence of crack patterns for homogenous and heterogeneous cases shown previously, one can observe that these specimens are all eventually split into two main large fragments. However, their failure processes are quite
different:

- When the strain rate is below 120 s$^{-1}$:
  For those homogeneous cases, failure is clearly due to the primary crack initiated from the disc center and its subsequent propagation in a straight way outwards toward the loading boundaries. Subsidiary cracks can also be observed at higher strain rate cases.

For heterogeneous cases below strain rate 1.0 s$^{-1}$, failure is roughly by the major cracks initiated at weaker zone around the disc center, dependent on the stochastic distribution of particle strengths. Crack propagation path is along a tortuous way. Above this strain rate level, disc is split mainly by the crack band formed by the coalescence of growing micro-cracks. The crack band appears wider when the loading strain rate is higher.

- For cases whose strain rate is above 120 s$^{-1}$
  Due to the rapid increasing boundary force, initial crack (in homogeneous case) or cluster of micro-cracks (in heterogeneous case) are observed near the regions of two loading boundaries instead of on the disc center. Disc loading capacities are lost before the well-developed major crack or the crack band.

Statistics of damaged particle numbers at the moment of peak load for all cases are given in Figure 4-27. Bars in each frame are in the sequence of the strain rate from 0.1 s$^{-1}$ to 200.0 s$^{-1}$. As can be observed, the damaged particle numbers are directly proportional to the strain rate below 120.0 s$^{-1}$. In these cases, stress equilibriums are roughly achieved before the peak load. Occasional exceptions in the homogeneous cases are caused by the developed subsidiary cracks in those cases. Besides, the different failure modes between the homogeneous cases and the heterogonous ones can also be depicted from the figure. The relatively bigger damaged numbers in the heterogeneous cases indicate that their failures are due to more micro-cracks, whereas in homogeneous cases are by major cracks. Generally speaking, at higher loading rates, more micro-cracks are activated and developed before the specimen’s failure. Such a conclusion is coincided to the simulation by Zhou and Molinari (2004). Furthermore, by comparisons between the two heterogeneous cases, we can see more damaged
particles in the more heterogeneous material under the same strain rate in all cases.

![Figure 4-27 Damaged particles vs. strain rate in homogenous and heterogeneous cases at the moment of their peak loads, accordingly.](image)

Remarkably, in all homogenous cases, all cracks are symmetric along the vertical diametric line. However, in heterogeneous cases, they are more randomly initialized and developed. Since real materials are more or less non-homogeneous. Evidently, the numerical simulation provides a wealth of information regarding the character of the evolving fracture patterns which is inaccessible to experimental diagnostics, which are for most part limited to the observation of the surface of the specimen. In this respect, the simulated failure processes and patterns can better reveal the inner mechanisms for real materials.

### 4.5.4 Apparent dynamic tensile strength and rate sensitivity

The predicted tensile strengths with the different loading rates for three specimens are plotted in Figure 4-28. As can be seen, the simulated apparent dynamic tensile strength increases with the increment of the loading rate for all specimens. Besides, we can also observe that, at the same loading rate, the predicted strength becomes higher when the material is more homogeneous.
Figure 4-28 Predicted tensile strengths against the loading rates for three specimens with different heterogeneous levels.

To further evaluate the material heterogeneity effects on the dynamic tensile strength, the dynamic increment factors of predicted specimen tensile strengths against the logarithm of real strain-rates are plotted in Figure 4-29. Tensile strengths are calculated using the Eq. (4.3). Dynamic increment factor (DIF) is defined as,

$$DIF = \frac{\sigma_{td}}{\sigma_i}$$

(4.9)

where $\sigma_{td}$ is the dynamic tensile strength, $\sigma_i$ is the quasi-static strength and here taken the value under the strain rate 0.1 s$^{-1}$.

Experimental results from the granite samples are also plotted for comparison. The experimental data can be referred in Appendix A, where the dynamic tensile strengths are obtained from Brazilian splitting tests on granite samples. The quasi-static test is performed under a strain rate $1.0 \times 10^{-5}$ s$^{-1}$.

It is seen that for both materials, the tensile strength of the specimen increases with the strain-rates as reported by many researchers. It bears emphasis that these features of the dynamic behaviors are predicted by, rather be built into, the theory. Indeed, parameters of the numerical constitutive model are all obtained from the static experiments, which are definitely rate-independent.
Figure 4-29 Comparisons of the dynamic increment factor of predicted tensile strengths for three specimens with different heterogeneous levels and experimental results with the logarithm of strain rate.

It has also been observed that when strain rates at 160 s$^{-1}$ and 200 s$^{-1}$, the increasing trend of DIF is not much obvious as those cases with strain rates below 160 s$^{-1}$. This is mainly caused by the non-equilibrium stress-distributions along the diameter line region as discussed previously on the failure processes. At such high loading rates, the analytical equation may be invalid to be applied on the dynamic tensile strength calculations.

Comparisons between the numerical and experimental results show that the increments of the numerical predicted result are not as sharp as those obtained by experiments. Such deviations may come from several sources. One is that the numerical heterogeneous microstructure model is not an exact replica one of real samples. It should be clearly understood that the microstructures of real material are much more complex. For instance, the voids, pre-existing cracks, etc. cannot be exactly modeled by the current method. Another important factor is that, the DIF of the numerical simulations takes the strength in strain rate 0.1s$^{-1}$ as the quasi-static value and will inevitably underestimate such rate increments. What more, since the experimental result under high-rate loadings has an extremely short duration; it may be difficult to obtain an accurate measurement. However, results still show good agreements in terms of the overall trend.
Since our model does not explicitly account for the strain rate effects, a question may arise here on what cause the strength increment under dynamic loadings.

The rate dependent-effect is often accounted for the inertia effect as pointed by Bischoff and Perry (1995) and Donze et al. (1999). During high strain rate loading, micro-cracks have less time available for their development or propagation. When local equilibrium is not attained, the inertial forces will increase the apparent resistance in opposition to the movement. Thus, higher load will be required before cracking becomes prominent enough to make the specimen failure. However, since strain rates in the current simulation are below 200 s\(^{-1}\), inertia effect is not obviously compared with those in very high strain rate cases up to 1000 s\(^{-1}\). Furthermore, we obtain the increasing trends in the cases of strain rate 160 s\(^{-1}\) and 200 s\(^{-1}\) are not as sharp as those in lower cases.

It is commonly recognized that geo-material strength is greatly affected by the hydrostatic pressure. In our program, we employ a pressure dependent model. This rate-dependent effect may be attributed to the pressure increment due to the rapid loading.

To investigate the pressure effects on the strain rate dependency of the specimen’s predicted tensile strength, the \( DIF \) of average pressure is defined as the dynamic average pressure divided by the average pressure in quasi-static loading, as

\[
DIF_p = \frac{P_d}{P_0} \tag{4.10}
\]

Again, we take the value of strain rate 0.1 s\(^{-1}\) case as a reference to calculate \( P_0 \).

By considering the facts that the failure particles mostly occur within a narrow strip along the disc diameter in the numerical simulations, the calculation of the \( DIF_p \) is defined over particles within such a region. The strip width is equal to the length of the specimen’s loading boundary, which is 12% of the disc diameter as shown in the Figure 4-30 –a). The \( DIF_p \) as well as the \( DIF \) of the pre-
dicted tensile strength with the logarithm of strain rate for all cases are plotted in Figure 4-30–b) for comparisons.

Figure 4-30 a) Illustration of the calculation region of average pressure in specimen; b) Comparisons of the DIF of the average pressures and DIF of tensile strength with the logarithm of strain rates.

It is very interesting to see that the trend of DIF of tensile strength curves remarkably match that of DIF of the average pressure except for the anomalies for those strain rates above 120 s⁻¹. Such a good agreement attests that the pressure increment caused by the loading rate plays an important role for the rate-dependent dynamic strength. The phenomena of pressure increment due to the high strain rate is also reported by Brace and Jones (1971), Bischoff and Perry (1991) for concrete and Janach (1976) for rock. They explained that an apparent effective confining stress would be caused by the lateral inertial restraint for the specimen is unable to expand instantaneously during the rapid loading. Since the adopted strength criterion is pressure dependent, particles under the higher confining compressive pressure will have higher failure strength. Consequently, the specimen will have a higher loading capacity. Hence, the predicted tensile strength of Brazilian specimen will be larger according to Eq. (4.3).

From the DIF of the strength curves, one can also observe that this rate-dependence is also affected by the material heterogeneity. For homogene-
ous cases, strain rate effect on the strength is not evident. As can be seen, the $DIF$ value is smaller than 1.5. At the same strain rate, the $DIF$ value of more heterogeneous material (as homogeneous index 5) increases shaper than that in less heterogeneous one (as homogeneous index 10). This may be explained by the micro-cracking effect manifested in the previous discussion on failure processes. In the heterogeneous specimens, material failure is caused by micro-cracks initiation, propagation and coalescence. Because the extension of the micro-cracks takes time, other micro-cracks may be activated before a neighboring activated micro-crack extends and unloads them. As a result, the specimen breaks into more cracks at higher loading rates; while at lower loading rates, a single main crack may cause catastrophic failure. As may be seen from Figure 4-27, it is clear that more heterogeneous cases have more micro-cracks formed than those in the less ones at the same strain rates. On one hand, this would cause stress releasing during the formation of these cracks and consume considerable energy. On the other hand, the formation of cracks delays the specimen’s failure and will be helpful for the load to be further increased. As a result, the dynamic average pressure highly depends on heterogeneous conditions.

### 4.5.5 Effects of strength criterion coefficient $b$

As mentioned previously, the adopted UTSS criterion can produce a full spectrum of new criteria when the value of $b$ varies between 0 and 1, to reflect the characteristics of various different materials. When $b = 0$, it becomes the single-shear criterion (e.g., the Mohr-Coulomb) to give the lower limit convex shape function, and becomes to the Twin-Shear Strength criterion when $b = 1$, which gives the upper limit convex shape function.

To examine the effects of $b$ on the predicted tensile strength, two series of compressive simulations on the heterogeneous specimens of homogeneous index 10 with same loading rates were performed with $b = 0$ and $b = 1$, respectively. The simulated loading forces with different strain rates for these two cases are plotted in Figure 4-31. These two series of curves are generally similar to the ones of $b = 0.6$ as described previously. In all cases, when the strain rate is above a certain value, the disc loading capacity deviates with respect to dif-
different strain rates. Thus, the value of $b$ has much more influences under the higher loading rates.

![Diagram](image.png)

Figure 4-31 Profiles of loading force vs. displacement for the specimens with homogeneous index 5 under different strain rates, $b=0$ (top) and $b=1$ (bottom). As shown more clearly in Figure 4-32 a), the predicted apparent tensile strength is affected by the $b$ value adopted in the strength criterion. In general, the strength increases with a bigger value of $b$ under the same strain rate. This coincides with the UTSS theory in that the larger $b$ value corresponds to a bigger convex failure surface. Besides, we can observe that, the influence of $b$ on the predicted strength becomes significant when the strain rate is above a certain value, for example, 60 s$^{-1}$ in our simulation results. Such a phenomenon can be ascribed to the effect from the specimen’s internal pressure under the dy-
namic load. As shown in Figure 4-32 b), for different b values, the average pressure values at the specimen’s peak load are much close in cases when strain rate is not high. However, under the higher strain rate cases, they differ remarkably. Therefore, the predicted tensile strengths are greatly affected by the b value in the strength criterion under higher loading cases.

Figure 4-32 Predicted tensile strengths (left) and their average pressures at peak loads (right) under different strain rates for the homogeneous index 10 specimens with different b values

Figure 4-33  *DIF* of the simulated tensile strength with the logarithm of strain rate for different values of strength criterion parameter b

The *DIFs* of the simulated tensile strength and the average pressure are also plotted in Figure 4-33 and Figure 4-34, respectively, and show good agreements. Similarly, in higher loading rate cases, the *DIF* value of the predicted tensile strength increase faster for cases with the larger *b* value. However, at low
strain rate cases, the influence from $b$ is not obvious.

![Figure 4-34](image)

Figure 4-34 $DIF$ of the average pressure at specimen’s peak load with the logarithm of strain rate for different values of strength criterion parameter $b$

### 4.6 Summary

In this chapter, the developed SPH program has been applied to simulate the indirect tensile strength determination method via the Brazilian splitting test on rock-like heterogeneous materials with the statistical Weibull distribution model. A series of numerical simulations are performed. Focuses are concentrated on the effects of the material heterogeneity as well as the strain rate on the fracture process and dynamic response characteristics in terms of the predicted tensile strength.

Differences of the fracture process in these cases are compared and analyzed. Results show that the material heterogeneity has significant influences on the fracture processes as well as their predicted dynamic tensile strengths. Such differences come from the non-uniform strength distribution in microstructures controlled by the different material heterogeneity levels. Results also manifest that the predicted tensile strengths increase when the material becomes more homogeneous.

The strain rate has significant influence on the Brazilian fracture process and its
tensile strengths. Generally speaking, the higher strain rate will produce more micro-cracks in the specimen. Beside, the predicted dynamic tensile strengths increase with the increasing strain rates. Moreover, such increments are more obvious in material that is more heterogeneous. The predicted tensile strength increments are compared with those obtained from experiments. Results show a good agreement in the overall trend. Further studies reveal that the increasing pressure due to the rapid loading is one of the major reasons accounting for such effects.

Effects of the coefficient \( b \) employed in the failure criterion are also investigated. Result shows that the predicted tensile strengths are highly influenced by the value of \( b \) under higher strain rate cases.

Result in the current research also shows that the equation to determine the indirect tensile strength in the Brazilian splitting test by SHPB may be invalid above a certain higher loading rate due to it violate the prescribed assumption.
Chapter 5  Rock Dynamic Failure under Compressive Loading

5.1 Introduction

The mechanism of dynamic compressive failure of rock-like materials is of particular importance from both theoretical and practical aspects. Many experimental and numerical studies, such as Kumar (1968), Brace and Jones (1971), Grady and Kipp (1979), Lankford (1981), Masuda et al. (1987), Olsson (1991), Li and Lambros (1999), Zhao et al. (1999), have been conducted on the dynamic properties of rock and rock-like materials under the compressive loadings. These studies showed that the strength of rock and rock-like materials are rate dependent, e.g., the strength becomes higher as the applied strain rate increases.

Rock material is heterogeneous, containing pre-existing defects, such as grain boundaries, micro-cracks and pores. Under the compressive loading, these defects evolve and macroscopic damage will be induced. The inherent heterogeneities play a very important role in the failure process, especially in a dynamic loading condition. Through scanning electron microscope (SEM) and acoustic emission (AE) examinations, it is realized that the growth and nucleation of these defects dominate the failure and the macroscopic mechanical properties of rock material. With these observations, researchers began to pay more attention to analyze the behavior of cracks by experimental and numerical methods in studying the mechanical properties of rock materials under compressive loading.

In this chapter, the developed SPH code by considering heterogeneity of rock-like material is applied to investigate the dynamic failure behavior under compressive loading. Effects of the strain rate as well as the material hetero-
geneity are examined by numerical parametric studies. Besides, influences of the parameter $b$ employed in the yield criterion on the specimen’s dynamic compressive strength is also being examined by adopting the different values of 0, 0.6 and 1, respectively.

## 5.2 Numerical model

### 5.2.1 Specimen geometry and loading conditions

The geometry and loading conditions for the rock specimen used in the numerical simulations are shown in Figure 5-1. The specimen has a width of 5 cm and a height of 3 cm. In the simulation, the specimen is sandwiched between two rigid walls which are loaded by prescribed boundary velocities. The velocity $v(t)$ at the upper and bottom boundaries are given by,

$$v(t) = \begin{cases} \frac{t}{t_0} v_0, & \text{when } t \leq t_0 \\ v_0, & \text{when } t > t_0 \end{cases}$$

(5.1)

where, $t_0 = 5.0 \times 10^{-3}$ s can guarantee the specimen to achieve a stress equilibrium state. The velocity ramp when $t < t_0$ is specially included which can help to achieve the stress equilibrium and prevent the premature failure due to the stepwise increasing force on the loading boundaries. After $t_0$, the prescribed velocities on the boundary are kept at a constant value $v_0$. The strain rate $\dot{\varepsilon}$ is a constant after the time $t_0$ which can be defined as $\dot{\varepsilon} = 2v_0/L$, where $L$ is the specimen height. The loading cases and their corresponding strain rates used in the numerical simulation are shown in Table 5-1.

Along with the specimen’s deformation, the compressive stresses on the two boundaries increase and drop down once the specimen fails. The average peak value of the compressive stresses on the two boundaries is taken as the representative uniaxial compressive strength of the specimen.
Figure 5-1 Geometry and loading condition for rock specimen under dynamic compressive loading, ratio of length to width is 0.6

<table>
<thead>
<tr>
<th>Loading cases</th>
<th>Quasi</th>
<th>Low</th>
<th>Medium</th>
<th>High</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
<td>2 3</td>
<td>4 5</td>
<td>6 7 8</td>
</tr>
<tr>
<td>$v_0 (m/s)$</td>
<td>$1.5 \times 10^{-3}$</td>
<td>0.015</td>
<td>0.15</td>
<td>0.45</td>
</tr>
<tr>
<td>$\dot{\varepsilon} (s^{-1})$</td>
<td>0.1</td>
<td>1</td>
<td>10</td>
<td>30</td>
</tr>
</tbody>
</table>

5.2.2 Numerical approach and parameters

The developed SPH code is applied to simulate the dynamic compression test. The elasto-plastic damage model with the Twin Shear Strength Theory failure criterion is again employed as the constitutive model of the material. To investigate the material heterogeneity effects, two specimens are configured to represent different degrees of heterogeneity by using two normalized Weibull distributions with the homogeneous index 10 and 5, respectively.

For each heterogeneous specimen, firstly, all particles are assigned with the same model parameter values given in Table 3-2. After that, each particle is assigned a random number from the generated Weibull distribution data. The assigned number is further multiplied with its strength related model parameter values, such as $E$, $\sigma_c$, $\sigma_t$ and $D_t$ to obtain the heterogeneous strength values of particle $i$ according to Eq. (3.100).

Two specimens are shown in Figure 5-2. Obviously, the specimen with the homogeneous index 5 has a more heterogeneous distribution of the particles than the homogeneous index 10 one. Each specimen contains 9375 particles, 75 in
height and 125 in width. These particles are evenly distributed in a lattice manner. The SPH particle smoothing length in both specimens is 0.4 mm.

Figure 5-2 Illustration of two numerical specimens with different degrees of heterogeneity having the homogenous indices of 10 and 5, from left to the right, respectively. Intense of the gray scale indicates the magnitude of the particle strength.

Unless it is specifically stated, the parameter $b$ employed in the simulations takes 0.6

5.3 Axial stress-strain curves and fracture processes

The simulated profiles of the average response stress with the axial strain for the eight cases are plotted and compared in Figure 5-3. It can be seen that the uniaxial stress-strain curve is sensitive to the strain rate. The following conclusions can be drawn based on the simulated results:

- The specimen’s axial stress-strain curve exhibits an ideal brittle response when the strain rate is low. The axial stress increases linearly and drops sharply after the peak strength. When the strain rate becomes higher, the curve exhibits three stages: the linear elastic, the non-linear and the post-peak softening.

- Clearly, the specimen’s uniaxial dynamic compressive strength and the sustained maximum strain increase as the strain rate increases.
Numerical Simulation of Heterogeneous Material Failure by using the SPH Method

Figure 5-3 Axial stress vs. axial strain for the heterogeneous rock specimen with the homogeneous index 10 under different strain rates

The specimen’s fracture processes under different strain rates are depicted in Figure 5-4 by plotting the specimen’s damage distributions at their representative frames in the sequence with the loading steps.

For the strain rate 0.1 s\(^{-1}\) case, it can be observed that several isolated micro-cracks occurred close to the specimen’s left side at the mid-height plane at about 80% of its peak stress. Those micro-cracks become more with the increasing applied load and form a short vertical crack close to the left side of the specimen at the peak stress. In the post-peak stage, the previously formed vertical crack grows rapidly towards the top and bottom end, leading to one major traversing crack parallel to the loading axis at 94% of its peak stress. This major crack eventually splits the specimen. Since the specimen’s failure from partially fracture (at its peak stress) state to the complete fracture stage (at 94% stress in the post-peak stage) is very rapid, the specimen suddenly loses its carrying capacity. Therefore, the stress-strain curve drops steeply as shown in Figure 5-3.

For the strain rate 1.0 s\(^{-1}\) case, three macro-cracks can be observed at its peak stress. Among them, the one close to the middle plane appears as the most competitive one. After the peak stress, this crack proliferates and leads to a vertically aligned macro-crack that splits the specimen in the axial loading direction.
The fracture process in the strain rate 10.0 s\(^{-1}\) case is similar to those in the previous two cases except that the developed macro cracks appear wider.

For the cases with the strain rates of 30 s\(^{-1}\) and 50 s\(^{-1}\), it can be seen that the activated micro-cracks are getting more and more. These micro cracks coalesce to form many macro cracks. Finally, the specimen split into many fragments.

In the higher strain rate cases of 120 s\(^{-1}\), 160 s\(^{-1}\) and 200 s\(^{-1}\), many more elongated short-length micro cracks can be observed before their peak stresses. These cracks are evenly distributed within the specimen. At the post-peak stage, the interactions and coalesce of these short-length cracks produce many more oblique macro cracks.

From the numerically simulated results, it can be concluded that the failure processes are remarkably influenced by the strain rate. When the strain rate is low, the specimen’s failure is due to one or few traversing macro-cracks parallel to the loading direction. Therefore, the specimen is split into two or a few parts along with these macro cracks. Since those cracks grow very rapidly after the peak stress, the specimen loses its capacity suddenly and the stress-strain curve drops steeply. When the strain rate becomes higher, specimen’s failure is resulted by many short-length macro-cracks. More fragments are produced during the specimen’s post-peak failure stage. Since these cracks are still growing and interacting after the peak stress, the specimen’s loading capacity does not lose immediately as that in the lower strain rate case. Correspondingly, the stress-strain curve exhibits a strain-softening phenomenon.
Numerical Simulation of Heterogeneous Material Failure by using the SPH Method

strain rate 0.1 s$^{-1}$

strain rate 1.0 s$^{-1}$

strain rate 10 s$^{-1}$
Chapter 5 Rock Dynamic Failure under Compressive Loading

Strain rate $30.0 \, \text{s}^{-1}$

Strain rate $50.0 \, \text{s}^{-1}$

Strain rate $120.0 \, \text{s}^{-1}$
Figure 5-4 Fracture process of the heterogeneous specimen with a homogeneous index 10 under compressive loadings with the strain rate from $1.0 \text{ s}^{-1}$ to $200 \text{ s}^{-1}$.

For the specimen with the homogenous index of 5, the simulated compressive stress-strain curves for the eight cases are plotted and compared in Figure 5-5. Similar to the results of the homogenous index 10 specimen, these stress-strain curves demonstrate a transition from an ideal brittle failure response to the ductile one with the increasing strain rate. The specimen’s dynamic uniaxial strength increases consequently. Their failure processes are plotted in Figure 5-6. As can be seen, they are similar to those of the homogenous index 10 specimen and will not be described elaborately herein.
Figure 5-5 Axial stress-strain curves for the heterogenous specimen with the homogeneous index 5 with the strain rate from $1.0 \text{ s}^{-1}$ to $200 \text{ s}^{-1}$. 

Strain rate 0.1 $\text{s}^{-1}$

1. Strain rate 0.1 $\text{s}^{-1}$
2. Strain rate 1 $\text{s}^{-1}$
3. Strain rate 10 $\text{s}^{-1}$
4. Strain rate 30 $\text{s}^{-1}$
5. Strain rate 50 $\text{s}^{-1}$
6. Strain rate 120 $\text{s}^{-1}$
7. Strain rate 160 $\text{s}^{-1}$
8. Strain rate 200 $\text{s}^{-1}$

Strain rate 1.0 $\text{s}^{-1}$

363601 67% peak
530101 97% peak
569901 100% peak

548101 93% peak
543101 95% peak
549301 80% peak

57501 67% peak
56301 96% peak
56701 100% peak

57001 99% peak
57501 96% peak
56201 82% peak

Strain rate 1.0 $\text{s}^{-1}$
Numerical Simulation of Heterogeneous Material Failure by using the SPH Method

- Strain rate 10.0 s$^{-1}$
  - 05301 67% peak
  - 07501 95% peak
  - 07901 100% peak
  - 08201 98% peak
  - 08401 92% peak
  - 08801 67% peak

- Strain rate 30.0 s$^{-1}$
  - 02301 70% peak
  - 03001 95% peak
  - 03301 100% peak
  - 03451 97% peak
  - 03701 83% peak
  - 03851 67% peak

- Strain rate 50.0 s$^{-1}$
  - 01701 66% Peak
  - 02301 95% Peak
  - 02501 100% Peak
  - 02651 95% Peak
  - 02701 92% Peak
  - 02901 72% Peak
Figure 5-6 Failure process of the heterogeneous specimen with the homogeneous index 5 under compressive loadings with strain rate from 0.1 s\(^{-1}\) to 200 s\(^{-1}\)
5.4 Result discussions

5.4.1 Mechanism of the dynamic fracture process in heterogeneous material

Result in the previous section shows that the fracture processes of heterogeneous rock specimens under compression are influenced by the strain rate. In the case of quasi-static or low strain rate, specimen’s failure is controlled by one or several large macro-cracks roughly aligned to the loading direction. These cracks are originated from those relative ‘weak strength’ zones in the heterogeneous specimen. Consequently, the specimen ruptures into several large fragments. However, in the higher strain rate case, more fractures are activated almost simultaneously during the fracture process. Specimen’s failure is dominated by the interactions of many short length macro-cracks. As a result, the specimen is split into many pieces of small fragments.

Generally, the simulation results agree well with the observations from other researchers such as by Klepaczko (1990) and Li et al. (2005). Figure 5-7 gives the failure patterns of the granite samples from the SHPB tests under different strain rates by Li et al. (2005).

Figure 5-7 Different failure patterns with increasing loading rates (from a to d) for granite samples (after Li et al., 2005)

In the homogeneous index 10 specimen, it is very interesting to note that the locations of the developed macro-crack are different in the strain rate 0.1 s⁻¹ and 1.0 s⁻¹ cases. However, in the homogeneous index 5 specimen, the two cracks take place almost at the same place in the specimen. The difference is mainly due to the specimen’s strength heterogeneity effect. In a relatively homogeneous-
ous specimen, one or few weak zones may cause a catastrophic failure. Therefore, the activations of the micro-cracks at these defect locations are more sensitive to the loading conditions and may result in different phenomena under different strain rates.

Evidently, the predicted results provide a wealth of information regarding the characteristics of the evolving fracture process and the failure pattern that is relatively difficult to be obtained by the experiments. For instance, in those tests, acquired information is mostly limited to the observation from the specimen’s surface. In this respect, the simulated failure processes is greatly useful for better understanding the specimen’s failure mechanisms.

To quantitatively assess the strain rate effect on the specimen’s failure process, statistics of the damaged particle numbers at their peak stresses under different strain rate cases for the two heterogeneous specimens are shown in Figure 5-8. As can be seen, the number of damaged particles increases with the increasing strain rate in both cases. One can also observe that, when the strain rate is above $120 \, \text{s}^{-1}$, the increments are not so obvious. As the strain rate becomes higher, more weak particles in the heterogeneous specimen will damage. In the heterogeneous specimen, those weak particles are limited to a certain number. Hence, there is not much chance to develop further damages once all those weak particles fail.

Figure 5-8 The accumulated damaged particle numbers vs. different strain rates in two heterogeneous specimens at the moment of their peak stresses, accordingly
By comparing the two heterogeneous specimens, one can also find that the number of damaged particles for the relatively homogeneous case (index 10) is fewer than that for the homogeneous index 5 case at the same strain rate. Therefore, the more heterogeneous specimen generates more micro-cracks under the same loading condition. Same conclusion can also be obtained by comparing the failure processes of these two specimens.

Figure 5-9 Frequency counts of all damaged particles by means of their normalized strengths at the moment of the peak stress in specimen with heterogeneous index 10 under different loading rates.

Figure 5-9 compares the frequency counts of all damaged particles at the moment of the peak stress by means of their normalized strengths in specimen with heterogeneous index 10 under four different strain rates. The specimen’s initial strength distribution is also plotted in the figure. It can be found that, under the low strain case, most of the damaged particles are those with lower strengths. However, with the increase of the strain rate, many particles with higher strengths are involved and may contribute to a higher specimens’s macro compressive strength. Besides, we can find that the strength distributions of these damaged particles are not much different when the strain rate is above a certain value, for example, of 50 s\(^{-1}\) in our simulations. Such an observation is helpful
to understand the strain rate effects on the heterogeneous specimen’s dynamic strength and will be discussed later.

5.4.2 Predicted dynamic compressive strength in heterogeneous materials

The predicted dynamic uniaxial compressive strengths with the logarithm of strain rate for the two different heterogeneous specimens are plotted in Figure 5-10. To investigate the influence of the strength criterion parameter \( b \) on the dynamic strength, similar simulations are also performed on the homogeneous index 10 specimen with \( b = 0 \) and \( b = 1.0 \). Results are also plotted in the figure for a comparison.

![Figure 5-10](image_url)

Figure 5-10 Comparison of simulated apparent uniaxial compressive strengths with the logarithm of strain rate between two different heterogeneous specimens.

The material heterogeneity as well as the strain rate effects on the specimen’s compressive strength is discussed as following:

- Effect of the specimen’s heterogeneity

From Figure 5-10, one can observe that the material heterogeneity has notable influence on the specimen’s compressive strength. Generally, the specimen ex-
hibits a higher strength when it is more homogeneous.

It can also be observed that, as the strain rate becomes higher, the strength difference between these two specimens appears smaller. As discussed previously, in the low strain rate cases, the specimen’s failure is controlled by a single or few macro-cracks initiated usually from its weakest part. However, under higher loadings, the specimen’s failure is dominated by many cracks. Therefore, the specimen’s strength reflects a collective response by many particles, which results in a relatively smaller difference on the strength of the two specimens.

- **Effect of the strain rate**

The predicted dynamic uniaxial compressive strengths of the two heterogeneous specimens demonstrate obvious rate dependence as shown in the Figure 5-10. Result from the simulations agrees well with those done by other researchers on rock and concrete. We also observe that, when the strain rate is above a certain value, the strength increases sharply with the strain rate as reported in experiments by Kumar (1968), Olsson (1991) and other researches.

![Figure 5-10](image)

Figure 5-10 shows the predicted dynamic uniaxial compressive strength of the two heterogeneous specimens. The predicted strength is compared with the experimental results. The DIF values are plotted against the logarithm of the strain rate. The figure demonstrates the rate dependence of the predicted strengths.

![Figure 5-11](image)

Figure 5-11 Comparisons of the DIF values of the predicted compressive strength for two specimens with different heterogeneous levels and experimental results with the logarithm of strain rate.

Figure 5-11 compares the numerical predicted apparent dynamic compressive strength in terms of the dynamic increment factor (DIF) with experimental tests.
using granite samples. The dynamic increment factor \((DIF)\) is defined in Chapter 4. For numerical results, it takes the strength at strain rate \(0.1\text{s}^{-1}\) as the quasi-static reference value. Experimental data are obtained by using the SHPB tests and can be referred in the Appendix B. The \(DIF\) takes the compressive strength at the strain rate \(5\times10^{-5}\text{s}^{-1}\) as the referred quasi-static value.

Comparisons between the numerical and experimental results show that they both have the same incremental trend as the strain rate increases. It seems that the result from the specimen homogeneous index 10 matches the experimental result better.

Since our model is strain rate insensitive, where its parameters are determined by the static tests, such a dynamic strength enhancement should come from other sources. Several theories have been put forwards to account for such phenomena. For instance, the hypothesis proposed by Gopalaratnam et al. (1996) attributes such effect to the material viscoelastic behaviors. The inertial based hypothesis, proposed by Brace and Jones (1971), Janach (1976), Bischoff and Perry (1991), Bischoff and Perry (1995), Donze et al. (1999), etc, suggests that the strain rate effect on the dynamic strength is mainly due to the increasing hydrostatic confinement caused by the lateral inertial effect. Li and Meng (2003) validated the hypothesis in their numerical simulations, where the strain-rate insensitive constitutive models were employed and the simulated dynamic strength exhibited strain rate effects. They concluded that the lateral confinement mainly come from the radial inertia in dynamic loading. However, it may be caused by various reasons, such as the interface friction constraints between the sample ends and the SHPB pressure bars.

Based on our previously predicted micro-cracking activities in the failure processes and discussions on the failure mechanism, the inertial based hypothesis is reasonable. Under the high strain rate loading, many micro-cracks are produced and there have limited time for their development or propagation. On one hand, in the axial loading direction, the inertial forces will increase the apparent resistance opposite to the movement when local stress equilibrium is not achieved. Higher load will be needed before cracks become prominent enough.
to rupture the specimen. On the other hand, when the expanding lateral strain is inhibited, the inertia will also act on the lateral direction to cause an apparent effective pressure confinement.

Beside the inertial effects, the material heterogeneity also contributes to the strength enhancement. As illustrated by Figure 5-9, under the low strain rate cases, the macro strength of heterogeneous specimen is controlled by few particles with relatively weak strength. With the increasing strain rate, its strength can be enhanced since there will be more chances for relatively strong particles to be involved and contribute. Such a heterogeneous effect may be mainly responsible for the strength increase when the strain rate is not high. As recalled from Figure 5-8 and Figure 5-9, the total number of damaged particles and their distributions seems not much difference when strain rate is above 50 s\(^{-1}\). It implies that the apparent strain rate effects mainly come from the inertial effects at the higher loading rate cases. All the above reasons will result in the internal pressure increase.

![DIF of average pressure with the logarithm of strain rates for two heterogeneous specimens with different b values](image)

**Figure 5-12 DIF** of the average pressure with the logarithm of strain rates for two heterogeneous specimens with different \( b \) values

To elucidate the inertial induced confining effects on the rate-dependent phenomena, the DIF values of the average pressure for those cases with the loga-
rithm of strain rate are plotted in Figure 5-12. The $DIF$ of the average pressure is defined as the ratio of the average pressure in the specimen at its peak stress to the pressure in the static case at strain rate $0.1 \text{ s}^{-1}$.

By comparing Figure 5-11 with Figure 5-12, it is very interesting to see that the trend of these two $DIF$ curves remarkably match each other. Such a good relation manifests that the rate-dependent dynamic strength come mainly from the specimen’s internal pressure increase. It is also found that, when the strain rate is above a certain higher value, the internal pressure increases sharply. This confirms our previous deduction and supports the conclusion by Li and Meng (2003) and others.

- Effects of the strain rate as well as the material heterogeneity

The aforementioned inertia effect and the fracture mechanism can well explain the rate–dependence of the dynamic strength. From the $DIF$ of strength curves, we can also observe that this rate-dependence is affected by the material heterogeneity. It is clear that, at the same strain rate, the $DIF$ value of more heterogeneous specimen (homogeneous index 5) increases faster than that in the less heterogeneous one (homogeneous index 10).

This can be explained by the micro-cracking effect manifested in the previous discussion on failure processes. In heterogeneous specimens, failure is caused by micro-cracks initiation, propagation and coalescence. Because the extension of the micro-cracks takes time, other micro-cracks are activated before a neighboring activated micro-crack extends and unloads them. As a result, the specimen breaks with more cracks at higher loading rates; while at lower loading rates, a single or few major cracks cause catastrophic failure. As can be seen from Figure 5-8, it is evident that more heterogeneous specimen forms more micro-cracks than the less one does at the same strain rate. On one hand, this would cause stress releasing during the formation of these cracks and consume considerable energy. On the other hand, the formation of these cracks delays the specimen’s failure that is helpful for the load to be able to further increase. Thereafter, the dynamic average pressure is highly dependent on heterogeneous conditions.
• The coefficient $b$ in UTSS strength criterion

As mentioned previously, the adopted UTSS criterion can produce a full spectrum of new criteria to reflect the characteristics of various materials by varying the value of $b$ between 0.0 and 1.0. When $b=0$, it becomes the single-shear criterion (e.g., the Mohr-Coulomb) to give the lower limit convex shape function. When $b=1$, it becomes the Twin-Shear Strength criterion, which gives the upper limit convex shape function.

To examine effects of $b$ on the compressive strength, two series of compressive simulations on the heterogeneous specimens of homogeneous index 10 with the same loading rates were performed with $b=0$ and $b=1$, respectively.

The simulated axial stress-strain curves for these two cases are plotted in Figure 5-13 and Figure 5-14 under different loading rates, respectively. These two series of curves are generally similar to those of $b=0.6$ as described previously. As can be seen, the peak stresses and their corresponding axial strains slightly increase when the value of $b$ becomes from 0 to 1.0 at the same strain rate. A more clear observation from Figure 5-10 also shows such a strength increment trend as the value of $b$ becomes larger. The result coincides to the UTSS theory in that a larger $b$ value corresponds to a bigger convex shape.

![Figure 5-13 Axial stress vs. axial strain for the heterogeneous specimen with the homogeneous index 10 under different strain rates with $b=0$](image)
Figure 5-14 Axial stress vs. axial strain for the heterogonous disc with homogeneous index 10 under different strain rates with $b=1.0$

We can also observe the strain rate effect on the DIF of the compressive strength as in Figure 5-11. The DIF value of $b=0.6$ is nearly between those values of $b=0.0$ and $b=1.0$, which is coincident to its DIF value of average pressure as plotted in Figure 5-12.

5.5 Summary

In this chapter, the developed SPH program is applied to simulate the dynamic uniaxial compressive failure on rock-like heterogeneous specimens. Investigations are concentrated on the effects of the material heterogeneity as well as the strain rate on the specimen’s fracture process and the dynamic response characteristics. Simulation results from two specimens with different degrees of heterogeneity are compared in terms of their fracture processes and predicted compressive strengths.

Results show that material heterogeneity has significant influences on the fracture processes as well as the predicted dynamic compressive strengths. Such differences come from the heterogeneous strength distribution in the specimen controlled by the different degrees of material heterogeneity. Results also manifest that the predicted compressive strength increases as the specimen be-
comes homogeneous in all strain rate cases.

The strain rate effect on the specimen’s fracture process and its dynamic compressive strength is also examined. Result shows that the fracture mechanism under the higher strain rate cases is different from that in the lower cases. In addition, it also shows that the predicted dynamic compressive strength has clear strain rate dependences as demonstrated in the experimental results. Further studies reveal that the increasing pressure due to the rapid loading is one of the major reasons accounting for such effects.

The strain rate dependent dynamic compressive strength is affected by the material heterogeneity. Result shows that the strength increases faster for the more heterogeneous specimen.

Effects of the parameter b employed in the strength criterion are also examined. Result shows that the predicted compressive strength increases as the value of b becomes larger.
Chapter 6 Heterogeneous Rock Failure under Uniaxial Compressive Loading and Biaxial Loading Conditions

6.1 Introduction

The study of rock brittle failure under compression is essential for an understanding of many processes in rock engineering and earth sciences. Researchers have performed many experimental and numerical studies to obtain better knowledge on the failure mechanism and the fracture process. A considerable literatures has been yielded on this topic, such as those by Hegemier and Read (1984), Nemat-Nasser (1985) and Andreev (1995).

Figure 6-1 illustrates several typical failure modes for rock material under compression by Jaeger et al. (2007). Under unconfined uniaxial compression, rock sample tends to appear the brittle failure featured by that the failure happens abruptly. The failure is usually accompanied irregular longitude axial splitting as shown in Figure 6-1 (a). With the moderate confinement, failure occurs along a clearly defined fracture plane as shown in Figure 6-1 (b), characterized by shearing displacement along its surface. Usually the shear fracture plane is inclined at an angle less than 45° from the direction of the axial loading plane. With the increment of the confining pressure, the rock becomes relatively ductile. Usually a network of small shear fractures appears, accompanied by the plastic deformations as shown in Figure 6-1 (c).

Although the axial splitting failure is the mostly common one in the unconfined compression tests, in reality, the failures exhibit diversity. As can be seen from Figure 6-2, the marble specimens may fail in splitting, faults or the combined modes as reported by Andreev (1995). What’s more, even with the same failure mode, the specimens’ failures may quite differ from one another.
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Figure 6-1 Illustration of different failure modes of rock samples under compression (after Jaeger et al., 2007)

Figure 6-2 Marble specimens failed under uniaxial compression by a) Axial splitting; b) fault; c) and d) Combined failure patterns (after Andreev, 1995)

Figure 6-3 gives the schematics for the states of micro-cracking initialization and shear crack formation observed on quartzite specimens under the triaxial test by Hallbauer et al. (1973). Initially, the visible elongated micro-cracks appear. Then, the number of micro-cracks increased drastically, and these cracks began to coalesce along a plane located in the central region of the specimen. At the point of the peak axial stress, the micro-cracks begin to link up to form a macroscopic fracture plane. Finally, the fracture plane has extended through the entire specimen, and shear displacement begins to occur across the two ends of the specimen.

The above descriptions manifest the failure modes are dependent on the loading conditions and closely related to the micro-cracks activities. Those micro-cracks activities involve their initiations, growths and accumulations during the failure process. Although these observations can give physical descriptions
of fracture phenomena, an accurate prediction of these phenomena remains one of the most difficult tasks. Fracture mechanics theory is very successful in predicting fracture generations and propagations. However, in the classic fracture mechanics extent, it is difficult to determine micromechanical parameters such as crack density and roughness for different mode cracks. Recently, several numerical models based on the continuum damage mechanics have achieved success in predicting heterogeneous fracture processes. For instance, Tang et al. (2000a) successfully simulated heterogeneous effects on rock failures under the uniaxial compression. Fang and Harrison (2002) developed the local degradation model based on FLAC and simulated the rock fracture under triaxial loading conditions. Although these methods are successful in some aspects, they may have limitations in processing the large deformations, crack propagations and fragmentations.

Figure 6-3 Schematics of the states of micro-cracking initialization and shear the crack formation observed on quartzite specimens by Hallbauer et al. (1973) under triaxial test

The developed SPH program can handle both continuity and discontinuity. Therefore, it is suitable to be applied to examine the rock compressive failures.
6.2 Numerical model

6.2.1 Specimen geometry and loading conditions

The geometry and loading conditions for the rock specimen are shown in Figure 6-4. The specimen’s width is 0.05 m and height is 0.1 m. In the figure, the left one represents the unconfined uniaxial compression test under 2D plane strain or plane stress condition.

In the simulation, the specimen is sandwiched into two rigid walls loaded by boundary velocities without end frictions. Loading velocity is constant at -0.1 m/s. The right graph represents a biaxial compression test under the plane strain condition. The prescribed initial stress is firstly applied to the two sides of the specimen and the outer surface of top and bottom sides to achieve a hydrostatic stress state at a level of specific confining pressure. After that, an axial velocity boundary condition at -0.1 m/s is applied to produce an additional axial force.

The dynamic relaxation method implemented in AUTODYN (2005) is adopted to apply the initial confining stress. By introducing a static damping coefficient $R_d$, the particle’s velocity will be,

$$
(v_a)^{(n+1)} = (1 - 2\pi R_d)(v_a)^{(n)} + (1 - \pi R_d)(a_a)^{(n)} \Delta t^{(n)}
$$

(6.1)

where, $(a_a)^{(n)}$ and $(v_a)^{(n)}$ are the particle’s accelerations and velocities at the
time integration of $n^{th}$ loop, $\Delta t^{(n)}$ is the time step and $R_d$ is the static damping coefficient. The value of $R_d$ for critical damping of the lowest mode is,

$$R_d = \frac{2 \Delta t}{T} \frac{1}{1 + 2\pi \frac{\Delta t}{T}}$$

(6.2)

where, $T$ is the period of the lowest mode of vibration of the system. It is commonly believed that the solution to converge to the static equilibrium state in a time roughly $3T$ if the value of $T$ is that for critical damping.

Since $\frac{\Delta t}{T} \approx 0$, Eq. (6.2) can be simplified as,

$$R_d \approx \frac{2\Delta t}{T}$$

(6.3)

The confining stress is applied as a ramp function to those boundary particles as,

$$p(t) = \begin{cases} \frac{t}{T}p_0, & \text{when } t \leq T \\ p_0, & \text{when } t \geq T \end{cases}$$

(6.4)

where $p_0$ is the specific confining stress.

After the $3T$ time, the axial velocity boundary conditions will be applied to produce the deviatoric axial stress.

For the single freedom system, the critical damping $T$ is,

$$T = \frac{2\pi}{\omega_n} = \frac{2\pi}{\sqrt{\frac{K}{m}}} = \frac{2\pi}{\sqrt{\frac{EA}{lm}}}$$

(6.5)

where $E$ is the Young’s modulus, $A$, $l$ and $m$ are specimen’s cross-section area, length and mass, respectively.

Along with the specimen’s deformation, reaction forces on the two boundaries increase and then drop down when the specimen fails. The average value of the stresses on the two boundaries is taken as the specimen’s macroscopic response.
Chapter 6 Heterogeneous Rock Failure under Uniaxial Compressive Loading and Biaxial Loading Conditions

6.2.2 Numerical approach and material parameters

The developed SPH program is applied to simulate the uniaxial and biaxial compressive test. Three specimens are configured to represent different degrees of heterogenous rock materials as shown in Table 6-1. The generated specimens are shown in Figure 6-5.

<table>
<thead>
<tr>
<th>Homogeneous index</th>
<th>3</th>
<th>5</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specimen</td>
<td>H03-1</td>
<td>H03-2</td>
<td>H05-1</td>
</tr>
<tr>
<td>Heterogeneity</td>
<td>More</td>
<td></td>
<td>Less</td>
</tr>
</tbody>
</table>

Figure 6-5 Numerical specimens with the increasing homogenous index $\beta$, from left to right. Intense of the gray scale indicates the magnitude of the particle strength.

Each specimen is discretized into 20000 SPH particles, 100 in width and 200 in height. The SPH particle smoothing length is 0.5 mm. For each heterogeneous specimen, firstly, all particles are assigned with the same model parameter values given in Table 3-2. After that, each particle is assigned a random number from the generated Weibull distribution data. The assigned number is further multiplied with its strength related model parameter values, such as $E$, $\sigma_c$, $\sigma_t$, and $D_1$ to obtain the heterogeneous strength values of particle $i$ according to Eq.(3.100). For each specimen, simulations under both plane strain and plane stress conditions are preformed. Later on, simulations on the biaxial compres-
sion tests with different confining pressures under the plane strain condition are carried on for the H05-02 specimen.

6.3 Results under the uniaxial compression simulation

6.3.1 Results for homogeneous index 3 specimens under plane strain condition

The axial stress-strain curve for the specimen H03-01 is plotted in Figure 6-6.

![Simulated axial stress-strain curve and the profile of damaged particles profiles for homogeneous index 3 specimen H03-01 under plane strain condition](image)

The profile of simulated AE (acoustic emission) counts is also plotted in the figure by recoding the number of damaged particles according to the incremental axial strain. The monitoring of the AE produced during the deformation has been widely used as an effective method to observe crack activities during rock deformation experiments by many researchers such as Cox and Meredith (1993). It is commonly believed that, during the specimen’s deformation process, a variety of micro mechanisms activities, including dislocation, twin and crack formations, will cause such AE events. For the brittle failures, crack formation is of the most importance in the above micromechanical activities. Therefore, by associating the single AE event with the micro crack formation, one can deduce the specimen’s damage by the AE event record. Numerical approach to simulate
AE events on rock failure studies has been used by many researchers, such as in Tang et al. (2000b). When the particle fails from the intact, strain energy is released accordingly. Therefore, each particle failure event can be regarded as one AE count. It is found that, initially the stress-strain curve slightly fluctuates with more damaged particles during the loading. With the incremental strain, the curve exhibits non-linear characteristics before the maximum stress. After that, the curve drops down to a low stress level and exhibits the strain-softening characteristic. From the profile of damaged particles, as can be seen, before the 75% peak stress (marked by point a), few particles fail. After that, more damaged particles occur with the increasing load. Dramatically, a large volume of damaged particles occurs shortly after the peak stress along with that the stress quickly drops down. It can be deduced that a large number of macro-cracks are being formed during such a period. Many researchers in their studies have evidenced the phenomenon. For instance, Maher and Darwin (1982) describes, “crack begin to appear in the specimens shortly after crossing the peak of the stress-strain curve.”

The distributions of the damaged particles of H03-01 specimen at different stages are plotted in Figure 6-7 in sequence corresponding to the moment marked as “a” to “f” in Figure 6-6. Each circle represents one AE event. Circles in dark indicate AE locations in the previous frame.

At stage a, it seems that the damaged particles are randomly distributed throughout the specimen. Following at stage b, we can observer that more events take place and some are clustered. At the moment of its peak stress, it can be seen more events happen along the previous clusters by those damaged particles. It seems that potential damaged zones will be formed near these clusters. However, at stage e, we observe that more events happened and intend to coalesce with the previous isolated zone into inclined crack zones close to the left side. Finally, at the stage f, these damaged particles forms two inclined zones cut through the specimen. The migrations of damaged zone reflect the heterogeneous stress distribution in the specimen and its consequent redistribution due to the local failures.
Figure 6-7 Simulated distributions of damaged particles for the heterogeneous specimen H03-01 during the fracture process.

Figure 6-8 plots the failure process of specimen H03-01 and the final failure pattern. Cracks are represented by plotting the damaged particles in dark black. When specimen fails, those damaged particles can separate according to the governing equations and fragmentations will be formed consequently. The final failure pattern is obtained by plotting the particles according to their locations.

Figure 6-8 Simulated failure process and final failure pattern of specimen H03-01 under plane strain corresponding to stages from a) to f) in Figure 6-6. Initially, the isolated micro-cracks are distributed throughout the specimen ran-
domly. Next, these micro-cracks start to form a cluster. Their nucleation controls the formations and evolutions of macro-cracks in the future stage. At last stage, those macro-cracks interact and coalesce to form two major shear faults. In the final failure pattern, one can clearly observe these two major faults in white and those fragments caused thereafter. Small flying fragments can also be observed at the left and right sides of the specimen. Hence, the specimen’s fracture looks like the rock burst. The developed SPH code can well capture the failure process and represent the real cracks and fragmentations induced by large deformations vividly. Moreover, the whole process does not need any special treatments, such as remeshing, to handle such large deformations or any assumption in presenting the cracks and fragments. From the view of this point, the SPH code has obvious advantages over other methods in rock-like brittle material failure simulations.

The phenomenon that most macro-cracks are formed shortly after the post-peak stage agrees well with the simulated profiles of the damaged particles shown in Figure 6-6. Although the exact locations of major faults can only be known until its final failure stage, one can still predict the major one at the earlier stage as shown by the arrow at the specimen’s peak stress stage in Figure 6-8 c). Furthermore, it is worth noting that most of the macro-cracks are parallel to the applied stress before the faults form.

Figure 6-9 shows the stress-strain curve and the simulated profile of the damaged particles along with the strain for the specimen H03-02. The specimen’s failure process and final failure pattern are plotted in Figure 6-10.

The specimen H03-02 has the same degree of the heterogeneity with H03-01. As can be seen, due to different spatial distributions of the particles, the failure process of them may differ from one another. Again, we can clearly observe the major faults and fragments in the plot of specimen’s failure pattern.
Numerical Simulation of Heterogeneous Material Failure by using the SPH Method

Figure 6-9 Simulated axial stress-strain curve and the profile of the damaged particles for homogeneous index 3 specimen H03-02 under plane strain condition

![Simulated axial stress-strain curve and the profile of the damaged particles](image)

Figure 6-10 simulated failure process and failure pattern of specimen H03-02 under plane strain

In Figure 6-11, the stress-strain curves and the profiles of accumulated damaged particle numbers with the incremental strain for these two specimens are plotted together. Although these two specimens are quite different in their heterogeneous microstructures and failure processes, their mechanical responses are similar. Characteristics of these two curves match well with those from experimental results by Wawersik and Fairhurst (1970). Two curves appear almost same during the small strain stage. In this period, randomly distributed micro-cracks have little influence on the whole stress filed. Following with the more micro-cracks activations and their coalitions, curves become different and nonlinear behaviors are pronounced. Stresses distributions at this stage are remarkable inhomogeneous. Potential macro-cracks are formed depending on their different microstructures, which may lead to the different peak strengths. After that,
specimens are in post failure stages and become unstable. More macro-cracks appear with stress redistributions. Their interactions lead to faults or splitting planes, which cause curves to drop down in different manners. One can also deduce this difference by comparing the accumulated damaged particles curves in this stage. Finally, we see that two curves approach to a similar residue strength.

![Graph](image)

**Figure 6-11** Comparison of the stress-strain curves and the accumulations of damaged particles for the specimens H03-01 and H03-02 with the same degree of heterogeneity under plane strain condition

### 6.3.2 Simulation results for other specimens and discussions

Based on previous compressive simulation results for the H03-01 specimen under plane strain condition, it can be found that both the macro mechanical response and the failure process can be well modeled using the developed program. In this section, other simulation results are presented. Discussions are focused on the differences in their stress-strain curves, failure processes and failure patterns.

- **Stress-strain curves and uniaxial compressive strength (UCS)**

Axial stress-strain curves of all specimens both under plane strain and plane stress conditions are shown in Figure 6-12. The shapes of these curves are typical brittle response ones similarly as those by H03-01 and H03-02. The stress-strain keeps nearly linear with the incremental strain until certain stress
levels. With the local failures and stress redistributions, these curves exhibit non-linear somehow. After the peak stress, they fall down rapidly to a certain residual stress like the brittle failures.

Effect of material heterogeneity on the macro stress-strain can be found from Figure 6-12. For specimens with different degrees of heterogeneity, their apparent Young’s modulus in linear regions increases when the specimen becomes more homogeneous. For specimens with same degree of heterogeneity, their apparent Young’s modulus values evaluated from their linear stage of stress-strain curves are almost identical regardless of under plane strain or plane stress conditions.

As can also be found, the curve behaves more brittle when the specimen becomes more homogeneous. For the plane strain conditions, due to the strain constrained along the out-of plane direction, the specimen will have a residual stress.

Figure 6-13 shows all the simulated UCS values. Material heterogeneity effects on the material strengths can be seen evidently. The UCS values of heterogenei-
ous specimens are far smaller than the assigned seed value in the model. The more heterogeneous the specimen is, the smaller its UCS value. Besides, the UCS values of different specimens, even with the same degree of heterogeneity, may be different. The more homogenous these specimens are, the scatter their UCS values. Due to the material heterogeneity, each specimen has its own properties and exhibits unique macro mechanical response in experiments. While, for those with same degree of heterogeneity, their macro mechanical characteristics are similar.

Figure 6-13 Simulated uniaxial compressive strengths for heterogeneous specimens under plane strain and plain stress conditions

In numerical simulations, the specimen is commonly assumed to be under the plane strain or plane stress conditions dependent on the situation. In the simulations, we find that the UCS value under the plane strain condition is smaller than that of the same specimen under plane stress condition. This phenomenon manifests the employed strength criterion in the numerical model is sensitive to the middle principal stress.

- Profiles of accumulated damaged particle occurring numbers with strains
  Profiles of heterogeneous specimens’ accumulated damaged particles against the incremental strains are plotted in Figure 6-14.
Numerical Simulation of Heterogeneous Material Failure by using the SPH Method

Figure 6-14 Simulated damage particle accumulation curves for all heterogeneous specimens under plane strain and plane stress conditions

Compared with those more homogeneous specimens, the less homogenous specimens have more damage particles before their peak stresses due to local failures of more weak particles. As described previously, a large volume of damaged particles indicate formations of rapid growing macro-cracks. For those relatively homogenous specimens, majority of these damaged particles occurs during the short time after its peak stress. Thus, once a few clusters of micro-cracks emerge, they will propagate rapidly to form macro-cracks and result in the failures in a catastrophic way. In those relatively homogeneous specimens, a few “weak” regions may arouse the crack initializations. Hence, their failures are more difficult to be predicted. Such a fact also can be account for why strengths are more scattered in those more homogeneous specimens as mentioned previously.

- Failure processes and failure patterns

Failure processes of two specimens with the homogeneous index 3 and their fracture patterns the under plane stress condition are plotted in Figure 6-15.
Chapter 6 Heterogeneous Rock Failure under Uniaxial Compressive Loading and Biaxial Loading Conditions

Figure 6-15 Failure processes and failure patterns of homogeneous index 3 specimens of H03-01, H03-02 under the plane stress, respectively

It is clear that the crack activities become evident only when the axial stress approaches the peak value. At this stage, the specimen’s fracture is characterized by the formation of different populations of isolated macro-cracks. After the peak strength, macro cracks become extremely pronounced and clearly predominated along the direction of the loading. Consequently, these macro cracks join together and lead to many axial cracks predominantly along cleavage planes. It is noteworthy that some short beam-like axial cracks form the shear faults due to the bulking as described by Peng and Johnson (1972) and Janach (1977). Failure patterns for these two specimens under plane stress are more like a combination modes of axial splitting and shear faults.

The crack developments for the specimen H05-01 and H05-02 under plane strain and plane stress conditions are depicted in Figure 6-16, where the final failure patterns of these specimens are darkened for better visual effects. As can be seen, failure processes are evidently distinct in these two samples though the general characteristics at different stages are similar. For H05-01 under the
plane strain condition, at the stage near its peak stress, one shear macro crack at
the lower left corner is formed. In its post-failure stage, this primary major
crack grows fast along the specimen’s central part and propagates towards the
bottom and top sides almost parallel to the loading direction. Its final failure
pattern appears to be the combination one. However, under the plane stress
condition, the axial cracking is more obvious and precedes the faults formations.
Again, such differences manifest that failures are highly dependent on the stress
conditions.

For H05-02 under the plane strain condition, although the failure is by faulting,
one can observe that axial cracks are also well developed earlier. In the plane
stress condition, the axial cracking is predominant.
Figure 6-16 Failure processes and final failure patterns of homogeneous index 5 specimens under plane strain and plane stress.
Failure developments for the specimen H10-01 and H10-02 under plane strain and plane stress conditions are shown in Figure 6-17. Again, the final failure patterns of these specimens are darkened for better visual effects. As can be observed, failures of these specimens are mostly induced by major cracks. Once the preferred macro crack is formed, it propagates rapidly toward both ends of the specimen. Large volumes of micro-cracks grow intensely after the major crack is well developed. Their activities such as interactions and twisting influence the failure pattern as shown in the plot.
Figure 6-17 Failure processes and failure patterns of the homogeneous index 10 specimen under the plane strain and plane stress conditions

The simulation results show that failure developments for these brittle specimens have some common characteristics. First, conspicuous cracks are formed near their peak stresses and mostly parallel to the loading directions as reported by other researchers, for instance, Wawersik and Fairhurst (1970). Second, axial cracks or faults are formed during their post-failure regions. In some cases, these faults are caused by the bulked “beams”. Furthermore, although the shear faulting and the cleavage are the two major modes in rock failures, simulation results show most failure patterns are the combination one.

Results of the simulated failure processes manifest that rock failure and its mode are highly affected by its material heterogeneity as well as the different stress conditions. For the specimens with different degrees of heterogeneity, one can clearly observe that the major crack will dominate the failure in a more homogeneous specimen. On the contrary, in less homogenous one, activities of many macro cracks will cause the failure. Even for specimens with the same degree of heterogeneity, the initial cracks and their consequent developments are highly affected by their microstructures due to the local stress severities. In 2D numerical simulations, the plane strain and plane stress condition assumptions are commonly used to simplify the real cases. However, simulation results show that they lead to different answers and may cause misrepresentations even for the same specimen.
6.4 Fracture process by the compressive load under different confining pressure in the plane strain condition

6.4.1 Failure processes

The failure of the heterogeneous rock-like specimen H05-02 is studied in terms of the failure process and the stress-strain characteristics with different confinements under the plane strain condition. The confining stress is applied as described previously, at 0, 2.5, 5.0, 10 and 20 MPa. Fracture processes for these cases are shown at Figure 6-18.

![Fracture process images](Figure 6-18)
Chapter 6 Heterogeneous Rock Failure under Uniaxial Compressive Loading and Biaxial Loading Conditions

with confinement of 5.0 MPa

Figure 6-18 Failure process for the homogeneous index 5 specimen H05-02 under compression with different confinements

The specimen’s uniaxial failure process without confinement is depicted previously. At the 98% peak stress, an oblique macro-crack forms and subsequently propagates rapidly aligned with the loading direction toward both ends of the specimen at the peak stress. During the post-failure region, the forenamed crack continues to develop and suggests an axial splitting failure mode. More micro-cracks appear along the sides of the major crack and a set of shear crack oriented at the upper right side of the specimen with an angle of about 45° to the loading direction by many bulking short ‘beams’. Finally, it is interesting to note the set of shear crack join the previously developed cracks and form the shear plane.

Under the low confining stress of 2.5 MPa, the first conspicuous crack takes
Numerical Simulation of Heterogeneous Material Failure by using the SPH Method

place almost at the same place as the uniaxial compression one near the peak stress. However, its propagation along the loading direction is prohibited by the lateral confining stress. As can be seen at the post-failure stage around its 73% peak stress, besides the shear crack at the upper right part, another two isolated sets of shear cracks appear at the lower half part along the same oblique plane. Subsequently, they grow and coalesce together to form the second shear fault plane that is shorter than the previous one. For the confinement of 5.0 MPa case, it is clear to see that the axial crack is further inhabited by the incremental lateral stress. It is noteworthy to observe that the first short shear fault become the primary shear fault after peak stress.

Failure propagation for the confinement of 10 MPa is similar to that of the 5MPa one. When confining stress becomes 20MPa, before the peak stress, the crack development is identical to previous ones. During the post-peak stage, shear faults become wider. Furthermore, the short shear fault has a larger angle to the vertical plane than those in other cases as indicated by the arrows in Figure 6-19.

In the unconfined case, there is only one shear fault. For cases with confinement, specimens have two major faults. For these cases, relatively few cracks form in the early stage. Near the peak load, major crack appears and tends to be aligned with the direction of maximum compression. After the peak stress, two macroscopic failure planes develop and cut across the specimen. As the confinement increases, the developments of axial cracks are inhibited. Besides, both shear cracks appear wider. The angle of the short shear crack to the vertical plane also increases slightly. Failure development at peak load is quite similar for all confining cases, and most damage occurs after peak load as the specimen expands along lateral direction. For the above discussions, it seems that the post-peak failure process is affected by the confinement. It is concluded that, with the increment of confinement, the tensile stress perpendicular to the maximum compressive plane decrease. Therefore, axial cracks are restrained and more shear cracks developed to form shear faults.
6.4.2 **Macroscopic axial stress-strain curves**

The axial stress-strain curves for the specimen H05-02 with confinement from 0.0 to 20 MPa under plane strain are plotted in Figure 6-20. Although simulations are not the real triaxial test, it is still clear to be seen that the peak strength increases with the incremental confining stress.

![Figure 6-19 Failure patterns of H05-02 under different confining stress](image)

Such a conclusion is consistent to the results by other researchers, such as Wawersik and Fairhurst (1970) and Zhao (1999). Apart from the expected increase in axial peak strength, higher lateral stress also leads to the peak strength occur-
ring at a larger axial displacement. One difference from those triaxial experimental results is that the nonlinear behaviors and the flattening from the curves are not obvious. However, as also pointed by Hallbauer et al. (1973), the nonlinear behavior is mainly attributed to and dependent on the formation and the density of micro-cracks conducted under the low confinement stress part. Since the crack density is highly influenced by the degree of material heterogeneity, the nonlinear behavior may differ from one material to another one. As shown previously in the uniaxial compression simulations for specimens with different degrees of heterogeneity, the nonlinear characteristic in more heterogeneous specimens is more pronounced than in those less heterogeneous ones. However, as can be seen, the residual stress increases with the incremental confinement. It exhibits the same trend as can be observed in triaxial tests.

6.5 Summary

In this chapter, the developed SPH code has been applied to simulate the compressive failure on heterogeneous rock-like materials under plane stress and plane strain conditions. The specimen’s heterogeneity is characterized by using the statistical Weibull distribution method. A series of simulations have been performed to investigate the mechanical characteristics and failure process for different degrees of heterogeneous specimens. The influences of the confining stress have also been explored by the biaxial compression test simulations on a heterogeneous specimen under the plane strain condition.

Result shows that the material heterogeneity has a great influence on the material’s macro mechanical response. For specimens with different degrees of heterogeneity, the predicted uniaxial compressive strength (UCS) and the corresponding axial strain increase as the specimen becomes homogenous. For those specimens having the same degree of heterogeneity, their macro mechanical responses are similar while still exhibits unique characteristics due to the spatial variations in the heterogeneous microstructure.

Simulation results also show that failure developments in the brittle materials have common characteristics. First, conspicuous cracks are formed near their
peak stresses and mostly parallel to the loading directions. Second, axial cracks or faults are formed during the post-failure regions. Although the shear faulting and the cleavage are the two major modes in rock failures, results show most failure patterns in these specimens are the combination one.

The simulated failure processes also manifest material heterogeneity effects. In a more homogeneous specimen, the major crack will dominate the failure. On the contrary, in a less homogenous one, activities of many macro cracks will cause the failure. Even for specimens with the same degree of heterogeneity, the initial cracks and their consequent developments are highly affected by the different local stress severities due to their microstructures.

In numerical simulations, the specimen is commonly assumed to be under the plane strain or plane stress conditions. Simulations show that the UCS value under the plane strain condition is smaller than that of the same specimen under plane stress condition. This phenomenon manifests the employed strength criterion in the numerical model is sensitive to the middle principal stress.

Simulation results from the biaxial test under different lateral confining stress show that the specimen’s carrying capacity increases as the applied lateral stress increases. Specimen’s post failure pattern is also affected by the magnitude of the applied stress. Due to the lateral confinement, the axial cracks are restrained and more shear cracks developed to form shear faults. Moreover, the higher applied confinement will induce the shear fault wider and its angle to the vertical plane slightly bigger.

The developed SPH code can well capture the failure sequences and represent the real cracks and fragments induced by large deformations vividly. Moreover, the whole process does not need any special treatments or assumption in presenting the cracks and fragments. From the view of this point, the SPH code has obvious advantages in rock-like brittle material failure simulations.
Chapter 7  A Heterogeneous Microstructure Modeling Method for Multiphase Materials and Its Applications in the Polycrystalline Granite Rock Failure Simulations

7.1 Introduction

The heterogeneous modeling method in the previous chapters does not well account for the aggregates in the specimen’s microstructure. However, the polycrystalline rocks are multiphase composites. The microstructures in them usually consist of several mineral components and some pre-existing defects, such as the void and cracks. With the advance of experimental techniques, close observations on the specimen’s activities towards its microstructures during the failure process become possible. For instance, Tapponnier and Brace (1976) investigated stress-induced micro cracks developments within different mineral components in the Westerly granite. They noted that new cracks appeared firstly at grain boundaries. With a subsequent load, the transgranular cracks are developed. Around the peak stress, biotite failure including the kinking and sliding can be observed. They also suggested that biotite grains might control the strength of the granite. Wong (1982) further investigated the faulting mechanisms of different minerals in Westerly granite with the confining pressure and temperature. He concluded that the failure mechanisms were related on both mineralogy and the mineral grain orientation. The tremendous contributions by various researchers can be very helpful to understand the failure mechanism in those polycrystalline rocks. Even with the great improvements, the understand-
ing on the failure mechanism is not yet a trivial work.

On the other hand, due to the complexity of its microstructure, it is very difficult to model and perform numerical simulations in order to obtain the detailed features on such a multiphase material. Consequently, most of the conventional computation models treat the material as a homogeneous one by obtaining their model parameters from the macroscopic experiments. However, such simulation results cannot reflect the features of the microstructure in these multiphase materials.

The study presented in this chapter is concentrated on the microstructure characteristics in the polycrystalline granite failure using the numerical approach. One microstructure modeling method is addressed to construct the artificial specimens for the multiphase material, for example, the polycrystalline rocks. Later on, the method is applied to generate the artificial granite specimens. Numerical simulations are performed on the failure processes of these specimens by using the developed SPH code. Studies are not only on the macro mechanic response of the specimens, but also on the characteristics of cracks developments during the failure process.

### 7.2 Method to generate the artificial microstructure for multiphase materials

Microscopically, the undisturbed rock is a multi-phase composite consisting of a variety of mineral grains or aggregates with different sizes. Traditionally, by using the SEM (scanning electronic microscope) or X-ray CT, one can capture the sample’s internal microstructure information such as the components’ shapes and spatial distributions, etc. Numerical specimens can be reconstructed by using those already acquired digital images. However, presently, these techniques are still costly for the practical using. In addition, the generated numerical specimen by using these techniques can only reflect the characteristics on the given small piece of the real material. Sometimes, it might cause problems such as the loss of some general features of the material.
If the statistical microstructure information for these multiphase materials, for example, their statistical components sizes and contents, can be acquired, the artificial microstructure of the specimen can be numerically constructed based on these data to resemble the real material while without loss of its general characteristics.

### 7.2.1 2D discretization of domain based on Voronoi diagram

The discretization process takes a square domain as an example. The Voronoi diagram composed by many convex polygons is employed to explicitly discretize the physical domain. Those polygons are constructed by a set of spatial points \{\tilde{p}\} filled in the domain. Each cell \(V_i\) is associated with one point \(\tilde{p}_i\) in that any point in such a cell is almost closer to a point \(\tilde{p}_i\) than to any other point \(\tilde{p}_j\) in \{\tilde{p}\}. The word "almost" is used to indicate the exceptions where this point may be equally close to two or more points in \{\tilde{p}\}. Such a relationship can be described as,

\[
V_i(x) = \bigcap_{j \neq i} \left\{ \tilde{x} \mid s(\tilde{x}_i, \tilde{x}) \leq s(\tilde{x}_j, \tilde{x}) \right\}
\]  \(\text{(7.1)}\)

where, \(x_i\) are the coordinates of \(\tilde{p}_i\); \(s(\tilde{x}_i, \tilde{x})\) is the Euclidean distance between \(\tilde{p}_i\) and any point at interior of \(V_i\).

The Voronoi diagram can be directly constructed from a set of points by using the software Matlab as illustrated in Figure 7-1. Obviously, the coordinates of these points are vital because they control the shapes as well as the area of generated polygons. In order to guarantee the areas of those arbitrarily generated polyhedrons within a prescribed range, the distance of any two spatial points in \{\tilde{p}\} must be checked to meet,

\[
L_{\text{min}} \leq s(\tilde{x}_i, \tilde{x}_j) \leq L_{\text{max}}
\]  \(\text{(7.2)}\)
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Figure 7-1 illustration of a 2D Voronoi diagram (right) construction process using the random spatial points (left).

One simple method to generate those set of points is to insert random generated points sequentially until they eventually saturate the whole domain. When a new point is to be inserted, Eq. (7.2) must be performed against all the accepted points. When domain is nearly saturated, the probability of the acceptable point becomes low and more trial points may be rejected. Hence, the insertion of new points may become difficult. When there is no satisfied point after a fair long time, Voronoi diagram can be constructed based on these selected points.

7.2.2 The artificial components generation and their heterogeneities treatment

After the Voronoi diagram is ready, the generated polygons can be classified to represent different types of components, for example, different mineral grains according to their ratios in the rock. Considering the spatial variations in the distributions of these components, the current work takes a stochastic approach.

A series of pseudo-random numbers is generated corresponding to those polygons one by one. According to the statistical contents of those minerals in the polycrystalline rock, these pseudo-random numbers can be divided into several groups by their values. Each group corresponds to one type of mineral. Thus, each polygon is specified to be one type of artificial component according to its associated pseudo-random number value. Once the ratio of these generated artificial components meets the prescribed one, such a process can stop. Otherwise, it needs repeating several times.
Even for the same kind of component in the specimen, their mechanical properties are not homogeneous due to many reasons, i.e., the pre-existing defects in them. A treatment with spatially varying the values of these properties within the specification of properties ranges would be more realistic. Such component strength variations can be incorporated in the analysis by assuming their properties to obey a statistical distribution, for example, the Weibull distribution. Each kind of components can have an independent degree of heterogeneity. Thus, the material heterogeneity in its microstructures can be reflected by those heterogeneous components.

7.2.3 Representation of the physical domain microstructure by the SPH particles

In order to use the SPH particles to represent the physical domain’s microstructure, one must determine to which polygons each particle belongs. If the particle’s center falls inside the polygon, it is assigned to the component’s properties represented by this polygon.

There are many methods to judge a point is inside or outside a 2D polygon, such as the ”crossing test” method by Shimrat (1962), the “triangle test” method by Didier (1990) and the well known “angle summation test” method, etc. Implementations of these methods can be referred in Haines (1994).

The current work employs the “crossing test” method as shown in Figure 7-2 for its efficiency. In the method, a ray is shot from the test point in any direction. If the number of the crossings of the ray and the polygon’s edge is even, the test point is outside the polygon. Otherwise, it is inside.

By using the above method, each particle can find its polygon container by traversing all these polygons. The material domain can be represented by those clusters of particles to resemble the real specimen’s microstructure. Figure 7-3 gives an illustration of such a process by using the regularly arranged particles.
7.2.4 Application of the method on the 2D granite microstructure generation

The granite is generally light grey and medium grained which can be discerned easily by the naked eye. Statistical data from Geological Unit of Singapore (1976) show that the Bukit Timah granite in Singapore is mainly composed by the feldspar, quartz and biotite grains and their volumes in a ratio of around 6:3:1. The grain size generally ranges from 3.0 mm to 5.0 mm. Table 7-1 presents the mineral contents and their properties in the Bukit Timah granite. Figure 7-4 shows one cross-section image of such a granite sample.
Table 7-1 Statistical mineral components contents and their properties of the Bukit Timah granite

<table>
<thead>
<tr>
<th>Mineral type</th>
<th>Ratio</th>
<th>Density (kg/m³)</th>
<th>Mohs’ Hardness scale</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feldspar</td>
<td>60%</td>
<td>2570</td>
<td>6</td>
</tr>
<tr>
<td>Quartz</td>
<td>30%</td>
<td>2648</td>
<td>7</td>
</tr>
<tr>
<td>Biotite</td>
<td>10%</td>
<td>2800</td>
<td>3</td>
</tr>
</tbody>
</table>

Figure 7-4 One cross-section image of the typical Singapore Bukit Timah granite sample.

Two rectangle artificial rock specimens in different microstructures are constructed based on the above-described approaches to resemble the Bukit Timah Granite. These two specimens have the same size, with a width in 5.0 cm and a height in 10.0 cm. Each specimen is discretized by the regularly distributed 31250 SPH particles with the same smoothing length in 0.4 mm.

The spatial points prepared for the Voronoi diagram are firstly generated to fill the domain according to the Eq. (7.2). In the equation, the $L_{\text{Min}}$ and $L_{\text{Max}}$ are specified to be 0.3 mm and 0.5 mm, respectively, to meet the requirement of the typical granite grain size. After these polygons are ready, they are classified into different mineral types by the values of the pseudo-random numbers associated with them according to the prescribed ratio of three kinds of minerals. Heterogeneities of three kinds of minerals are assumed to follow the Weibull distributions with the different homogeneous index values for feldspar, quartz and biotite, respectively.

Figure 7-5 shows these two granite samples, named N1 and N2. In the figure, those grains in dark black are biotite. Quartzite grains are in grey white and the
feldspar ones are in grey. The mineral contents in the two artificial granite samples are presented in Table 7-2. As can be seen, they are very close to the expected ratio. The microstructures of these two artificial samples resemble the real one by having the common features in the mineral components contents and their grain sizes. Their different microstructures reflect the spatial variations existing in the reality.

Table 7-2 Ratios of mineral grains in the two artificial granite samples

<table>
<thead>
<tr>
<th>Specimen</th>
<th>Feldspar</th>
<th>Quartz</th>
<th>Biotite</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1</td>
<td>59.52%</td>
<td>29.94%</td>
<td>10.54%</td>
</tr>
<tr>
<td>N2</td>
<td>61.77%</td>
<td>29.38%</td>
<td>8.85%</td>
</tr>
</tbody>
</table>

Figure 7-5 Two artificial granite samples N1 (left) and N2 (right), their microstructures resemble the real Singapore Bukit Timah granite sample.

7.3 Numerical approach and model parameters

The developed SPH code is applied to simulate the uniaxial compression test. The elasto-plastic damage model is employed as the constitutive law. Due to the
difficulties in obtaining the mechanical properties of these minerals directly, their parameters in the model are determined indirectly.

It is assumed that these properties related to the mineral’s strengths (\(E, K, G, \sigma_f, \sigma_c, p_r, D_1, A, B\)) are in a proportional relationship with its Mohs’ hardness scale value. Thus, the ratio of those strength related parameters’ values for the certain mineral to their corresponding macroscopic ones in the granite can be determined by

\[
r_{\text{mineral}} = \frac{\text{Mineral's Mohs' hardness value}}{\text{The average Mohs' hardness value of all mineral components}}
\]

The average Mohs’ hardness value for all the three types of minerals is 5.33. Hence, the above-mentioned ratio values are 1.125, 1.3125 and 0.5625 for feldspar, quartz and biotite, respectively. Table 7-3 shows model parameter values of these three kinds of mineral grains in the granitic rock.

To consider the heterogeneity for the certain mineral’s property, the statistical model based on the Weibull distribution law is used. Heterogeneity among the same type of mineral grains can be introduced by assuming their properties to follow a certain normalized Weibull statistical distribution. Hence, each mineral can have a dependent distribution. Assume that the three normalized Weibull distributions for feldspar, quartz and biotite are \(W_F\), \(W_Q\) and \(W_B\), respectively, ratios of their containing particle’s parameters to the according granite macroscopic ones can be obtained as presented in Table 7-4.
Table 7-3 Model parameters for the three mineral grains in the granitic rock

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Granite</th>
<th>Feldspar grain</th>
<th>Quartz grain</th>
<th>Biotite grain</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho$ (kg/m$^3$)</td>
<td>2670</td>
<td>2570</td>
<td>2648</td>
<td>2800</td>
</tr>
<tr>
<td>$E$ (GPa)</td>
<td>75.20</td>
<td>84.6</td>
<td>98.7</td>
<td>42.3</td>
</tr>
<tr>
<td>$\nu$</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
</tr>
<tr>
<td>$K$ (GPa)</td>
<td>41.78</td>
<td>47.00</td>
<td>54.84</td>
<td>23.50</td>
</tr>
<tr>
<td>$G$ (GPa)</td>
<td>31.33</td>
<td>35.25</td>
<td>41.12</td>
<td>17.62</td>
</tr>
<tr>
<td>$\sigma_t$ (MPa)</td>
<td>16.1</td>
<td>18.1</td>
<td>21.1</td>
<td>9.06</td>
</tr>
<tr>
<td>$\sigma_c$ (MPa)</td>
<td>157.0</td>
<td>176.6</td>
<td>206.1</td>
<td>88.3</td>
</tr>
<tr>
<td>$P_T$ (MPa)</td>
<td>5.367</td>
<td>6.038</td>
<td>7.044</td>
<td>3.019</td>
</tr>
<tr>
<td>$A$</td>
<td>0.1334</td>
<td>0.1501</td>
<td>0.1751</td>
<td>0.07504</td>
</tr>
<tr>
<td>$B$</td>
<td>0.04446</td>
<td>0.05002</td>
<td>0.05835</td>
<td>0.02501</td>
</tr>
<tr>
<td>$r_c$</td>
<td>0.5831</td>
<td>0.5831</td>
<td>0.5831</td>
<td>0.5831</td>
</tr>
<tr>
<td>$N$</td>
<td>0.8536</td>
<td>0.8536</td>
<td>0.8536</td>
<td>0.8536</td>
</tr>
<tr>
<td>$M$</td>
<td>0.8536</td>
<td>0.8536</td>
<td>0.8536</td>
<td>0.8536</td>
</tr>
<tr>
<td>$D_1$</td>
<td>$1.748 \times 10^{-4}$</td>
<td>$1.97 \times 10^{-4}$</td>
<td>$2.29 \times 10^{-4}$</td>
<td>$9.83 \times 10^{-5}$</td>
</tr>
<tr>
<td>$D_2$</td>
<td>0.9326</td>
<td>0.9326</td>
<td>0.9326</td>
<td>0.9326</td>
</tr>
</tbody>
</table>

It is found from the previous experimental studies that the quartz grains have more pre-existing micro-cracks than those in biotite and feldspar grains. To consider this fact in the analysis, the quartz grains are given a more heterogeneous Weibull distribution than that in the other two mineral grains.
Table 7-4 Determination of model parameters’ values for particles in different mineral grains

<table>
<thead>
<tr>
<th>Mineral components</th>
<th>Ratio of mineral’s parameter value to that of the according granite macroscopic one</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feldspar grains</td>
<td>$1.125 , W_F$</td>
</tr>
<tr>
<td>Quartz grains</td>
<td>$1.3125 , W_Q$</td>
</tr>
<tr>
<td>Biotite grains</td>
<td>$0.5625 , W_B$</td>
</tr>
</tbody>
</table>

The different microstructures in the previous two generated artificial specimens reflect the possible spatial distribution variations of granite components in reality. For the real granite samples, they might also be subjected to other conditions, such as weathering, which can cause their strengths varying. To consider this fact, each artificial specimen is incorporated with two different systems of heterogeneity. Their configurations are listed in Table 7-5. Of them, N1-1 and N1-2 have the same microstructure with N1. Similarly, the microstructures in N2-1 and N2-2 are same with that of N2.

Table 7-5 Heterogeneous configurations in mineral grains of specimens

<table>
<thead>
<tr>
<th>Specimen</th>
<th>Homogeneous index value in mineral grains</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Feldspar</td>
</tr>
<tr>
<td>N1-1</td>
<td>10</td>
</tr>
<tr>
<td>N1-2</td>
<td>50</td>
</tr>
<tr>
<td>N2-1</td>
<td>10</td>
</tr>
<tr>
<td>N2-2</td>
<td>50</td>
</tr>
</tbody>
</table>

Obviously, N1-1 and N2-1 are more heterogeneous than N1-2 and N2-2. Figure 7-6 shows the strength distributions in different mineral grains in the specimen N1-1 and N1-2.

It is noteworthy that, when the statistical models are introduced, the predicted
results will give lower response values than the macroscopic ones determined in the experiments are as shown in the results from previous chapters. To make the simulation results more realistic, the trail tests should be performed to get the relationship between the macroscopic parameters values and the ones applied in the statistical model. The uniaxial compression tests are carried on these four specimens in the plane stress condition to determine such a relationship. In the simulation, the specimen is sandwiched into two rigid walls loaded by boundary velocities without the friction between the wall and specimen’s ends as sketched in Figure 7-7. Loading velocity keeps a constant value at 0.01 m/s. The average compressive stress in the specimen’s two end boundaries is taken as the trail specimen’s macroscopic compressive stress.

![Normalized strength distributions](image)

Figure 7-6 The normalized strength distributions in the different mineral grains in two of heterogeneous specimen a) N1-1 and b) N1-2
The simulated macroscopic axial stress-strain curves for these four trail specimens are shown in Figure 7-8.

Figure 7-8 Axial stress-strain curves for these four trail specimens

It can be seen that responses of these trial specimens are influenced by the spatial distributions in the mineral grains as well as their heterogeneous configurations. For the specimens with the same microstructure, those relatively more homogeneous specimens exhibit the larger compressive strengths and the larger axial failure strains. For the specimens with the same degree of heterogeneity, their response curves are also different and mainly affected by those mineral grains spatial distributions, such as their ratio, orientations and shapes, etc.

The Predicted uniaxial compressive strengths in the two degrees of homogeneous trail specimens are listed in Table 7-6. The ratios of these two different heterogeneous specimens’ average strength to the macroscopic real granite’s strength (taken as 157 MPa) are given in the table. The ratio $R$ is incorpor-
rated to the model parameters to make the simulations more realistic for these two degrees of heterogeneous specimens. Therefore, model parameters’ values for different mineral grains can be obtained as given in Table 7-7.

Table 7-6 Predicted uniaxial compressive strengths in the two degrees of homogeneous trail specimens and their ratios to the macroscopic real granite samples

<table>
<thead>
<tr>
<th>Heterogeneity</th>
<th>Specimen</th>
<th>Strength (MPa)</th>
<th>Average strength (MPa)</th>
<th>Ratio to the macroscopic strength</th>
</tr>
</thead>
<tbody>
<tr>
<td>More</td>
<td>N1-1</td>
<td>33.27</td>
<td>38.27</td>
<td>4.4</td>
</tr>
<tr>
<td></td>
<td>N2-1</td>
<td>35.72</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Less</td>
<td>N1-2</td>
<td>82.87</td>
<td>77.12</td>
<td>2.0</td>
</tr>
<tr>
<td></td>
<td>N2-2</td>
<td>71.37</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 7-7 Determination of the model parameters’ values for different mineral grains to represent the real granite

<table>
<thead>
<tr>
<th>Mineral components</th>
<th>Ratio of mineral’s parameter value to that of the according Granite macroscopic one</th>
</tr>
</thead>
<tbody>
<tr>
<td>σ₁, σₑ, K, G, σᵣ, Pᵣ, Dᵣ, A, B</td>
<td>N, M, D₂, rₑ</td>
</tr>
<tr>
<td>Feldspar grains</td>
<td>1.125WᵢR</td>
</tr>
<tr>
<td>Quartz grains</td>
<td>1.3125WᵢR</td>
</tr>
<tr>
<td>Biotite grains</td>
<td>0.5625WᵢR</td>
</tr>
</tbody>
</table>

7.4 Simulations on the uniaxial compression tests

7.4.1 Results for more heterogeneous specimen N1-1 and N2-1

The axial stress-strain curve of specimen N1-1 is plotted in Figure 7-9. The profile of AE (acoustic emission) count is also plotted by taking each damaged particle as an AE event during the fracture process.
Figure 7-9 Simulated axial stress-strain curve and AE record in specimen N1-1. The predicted compressive strength is 146 MPa with the corresponding axial strain of $4.5 \times 10^{-4}$. The curve exhibits some typical features of a brittle failure. It almost keeps linear until the peak stress and then drops down abruptly. The number of the damaged particles increases at about the 68% peak stress (marked as the first circle on the stress-strain curve). Most of these damaged particles appear around its peak stress as evidenced by other researchers in their experimental studies.

In Figure 7-10, the specimen’s fracture process is depicted in different frames as indicated by those circle marks in Figure 7-9.

The simulated cracks are represented by those damaged particles in white color. The final failure pattern is also given by plotting those particles as squares according to their coordinates. Hence, the white gaps between the fragments are predicted fracture zones. It should be mentioned here that the failure pattern might be a little different from that in the experiments. Unlike the well-controlled test apparatus in the experiments, the incremental displacement applied on the specimen is constant during its whole fracture process.
From the first graph, it can be seen that the cracks first occur at the quartz grains and the boundaries between the quartz and feldspar grains, as indicated by the open white circles. With the increasing load, those cracks propagate along the loading direction. Subsequently, they become the transgranular cracks. At the peak stress, besides previous well-developed cracks, some new cracks are initiated at the quartz grains and the boundaries of quartzes and biotites. At the post-peak stage, those cracks on the right side of the specimen propagate rapidly and extend over several grains. At the 95% of peak stress, many long cracks can be found in arrays and some begin to cluster. Finally, we can observe that several vertical cracks split the specimen. It is evident that the failure is the axial cracking mode. The specimen falls into several large fragments eventually. Spalling phenomena can be observed at the specimen’s edges. Further observation can find that, in the pre-peak stress stage, few cracks are developed in the biotite grains. Beyond the peak strength, the crack kinking can be clearly ob-
served in some biotite grains. Finally, it leads to small shear faults in the specimen as can be found in the final failure pattern.

Because the quartz grains are more heterogeneous, cracks may be firstly initiated among these grains. The phenomena that cracks are more like to occur along the grain boundaries can account for the stiffness mismatches between the different mineral grains as reported by Janach (1977). Figure 7-11 shows the effective stress ($\sqrt{J_2}$) distribution at different loading level. The stress concentration on the stiffer grain can be clearly observed. This can also account for one reason why those initial stress-induced cracks seldom appear in the soft biotite grains and often at the boundaries of quartzes and feldspars instead.

![Figure 7-11 Variations of effective stress distribution in specimen’s fracture process. Intense of the gray scale indicates the stress magnitude. Open circles indicate locations where cracks are initialized and developed. Specimen N2-1 has a different microstructure with the N1-1. Its axial stress-strain curve and the profile of the damaged particles are plotted together in Figure 7-12. Not surprisingly, they are qualitatively similar to those of the specimen N1-1 since both have the same degree of heterogeneity. The predicted compressive strength is 168 MPa with the corresponding axial strain of $5 \times 10^{-4}$. Both are larger than those in N2-1. It demonstrates that the spatial variation in the specimen’s microstructure has slight effect on the specimen’s macroscopic mechanical responses.](image-url)
Figure 7-12 Simulated axial stress-strain curve and profile of the damaged particles in specimen N2-1.

Figure 7-13 Fracture process and the final failure pattern of specimen N2-1. The failure process and its final failure pattern of specimen N2-1 are plotted in Figure 7-13 in sequence. At the 96% of the peak stress stage, the crack appears at the boundaries of quartz and feldspar grains. With a further load at the peak...
stress, another crack occurs within the quartzes near the specimen’s middle height plane close to the left side. More cracks are initiated in the post-peak region. They propagate rapidly predominately along the loading direction. It can be seen that crack’s propagation is more difficult in relatively hard and homogeneous feldspar grains than in other mineral grains. As it can be seen from the plot, the first two cracks are almost halted when they enter the feldspar grains. The kinking and coalitions of these cracks can also be observed. The appearance of a parallel array with step-like propagation paths of these cracks strongly suggests that the failure is the axial splitting one with some small shear faults.

Although the specimens N1-1 and N2-1 have different microstructures, their mechanical responses and the final failure patterns are similar.

**7.4.2 Results of the more homogeneous specimens N1-2 and N2-2**

The simulated axial stress-strain curve and the profile of the damaged particles of the specimen N1-2 are shown in Figure 7-14. Since the specimen N1-2 has the same microstructure with N1-1, the curves of these two specimens are plotted together for a comparison.

![Figure 7-14](image)

Figure 7-14 Comparisons of the simulated axial stress-strain curves and the profile of the damaged particles between the specimen N1-2 and N1-1

The predicted compressive strength of the specimen N1-2 is 168 MPa, which is higher than that of the specimen N1-1 of 146 MPa. The axial strain corres-
ponding to the peak stress is 0.001, which is almost two times of the less homogenous specimen N1-1. The profiles of the damaged particles are also different. Since the strength distribution is more homogeneous in the mineral grains of the specimen N1-2, a substantial volume of particles fail almost concurrently.

The fracture process and its final failure pattern of N1-2 are plotted in Figure 7-15. The cracks appear firstly at quartz grains at the 99% of its peak stress. With the further compressive load close to the specimen’s peak stress, the transgranular cracks among the quartz and biotite grains can be found. The formed major crack propagates rapidly parallel to the loading direction in the post-peak region. The cracks nucleation can be observed within quartz grains at the 82% peak stress in the post-peak stage. Subsequently, many single isolated axial cracks are initiated. These cracks tend to cluster around the well-developed major crack and eventually form a fault as shown in the final failure pattern.

Figure 7-15 The fracture process and the final failure pattern of the specimen N1-2
The predicted fracture process agrees well with the observations from other researches. For instance, Hallbauer et al. (1973) described that a fault is formed by stepwise joining of the growing fractures with the existing macro-cracks close to the specimen’s failure. Janach (1977) also proposed a failure model to account for the granite specimen’s failure process. He explained that the observed shear fault was caused by the formation of a diagonal array of tipped elements due to the stiffness mismatches among those different mineral components as shown in Figure 7-16.

Figure 7-16 Illustration of the failure model for the granite sample under compression (after Janach, 1977). a) the column distortion by the stiffness mismatches among different components; b) shear fault developed by the formation of a diagonal array of the tipped elements

The simulated stress-strain curve and the profile of damaged particles for the specimen N2-2 are given in Figure 7-17.

Figure 7-17 Simulated axial stress-strain curve and the profile of damaged particles in the specimen N2-2
The compressive strength of N2-2 is about 145 MPa with the corresponding axial strain of 0.0089. Its stress-strain curve and the profile of the damaged particles are similar to those of the specimen N1-2 as these two specimens have the same degree of heterogeneity.

Figure 7-18 Fracture process and the final failure pattern in the specimen N2-2

Figure 7-18 presents the fracture process and the final failure pattern of the specimen N2-2. As can be observed, the first evident crack appears at the quartz grains at the pre-peak stage around the 99% of its peak stress. It propagates into different mineral grains rapidly along the loading direction after the peak stress. At the 99% of its peak stress in the post-peak stage, one can observe that the crack deviated from its original path as indicated by the open circles in the graph. Such deviations might be resulted by the stress concentrations and redistributions due to the mismatched properties among these different mineral grains. The failure is mainly due to the axial splitting crack. However, the clusters and nucleation of micro-cracks also result in some small shear faults.
7.4.3 Comparisons and discussions

The axial stress-strain curves for all the specimens are plotted in Figure 7-19. Obviously, the more homogeneous specimens N1-2 and N2-2 have larger sustainable axial strains than the other two less homogeneous specimens do. Previous failure processes demonstrate that failures in these more homogeneous specimens are more abrupt accompanied with a large numbers of damaged particles almost concurrently. The specimen’s failure is usually due to one major axial crack and the consequent shear faults by the nucleation of an array of short cracks mainly in biotite grains. Results also show that the failure process is influenced by the spatial distributions of the different grains in their microstructures.

Figure 7-19 simulated axial stress-strain curves for all specimens

However, for those more heterogeneous specimens, their failures appear more progressively. Due to the existence of many weak grains, the specimen is split into many pieces by many parallel vertical cracks. The cracks are more often developed in the more heterogeneous quartz grains. In addition, they may take place at the boundaries between different grains due to the mismatching stiffness induced stress concentrations. The transgranular cracks can be intensively observed during the post-peak stage. We can also observe that most biotite grains keep intact till specimen fails. While, some may kink and slide to form shear faults. Such features agree with the results by other researches as dis-
cussed previously.

The predicted final failure patterns of these specimens are plotted in Figure 7-20. Their differences reflect the variations in the real rock samples in terms of the spatial distribution in the microstructure as well as the heterogeneous strength distributions among their mineral components. As can be seen, these failure patterns agree well with those observed in the experiments by Andreev (1995) qualitatively.

![Figure 7-20 Predicted final failure patterns in specimens N1-1, N1-2, N2-1 and N2-2, from the left to the right (top); Rock uniaxial compression test results (bottom, after Andreev, 1995)](image)

The simulation results demonstrate that the developed microstructure modeling method can well present those cracking features in the polycrystalline granite rock compressive failure process.

### 7.5 Simulation results in the Brazilian splitting test

#### 7.5.1 Numerical approach description

Two artificial granite specimens named B1 and B2 are generated by taking the central part from the previously constructed specimen N1-2 and N2-2, respec-
Numerical Simulation of Heterogeneous Material Failure by using the SPH Method

Their microstructures are shown in Figure 7-21. In these figures, dark black grains are biotite mineral and feldspar grains are grey serving as the matrix. Quartz grains are in light bright color. The ratios of mineral components in these two specimens are given in Table 7-8. These two specimens inherit the heterogeneities of their parents. The homogenous index values of the feldspar and biotite grains are 50 and the quartz’s is 5. The magnitude of their relative grain strengths is indicated by the intensity in gray scale.

![specimen B1](image1.png)  ![specimen B2](image2.png)

Figure 7-21 Two artificial granite specimens B1 and B2 based on the specimen N1-2 and N2-2 shown in Figure 7-5; Intensity in the gray scale indicates the magnitude of the relative grain strength.

Each specimen contains 12281 SPH particles with the same smoothing length of 0.4 mm. The geometry and loading conditions for these two specimens are illustrated in the Figure 7-22. In the simulation, the specimen is sandwiched into two rigid walls loaded by the boundary velocities symmetrically. Particles within the upper and bottom boundaries were directly given the constant velocity at 0.0025 m/s.

<table>
<thead>
<tr>
<th>Specimen</th>
<th>Feldspar</th>
<th>Quartz</th>
<th>Biotite</th>
</tr>
</thead>
<tbody>
<tr>
<td>B1</td>
<td>57.69%</td>
<td>31.71%</td>
<td>10.60%</td>
</tr>
<tr>
<td>B2</td>
<td>61.10%</td>
<td>28.90%</td>
<td>10.00%</td>
</tr>
</tbody>
</table>
Along with the specimen’s deformation, the average compressive force on the two boundaries is recorded and taken as the loading force. The predicted tensile strength can be obtained using Eq. (4.3).

The developed SPH code is applied to simulate the Brazilian splitting test described previously. Parameters for these two specimens follow their parent specimens N2-1 and N2-2, respectively.

### 7.5.2 Simulation results

The loading force with the loading displacement curve as well as the record of the damaged particle numbers record with the displacement is plotted in Figure 7-23. The loading force increases almost linearly with the loading displacement. When attaining the peak value, it drops down abruptly. As can be observed, the damaged particles are predominately concentrated near the peak force region.

Figure 7-24 shows the process of crack initiation and propagation and the final failure pattern of specimen B1. The crack occurs at the 98% of the peak force. It is located on the boundaries between the quartz and biotite grains around the disc center, as indicated by the open circle. Unlike the homogeneous case where the crack occurs exactly at the disc center, situation in the heterogeneous case is more dependent on the local stress conditions affected by the interactions of mineral grains and their mechanical properties. Therefore, the first crack does not need to occur as theoretically predicted. Instead, it may take place where the stress condition is most severe as discussed in Andreev (1995). With the further
increasing load, the crack propagates rapidly towards the both ends of the disc along the loading diameter plane until it splits the whole disc. Again, it is very interesting to observe that the crack deviates from its original path at the 92% of the peak load in post-peak region due to the specimen’s heterogeneity. After the specimen is completely failed, those damaged particles may separate naturally and form the real “crack” under the governing equations. The final failure pattern is given by plotting all particles in a square according to their coordinates. One can observe that the predicted real crack in blank eventually splits the disc into two halves.

![Graph showing the simulated response force-loading displacement curve and the damaged particles record for the specimen B1](image)

**Figure 7-23** Simulated response force-loading displacement curve and the damaged particles record for the specimen B1

![Failure process and the final failure pattern of specimen B1](image)

**Figure 7-24** Failure process and the final failure pattern of specimen B1
Figure 7-25 presents the profiles of the horizontal and vertical stress components distributions along the loading diameter during the specimen’s fracture process.

As shown in the first plot in Figure 7-24, the first crack appears at the 98% of the peak load. It is evident that the crack is not exactly located along the disc center since the horizontal and vertical stresses do not vanish as indicated in Figure 7-25. Distributions of stresses fluctuate along their theoretical values (in solid lines), which demonstrate the heterogeneous effects in the specimen’s microstructure. Since crack will create new open boundaries, those particles adjacent to the open boundaries may lose their stresses. As can be seen at the peak load, horizontal stresses of some particles near the disc middle part appear to be zero. In the post-peak region, more and more particles along the loading diameter plane are affected by the developing opening boundaries, as can be seen from the subsequent graphs. As can be concluded, features in such a heterogeneous specimen are significantly different from those in the homogeneous one.

Figure 7-25 Profiles of stress distributions along the loading diameter plane for specimen B1 during the splitting process
Specimen B2 has a different microstructure with B1. It has the same degree of heterogeneities in the mineral grains. The simulated curve of response force with the loading displacement is similar to that of B1 as shown in Figure 7-26. The force increases steadily with the applied displacement and falls down rapidly during the post-peak region. Particles fail mostly around the specimen’s peak force region.

The failure process shown in Figure 7-27 is different from that by B1 due to their different microstructures of mineral grains and the according heterogeneities. The crack occurs firstly along the boundaries between biotite and quartz grains when force approaches its 98% peak. During its propagation towards the bottom end in post-peak region, another crack occurs near the first one and propagates towards the disc top end. It can be seen that these two cracks are not located exactly along the loading diameter plane. The disc finally ruptures by those cracks as shown in the final failure pattern. Besides, a large block of fragment at the upper half is also formed. Profiles of the horizontal and vertical stresses distributions along the loading diameter for specimen B2 during the splitting process are given in Figure 7-28. As can be seen, the stress states are more complex than those in the homogeneous case are.

Figure 7-26 Simulated loading force against the loading displacement as well as the profile of the damaged particles in specimen B2
Chapter 7 A Heterogeneous Microstructure Modeling Method for Multiphase Materials and Its Applications in the Polycrystalline Granite Rock Failure Simulations

Figure 7-27 Failure process and the failure pattern of specimen B2

Figure 7-28 Profiles of stresses distributions along the loading diameter for specimen B2 during the splitting process

The numerical results on these two specimens have shown that the failure mechanics is significantly different from that in the theoretical one and appears more complex. The simulated loading force-loading displacement curves and their damage particles count records of these two specimens are qualitatively
comparable. The predicted tensile strengths for two specimens B1 and B2 are 7.93 MPa and 9.28 MPa, respectively. Although these two specimens have different microstructures, their macroscopic responses are similar. However, such a difference in the specimen’s microstructures and their heterogeneous conditions can have more influence on the specimen’s failure process in terms of the crack initiations and propagations.

7.6 Summary

In this chapter, one statistical microstructure modeling method for the multiphase material has been presented by taking account into the actual contents of different components and their characteristic sizes. A treatment of the heterogeneities in these components is also addressed by introducing the statistical method using the Weibull distribution law. The proposed method can reflect the spatial variations of the components distributions as well as their strengths distributions without losing the generality.

The modeling method has been applied to construct the artificial polycrystalline granite specimen. Numerical simulations of the uniaxial compression test and Brazilian tensile test are further performed on these artificial specimens to investigate the granite failure behaviors. Results demonstrate that both the microstructure and mineral components heterogeneities have influence on the specimen’s failure process and macroscopic mechanical response.

Although the proposed microstructure modeling method can only be regarded as an approximation of a real complex material, it shows potential advantages as an efficient approach to extend the conventional numerical methods in the analysis of real materials. The approach presented here can be further extended to the 3D applications.
Chapter 8 Dynamic Simulations on 2D Granite Failure Process Using the Microstructure Modeling Method

8.1 Introduction

In Chapter 7, a heterogeneous microstructure modeling method for the multiphase materials has been proposed and applied to construct the artificial microstructure specimens for the polycrystalline granite. By using those generated artificial specimens, the granite failure behaviors under the low loading strain rate are investigated. In this chapter, we continue the previous studies. The analyses will be concentrated on the granite dynamic failure characteristics.

8.2 Numerical model configuration

8.2.1 Specimen geometry and loading conditions

Based on the previous generated artificial specimen N1-2 by the proposed microstructure modeling method, two granite samples are constructed by intercepting the central part of specimen N1-2 as illustrated in Figure 8-1. Of them, one is used to conduct the Brazilian splitting test simulation with a diameter of 0.05 m; the other is for the uniaxial compression test with a width of 0.05 m and a height of 0.03 m. The mineral contents for these two specimens are listed in Table 8-1. Figure 8-2 shows their boundary conditions and loading conditions, respectively.
Figure 8-1 Illustration for the preparations of the Brazilian splitting test and the uniaxial compression test specimens; a) specimen N1-2; b) specimen for the Brazilian splitting test; c) specimen for the uniaxial compression test.

Table 8-1 Mineral components contents in the generated granite specimens

<table>
<thead>
<tr>
<th>specimen</th>
<th>Feldspar</th>
<th>Quartz</th>
<th>Biotite</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1-2</td>
<td>59.52%</td>
<td>29.94%</td>
<td>10.54%</td>
</tr>
<tr>
<td>Brazilian</td>
<td>57.69%</td>
<td>31.71%</td>
<td>10.60%</td>
</tr>
<tr>
<td>Uniaxial compression</td>
<td>57.38%</td>
<td>31.18%</td>
<td>11.44%</td>
</tr>
</tbody>
</table>

Figure 8-2 Geometry and loading conditions for: a) Brazilian splitting test; b) uniaxial compression test.

In both simulations, the samples are sandwiched between two rigid walls with the prescribed velocities defined as,
\[ v(t) = \begin{cases} \frac{t}{t_0} v_0, & \text{when } t \leq t_0 \\ v_0, & \text{when } t > t_0 \end{cases} \] (8.1)

where \( t_0 = 5.0 \times 10^{-5} \) s. The velocity ramp can help to achieve the stress equilibrium and prevent the premature failures due to the stepwise increasing force on the loading boundaries. After \( t_0 \), the prescribed velocities on the boundary are kept at a constant value \( v_0 \). Strain rate \( \dot{\varepsilon} \) is constant after the time \( t_0 \) as \( \dot{\varepsilon} = 2v_0/L \), where \( L \) is the nominal length of specimen along the loading direction. The loading cases and their corresponding strain rates for these two kinds of tests are presented in Table 8-2 and Table 8-3.

It should be noted that the strain strain in Brazilian splitting simulations is the nominal strain rate as mentioned in chapter 4.

<table>
<thead>
<tr>
<th>( v_0 ) (m/s)</th>
<th>0.0025</th>
<th>0.025</th>
<th>0.25</th>
<th>1.25</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \dot{\varepsilon} ) (s(^{-1}))</td>
<td>0.1</td>
<td>1</td>
<td>10</td>
<td>50</td>
<td>120</td>
</tr>
</tbody>
</table>

Table 8-3 Loading conditions for the uniaxial compression simulations

<table>
<thead>
<tr>
<th>( v_0 ) (m/s)</th>
<th>0.0015</th>
<th>0.015</th>
<th>0.15</th>
<th>0.75</th>
<th>1.8</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \dot{\varepsilon} ) (s(^{-1}))</td>
<td>0.1</td>
<td>1</td>
<td>10</td>
<td>50</td>
<td>120</td>
</tr>
</tbody>
</table>

8.2.2 Numerical approach and model parameters

The developed SPH code is applied to conduct the Brazilian splitting test and uniaxial compression test simulations under the plane stress condition. Model parameters follow those of their “parent” specimen N1-2, in which feldspar, quartz and biotite grains are assumed to have the independent Weibull distributions with the shape values of 50, 5 and 50, respectively. The SPH particles in these two specimens have the same smoothing length of 0.4 mm. The total particle numbers in the Brazilian test and compression test samples are 12281 and 9375, respectively.
8.3 Simulation results of the Brazilian splitting tests

8.3.1 Simulated loading force-displacement curves and the fracture processes under the different strain rates

The compressive loading force with the loading displacement curves for the cases with the strain rate from $0.1 \text{ s}^{-1}$ to $120 \text{ s}^{-1}$ are shown in Figure 8-3. In the figure, the dashed, dotted and solid lines are the profiles of the upper boundary force, the bottom boundary force and their average one, respectively. The corresponding simulated fracture processes and the final failure patterns of the specimen under those strain rates are depicted in Figure 8-4. The failure process is presented by a series of damage distribution plot frames starting from the moment when the first visible crack occurs. These frames are indicated by the white circle marks on the loading force curve in each case as shown in Figure 8-3.

For the two cases with the strain rate $0.1 \text{ s}^{-1}$ and $1.0 \text{ s}^{-1}$, their loading force profiles are similar. The loading force increases almost linearly until the peak load and then drops suddenly once the sample loses its bearing capacity. Their fracture processes are almost identical. It can be seen that the crack initiated near their peak loads on the quartz and biotite grain boundaries around the disc center, as indicated by those open circles. Due to the effect of specimen’s heterogeneous microstructure, the initiated crack might not occur at the disc center but would take place where the stress condition is most severe as discussed by Andreev (1995). With the further increasing load, the crack propagates rapidly towards the both ends of the disc along the loading diameter until it cuts through the whole disc. As can be seen from the failure pattern, the predicted real crack in blank splits the disc into two halves.

For other higher strain rate cases, the shapes of the loading force curves differ remarkably from those in the two lower cases. In these higher strain rate cases, the curve exhibits somewhat nonlinear characteristic after the first visible crack occurs, as marked by the first white circle.
Numerical Simulation of Heterogeneous Material Failure by using the SPH Method

Figure 8-3 Curves of the response loading force with the loading displacement; Figures from a) to e) correspond to the strain rate from $0.1 \text{s}^{-1}$ to $120 \text{s}^{-1}$, respectively.

For the strain rate $10.0 \text{s}^{-1}$ case, the first visible crack occurs around the 87% of its peak force and then propagates towards both ends. At its peak force, another crack appears along the boundary between quartz and biotite grains.
The propagations and interactions of these two major cracks result in the oscillation of the response force in the subsequent stages.

The failure processes in the cases of the strain rate 50.0 $s^{-1}$ and 120.0 $s^{-1}$ are much alike. In both cases, the initiated crack happens much earlier before their peak forces (around 58% in the strain rate 50.0 $s^{-1}$ case and 61% for the 120.0 $s^{-1}$ case). Their failure processes can be featured by the developments and interactions of many short cracks near the loading diameter plane. Their loading force curves behave much more fluctuant due to the intensive crack activities. In addition, the bending cracks can be clearly observed along the disc edge.

From Figure 8-3, it can be seen that in all cases, the reaction forces on both loading sides are almost identical before their peaks. After their peaks, the specimen’s failure becomes unstable and the force oscillations can be observed especially in those higher strain rate cases.
Numerical Simulation of Heterogeneous Material Failure by using the SPH Method

strain rate 1.0 s$^{-1}$

strain rate 10.0 s$^{-1}$

strain rate 50 s$^{-1}$
Figure 8-4 Fracture processes and the final failure patterns for the Brazilian splitting test sample under the strain rate from $0.1 \ s^{-1}$ to $120 \ s^{-1}$.

### 8.3.2 Strain rate effects on the loading force profiles and their failure patterns

The predicted fracture processes shown in the previous section manifest that their failure processes are influenced by the strain rates notably. In the lower strain rate cases with the strain rate $0.1 \ s^{-1}$ and $1.0 \ s^{-1}$, specimen’s failure is roughly due to the development of one major crack initialized at the weaker zone around the disc center. On the contrary, in those higher strain rate cases, more short cracks are developed. Consequently, the coalescence of those short cracks forms the crack band, which finally causes the specimen to rupture.

The loading force profiles in Figure 8-5 show that the specimen’s macro mechanical behavior differs considerably under different strain rates. The difference takes the form of the specimen’s increasing loading capacity and sustained maximum loading displacement exhibited by the specimen as the strain rate becomes higher. The applied forces increase almost linearly with the loading displacement until the first visible crack occurs. In the lower loading cases of strain rate $0.1 \ s^{-1}$ and $1.0 \ s^{-1}$, the major crack propagates fast and the disc thoroughly losses its bearing capacity shortly after its peak. However, in those
higher strain rate cases, response forces can still increase until those isolated short cracks coalesce to form the crack band. The interactions of those short cracks during such processes cause fluctuations of the loading force curve.

Figure 8-5 Curves of loading force vs. loading displacement for the Brazilian tests under the strain rate from 0.1 s\(^{-1}\) to 120 s\(^{-1}\).

As mentioned earlier, the SPH particles can separate naturally under the large deformations. This advantage makes the method easier to process the fractures and fragmentations compared with other conventional grid based methods. Figure 8-6 shows the predicted failure patterns in the strain rate of 0.1 s\(^{-1}\), 50.0 s\(^{-1}\), and 120 s\(^{-1}\), respectively. Those blank areas in the plotted graph are real cracks formed by the particle separations. As can be seen, these failure patterns resemble those obtained in the quasi-static and SHPB dynamic experimental tests. When the strain rate approaches to the quasi-static condition, the specimen ruptures into two pieces by one major crack. However, the higher strain rate loading will cause more fragments and conspicuous crashed zones near the two loading boundaries.
Chapter 8 Dynamic Simulations on 2D Granite Failure Process Using the Microstructure Modeling Method

8.4 Simulation results of the uniaxial compression test

8.4.1 Axial stress-strain curves and fracture processes under different strain rates

Figure 8-7 plots the specimen’s axial compressive stress-strain curves with the strain rate from 0.1 \( s^{-1} \) to 120 \( s^{-1} \). In each case, profiles of the upper boundary stress, the bottom boundary stress and their average are plotted in the dashed, dotted and solid lines, respectively. The corresponding fracture processes and the final failure patterns of the specimen under these strain rates are depicted in Figure 8-8. Similarly, the first failure process frame in each case corresponds to the first visible crack in the specimen. These frames are indicated by the white circle marks on the curve shown in Figure 8-7.

For cases with the strain rate from 0.1 \( s^{-1} \) and 1.0 \( s^{-1} \), their stress-strain curves are similar resembling a typical brittle failure response. The axial stress increases almost linearly until its peak value and then drops suddenly. Their
fracture processes are almost identical. The crack initiates at the peak stress at the boundary between the quartz grain and biotite grain, as indicated by the open circle. The crack propagates rapidly in the post-peak region and coalesces with another developed crack. Finally, these cracks form one vertical macro transgranular crack across the specimen. More cracks occur and propagate rapidly in the direction parallel to the loading axis. Besides, kinking in suitably oriented biotite grains can be evidently observed. Some of them form the small shear faults as shown in the specimen’s failure pattern plot.

For other higher strain rate cases, their axial stress-strain curves exhibit three recognized regions: the linear elastic, the non-linear and the post-peak softening region.

In the case of strain rate $10.0 \ \text{s}^{-1}$, the initiated crack occurs around the 98% of its peak stress. The macro-crack propagates across the specimen at 98% of its peak stress in the post-peak stage. For the strain rate $50.0 \ \text{s}^{-1}$ and $120.0 \ \text{s}^{-1}$ cases, their fracture processes resemble one another. In both cases, the cracks appear much earlier compared with other lower strain rate cases (around 85% of its peak stress in the strain rate $50.0 \ \text{s}^{-1}$ and 75% in the $120.0 \ \text{s}^{-1}$ one). The major cracks are formed at their peak stresses. In the subsequent post-peak stage, more short cracks are developed predominantly along the loading direction. These cracks, together with the kinking in biotite and other grains, form several faults and divide the specimen into many fragments.

As can be seen from Figure 8-7, in all cases, the response compressive stresses on the two loading boundaries are in an equilibrium state.
Figure 8-7 Profiles of compressive stress on the upper boundary, the bottom boundary and their average with the axial strain; in the cases of the strain rate from 0.1 s\(^{-1}\) to 120 s\(^{-1}\).
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- Strain rate 0.1 $s^{-1}$
- Strain rate 1.0 $s^{-1}$
- Strain rate 10.0 $s^{-1}$
8.4.2 Strain rate effects on the axial strain-stress curves and the final failure patterns

The compressive axial stress-strain curves under different strain rate cases are plotted together in Figure 8-9, where the stress is taken the average between the upper’s and bottom’s. Result shows that the specimen’s macro mechanical behaviors are remarkably affected by the strain rate. It is clearly observed that the maximum stress and the maximum sustained strain exhibited by the specimen increase when the strain rate is getting higher. When the strain rate is low, the sample experiences little plasticity before a brittle failure happens. The stress reaches to the peak linearly and drops down sharply after its peak. Whereas, for the higher strain rate cases, the curves experience linear elastic, non-linear and the post-peak softening stages.
Figure 8-9 Compressive axial stress vs. axial strain under the strain rate from 0.1 s\(^{-1}\) to 120 s\(^{-1}\).

Figure 8-10 shows the simulated final failure patterns of cases with strain rate 0.1 s\(^{-1}\), 50.0 s\(^{-1}\) and 120 s\(^{-1}\), respectively. As can be seen, the sample fractures into more small fragments when subjected to a higher strain rate loading.

8.5 Strain rate effect on the predicted dynamic tensile and compressive strengths

The predicted dynamic tensile strength (\(\sigma_{td}\)) and compressive strength (\(\sigma_{cd}\)) under the different strain rates are presented in Table 8-4. \(\sigma_{td}\) is calculated using Eq. (4.3) by taking the maximum average compressive force on two loading boundaries as the peak force. \(\sigma_{cd}\) directly takes the maximum average response stress on the two loading boundaries.
Table 8-4 Predicted dynamic tensile strength ($\sigma_{td}$) and compressive strength ($\sigma_{cd}$) with the strain rates

<table>
<thead>
<tr>
<th>$\dot{\varepsilon}$ (s$^{-1}$)</th>
<th>0.1</th>
<th>1.0</th>
<th>10.0</th>
<th>50.0</th>
<th>120.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_{td}$ (MPa)</td>
<td>7.93</td>
<td>8.26</td>
<td>10.05</td>
<td>18.27</td>
<td>28.51</td>
</tr>
<tr>
<td>$\sigma_{cd}$ (MPa)</td>
<td>165.62</td>
<td>165.75</td>
<td>174.96</td>
<td>209.75</td>
<td>243.94</td>
</tr>
</tbody>
</table>

As can be seen, both $\sigma_{td}$ and $\sigma_{cd}$ exhibit the strain rate sensitivity in a sense that they increase as the applied strain rate increase. Such a relationship is coincident with the results reported by many researches as mentioned in the previous chapters. However, to quantitively validate these predicted results with the experimental results is difficult. It is simply because that the artificial specimens used in the current analyses are constructed by the statistical heterogeneous microstructure model. Although their microstructures have been entitled with the common features to resemble those of the real granite, these artificial specimens are not the replicas of those samples using in the experimental tests. In addition, the mechanical parameters of those mineral components are based on an approximation method with some assumptions due to the difficulties in obtaining them from measurements directly.

A question may arise on how representative the result of a particular simulation for specific real samples. While it is not of much practical importance to concentrate on the specific value of a certain field quantity because materials in reality are heterogeneous and their mechanical characters and microstructures differ from one another. Of course, one can perform more simulations on those artificial specimens with different microstructures and heterogeneities to get a full evaluation as doing in the experimental tests. However, it will inevitably bring into many difficulties, such as the considerable computational effort and large scatters of these results. Therefore, the use of the same typical microstructure specimen to investigate the general characteristics of its representative material under the different strain rate loadings will circumvent those draw-
backs to some extent without losing the general trends.

Figure 8-11 and Figure 8-12 compare the numerical predicted dynamic tensile and compressive strengths with those obtained from the experimental tests on the granite samples, respectively. The comparisons take the forms of their dynamic increment factor (DIF) values for these strengths. The DIF value is calculated by normalizing the dynamic strength with respect to their quasi-static values (at a strain rate around \(10^{-5} \text{ s}^{-1}\)). Due to the expensive computational effort to perform the quasi-static analysis using the SPH code, the DIF values of the numerical predicted strengths are normalized with their strain rate 0.1 \(\text{s}^{-1}\) values instead. The experimental results of the granite samples are given in the Appendix A and Appendix B, where the dynamic tensile and compressive strengths are obtained from the Brazilian splitting tests and uniaxial compression tests using the HSPB apparatus. Similarly, the DIF values of the specimen’s average pressure (\(DIF_p\)) in the numerical simulations are also calculated under the different strain rates. These values are plotted in the both diagrams and will be explained next.

![Figure 8-11 Comparison of the numerical and experimental dynamic tensile strength with the logarithm of strain rate](image)
Figure 8-12 Comparison of the numerical and experimental dynamic compressive strength with the logarithm of strain rate

As can be seen from these two diagrams, the experimental and numerical results demonstrate the similar trends in the sense that both the tensile and compressive strengths increase with the applied strain rate. We can also observe that the increments of numerical predicted two kinds of strengths are generally not so sharp as those obtained by experiments. Such deviations may come from several sources. One very important factor is due to the limitations in the current model as explained previously. It should be clearly bear in mind that the real material structures are much more complicated. Another important factor is that, the DIF values of the predicted strengths are normalized by the higher strain rate values instead of those at the quasi-static conditions. This will inevitably underestimate the predicted DIF values. Moreover, since the experimental test under the high strain rates has an extremely short duration, it may be difficult to obtain accurate measurements. However, in spite of those reasons, the comparisons still show good agreements in the overall trends.

Since our model does not explicitly account for the strain rate effects, it should be clear to know what cause the strength increment under the dynamic loadings here. Some researches account the rate dependent effect for the inertia effect as reported by Bischoff and Perry (1995) and Donze et al. (1999). During high strain rate loading, micro-cracks have less time available for their development or propagation. When the local equilibrium state is not attained, the inertial
forces will increase the apparent resistance in opposition to the movement. Thus, a higher load will be required before cracking becomes prominent enough to make the specimen failure. Others, such as Brace and Jones (1971), Bischoff and Perry (1991) and Janach (1976), reported that the phenomena of the pressure increment due to the high strain rate may also be responsible for the strain rate effects on geomaterial. They explained that an apparent effective confining stress might be caused by the inertial restraint in lateral direction for it is unable to expand instantaneously in the rapid loading. Since geomaterial strengths are greatly affected by the hydrostatic pressure. This rate-dependent effect might be attributed to the pressure increment due to the rapid loading.

It is very interesting to observe that the trends of $DIF$ of tensile and compressive strengths curves remarkably match those $DIF$ values of their average pressure, as shown in Figure 8-11 and Figure 8-12. Such a good agreement clearly attests that the pressure increment caused by the strain rate plays an important role for the rate-dependent dynamic strength.

Besides the lateral inertial effect, the crack activities can also be one of the factors to cause the increment of the specimen’s internal pressure during the dynamic loadings. As depicted in the fracture processes of the Brazilian splitting and uniaxial compression simulations (see Figure 8-4 and Figure 8-6), the specimen’s failure is closely related to the activities of the cracks, including their initiations, propagations and coalescence. At the lower loading rate cases, only few micro cracks are activated before the maximum load (or stress) is reached. One single macro crack may cause the specimen a catastrophic failure. On the contrary, at the higher loading rate cases, it is clear that substantially more micro cracks are developed before the maximum load. Because the extension of the micro-cracks takes time, other micro-cracks might be activated before a neighboring activated micro-crack extends and unloads them. Consequently, the specimen breaks into more pieces. The formation of these cracks, will not only delay the specimen’s failure, also cause the stress releasing and consume considerable energy. All these will be much helpful for the specimen’s internal pressure to be further increased.
8.6 Summary

In this chapter, the granite rock dynamic failures are further examined by using the artificial specimens, which are constructed by the heterogeneous microstructure modeling method proposed in the last chapter. Numerical simulations on Brazilian splitting tests and uniaxial compression tests have been conducted using the developed SPH code. The numerical results are compared with those from the experiments in terms of the final failure patterns and the dynamic strength increments. Results demonstrate that they have good qualitative agreements.

The predicted fracture sequences in both Brazilian splitting tests and uniaxial compression tests manifest their failure processes are notably influenced by the applied strain rates. In the lower strain rate cases, the failure is roughly due to the development of few major cracks initialized at weaker zone. On the contrary, under the higher strain rate cases, the specimen’s failure is resulted by the coalescences and interactions of many short cracks.

Specimen’s macro mechanical behaviors exhibit pronounced strain-rate sensitivities. As the strain rate becomes higher, both the specimen’s loading capacity and its sustained maximum displacement (or strain) also becomes larger. Finally, the strain rate effect on the strength are analyzed and compared with the experimental results. It seems that such an effect might be attributed to the internal pressure changes due to the inertial effects as well as the specimen’s crack activities under the different strain rates.
Chapter 9 Dynamic Simulations on 3D Direct Compression Test

9.1 Introduction

All the numerical simulations in the previous chapters are performed under the 2D plane strain or plane stress conditions. Obviously, the 2D analysis is simpler and faster compared with those in 3D. For most situations, the 2D analysis can yield the satisfied result. However, sometimes, its simplified assumptions may affect the accuracy of the results due to all problems are generally 3D in nature. The 3D analysis would be more rigorous and theoretically more accurate especially for those mechanical problems related with the material heterogeneity, such as its microstructure and its crack activities. In this chapter, we change our study to the 3D scope to reinvestigate the uniaxial granite compression failure by using a 3D heterogeneous microstructure modeling method.

9.2 Method to generate the 3D microstructure of multiphase materials

In Chapter 7, we proposed a microstructure modeling method for the multiphase materials by using the 2D Voronoi diagram. In this section, we extend the method to 3D. Firstly, the physical domain is discretized into many polyhedrons by using the 3D Voronoi diagram. After that, those polyhedrons are categorized into different kinds of components according to the statistical content of these components. Finally, the SPH particles are further discretized to represent the real material microstructure.
9.2.1 3D domain discretization method based on the Voronoi diagram

The discretization process takes a rectangular prism as an example. The 3D Voronoi diagram is composed by many convex polyhedrons that explicitly discrete the domain. Similar to the 2D case, those polyhedrons are constructed by a set of 3D spatial points \( \{ \vec{p} \} \).

The Voronoi diagram can be directly constructed from a set of 3D points by using the software Matlab as illustrated in Figure 9-1. Obviously, the coordinates of these points are vital because they control the shapes as well as the volumes of these generated polyhedrons.

In order to guarantee the volumes of those arbitrarily generated polyhedrons within a prescribed range, the distance of any two spatial points in \( \{ \vec{p} \} \) must be checked to meet,

\[
L_{\text{min}} \leq s(\vec{x}_i, \vec{x}_j) \leq L_{\text{max}}
\]

(9.1)

where, \( s(\vec{x}_i, \vec{x}_j) \) is the Euclidean distance between \( \vec{p}_i \) and \( \vec{p}_j \) in \( \{ \vec{p} \} \); \( L_{\text{min}} \) and \( L_{\text{max}} \) are the minimum and maximum allowable distance. One simple method to generate those set of points is to insert random generated points sequentially until they eventually saturate the whole domain as we do in Chapter 7. Obviously, the method is very time consuming since Eq. (9.1) must be performed for all acceptable points in the new point insertion process. The compu-

\[\text{Figure 9-1 Illustration of the 3D Voronoi diagram construction using the 3D spatial points}\]
Numerical Simulation of Heterogeneous Material Failure by using the SPH Method

tational expense can be reduced by using a grid search algorithm. This algorithm is similar to the link-list searching approach used in the SPH method to search the particle’s neighborhoods. Since all existing points have been placed in the different boxes, the new trail point only needs to be checked against the points contained by its nearby neighboring boxes using Eq. (9.1). However, when domain is nearly saturated, the new point insertion still consumes a lot of computational time.

Figure 9-2 A body-centered cubic lattice (left) and generated truncated octahedral tessellation (right).

The current work uses a semi-random point generation method. The points are arranged as the body-centered cubic lattice as illustrated in Figure 9-2. The body centered cubic system has one lattice point in the center of the unit cell in addition to the eight corner points. Such a unit lattice will give a tessellation of space with the truncated regular octahedral shown in Figure 9-2. In order to make the generated truncated octahedral more irregular, the coordinates of each points in \( \{ \tilde{p} \} \) are applied to a pseudo-random disturbance. By limiting the bounds of these random disturbances, volumes of those generated tessellations can be roughly controlled within a prescribed range.

Once the domain’s dimensions and the prescribed bounds for the tessellation’s volumes are given, the coordinates of points of \( \{ \tilde{p} \} \) can be constructed using this semi-random method. Consequently, the 3D Voronoi diagram can be produced based on those generated spatial points in \( \{ \tilde{p} \} \) using the Matlab.
9.2.2 Artificial components generation and their heterogeneities treatments

After the Voronoi diagram is ready, the generated polyhedrons can be classified to represent different types of material’s components, for example, different mineral grains according to their ratio in the rock sample. Considering the spatial distribution variations of these components, the current work takes a stochastic approach similarly as that in the 2D case.

A series of pseudo-random numbers is generated corresponding to those polyhedrons one by one. According to the statistical content of those components, these pseudo-random numbers can be divided into several groups by their values. Each group corresponds to one type of component. Thus, each polyhedron is specified to be one type of the component according to its associated pseudo-random number. Once the ratio of these generated components meets the prescribed one, such a process can stop. Otherwise, it needs repeating several times.

Even for the same kind of components in the specimen, their mechanical properties are not homogeneous due to many reasons, i.e., the pre-existing defects in them. A proper treatment that can spatially vary the values for these properties within the specification of properties ranges would be more realistic. Such variations can be incorporated in the analysis by assuming their properties to obey a statistical distribution, for example, the Weibull distribution. Each kind of components can have an independent degree of heterogeneity. Thus, the heterogeneities of these components can be implemented.

9.2.3 Representation of the physical domain microstructure by the SPH particles

In order to use the SPH particles to represent the physical domain’s microstructure, one must determine to which polyhedron each particle belongs. If the particle’s center falls inside the polyhedron, it is assigned to the component’s properties represented by this polyhedron.

There are many methods to judge a point is inside or outside a 3D polyhedron.
The current work uses the one proposed by Pinto and Paulo (1995) for its simplicity.

Figure 9-3 Projecting one face of a polyhedron onto a unit sphere of center $p$ (after Pinto and Paulo, 1995)

The approach is to project each face of the polyhedron onto a unit sphere of the center $p$ (see Figure 9-3) and compute the signed area of the spherical polygon thus determined. The sign is positive if the spherical polygon has counterclockwise orientation and negative otherwise. The summation of the signed areas of the projections of all faces of the given polyhedron onto the unit sphere of $p$ is $0$, $4\pi$ or $-4\pi$. If the summation is $0$, then $p$ is exterior to the polyhedron. Otherwise, it is interior.

By using the above method, each particle can find its polyhedron container by traversing all these polyhedrons. The material domain can be represented by those clusters of particles to resemble the real specimen’s microstructure.

### 9.2.4 Application of the method on the 3D granite microstructure generation

One 3D microstructure of the Bukit Timah Granite prism is constructed by using the proposed approach. The prism has a cross section of $5 \, \text{cm} \times 5 \, \text{cm}$ and a height of $10 \, \text{cm}$. Statistical data show that Bukit Timah granite is composed mainly by feldspar, quartz and biotite with a ratio of around 6:3:1. The grain size of these mineral grains is within a range from 3 mm to 5 mm.

A set of points arranged in the body-centered cubic lattices with the edge length of $4.0 \, \text{mm}$ are constructed for the Voronoi diagram generation. To make these
constructed tessellations irregular, the pseudo-random disturbances are added to the coordinates in those points. The disturbances are limited within -1.0 mm to 1.0 mm to meet the grain size requirement.

After these tessellations are ready, they are classified into different mineral types by the values of the pseudo-random numbers associated with them according to the prescribed ratio of three kinds of minerals. Heterogeneities of three kinds of minerals are assumed to follow the Weibull distributions with the different homogeneous index values of 10.0, 3.0 and 10.0 for feldspar, quartz and biotite, respectively.

The SPH particles to represent the domain are discretized by those polyhedrons. These particles have the same smoothing length of 0.625 mm.

Figure 9-4 3D microstructure of Bukit Timah granite prism; a) granite composed by mineral grains; b) feldspar grains; c) quartz grains; d) biotite grains.

The generated 3D microstructure of the Bukit Timah granite prism is shown in
Figure 9-4. The images of its each mineral component are also given in the diagram. The ratio of feldspar, quartz and biotite in the generated sample are 59.28%, 30.54% and 10.18%, respectively, which is very close to the statistical value. In order to give a better internal view, the microstructure images in different layers along the three orthogonal planes are plotted in Figure 9-5.

Figure 9-5 Plots of the granite microstructure images in different layers; a) along the x coordinate axis; b) along the y coordinate axis; c) along the z coordinate axis.

Figure 9-6 plots the statistical frequency counts in the mineral’s heterogeneous strength distributions. As can be seen, the strength distribution in the quartz grains is more heterogeneous.

Figure 9-6 Plots of the strength heterogeneities in three minerals of the generated granite prism by their statistical frequency counts.
9.3 Numerical model configuration

9.3.1 Specimen geometry and loading conditions

The granite uniaxial compression failure simulations are conducted under 3D. Two samples are constructed by intercepting from the top and bottom parts of the inscribed cylinder from the generated 3D granite prism, as illustrated in Figure 9-7. Diameters of these two cylinder samples are 0.05 m. Their heights are both in 0.03 m. Their Mineral contents are given in Table 9-1.

![Illustration for the preparations of the granite compression test samples. a) the granite prism b) sample 1 intercepted from the top part of the prism; c) sample 2 intercepted from the bottom part of the prism.](image)

<table>
<thead>
<tr>
<th>specimen</th>
<th>Feldspar</th>
<th>Quartz</th>
<th>Biotite</th>
</tr>
</thead>
<tbody>
<tr>
<td>Prism</td>
<td>59.28%</td>
<td>30.54%</td>
<td>10.18%</td>
</tr>
<tr>
<td>Sample 1</td>
<td>59.77%</td>
<td>30.44%</td>
<td>9.79%</td>
</tr>
<tr>
<td>Sample 2</td>
<td>59.73%</td>
<td>29.94%</td>
<td>10.33%</td>
</tr>
</tbody>
</table>
Figure 9-8 shows the specimen’s boundary condition and loading conditions. The sample is sandwiched between two rigid walls with the prescribed velocities defined in Eq.(9.2),

\[
v(t) = \begin{cases} 
\frac{t}{t_0} v_0, & \text{when } t \leq t_0 \\
v_0, & \text{when } t > t_0 
\end{cases}
\]  

(9.2)

where \( t_0 = 5.0 \times 10^{-5} \text{ s} \). The loading cases and their corresponding strain rates are presented in Table 9-2.

![Figure 9-8 Illustration of the specimen's geometry and loading conditions](image)

Table 9-2 Loading conditions for numerical uniaxial compression simulations

<table>
<thead>
<tr>
<th>( v_0 \text{ (m/s)} )</th>
<th>0.015</th>
<th>0.15</th>
<th>0.9</th>
<th>1.8</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \dot{\varepsilon} \text{ (s}^{-1}) )</td>
<td>1</td>
<td>10</td>
<td>60</td>
<td>120</td>
</tr>
</tbody>
</table>

9.3.2 Numerical approach and parameters

The developed SPH code is applied to carry out the 3D uniaxial compression test simulations. All model parameters follow to those in the specimen N2-2 in Chapter 7, in which feldspar, quartz and biotite grains are assumed to follow the independent Weibull distributions with the shape values as 10, 3 and 10, respectively. The SPH particles of these two specimens have the same smoothing length of 0.625 mm. Each specimen contains 241152 SPH particles.
9.4 Simulation results

The numerical simulations have been performed under the four different strain rates as given previously for both samples. The result from the sample 2 will be presented in details firstly and compared with those from sample 1 next.

9.4.1 Stress-strain curves and dynamic stress balance

Figure 9-9 plots the axial stress-strain curves under the different strain rates from 1.0 s\(^{-1}\) to 120 s\(^{-1}\), where the axial stresses are expressed in terms of the response compressive stress on the upper boundary, the bottom boundary and their average. The dashed, dotted and solid lines are the stress profile on the upper boundary, the bottom boundary and their average, respectively. Profiles of the damaged particle count with the axial strain for those four strain rate cases are also plotted in the figure.

Figure 9-9 Profiles of the damaged particles count as well as the axial response compressive stress with the axial strain; Figures from a) to d) correspond to those cases with the strain rate from 1.0 s\(^{-1}\) to 120 s\(^{-1}\), respectively.
It can be seen that the dynamic response stresses on the both sides of the specimen are almost identical during the whole loading duration in all cases. Such a stress balance state is vital to ensure the credibility of numerical simulation result especially under the dynamic loadings.

Both the damaged particles count records and the axial stress-strain curves are quite different for the different strain rate cases. As can be seen in the low strain rate 1.0 s\(^{-1}\) case, before its peak stress, few particles fail. Instead, a substantial number of the damaged particles intensively appear shortly after its peak stress. The stress almost linearly increases and then drops down suddenly. The stress-strain curve resembles a typical brittle failure. With the increasing strain rate, it is clearly to be observed that these damaged particles occur at a much lower percentage of the peak stress. The damaged particles become more and more before the peak stress as the strain rate increases. Such phenomena are more evident in the diagrams of the accumulated damaged particles count shown in Figure 9-10. With the failures of those particles, the strain-stress curve becomes nonlinear.

![Figure 9-10 Profiles of accumulated damaged particles count with the axial strain under the different strain rates of sample 2.](image)

### 9.4.2 Failure patterns

The damage distributions of the specimen 2 under the four strain rates are plotted together in Figure 9-11. In the plot, those damaged particles are in white. To
give a better internal view, the specimen’s damage distributions at the different layers along the three orthogonal planes are also plotted in the figure.

For the cases with the strain rate 1.0 and 10.0 \( s^{-1} \), it can be seen that a visible crack appears on the top surface. From their internal layers, one can observe that, in the front right side, a portion of severely damaged fragment was formed by those traversing cracks along the loading direction. The specimen is roughly split into two or three few large fragments.

With the increasing strain rate, the visible cracks on the specimen become more. Consequently, the specimen is broken into more fragments. As can be seen, in the case of the strain rate 120.0 \( s^{-1} \), the specimen has an irregular circumferential like crack at specimen’s inner part and the radial cracks at its outer part. Those cracks cause the sample to rupture into one large fragment in the center part and many small ones along the edge as shown in the figure.

Those damage patterns are comparable to those obtained from the experiments qualitatively as shown in the previous chapters.
Numerical Simulation of Heterogeneous Material Failure by using the SPH Method

strain rate $0.1\, s^{-1}$ at the 70.0% of its peak stress in the post-peak stage

strain rate $10.0\, s^{-1}$ at the 70.0% of its peak stress in the post-peak stage
strain rate 60.0 s\(^{-1}\) at the 65.0% of its peak stress in the post-peak stage

strain rate 120.0 s\(^{-1}\) at the 65.0% of its peak stress in the post-peak stage

Figure 9-11 Plots of specimen’s damage pattern under the different strain rates of sample 2.
9.4.3 Comparisons of the results from the two samples

Since both are from the same parent, sample 1 and sample 2 have the same degree of heterogeneity while different microstructures. To examine such a spatial variation effect in the microstructure, those aforementioned simulations on the sample 2 are also performed on the sample 1.

The stress-strain curves of these two specimens under the different strain rates are plotted together in Figure 9-12. It can be seen that macro mechanical behaviors of both specimens are affected remarkably by strain rates and have same characteristics. The maximum stress and sustained maximum strain exhibited by the specimen increase as the strain rate is getting higher. Shapes of the curves are also different under different strain rates. When strain rate is low, the sample experiences little plasticity before a brittle failure happens. Whereas, for the higher strain rate cases, curves exhibit three stages: the linear elastic, non-linear and the post-peak softening region.

![Comparison of the stress-strain curves of the two specimens under the different strain rates](image)

Figure 9-12 Comparison of the stress-strain curves of the two specimens under the different strain rates

Although these two specimens are quite different in their microstructures, their mechanical responses are in a very similar shape and match well. Under the lower strain rates, the curves from the two samples have a slightly difference. When strain rate increases, the deviations decrease and the curves of the two
specimens are almost identical. Such phenomena are due to the different failure mechanisms affected by the strain rate. Under the low strain rate cases, the specimen’s failure is controlled by few relatively “weak” zones. Once a crack is formed, its rapid propagation can ruin the specimen’s load carrying capacity. Therefore, its mechanical response is more dependent on the specimen’s heterogeneous microstructure condition. However, under the higher loading rate, the specimen’s failure is dominated by the interactions of many cracks. Thus, its mechanical behavior is more likely to be a collaborative response.

Figure 9-13 Comparison of the damage distributions of two specimens under different strain rates; a)-d) specimen 2 under strain rate from $1.0 \text{ s}^{-1}$ to $120 \text{ s}^{-1}$; e)-f) specimen 1 under strain rate from $1.0 \text{ s}^{-1}$ to $120 \text{ s}^{-1}$.

Figure 9-13 plots the damage patterns of these two specimens under different strain rates. We can see more visible cracks and fragments under the higher strain rate cases.

### 9.4.4 Strain rate effect on the predicted dynamic compressive strength

Similar to the results in the previous chapter, the predicted compressive strength also exhibits the strain rate sensitivity in that the dynamic strength increases as the strain rate becomes higher. As discussed previously, the validation of these predicted results in quantitative with those of experimental results is difficult.
Again, instead of concentrating on the specific value of a certain field quantity of the results, we do care the general characteristics that those artificial samples behave.

Figure 9-14 compares the numerical predicted apparent compressive strength with those obtained from the granite experimental tests, respectively. Experimental result 1 can be referred in Appendix A and Appendix B, where the dynamic strengths are obtained from SHPB tests. Results of the experiment 2 are from Xia et al. (2008). The comparisons take the forms of their dynamic increment factor (DIF) values for these strengths. The DIF value is calculated by normalizing the dynamic strength with respect to its quasi-static value (at a strain rate around $10^{-5}$ s$^{-1}$). Due to the expensive computational effort to perform the quasi-static analysis using the SPH code, the DIF values of the numerical predicted strengths are normalized with the strain rate 1.0 s$^{-1}$ value instead. In the diagram, the DIF values of the numerical predicted average pressure $DIF_p$ under the different strain rates are also plotted.

![Graph showing DIF values for apparent compressive strength and average pressure](image)

**Figure 9-14** Comparison of numerical and experimental dynamic compressive strength with the logarithm of strain rate

As can be seen from the diagram, the experimental and numerical results both demonstrate the similar trends in the sense that their compressive strengths in-
crease with the applied strain rate. It seems that the predicted increment is sharper around the strain rate $10 \text{ s}^{-1}$. Such a deviation may come from several sources and has been analyzed in the previous chapter.

As discussed previously, the possible reasons for such a strain rate sensitivity phenomenon in the specimen’s compressive strength may come from the inertial effect caused by the micro crack activity, the dynamic failure mechanism in the heterogeneous materials and the lateral inertial effect. Those effects will cause the pressure increments under the dynamic loading and finally result in the specimen’s higher strength. As can be seen in Figure 9-14, the DIF curve of the predicted specimen’s average pressure agree well with that of the compressive strength.

9.5 Summary

In this chapter, the 2D heterogeneous microstructure modeling method is extended to the 3D cases and applied to generate the 3D artificial microstructure granite specimens.

The 3D uniaxial compression test simulations have been conducted on these artificial specimens by using the developed SPH code under the different strain rates from $0.1 \text{ s}^{-1}$ to $120 \text{ s}^{-1}$. The specimen’s dynamic mechanical responses under these cases are examined and their damage patterns are discussed. The strain rate sensitivity of the specimen’s dynamic compressive strength is analyzed and compared with the experimental result. The comparison result shows that they are in good agreement in the overall trend. It seems that the proposed 3D modeling method can better resemble the real rock microstructure and can be further used in other applications.
Chapter 10 Conclusions and Recommendations

10.1 Conclusions and discussions on the current work

The study presents a new progress in the heterogeneous micromechanical modeling method and a 3D solver based on the novel mesh-free method to simulate the dynamic failure on heterogeneous brittle materials by capturing the detailed fracture sequence of the microscopic crack activities and the macro mechanical response.

10.1.1 The proposed heterogeneous micromechanical modeling method and the developed SPH code

In the method, an elasto-plastic damage constitutive model is proposed to describe the mechanical characteristics of the brittle material during the failure process. Since the Unified Twin Shear Strength theory has the advantage to unify the existing criteria through a weighting coefficient \( b \), a generalized multi-parameter unified yield criterion based on the UTSS theory is adopted. It is further extended to include the empirical pressure dependent tensile and compressive meridians by regressing the static uniaxial and triaxial compression tests results. To account for the compression and tension induced strength degradation, a scalar damage variable induced by the effective plastic strain is adopted in conjunction with a pressure-cutoff failure criterion.

The statistical approach has been utilized to characterize the material heterogeneity by associating the specimen’s microstructure strengths with the Weibull distribution. Therefore, material with a certain degree of heterogeneity can be described by using one defined homogeneous index parameter \( \beta \). Initially, the heterogeneous Weibull distribution is directly applied on each computational
“element” (SPH particle) which is suitable for material with fine grains (heterogeneous model I). Later on, an advanced 2-D and 3-D microstructure modeling approach for the multi-phased material is proposed to better model the geomaterial usually composed by different kinds of components with irregular aggregates (heterogeneous model II). A treatment of the heterogeneities in these components is also addressed by using the Weibull distribution law. The proposed method can reflect the spatial variations of the components distributions as well as their strengths distributions without losing the generality. Although the proposed microstructure modeling method can only be regarded as an approximation of a real complex material, it shows potential advantages as an efficient approach to extend the conventional numerical methods in the analysis of real materials.

A 3D computer program is developed to implement the new micromechanical model based on the novel mesh-free Smoothed Particle Hydrodynamics (SPH) method. The adopted SPH method provides an efficient and robust solver in processing the discontinuous problems, such as the large deformation and fragments during the failure process simulation. The core part of the developed program is calibrated using the commercial software AUTODYN 2D. Results demonstrate a satisfactory accuracy.

10.1.2 Simulations on the brittle material failures

The developed 3D SPH code has been applied to examine the failure characteristics on heterogeneous rock-like materials. A series of numerical simulations are performed on the Brazilian tensile test, uniaxial and biaxial compression test under different strain rates. Investigations are concentrated on the material heterogeneity as well as the strain rate effects on the fracture process and the macroscopic mechanical response.

- Simulation results on the Brazilian splitting test and compression test with the heterogeneous model I under different strain rates:

Results show that specimen’s heterogeneity influences the dynamic tensile and compressive strengths in that the predicted tensile and compressive strengths
increase as the specimen gets more homogeneous. The strain rate can affect the specimen’s fracture process in a sense that the higher strain rate will cause more micro cracks in the specimen. It can also influence specimen’s strength. The predicted dynamic tensile and compressive strengths will increase with the increasing strain rates. In addition, such increments are more obvious in more heterogeneous specimen. The predicted tensile strength increments are compared with those obtained from experiments. Results show good agreements in the overall trend. Since the constitutive model does not explicitly consider the strain rate effects, further studies indicate that the increasing pressure due to the rapid loading is one of the major reasons for such effects. The effect of the coefficient $b$ on the specimen’s strengths is also examined. Result shows the predicted strengths increase as the $b$ becomes larger.

- Simulations of compressive failure on rock-like specimens with the heterogeneous model I under a low strain rate:

Result shows that the material heterogeneity has a great influence on the material’s macro mechanical response. For specimens with different degrees of heterogeneity, the predicted uniaxial compressive strength (UCS) and the corresponding axial strain increase as the specimen becomes more homogenous. Simulation results also show that failure developments in the brittle materials have common characteristics. First, conspicuous cracks are formed near their peak stresses and mostly parallel to the loading directions. Second, axial cracks or faults are formed during the post-failure regions. Although the shear faulting and the cleavage are the two major modes in rock failures, results show that most failure patterns in these specimens are the combination one. The simulated failure processes also manifest the material heterogeneity effects. In a more homogeneous specimen, the major crack will dominate the failure. On the contrary, in a less homogenous one, activities of many macro cracks will cause the failure. Even for specimens with the same degree of heterogeneity, the initial cracks and their consequent developments are highly affected by the different local stress severities due to their microstructures.

- Simulation results from the biaxial test under different lateral confining
stress with the heterogeneous model I:

Result show that the specimen’s load carrying capacity increases as the applied lateral stress increases. Specimen’s post-failure pattern is also affected by the magnitude of the applied stress. Due to the lateral confinement, the axial cracks are restrained and more shear cracks developed to form shear faults. In addition, the higher applied confinement will induce the shear fault wider and its angle to the vertical plane slightly bigger.

- The heterogeneous model II and its applications in the Brazilian splitting test and compression test simulations at a low strain rate:

The heterogeneous model II is proposed for multi-phased material by taking account into the actual contents of different components and their characteristic sizes. The modeling method has been applied to construct the artificial polycrystalline granite specimen. Numerical simulations of the uniaxial compression test and Brazilian tensile test are further performed on these artificial specimens to investigate the granite failure behaviors. Results demonstrate that both the microstructure and mineral components heterogeneities have influences on the specimen’s failure process and macroscopic mechanical response.

- Simulation results on the Brazilian splitting test and compression test with the heterogeneous model II under different strain rates:

The predicted fracture sequences in both Brazilian splitting tests and uniaxial compression tests manifest their failure processes are notably influenced by the applied strain rates. In the lower strain rate cases, the failure is roughly due to the development of few major cracks. On the contrary, under the higher strain rate cases, the specimen’s failure is caused by the coalescences and interactions of many short cracks. Specimen’s macro mechanical behaviors exhibit pronounced strain-rate sensitivities. As the strain rate becomes higher, both the specimen’s loading capacity and its sustained maximum displacement (or strain) also becomes larger. The strain rate effect on the specimen’s strength is analyzed and compared with that obtained from the experimental results. It seems that such an effect might be attributed to the internal pressure changes due to the inertial effects as well as the specimen’s crack activities under the different
Numerical Simulation of Heterogeneous Material Failure by using the SPH Method

strain rates.

- Simulation results on the 3D compression test with the heterogeneous model II under different strain rates:

The 3D uniaxial compression test simulations have been conducted on the artificial specimens by using the developed SPH. The specimen’s dynamic mechanical responses under these cases are examined and their damage patterns are discussed. The strain rate sensitivity of the specimen’s dynamic compressive strength is analyzed and compared with the experimental results. The comparison shows that they are in good agreement in the overall trend. It seems that the proposed 3D modeling method can better resemble the real rock microstructure and can be further used in other applications.

The above simulations manifest that the developed SPH code can well capture the failure sequences and represent the real cracks and fragments induced by large deformations. Moreover, the whole process does not need any special treatments or assumption in presenting the cracks and fragments. From the view of this point, the SPH code has obvious advantages in rock-like brittle material failure simulations.

10.2 Recommendations on the future work

The developed 3D SPH code can predict most of the experimentally observed phenomena. The potentials of utilization for the proposed model in future research are very broad. Of course, there exist some shortcomings. Therefore, the following recommendations are given for future research:

- To apply the current program on large dynamic deformation analysis

Since the developed SPH code is very suitable to simulate problems with large deformations, further applications can be carried out on those fields such as the rock blasting and high-speed penetrations.

- To improve the current micromechanical modeling method

The heterogeneous microstructure in real materials is definitely more complex than what the current proposed models can provide and can be improved in the
future towards representing the real ones, such as considering the void, the pre-existing cracks and the interface modelling between the mineral grain boundaries, etc. Besides, parameters in the micromechanical modeling need to be further analyzed to better reflect the macro mechanical of real materials.

- To improve the current SPH solver

The higher accuracy of the current SPH method can be achieved by using some “corrective” or “restoring” methods towards its kernel and derivative approximations and a proper boundary treatment method.

Due to the expensive computational effort of the SPH solver in performing the large-scale calculations especially under 3D cases, the current SPH code can be coupled with the other Lagrangian method to improve its efficiency.
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Appendix A  Experimental Results on the Dynamic Tensile Strengths of Granite under Different Strain Rates

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Appendix B  Experimental Results on the Dynamic Compressive Strengths of Granite under Different Strain Rates

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