Three-dimensional multi-scale hydraulic fracturing simulation in heterogeneous material using Dual Lattice Model

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This dissertation is submitted for the degree of
Doctor of Philosophy

Churchill College January 2018
I would like to give the glory to the almighty God.

*I am the way and the truth and the life.*

(John 14:6, Holy Bible)
Declaration

I hereby declare that except where specific reference is made to the work of others, the contents of this dissertation are original and have not been submitted in whole or in part for consideration for any other degree or qualification in this, or any other university. This dissertation is my own work and contains nothing which is the outcome of work done in collaboration with others, except as specified in the text and Acknowledgements. This dissertation contains fewer than 65,000 words including appendices, bibliography, footnotes, tables and equations and has fewer than 150 figures.

John Kam Wing Wong
January 2018
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Abstract

Hydraulic fracturing is a multi-physics and multi-scale problem related to natural processes such as the formation of dikes. It also has wide engineering applications such as extraction of unconventional resources, enhanced geothermal energy and carbon capture and storage. Current simulators are highly simplified because of the assumption of homogeneous reservoir. Unconventional reservoirs are heterogeneous owing to the presence of natural fracture network. Simulators that considered heterogeneous reservoirs are needed.

Different numerical methods have been suggested for hydraulic fracture simulations. They focus on the multi-physics nature of the problem. Because of high computational effort, three-dimensional multi-scale simulations are uncommon, in particular, modelling material as a heterogeneous medium. Lattice Element Method (LEM) is therefore proposed for multi-scale simulation of heterogeneous material.

In LEM, material is discretised into Voronoi cells and their interactions are modelled by lattices, hence a three-dimensional model is simplified to a network of one-dimensional lattice. Normal, shear and rotational springs are used to define the constitutive laws of a lattice. Lattice models are solved implicitly, giving high computational performance that enables desktop computers for simulation of a lattice model that consists of millions of lattices.

From simulations, normal springs govern the macroscopic bulk deformation while shear springs govern the macroscopic distortion. Rotational springs have negligible effects on both the macroscopic and the microscopic behaviour. There is fluctuation of stresses even under uniform loading which is one of the characteristics of a lattice model. The magnitude increases with the stiffness ratio of shear spring to normal spring. Additional heterogeneity can be applied by introducing statistical distributions on lattice parameters.

Fracturing process can be modelled by LEM by introducing a microscopic tensile strength and a microscopic shear strength to the lattice properties. The strength parameters can be related to the fracture toughness with the length scales of cells. From simulations, the relationships between model parameters and macroscopic parameters that are measurable in experiments are identified.
From the simulations of uni-axial tension tests, both the spring stiffness ratio and the applied heterogeneity govern the fracturing process. The heterogeneity increases the ductility of a lattice model at the expense of the reduction on the macroscopic strengths. Different stages of fracturing are identified which are characterised by the model heterogeneity. Heterogeneous models go through the stages of the spatially distributed microcrack formation, the growth of multiple fracture clusters to the dominant fracture propagation. For homogeneous models, one of the microcracks rapidly propagates and becomes a dominant fracture with the absence of intermediate stages. From the uni-axial compression test simulations, a linear relationship is established between the macroscopic compressive strength to the microscopic strength ratio of shear spring to tensile spring. The peak compressive stress is reached at the onset of the microscopic shear crack formation. Ductility is mainly governed by the stiffness reduction ratio of a lattice in closed fractured stage to its unfractured stage.

A novel Dual Lattice Model (DLM) is proposed for hydraulic fracture simulation by coupling a solid lattice model with a fluid lattice model. From DLM simulations of hydraulic fracturing of the classical penny shape crack problem under hydrostatic condition, the heterogeneities from both the fracture asperity and the applied heterogeneity increase the apparent fracture toughness. A semi-analytical solution is derived to consider the effect of fluid viscosity in the elastic deformation regime. Two asymptotes are identified that give steep pressure gradients near the injection point and near the fracture tip. These two asymptotes are also identified in the DLM simulations. The DLM simulations also show three evolving regimes on energy dissipation/transfer mechanisms of hydraulic fracturing: from the viscosity dominant, the elastic deformation dominant and the mixture of elastic deformation and toughness.
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3 Analytical and numerical methods in hydraulic fracturing simulation

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Nomenclature

Roman Symbols

$A_l$  Area of lattice facet

$A_P^{}$  projected area of facet perpendicular to the resultant force of lattice

$a_{RVE}$  RVE size

$A_s$  Shear area

$B$  Brittle index

$C_{ijkl}$  Stiffness tensor

$C_L$  Leak off coefficient

$D$  Structural size

$d_r$  Fracture surface roughness

$E$  Macroscopic Young Modulus

$E_{micro}$  Microscopic Young Modulus

$E_{s,micro}$  Microscopic secant Young modulus

$\sigma_{ij}^n$  Nodal stress

$F_f$  Lattice force

$F_n$  Lattice axial force

$F_R$  Resultant force of lattice axial force and shear force
Nomenclature

- $f_{r,t}$: Residual macroscopic tensile strength
- $F_s$: Lattice resultant shear force
- $F_{s1}$: Lattice shear force along local axis 1 (3D case)
- $F_{s2}$: Lattice shear force along local axis 2 (3D case)
- $f_{sc}$: Microscopic compressive strength
- $f_{ss}$: Microscopic shear strength
- $f_{st}$: Microscopic tensile strength
- $f_t$: Macroscopic tensile strength
- $F_{tn}$: Threshold for lattice tensional force
- $F_{ts}$: Threshold for lattice shear force
- $G$: Macroscopic shear modulus
- $G_c$: Critical strain energy release rate
- $G_{micro}$: Microscopic shear modulus
- $G_e$: Strain energy release rate
- $h_{ij}$: Permeability tensor
- $I_{11}$: Principal moment of area
- $I_{22}$: Principal moment of area
- $J_p$: Polar second moment of area
- $K$: Consistency index (Power law model of fluid)
- $K$: Macroscopic bulk modulus
- $k$: Hydraulic permeability
- $K_f$: Bulk modulus of pore fluid
- $K_I$: Stress intensity factor (Mode I)
- $K_{Ic}$: Fracture toughness, critical stress intensity factor (Mode I)
Nomenclature

$K_{micro}$ Microscopic bulk modulus

$k_n$ Axial spring stiffness

$k_{\phi n}$ Torsional spring stiffness

$k_{\phi s}$ Rotation spring stiffness along principal direction $s$

$k_{\phi t}$ Rotation spring stiffness along principal direction $t$

$K_f$ Bulk modulus of solid skeleton

$k_s$ Shear spring stiffness

$l_{FPZ}$ Length of fracture process zone

$l_k$ Length scale for toughness

$l_l$ Lattice length

$l_t$ Lattice length

$l_m$ Length scale for viscosity

$l_{\overline{m}}$ Length scale for leak-off

$l_{min}$ Minimum distance between any two nodes

$M_b$ Lattice bending moment (2D case)

$M_n$ Lattice torsional moment (3D case)

$M_t$ Threshold for lattice moment

$M_{tb}$ Threshold for lattice bending moment

$M_u$ Lattice out of plane moment (3D case)

$M_v$ Lattice out of plane moment (3D case)

$N$ Number of node

$n$ Node density expressed as a fraction to closest possible packing of equal spheres

$n = \frac{N}{N_{HCP}}$
Nomenclature

\begin{itemize}
  \item $n^*$ Saturated node density expressed as a fraction to closest possible packing of equal spheres $N_{HCP}$
  \item $n_{\text{coord}}$ Coordination number of node
  \item $N_{\text{DOF}}$ Number of DOF
  \item $N_{\text{HCP}}$ Number of node corresponding to closest possible packing of equal spheres of HCP
  \item $N_{\text{lattice}}$ Number of lattice
  \item $N_{\text{rej}}$ Number of successive rejection of trial node in random node generation
  \item $p$ Pore fluid pressure
  \item $p_L$ Applied uniform pressure
  \item $q$ Flow rate/Injection rate
  \item $q_{ij}$ Specific discharge
  \item $f$ Friction factor (Fluid mechanics)
  \item $Re$ Reynolds number
  \item $\sigma_{ss}$ Microscopic shear stress
  \item $t_c$ Characteristic time
  \item $t_{\text{exp}}$ The time when fracture was exposed to fracturing fluid
  \item $t_{mk}$ Dimensionless time related to relative importance of toughness and viscosity
  \item $t_{mk}$ Time scale for evolving from viscosity to toughness regime in hydraulic fracturing assuming zero lag
  \item $t_{m\tilde{m}}$ Time scale for evolving from storage to leak-off regime in hydraulic fracturing assuming zero toughness
  \item $t_{om}$ Dimensionless time related to \textit{in-situ} stress
  \item $u_L$ Leak off velocity
  \item $V_{cell}$ Volume of cell
  \item $Y$ Geometry factor for calculation of stress intensity factor
\end{itemize}
**Greek Symbols**

- $\alpha$: Ratio of stiffness between axial spring and shear spring in RBSN
- $\alpha^+$: Load increment factor
- $\alpha^-$: Load decrement factor
- $\alpha_B$: Biot coefficient
- $\alpha_b$: Dimensionless value accounting the effect on bending in lattice failure criterion
- $\beta$: Factor to modify the contribution of rotation stiffness in RBSN
- $\delta$: Fracture aperture
- $\gamma$: Lattice reconnection factor
- $\sigma_1$: Statistics: skewness
- $\sigma_2$: Statistics: excess kurtosis
- $\gamma_f$: Specific fracture surface energy
- $\gamma_{sf}$: Micro-ductility
- $\dot{\gamma}$: Shear rate of fluid
- $M_i(x)$: Local enrichment function
- $\mu$: Newtonian fluid viscosity
- $\mu$: Statistics: mean
- $N_i(x)$: Conventional FE shape functions
- $\nu$: Macroscopic poisson ratio
- $\nu_{micro}$: Microscopic Possion ratio
- $\omega$: Scalar damage variable
- $\Phi_f$: Threshold for total potential energy of lattice
- $\Psi(x)$: Global enrichment function
- $\Psi_{cell}$: Cell sphericity
\( \rho \)  
Load capacity ratio of a lattice

\( \rho_{l, \text{max}} \)  
Maximum load capacity ratio among all lattices

\( \sigma \)  
Statistics: standard deviation

\( \sigma_1 \)  
Minimum principal stress

\( \sigma_2 \)  
Intermediate principal stress

\( \sigma_3 \)  
Maximum principal stress

\( \sigma_{ij} \)  
Stress tensor

\( \sigma'_{ij} \)  
Effective stress

\( \sigma_\infty \)  
Far field stress

\( \sigma_{sn} \)  
Microscopic axial stress

\( \sigma_{ys} \)  
Microscopic yield stress

\( u^h(\mathbf{x}) \)  
Enrichment shape function

\( \varphi_i(\mathbf{x}) \)  
Partition function (XFEM)

\( \varepsilon_A \)  
Minimum area of facet to be represented by a lattice

\( \varepsilon_{kl} \)  
Strain tensor

\( \varepsilon_{sf} \)  
Microscopic failure strain

\( \varepsilon_{st} \)  
Microscopic yielding strain

\( \varphi \)  
Trajectory parameter for evolving regimes for penny-shape hydraulic fracturing propagating in an impermeable elastic medium

\( \xi \)  
correlation length

**Other Symbols**

\( C_m \)  
Dimensionless parameter for leak-off

\( K \)  
Dimensionless toughness

\( \mathcal{M} \)  
Dimensionless viscosity
### Nomenclature

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<td>$\mathcal{O}_m$</td>
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<td>$Z$</td>
<td>Dimensionless far field stress</td>
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### Acronyms / Abbreviations

- **3DEC**: Commercial package of 3D version block type DEM developed by Itasca Consulting Group
- **AE**: Acoustic Emission
- **BEM**: Boundary Element Method
- **BPM**: Bonded Particle Model
- **CDM**: Continuum damage mechanics
- **CFD**: Computational Fluid Dynamics
- **CPU**: Central Processing Unit
- **DDA**: Discontinuous Deformation Analysis
- **DD**: Displacement Discontinuity
- **DBEM**: Dual Boundary Element Method
- **DDM**: Displacement Discontinuity Method
- **GBEM**: Galerkin Boundary Element Method
- **DEM**: Discrete Element Method
- **DIANE**: Discontinuous, Inhomogeneous, Anisotropic and Non-Elastic
- **DLM**: Dual Lattice Model
- **DOF**: Degree of Freedom
- **DRFM**: Ductile Random Fuse Model
- **LSM**: Lattice Spring Model
<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
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<tbody>
<tr>
<td>EGS</td>
<td>Enhanced Geothermal System</td>
</tr>
<tr>
<td>FCC</td>
<td>Face Centre Cubic</td>
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<tr>
<td>FEM</td>
<td>Finite Element Method</td>
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<tr>
<td>FMM</td>
<td>Fast Multipole Method</td>
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<tr>
<td>FPZ</td>
<td>Fracture process zone</td>
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<tr>
<td>GPU</td>
<td>Graphics Processing Unit</td>
</tr>
<tr>
<td>HCP</td>
<td>Hexagonal Close Packing</td>
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<tr>
<td>HF</td>
<td>Hydraulic Fracture</td>
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<tr>
<td>KGD</td>
<td>Khristianovich-Geertsma-de Klerk hydraulic fracturing model</td>
</tr>
<tr>
<td>LBM</td>
<td>Lattice Boltzmann Method</td>
</tr>
<tr>
<td>EPFM</td>
<td>Elastic-Plastic Fracture Mechanics</td>
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<tr>
<td>LEFM</td>
<td>Linear Elastic Fracture Mechanics</td>
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<tr>
<td>LEM</td>
<td>Lattice Element Method/Model</td>
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<tr>
<td>LSM</td>
<td>Lattice Spring Model</td>
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<tr>
<td>LVDT</td>
<td>Linear Variable Differential Transformer</td>
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<tr>
<td>MPI</td>
<td>Message Passaging Interface</td>
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<td>NF</td>
<td>Natural Fracture</td>
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<td>P3D model</td>
<td>Pseudo-3D hydraulic fracturing model</td>
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<tr>
<td>PCG</td>
<td>Preconditioned Conjugate Gradient</td>
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<tr>
<td>PDF</td>
<td>Probability Density Function</td>
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<tr>
<td>PFV</td>
<td>Pore-scale Finite Volume</td>
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<td>PKN</td>
<td>Perkins-Kern-Nordgren hydraulic fracturing model</td>
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<tr>
<td>PL3D model</td>
<td>Planar-3D hydraulic fracturing model</td>
</tr>
</tbody>
</table>
Nomenclature

RBSM  Rigid Body Spring Model
REV   Representative Elementary Volume
RFM   Random Fuse Model
RMR   Rock Mass Rating
RQD   Rock Quality Designation
SJM   Smooth Joint Model
SRM   Synthetic Rock Mass

UDEC  Commercial package of 2D version block type DEM developed by Itasca Consulting Group
DFN   Discrete Fracture Network
UFM   Unconventional Fracture Model
XFEM  Extended Finite Element Method
Chapter 1

Introduction

1.1 Background

Hydraulic fracturing is a technique which aims to enhance the permeability of rock by injecting highly pressurised fluid to create fracture surfaces. It is termed as stimulation in reservoir engineering and sometimes is referred as hydrofracturing. It is often called fracking by the general public.

Hydraulic fracturing was first introduced in the 1950s by the oil industry to enhance the productivity of wells (Economides and Nolte, 2000). Later, it has been extended to other applications such as extraction of unconventional resources (Li et al., 2015), enhanced geothermal system (EGS) (Kohl and Megel, 2007), disposal of radioactive waste (Brown, 2014), mining (van As and Jeffrey, 2000), Carbon Capture and Storage (Ishida et al., 2012) and in-situ stress measurement of rock (Stock et al., 1985). Hydraulic fracturing is also involved in natural processes such as formation of dikes by magma (Lister and Kerr, 1991; Rubin, 1995) and crack propagation at glacier beds (Tsai and Rice, 2010).

1.2 Brief description on process of hydraulic fracturing

Figure 1.1 illustrates a hydraulic fracturing process for the extraction of unconventional resources. The process starts with drilling from surface. Horizontal drilling starts once the well reaches the target reservoir (called pay zone or production zone). Steel casing is provided at shallow depth and a cementitious annulus is cast around the whole length of the well to prevent contamination of ground water.

At the location of the target zone where hydraulic fracturing to be applied, perforation is formed by explosives or hydro-jets to create finger-like holes or weak points at a given
orientation. After that, packers are placed at two ends and high pressure fracturing fluid is injected in between. Pressure is increased until the rock near the wellbore fails and fracture initiates (breakdown).

Clean fluid is first injected to create fractures with sufficient aperture for proppants to pass through (a pad). The slurry-like fracturing fluid carrying proppants is then pumped at the later stage. Pumping is stopped (shut-in) and fluid pressure is maintained for the fracture to grow and for the proppants to fill the fracture. The duration of shut-in varies from less than an hour to more than 10 hours (Davies et al., 2012), depending on the design. Then, the well is de-pressurized and part of the fracturing fluid returns to the surface (flow back or bleed off) and the remaining fluid seeps into the porous rock matrix (leak off). Fractures try to close and the pressure in the fracturing fluid is transferred to the proppant which keeps the fracture open.

Fig. 1.1 An illustration of hydraulic fracturing (after de Pater and Baisch, 2011)

Nowadays, multi-stage hydraulic fracturing is usually employed. Smaller volume of fracturing fluid is first injected at lower pressure. The injection volume and pressure increase at later stages. Mini-frac or pre-pad may be carried out by injecting a small amount of fluid for observation and analysis of the fracturing design.
1.3 Motivation

In the oil and gas industry, hydraulic fracturing is mainly deployed to increase the productivity for conventional resources. Because the properties of the reservoir rock, mainly sandstone, is uniform, the design of hydraulic fracturing relies mostly on empirical formula and assists by highly idealised and simple simulators. Within the same project, the design of hydraulic fracturing operation can be done by back analysis of the previous operations.

Starting from the 1990s, the development on hydraulic fracturing, together with horizontal drilling, enable the extraction of unconventional resources. The reservoir, mainly Shale, has very low permeability and hydraulic fracturing is the key process to enhance its permeability. The reservoir is heterogeneous because of the presence of network of natural fractures. Hydraulic fracture needs to interact with natural fractures and to connect them to achieve the permeability required for economic production.

Because of the heterogeneity of the reservoir rock, empirical formula cannot be formulated and is useful for hydraulic fracturing design. Design of hydraulic fracturing in unconventional resources requires more in-depth understanding on the geomechanics of the reservoir, in particular the effects of natural fractures. Under the current monitoring techniques, field tests can only provide limited data about the reservoir. It is also impractical to obtain a representative sample for laboratory tests. Numerical simulation becomes an important tool to understand the complex interaction between hydraulic fracture and natural fracture.

However, conventional hydraulic fracturing simulators used by the industry were developed assuming reservoir is homogeneous and hydraulic fracture generated does not interact with natural fractures. There is a need to develop a more advanced numerical model that can simulate hydraulic fracture in heterogeneous reservoir.

1.4 Problem statement

Hydraulic fracturing is a multi-physics, multi-phase and multi-scale process. It is a multi-physics process because it involves mechanical deformation of rock, fracturing of rock and fluid flow along fracture. All these processes coupled one another. Hydraulic fracturing is also a multi-phase process as it involves solid rock matrix, groundwater, fracturing fluid and proppant. Its multi-scale nature comes from the presence of discontinuities (i.e. faults, joints and fissures) with length scales across several orders of magnitude.

The assumption of homogeneous reservoir leads to the use of continuum based numerical methods such as Finite Element Method (FEM). Fracturing simulation using FEM is chal-
lenging because of the dependence of fracture path on meshing. eXtended Finite Element Method (XFEM) has been developed to overcome the above challenges. Researches on hydraulic fracturing using continuum based methods focus on the understanding of hydraulic fracturing in the context of a multi-physics process. More recently, there are researches on modelling of hydraulic fracturing in material with a few natural fractures. But these models are incapable of simulating complex fracturing processes such as fracture clustering and coalescence that are observed in the fracturing of heterogeneous material.

Discontinuum based numerical methods have been developed considering material as an assemblage of discrete elements. They are suitable in modelling heterogeneous material. Particle-type Discrete Element Method (DEM) was developed to study the mechanics of granular material. It has been extended to Bonded Particle Model (BPM) to model rock mass by introducing breakable bonds between particles. Block-type DEM is also proposed to model fractured rock mass as an assemblage of blocky elements to study the stability of rock slopes and rock tunnels. The above models were developed to consider the kinematics of discrete elements in which large deformation at local level is involved.

By using high performance computers (HPCs), multi-scale modelling of heterogeneous material becomes feasible by building models composed of as many as 100,000 particles. However, for the hydraulic fracturing simulation that involves interaction between multiple physical processes, computational resources required for multi-scale simulations are prohibitively expensive. An efficient numerical method is therefore required to study the multi-physics and multi-scale problem of hydraulic fracturing.

The computational efficiency of the new numerical method can be enhanced by making simplifications that apply for hydraulic fracturing. One of the directions is developing a discontinuum method that assumes small displacement at element level.

The fluid model chosen should be able to handle evolving fluid front and complex geometry of hydraulic fracture formed in a heterogeneous reservoir. This leads to the preference on selecting a fluid model that simplifies the fluid flow at local level. This is also important for multi-scale simulation to reduce the computational effort.

To limit the scope of this research, the following are the major assumptions made for the simulations presented in this thesis.

- Rock is elastic, isotropic and impermeable.
- Fracturing fluid is Newtonian
- Effects on proppant is not explicitly modelled.
- Mulit-phase flow between fracturing fluid, groundwater and oil/gas is ignored.
• Leak off is ignored.

However, the new numerical model can be extended to relax some of the above assumptions. In particular, leak off is included in the numerical code developed for the simulations presented in this thesis.

1.5 Research objectives

Three research objectives are formulated by progressively adding complexity in each objective, leading to the ultimate aim of the development of a numerical method for multi-scale and multi-physics hydraulic fracturing simulation.

• Development of a numerical model for intact heterogeneous material and study how model parameters govern both the macroscopic and the microscopic behaviour.

• Simulations of the fracturing process in heterogeneous materials and exploration on how model parameters relate the fracturing behaviour.

• Development of a solid-fluid coupled model for hydraulic fracturing simulation in heterogeneous material. Simulations of hydraulic fracturing to identify different regimes of hydraulic fracturing.

1.6 Outline of thesis

The first two chapters are literature review.

Chapter 2 provides a background knowledge of the physics involved in hydraulic fracturing - rock mechanics, fracture mechanics and fracture flow. Theoretical research studying different regimes of hydraulic fracturing are summarised to help the understanding on the complexity of the multi-physics nature of hydraulic fracturing. Experimental studies exploring different mechanisms in hydraulic fracturing are reviewed. Also, a review on recent research on hydraulic fracturing modelling considering the effects on natural fractures is presented.

After giving the background knowledge for the understanding of the complex process of hydraulic fracturing, Chapter 3 reviews models that idealise hydraulic fracturing in different ways. The early development of analytical and numerical models are reviewed. Then, different numerical methods are reviewed in detail for modelling rock and hydraulic fracturing process, treating rock as a continuum or discontinuum. Comparisons are made on the strengths and weaknesses among these numerical methods.
Chapters 4 to 6 present the research work done in the development of a new multi-scale hydraulic fracturing numerical model.

**Chapter 4** proposes Lattice Element Method (LEM) to model heterogeneous material. It covers the generation of a disordered lattice network. The relationships between microscopic model parameters and macroscopic parameters are explored for model calibration.

**Chapter 5** focuses on fracturing simulations by LEM. Relationship is established between material parameters in Linear Elastic Fracture Mechanics (LEFM) and microscopic model parameters in LEM. Simulations on uni-axial tensile tests and uni-axial compression tests are presented. Analysis including stress-strain curves, fracture statistics and microscopic stress statistics are reported. Relationships among macroscopic strengths, ductility and various microscopic parameters are identified. They can be used for model calibration given the macroscopic parameters which are measurable by experiments.

**Chapter 6** introduces a novel Dual Lattice Model (DLM) for solid-fluid coupling problems, including hydraulic fracturing, in heterogeneous material. The formulation of DLM and numerical techniques are covered. Classical problem of the hydraulic fracturing of a penny shape crack is simulated in DLM and compared with the analytical solution for hydrostatic pressure. Simulations are carried out to study the effects on the heterogeneity arisen from fracture asperity and statistical distributions on lattice parameters. A semi-analytical model is derived and compared with DLM simulations when the effect of fluid viscosity is taken into account. Different flow regimes are identified in hydraulic fracturing.

**Chapter 7** summarises the findings in this thesis. Future work is proposed and the future visions on the applications of LEM and DLM are outlined.
Chapter 2

Fundamentals in hydraulic fracturing

This Chapter provides the background knowledge in hydraulic fracturing to understand the complexity of the problem. Chapter 3 reviews the available numerical techniques in simulation of hydraulic fracturing.

Hydraulic fracturing is a multi-physics and multi-scale problem as illustrated in Figure 2.1. At least three physical processes are involved (Adachi et al., 2007) - (1) mechanical deformation of rock mass, (2) fracture propagation and (3) fluid flow along fracture. Hydraulic fracturing is further complicated by the leak off of the fracturing fluid into the rock matrix and the transportation of proppant in fracturing fluid. Therefore, hydraulic fracturing is a challenging problem for researchers because of many interdependent processes involved.

Fig. 2.1 Illustration of multi-physics and multi-scale of hydraulic fracturing problem
Hydraulic fracturing is further complicated by its multi-scale nature because of the presence of natural fracture with length scale across several orders of magnitude. All three physical processes described above are highly affected by these discontinuities.

This Chapter starts with a review on the theoretical background of three key physics involved in hydraulic fracturing: rock mechanics, fracture mechanics and fluid mechanics. This gives an understanding of each physical process involved in hydraulic fracturing before considering their coupled effects.

Linear elasticity in continuum mechanics is the core assumption in rock mechanics. However, rock is heterogeneous and regarded as a discontinuum because of the presence of discontinuities. This review focuses on the effects of discontinuities and the techniques usually used to account for such effects under the assumption of linear elasticity. The scale effects are originated from the multi-scale nature of discontinuities. Continuum Damage Mechanics (CDM) was developed to model the progressive loss of integrity of intact rock under loading due to the growth of features in small length scales such as fissures and voids. The effects of groundwater assuming rock as a porous material is handled by poroelasticity theory.

Classical Linear Elastic Fracture Mechanics (LEFM) is summarised which assumes material as a homogeneous, elastic and brittle medium. For quasi-brittle material like rock, LEFM is modified by considering the complex response of material near the fracture tip.

Fluid flow in reservoir can be categorised into (a) the flow within fracture, (b) the flow within porous rock matrix and (c) the flow between fracture and matrix (leak-off). There should be some interaction among them but the current theories treat them as uncoupled process. Flow within fracture is usually modelled by the so-called cubic law. Permeability of fracture is very sensitive to fracture aperture. The leak-off is often modelled by Carter one-dimensional model. Dracy’s law is used to model the combined fluid flow in rock matrix and fracture assuming rock as an equivalent porous medium. Dual Porosity Model has been proposed to couple the fluid flow in fracture and the leak-off. For hydraulic fracturing, the fluid flow in fracture and the leak-off are the dominant processes and the fluid flow within rock matrix is usually ignored.

After reviewing the theories for individual physical process, more complicated issues such as the coupling among physical processes and their interaction with natural fractures are investigated.

There are theoretical studies on the coupling of different physical processes involved in hydraulic fracturing. Different regimes of hydraulic fracturing has been identified which is determined by dimensionless parameters. This provides a guidance on the development
of idealised models focusing on the dominant physics processes for different hydraulic fracturing problems.

There are some experimental studies on hydraulic fracturing despite some major limitations to mimic the actual site condition. Some topics have been studied including the fracture containment mechanism that limit the growth of fracture in certain direction and the interaction of hydraulic fracturing with a single natural fracture.

There is a lack of theories explaining the observations from experiments. However, numerical models have been used to simulate some of the problems, in particular the interaction between hydraulic fracture and existing natural fracture.
2.1 Rock Mechanics

Rock is regarded as a discontinuous, inhomogeneous, anisotropic and non-elastic (DIANE) material but is often modelled as homogeneous, isotropic and linear elastic material (CHILE) (Harrison and Hudson, 2000).

So, continuum approach is often used to idealise rock as an equivalent continuum. Well established theories in continuum mechanics such as theory of elasticity can be applied to model the mechanical behaviour of rock.

2.1.1 Linear elasticity in rock mechanics

In linear elasticity, the relationship between stress $\sigma_{ij}$ and strain $\varepsilon_{kl}$ is given by

$$\sigma_{ij} = C_{ijkl} \varepsilon_{kl} \quad (2.1)$$

where $C_{ijkl}$ is a forth-order tensor called stiffness tensor. For an isotropic material, only two constants, for example Young Modulus $E$ and Poisson ratio $\nu$, are required to define the entire stiffness tensor.

Fig. 2.2 Illustration on the effect of joints on the anisotropy of rock: (a)Isotropic rock, (b) Transversely isotropic rock, (c) Orthotropic rock and (d) Completely anisotropic rock (after Harrison and Hudson, 2000)

One of the important characteristics of rock is anisotropy. It can be originated from discontinuities of rock (see Figure 2.2) and inhomogeneity of matrix material. The discon-
tinuities provide the material a preferred orientation to deform. In linearly elasticity, the anisotropy can be represented by giving different elastic moduli in different directions. Hence, more parameters are required for constitutive laws of an anisotropic material. For completely anisotropic material in linear elasticity, 21 constants are required to define the stiffness matrix $C_{ijkl}$. Simpler models that are used in rock mechanics to address the anisotropy are orthotropic isotropy and transverse isotropy. However, the highly anisotropic rock may not be described sufficiently by a stiffness tensor because the assumptions of continuum mechanics are no longer valid.

A large number of rock models have been derived in rock physics for geophysicists and petroleum engineers to interpret data from geophysics measurement. The book from Mavko et al. (2008) provide a comprehensive collection of anisotropy rock models that determine the effective parameters required using the framework of linear elasticity.

Continuum mechanics can be extended to cover more complicated material behaviour such as non-linearity and plasticity (Fjaer et al., 2008; Harrison and Hudson, 2000). One may argue that more sophisticated continuum model and more advanced constitutive laws can be deployed to describe the fractured rock mass. However, more parameters are required which are difficult to be quantified. Direct site measurements are highly restrictive and are often impractical whilst laboratory experiments are hardly representative given the heterogeneous nature of rock and its scale effects. These issues are more apparent for reservoir engineering. Even the most basic parameter required by linear elasticity, the Young’s modulus, has to be interpreted by geophysical techniques rather than measured directly.

This introduces another reason for the extensive use of linear elasticity in reservoir engineering - the use of geophysics to characterize reservoir kilometres from the surface. The mechanical properties of rock are measured indirectly by the response of rock under acoustic waves. Under small disturbance induced by acoustic wave, rock only responds linear elastically.

The only possible ways of measuring non-linear and plastic rock behaviour are laboratory testing of intact rock or hydraulic fracturing test on site. The former is hardly representative of the field while the latter only provides limited information.

### 2.1.2 Representative Elementary Volume

The existence of Representative Elementary Volume (REV) is an important assumption for the validity of continuum-based rock mechanics. The extent of the problem in which the use of continuum rock mechanics is valid rests on the concept of REV, which is illustrated in Figure 2.3. It is a concept from statistical mechanics that the randomness of molecular effects can be neglected by averaging a large number of them. In other words, the REV is the volume
Fig. 2.3 The concept of Representative Elementary Volume: change of measured property with sample volume (from Bear, 1972)

at which the size of the sample tested contains a sufficient number of inhomogeneities such that its average value is reasonably consistent under repeated testing (Hudson and Harrison, 1997). However, when the sample volume increases, the macroscopic inhomogeneity starts to affect the average value. For instance, a large planar fracture may affect the strength of rock mass. The concerned problem and the sampling should not be affected by both limits (i.e. stay on the ‘flat’ region between the upper and lower bound of REV in Figure 2.3).

Long et al. (1982) discussed the homogeneity of groundwater flow problem related to REV and claimed that there was no guarantee of the existence of REV for every permeable system. They supported this claim by referencing the theoretical and experimental work of Snow (1969) which showed an increasing trend of permeability of fractured rock with sampling volume.

2.1.3 Scale Effects

The scale effects are well-documented in the literature (da Cunha, 1990). They are related to the inhomogeneity of rock. Also, it is observed that the uniaxial compressive strength of rock decreases with the increase in sampling size. Scale effects are observed even in a laboratory rock sample. For instance, Hoek and Brown (1980) expressed the relationship between uniaxial compression strength and specimen diameter.

The scale effects have the following implications on rock characterization (Jing, 2003):

- Rock properties measured in the laboratory may not be representative at a larger scale
• Rock properties at larger scale cannot be measured directly

• Rock properties may have to be estimated from empirical methods

• The uncertainty in the estimated rock property cannot be quantified easily

This suggests the use of geophysics and *in-situ* testing in reservoir engineering in which there are no scale effects.

### 2.1.4 Accounting discontinuities in continuum rock mechanics

The effect of discontinuities on the geomechanics of reservoir is concerned in recent years (Dusseault, 2013). It is believed that natural fracture network plays a significant role in the success of hydraulic fracturing for shale gas extraction. Hydraulic fracture connects the existing natural fracture network to form an inter-connected network to reach out more gas in low permeability reservoir. The following provides a review of two existing approaches in accounting discontinuities and inhomogeneity in the framework of continuum rock mechanics.

**Rating systems**

The presence of discontinuities in rock mass could greatly alter its mechanical and hydraulic properties. Parameters used to describe discontinuities include spacing, orientation, persistence, roughness and aperture. Since three dimensional characterization of all the discontinuities in rock mass is impractical, deterministic analysis is not feasible. Different rock rating systems have been developed to provide an aggregated effects of discontinuities. Rock mass can be analysed as an effective continuum.

Commonly used rating systems are Rock Quality Designation (RQD), Rock Mass Rating (RMR) (Bieniawski, 1973) and Q-system (Barton et al., 1974).

Some empirical relationships between these rating and mechanical properties of rock have been established. For example, Serafim and Pereira (1983) related RMR with Young modulus of rock mass. The RMR can also be used to estimate the strength parameters (Hoek and Brown, 1988). Rock can be treated as continuum for numerical analysis with the equivalent parameters estimated from these rating systems.

These rating systems are mainly applied in civil engineering such as designing a supporting system for tunnel and slope stabilization works. They require a lot of information about discontinuities which is not available for reservoir engineering. Therefore, relevant rating systems for reservoir engineering are not available.
Continuum Damage mechanics

In continuum mechanics, the fracture of quasi-brittle materials is studied from two different perspectives: continuum damage mechanics (CDM) and fracture mechanics. The later which models explicitly how a pre-existing crack propagates which is covered in Section 2.2.

CDM, sometimes referred as smeared crack model, deals with the study of crack formation and growth from an initially flaw or defect-free structure. It describes the progressive loss of material integrity due to propagation and coalescence of microcracks and microvoids. It has widespread applications in simulating macroscopic responses of heterogeneous material (Yuan and Harrison, 2006). The model assumes that micro-defects in rock change the macroscopic mechanical properties as well as the strength of a rock. The aim of CDM is to homogenize the heterogeneous properties of a solid arisen by the existence and evolution of micro-defects into an equivalent continuum that exhibits the similar macroscopic behaviour as the actual material (Krajcinovic, 1996).

The effects of micro-defects are modelled by one or more damage variables. Damage evolution laws are introduced to model the aggregated effects on the growth of micro-defects. Constitutive relationship between macroscopic properties and damage is also established to relate their effects on macroscopic properties. Suitable element size or RVE has to be chosen. For statistically homogeneity within element, the RVE should be large enough to contain sufficient number of cracks. The RVE should also be small enough such that variation of macroscopic variable among neighbour elements is small. The size required for element can vary from 0.1 mm for metal to 100 mm for concrete (Murakami, 2012).

The most simple 1D case of damage mechanics model can be formulated by introducing a scalar damage variable $\omega$:

$$\sigma = (1 - \omega)E\varepsilon \quad (2.2)$$

$\omega$ is related to strain $\varepsilon$ by a damage evaluation law which is determined by experiments. The damage variable represents the extent of damage or density of micro-cracks of the continuum material. Crack closure can also be simulated by restoring elastic modulus of material. The model can be extended by using a damage tensor instead of a scalar as damage variable for more complicated cases, such as anisotropic damage.

2.1.5 Poroelasticity

The review in the previous sections assumes rock as a single phase material. This section considers rock as a porous and permeable material with water filled pores. van Terzaghi (1923) first introduced the effective stress concept in soil mechanics that describes the role of
pore water pressure in the one dimensional consolidation theory of a two phase material (soil skeleton and pore water). The poroelasticity theory was then introduced by Biot (1941) that provides a consistent theory coupling hydraulic and mechanical processes for a fluid-saturated porous medium. In simple terms, it describes the interaction between two mechanisms:

- Dilation of solid due to the increase in pore fluid pressure
- Increases in pore fluid pressure due to compression in solid

It is derived from the linear elastic theory, the Navier-Stoke equations and the Darcy’s Law for fluid flow in porous medium.

This section only briefly introduces the poroelastic concept for understanding on the effect of pore fluid. Detournay and Cheng (1993) provides more thorough exposition of poroelasticity theory. Poroelasticity has also been applied to model rock matrix in hydraulic fracture simulation which is discussed in Detournay and Cheng (1988).

**Effective Stress Concept**

The effective stress $\sigma'_{ij}$ is defined as

$$\sigma'_{ij} = \sigma_{ij} - \delta_{ij}\alpha_B p$$

(2.3)

$p$ is pore fluid pressure and $\alpha_B$ is Biot coefficient which is defined as

$$\alpha_B = \frac{K_f}{K_s}$$

(2.4)

$\alpha_B$ is a measure of the relative bulk moduli between pore fluid $K_f$ and solid skeleton $K_s$ and indicates the efficiency of pore fluid to take up applied stress. In soil mechanics, the bulk modulus of soil skeleton is much smaller than that of water and hence water is assumed to be relatively incompressible. This gives $\alpha_B = 1$. In rock, the compressibility of water should be taken into account, especially for rock at large depth which is under high stress. Typical value of $\alpha_B$ is about 0.7 for petroleum reservoir (Economides and Nolte, 2000) but it varies a lot among different rock types (Detournay and Cheng, 1993).
2.2 Fracture Mechanics

Fracture mechanics is first developed in mechanical engineering to study how material fails. It assumes that microcracks exist in the material and failure occurs as a result of fracture growth in an uncontrolled manner. Fracture mechanics does not describe how cracks initiate but provides the criteria of crack propagation.

The Linear Elastic Fracture Mechanics (LEFM) is the foundation of fracture mechanics. It is suitable for brittle material such as glass. LEFM assumes linear elastic behaviour including the highly concentrated stress at crack tip. Elastic-Plastic Fracture Mechanics (EPFM) considers the plasticity near crack tip. Rock is considered as quasi-brittle material. Non-linear fracture mechanics has been introduced to model the process zone ahead of the fracture tip.

2.2.1 Griffith’s Energy Approach

Fracture mechanics was first developed by Griffith (1921). His theory proposes an energy based crack propagation criteria

\[ \partial U_t = \partial U_s + \partial W_r + \partial U_e \]  

(2.5)

where

- \( \partial U_t \) total change in energy
- \( \partial U_s \) surface energy need to create new fracture surface
- \( \partial W_r \) change in work done in boundary tractions
- \( \partial U_e \) change in the strain energy of the material

Griffith’s energy conservation approach assumes that the total energy of the material-crack system \( \partial U_t \) should be unchanged when fracture propagates. Also, it is assumed that the surface energy \( \partial U_s \) required to create a new fracture surface is proportional to the fracture area created.

\[ \partial U_s = -2\gamma_f \partial A \]  

(2.6)

where

- \( \gamma_f \) fracture surface energy of the solid per unit area
- \( \partial A \) fracture area extended

The factor of 2 arises because of the 2 surfaces created during fracturing. Griffith introduced a term called strain energy release rate \( G_s \) which is the change of mechanical energy per area
2.2 Fracture Mechanics

of crack surface extended $\partial A_f$.

$$G_s = -\frac{\partial \gamma_f}{\partial A_f}$$  \hspace{1cm} (2.7)

For plain strain problems, the crack surface extended refers to the crack length extended $dl$. When $G_s$ reaches a critical value $G_c$, crack propagates. The energy released includes energy dissipated by plastic deformation, micro-cracking, friction, craze formation, void growth etc.

2.2.2 Modes of Fracture

There are 3 modes of fracture which are determined by the stress field at the crack tip: opening (tensile), sliding (in-plane shear) and tearing (out of plane shear).

It is widely accepted that the fracture generated by hydraulic fracturing is largely tensile mode failure (Mode I). Large seismicity is mainly caused by shear model failure (Mode II) at faults as larger amount of energy is released during Mode II failure.

![Fig. 2.4 Three modes of fracture](image)

2.2.3 Irwin’s stress approach

Irwin (1957) expressed the fracture propagation criterion in terms of the stress concentration at the fracture tip rather than energy. A stress intensity factor $K_I$ describes the stress concentration at the crack tips where subscript $I$ denotes mode I failure. The stress field near the crack tip $\sigma_{ij}$ is expressed as

$$\sigma_{ij} = \frac{K_I}{\sqrt{2\pi r}} f_{ij}(\theta)$$  \hspace{1cm} (2.8)

where $r$ distance from crack tip

$\theta$ angle in polar coordinate if crack tip is the origin
\( f_{ij}(\theta) \) a geometric function depends on fracture mode

The subscript \( I \) denotes fracture mode I. The stress intensity factor \( K_I \) is written as

\[
K_I = Y \sigma_\infty \sqrt{\pi a}
\]

(2.9)

where

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<tr>
<th>Symbol</th>
<th>Description</th>
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<tr>
<td>( \sigma_\infty )</td>
<td>far field stress</td>
</tr>
<tr>
<td>( a )</td>
<td>half crack length</td>
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<tr>
<td>( Y )</td>
<td>geometry factor</td>
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</tbody>
</table>

Similar equations follow for Mode II and Mode III fracture modes. The geometry factor \( Y \) is related to crack geometry. Closed form solutions only exist for a few geometry factors and numerical integration is often required to obtain the stress intensity factor.

When the stress intensity factor reaches a critical value \( K_{Ic} \), crack propagates. This critical value is called fracture toughness and is a material property.

The relationship between energy release rate \( G_I \) and stress intensity factor \( K_I \) in plain strain condition is as follow:

\[
G_I = \frac{1 - \nu^2}{E} K_I^2
\]

(2.10)

Both Griffith and Irwin models assume linear elastic material so the zone of plasticity should be small compared with the width of the crack.

### 2.2.4 Applicability of LEFM

Plastic region does exist near the fracture tip in real material but it is the region where LEFM focuses on. If LEFM is applicable, such plastic region has to be small compared to the fracture size. Also, plain strain conditions are usually applied to simplify the calculation but the crack does have finite dimension out of the plane under analysis. This two criteria mean both dimensions, the crack length \( a \) and out of plane length, or breadth \( B \) should be large enough. From (ASTM, 1983),

\[
a > 2.5 \left( \frac{K_{Ic}}{\sigma_{ys}} \right)^2
\]

(2.11)

\[
B > 2.5 \left( \frac{K_{Ic}}{\sigma_{ys}} \right)^2
\]

(2.12)

where \( \sigma_{ys} \) is the yield stress of material. Clearly, LEFM is a good approximation for brittle material with low fracture toughness and high yield stress. Also, the second order relation in
the above equations also means that the plastic zone is sensitive to material yield stress and fracture toughness.

2.2.5 Elasto-Plastic Fracture Mechanics

The linear elastic fracture mechanics (LEFM) simplifies the actual mechanics of fracture as the fracture tip is elastic rather than plastic assumed in LEFM. The stress increases indefinitely towards the crack tip and becomes singular at the crack tip. However, the stress near crack tip cannot reach this singularity without yielding first. The LEFM can predict fracture propagation for small toughness material such as glass. For large toughness material such as steel, the plasticity plays an important role in fracture mechanics. For quasi-brittle material like rock and concrete, microcracks form ahead of fracture to prevent stress to continue to build up near crack.

2.2.6 Plastic Zone

Fig. 2.5 Different assumptions on plastic zone geometry ahead of fracture tip in Elasto-Plastic Fracture Mechanics. (a) Assumption of circular disk plastic zone ahead of fracture tip and (b) Assumption of thin line plastic zone ahead of fracture tip in Dugdale-Barenblatt cohesive model

If the plastic zone assumed ahead of crack tip is a circular plastic disk (Figure 2.5a) as proposed by Irwin (1957), it can be shown that, in mode I fracture, the diameter of disk \( r_p \) is given by

\[
r_p = \frac{1}{\pi} \left( \frac{K_I}{\sigma_{ys}} \right)^2
\]  

(2.13)
Alternatively, Dugdale (1960) and Barenblatt (1962) proposed a cohesive model which is now referred as Dugdale-Barenblatt cohesive model. Only a strip ahead of crack tip is assumed to be plastic where there exists a constant cohesive force trying to bring the fracture surfaces together. If the cohesive zone is denoted by $\rho$ as shown in Figure 2.5b.

The cohesive zone $\rho$ is obtained from the equation below:

$$\rho = \frac{\pi}{8} \left( \frac{K_I}{\sigma_{ys}} \right)^2$$

(2.14)

The plastic zones calculated by the two different assumptions differ by about 23%. The introduction of plastic zone eliminates the singularity at fracture tip. When the crack aperture is smaller than a threshold value $\delta_c$, there is a cohesive force trying to close the crack.

In rock and concrete fracturing, the cohesive zone is called fracture process zone (FPZ). There are some bridging mechanics to keep the fracture closed in the process zone. It is developed where micro-cracking and grain bridging occur to weaken the process zone. Labuz et al. (1985) investigated FPZ experimentally and suggested that FPZ is larger for larger grain-size rock.

Different cohesive stress profiles have been used instead of the constant yield stress. Hillerborg et al. (1976) proposed a linear variation of cohesive stress decreased with the fracture aperture to model the fracture propagation in concrete. It has been adopted for hydraulic fracturing simulation considering FPZ (Carrier and Granet, 2012; Chen, 2012; Gonzalez et al., 2015; Papanastasiou, 1997; Salimzadeh and Khalili, 2015; Sarris and Papanastasiou, 2011).

### 2.2.7 Non-linear Fracture Mechanics

The LEFM is applicable for brittle material such as glass while elasto-plastic fracture mechanics is suitable for metal. Bazant (1984) developed blunt crack band theory to describe the fracture propagation for quasi-brittle material such as rock and concrete. It is also called non-linear fracture mechanics. Crack band theory assumes that FPZ can be regarded as crack band with a fixed width where microcracks are uniformly distributed.

The applicability of this theory depends on the relative length of FPZ $l_{FPZ}$ to structural size $D$ as shown in Figure 2.6a. Bazant (2002) provided a rough delineation of different theories in analyzing fracturing. For $D/l_{FPZ} \geq 100$, LEFM should be used. For $5 \leq D/l_{FPZ} < 100$, non-linear fracture mechanics should be used. For $D/l_{FPZ} < 5$, non-local damage, discrete element models or plasticity models should be used.
2.2 Fracture Mechanics

![Graphs showing size effects in fracture mechanics. (a) Strength or yield criterion compared to linear or non-linear fracture mechanics according to Bazant (1984). (b) Experimental result of cross-ply glass fiber reinforced composite experiment showing relationship of scale effect and strength and toughness failure criteria. Solid line denotes toughness criterion and dotted line denotes strength criterion. (after Parvizi et al., 1978)]

2.2.8 Stress criteria and energy criteria

There are two criteria for material failure: strength criterion and toughness criterion. Strength criterion refers to material fails when stress reaches a certain level while toughness criterion refers to the material failure by fracture propagation of a given pre-existing crack. Leguillon (2002) used an example of a homogeneous isotropic bar under increasing applied strain to illustrate the contradiction between the above two criteria. Using toughness criterion, the failure stress $\sigma_f$ of the bar is inversely proportional to square root of bar length $L$.

$$\sigma_f \geq \sqrt{\frac{2EG_c}{L}}$$  \hspace{1cm} (2.15)

There is a length scale in the toughness criterion while no length scale in the strength criterion. Stress criterion prevails for most engineering applications. From the cross-ply glass fiber reinforced composite experiment conducted by Parvizi et al. (1978), the failure strain is related to the thickness of inner ply, but only up to certain thickness, beyond which the failure strain remains constant as shown in Figure 2.6b.

Leguillon (2002) pointed out that fracture onset criterion requires two parameters, toughness and strength, or one of the above parameters plus a characteristic length. This aligns with crack band theory (Section 2.2.7) that includes the size effect in the previous section.
2.3 Fluid modelling

This section first gives some background information about fracturing fluid which has complex rheology. Fluid flow can be categorized into (a) flow within fracture (fracture flow), (b) flow within porous matrix and (c) flow between fracture and matrix (leak off). Flow within fracture is usually modelled by so-call cubic law. Flow within porous matrix is modelled by Darcy law. Leak-off is commonly modelled by Carter model (Carter, 1957). A brief review is given on these three models. Dual porosity model that considers all three types of fluid flow is also reviewed.

2.3.1 Properties of fracturing fluid

Fracturing fluid used in stimulation is specially designed to create optimal fractures. The objectives of fracturing fluid design are summarized (Pandey, 2010):

- Reservoir Compatibility
- Low friction loss
- Low leak off rate
- Proppant carrying ability
- Ease of removal from the formation

The commonly used fracturing fluid is water-based in which water is composed of about 95% by volume. Sand (5%) is added as a proppant to keep fracture open. Various chemicals (called additives, 0.17%) are also added such as friction reducer, surfactant and acid.

The rheology of fracturing fluid is complex, even for water-based fracturing fluid. Newtonian fluid model is insufficient to characterise the fluid. The rheology of fracturing fluids including polymers, viscoelastic surfactants and proppant is commonly approximated by a power law model. Shear stress $\tau$ is related to shear rate $\dot{\gamma}$ as follow:

$$\tau = K\dot{\gamma}^n$$  \hspace{1cm} (2.16)

where $K$ is called consistency index and $n$ is called flow behaviour index. When $n = 1$, it reduces to Newtonian fluid model. Properties of fracturing fluid depends on other factors such as temperature. More about different fluid rheology in modelling hydraulic fracturing can be found in (Valkó and Economides, 1995). Most of the fracturing fluids used in oil and gas industry are shear thinning as their apparent viscosity decreases with $\dot{\gamma}$ (i.e. $n < 1$).
However, the majority of analytical and numerical studies in the literature model fracturing fluid as Newtonian.

Usually, the proppant is not explicitly modelled. The transport and placement of proppant within the fracture is usually modelled as two-component inter-penetrating continuum. The distribution of proppant is represented by volumetric concentration. The proppant particles are regarded as negligible compared with fracture aperture (Adachi et al., 2007).

### 2.3.2 Dracy’s Law

Darcy’s law describes fluid flow in porous medium. It is the fundamental law for seepage flow in soil mechanics and groundwater flow in hydro-geology. It is first discovered experimentally by Darcy and can also be derived from the Navier-Stokes equations (Hall, 1956; Hubbert, 1956).

If the rock is treated as a continuous porous material, Darcy’s law can be used to predict fluid flow through pores. It is also used when a fractured rock mass is treated as an equivalent porous material.

By Darcy’s law, the specific discharge $q_{ij}$ is given by

$$q_{ij} = h_{ij} A \frac{\mu}{\nabla p}$$

where

- $k_{ij}$ permeability of porous medium
- $A$ cross-sectional area
- $\mu$ Newtonian fluid viscosity
- $p$ fluid pressure equivalent to pressure head

The permeability $h_{ij}$ is a tensor quantity which describes the anisotropy of fluid flow in a fractured rock mass. If the porous medium is isotropic, the permeability tensor is reduced to a scalar and the Darcy’s Law is further simplified to a form commonly used in soil mechanics.

$$q = k A \frac{dp}{dx}$$

The fluid viscosity $\mu$ and the material permeability are lumped into a single term called hydraulic permeability $k$.

Darcy’s law states that there is a fluid flow if there are pressure difference (hydraulic gradient) and flow rate is proportional to the permeability $k$.

The important assumptions of Dracy’s law are laminar and uniform flow. However, it is well recognised in hydro-geology field that fluid flow in fractured rock is highly tortuous
even in a large scale. The permeability tensor $h_{ij}$ may not be adequate to describe such flow in a reasonable accuracy.

### 2.3.3 Cubic flow law for fracture flow

The lubrication theory governs fluid flow between two narrow surfaces. It is widely used in mechanical engineering to describe fluid film lubrication (i.e. lubricant between contacting interfaces). The dimension of flow depth (fracture aperture) $\delta$ between two surfaces is significantly smaller than another two dimensions. This assumption applies to fluid flow between fractures in rock where the fracture aperture is several orders of magnitude smaller than the fracture planes. Therefore, the lubrication theory is widely used in hydraulic fracturing.

Apart from the assumption of narrow surface, the lubrication theory also assumes the following:

- Steady flow conditions
- Constant pressure through fracture
- Laminar flow
- Newtonian fluid
- Rigid and smooth solid surfaces
- Constant viscosity

Consider fluid flow between two parallel plates separated by distance $\delta$ along $z$-direction. The plates are assumed to be wide and long so that fluid mainly flows along $x$-direction and is driven by the pressure gradient $dp/\ dx$. With the above assumptions, the Navier-Stokes equations are simplified to a second order ordinary differential equation:

$$\frac{dp}{dx} = \mu \frac{d^2u}{dz^2}$$

Integrating twice with respect to $z$ gives

$$u(z) = \frac{1}{2\mu} \frac{dp}{dx} x(z - \delta)$$
2.3 Fluid modelling

This is the well-known Hagen-Poiseuille equation. The flow rate \( q \) is obtained by integrating the fluid velocity \( u \) along depth \( z \)

\[
q = \int_0^\delta u \, dz = -\frac{\delta^3}{12\mu} \frac{dp}{dx}
\]  

(2.21)

This is so-called cubic law model which has been used extensively in modelling hydraulic fracture.

This equation provides an insight of fracture flow in rock. The flow rate \( q \) is proportional to the cubic of fracture aperture \( \delta \). The fluid flow is concentrated at the most conductive channel where the fracture aperture is the largest. The highly sensitivity of the fracture aperture to the flow rate imposes a great challenge of hydraulic fracturing simulation as the fracture aperture in rock cannot even be roughly determined.

2.3.4 Validity of cubic flow law

Louis (1969) carried out a series of experiments to study steady flow of water in a single fracture of constant aperture. He proposed different regimes delineated by friction factor \( f = d_r/(2\delta) \) and Reynolds number \( Re = 2\delta u/\mu \) as shown in Figure 2.7. \( d_r \) is the fracture surface roughness, \( u \) is the average velocity of fluid. There are five regimes (I to V) governed by different flow laws as summarized in Table 2.1. Cubic flow law is applicable for regime I. For turbulence flow, the linearity between flow rate \( q \) and hydraulic gradient \( \frac{dp}{dx} \) does not hold

\[
q = KA \left[ \frac{dp}{dx} \right]^n
\]  

(2.22)

For narrow fracture aperture and low discharge rate, flow remains laminar. The asperity of the fracture has an effect when the relative roughness reaches a certain value.

<table>
<thead>
<tr>
<th>Regime</th>
<th>Hydraulic conductivity ( K )</th>
<th>Exponent ( n )</th>
<th>Flow condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>( w^2/12\mu )</td>
<td>1.0</td>
<td>Laminar</td>
</tr>
<tr>
<td>II</td>
<td>( 1/w[83.4/\mu^{0.25} + w^3]^{4/7} )</td>
<td>4/7</td>
<td>Turbulent</td>
</tr>
<tr>
<td>III</td>
<td>( 12.5 \log[3.7/(d_r/2w)]\sqrt{w} )</td>
<td>0.5</td>
<td>Turbulent</td>
</tr>
<tr>
<td>IV</td>
<td>( w^2/(12\mu[1 + 8.8(d_r/2w)^{1.5}]) )</td>
<td>1.0</td>
<td>Laminar</td>
</tr>
<tr>
<td>V</td>
<td>( 12.5 \log[1.9/(d_r/2w)]\sqrt{w} )</td>
<td>0.5</td>
<td>Turbulent</td>
</tr>
</tbody>
</table>

Table 2.1 Hydraulic conductivity and degree of non-linearity for fracture flow in different regimes
Fig. 2.7 Different regimes of fracture flow laws for a single parallel fracture compiled by Kim et al. (1999). The dashed lines represent mathematical boundaries (Amadei et al., 1995) and the solid lines the boundaries as determined by experiments (Louis, 1969)
On the other hand, Witherspoon et al. (1980) has carried out laboratory tests on artificially induced tension fractures in homogeneous samples of granite, basalt and marble. The aperture varies from 4 to 250 $\mu$m under normal stresses up to 20 MPa. Figure 2.8 shows the comparison of the cubic flow law with laboratory results. It is found that fracture permeability is uniquely defined by a fracture aperture. Cubic law is valid no matter fracture is open or closed, rock type and loading path. The fracture asperity causes a reduction in flow rate and can be taken into the consideration by a factor which varies from 1.04 to 1.65.

For closed fracture, the asperities in contact are able to withstand significant stresses that provide space for fluid to flow as illustrated in Figure 2.9 (Witherspoon et al., 1980).

The fracture surfaces in reality are neither parallel nor have infinite extent. The cross sections may vary and channels could be formed in a single fracture as revealed by field tests (Tsang and Tsang, 1987) and laboratory tests (Haldeman et al., 1991). This phenomenon is called channelling as illustrated in Figure 2.10.

Moreover, Warren and Root (1963) observed that the time required to reach quasi-state flow in fractured reservoir is one to two orders longer than that of homogeneous system. Furthermore, the flow along fracture intersections alone may have a greater influence to the flow along fracture surface (Neuman, 2005).
Fig. 2.9 Idealised fracture showing the effect of asperities when fracture is closed under stress (after Witherspoon et al., 1980)

Fig. 2.10 Schematic diagram of channelling in a between two fracture planes. (a) Several channels formed inside a single fracture and (b) close-up of a single channel. (after Tsang and Tsang, 1987)
2.3 Fluid modelling

2.3.5 Leak-off

Leak-off is the fluid loss from fracture to the surrounding rock. There are different models developed to model leak-off. Settari (1985) provided a review of the classical leak-off models. Among them, Carter (1957) model is the most widely used in numerical modelling. He developed a time-dependent leak off term by relating the leak-off velocity $u_L$ at time $t$ on the fracture wall

$$u_L = \frac{C_L}{\sqrt{t - t_{exp}}}$$

(2.23)

where $C_L$ Leak off coefficient

$t_{exp}$ The time when fracture was exposed to fracturing fluid

This is called one-dimensional leak-off model assuming that the fracture length is much greater than the invasion depth. The inverse square-root of time arises from the solution of a 1D diffusion problem. The leak-off term is the aggregated effects of three mechanisms of leak-off resistance in different region as shown in Figure 2.11:

- wall-building characteristics (filter cake) of the fracturing fluid
- the effect of filtrate (fracture fluid behind filter cake) characterized by the relative permeability of the formation to the fracturing fluid filtrate
- displacement and compressibility of reservoir fluid. The leak-off term can be determined by mini-fracture treatment at field

The leak-off term can be determined by mini-fracture treatment at field. The usual assumptions of Carter’s model are: (a) filter cake has a relatively low permeability and its deposition rate is proportional to the leak-off rate and (b) the filtrate has enough viscosity to fully displace the reservoir fluid.

Limitations

Fluid loss into natural fissures may result in deep filtrate invasion that invalidates the linear flow assumption. The leak-off is independent of fluid pressure which may not be true for leak off in natural fissures as well (Economides and Nolte, 2000). The Carter leak-off model is only applicable a distance away from the tip in the intermediate-tip region (Mitchell et al., 2007).
2.3.6 Fluid Lag

Fracturing fluid can only fill the fracture to a certain extent. The difference between fluid front and fracture tip is called fluid lag as illustrated in Figure 2.12. Fluid lag is a cavity filled with fluid vapors and its pressure is negligible. The effect of fluid lag is significant when the fracture toughness is small (Garagash, 2006; Lecampion and Detournay, 2007). Fluid lag was also observed at the field scale (Warpinski et al., 1985). For deep hydraulic fracturing (>1000m), it is estimated that fluid lag is no larger than a few centimeters because of high confining pressure (Detournay, 2016). It is because high fluid pressure are required to open the fracture and such high pressure pushes the fluid towards the tip.

2.3.7 Dual Porosity Model

Dual porosity model was introduced by Barenblatt et al. (1960) and Warren and Root (1963) which have been used in petroleum industry to model fractured rock. Dual porosity model divides the problem into two domains - the intact rock matrix and fracture network. The rock matrix is simplified into cubic blocks separated by a distance. Fractures are represented by parallel faces of matrix blocks.
2.3 Fluid modelling

Fig. 2.12 An illustration of fluid lag

Fig. 2.13 Illustration of dual porosity model
The rock matrix and fracture network have two distinct porosities and two distinct permeabilities. Most of the fluid flow is contributed by the fracture as the permeability of fracture is much higher than that of matrix by several orders of magnitude. However, most of the fluid storage is provided by the porous rock matrix.

There is no net flux in matrix as assumed. Flux of the model is provided by fractures only. Rock matrix is treated as sources or sinks in the dual porosity system. The transfer of fluid between matrix and fracture is represented a transfer term, which is done by changing the volume of the rock matrix.

The model can be uncoupled or coupled to the deformation of matrix. If uncoupled, the permeability of fracture is a constant value and the flow of both the fracture and matrix are governed by Darcy’s Law. For coupled mechanical and hydraulic model, cubic law model is used to describe the flow in fracture while Darcy’s law is used to describe the flow in rock matrix. Poroelastic model can be used to model the effect on the deformation of rock matrix.

**Upscaling**

The size of reservoir and the size of fractures that governs the flow can be differed by several orders of magnitude. Upscaling techniques have been developed to model the reservoir across several length scales. The reservoir is first discretised into coarse grids. Each of the matrix block in coarse grid model is made up of intermediate grids and each matrix block in intermediate grid is built up by local fine grids that is small enough to model the fractures presence in the reservoir. Local fine grids are analysed first to provide the boundary conditions of one of intermediate matrix blocks. Same procedure follows to analyse the coarse grid dual porosity model.

The coupling between different grid systems involves large number of iterations. Substantial computational power is therefore required but the model can be parallelised easily to boost the computational performance.
2.4 Regimes on hydraulic fracturing

In the past 30 years, numerous fundamental research studies on simple geometry were published and such research is still carrying on. However, a full analytical solution is still unavailable. Instead, different scaling laws are studied on different regimes of the problem in different limiting cases. They are called asymptotic solutions. Progress has been made by considering more parameters and relaxing some of the assumptions.

![Illustration of different physical processes involved in hydraulic fracturing.](image)

The following lists some of the assumptions:

- Rock is homogeneous, linear elastic, brittle, and of infinite extent and follows LEFM
- Rock is either assumed to be impermeable or 1D Carter’s model is used to model leak-off
- Fracturing fluid is incompressible and Newtonian
- Orientation of minimum in-situ compressive principal stress is uniform

Even with highly idealisation, it is still a highly challenging problem due to the interaction between different competing processes of viscous fluid flow, creation of fracture, elastic deformation and leak-off. The physical processes considered in this review are illustrated in Figure 2.14. There are also multiple timescales in the fracture propagation (Detournay, 2016). The relative influence among controlling physical processes changes with time. So the regimes of hydraulic fracturing problem also change with time.

Dimensionless groups have been extensively used to generalize the solution. Dimensionless parameters for different physical processes have been derived and governing equations and solutions are expressed in terms of dimensionless parameters.
These analytical solutions can serve as benchmark of numerical codes for hydraulic fracture simulations (Carrier and Granet, 2012; Chen, 2012; Hunsweck et al., 2012; Salimzadeh and Khalili, 2015). They have also been validated by experiments (Bunger and Detournay, 2008; Bunger et al., 2005; Lai et al., 2015).

In this section, the following parameters are used to simplify the equations

\[ E' = \frac{E}{1 - v^2}, \quad K' = 4 \left( \frac{2}{\pi} \right)^{1/2} K_{fc}, \quad \mu' = 12 \mu, \quad C' = 2C_L \]  

(2.24)

where \( E \) is Young Modulus, \( K_{fc} \) is fracture toughness, \( \mu \) is viscosity and \( C_L \) is Carter’s leak off coefficient.

The solutions of both the plain strain condition and the penny shape crack are reported in the literatures. This review focuses on the penny shape crack problem.

### 2.4.1 Overview on the interactions between regimes

There are three competing energy dissipation processes in hydraulic fracturing: viscosity, toughness and leak-off. They are characterised by different sets of dimensionless groups according to the dominant energy dissipation process. This review focuses on the penny shape hydraulic fracturing.

When rock is assumed impermeable and the fluid lag is negligible, there is an interaction between viscosity and toughness which can be characterised by a dimensionless toughness (or dimensionless viscosity). The dimensionless parameters are time variant. Hydraulic fracturing starts from viscosity dominant to toughness dominant and a time-scale can be introduced to relate this transition.

When fluid lag is considered, another time-scale is involved which is related to the rate of reducing fluid lag. At the start of hydraulic fracturing, fluid lag is large. It eventually vanishes and hydraulic fracturing becomes toughness dominant. Whether most of the fluid lag is reduced in viscosity regime or toughness regime depends on the ratio of two time-scales.

When leak-off is considered under zero-lag assumption, the fracturing process involves two time scales. One of them governs the interplay between energy dissipation mechanisms by viscosity and toughness. Another one governs the interplay between fluid storage and leak-off regimes. Hydraulic fracturing always starts from the viscosity-storage regime and eventually reaches the toughness-leak off regime. The intermediate regime, either the toughness-storage or the viscosity-leak off regime, depends on the ratio of two time-scales.
2.4 Regimes on hydraulic fracturing

2.4.2 Toughness dominant and viscosity dominant regimes

The analytical study of hydraulic fracturing was started by Spence and Sharp (1985). Early analytical solutions ignore the effect of leak-off in hydraulic fracturing (i.e. assuming impermeable rock). These studies focus on two regimes: viscous-dominant and toughness-dominant regimes characterised by a single parameter, dimensionless toughness. Solutions of different limiting cases are derived, such as zero (Adachi and Detournay, 2002; Savitski and Detournay, 2002), small (Garagash and Detournay, 2005) and large (Garagash, 2006; Savitski and Detournay, 2002) toughness.

![Illustration of the evolving regimes of viscosity dominant and toughness dominant.](image)

**Fracturing assuming zero leak-off**

Detournay (2004) introduced dimensionless groups, $K$ and $M$ characterising the effect of rock toughness and fluid viscosity respectively. The competing and evolving regimes of the viscosity dominant and toughness dominant are illustrated in Figure 2.15.

\[
K = K' \left( \frac{t^2}{\mu' Q_o E'_{13}} \right)^{1/18} \sim t^{1/9} \quad (2.25)
\]
\[
M = \mu' \left( \frac{Q_o^3 E'_{13}}{K' t^2} \right)^{1/5} \sim t^{-2/5} \quad (2.26)
\]

$K$ and $M$ are dependent ($M = K^{-18/5}$). Time element is included in both $K$ and $M$, meaning that hydraulic fracturing may go through a transition from viscosity-dominated to...
the toughness-dominated given sufficient amount of time. The time scale \( t_{mk} \) characterising such transition is given below

\[
t_{mk} = \left( \frac{\mu^o Q_o^3 E''_o}{K'_{18}} \right)^{1/2}
\]  

(2.27)

As \( t \leq t_{mk} \), HF would be viscosity-dominated. In other words, hydraulic fracture always starts with viscosity-dominated regime in penny shape crack problem.

### 2.4.3 Fluid lag

The above discussions focus on zero fluid lag assumption. Theoretically, fluid lag must exist unless for zero toughness or infinite toughness (zero viscosity) solutions. Otherwise, the fluid pressure at crack tip would become singular (The SCR Geomechanics Group, 1993). Garagash and Detournay (2000) recognised that no fluid lag assumption causes incompatibility between fluid flow equation and asymptotic stress field near crack tip as given by LEFM.

If fluid lag is considered, fracture propagation is more complicated which is characterised by two time-scales \( t_{om} \) and \( t_{mk} \) (Bunger and Detournay, 2007).

\[
t_{om} = \frac{E''_o \mu'}{\sigma_o^3}, \quad t_{mk} = \left( \frac{E''_o \mu^o Q_o^3}{K'_{18}} \right)^{1/2}
\]  

(2.28)

Time-scale \( t_{om} \) characterises the vanishing of fluid lag and \( t_{mk} \) from Eq. (2.27) relates to the evolution from viscosity dominant to toughness dominant regimes which has been discussed in Section 2.4.2.

\( \text{OMK} \)-triangle (Figure 2.16) represents the evolution of different regimes of the penny-shape fracture problem with dimensionless parameters \( Z \) and \( K' \):

\[
Z = \left( \frac{t}{t_{om}} \right)^{1/3} \propto \sigma_o, \quad K' = \left( \frac{t}{t_{mk}} \right)^{1/9} \propto K'
\]  

(2.29)

\( Z \) measures the contribution of confining pressure and \( K' \) measures the contribution of toughness in vanishing the fluid lag. In this triangular space, the regime evolves from \( O \)-vertex (large fluid lag regime, when \( Z = K' = 0 \)) to the \( K \)-vertex (zero fluid lag in toughness regime when \( Z \to \infty \) and \( K' \to \infty \)). In simple terms, the \( \text{OMK} \)-triangle illustrates how the fluid lag diminishes under the evolving regimes from viscosity dominant to toughness dominant. Figure 2.17 summarises the relationship between the large fluid lag regime, the viscosity regime and the toughness regime.
Fig. 2.16 Parametric space OMK with the three vertices representing the small-time ($O$), intermediate-time ($M$) and large-time ($K$) similarity solutions for a penny-shape hydraulic fracturing propagating in an impermeable elastic medium. (after Bunger and Detournay, 2007)
Fig. 2.17 Relationship between the evolving regimes of the large fluid lag, viscosity and toughness regime as illustrated in $OMK$-triangle
If the fluid lag is assumed to the zero, as discussion in Section 2.4.2, there is no $O$-vertex. The triangle reduces to $MK$-edge only and the regimes evolves from viscosity dominant ($M$-vertex) to toughness dominant ($K$-vertex) with the time-scale $t_{mk}$ only. Similarly, edges $OM$ and $OK$ corresponding to the case of $K = 0$ (reducing fluid lag in viscosity regime) and $Z = 0$ (reducing fluid lag in toughness regime) respectively.

For a full picture, the evolving of regimes from $O$-vertex (large fluid lag) to $K$-vertex (toughness dominant) is determined by a trajectory parameter $\varphi = t_{om}/t_{mk}$. Only when $\varphi \ll 1$, there are transitional regime of $M$-vertex for small lag and viscosity dominant.

**Solutions**

The early-time solution near $O$-vertex is given by Garagash (2006) for the plane strain problem and Bunger and Detournay (2007) for the penny-shape crack problem. The intermediate solution near $M$-vertex (small toughness) is given by Garagash and Detournay (2000, 2005) and the early-time and late-time solutions along $MK$-edge is given by Lecampion and Detournay (2007).

**Remarks**

For deep reservoirs, hydraulic fracturing is characterised by $\varphi \ll 1$ and $O$-solution is irrelevant as the treatment time is much longer than $t_{om}$ (Bunger and Detournay, 2007). Fluid lag matters only for fracture initiation near wellbore which happens at the timescales close to $t_{om}$ (Detournay, 2016). By ignoring fluid lag, the solution regime is reduced to toughness dominant and viscosity dominant regimes as discussion in Section 2.4.2.

### 2.4.4 Competing regimes of toughness and leak-off

Hydraulic fracturing is governed by two competing energy dissipative processes by fluid viscosity and rock toughness. When leak-off is considered, there are also competition between two fluid balance components associated with fluid storage in fracture and leak-off into surrounding rock. The relationship between the effects of leak-off, viscosity and toughness are illustrated in Figure 2.18. When fluid lag is ignored, these two dimensions of competing mechanism which can be visualized in a rectangular phase diagram $M\overline{M}K\overline{K}$ as shown in Figure 2.19. The vertices of the diagram correspond to four regimes where there exists one dominant fluid storage mechanism and one dominant energy dissipation process:

- storage-viscosity $M$ regime ($C' = K' = 0$)
- storage-toughness $K$ regime ($C' = \mu' = 0$)
Fig. 2.18 Illustration of the relationship between the evolving regimes of viscosity-storage, toughness-storage, viscosity-leak-off and toughness-leak-off

- leak-off-viscosity $\widetilde{M}$ regime ($C' \to \infty$, $K' = 0$)
- leak-off-toughness $\widetilde{K}$ regime ($C' \to \infty$, $\mu' = 0$)

Four edges of the phase diagram correspond to the four secondary regimes where either one fluid storage mechanism or one energy dissipation process is vanishing:

- storage $MK$ regime ($C' = 0$)
- leak-off $\widetilde{M}\widetilde{K}$ regime ($C' \to \infty$)
- viscosity $MM$ regime ($K' = 0$)
- toughness $\widetilde{K}\widetilde{K}$ regime ($\mu' = 0$)

For the penny-shape hydraulic fracture assuming zero fluid lag, the solution evolving from $M$ (storage-viscosity regime) to $\widetilde{K}$ (leak-off-toughness regime) and fracture evolution is governed by two independent timescales $t_{mk}$ (Eq. 2.27) and $t_{m\widetilde{m}}$

$$t_{mk} = \left( \frac{E^3 Q^2}{\mu' K^{18}} \right)^{1/2}$$
$$t_{m\widetilde{m}} = \left( \frac{\mu' Q_0^6 C}{E^{13/7} \mu'^{1/7}} \right)^{1/7}$$

(2.30)
2.4 Regimes on hydraulic fracturing

Fig. 2.19 Parametric space $MK\tilde{K}\tilde{M}$ for a zero-lag hydraulic fracture propagation of the penny shape crack. The system evolves with time along a $\phi$-trajectory, starting from $M$-vertex (viscosity-storage regime) and ending at the $\tilde{K}$-vertex (toughness-leak-off regime). For small $\phi$, the trajectory is attracted by the $\tilde{K}$-vertex and, conversely, by the $\tilde{K}$-vertex for large $\phi$. (after Detournay, 2016)
Timescale $t_{mk}$ gives the time required to evolve from viscosity to toughness regime (See Section 2.4.2) while $t_{m\bar{m}}$ characterises the transition between storage and leak-off regime. $M$-vertex corresponds to the early-time regime and $\bar{K}$-vertex to the large-time regime. Another two vertices are intermediate time regimes. The evolution of regimes is related to the ratio of two characteristic times

$$
\phi = \frac{E'^{11} \mu^3 C' \nu^4 q_o}{K'^{\frac{14}{3}}} = \left( \frac{t_{mk}}{t_{m\bar{m}}} \right)^{14/9}
$$

The trajectory is attracted to the $K$-vertex for small value of $\phi$ and $\bar{M}$-vertex for large $\phi$. The growth of the penny shape crack radius $R \sim t^n$ decreases with time with exponent $n$ which changes from $4/9$ at $M$-vertex, $2/5$ at $K$-vertex and eventually $1/4$ at both $\bar{M}$ and $\bar{K}$-vertex (Detournay, 2016). So, when the regimes evolve with time, the rate of growth of fracture radius is decreasing.
2.5 Experimental studies

Experiments in laboratory environment have been carried out to gain basic understanding on the governing parameters that influence the geometry and propagation characteristics of hydraulic fracture.

The major limitation of experimental studies is to extract a large rock sample from reservoir at great depth. Consequently, rock specimens used in tests mainly are near surface rock or artificial rock (Yew and Weng, 2014). Cement, gypstone and hydrostone are some of the example of artificial rocks used as test samples.

High confining stress (>10MPa) is applied to model the in-situ stress in field which could be more than 1km depth. Heavy loading machinery is required to apply such a high stress (Figure 2.20a-b). The sample may be cubic (typically 0.3m length, Figure 2.20c), rectangular or cylindrical (5-20cm radius). Test on larger shale sample of 762x762x914mm has also been carried out (Suarez-Rivera et al., 2013; Wang et al., 2015).

Given the significant difference between sample size and field scale where fracture generated can be extended to several hundred meters, the size effects have to be taken into consideration in interpretation of laboratory results. Hydraulic fracturing is toughness dominant in laboratory test while hydraulic fracturing in field scale is viscosity dominant (for details see Section 2.4). Therefore, high viscosity fluid has often been used in experiments to mimic the field environment and to reduce leak off. Scale laws using non-dimensional groups have also been developed to relate small scale laboratory tests to field scale (de Pater et al., 1994). However, laboratory sample cannot represent the heterogeneity in a larger scale. The effect of mulit-scale fracture network in reservoir cannot be easily modelled in laboratory test.

Another limitation of experimental studies is boundary effects. When hydraulic fracture in the rock becomes approximately one-third or the specimen dimension, fracture will grow towards the boundary causing unstable fracture propagation (Yew and Weng, 2014).

Visualisation of fracture is one of the challenges. To inspect fracture surface, samples need to be cut along fracture plane or chiselled into blocks for non-planar fracture (Olson et al., 2012). Transparent materials such as PMMA were used (Rubin, 1981; Wu, 2006) with coloured fractured fluid for visualisation of the whole fracturing processes but the homogeneous PMMA material cannot be easily compared with natural rock. Chen et al. (2015) mixed fracturing fluid with fluorescent paint so that fracture in a microscopic scale can be observed clearly. As shown in Figure 2.21, the fracture path is tortuous with branches in microscopic scale but the fractures in macroscopic scale appear straight and do not show branches. The fracture can also be visualised by CT scan (Jia et al., 2013) or approximated by AE detection (Bunger et al., 2015; Ishida, 2001).
Fig. 2.20 Photos of hydraulic fracture experiments. (a) True triaxial loading machinery in Delft University of Technology (from Weijers, 1995) (b) Triaxial compression apparatus with flat jacks installed along 4 sides (from Blanton, 1982) (c) A 305x305x305mm Shale sample mounted with six acoustic transducers (from Zhang and Fan, 2014)
Fig. 2.21 Hydraulic fracture experiment in shale as observed at different scale. (a) Macroscopic scale. The diameter of injection hole is 10mm (b) Microscopic scale (from Chen et al., 2015)
2.5.1 General observations

Medlin and Masse (1984) measured fracture width and length verse time in addition to fluid pressure in hydraulic fracture experiments of over 200 limestone and sandstone samples. Fracture width at borehole was measured by capacitance method and fracture length was measured by ultrasonic transducers. Power law relationship of fluid pressure, fracture length and width with time was observed. It was observed that fluid lag, which is only several percent of total fracture length, decreases with increasing confining pressure. This agrees with the analytical study in Section 2.4.3.

Guo et al. (1993) carried out experiment on gypstone, an artificial rock which is homogeneous and isotropic. The rate of fracture propagation decreased with increases in minimum principal stress. Under high stress, fracture propagated slowly and more stable, resulting in smaller boundary displacement. Injection rate had great influence on the breakdown pressure in low stress. Fluid efficiency (i.e. volume of fluid used to create fracture to total injected fluid) increased with higher injection rate.

Ishida (2001) studied the effects on grain size in granitic rock and acoustic emissions (AE) were measured. The number of AE event increased with increasing grain size due to greater roughness of induced crack surface. Fracture mechanism was governed by grain size and viscosity of fracturing fluid. Shear fracturing was dominant in large grain specimens using viscous fluid while tensile fracturing was dominant in small grain size specimens using low viscosity fluid.

If the effect of leak off is negligible, the pressure at which tensile fracturing initiated was independent of pressurization rate but it affected the breakdown pressure. (Zoback et al., 1977).

2.5.2 Fracture containment mechanism

It is commonly assumed that fracture containment mechanism exists to limit the vertical growth of hydraulic fracture in field and terminates at the formation interface between two different materials. It is also the assumption of PKN solution in which fracture height is kept constant. Warpinski et al. (1982b) carried out more than 200 field scale experiments to study fracture containment in layered rock. Increase in minimum principal stress had predominant influence on fracture containment. The level of stress increment required for containment is only 1.4-3.5 MPa which is further verified by other experiments (Warpinski et al., 1982a; Zhou et al., 2008). Teufel and Clark (1984) suggested that minimum of 4MPa stress increment was required but greater value was expected in hydraulic fracturing in deeper formation and for larger scale fracture. From mineback experiments reported in
Warpinski (1985), high-stress regions have resulted in a nearly rectangular-shape fracture for low-viscosity, low-flow rate tests. Higher viscosities and flow rates, which induced higher fracture pressures, resulted in greater heights and less rectangular shape.

Both Warpinski et al. (1982b) and Teufel and Clark (1984) pointed out that the difference of Young’s modulus alone was not effective to restrict fracture growth, but the difference might induce changes in stress distribution and arrest crack growth. Hydraulic fracture tends to cross natural fracture with small aperture. Natural fracture with large aperture tends to dilate and diverts the fracture propagation (Zhou et al., 2008).

Laboratory experiments showed that fracture may be terminated at weak and unbounded interface (Anderson, 1981; Teufel and Clark, 1984). Teufel and Clark (1984) demonstrated experimentally that interface shear strength also contributed to fracture containment. When interface shear strength was less than tensile strength and minimum horizontal compressive stress, fracture was diverted along the interface. This happened at low overburden pressure. At deeper formation, shear resistance of interface increases with overburden pressure such that the effect of interface can be neglected.

Bruno and Nakagawa (1991) carried out experiment on square slabs of highly porous limestone and sandstone to study the role of pore water pressure in hydraulic fracturing. It affected fracture initiation pressure and orientation. They found that fracture propagate towards the regions of higher local pore pressure.

### 2.5.3 Effect of existing fracture

Medlin and Masse (1984) observed that the influence of existing fracture depended on confining stress. At low confining stress (3.4-6.9MPa), natural fracture might stop growing. High confining stress (13.8-20.7 MPa) has little effect on the growth of existing fractures.
Blanton (1982) studied the effect of existing fracture in hydrostone experiments. Hydraulic fracture opened the existing fracture and diverted the fracturing fluid or the propagation was arrested when differential stress and angle of approach are small. Hydraulic fracture crossed the existing fracture when differential stress and angle of approach is high. It showed similar trend in hydraulic fracturing in Devonian shale. Fracture was either diverted or arrested by existing fracture when differential stress was small. Fracture propagation was unaffected when differential stress was high.

Beugelsdijk et al. (2000) studied the effect of natural fracture by cement block with shrinkage crack induced by heat treatment. They drew similar conclusion that hydraulic fracture is unaffected by existing crack under high differential stress, creating less tortuous fractures. They found that increasing the product of fluid viscosity and flow rate reduced the effect of existing fractures. Also, fracture with larger aperture showed more interaction with the hydraulic fracture. Similar findings were also reported by hydraulic fracturing of large sample (762x762x914mm) of Shale outcrop (Wang et al., 2015). Casas et al. (2006) studied how infill material (epoxy and grout) in existing fracture affected the interaction with hydraulic fracturing in Colton sandstone, rock with low stiffness and permeability. Low stiffness and viscoelastic behavior of epoxy modelled the clay rich infill material in crack that resulted in the arrest of hydraulic fracturing. Grout infill which has much higher stiffness than Colton sandstone did not arrest fracture propagation.

On effect on stress shadowing, Kear et al. (2013) carried out experiments on 4 closely spaced hydraulic fracture in South Australian Gabbro. Curving of fracture was observed but it was suppressed when the minimum stress increased. Initial notch which was favourably oriented had a profound effect on maintaining hydraulic fracture to be horizontal.
2.6 Hydraulic fracturing in naturally fractured formation

As the interaction between hydraulic fracture (HF) and natural fracture (NF) has been observed in both field and experiment, it is important to include its effect in numerical simulations. This section gives a review on the effect of a single planar fracture and more complicated fracture network affecting the hydraulic fracturing.

2.6.1 Interaction of hydraulic fracturing with single natural fracture

![Fig. 2.23 Different interactions between hydraulic fracture (HF) and natural fracture (NF) (from Yew and Weng, 2014)](image)

Different possibilities of interaction between hydraulic fracture and natural fracture are illustrated in Figure 2.23. When the tip of hydraulic fracture approaches natural fractures, the hydraulic fracture is under the influence of the stress field produced by the natural fracture. There are three possible scenarios: (1) Natural fracture slips under shear stress and arrests the hydraulic fracture (Figure 2.23b), (2) Hydraulic fracture crosses natural fracture directly (Figure 2.23c) or (3) hydraulic fracture crosses natural fracture with an offset (Figure 2.23d).
In case 1 in which hydraulic fracture is arrested, fluid flows into the natural fracture and it dilates if the fluid pressure exceeds the closure stress of the natural fracture. The dilated natural fracture may become part of the hydraulic fracture network as shown in Figure 2.23e.

If a hydraulic fracture crosses a natural fracture as in Case 2 and 3, there are two possibilities depending on whether the natural fracture is open or closed. When fluid pressure is smaller to closure stress, the natural fracture remains closed and the hydraulic fracture becomes planar (Figure 2.23f). Tortuous flow path may be formed if hydraulic fracture crosses natural fracture with an offset, which reduces the permeability of hydraulic fracture. When fluid pressure exceeds closure stress, natural fracture opens and becomes part of complex fracture network of hydraulic fracture (Figure 2.23g).

### 2.6.2 Crossing criterion

Blanton (1982) developed a criterion of a hydraulic fracture crossing a planar natural fracture with angle of approach and horizontal differential stress as parameters. It assumes the hydraulic fracture as a penny shaped crack under hydrostatic fluid pressure and the reservoir has zero tensile strength. A series of experiments in Devonian shale and hydrostone blocks have been carried out and the results matched reasonably well with the prediction from the above criterion.

Renshaw and Pollard (1995) developed analytically a simple criterion for a hydraulic fracture crossing a perpendicular natural fracture based on Linear Elastic Fracture Mechanics (LFEM). The criterion was verified experimentally. Hydraulic fracture is considered as an unbonded frictional interface.

Yew and Weng (2014) extended the above criterion for different intersecting angles between hydraulic fracture and natural fracture. It is more difficult for hydraulic fracture to cross natural fracture when the intersecting angle is small. This has been demonstrated experimentally. Chuprakov et al. (2014) developed a so-called OpenT model, a semi-analytical model that included the effect of fluid viscosity. Cubic law was used to model fluid flow and energy release in fracture propagation was considered as well. The model captured the tendency of hydraulic fracture crossing natural fracture under high flow rate and high fluid viscosity. This has been observed in experiments (Beugelsdijk et al., 2000).

Figure 2.24 compares different criteria and numerical simulations using code MineHF2D. Sarmadivaleh et al. (2011) and Sarmadivaleh (2012) carried out Discrete Element Method (DEM) simulations using PFC2D and showed that hydraulic fracture could not cross natural fracture in any circumstance when the approaching angle is less than 30°.

For cemented natural fracture, Taleghani and Olson (2013) proposed an energy based crossing criterion from 2D XFEM simulation results. Hydraulic fracture crosses a natural
2.6 Hydraulic fracturing in naturally fractured formation

fracture if the critical energy release rate of cemented material is at least 25% that of the matrix material. The ratio required increases for oblique intersecting angle.

![Comparison of hydraulic fracture - natural fracture crossing-arresting behaviour between analytical models and numerical models](image)

Fig. 2.24 Comparison of hydraulic fracture - natural fracture crossing-arresting behaviour between analytical models and numerical models (from Chuprakov et al., 2014). The red crosses and squares denote crossing and arresting of hydraulic fracture in MineHF2D code respectively. Solid green, dashed yellow and dashed blue curves correspond to OpenT criterion (Chuprakov et al., 2014), Blanton criterion (Blanton, 1982) and R&P criterion (Renshaw and Pollard, 1995) respectively. The effect of injection rate and relative stress difference for two approaching angles 90° and 60° are shown in (a) and (b) respectively.

2.6.3 Shear slip of natural fracture

For unconventional shale reservoirs, the permeability of the formation is very low (in the order of 0.1 \( \mu \)D). However, the formation contains a lot of natural fractures. They are mostly mineralized with no initial permeability. They are often weaker compared with matrix rock and are easily failed by shear when interacting with a hydraulic fracture.

Shear-induced dilation enhances the conductivity of natural fractures and increases fluid pressure in fracture. Shear force in the slipped part of natural fracture reduces and redistributes to not-yet-slipped part of natural fracture, causing propagation of slip front further in natural fracture. Such dilation can cause significant pressure-dependent leak off in hydraulic fracturing in unconventional shale reservoir (Yew and Weng, 2014).

Yew and Weng (2014) formulated an analytical solution for interaction between hydraulic fracture and natural fracture. In unconventional reservoir, hydraulic fracturing is first dominated by hydraulic fracture permeability growth and transits to natural fracture
growth dominant due to shear induced dilation in natural fracture. The solution suggests that formation subjected to high stress anisotropy is more favourable for shear dilation of natural fracture.

2.6.4 Interaction between hydraulic fracture and a single natural fracture

There are various factors affect the interaction between hydraulic fracture and natural fracture such as stiffness and toughness of formation, stress anisotropy, approaching angle, strength and frictional coefficient of natural fracture, fluid viscosity and injection rate. There are experiments investigating some of the above factors affecting the interaction (see Section 2.5.3). Semi-analytical models have been developed to describe how a few factors affecting the intersection behaviour. Numerical modelling provides a convenient way to explore more comprehensively how these factors govern the interaction between hydraulic fracture and natural fracture.

Cooke and Underwood (2001) modelled dry fracture propagation through a perpendicular bedding plane under in-situ stress in sedimentary rock. There are three possibilities: arrest, crossing with or without an offset. Fracture arrest happens in very weak bedding contacts while fracture crossing happens in strong contacts. Fracture might be arrested or might cross with an offset if the bedding plane has moderate strength, depending on how strong the in-situ stress is.

Zhang and Jeffrey (2006, 2008); Zhang et al. (2007) studied hydraulic fracture and natural fracture interaction in hydraulic fracturing. Zhang and Jeffrey (2006) simulated hydraulic fracturing crossing a perpendicular natural fracture. They showed that there was an increase in fluid pressure during the hydraulic fracture and natural fracture interaction and its magnitude depended on frictional coefficient of natural fracture and distance from injection point to natural fracture. Hydraulic fracture could be arrested or retarded in growth because of fluid flow diversion into natural fracture and frictional sliding along natural fracture. Fluid penetration into natural fracture required higher injection pressure for weak bedding. Zhang et al. (2007) and Zhang and Jeffrey (2008) modelled hydraulic fracturing across a perpendicular bedding plane separating two formations of different elastic moduli, in-situ stress and interface frictional coefficient. It showed that predicted hydraulic fracturing offset was in the order of centimetre and hydraulic fracture propagated perpendicular to the bedding plane. A large modulus or toughness contrast across the interface could lead to containment of the HF. Also, there were competition among fracture branches to become the main one.
2.6 Hydraulic fracturing in naturally fractured formation

Chuprakov et al. (2011) studied three stages of interactions between hydraulic fracture and natural fracture in hydraulic fracturing: (1) hydraulic fracture approaching, (2) contact and (3) subsequent infiltration of natural fracture. Different intersecting angles were modelled. Fluid was assumed to be hydrostatic and decoupled with mechanical deformation. The numerical results agreed well with the experimental results reported by Blanton (1982); Renshaw and Pollard (1995) that both high stress anisotropy and large approaching angle are in favour of the crossing of hydraulic fracture. Sesetty (2012) considered fluid flow in the simulation and found that injection pressure decreased when hydraulic fracture approached natural fracture and it might increase or decrease depending on various factors such as the distance between hydraulic fracture and natural fracture, fluid viscosity and injection rate.

2.6.5 Stress shadowing effects in parallel fractures

The presence of fractures alters the stress condition in their vicinity. Such effect is called stress shadowing. Within the shadow, the compressive stress of rock is increased by fluid pressure which suppresses the growth of fracture. Stress change in shadow can be so substantial that the orientation of maximum and minimum stress is changed or even reversed, called stress reversal. This causes reorientation of hydraulic fracture.

For multi-stage hydraulic fracturing, multiple cluster perforations are done to create fractures in a single stage. How to place these perforations is a critical issue because the number of perforation clusters to be used and the their spacing significantly impacts how effective fractures can be created.

Cheng (2009, 2012) carried out simulations of simultaneous multiple parallel hydraulic fractures with constant spacing. They showed that for two fracture system, fracture apertures were only slightly reduced. For three fracture system, the edge fractures were only slightly affected by stress shadowing. For the middle fracture, both its fracture aperture and extent were greatly reduced. As illustrated by Figure 2.25, the stress shadowing effect decreases with increasing spacing of parallel hydraulic fracture and the edge fractures curve slightly outward while the inner fractures keep straight (Kresse et al., 2013b; Sesetty, 2012). Under anisotropic stress, stress shadowing may cause complex fracture surface if there are no fracture containment mechanism (Castonguay et al., 2013).

Peirce and Bunger (2015) modelled simultaneous hydraulic fracturing in 3D. A cluster of 5 or 6 parallel fractures was simulated and they are only allowed to propagate in planar direction. The result was similar to 2D simulations mentioned above. As shown in Figure 2.26, non-uniform spacing of hydraulic fracture could increase up to 74% in fracture area as compared with even spacing hydraulic fracture.
Fig. 2.25 Comparison of fracture geometry and fluid pressure for five perforation clusters propagation with different perforation spacing from horizontal well: (a) 10m, (b) 20m and (c) 40m (from Kresse et al., 2013b)

Fig. 2.26 Comparison of the effect of stress shadowing of five parallel perforation clusters propagation from horizontal well on uniform and non-uniform perforation spacing: (a) uniform spacing and (b) non-uniform spacing (from Peirce and Bunger, 2015)
Bunger et al. (2012) carried out parametric study of two parallel fracture system, one was formed before another. They proposed a group of 4 non-dimensional parameters that governed the stress shadowing behaviour: dimensionless differential stress, dimensionless confining stress, dimensionless viscosity and dimensionless propped opening. Fracture path might curve away or towards the adjacent fracture (attractive or compulsive curving) depending on these non-dimensionless parameters. Such fracture curving was a result of stress redistribution and reorientation of principal stress and might lead to mixed Mode I and Mode II fracturing (Gholami et al., 2015). Zeeb and Konietzky (2015) showed that allowing backflow out of finished fractures could reduce the effect of stress shadowing.

### 2.6.6 Large-scale complex fracture

From simulation of natural fracture network, the observation of field during hydraulic fracturing of unconventional reservoir such as the high net pressure, relatively short fracture length and extensive region of microseismicity can be explained (McClure et al., 2015).

![Hydraulic fracture network simulation with multiple natural fractures](image)

**Fig. 2.27** Hydraulic fracture network simulation with multiple natural fractures for a Barnett case with different fracturing fluid. Thin blue lines denote natural fracture and the contour indicates aperture of hydraulic fracture (from Kresse et al., 2013a)

Kresse et al. (2013a) modelled a fractured reservoir with one set of natural fracture to study how flow rate and viscosity of fracturing fluid affected the geometry of fracture network produced by hydraulic fracturing. The result is illustrated in Figure 2.27. They also simulated staged hydraulic fracturing and showed that due to stress shadowing, fracture could even turn 90 degrees to propagate along maximum stress direction if stress anisotropy was small in formation.

Taleghani and Olson (2013) simulated 2D hydraulic fracturing in a fractured reservoir with one set of natural fracture to investigate the sensitivity of fracture geometry to stress
anisotropy and natural fracture orientation with respect to the *in-situ* minimum compressive stress. The graphical results are shown in Figure 2.28. The hydraulic fracture formed was linear without branches. Natural fractures diverted hydraulic fracture from its original alignment but stress anisotropy suppressed the nonalignment of hydraulic fracture. So, hydraulic fracture propagated further when natural fractures aligned favourably along with *in-situ* stress.

![Figure 2.28 Fracture network in hydraulic simulation in fractured formation under different degrees of stress anisotropy and orientation of natural fracture: (a) Isotropic in-situ stress and natural fracture is $30^\circ$ from horizontal and (b) isotropic in-situ stress and natural fracture is $45^\circ$ from horizontal and (c) anisotropic in-situ stress and natural fracture is $45^\circ$ from horizontal (from Taleghani and Olson, 2013)](image)

Riahi and Damjanac (2013) simulated hydraulic fracturing in fractured reservoir and showed that well-connected natural fractures created a more extensive hydraulic fracture network. Similar observation was obtained from Savitski et al. (2013). For equal injection volume, smaller injection rate leads to greater total area of hydraulic fracture network (Riahi and Damjanac, 2013). Fu et al. (2013) simulated hydraulic fracturing in a reservoir with natural fracture in random orientations. From Figure 2.30, isotropic *in-situ* stress produced more complex fracture network. With stress anisotropy, fracture propagation perpendicular to maximum stress direction was suppressed and produced more linear hydraulic fracture. Similar result was obtained by Torres and Castaño (2007).

Savitski et al. (2013) modelled natural fractures by statistically generated fractures. Significant leak off into natural fracture network could be achieved even if the natural fractures did not completely open. Shearing of natural fractures lead to crossing of the hydraulic fracture. This resulted in highly non-uniform aperture distribution. Injection rate was a crucial factor for the distribution of fluid between hydraulic fracture and natural fracture network. Lower injection rate increased the area of stimulated fracture network but it caused slower propagation of main hydraulic fracture and reduced aperture. Lower stress anisotropy
Fig. 2.29 Effect of natural fracture connectivity on hydraulic fracturing (from Riahi and Damjanac, 2013)
Fig. 2.30 Fracture network in hydraulic simulation in fractured formation under different degrees of stress anisotropy. (a) Anisotropic in-situ stress and (b) Isotropic in-situ stress. (from Fu et al., 2013)

increased the area of stimulated natural fracture network. Higher dilation angle of fracture increased leak off and reduced hydraulic fracture aperture.
2.7 Conclusion

Hydraulic fracturing is a multi-physics and multi-scale process. This Chapter reviews the three major physical processes involved in hydraulic fracturing, namely rock mechanics, fracture mechanics and fluid mechanics.

Rock is often modelled as a continuum and which follows linear elasticity. Under this assumption, fracturing can be modelled by continuum damage mechanics (CDM) without explicitly modelling of fractures. Poroelasticity is used to model rock as a two phase porous medium. Because of the presence of discontinuities (faults, joints, fractures and fissures), there are scale effects on rock which violates the assumption of treating rock as a continuum. The discontinuities are also the major source of heterogeneity.

Fracture mechanics studies how a fracture propagates. Linear Elastic Fracture Mechanics (LEFM) is the foundation of fracture mechanics that gives a fracture propagation criterion by considering stress intensity factor which measures the stress singularity at the fracture tip. However, LEFM is not applicable for rock as a quasi-brittle material because the fracture process zone (FPZ) at crack tip. It is handled by introducing a cohesive zone where there are some bridging mechanisms trying to close the crack. FPZ is weakened by micro-cracking and the growth of voids. The rock is assumed as a continuum except the fracture modelled. Also, heterogeneity is ignored in the fracture mechanics.

For fluid modelling, Darcy’s law is used to describe the fluid flow in rock if it is assumed as a porous continuum. The fluid flow along fracture is modelled by the cubic law in which the permeability of fracture is very sensitive to the aperture of fracture. Fluid flow from fracture to rock matrix (leak-off) is usually modelled by Carter’s model where the flow rate to rock matrix decreases with the exposure time of fracture to fluid. In the above modelling, rock is assumed as an equivalent continuum of a fractured and homogeneous rock.

There are studies on the different regimes in hydraulic fracturing assuming rock as homogeneous, linear elastic and brittle. These regimes are identified by different dimensionless parameters describing the interactions between different energy dissipation mechanisms between viscosity, toughness and leak-off. These regimes are time-variant so they evolve from one another as characterised by several dimensionless time-scales.

Hydraulic fracturing were investigated experimentally using large rock samples or artificial rocks. Topics studied are fracture containment and the interactions between the hydraulic fractures and the existing planar fractures.

The theoretical and experimental studies mentioned above assumed rock as a continuum and homogeneous. Recently, the effects of natural fractures have been studied numerically. Simulations were carried out to investigate the interactions between a single natural or a
natural fracture network. The presence of natural fractures has significant effects on the fracture path and extent of hydraulic fracture.
Chapter 3

Analytical and numerical methods in hydraulic fracturing simulation

The previous chapter gives a review on different theories on the physical processes involved in hydraulic fracturing. It also covers some theoretical studies on the coupled effects among the physical processes involved and the regimes of hydraulic fracturing in an idealised condition. These theoretical studies assume rock as a homogeneous material. Rock is treated as a continuum and the effects of discontinuities (natural fractures) have not been properly accounted for.

From experimental studies on the hydraulic fracturing, only simple interaction between the role of natural fracture is investigated. The role of natural fractures is understood by numerical studies.

This Chapter first reviews early analytical models that are commonly used in oil and gas industry for the extraction of conventional reservoir. The most classical analytical models are called PKN and KGD models. Simulators used by the industry for fracture design based on pseudo-3D (P3D) and planar-3D models (PL3D) are reviewed. These models are not truly 3D models but they transform a 3D problem into a 2D one. Since the reservoirs for conventional reservoir are homogeneous and the presence of fractures has negligible effect on hydraulic fracturing, the above models assume reservoir as a continuum.

This Chapter mainly reviews different numerical methods used in rock mechanics and their applications on hydraulic fracturing simulation.

In the early age, numerical methods in rock mechanics are based on continuum approach like Finite Element Method (FEM) and Boundary Element Method (BEM). eXtended Finite Element Method (XFEM) is proposed to overcome some limitations on modelling fracture propagation.
To account for the discontinuities in rock, discontinuum methods are also used to model rock. For example, Discrete Element Method (DEM) and Discontinuous Deformation Analysis (DDA) are often used to assess the stability of blocks of rock for tunnelling and slope work. Discrete Fracture Network (DFN) is proposed to study the fluid flow and transportation in reservoir. Finally, Lattice Element Method (LEM) is reviewed which has been used to model heterogeneous material such as concrete.
3.1 Early analytical models for hydraulic fracturing

The development of analytical models started in the 1950s. One of the earliest models were developed by Perkins and Kern (1961) and later Nordgren (1972) further developed it to formulate the well-known PKN Model. Khristianovich and Zheltov (1955) and Geertsma and de Klerk (1969) independently developed another model called KGD model. These models were developed to calculate the fracture geometry, width in particular, for a specified length and flow rate. The volume balance was not taken into account. Both PKN and KGD use the work of Carter (1957) to include the effect of leak off.

Both PKN and KGD models are applicable to fully confined fractures. The difference lies on the approach to convert a 3D problem into a 2D one. KGD model assumes plane strain in horizontal direction while PKN model treats each vertical cross section independently. For PKN model, pressure at any section is dominated by the height of the section rather than the length of the fracture. Therefore, PKN model is applicable to long fractures of limited height with elliptical vertical cross-section whereas width calculation in the KGD model is height independent. If there is no confinement of fracture, radial model can be used.

In terms of fracture mechanics, PKN model does not consider fracture mechanics and the effect of crack tip. KGD model, however, considers the crack tip region which governs the fracture propagation.

3.1.1 PKN Model

Perkins and Kern (1961) assumed a fixed height vertical fracture propagating in a well-confined pay zone (i.e. some confinement mechanism exists to prevent fracture growth out of pay zone). Another assumption of PKN model is elliptical fracture cross-section (Figure 3.1a) with maximum width proportional to the net pressure. The model assumes plane strain condition in every vertical plane, but the stress and strain are not exactly the same in adjacent planes. The model is said to be quasi-plane strain assumption (Valkó and Economides, 1995).

Perkins and Kern pointed out that the pressure required for fluid flow was far greater than the pressure required to extend a fracture. This justified the zero fracture toughness assumption in PKN model. Also, fracture would continue to extend after pumping was stopped, until the pressure was dissipated by leak-off and reached the minimum pressure for fracturing.

Nordgren (1972) included the effect of leakoff and fluid storage in fracture in the Perkins and Kern model to form a well-known PKN model. The leakoff model provides the fracture length and Perkins and Kern model provides the fracture width.
3.1.2 KGD Model

Khristianovich and Zheltov (1955) provided a solution for propagation of a hydraulic fracture by assuming the width of the crack is independent of its vertical position (Figure 3.1). This means that it is applicable for a tall fracture. Their solution considers the fracture mechanics at crack tip. To simplify the solution, the flow rate in the fracture is assumed to be constant and fluid pressure is constant except near the fracture tip. This recognises that most of pressure change occurs near crack tip region as pressure change is very sensitive to fracture aperture according to cubic law (See Section 2.3.3). Also, they assumed no fluid lag near crack tip region. They showed that the dry part is only a few percentage of the total length in fluid.
3.2 Further development of hydraulic fracturing simulators

The early fracture models based on analytical methods cannot be applied to layered reservoirs because the fracture footprint is sensitive to the changes in confining stress across layer interfaces (Adachi et al., 2007). More refined models were therefore developed to overcome this limitation. These numerical models can be categorised into (a) Pseudo-3D (P3D) and (b) Planar-3D (PL3D).

Most of the commercial software use P3D or PL3D models for fracture design. Despite PL3D models are more accurate, they are computationally expensive for day-to-day fracture design so faster P3D models are more popular for commercial software.

3.2.1 Pseudo 3D Models

PKN or KGD models are not able to simulate both vertical and lateral propagation. Settari and Cleary (1986) first introduced P3D models to model multi-layers reservoir with different in-situ stress and stiffness. P3D models can be further classified into two types: lumped-based and cell-based models (Economides and Nolte, 2000).

**Lump-based Model**

In lumped-based (elliptical) models, the vertical profile of the fracture is assumed to consist of two half-ellipses connected at the centre (Figure 3.2a). The height and length of hydraulic fracture are calculated at each time step. It is assumed that their shape are compatible at the
connection. This model assumes that fluid flow is along streamlines from the perforations to the edges of the fracture. The shape of the streamlines are obtained from analytical solutions.

**Cell-based Model**

Cell-based models treat the fracture as a series of connected PKN-like cells along fracture length. Each cell has different height (Figure 3.2b). Each cell acts independently and fluid flow in the vertical direction are not fully coupled between cells. As such, fracture opening is only related to fluid pressure in individual cell and there are no interaction between adjacent cells. So, it is suitable for contained fractures, which are long relative to their height. This is considered as analogous of the PL3D model with the fracture which is discretised along horizontal direction only.

### 3.2.2 Planar 3D Models

Planar 3D (PL3D) models were also developed in 1980-2000. PL3D models are regarded as more accurate but computationally far more expensive than P3D ones. It uses technique from boundary element method to transform elasticity equations to integral equations by the use of Green’s function. Only the fracture surface is required to be modelled and discretised, which effectively reduces a 3D problem into 2D. Homogeneous and elastic medium is assumed. Homogenised elastic medium can be assumed fractured medium. PL3D for layered formation has also been developed (Siebrits and Peirce, 2002). However, it is difficult to consider non-linearity and anisotropy in PL3D models because of the use of Green’s function (Li et al., 2015).

In PL3D models, fracture footprints and the coupled fluid flow equations are described by a 2D mesh of cells, typically a moving triangular mesh, oriented in a vertical plane. A moving boundary element mesh (Clifton and Abou-Sayed, 1981; Siebrits and Peirce, 2002; Vandamme and Curran, 1989) or fixed grid approach (Siebrits and Peirce, 2002) have been used to model the planar fracture. In moving boundary mesh, fracture plane is discretised using automated grid generation scheme. Mesh is regenerated whenever fracture propagates. Special treatment is required to avoid highly distorted mesh. For fixed grid approach, fracture front is interpolated from the width obtained from interior nodes of the fracture.

For formulation of PL3D models, five groups of basic governing equations are required

- Elasticity equations for mechanical response of rock
- Fracture propagation criteria
- Fluid flow equations
3.2 Further development of hydraulic fracturing simulators

- Leak off equations
- Proppant transport equations

A lot of research effort has been deployed to develop a stable, robust and efficient algorithm to couple all the above equations.

3.2.3 Limitations on P3D and PL3D models

The major limitation of P3D and PL3D models is that the propagation of fracture is limited to plane perpendicular to direction of confining stress. They are built on the basic assumptions that the reservoir elastic properties are homogeneous. Only so-called bi-wing fracture is produced. Non-planar fracture growth cannot be modelled. Also, these models cannot simulate the complex stress field around wellbore. Fully 3D models have to be used to address the above limitations.

3.2.4 Comparison of different commercial simulators

Warpinski et al. (1994) provided a review of 12 hydraulic fracture simulators used by oil and gas industry which are summarised in Table 3.1. A field experiment data were used to compared the simulation results form these industrial simulators. With the same input parameters, these simulators gave a significant difference (as great as five-fold) in fracture geometries and net fluid pressure as shown in Figure 3.3. Moreover, ad hoc parameters were introduced in these simulators to attempt to model phenomenologically some of the complex processes occurring within fracture such as multiple fractures, increased frictional loss of fluid, micro-cracking and the complexity of formation including heterogeneity, nonlinearity, plasticity and dilatancy. The choice of these ad hoc parameters is based on experience of modellers.
<table>
<thead>
<tr>
<th>Numerical Models</th>
<th>Software</th>
</tr>
</thead>
<tbody>
<tr>
<td>Planar 3D</td>
<td>TerraFrac (TerraTek Inc.) HYFRAC3D (S.H. Advani of Lehigh U.)</td>
</tr>
<tr>
<td>Finite difference</td>
<td>GOHFER (Marathon)</td>
</tr>
<tr>
<td>Pseudo-3D Cell-based</td>
<td>STIMPLAN (NSI Inc.) ENERFRAC (Shell)</td>
</tr>
<tr>
<td></td>
<td>TRIFRAC (S.A. Holditch &amp; Assocs. Inc.)</td>
</tr>
<tr>
<td>lumped-based</td>
<td>FRACPRO (Reservoir Engineering Systems)</td>
</tr>
<tr>
<td></td>
<td>MFRAC-II (Meyer &amp; Assocs.)</td>
</tr>
<tr>
<td>PKN and GDK</td>
<td>PROP (Halliburton)</td>
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<tr>
<td></td>
<td>Chevron 2D model</td>
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<td></td>
<td>Conoco 2D model</td>
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<td></td>
<td>Shell 2D model</td>
</tr>
</tbody>
</table>

Table 3.1 Hydraulic fracturing simulators used by the oil and gas industry (from Warpinski et al., 1994).

Fig. 3.3 Comparison of industrial hydraulic fracture simulators by modelling a field experiment in a 3-layer case (a) fracture length growth and (b) fracture height growth (from Warpinski et al., 1994)
3.3 Continuum and discontinuum approaches

Early analytical solutions and later P3D and PL3D models idealise rock mass as a continuum without explicitly model the fractures in rock mass except the hydraulic fracture itself. For a continuum, it is assumed that the domain can be sub-divided infinitely and the same governing laws or equations apply to every sub-domains as if the undivided itself. The validity of continuum assumption hinges on the concept of REV. The effect of discrete fractures and other microscopic inhomogeneity can be averaged out in a REV (homogenisation).

These models also assume rock to be homogeneous, isotropic and elastic. The most common numerical method using continuum approach is Finite Element Method (FEM) which has wide applications across different fields of engineering. Apart from FEM, Boundary Element Method (BEM) and eXtended Finite Element Method (XFEM) are also continuum-based numerical methods where the later has been developed to overcome the limitations on modelling discontinuities in FEM.

However, rock is regarded as a ‘DIANE’ material - Discontinuous, Inhomogeneous, Anisotropic and Non-Elastic (Harrison and Hudson, 2000). The presence of pre-existing fractures contributes to DIANE nature of rock and greatly changes the mechanical and hydraulic properties of rock mass. Fluid flow in rock mass is heavily influenced by fractures because the majority of fluid flow in rock mass is in form of fracture flow rather than leak off into rock matrix. Therefore, discontinuum approaches are developed to model the effect of fractures on rock. The earliest discontinuum method in rock mechanics is Discrete Element Method (DEM) proposed by Cundall (1971).

As defined by Cundall and Hart (1992), discontinuum methods should have the following capabilities

- allow finite displacements and rotations of discrete bodies, including detachment.
- automatically recognizes new contacts between bodies during calculation.

Later development of numerical methods for rock mechanics diverges into continuum approaches and discontinuum approaches (Bobet et al., 2009; Jing, 2003). Figure 3.4 summarises the numerical methods used in rock mechanics. The choice of continuum and discontinuum methods depends mainly on the problem scale and fracture system geometry (Jing, 2003). Figure 3.5 gives an example of the choice of continuum or discontinuum method to model rock tunnel excavation. Continuum methods are suitable for rock masses with no fractures or with many fractures. Discontinuum methods are suitable for moderately fracture rock masses where there are too many fractures to be handled by continuum methods and large-scale displacement of blocks is possible (Jing, 2003).
Fig. 3.4 Numerical methods in rock mechanics

Fig. 3.5 Choice of different numerical methods for rock mass excavation. (a) Continuum method, (b) either continuum method with fracture element or discontinuum method, (c) Discontinuum method and (d) Continuum method with equivalent properties of fractured rock (from Jing, 2003)
Hybrid continuum discontinuum models were also proposed (Lorig et al., 1986) to enjoy the advantages of the two approaches. The near-field domain that rock is likely to exhibit discontinuous behaviour is modelled using discontinuum method while the far-field domain is modelled using continuum methods where the stress and deformation changes are small.
3.4 Finite Element Method

Finite Element Method (FEM) is the most popular numerical method in engineering, including rock mechanics and hydraulic fracturing simulation. Owing to its versatility, FEM has been developed not only for solving solid mechanics problems, but it has also extended to multi-physics hydraulic fracturing problem.

There have been different attempts to model fractured rock mass using FEM. The first attempt was the development of different joint elements. Joints parameters are required to establish constitutive relationship of joint in resisting both normal and shear. Interface elements have also been developed to solve contact problem using contact mechanics instead of continuum approach used in joint elements (Jing, 2003).

Very fine mesh is required for accurate calculation of stress intensity factor as shown in Figure 3.6. Special quarter point element around fracture tip has been developed to more accurately calculate stress intensity factor (Barsoum, 1976, 1977). Adaptive meshing technique (Azadi and Khoei, 2011; Schöllmann et al., 2003) is required to model fracture propagation in FEM to avoid using very fine mesh for the whole domain.

Numerical issues also arise by using joint element or interface element. Since the thickness of joint element is either assumed to be zero or a very small value, the aspect ratio of the element becomes high. This is commonly the source of numerical ill-conditioning of global stiffness matrix. The displacements of joints have to be limited to a small value due to small displacement assumption in continuum mechanics.

Fractures have to conform with element boundaries because they cannot cut across elements. The fracture path has to be pre-defined before analysis. This rises the mesh dependency issue, particular in regular mesh. Random mesh can be used to reduce the effect of mesh dependency in macroscopic scale. Without pre-defining fracture path, complicated adaptive mesh algorithm is required such that elements are aligned with the fracture path.

3.4.1 Applications on hydraulic fracturing

Single crack system

Because of the complexity involved and the limitation on computational power, FEM has been used to model a single crack system for fundamental research on hydraulic fracturing (Carrier and Granet, 2012; Chen, 2012; Hunsweck et al., 2012; Yao et al., 2015). Cohesive fracture model has been implemented by FEM software ABAQUS assuming formation as impermeable in 2D (Chen, 2012), 3D (Yao et al., 2015) or porous medium governed by poroelasticity (Gonzalez et al., 2015).
Secchi and Schrefler (2012) also performed 3D FEM simulation and the formation was modelled as a porous media and crack propagation modelled by cohesive model. No pre-determined fracture path is needed but continuous remeshing is still required.

**Continuum damage mechanics**

Using continuum damage mechanics (see Section 2.1.4), the effect of heterogeneity and the evolution of micro-defects in rock are implicitly modelled. Wang et al. (2009a) developed code RFPA2D to simulate hydraulic fracturing of heterogeneous stiff clay with a cylindrical cavity. The material properties follow Weibull distribution. Later, Li et al. (2012) further developed RFPA2D to RFPA3D-Parallel to simulate hydraulic fracturing in 3D. Two damaging evolution laws were used to describe the damage by tension and shear separately. Zhang et al. (2010) used FEM package ABAQUS for 3D simulation. Cohesive crack model was used as a 1D damage model to simulate fracture propagation. Ma et al. (2016) modelled reservoir by dual porosity model and fracturing by an elasto-plastic damage model.

The major advantage of the use of damage mechanics is neither remeshing nor refinement is required. However, the geometry of hydraulic fracturing cannot be obtained precisely. Otherwise, very small element has to be used.
3.5 Extended Finite Element Method

Extended Finite Element Method (XFEM), or General Finite Element Method (GFEM), has been developed to overcome the limitations on FEM in modelling discontinuities, mainly on the dependence of fracture propagation path on meshing and remeshing required during fracture propagation. XFEM was first proposed by Babuska and Melenk (1995) to model a fracture path that is independent to meshing. XFEM harvests the extensive research on meshfree methods, an approach that the domain is discretised by nodes only without providing any mesh to relate their connectivity.

It is called extended or general FEM because all the techniques in FEM are preserved in XFEM. On top of FEM, the geometry of discontinuities and its effects are represented within the framework of XFEM by mathematical techniques. The objective is to tackle discontinuities locally at element level by enrichment.

Same as other continuum methods, XFEM and meshfree methods have been developed under rigorous mathematical framework (Babuka et al., 2003). A lot of research effort has been put in XFEM development recently (Abdelaziz and Hamouine, 2008; Karihaloo and Xiao, 2003), particular in fracture mechanics which is the most mature field of XFEM applications (Belytschko et al., 2009). Reviews of using XFEM to model fracture propagation are provided by Abdelaziz and Hamouine (2008) and Rabczuk et al. (2010).

3.5.1 Brief description on XFEM formulation

The XFEM achieves its aim by introducing an additional term, called *enrichment* in shape functions $u^h(x)$ to take into account for the effect of discontinuities.

$$u^h(x) = \sum_{i \in I} N_i(x)u_i + \sum_{i \in I^*} M_i(x)a_i$$ \hspace{1cm} (3.1)

where

$N_i(x)$ conventional FE shape functions

$u_i$ conventional FE nodal degree of freedom

$M_i(x)$ local enrichment function

$a_i$ additional degree of freedom for enrichment

$I$ A set that contain all the nodes in a element

$I^*$ A set that contain all the enriched nodes in a element, $I^* \subset I$
The shape function is divided into two parts: the first part is same as the shape function in conventional FEM; the second part accounts for the effect from discontinuities. The concept of enrichment comes from Partition of Unity Method from meshless methods. The local enrichment functions $M_i(x)$ can be expressed as the product of partition function $\varphi_i(x)$ and global enrichment function $\Psi(x)$ as

$$M_i(x) = \varphi_i(x)\Psi(x)$$  \hspace{1cm} (3.2)

The contribution of the discontinuities are discretised across the entire domain into sub-domain by $\varphi_i(x)$, such that $\sum \varphi_i(x) = 1$. Such a way to discretise the influence from discontinuities allows the use of the principles of superposition. In fact, the effect of a crack influences over the entire domain, but enriching of the entire domain is not an ideal way. Discontinuous partition functions are chosen to have non-zero terms only in nodes in the vicinity of discontinuities. In other words, the effect of discontinuities to the entire domain is lumped to these enriched nodes. The extra degrees of freedom (DOFs) can be significantly reduced and the sparsity of the global stiffness matrix in conventional FEM can be preserved. Usually, shape functions for the standard approximation and the enrichment are the same functions (i.e. $\varphi_i(x) = N_i(x)$), but different functions may be used.

Sethian (1998) and Osher and Fedkiw (2004) proposed an implicit scalar function called level set function to represent the geometry of discontinuities in terms of nodal values. It has zero value at discontinuity and the domain $\Omega$ is divided into two sub-domains on either side of the discontinuity where the level-set function is either positive or negative. This method greatly simplifies the representation of discontinuities, especially in 3D cases and in complex fracture network.

Two different enrichment functions are required to represent crack segments that cut through elements and crack tips that estimate the near tip behaviour as illustrated in Figure 3.7.

### 3.5.2 Hydraulic fracturing simulation

Recently, there have been extensive research on the use of XFEM for hydraulic fracturing simulation. Enrichment functions including fluid flow in fracture are formulated.

Rethore et al. (2007) developed two scale approach for hydraulic fracturing simulation. Cubic law is used for microscopic flow in fracture and poroelasticity (Section 2.1.5) is used for macroscopic flow. The coupled equations are non-linear which are solved iteratively by Newton-Raphson method. Lecampion (2009) proposed that different asymptotic crack tip fields were required for hydraulic fracturing in toughness regime and viscous regime.
Meschke and Leonhart (2015) constructed enrichment functions from the analytical solution of 1D consolidation problem to approximate the fluid pressure near crack. The enrichment functions are space and time variant. Considerable reduction of error compared to other XFEM formulation is achieved. Gordeliy and Peirce (2015) researched on the convergence rate of different XFEM enrichment schemes for hydraulic fracturing and developed a scheme which achieves second order of convergence.

Formation was either assumed as impermeable (Chen, 2013; Gordeliy and Peirce, 2013b; Keshavarzi and Mohammadi, 2012; Lecampion, 2009; Weber et al., 2013) or modelled as a porous medium (Meschke and Leonhart, 2015; Mohammadnejad and Khoei, 2013; Rethore et al., 2008; Wang, 2015). Salimzadeh and Khalili (2015) developed a three phase model (fracturing fluid, pore fluid and solid). Two fluid phases are captured by capillary pressure-saturation relationship. Hydraulic fracture with fluid lag was also developed (Gordeliy and Peirce, 2013a; Mohammadnejad and Khoei, 2013; Weber and Fries, 2013). Most of these formulations are based on LEFM but cohesive crack model has also been proposed (Mohammadnejad and Khoei, 2013; Rethore et al., 2008; Wang, 2015).

Hydraulic fracturing using XFEM has been implemented in FEM software ABAQUS (Chen, 2013; Wang, 2015). Wang (2015) included Mohr-Coulomb plasticity model to simulate non-planar fracture propagation of deviated well. ABAQUS has also been used in more complicated simulations such as the interaction between hydraulic fracture and existing natural fractures (Dahi-Taleghani and Olson, 2011; Keshavarzi and Mohammadi, 2012; Taleghani and Olson, 2013). All of the above XFEM implementations are in 2D but
recently 3D implementations are also reported to model non-planar fracture propagation (Gupta and Duarte, 2014).

### 3.5.3 Remarks on XFEM

The main advantage of XFEM is the use of mature FEM framework that both researchers and engineers are familiar with. FEM codes *ABAQUS* and *LS-DYNA* have included the capacity of XFEM to model crack propagation problem. Fracture mechanics can be more easily applied to XFEM by enrichment and without the limitations from meshing. The approach to model rock in FEM such as heterogeneity by assigning different material parameters and anisotropic model can be applied to XFEM.

However, the level set equations are not polynomials in which conventional shape functions do. Discontinuities and singularities are involved in XFEM. The conventional FE techniques in evaluating integrations of the weak form solution cannot be directly applied. The moving of singularity (crack tip) inside the element causes instability in numerical solution (Richardson et al., 2009). Different techniques have been investigated such as high order Gaussian quadrature and spitting elements into sub-elements. A robust and efficient way to solve this enriched weak form solution is still under research.

Complex fractures such as intersecting and branching of fractures can be modelled in a limited way (Richardson et al., 2009). Mesh refinement is still required near fracture tip because of the singular stress around it. Adaptive meshing has been developed to reduce the computation cost, particular for 3D simulation (Gupta and Duarte, 2014).

Under the continuum approach, the singularity and discontinuities during formulation cannot be avoided and complicated mathematical treatments and numerical techniques are required. They are the sources of numerical instability and inaccuracy although they are better handled in XFEM compared with FEM. More research on robust numerical techniques is needed.
3.6 Boundary Element Method

The main difference between Boundary Element Method (BEM) and FEM is FEM discretise the entire domain but BEM only discretises its boundaries. BEM was first developed and called boundary integral equation method by Jaswon (1963) and Symm (1963). Therefore, BEM was called boundary integral method during its early development.

The application of BEM on rock mechanics started from the work of Brady and Bray (1978). BEM has become one of the popular numerical methods in rock mechanics. Large number of papers report the use of BEM in underground excavation, dynamic problems, in-situ stress and elastic properties interpretation and borehole tests for permeability measurements (Jing, 2003). The use of BEM in fracture mechanics was initiated by the work of Cruse (1978). A review of the use of BEM in fracture mechanics is provided by Maschke and Kuna (1985) and a review of BEM focusing on computational aspects is provided by Liu et al. (2012).

Same as FEM, BEM can tackle coupled mechanical processes such as coupled hydro-mechanical processes (Pan and Maier, 1997).

3.6.1 Brief description on BEM formulation

The concept of BEM lies on the principle that the changes at one point inside the domain affect other points inside the domain, including its boundaries. Such a relationship can be given by Green’s functions (or named kernel functions) which can be found in literature for different kinds of problems on various material models. If both the boundary conditions and how a source point influences the domain boundary are given, the solution inside the domain can be worked out.

BEM first seeks a weak solution at the global level through an integral statement, based on Betti’s reciprocal theorem and Somigliana’s identity. By discretisation of boundary and approximation of solution using shape functions, the integral form of the original problem can be expressed in matrix form

$$Ax = By$$  \hspace{1cm} (3.3)

where \(x\) are the unknown values and \(y\) are the known values from boundary conditions. The above system of equations becomes a typical \(Ax = b\) problem in linear algebra, but the matrix \(A\) is dense which is different from FEM where the stiffness matrix is sparse.
### 3.6.2 Computational Aspects

The advantages of BEM in computational aspects are summarised below:

- The dimensions of problem can be reduced by one
- High accuracy due to the nature of integrals used in the formulation
- Capable to model infinite domain problem (without boundary effects in FEM)

The main drawback of BEM comes from the dense matrix in contrast to the sparse global stiffness matrix in FEM. Efficient sparse matrix solvers used in FEM cannot be used in BEM. This offsets some of the edge of BEM that it reduces the dimension of problem by one. This shortcoming can be tackled by the development of new numerical approaches such as Fast Multipole Method (FMM). This enables BEM to handle large 3D problem with many DOFs. BEM can also be easily parallelised (Yokota et al., 2011) to take the advantage of multi-core CPU and Graphics Processing Unit (GPU) (Takahashi and Hamada, 2009) for larger scale problems.

### 3.6.3 Modeling discontinuities

One of the main applications of BEM is fracture mechanics. Liu et al. (2012) has summarized the advantages of the use of BEM to model fractures:

- Only the discretisation of boundary is required which simplifies preprocessing and remeshing when crack propagates.
- Improvements on the accuracy in solving stress concentration problems since there are no approximations imposed on the stress solution at the interior domain points.
- Fracture parameters (such as stress intensity factors \( K \) and energy release rates \( G \)) can be accurately determined in a straightforward manner.
- Modelling of problems involving infinite or semi-infinite domains is simple and accurate

In modelling fractures, special treatments are required to model fracture to avoid singularity in solution. Dual Boundary Element Method (DBEM) and Displacement Discontinuity Method (DDM) are some of the examples.

DDM was first developed by Crouch (1976). It is also referred as indirect or special type BEM because the unknowns do not have physical meanings. They are mapped values of
physical quantities on imaginary infinite domain that are used to facilitate the formulation of the integral solutions. In hydraulic fracturing simulation, DDM is often used to simulate the interaction between hydraulic fracture and natural fracture. This is discussed in detailed in Section 3.6.3. Fracture is modelled by a special displacement discontinuity (DD) element that can propagate in an impermeable and linear elastic medium.

Galerkin Boundary Element Method (GBEM) can be used to overcome the limitation on modelling sharp boundaries in conventional BEM.

3.6.4 Heterogeneity

BEM is suitable to model linear elastic and homogeneous material (Jing, 2003; Liu et al., 2012). The discontinuities are modelled explicitly as boundary elements while the domain remains linear elastic and homogeneous. To account for heterogeneity, the domain can be divided into several sub-domains. However, BEM cannot have as many sub-domains as in FEM. BEM can model anisotropic material (Ding et al., 2004; Pan and Amadei, 1996) and elasto-plastic material (Swedlow and Cruse, 1971). However, applying constitutive law in BEM is not as straightforward as in FEM. This restricts the use in BEM that requires complicated constitutive law and models the progressive failure by damage mechanics as in FEM (Tang, 1997).

3.6.5 Hydraulic fracturing simulation

Sousa et al. (1993) developed a 3D BEM hydraulic fracturing simulator HYFSYS capable to model non-planar fracture from arbitrarily oriented, perforated wellbores. Yamamoto et al. (2004) developed a 3D simulator considering the interaction between multiple fractures. BEM has been implemented to simulate hydraulic fracturing interacting with natural fracture or bedding interface (Zhang and Jeffrey, 2006, 2008; Zhang et al., 2007), closely spaced hydraulic fracture (Bunger et al., 2012) and multiple fracture initiation and propagation at a wellbore (Zhang et al., 2011). With some simplifications in modelling interaction between fractures, numerical codes based on BEM have been developed which are capable to model the interaction of hydraulic fracture with complex fracture network (Bérard et al., 2015; Kresse et al., 2013a). More discussion can be found in Section 2.6.6.
3.7 Discrete Fracture Network

The Discrete Fracture Network (DFN) was first proposed by Long et al. (1982) to study fluid flow and transport processes in fractured rock mass. It was originated from the field of rock hydro-geology but also in the interest of reservoir engineering (Karimi-Fard et al., 2004) in oil and gas industry (Meyer, 2009) and geothermal reservoirs (Watanabe and Takahashi, 1995). Other applications include assessing fractured aquifers and fractured zones in bedrock as a water resource in mountainous terrain (Mortimer et al., 2011; Reeves et al., 2013), controlling seepage in mining (Ouyang and Elsworth, 1993), rock tunnelling (Lee and Moon, 2004; Moon and Song, 1997), migration of pollutants such as toxic and radioactive waste (Dverstorp et al., 1992; Sun and Zhao, 2010) in geo-environmental engineering.

In a DFN, only fracture planes are modelled. The rock matrix is either assumed to be impermeable or its effects is described by simple laws. Hence, the effects of mechanical deformation (i.e. the change of aperture with stress) are often neglected or modelled in a simple way.

While other numerical methods focus on the mechanical response of rock, DFN mainly handles fluid flow and transport process problems. DFN is the only tool that can be applied to practical problems by modelling fractured rock in field scales.

DFN reduces a 3D problem into 2D by modelling fractures only. It can be further reduced to 1D if fracture planes are modelled using pipe models. A 3D problem can hence be analysed at a lower computational cost and large numbers of fractures can be included.

Among other numerical models, DFN provides the most representative fractured rock mass at field scale. It is often used to characterisation of the permeability of fracture rock. There is also attempt to derive equivalent elastic parameters of fractured rock using DFN (Min and Jing, 2003).

3.7.1 Generation of Fracture Network

Figure 3.8 shows two fracture networks generated by DFN. The geometry of fracture network need to be inputted explicitly. Fracture dimensions, spacing, orientation and aperture are required to define a fracture network. Hydraulic parameters such as transmissivity are also required. As the actual fracture network can never be fully revealed, fractures are generated by a random fracture generator following certain probability density functions (PDFs) with the input of fracture parameters: size, orientation, spacing and aperture. These parameters are estimated from boreholes, in situ tests and mappings. Stochastic methods such as Monte Carlo simulation (Andersson, 1984) have been used to reduce the effects due to uncertainty in modelling of fracture network.
In the early development of DFN, assumptions were made to simplify the generation of fracture network. For example, Andersson (1984) assumed that

- All fractures are planar
- All fractures are independent of one another
- Fractures are of infinite extent
- All fracture locations are equally probable
- All fracture orientations are independent of fracture location and are equally probable

Many of them are not valid. For example, the heterogeneous nature of rock means that the fracture locations are not totally random. Also, fracture orientation should have a correlation with in-situ stress.

The current development of DFN relaxes some of the assumptions listed above. The infinite extent of fracture is no longer assumed by adopting circular, rectangular or polygonal shape of fractures. The dependency among different fracture parameters can be tackled by fractal geometry (Watanabe and Takahashi, 1995) and geo-statistical methods (Chiles, 1988). However, non-planar fractures are not considered in DFN even in the latest literatures.

### 3.7.2 Explicit Fracture Network Input

The concern on the uncertainty of underground condition becomes more apparent in DFN as explicit input of fracture network is required. Neuman (2005) pointed out that the ability
to map discontinuities in rock was limited by the available geological and geophysical techniques. Quantitative information about fracture aperture, fracture shape and size could not be obtained.

The data limitation and the complexity of fracture flow make DFN models difficult to be validated. Given the efforts on fracture characterisation, Neuman (2005) mentioned that DFN did not outperform much simpler continuum or hybrid discrete-continuum methods.

### 3.7.3 Application on hydraulic fracturing simulation

The major drawback of DFN is that the influence of rock matrix on fluid flow in rock fractures cannot be properly accounted for since rock matrix is not modelled in DFN. It was developed in hydro-geology field to study fluid flow and transport process problems. These processes induce little stress change so that the hydro-mechanical coupling between rock matrix and fractures is usually ignored or is estimated in a simple way. For instance, Ouyang and Elsworth (1993) used a single parameter, modulus reduction factor, to estimate the combined impact of the permeability from joint apertures, joint spacing, joint stiffness and modulus of intact rock. However, stress changes in rock matrix affect the aperture of crack, which is very sensitive to flow rate and their relationship is highly non-linear (Willis-Richards and Wallroth, 1995).

To overcome this limitation, DFN can be combined with other numerical methods for hydraulic fracturing simulation. The most common way is combining block type DEM with DFN. DFN can be used for the tessellation of blocks for block type DEM as illustrated in Figure 3.9 (Riahi and Damjanac, 2013; Savitski et al., 2013). DFN models the fluid flow within fracture network and the mechanical deformation is solved by DEM. The apertures in fractures are updated. DFN can also be coupled with particle type DEM (Mas Ivars et al., 2011). They are discussed in details in the following section.
Fig. 3.9 A reservoir model with embedded DFN representing natural fractures modeled by 3DEC. (a) 3DEC base model with block geometry and zoning and (b) Fully-connected (top) and sparsely-connected (bottom) DFN realizations. Clusters of connected fractures share the same color (from Savitski et al., 2013)
3.8 Discrete Element Method

Distinct/Discrete Element Method (DEM) is classified as a discontinuum method. It was first proposed by Cundall (1971) to model geomaterial as rigid blocks and later rigid particles was proposed to model granular material (Cundall and Strack, 1979). DEM can be further categorised into block models and particle models. The former uses polygons (2D) or polyhedrons (3D) as elements while the later uses discs (2D) or spheres (3D). The particle model simplifies the detection of contacts.

Another branch of DEM is Discontinuous Deformation Analysis (DDA) which is referred as implicit DEM. It is discussed in detail in Section 3.9.

Complex macroscopic behavior such as non-linearity, hysteresis and damage evolution can be produced by DEM using simple constitutive relationship between particles/blocks. Not a single constitutive law in continuum models can produce all these behavior. Some of these behaviour can be reproduced but many ad-hoc parameters are required (Potyondy and Cundall, 2004). Also, the failure mechanism does not need to be inputted as a priori as the model automatically fails by the most critical mechanism.

The computation of DEM mainly composes of (1) neighbourhood and contact detection and (2) solving equilibrium positions. Time stepping algorithm is used to solve the law of motion applied to each particle and force displacement law are applied to each contact. DEM is computationally intensive, particular for block models, because of neighborhood search and contact detection. Time step selected has to be very small to ensure numerical stability. It should be chosen smaller than a critical time step which is depended on the minimum block size and the maximum shear contact stiffness (Hart et al., 1988). Longer time step can be chosen in DDA but the computation time in solving takes longer time compared with explicit method in each step.

3.8.1 Block models

In block models, the domain is discretised into blocks. Blocks can be specified by joint set parameters (dip angles, dip directions, spacing and apertures). Blocks can also be generated by a fracture set generators. The generators use probability density functions (PDFs) specified by users to create fractures. It can also be generated by Voronoi tessellation to minic the grains in rock (Ghazvinian et al., 2014; Hamidi and Mortazavi, 2014; Lan et al., 2010; Torres and Castaño, 2007).

One of the major tasks in DEM is the identification of neighbourhood and the determination of contact type. It is much complicated in block type DEM compared with particle type DEM. Also, interactions between blocks are governed by contact forces between them,
which depends on the type of contact also. There are three contact types for 2D problems: (1) vertex-vertex, (2) vertex-edge and (3) edge-edge. For 3D problems, the number of contact types is increased to 6: (1) vertex-vertex, (2) edge-edge, (3) face-face, (4) vertex-edge, (5) vertex-face and (6) edge-face. However, the determination of contact is not a simple task, especially in 3D case. A major research area in DEM is finding robust and fast algorithms to identify the neighbourhood and the contact type.

Blocks can represent intact and deformable rock material, while interfaces represent pre-existing discontinuous surface such as faults, joints and fractures. The major limitation is that fracture path has to be pre-defined by blocks and contact geometry.

Applications on Hydraulic Fracturing

Fig. 3.10 Block generation by Voronoi tessellation for hydraulic simulation by DEM. (from Preisig et al., 2015) (a) Voronoi tessellation with superposition of joints and (b) directional polygons approach to generate block with interfaces bias towards favorable orientation for fracture initiation

In the application of block type DEM in hydraulic fracturing, vast majority of simulations reported were implemented in commercial package UDEC (Itasca Consulting Group Inc., 2014b) in 2D and 3DEC (Itasca Consulting Group Inc., 2013) in 3D.

Block generation

This paragraph presents 2D hydraulic fracturing simulations using UDEC. Torres and Castaño (2007) modelled reservoir as Voronoi blocks. Interactions between blocks were modelled by
3.8 Discrete Element Method

elastic beams and the repulsive force between them is proportional to the overlapping area. Fluid was assumed to be hydrostatic and leak off was considered by specifying permeability of blocks that obeys Dracy’s law. Zangeneh et al. (2015) also generated blocks by Voronoi tessellation with superposition of joints with specified dip angles, spacing and persistence. However, using Voronoi blocks would introduce a large number of interfaces perpendicular to the major principal stress which might stop hydraulic fracture from propagating further. In this regard, Preisig et al. (2015) proposed directional polygon approach that controls the orientation of fracture to align at a favourable orientation for fracture initiation (see Figure 3.10).

Hamidi and Mortazavi (2014) used finite element mesh generator GMESH (Geuzaine and Remacle, 2009) to construct polyhedral blocks. Non-presistent joints were modelled by fictitious joint approach. Linear elastic perfectly plastic constitutive model with Mohr-Coulomb failure criterion (with tension cut-off) was applied for both intact rock and fictitious joints.

For 3D simulation using 3DEC, McLennan et al. (2010) modelled a reservoir with 2 joint sets orthogonal to each other. Although it is a 3D model, joint sets have constant height. There are several limitations on modelling. Hydraulic fracture only propagates along existing joints. Blocks are impermeable, meaning that leak-off is not considered. The computation time required for one simulation can reach several weeks.

DFN for natural fractures

Another way to generate blocks is tessellation by DFN that represents natural fracture or favourable fracture orientation. In the simulations reported by Riahi and Damjanac (2013), fractures can deform elastically, open and slip (by Coulomb slip law) as functions of pressure and total stress. Savitski et al. (2013) also modelled natural fracture by DFN. It showed that significant leak-off into the natural fracture could be achieved even if natural fractures do not completely open. Lower injection rate increases the stimulated fracture network area, with the cost of slower propagation of main hydraulic fracture and reduced aperture. Under lower stress anisotropy, more natural fractures are stimulated that enhances their shear dilatancy. The effect of dilation angle is found to be significant. With higher dilation angle, leak-off increases and aperture of main hydraulic fracture deceases.

3.8.2 Particle models/Bonded Particle Model

Using particle models to model rock was first proposed by Potyondy and Cundall (2004) which is referred as Bonded Particle Model (BPM). The concept of BPM is largely enlight-
ened by the research on DEM. The idea of BPM is that the macroscopic rock behaviour is driven by the mechanics of micro-structures such as pores and micro-cracks. They postulated that, similar to granular material, the macroscopic load in rock was transmitted by force chains that propagated from one grain to another by contact forces. In rock, such force chains were formed by grains and cement skeleton. So, BPM is suitable for modelling sedimentary rock.

In terms of modelling, particle models are similar to block models, as both of them discretise rock into distinct elements that can detach and interact with different neighbourhood. The simplification in discretised rock by particles provides better computational performance. More complex grain shapes can be modelled by using ellipse particles (Ting, 1992) or clamping particles together (Cho et al., 2007).

In addition to contact models, bonds are installed between neighborhood particles to mimic the cementation between particles. Damage process, fracture initiation and propagation can be modelled by removal of bonds. Figure 3.11 shows two bond models used in BPM: parallel bond model and flat joint model. Parallel bond model is the most commonly used model that bonds can resist rotation between particles. Recently, flat-joint model has been proposed to simulate angular, interlocked grains that can sustain partial or full damage of bonds (Potyondy, 2015).

BPM provides an unified framework that is able to produce anisotropy, heterogeneity and discontinuities of geomaterial. There are virtually no limitations on fracture paths and complexity of fracture patterns generated. Numerical stability problems often occur if continuum models are used instead. Growth of micro-cracks and their coalescence into macroscopic fractures are inherently considered in the model. It can produce some useful
output such as acoustic emissions (AE) during failure which are observed in rock testing. This is useful for simulation of induced seismicity in hydraulic fracturing.

Macroscopic discontinuities are \textit{explicitly} modelled in block type DEM whereas microstructures such as micro-cracks in geomaterial are \textit{implicitly} modelled as particles in BPM. Therefore, BPM is often used for simulation of laboratory test of intact rock sample. Discontinuity can be modeled explicitly in BPM by employing a technique called smooth joint model (SJM) proposed by Mas Ivars et al. (2011). Particle may overlap and ‘slide’ against each other along a specified joint orientation. This avoids the inherent roughness along the joint by being forced to move around one another.

Coupled with DFN, complex fracture network has been incorporated in BPM to simulate large scale rock mass (Damjanac et al., 2013; Mas Ivars et al., 2011). Such model is referred as Synthetic Rock Mass (SRM). Vallejos et al. (2016) mapped veins in core samples and modelled them as SRM. The simulations successfully reproduced laboratory results of uni-axial compression tests.

Particles in BPM do not correspond exactly to grains in geomaterial. Grain-based BPM model was developed to model deformable and breakable polygonal grains and grain interfaces (Potyondy, 2010). Models are constructed by overlaying a polygonal grain structure which completely fills space. Each grain is made up of clusters of lumped particles and grain boundaries are modelled by SJM. Therefore, the computation cost of grain-based models is much higher than that of conventional BPM models.

\textbf{Model calibration}

The macroscopic properties of rock come from the following microscopic parameters

\begin{itemize}
  \item Gain shape
  \item Gain size distribution
  \item Gain packing
  \item Gain-cement micro-mechanics
\end{itemize}

There is a calibration process to obtain a set of micro-mechanical parameters to match the macroscopic parameters that can be measured in laboratories. The calibration is a lengthy process. The macroscopic properties of the model can only be obtained by carrying out numerical experiments (such as triaxial test and Brazilian test). Fakhimi and Villegas (2007) produced non-dimensional graphs to assist the searching of suitable micro-mechanical parameters. Also, not all the macroscopic parameters can be duplicated in BPM. The ratio of
compressive to tensile strength of rock sample is unusually high whereas the friction angle is too low (Bobet et al., 2009).

Intact and compact rock can be modelled reasonably well in 2D using either grain-based or flat-jointed models in direct tension or direct compression tests (Potyondy, 2015). Intact rock in 3D can be modelled using parallel bonded model including a moment-contribution factor (Potyondy, 2011) or 3D flat-jointed model (Potyondy, 2015).

Applications on Hydraulic Fracturing

Fig. 3.12 Acoustic emission in hydraulic fracturing simulated by BPM. (a) Fracture propagation and fluid infiltration. The solid lines indicate cracks and the shade indicates the fluid pressure. (b) Crack types and magnitude of energy released from the cracks (from Shimizu et al., 2011)

The energy release by bond breakage can be converted to AE which is first reported by Hazzard and Young (2000). Al-Busaidi (2005) correlated the AE data from hydraulic fracturing of cylindrical samples of Lau du Bonnet granite. Hydraulic fracturing generated predominantly tensile failure which produced smaller AE events. Shear failure occurred by slipping on pre-existing fracture. Shimizu et al. (2011) studied the influence on fluid viscosity and particle size distribution in saturated or partial saturated BPM models. Figure 3.12 shows the graphical output of a simulation result. They showed that tensile cracks were dominantly generated and more shear failure occurred in heterogeneous models (models with widely distributed particle radii).

BPM simulation gives microscopic perspectives in hydraulic fracturing. Deng et al. (2014) investigated interaction between Shale and proppant. Proppants were modelled as unbonded particles and fluid was modelled by Computational Fluid Dynamics (CFD). However, large scale simulation can only be implemented by BPM with particle size much larger than grains in rock to study the induced seismicity in hydraulic fracturing. Damjanac et al. (2010) modelled 5x5 m modelled with the average particle size of 0.0225m. Natural
fractures were modelled by DFN. It was found that if all the fractures were modelled, the rock mass would become too soft. So, only some of fractures were included in the model.

Hazzard and Young (2002) simulated fluid injection test in granitic rock at Soult-sous-Forts, France, for an EGS project. The model generally produced fluid pressure and seismicity similar to observations in field. Yoon et al. (2014) modelled continuous and cyclic fluid injection in a 2x2 km reservoir of granitic rock with joints. Some field observations on induced seismicity were simulated including the reactivation of pre-existing joints and the post shut-in seismicity. Cyclic injection caused fewer numbers of both total and large magnitude events.

The above simulations were implemented in PFC2D. The most popular and simplest fluid model is pore network model as illustrated in Figure 3.13. Wang and Adhikary (2015) and Mora et al. (2015) implemented a coupled scheme between DEM and Lattice Boltzmann Method (LBM) using ESys-particle (Mora and Place, 1994) as DEM simulator. Wang et al. (2016) also implemented a DEM-LBM coupled scheme to capture the onset and the propagation of hydraulic fracture at grain scale in a great details, as shown in Figure 3.14. Papachristos et al. (2015) used open source DEM code YADE (Kozicki and Tejchman, 2008) to model solid part. This is the only literature from the knowledge of the author reporting 3D implementation. Fluid was modelled by pore-scale finite volume (PFV) to consider the fluid flow in both rock matrix and fractures.
Fig. 3.14 Hydraulic fracturing simulation in grain scale by coupling of BPM and LBM at different instants. (from Wang et al., 2016)
3.8.3 Remarks

Researches are undergoing to work on various unsolved issues in BPM. The unrealistic high compressive to tensile strength ratio can be reduced by using clamped particles to model the interlocking effect from irregular grains. Both the macroscopic strength and fracture toughness depend on particle sizes but no single particle size can be chosen to match both quantities.

There are several limitations on its application on hydraulic fracturing simulation.

- Assemblage of particles consists of large numbers of pores which applies only in very porous rock.

- Fluid flow in fracture cannot be easily modelled because the fracture geometry cannot be obtained.

- The micromechanical parameters used cannot be measured easily and are not fully understood

- Complex process required to prepare a model (such as material genesis)

- Lengthy calibration process is required but not all macroscopic parameters can be matched

- The highly expensive computational efforts limits its use on large scale 3D problem
3.9 Discontinuous Deformation Analysis

Discontinuous Deformation Analysis (DDA) was first developed by Shi and Goodman (1984, 1985) and was further developed for a complete analysis of block system (Shi, 1988). DDA is also referred as implicit DEM. Maclaughlin and Doolin (2006) provided a review on the validation of DDA against analytical solutions, other numerical methods as well as laboratory and field data.

DDA ensures force equilibrium implicitly by minimizing total potential energy of the global system. The potential energy has a broader scope than FEM. It includes the kinetic energy and the strain energy from contacts and the dissipated energy from friction. As a result, the solution of DEM is force based while that of DDA is displacement based. Another difference from DEM is that the interactions between blocks in DEM are arisen from contacts during overlapping but overlaps are prevented by adding very stiff springs between blocks in DDA. The elimination of overlaps enables DDA to model fracture flow by coupling a fluid model (Jing et al., 2001).

The major advantage of DDA is the use of mature FEM techniques to assemble global stiffness matrix and solve it. Well-developed FEM codes can be easily converted to DDA code. Compared to DEM, longer time step can be chosen without numerical instability or inaccuracy in the final result.

However, the computational cost is still high compared to continuum methods. The neighbourhood searching and contact detection is computationally intensive. The global stiffness matrix needs to be updated once contact condition has changed. Although 3D DDA has been developed (Beyabanaki, 2008) but most of the applications of DDA are still limited to 2D.

3.9.1 Applications on Hydraulic Fracturing

Compare with other numerical methods, DDA is rather undeveloped in hydraulic fracturing application. Kim et al. (1999) and Jing et al. (2001) have formulated a coupled hydro-mechanical model for fluid flow in fractures but fracture propagation was not modelled.

Ben et al. (2012) first reported the use of DDA in hydraulic fracturing simulation using square blocks. Morgan and Aral (2015) used finite volume fracture network model for the simulation of compressible fluid flow in fractures including one-dimensional Carter leak off model. Mohr-Coulomb failure criteria (shear failure) with a tension cut-off (tensile failure) was used to model fracture. There were 3 types of contact: locked (normal and shear spring), sliding (normal spring only) and open (no springs). 'Open-close’ iteration was performed to determine the type of contact. Few hundred iterations were required in each time step. The
numerical results have been verified by analytical solutions (penny shape fracture and KGD fracture) and by experiments (Rubin, 1981).

Jiao et al. (2015) generated joint network by Monte Carlo simulation and modelled heterogeneity by applying Weibull distribution on material properties. Sliding failure is governed by Mohr-Coulomb and tensile failure by cohesive model.

The above simulations assume blocks are rigid. Choo et al. (2016) proposed the use of deformable blocks by discretization them into FEM elements. As the flow in fracture is sensitive to its aperture according to the cubic law, considering the deformation of block can simulate fluid flow in fracture more realistically. Also, higher computational efficiency can be achieved as the number of blocks involved can be reduced substantially.

All the simulations presented above are two dimensional. There is no three dimensional DDA simulation for hydraulic fracture so far. Also, there are mesh dependency issues as fractures have to be conformed with the interfaces between blocks but such effect can be minimized by using a dense mesh (Choo et al., 2016).
3.10 Lattice Element Method

In the literature, Lattice Element Method (LEM) is also referred as lattice models or Lattice Spring Model. The term LEM is used to give the flexibility of using different models for lattice.

Figure 3.15 illustrates the basic components in LEM. The domain is discretised into cells. Each cell is represented by a node. All the information of a cell is stored in its corresponding node. When two cells share a common facet, they are neighbours and their nodes are linked by a lattice. Each lattice represents a common facet (common edge for 2D) between two neighboring cells. All the information of a common facet is stored in its corresponding lattice. Forces between neighbourhood cells are transmitted through lattices.

The basic element in LEM is a lattice. There are only two ways to specify the mechanical properties of a material, by specifying lattice network geometry and by specifying lattice properties. For a regular lattice network, the Poisson’s ratio depends on the choice of lattice element. The Poisson’s ratio is fixed at 1/3 for 2D and 1/4 for 3D if Hookean spring model is used for a regular triangular lattice. It can vary in a certain range if other lattice models are used. The issue of Poission’s ratio is discussed later in this Chapter.
The heterogeneity of material can be modelled in two ways: a regular lattice with voids or fractures or a disordered lattice.

LEM is often used to simulate fracturing process of a heterogeneous material which is difficult to be modelled using continuum methods. Also, fracture properties of material is known to be sensitive to the microstructure (H. Leibowitz, 1984).

Hrennikoff (1941) first proposed to discretise a continuum domain into a lattice composed of spring elements or beam elements. Elements cannot be further sub-divided. This is the analogy of an atomic structure of a material where a node represent an atom and a spring connecting two nodes represents the force between them. But the lattice has much coarse resolution than the atomic structure. LEM has caught little attention due to the lack of computational power to solve multi-DOF system and the later development of FEM.

If the kinematics of particles is less important and particles undergo small deformation, which is the case of solid geomaterial like rock, LEM is a suitable tool in microscopic modelling. LEM has been used to model geomaterial (Wong et al., 2014, 2015), concrete (Lilliu and van Mier, 2003; Liu and Liang, 2009; Schlangen and Garboczi, 1997; van Mier and van Vliet, 1999), cemented granular material (Topin et al., 2007), cellular material (Wang and Stronge, 1999), composite material (Sadhukhan et al., 2011; Snyder et al., 1992; Spagnoli, 2009) and biomaterial (Hansen et al., 1996). LEM is capable to represent heterogeneity by including micro-structures or by assigning heterogeneity (i.e. a probability density function) in lattice properties. Because of its simplicity and efficiency in computation, especially in modelling fracture propagation, large number of nodes and lattices can be modelled. LEM is therefore extensively used for statistical mechanics of fracture in disordered media (Chang et al., 2002; Chiaia et al., 1997; Gao and Klein, 1998; Prado and van Mier, 2003).

In this section, different applications of LEM are reviewed. The review starts at lattice network construction. Different methods of lattice network construction have been proposed for different materials for heterogeneous (or called disorder by physicists) material. Also, different lattice types have been proposed, including the most simple scalar model, different spring models and more complicated beam models. Different lattice failure criteria and post-peak behaviour of a lattice are also reviewed.
3.10.1 **Lattice network construction**

Most of the applications of LEM is modelling heterogeneous material. This can be achieved by two means: variation of lattice element parameters and variation of lattice geometry. The former approach will be discussed later. The latter is called geometric disorder and this section focuses on the generation of disordered lattice network.

**Structures in Ordered Mesh**

This is the most common approach to model heterogeneity. The structures are explicitly included in the lattice. For example, in modelling concrete fracturing processing, aggregate, cement paste and interface between them are included (Lilliu and van Mier, 2003; Liu et al., 2007; Liu and Liang, 2009; Schlangen and van Mier, 1992). Man and van Mier (2011) modelled a real concrete structure in a 3D lattice model with its structures obtained by CT scans (Figure 3.16). In material science, heterogeneity is incorporated by putting microstructures such as voids (Day et al., 1992), flaws (Ashurst and Hoover, 1976), grain boundaries and intrusions (Ostoja-Starzewski et al., 1996).

In this approach, a regular triangular, square or hexagonal mesh is first chosen. Spatially disordered structures are overlaid on the lattice. It can be generated by specifying a statistical model such as Gaussian distribution (Spagnoli, 2009). Lattice elements are removed to model voids or flaws. For multi-phase material such as concrete, different lattice element properties are assigned. Properties of lattice elements are usually identical within the same material without assigning a statistical distribution.
Disordered Mesh

Another approach to introduce geometric disorder is using a disordered mesh. There are several ways to generate a disordered mesh which are briefly mentioned below:

Modification from an ordered mesh  This is the simplest method to generate a disordered mesh. It is done by first generating an ordered mesh and assigning a random shift to each node. To maintain the same connectivity of node without intersections between lattice elements, the node can only be shifted within a certain region and the amount of shift indicates the geometrical randomness. The advantage of this method is that the number of node connectivity can be fixed and computation can be more efficient. However, this method cannot generate a highly disordered lattice with a wide variety of lattice length. Also, the coordination number is fixed.

From Connecting Disordered Nodes  In this method, spatially random nodes are first generated. Voronoi cell of each node is then tessellated. Non-intersecting lattice elements can be constructed by jointing nodes that share at least one edge in their Voronoi cell. This method is called Voronoi construction. There is a concern of generating unwanted anisotropy when disorder is introduced. Moukarzel and Herrmann (1992) provided an algorithm to generate a random lattice without anisotropy. Geometrical disorder introduced by random points is found to be negligible if physical disorder due to random distribution of lattice parameters is introduced (Grassl and Bažant, 2009).

From Particle Packing  This method is used for modelling cemented granular material (Affes et al., 2012; Topin et al., 2007). A packed granular particles are first generated by techniques available in DEM. The most simple way to construct a lattice is joining the particles in contact. The lattice models the aggregated effect of particle, matrix and particle-matrix interface. A more detailed modelling involves mapping the packed granular particles to a very fine regular lattice mesh. Different properties are assigned for different material and interface.

Other Approaches  There are other methods to produce a random lattice such as Delaunay triangulation used in Hansen et al. (1996). This method avoid producing skinny triangles by maximizing the minimum angle in triangles generated.


3.10.2 Statistical modelling

Continuum based finite elements are suitable for modelling progressive damage evolution or fracture in homogeneous material. Simulation of fracture in heterogeneous materials is complicated by the presence of disorder, that leads to statistical distribution of failure stresses, accumulated damage, acoustic activities and different crack shape (Alava et al., 2006). In the discrete lattice modelling of fracture, heterogeneity can be explicitly modelled while in continuum mechanics based numerical methods such as FEM, the heterogeneity is often implicitly modelled using the homogenisation concepts over RVE like continuum damage mechanics.

Statistical fracture mechanics aims to explore the role of disorder in fracture model and attempts to quantify the effect of disorder on damage distribution, size effects, damage localization, acoustic emissions, crack roughness and avalanches by means of scaling laws. One of the simplest and most studied numerical tools is Random Fuse Model (RFM).

3.10.3 Random Fuse Model

RFM is the simplest scalar model studied by physicists which is first proposed by Arcangelis et al. (1985). Each bond in the network is modelled as fuse with a electrical conductance and a breaking threshold. The local stress $\sigma_i$, strain $\epsilon_i$ and local elastic modulus $E_i$ are mapped to the current $I_i$, potential drop $V_i$ and local conductance $k_i$ respectively. Each fuse $i$ obeys Ohm’s laws ($I_i = k_iV_i$), the analogy of elasticity ($\sigma_i = E_i\epsilon_i$). Once a critical
current $I_c$ is reached, the conductivity becomes zero. The disordered can be introduced in three ways:

- random threshold $i_c$ according to a probability distribution function (Arcangelis et al., 1985; De Arcangelis and Herrmann, 1989)
- random dilution, removing a fraction $p$ of the fuses at the beginning of the simulation (Lennartz-Sassinek et al., 2013; Nukala et al., 2005).
- random conductivities $k_{ij}$ according to a probability distribution function (Sahimi and Goddard, 1986; Takayasu, 1985)

The random distribution of lattice strength can also be spatially correlated (Grassl and Bažant, 2009) as shown in Figure 3.18. The ratio of correlation length $l_a$ to size of RVE $l_{RVE}$ (or FPZ) is the main parameter that controls the statistical size effect in fracturing (Grassl and Bažant, 2009). Size effect is significant if $l_a \gg l_{RVE}$ and negligible if $l_a \ll l_{RVE}$.

![Spatial correlated field for correlation length](image)

Fig. 3.18 Spatial correlated field for correlation length (a) $l_a = 0.02$ m, (b) $l_a = 0.04$ m; (c) Nominal strength versus sample size for different correlation length (from Grassl and Bažant, 2009).

Lattice failure becomes more gradual with the presence of heterogeneity as not all the links fail at the same time. The use of irregular lattice network is analogous to a percolation-type heterogeneity in spring or beam lattice modelling. RFM is suitable for modelling of progressive damage evolution in quasi-brittle material (Alava et al., 2006) but ductile fracture of heterogeneity material has been modelled by using ductile random fuse model (DFRM) which is able to accumulate plastic deformation before failure (Picallo et al., 2010).
RFM is used to study the trend or phenomenon of fracturing in heterogeneous material rather than giving accurate prediction. Despite its simplicity, RFM simulations have been demonstrated to be very similar to more complicated Lattice Spring Model (LSM) (central force models) (Nukala et al., 2005) and lattice beam model (Herrmann et al., 1989). With the advancement of high-performance computing, 3D FRM has also been developed (Nukala et al., 2007; Zapperi and Nukala, 2006).

From large amount of RFM simulations carried out, different scaling laws are derived among different parameters such as damage density, fracture strength, acoustic emission, avalanches of local failure (e.g. number of failure lattice at one time) characterised by a system length \( L \) that represents the fineness of mesh. They are usually in the form of power law relationship with \( L \) (i.e. \( \propto L^\xi \)) and studies are focused on the comparison of exponent \( \xi \).

Also, damage accumulated prior to fracture follows Gaussian distribution, meaning the absence of long-range correlations. The strength distribution of model is found to be lognormal with size effect to the average strength, which is different from commonly used Gumbel distribution or Weibull distribution based on 'weakest-link' approach (Zapperi and Nukala, 2006).

![Fig. 3.19 Study of morphology of fracture using RFM](image)

(a) RFM simulation of a crack in triangular lattice of size \( L = 1024 \) and (b) the distribution of crack width for diamond and triangular lattices showing a lognormal distribution (shown by dashed line) (from Zapperi et al., 2005)

RFM has been used to analyse the morphology of fracture surface (i.e. roughness) in 2D (Hansen et al., 1991; Räisänen et al., 1998; Seppala et al., 2000; Zapperi et al., 2005) (Figure 3.19) and 3D (Batrouni and Hansen, 1998; Raisanen et al., 1998) by applying different kinds of heterogeneity. Crack surface is found to be self-affine in FRM simulations which is also
observed in experiments (Balankin and Sandoval, 1997). Scaling laws obtained from RFM simulations of heterogeneity material matches with the observation on the Earth’s crust as well (Girard et al., 2010), such as a power law distribution of earthquake energies (Gutenberg and Richter, 1956) and fractal clustering of hypocenters (Kagan, 2007).

### 3.10.4 Linear elasticity and lattice type

RFM is a scalar model in which local equilibrium and global stability cannot be guaranteed. More realistic tensorial models have been proposed. The simplest one is RSM that provides a central force system where nodes are connected by elastic springs.

It has been demonstrated in many literatures that a regular lattice network can represent a linear elasticity material in continuum mechanics, provided that lattice elements are also linearly elastic. Quantities such as stress tensor \( \sigma_{ij} \), strain tensor \( \varepsilon_{ij} \) and stiffness tensor \( C_{ijkl} \) can be derived from lattice geometry and constitutive relationship of lattice element.

Relationship between macroscopic parameters such as elastic modulus and spring parameters can be established. The standard technique is by equating the strain energy stored in a unit cell in lattice network to a continuum of the same volume. The derivation can be referred to (Ostoja-Starzewski, 2002) for 2D and (Wang and Mora, 2008) for 3D.

**Springs Elements**

The most simple element is Hookean spring that provides a central force interaction between 2 neighbourhood cells. For a regular triangular lattice of identical Hookean springs, it can be shown that the lattice is equivalent to a linear elastic isotropic material with \( \nu \) fixed at 1/3 for 2D case. For irregular lattice, \( \nu \) obtained closes to 1/3 (Jirásek and Bažant, 1994).

In Kirkwood spring model, rotation springs of rotational stiffness \( k_\phi \) are added at each node. The rotational springs do not affect the bulk properties. The Poisson’s ratio can be adjusted between 1/3 to -1 by adjusting the ratio \( \phi = k_\phi / (k_n l^2) \) where \( l \) is lattice length. Furthermore, Day et al. (1992) suggested to assign a three spring system with spring constants \( k_\alpha, k_\beta \) and \( k_\gamma \) in a special manner such that higher Poisson’s ratio from 1/3 to 1 can be modelled while preserving the isotropy of material. This is called triple honeycomb lattice as it is an overlay of three honeycomb lattice networks. Recently, Zhao et al. (2011) proposed distinct lattice spring model that included a normal spring and a multibody shear-type spring between two nodes. By using local strain-based technique rather than node displacement in calculating spring deformation, a full range of Poisson’s ratio of elastic solid can be modelled and rotational invariance can be preserved. High order model has been developed (Zhao and Zhao, 2012) for higher accuracy simulation.
Beam elements

The above models are called central force models. A popular non-central force model called Born spring model (Hassold and Srolovitz, 1989) has often been used in lattice model in which a shear spring $k_s$ is provided to penalise the rotation of spring. Poisson’s ratio can be adjusted between -1 and 1/3 by varying the ratio of normal to shear spring stiffness $\alpha = k_s/k_n$. However, the rotation invariance of the model cannot be preserved.

Beam elements that can resist axial force, shear force and bending moment have been used as lattice element as well. Additional DOFs for rotation are required. In 2D case, 3 DOFs are required (2 translation and 1 rotation) and 6 DOFs (3 translation and 3 rotation) for 3D case. For Euler-Bernoulli beam model, the axial stiffness $k_n$ and shear stiffness $k_s$ are given by $EA/l$ and $12EI/l^3$ respectively where $A$ and $I$ are area and second moment of area of beam cross section. For more general Timoshenko beam model, shear deformation of beam is considered and the shear stiffness of beam is modified as $k_s = 12EI/[(1 + b)l^3]$ where $b = 12EI/(GA_s l^2)$ and $A_s$ is shear area of cross section. For Timoshenko beam model with low shear stiffness (i.e. $b \to 0$), it reduces to Euler-Bernoulli beam model. The Possion ratio $\nu$ is control by the ratio of axial to shear stiffness of beam $\alpha = 12I/[Al^2(1+b)]$ but only $\nu \leq 1/3$ can be modelled.

In 3D, the maximum Possion’s ratio of lattice models of spring or beam can be achieved is reduced to 1/4. For the equivalent macroscopic elastic parameters from microstructure lattice properties for regular lattice in 3D, Wang and Mora (2008) is referred.

3.10.5 Lattice failure criteria

The most simple constitutive relationship of a lattice element is elastic-brittle for Hookean spring which has been extensively used in RSM. For 3D case, Hookean spring is more often used (Affes et al., 2012; Man and van Mier, 2011; Zhao et al., 2011). The lattice is removed when the microscopic axial stress $\sigma_{sn}$ reaches a specified microscopic tensile strength $f_{st}$.

$$\sigma_{sn} \geq f_{st}$$

(3.4)

$\sigma_{sn}$ can be calculated simply by dividing lattice axial force $F_n$ to area of facet $A_f$, i.e. $\sigma_n = F_n/A_f$. Wang et al. (2009b) did not consider the effect of bending in failure criteria, so the tensile stress in a beam element is the same as the Hookean’s spring one.

If beam model is used, the failure criteria become more complicated. A beam element can have all axial force $F_n$, shear $F_s$ (2 shear forces for 3D case) and bending moment $M_b$
(torsional $M_n$ and two out of plane bending $M_u$ and $M_v$ for 3D case). For the contribution of moment, different formula can be used.

Based on Tresca’s or von Mises’s general yielding criteria, the following lattice failure criterion was proposed by De Arcangelis et al. (1989):

$$\left( \frac{\sigma_n}{f_{st}} \right)^2 + \frac{\max(|M_i|, |M_j|)}{M_t} \geq 1 \quad (3.5)$$

where $M_t$ Threshold for lattice moment
$M_i, M_j$ Moments at nodes $i$ and $j$

From Schlangen and van Mier (1992)

$$\frac{F_n}{A_f} + \alpha_b \frac{\max(|M_i|, |M_j|)}{S_f} \geq f_t \quad (3.6)$$

where $\alpha_b$ dimensionless value accounting the effect on bending
$S_f$ Section modulus of facet represented by lattice

In modelling concrete fracturing, Schlangen and van Mier (1992) first took an arbitrary value $1/3$ for $\alpha_b$. Later, literatures have reported the use of a much smaller $\alpha_b$ value of 0.005 (Chiaia et al., 1997; Lilliu and van Mier, 2003; Liu and Liang, 2009; Prado and van Mier, 2003). It is not taken as zero as they observed that a small $\alpha_b$ value gave more realistic macroscopic load displacement curve and crack mechanism that matched experimental results.

For 3D lattice beam, Lilliu and van Mier (2003) proposed the following formula

$$\frac{F_n}{A_f} + \alpha_b \frac{\sqrt{M_u^2 + M_v^2}}{S_f} \geq f_{st} \quad (3.7)$$

The torsional moment $M_z$ was ignored. They tried a range of $\alpha_b$ from 0 to 0.005 and found that $\alpha_b$ was not sensitive to the result, so $\alpha_b = 0$ was used.

The above criteria do not consider the contribution of shear. Chang et al. (2002) proposed a criterion considering the combined effect of tension and shear.

$$\frac{\sigma_{sn}}{f_{st}} + \frac{|\sigma_{ss}|}{f_{ss}} \geq 1 \quad (3.8)$$
where $\sigma_s$ is microscopic shear stress which is given by $\sigma_s = F_s/A_f$ and $f_{ss}$ is microscopic shear strength. Bolander et al. (2001) proposed crack band model using RBSN model that resultant stress from axial force and shear forces is greater than $f_{st}$

$$\frac{F_R}{A^P} \geq f_{st}$$

(3.9)

where $F_R$ is the resultant translational forces of lattice and $A^P$ is the projected area of facet perpendicular to the direction of $F_R$. This criterion has also been applied to 3D RBSN model as well (Berton and Bolander, 2006). The RBSN model will be covered in more detail later in the next Chapter.

Wang et al. (2000) formulated a criterion that considered the combined effect of all axial force, shear force and moment of lattice

$$\frac{F_n}{F_{tn}} + \frac{|F_s|}{F_{ts}} + \frac{|M_b|}{M_{tb}} \geq 1$$

(3.10)

where $F_{tn}$ Threshold for lattice tensional force

$F_{ts}$ Threshold for lattice shear force

$M_{tb}$ Threshold for lattice bending moment

Mohr-Coulomb failure criterion was also adopted (Bolander and Saito, 1998; Kikuchi et al., 1992).

$$f_{ss} = c_f + \sigma_n \tan \theta_f$$

(3.11)

where $c_f$ cohesion

$\theta_f$ frictional angle

with the tension cut-off, the failure criterion becomes

$$\max \left( \frac{\sigma_n}{f_{st}}, \frac{\sigma_s}{f_{ss}} \right) \geq 1$$

(3.12)

Grassl and Jirasek (2010) proposed an elliptic stress envelop defined by microscopic tensile strength $f_{st}$, microscopic shear strength $f_{ss}$ and microscopic compressive strength $f_{sc}$.

Besides stress or force based failure criteria as proposed above, energy criterion was also proposed (Hassold and Srolovitz, 1989). Lattice fails when total potential energy of lattice reaches a threshold.
The above models assumed all springs (axial, shear and rotational) in a lattice fail at the same time once a single criterion is met. Different kinds of spring can have separate failure criteria and break separately (Zhao et al., 2011, 2012).

### 3.10.6 Post peak behaviour

For many LEM models, elastic-brittle lattice model is used that lattice satisfying the failure criteria is removed without any residual stiffness (Figure 5.1, curve a). This simple constitutive law is adopted for most of the statistical modelling of fracturing like RFM and RSM. For beam elements, only elastic-brittle constitutive relationship is found in the literature from the knowledge of the author.

Different constitutive laws have been proposed to describe the post peak behaviour of lattice element. By introducing a post peak behaviour, lattice can withhold certain amount of stress after reaching its yield stress. The stiffness of spring successively degrades afterwards until a larger failure strain is reached.

Elastic-perfectly plastic model (Figure 5.1, curve b) are used for fuse element in RFM (Hansen et al., 1991) and spring element (Seppala et al., 2000) in RSM.

The linear softening model (Figure 5.1, curve c) has been commonly used to model the cohesive zone or FPZ ahead of fracture tip (Jirásek and Bažant, 1994; Karihaloo et al., 2003; Mihashi, 1994; Spagnoli, 2009). Residual stress modelled the behaviour of cohesive FPZ in which material softens before the crack is fully opened. A microscopic yielding strain \( \varepsilon_{st} \) and a microscopic failure strain \( \varepsilon_{sf} \) are required to define a linear softening model. The ratio \( \gamma_{sf} = \varepsilon_{t}/\varepsilon_{f} \) is called micro-ductility (Jirásek and Bažant, 1994). When \( \gamma_{sf} = 1 \), it corresponds to elastic-brittle model while \( \gamma_{sf} \to \infty \) corresponds to elastic-perfectly plastic model. Such constitutive laws are applied to linear elastic spring model.

Bilinear softening constitutive law (Figure 5.1, curve d) which was first proposed by Petersson (1981) is commonly used to model the post peak strain softening of concrete as a quasi-brittle material (Bazant, 2002; Berton and Bolander, 2006; Bolander and Sukumar, 2005; Bolander et al., 2001). Yield strain and failure strain are needed to be specified. The shape of the softening curve can be obtained from a deformation controlled uni-axial tension test (Prado and van Mier, 2003).

Exponential softening (Figure 5.1, curve e) which was proposed by Hillerborg et al. (1976) was also used to model concrete by 2D RBSN (Grassl et al., 2012; Grassl and Jirasek, 2010; Grassl et al., 2014; Gregoire et al., 2015) and hydraulic fracturing simulation for quasi-brittle material using RBSN model in 2D (Grassl et al., 2015) and 3D (Grassl and Bolander, 2015).
Fig. 3.20 Different constitutive law modelling post peak behaviour of lattice. Stress-strain ($\sigma$-$\varepsilon$) law: (a) brittle, (b) perfectly plastic, (c) linear softening, (d) bilinear softening and (e) exponential decaying law.
Crack band theory (Bazant and Oh, 1983) has been used extensively to obtain the parameters required to define softening curves in modelling concrete fracturing. Fracture properties can be characterised by three material parameters, fracture energy $G_F$, uniaxial tensile strength $f_t$ and width of FPZ $l_{FPZ}$ which can be determined by experiments.

### 3.10.7 Fluid coupling and hydraulic fracturing simulation

The development of hydraulic fracturing simulation by LEM is primitive, especially full coupling between solid and fluid. There is a few literatures about solid-fluid coupling using LEM.

Holtzman and Juanes (2010) used a so-called block-spring network to study the displacement of one fluid by another (multi-phase flow) in a porous media. As illustrated in Figure 3.21, the skeleton of porous media was modelled by a square lattice of Hookean’s springs and the fluid flow was modelled by a pore-pipe model. Disorder was applied by varying the diameter of pores and the diameter of pipes that relates to their permeabilities. Hydro-mechanical coupling was achieved by changing pipe diameters due to the deformation of solid lattice network. This simple block-spring network was capable to simulate three different regimes of flow pattern that are observed in experiments.

Zhao and Khalili (2012) also used a similar model to stimulate behaviour of saturated soil. Coupling between soil skeleton and pore water was done by poroelasticity theory of Biot (1941).

Several literatures (Grassl, 2009; Grassl and Bolander, 2016; Grassl et al., 2015) reported the use of dual lattice network to model fluid mass transport in quasi-brittle material. As illustrated in Figure 3.23, structural deformation is modelled by a lattice network generated by Delanuay triangulation and mass transport is modelled by edges of Voronoi cell. Grassl (2009) modelled fluid flow in cracked concrete. Grassl et al. (2015) modelled hydraulic fracturing of a thick wall cylinder assuming fluid flow and mechanical deformation were not coupled. Grassl and Bolander (2016) extended the dual lattice network to 3D for mass transport in porous medium. Fluid flow along fracture was coupled with a mechanical lattice. Fracturing was induced by external force rather than fluid pressure.

Fully coupled hydraulic fracturing using LEM is reported by Wong et al. (2015). They performed a large scale 3D simulation for fluid injection in a fault. Lattices are modelled by normal Hookean’s springs. Rock was assumed impermeable and fluid flow in fracture was modelled by the cubic flow law.
Fig. 3.21 Block spring model for simulation of multi-phase fluid flow in disordered porous medium (a) Schematic of block-spring model and (b) simulation result of an inviscid non-wetting fluid injection at the center displacing a viscous wetting fluid (from Holtzman and Juanes, 2010).

Fig. 3.22 Hydraulic fracturing of thick wall porous cylinder (from Grassl et al., 2015).
Fig. 3.23 Dual lattice network for coupling of fracture and mass transport in quasi-brittle geomaterial. (a) Mechanical lattice and (b) fluid transport lattice (from Grassl et al., 2015).
3.11 Conclusion

3.11.1 Summary of numerical methods

The potential of different numerical methods in handling challenges in hydraulic fracture simulation is summarised here. The challenges considered are explicit modelling of fracture, including non-planar one, modelling rock as a heterogeneous material, ability of full coupling of multi-physics processes, modelling complex fracturing process, interaction with existing fractures and computational performance for multi-scale simulation.

**FEM**  
FEM is the most mature field in numerical modelling and has developed for multi-physics and multi-phase simulation. As a continuum model, the major limitation lies on the explicit modelling of fracture. Fractures have to conform with mesh, leading to mesh dependency issues. As a result, fracture path has to be pre-defined that limits the ability to model complex fracturing and fracturing in 3D. Very fine mesh is required to model the singular stress at crack tip. Adaptive meshing is required to refine the mesh when crack tip propagates. The computation cost is therefore very expansive. As a continuum model, heterogeneity in local scale cannot be conveniently modelled.

**XFEM**  
XFEM solves the major limitation of FEM on mesh dependency issue by allowing fracture paths to cross an element. More complex fracture, such as non-planar and interacting fractures can be modelled. However, some of the limitations of FEM and other continuum based numerical methods cannot be resolved such as modelling fracture initiation and fracture coalescence. Because of the use of enrichment functions, heterogeneity is more difficult to be modelled compared with FEM. The computational performance is better than FEM but still high for simulation of solid-fluid coupled problem.

**BEM**  
The major advantage of BEM is reducing the dimensions of problem by one. This substantially reduces number of DOFs of a model and allows 3D large scale simulation. There is no mesh dependency problem. Since the domain is not discretised, the heterogeneity inside the domain cannot be modelled. Same as other continuum based numerical models, fracture initiation and complex fracturing process cannot be handled.

**DFN**  
DFN gives realistic representation of fractured rock mass in field scale. It is developed for reservoir engineering and hydro-geology. Only fractures are modelled so hydro-mechanical coupling is ignored. DFN need to be coupled with other models, such as block-
3.11 Conclusion

DEM and BPM for a coupled simulation. The ability to model fracturing propagation and heterogeneity of rock depend on the coupling models with DFN.

**DEM-particle based (BPM)** BPM is a discontinuum model that can simulate complex fracturing process and interaction among fractures. Fracture path does not input as *a priori*. Large deformation and fragmentation can be modelled. The major limitation is modelling rock as a assemblage of circular disks or spheres that is only suitable for highly porous rock. The morphology of crack cannot be represented by pores and particles in a solid rock with low porosity. As a result, fracture flow cannot be properly modelled. Heterogeneous can be easily be modelled by assigning PDFs on microscopic parameters. Model parameters need to be calibrated to match with macroscopic response. BPM is computationally expensive, in particular a wide range of particle diameters is modelled or heterogeneity is applied to spring and bond parameters.

**DEM-block based/DDA** DDA is similar to DEM block based model. The model is solved implicitly for the former and explicitly for the latter. Unlike BPM, they model solid rock without pores by tessellation of the domain into blocks. It is suitable for large deformation problems as blocks can detach and establish new contact with another blocks. Unlike BPM, fractures are well defined and fluid flow can be properly modelled and coupled with solid blocks. However, fractures can only form at the interface of blocks so complex fracturing cannot be handled unless large number of blocks are used for simulation. Block type DEM is computationally more expensive than BPM due to complex contact detection.

**LEM** LEM has been developed in statistical physics to study fracturing in heterogeneous material. Heterogeneity can be introduced in different ways, such as applying PDFs in lattice parameters, percolation, putting structures like voids and intrusion in lattice models. Mesh dependency can be overcome by using disordered lattice network or introducing heterogeneity. Fracturing is modelled in a straight forward way and realistic morphology of fracture can be simulated. Fracture initiation and complex interaction of fractures can be modelled which can be only achieved by particle based DEM.

LEM has the flexibility to apply different constitutive laws for lattice and it can be done easily. This means that some microscopic parameters need to be calibrated but the relationships between microscopic parameters and macroscopic response are easier to be established compared with particle type DEM. The neighbourhood is fixed in LEM that eliminates computationally expensive contact detection. However, under this assumption, LEM is applicable for small displacement problems including hydraulic fracturing. Large deformation problems
and rock fragmentation cannot be modelled. The computation performance is the best among other numerical methods so 3D multi-scale simulation can be done. Geometry of fracture is well-defined which allows full hydro-mechanical coupling for fluid flow in fracture. The computation performance for hydraulic fracturing simulation can be further enhanced if fluid flow is modelled by lattice model as well which is introduced in Chapter 6.

3.12 Comparison of discontinuum approaches

This Chapter reviews several discontinuum methods in rock mechanics - DEM (particle based or block based), DDA, DFN and LEM. Particle type DEM is first used to model the granular material like sand and each grain is modelled by a particle. Rock is treated as particles that are bounded one another so it is called Bounded Particle Model (BPM). DDA is the implicit form of block type DEM. LEM is regarded as a simplified version of DEM that assumes small displacement between elements so that the neighbourhood of cells are fixed.

Discontinuum approaches recognise rock as heterogeneous material and discontinuities (fractures, joints and fissures) play an important role in mechanical and hydraulic properties of rock.

DFN only models the fluid transportation in fractured rock and mechanics of the rock is ignored. In order to consider the change of fracture aperture due to the mechanical deformation of rock and, DFN needs to couple other discontinuum methods. So, only DEM, DDA and LEM are compared in this section.

3.12.1 Model set-up

![Fig. 3.24 The change of contact during the shear of two agglomerates in BPM. Green dot denotes contact between two](image)

BPM models rock as an assemblage of spheres or cylinders (particles). It is suitable for porous sandstone which is formed by the cementation of sand grains. BPM is also used
for modelling laboratory test of intact rock sample in which micro-structures are implicitly modelled. For natural rock, joint sets tessellate the rock into blocks. Blocks can modelled by lumping particles using unbreakable bounds to form agglomerates. This is a common technique for more realistic modelling of soil grains and for the modelling of soil grain crushing.

Realistic modelling of discontinuities in rock is a great challenge. Agglomerates do not model well the blocks tessellated by discontinuities. Agglomerates have bumpy surfaces but surfaces of rock blocks are mostly planar. In Figure 3.24 showing the shearing of two amalgamates in BPM, the contact points between amalgamates change with the shear displacement. So, the ‘contact stiffness’ between two amalgamates can change rapidly with displacement.

Block type DEM and DDA explicitly tessellate the rock mass by discontinuities. Unlike BPM that there is one type of contact - particle to particle, the contact between blocks is more complicated. The contact between two blocks can be: (1) vertex to vertex, (2) vertex to edge, (3) vertex to surface, (4) edge to edge, (5) edge to surface and (6) surface to surface. Different constitutive laws are required to model different types of contact. Overlap between blocks is allowed and the contact force is proportional to the overlapping area. Another difficulty is distinguishing between normal force and shear force in which different constitutive laws apply. The applications of block type DEM and DDA focus on large deformation problem where the kinematics of blocks is important. The modelling of contact that governs a much smaller displacement is often roughly estimated.

In BPM, particles are rigid and the deformation of amalgamates solely comes from contact springs between particles. For block type DEM and DDA, blocks can be either rigid or deformable. Deformable blocks are modelled by FEM elements.

For LEM, the material can be tessellated into cells by discontinuities. There is only face to face contact between cells. The contact force between cells are modelled by lattice elements. Lattice elements can model the deformation solely from discontinuities or the combined deformation from cells and discontinuities.

### 3.12.2 Model parameters

To set up a BPM, parameters for constitutive laws of contact and the breaking threshold of bond are required. The breaking threshold is related to the particle size (Potyondy and Cundall, 2004). Because particles are used to model rock which cannot mimic the actual geometry of blocks, the model parameters may not bear any physical meaning. The model parameters are determined by calibration.
For block type DEM and DDA, spring stiffness between contact type does not affect much in the determination of kinematics of blocks. For hydraulic fracturing in which fracture aperture is important, the contact between block has to be restricted to surface to surface only. An appropriate joint model should be applied to fracture surface. For the strength parameters, Mohr-Coulomb criterion is often used.

### 3.12.3 Computation

Both BPM and block-type DEM are explicit methods. The DDA can be regarded as implicit form of block-type DEM. Although DDA is an implicit method, a time step is still required but the time step selected can be longer than BPM. The computation effort of block type DEM is more expensive than particle type BPM because of more complex contact detection.

LEM can be an implicit method or an explicit method. Implicit method is often used for quasi-static that often gives better computational performance.

### 3.13 Research gap and directions

Most of the theoretical studies on different physical process involved in hydraulic fracture and their interactions are based on the assumptions that rock is homogeneous and can be treated as a continuum. Some experimental studies and recent numerical studies demonstrate the significant influence on the heterogeneity from natural fractures. So, the recent trend of hydraulic fracturing research is the understanding on natural fractures considering the effects on the heterogeneity of rock.

The effect of existing fracture on hydraulic fracturing are studied by simulations using different numerical methods. Discontinuum numerical methods have caught attention in modelling heterogeneous material.

There is a lack of research focusing on the multi-scale nature of discontinuities, especially using three-dimensional model. To model a big model to include many discontinuities, a computationally efficient numerical method is required. LEM is a promising discontinuum numerical method for this purpose.

Therefore, this thesis examines the three-dimensional modelling of fracturing processes using LEM. An efficient coupling scheme of a solid lattice and a fluid lattice, called Dual Lattice Model (DLM) is proposed for hydraulic fracturing simulation.
Chapter 4

Lattice Element Method

Lattice Element Method (LEM) is proposed in this thesis to model heterogeneous rock for hydraulic fracture simulation. Mesh dependency issue is minimised by using disordered lattice network. Rigid Body Spring Model (RBSM) is proposed for lattice model and its formulation is covered. Computation performance is one of the major advantages of LEM which is critical for 3D simulations.

A C++ code named LEM3D is developed and validated by modelling a cantilever beam under lateral load. Statistical analyses on lattice network are presented to understand the characteristic of different lattice models. The micro-macro relationships of LEM are explored by parametric studies. Finally, the stress heterogeneity is studied in both nodal and facet levels. This Chapter also studies the behaviour of lattice model if heterogeneity is applied to lattice model parameters.

4.1 Proposed LEM formulation

In this thesis, a disordered lattice network is proposed for LEM simulation. Voronoi tessellation and Delaunay triangulation are used to construct a lattice network from random nodes. Some statistical analysis on lattices and cells are carried out.

Rigid Body Spring Model (RBSN) is proposed to model lattices and their model parameters are derived from geometrical properties of cells and lattices. The formulation of RBSM is covered in this Section.

4.1.1 Disordered lattice network generation

One of the major issues in mesh generation is mesh dependency of fracture path as illustrated in Figure 4.1. For regular lattice, fracture path is only allowed in several orientations. To
Fig. 4.1 Illustration of mesh dependency for a notched sample under uniaxial tension. Regular triangular lattice is used. Only three orientation are allowed for fracture to propagate. Fracture path deviates from theoretical horizontal path by 60°. (Wong et al., 2014)
conform the lattice geometry, the fracture path may deviate from its correct path. In FEM, this is tackled by either pre-defining the fracture path or using adaptive re-meshing which is difficult to be implemented and is only possible for simple fracture propagation.

To minimize the effect of mesh dependency, a disordered mesh is used. This is simple to implement and introduces local heterogeneity in the model which reflects rock in nature with a scale related to local heterogeneity. For an isotropic rock, lattice orientations are uniformly distributed such that lattice breakage is not favoured in certain orientation. For anisotropic rock, the lattice orientation can be biased to a weaker orientation such that fractures are more easily formed along that orientation.

To generate a disordered lattice network, 3 processes are involved: random node generation, Voronoi tessellation and Delaunay triangulation as illustrated in Figure 4.2.

**Random node generation**

This process generates nodes that fill up the domain with the constraint that separation between any two nodes is greater than a specified value \( l_{\text{min}} \). It is an analogy of putting spheres into a domain with diameter \( l_{\text{min}} \) without overlapping one another. Trial node is first generated with coordinates from a pseudo-random number generator. Distances between the trial node and nodes already in the domain are checked. The trial node is rejected if the minimum distance criterion is not fulfilled.

To speed up the checking of minimum distance criterion, partitioned domain search (Greengard and Rokhlin, 1987) is used to limit the number of nodes subjected to distance checking.
Fig. 4.3 (a) Relationship between node density $n$ and normalised limit of successive rejection of trial node $N_{rej}/N_{HCF}$ for different fineness of cubic model of size $L$ with $L/l_{min} = 50$ and $L/l_{min} = 100$. Voronoi cells generated by (b) high node density ($n \approx n^*$) and (c) low node density $n \rightarrow n^*$ in 2D.
The density of node is expressed as the fraction \( n = N/N_{HCP} \) where \( N \) is the total node number and \( N_{HCP} \) is the node number corresponding to the closest possible packing of equal spheres (i.e. Hexagonal Close Packing (HCP)).

The node generation stops when the number of node reaches a desired value or the number of successive rejection of trial node has reached a specified limit \( N_{rej} \). When a domain is filled with more and more nodes, the likelihood of a random trial node to be placed reduces. The domain is called saturated when it cannot accept any more nodes (\( n \to n^* \) when \( N_{rej} \to \infty \)). The relationship between \( n \) and \( N_{rej} \) is shown in Figure 4.3a. The practical \( n^* \) can be achieved is approximately 0.533 (with \( N_{rej}/N_{HCF} = 2000 \)). When \( n \to n^* \), nodes are uniformly distributed and cells generated by Voronoi tessellation are more regular compared with model with low node density.

Fig. 4.4 Illustration of lattice model with different node density. (a) D10 model \((n = 0.5)\), (b) M10 model \((n = 0.25)\) and (c) S10 model \((n = 0.1)\)

In this thesis, three different node densities are used: \( n = 0.1, 0.25, 0.5 \) which are denoted as Dense (D), Medium (M) and Sparse (S) models respectively. The examples of these three models are illustrated in Figure 4.4.

**Voronoi tessellation**

Using the random node generated, Voronoi tessellation is carried out for partitioning the domain into convex polyhedrons. Each node corresponds to one polyhedron (cell). For a set of nodes in a domain, the tessellation is defined by associating a cell of space \( V_i \) to each node \( x_i \), that corresponds to the section of the domain which is closer to that point than any other \( x_j \) such that

\[
V_i = V(x_i) = \bigcup_{i \neq j} \{ x | d(x_i, x) \leq d(x_j, x) \} \quad (4.1)
\]
where $x_i$ are the coordinates of point $i$; $d(x_i, x)$ is the distance between point $i$ and a location with coordinates $x$ and $j$ counts all the points except $i$.

The facet of the Voronoi diagram is a plane that is equidistant to the two nearest nodes. Each cell is obtained from the intersection of half-spaces partitioned by these facets and hence it is a convex polygon. The vertices of Voronoi cell are the points equidistant to three (or more) nodes.

**Delaunay triangulation**

A lattice network is generated by Delaunay triangulation of nodes. The Delaunay triangulation is the dual graph of Voronoi diagram. Delaunay triangulation maximizes the minimum angle of all the angles of triangles such that skinny triangles can be avoided. It has been widely used in mesh generation for FEM.

A lattice is formed between two neighborhood nodes. It also corresponds to a common facet of two neighborhood cells. The lattice properties are also scaled with the geometrical properties of facet which is discussed later. There are small number of facets which have very small area. The lattices with corresponding area of facet smaller than a threshold $\varepsilon_A l_{\text{min}}^2$ are rejected. $\varepsilon_A$ is set to be $10^{-4}$ for all models presented in this thesis, which accounts for about 2% of rejection of lattice.

**4.1.2 Generation of pre-existing fracture**

Figure 4.5 illustrates the generation of a pre-existing fracture in a lattice model. The node generation consists of two stages. Special nodes with a pattern determined by the geometry of fracture are first generated. For a planar fracture, the nodes can be in a square or rectangular grid with an offset from the fracture. After Voronoi tessellation, a planar facet surfaces that match the fracture geometry are formed. The separation between these special nodes should be smaller than $l_{\text{min}}$.

Random nodes are then generated as described in Section 4.1.1 (i.e. keeping separation of nodes to be greater than $l_{\text{min}}$). Since the spacing between special nodes is less than $l_{\text{min}}$, these random nodes do not interfere in the geometry of the fracture surface generated. Voronoi tessellation and Delaunay triangulation are carried out. Finally, the lattices corresponding to the pre-existing fracture are removed by assigning zero stiffness to them.
4.1 Proposed LEM formulation

Fig. 4.5 Illustration of the generation of a pre-existing fracture in lattice model.

(1) Generation nodes with regular pattern for pre-existing joint geometry
(2) Generation of random nodes
(3) Voronoi tessellation
(4) Delaunay triangulation
(5) Assign zero stiffness to lattices corresponding to the pre-existing joint
4.1.3 Statistical analysis on lattice network

The geometrical properties of a lattice network can be controlled by node density $n$. It can be considered as a parameter governing the geometrical heterogeneity of a lattice network. The fineness of the lattice does not affect the geometry of lattice.

The PDFs of lattice length are shown in Figure 4.6a. For the lattice length distribution, dense lattice models ($n \to n^*$) shows a vertical asymptote to $l_{\text{min}}$. It shows uniform distribution between $0.5$ and $1.5\ <l_l>-l_{\text{min}}$ (where $<\cdot>$ denotes mean value) and the population of the longer lattice starts to decline. When $n \to n^*$, the PDF stops at $2l_{\text{min}}$ because an additional node can be inserted between two nodes with separation greater than $2l_{\text{min}}$ to create a more dense model. Sparse models do not show the asymptote towards $l_{\text{min}}$. For $n \ll n^*$, node can be placed quite freely with minimal restraint by $l_{\text{min}} < l_l$ requirement, so $l_l$ shows a normal distribution when $n$ is sufficiently small.

For the distribution of lattice facet area $A_{\text{lattice}}$ shown in Figure 4.6b, all the lattice model shows the asymptote to $y$-axis because Voronoi tessellation generates a lot of very small facets. Some of them are eliminated by rejection of facets smaller than a tolerance $\varepsilon A_{l_{\text{min}}}^2$. However, these small facets do not affect much on the overall mechanical and hydraulic properties of lattice network.

Regarding the statistics on nodes, Figure 4.6c shows the distribution of volume of cell $V_{\text{cell}}$. A dense model shows a shorter tail and has less spread. The distribution of $n = 0.5$ model is similar to $n \to n^*$ model.

For the cell sphericity $\Psi_{\text{cell}}$ which is defined as

$$\Psi_{\text{cell}} = \frac{\pi^{1/3}(6V_{\text{cell}})^{2/3}}{\sum A_{\text{lattice}}}$$

(4.2)

$\Psi_{\text{cell}}$ has a range from 0 to 1 and $\Psi_{\text{cell}} = 1$ corresponds to a perfect spherical cell. A tetrahedron cell and cubical cell has a value $\Psi_{\text{cell}}$ of 0.671 and 0.806 respectively. Similar to $V_{\text{cell}}$, $\Psi_{\text{cell}}$ shows skewed distribution towards the left as illustrated in Figure 4.6d. Dense lattice models are composed of more spherical cells ($<\Psi_{\text{cell}}>$≈ 0.87) and are closer to the normal distribution with smaller spread while sparse model are composed of more angular cells ($<\Psi_{\text{cell}}>$≈ 0.81) and show longer tail.

For disordered lattice network generated by different $n$, coordination number $n_{\text{coord}}$ has a mean of 15.1 and decreases slightly with $n$. This is close to the value $<n_{\text{coord}}>$≈ 15.54 reported by Meijering (1953). For regular packings, the coordination numbers of HCF, BCC and simple cubic are 12, 8 and 6 respectively. The high coordination number of disordered lattice network is due to the presence of lattice with small area. $n_{\text{coord}}$ can vary from 7 to 28 and the spread of $n_{\text{coord}}$ increases with decreasing $n$. 
4.1 Proposed LEM formulation

Fig. 4.6 Lattice statistics in disordered lattice network against $n$. (a) Lattice length $l_{\text{lattice}} - l_{\text{min}} / \langle l_{\text{lattice}} - l_{\text{min}} \rangle$. Open circle indicate the location of $2l_{\text{min}}$ in PDF. (b) Lattice facet area $A_{\text{lattice}} / \langle A_{\text{lattice}} \rangle$, (c) node volume $V_{\text{cell}} / \langle V_{\text{cell}} \rangle$ and (d) cell sphericity $\Psi_{\text{cell}}$. (e) Coordination number $n_{\text{coord}}$ and (f) $\langle n_{\text{coord}} \rangle$ and $\langle \Psi_{\text{cell}} \rangle$. 
4.1.4 Generation of pre-existing fracture

4.1.5 Rigid Body Spring Model

The interaction between cells is modelled by Rigid Body Spring Model (RBSM), as first proposed by Kawai (1978). The formulation of 3-dimensional cases was developed by Kikuchi et al. (1992) and Berton and Bolander (2006). In RBSM, cells are assumed to be rigid, and the deformation solely comes from the interface between cells (facets). Deformation at facet is resisted by 3 translational springs and 3 rotational springs at its centroid. The local axes $n$-$s$-$t$ are defined by normal direction ($n$) and two principal directions ($s$ and $t$) of facet.

The axial spring stiffness $k_n$ is given by

$$k_n = \frac{E_{\text{micro}}A_{ij}}{h_{ij}} \quad (4.3)$$

where $E_{\text{micro}}$ is the microscopic Young’s modulus, $A_{ij}$ is the area of common facet of node $i$ and $j$ and $h_{ij}$ is the distance between node $i$ and $j$. $E_{\text{micro}}$ is different from the macroscopic Young’s modulus $E$ of the entire model. This will be further discussed in the next section.

The shear spring stiffness $k_s$ is given by

$$k_s = \alpha k_n \quad (4.4)$$
where parameter $\alpha$, the ratio of stiffness between axial spring and shear spring, is introduced which is studied in the coming sections. The stiffness of three rotational springs are given by

$$k_{\phi n} = \frac{\beta E_{\text{micro}} J_p}{h_{ij}}, \quad k_{\phi s} = \frac{\beta E_{\text{micro}} I_{11}}{h_{ij}}, \quad k_{\phi t} = \frac{\beta E_{\text{micro}} I_{22}}{h_{ij}}$$

(4.5)

where $J_p$ is the polar second moment of area of facet and $I_{11}$ and $I_{22}$ are the two principal moments of area of facet. An additional parameter $\beta$ is introduced to modify the contribution of rotational springs.

The relationship between the generalised spring displacement $d$ and the generalised nodal displacement $u$ is given by a $6 \times 12$ matrix $B$

$$d = Bu$$

(4.6)

where $B$ is expressed as

$$B = \begin{bmatrix} -I & -B_{12} & I & B_{14} \\ 0 & -I & 0 & I \end{bmatrix}$$

(4.7)

submatrices $B_{12}$ and $B_{14}$ are

$$B_{12} = \begin{bmatrix} 0 & -t_c & s_c \\ t_c & 0 & -h/2 \\ -s_c & h/2 & 0 \end{bmatrix}, \quad B_{14} = \begin{bmatrix} 0 & -t_c & -s_c \\ -t_c & 0 & -h/2 \\ s_c & h/2 & 0 \end{bmatrix}$$

(4.8)

where $s_c$ and $t_c$ are the offset of the facet centroid $C$ from the intersection $I$ between lattice and facet in local $s$ and $t$ directions respectively, as indicated in Figure 4.7. $I$ is the identity matrix and $0$ is the zero matrix. The element stiffness matrix $k_{\text{local}}$ in the local coordinate system is formulated using the virtual work theorem.

$$k_{\text{local}} = B^TDB$$

(4.9)

The material matrix $D$ ($6 \times 6$) is given by

$$D = \text{diag} [k_n, k_s, k_s, k_{\phi n}, k_{\phi s}, k_{\phi t}]$$

(4.10)
A coordinate transformation matrix $T$ is required to rotate the element stiffness matrix $k_{local}$ to the global x-y-z system before assembly of the global stiffness matrix

$$k_{global} = T^T B^T D B T$$

(4.11)

Now, the global stiffness matrix $k_{global}$ can be assembled from the local stiffness matrix $k_{local}$ of each lattice. Not that the system is elastic as all the springs are elastic. With the boundary conditions and external forces exerted on node, the system of equations is formed and the displacement of node can be solved. For regular square lattice with $\alpha = \beta = 1$, the RBSN reduces to a beam bending model (Bolander and Saito, 1998).
4.2 Computation

One of the merits of LEM is implicit formulation. After assembling the global stiffness matrix \( [K] \), the system of linear equations is formulated with nodal displacement \( \{u\} \) and nodal external force \( \{f\} \)

\[
[K] \{u\} = \{f\}
\] (4.12)

The computation efficiency of solving the above equations is crucial as it takes up most of the overall computational time. In LEM simulation, large number of nodes are involved, particular in 3D simulations. An efficient Preconditioned Conjugate Gradient (PCG) method is used to solve systems of linear equation. Also, the solver is parallelised for mult-core CPU to further speed up the computation.

4.2.1 Preconditioned Conjugate Gradient Method

In LEM3D, an iterative method PCG is used. A good reference is provided by Shewchuk (1994). The stiffness matrix \( [K] \) is sparse, symmetric and positive definite that fulfils the requirement of PCG. It has a complexity of \( \mathcal{O}(m\sqrt{k}) \) where \( m \) is the number of non-zero entries in \( [K] \) and \( k \) is its condition number. The complexity of 3D problem is \( \mathcal{O}(n^{4/3}) \) for number of DOFs \( n \). PCG is by far the most computationally efficient method for large scale problem.

In order to reduce \( k \) and the number of iteration required, a pre-conditioner \( [M] \) can be applied. In the study, Jacobi pre-conditioner is used which is given by \( [M] = \text{diag}([K]) \)

All the diagonals have to be positive which is the case. It is the simplest pre-conditioner which is efficient for diagonally dominant matrices. It is also fast to compute and save storage space as it is stored as a vector.

The convergence of solution is measured by the residual \( \{r\} = \{f\} - [M] \{d\} \) and it can be expressed as a scalar \( \delta = \{r\}^T \{r\} \). The tolerance \( \varepsilon \) is selected such that iteration stops when \( \delta_n < \varepsilon_{CG}^2 \delta_0 \) where \( \delta_0 \) is initial residual and \( \delta_n \) is current residual. \( \varepsilon_{CG} \) is set to be 0.00025 for all the simulations presented in this thesis.

In PCG, the information only pass from one node to its adjacent nodes in one iteration. A minimum iteration number \( i_{min} \) is set to guarantee the information can pass among all nodes and to avoid pre-mature termination of iteration, particular for large tolerance \( \varepsilon_{CG} \) cases. \( i_{min} \) is set as \( 1.5 \max(N_x, N_y, N_z) \), where \( N_x = L_x/l_{min} \) in direction \( x \).
4.2.2 Parallel computing

To benefit the computing capacity of multi-core CPU, the solver is further optimised for parallel computing. In LEM3D, linear algebra library Eigen++ (Guennebaud et al., 2010) is used but the library only supports serial computation.

OpenMP is implemented in the linear algebra module in LEM3D using shared memory system. It is applicable for personal computers or workstations running a single multi-core CPU. However, full capacity of high performance computers using a cluster of CPUs cannot be utilised. It can be done by parallelisation by Message Passing Interface (MPI) using distributed memory system.

Table 4.1 shows the computation time required to solve a uniaxial tension test of M100 lattice model and a cantilever beam problem of D20 lattice model. The simulations were run in a computer with 8-core Intel Xeron E5-2670 (2.6GHz) CPU. The OpenMP parallelisation gives a maximum of 4.33x speed-up. A 2.6 million DOFs problem can be solved within 1 minute.

<table>
<thead>
<tr>
<th>Model</th>
<th>$N_{\text{node}}$</th>
<th>$N_{\text{lattice}}$</th>
<th>$N_{\text{DOF}}$</th>
<th>Thread no.</th>
<th>Iteration no.</th>
<th>Time (s)</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>M100 cubic model</td>
<td>353,553</td>
<td>2,116,456</td>
<td>2,623,300</td>
<td>8</td>
<td>495</td>
<td>56.03</td>
<td>3.76x</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>4</td>
<td>491</td>
<td>94.71</td>
<td>2.20x</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2</td>
<td>494</td>
<td>133.92</td>
<td>1.57x</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1</td>
<td>492</td>
<td>209.21</td>
<td>1.00x</td>
</tr>
<tr>
<td>D20 Cantilever beam</td>
<td>56,851</td>
<td>394,739</td>
<td>339,120</td>
<td>8</td>
<td>2285</td>
<td>24.06</td>
<td>4.33x</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>4</td>
<td>2285</td>
<td>56.56</td>
<td>1.84x</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2</td>
<td>2285</td>
<td>78.86</td>
<td>1.32x</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1</td>
<td>2285</td>
<td>104.15</td>
<td>1.00x</td>
</tr>
</tbody>
</table>

Table 4.1 Computation time for solving lattice in LEM3D for 8-core Intel Xeron E5-2670 (2.6GHz) CPU
4.3 Validation on linear elasticity of LEM

To verify the elastic part of the LEM code, two simulations were carried out. The first one is applying uni-axial loading of a cubic sample and the second one is cantilever beam under lateral force. $E_{\text{micro}}$ is assumed to be $2 \times 10^7$ kPa in this thesis unless otherwise specified. Table 4.2 lists the statistics of the lattice models used in this Chapter. Simulations of different $\alpha$ and $\beta$ are carried out. Lattice networks generated from different node densities, fineness and packing are studied as well.

<table>
<thead>
<tr>
<th>Lattice model</th>
<th>$l_{\text{min}}$ (m)</th>
<th>$&lt;l&gt;$ (m)</th>
<th>$n$</th>
<th>$N_{\text{node}}$</th>
<th>$N_{\text{lattice}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cubic model (100 × 100 × 100m³)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>D100</td>
<td>1.0</td>
<td>1.358</td>
<td>0.5</td>
<td>707,106</td>
<td>5,141,953</td>
</tr>
<tr>
<td>D50</td>
<td>2.0</td>
<td>2.716</td>
<td>0.5</td>
<td>88,388</td>
<td>631,147</td>
</tr>
<tr>
<td>M50</td>
<td>1.587</td>
<td>2.733</td>
<td>0.25</td>
<td>88,388</td>
<td>646,023</td>
</tr>
<tr>
<td>S50</td>
<td>1.170</td>
<td>2.746</td>
<td>0.1</td>
<td>88,388</td>
<td>655,051</td>
</tr>
<tr>
<td>D25</td>
<td>4.0</td>
<td>5.432</td>
<td>0.5</td>
<td>11,048</td>
<td>79,101</td>
</tr>
<tr>
<td>D10</td>
<td>10.0</td>
<td>13.58</td>
<td>0.5</td>
<td>707</td>
<td>4,313</td>
</tr>
<tr>
<td>D5</td>
<td>20.0</td>
<td>27.16</td>
<td>0.5</td>
<td>88</td>
<td>437</td>
</tr>
<tr>
<td>Cantilever beam model (10 × 10 × 100m³)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>D50c</td>
<td>0.2</td>
<td>0.272</td>
<td>0.5</td>
<td>885,561</td>
<td>6,393,825</td>
</tr>
<tr>
<td>D20c</td>
<td>0.5</td>
<td>0.679</td>
<td>0.5</td>
<td>56,851</td>
<td>394,739</td>
</tr>
<tr>
<td>D10c</td>
<td>1.0</td>
<td>1.358</td>
<td>0.5</td>
<td>7,141</td>
<td>48,244</td>
</tr>
<tr>
<td>D5c</td>
<td>2.0</td>
<td>2.716</td>
<td>0.5</td>
<td>901</td>
<td>5,323</td>
</tr>
<tr>
<td>2D Rec. model (40 × 80 × 3m³)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>D80p</td>
<td>1.0</td>
<td>1.454</td>
<td>0.5</td>
<td>6,788</td>
<td>41,392</td>
</tr>
<tr>
<td>S80p</td>
<td>0.585</td>
<td>1.454</td>
<td>0.5</td>
<td>6,788</td>
<td>41,392</td>
</tr>
<tr>
<td>3D Rec. model (40 × 80 × 40m³)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>D80</td>
<td>1.0</td>
<td>1.358</td>
<td>0.5</td>
<td>90,509</td>
<td>646,049</td>
</tr>
</tbody>
</table>

Table 4.2 Details of lattice models used in LEM simulations presented in this thesis

4.3.1 Uniaxial loading

Uniaxial tension tests of a $100 \times 100 \times 100m³$ cube are simulated. The cube is subjected to a constant normal pressure of 250kPa on the top face and vertical ($z$) translation restrain on the bottom face. All other faces are free for translation and rotation. These simulations are aimed to study the macroscopic response of the lattice models under simple uni-axial loading. Figure 4.8 shows the displacement of lattice model D50 with $\alpha = 0.3$. The LEM simulations correctly calculate the nodal displacement and the lattice model shows Possion’s effect. This will be further explored in the next section.
Fig. 4.8 LEM simulation of uni-axial loading on D50 model with $\alpha = 0.3$ and $\beta = 1.0$. (Top left) The model configuration. The nodal displacement along x (top right), y (bottom left) and z (bottom right)
4.3.2 Cantilever beam under transverse load

For a cantilever beam of 100m long with a square cross section of 10x10m, a constant transverse pressure of 250 kPa along $x$ direction is applied on the top face and fully fixed restraint applied on the bottom face. This is a more complicated loading condition as the lattice model has to resist axial, shear and bending loading. The model configuration, deflection profiles and flexural stress distributions are shown in Figure 4.9. Both $\alpha$ and $\beta$ are taken as 1.0.

From the beam theory, the deflection $\delta_{tot}$ is given by

$$\delta_{tot} = \delta_{flexural} + \delta_{shear} = \frac{Pl^3}{3EI} + \frac{Pl}{GA_s}$$

(4.13)

where $l$ is the span of beam and $A_s$ is the shear area which is $5A/6$ for rectangular section of area $A$. By taking $E = E_{\text{micro}}$ and $G = E_{\text{micro}}/2$ (i.e. $\nu_{\text{micro}} = 0$), the flexural $\delta_{flexural}$ and shear $\delta_{shear}$ deflections of the cantilever beam is 0.5m and 0.03m respectively. The stick model composed of lattices stacking up correctly predicts the tip deflection from flexure. When cubical lattice (C10c model) is used, the shear deflection is also taken into account and gives the total deflection exactly the same as given by the beam theory. By using a disordered lattice (D10c model), the deflection is slightly smaller (0.5018m) but the difference between the simulation result of the lattice model and the beam theory diminishes when a finer lattice model is used (0.503m for D50c model).

The maximum flexural stress is 15000kPa from the beam theory. C10 model correctly predicts the flexural stress profile. For disordered lattices (D5c to D50c), the flexural stress profiles are similar with small local fluctuation observed, which decreases with increasing model fineness.
Fig. 4.9 LEM simulation of cantilever beam under lateral load. (a) Model configuration, (b) Deflection profile, the figure on the top shows tip lateral displacement, and (c) Flexural stress distribution.
4.4 Parametric studies on key parameters

4.4.1 $\alpha$ and $\beta$

This section explores the factors affecting the macroscopic properties of a lattice model. The physical significance of parameters $\alpha$ and $\beta$ given in Eqs. (4.4) and (4.5) is first explored. A series of simulations of a cubic lattice under uni-axial loading are carried out.

Figures 4.10(a,b) show the variation of the normalised macroscopic Young’s modulus $E/E_{\text{micro}}$, the normalised macroscopic shear modulus $G/G_{\text{micro}}$ and the normalised macroscopic bulk modulus $K/K_{\text{micro}}$ with various $\alpha$ and $\beta$ values, taken microscopic Possion ratio $\nu_{\text{micro}}$ as 0 because there is no coupling between translational springs. In all three macroscopic parameters, the effect of $\beta$ is small, meaning that the contribution of rotational springs to macroscopic stiffness is minimal for the uniaxial loading case. This also conforms the finding by Buxton and Clarke (2007). They used Born spring as lattice model in disordered lattice network and concluded that for high coordination number ($n_{\text{coord}} \leq 15$), lattice sketching dominant and the sketching-bending transition happens at $n_{\text{coord}} \approx 7$.

Both $E/E_{\text{micro}}$ and $G/G_{\text{micro}}$ drop significantly when $\alpha$ reduces. $K/K_{\text{micro}}$ remains almost constant when $\alpha$ varies. Therefore, $K$ is governed by normal spring stiffness $k_n$ while $G$ is governed by $k_s$. In other words, the bulk deformation of lattice model is governed by $k_n$ and distortion of model is governed by $k_s$.

From Figure 4.10c, $\alpha$ can be used to specify the Poisson’s ratio $\nu$ of the model. It also depends slightly on the density of node $n$. The value of $\nu$ becomes negative when $\alpha > 1$. Since $\alpha$ and $\beta$ cannot be negative, the largest $\nu$ for a lattice model that can be obtained is about 0.33.

4.4.2 Node density $n$

There are two parameters controlling the lattice geometry: node fineness and node density $n$. The former is controlled by $N_{\text{node}}$ and the later is controlled by $n$. This section explores the effect of both parameters on the macroscopic properties of lattice models.

Figures 4.11a,b show the relationship between $E/E_{\text{micro}}$ and mesh fineness in cubic lattice under uni-axial load and cantilever beam bending simulations. In both cases, mesh fineness does not influence the macroscopic behaviour except for very coarse model such as D5 model.

The macroscopic properties of a lattice model are also affected by $n$ but in a less extent comparing to that of $\alpha$. Figures 4.10c,d demonstrate the effect of $n$ on $\nu$ and $E/E_{\text{micro}}$. The effect of $n$ is insignificant when $\alpha > 0.3$. When $\alpha \leq 0.3$, lower $n$ gives a slightly stiffer
Fig. 4.10 Effect of \( \alpha \), \( \beta \) and node density \( n \) on macroscopic parameters in LEM simulation of uniform tensile test in D50 model.

Effect on normalised Young modulus \( E/E_{\text{micro}} \), normalised shear modulus \( G/G_{\text{micro}} \) and normalised bulk modulus \( K/K_{\text{micro}} \) by varying (a) \( \alpha \) and (b) \( \beta \). Effect of \( \alpha \) and \( n \) on (c) Poisson’s ratio \( \nu \) and (d) \( E/E_{\text{micro}} \).
4.4 Parametric studies on key parameters

Fig. 4.11 Effect of mesh fineness on macroscopic parameters in LEM simulation. Effect of mesh fineness on $E/E_{\text{micro}}$ in (a) cubic lattice model under uniaxial load and (b) cantilever beam under lateral load.

model and higher $\nu$. Such trend appears in both uniaxial tension case and cantilever beam bending case.
4.5 Stress heterogeneity

Stress heterogeneity refers to the stress fluctuation at local level. LEM shows stress heterogeneity even under uniform loading. In this section, cubic lattice models under two extreme loading cases: isotropic loading and uni-axial loading are studied. Stress heterogeneity of other loading should behave between these two extreme cases and can be analysed by superposition. Stress heterogeneity is studied at two levels: facet level and nodal level. The former is a scalar quantity and the latter is a tensor quantity.

4.5.1 Nodal stress calculation

In LEM, the nodal stress \( \sigma_{ij}^n \) is calculated by summing all forces from all its neighbors (Cambou et al., 2009):

\[
\sigma_{ij}^n = \frac{1}{2V_{cell}} \sum_{f=1}^{N_f} F_i^f l_j^f
\]  

(4.14)

where \( F_i^f \) is the \( i \)-component of the force exerted on the facet of lattice \( f \), \( l_j^f \) is the \( j \)-component of the branch factor (vector joining the centroids of cells \( i \) and \( j \)) and \( V_{cell} \) is the volume of cell. Nodal stress is regarded as stress homogenisation at nodal level.

The mean stress \( p^n \) and deviatoric stress \( q^n \) are called stress invariant as they do not depend on the choice of axes. They are calculated from principal stresses \( \sigma_{1}^n, \sigma_{2}^n \) and \( \sigma_{3}^n \)

\[
p^n = \frac{\sigma_{1}^n + \sigma_{2}^n + \sigma_{3}^n}{3}
\]  

(4.15)

\[
q^n = \sqrt{\left(\sigma_{1}^n - \sigma_{2}^n\right)^2 + \left(\sigma_{1}^n - \sigma_{3}^n\right)^2 + \left(\sigma_{2}^n - \sigma_{3}^n\right)^2} / 2
\]  

(4.16)

\( p^n \) and \( q^n \) indicate the cell volumetric change and the cell distortion respectively.

4.5.2 Isotropic loading

Table 4.3 shows the mean and the SD of facet normal stress \( \sigma_{fn}^f \) and facet shear stress \( \sigma_{fs}^f \) under isotropic stress \( p_L \) with different \( \alpha \) and \( n \). Shear springs are not mobilised in resisting isotropic loading for all lattice models. Only normal springs are mobilised in resisting isotropic load and \( \sigma_{fn}^f \approx p_L \) for all facets. This means that there are only stretching in lattices.

Figure 4.12 shows the different nodal stress \( (\sigma_{zz}^n, \sigma_{xy}^n, p^n \) and \( q^n ) \) distributions with different values of \( \alpha \) and \( n \) under isotropic pressure. All nodal stresses are insensitive with \( \alpha \) as shear
Fig. 4.12 Nodal stress distributions under isotropic loading \( p_L \) with different \( \alpha \) and \( n \). (a) normalised nodal normal stress \( \sigma_{zz}^n / p_L \), (b) normalised nodal shear stress \( \sigma_{xy}^n \), (c) normalised nodal mean stress \( p^n / p_L \) and (d) normalised deviator stress \( q^n / p_L \).
springs are not mobilised under isotropic loading. The distribution of nodal normal stress $\sigma_{zz}^n$ is almost the same as that of $\sigma_{xx}^n$ and $\sigma_{yy}^n$. Similarly, the distribution of nodal shear stresses $\sigma_{xy}^n, \sigma_{xz}^n, \sigma_{yz}^n$ are very similar. This shows that there is no anisotropy in the lattice models. It is interesting to note that there is nodal shear stress given that there is no facet shear stress. There are only normal stresses acting on cells. It is because the normal vectors at facet centroids of a Voronoi cell do not coincide at a point. Normal stress on facet alone can induce shear deformation (distortion) at nodal level. For lower $n$ value, larger spreads of both nodal normal stress and nodal shear stress increase because cells are more elongated and irregular. Larger shear stress is more likely to be induced and deviation of normal stress from the homogenised value also increases.

The spread of both nodal normal stress and nodal shear stress distribution increase with decreasing node density $n$ that governs the geometry of cell. As shown in Figure 4.6, cell sphericity $\Phi_{cell}$ decrease with $n$, meaning that cells are more angular and elongated with lower $n$. The deviation of node and centroid of cell is larger for smaller $n$ lattice model so higher nodal shear stress is induced.

$n$ also affects the distribution of nodal mean stress $p^n$ and nodal deviator stress $q^n$. $<p^n> \approx p_L$ which is close to the homogenised mean stress of $p_L$. Similar to nodal normal stress and nodal shear stress, the spread of $p^n$ distribution increases with decreasing $n$. The bulk deformation of cells varies with one another. For denser model, the deviation of nodal mean stress from macroscopic (homogenised) value of $p_L$ is smaller.

For nodal deviator stress $q^n$, its mean and variance increases with decreasing $n$. The macroscopic deviator stress $q$ is zero under isotropic stress, meaning that there is no distortion in macroscopic level. Larger mean and variance of $q^n$ means higher stress heterogeneity for
lattice model with smaller $n$. Cells are undergo larger distortion with smaller $n$. This is also explained by more elongated and angular cells in small $n$ lattice model.

### 4.5.3 Unaxial loading

#### Facet stresses

For all the lattice models under uni-axial load, $<\sigma_n^f> / p_L \approx 1/3$. The contribution of normal and shear spring are equally split with $<\sigma_s^f> / <\sigma_n^f> \approx 1$ when $\alpha = 1$, meaning that normal springs and shear springs have equal contribution in resisting uni-axial loading.

The case of uniaxial loading is more complicated than the isotropic case because of the macroscopic stress anisotropy. Figure 4.13 shows the distribution of $\sigma_n^f$ and $\sigma_s^f$ on lattice facets under uni-axial loading. $\sigma_n^f$ distribution for $\alpha = 1.0$ is featured by two distinct cut off at 0.0 and 1.0$p_L$. The large number of lattice with $\sigma_n^f \approx 0.0$ comes from unfavorably oriented lattices (0° or 180°) which are immobilised in taking loading, neither by normal springs nor by shear springs as shown in Figure 4.13. There is almost no tension lattice for $\alpha = 1.0$ lattice models as $\nu$ and $\nu_{micro}$ are zero theoretically. There is no transverse deformation in both macroscopic level and microscopic level. This means that horizontal lattices are subjected to zero strain and the overall model does not deform laterally as well.

These two cut offs diminish with decreasing $\alpha$. The spread of $\sigma_n^f$ significantly increases with decreasing $\alpha$ while $<\sigma_n^f>$ remains almost constant at $1/3p_L$. A lot of tensile lattices are formed for lattice models of $\alpha = 0.0$. Without shear springs to take loading, lattice network needs a more tortuous loading path (force chain) to transfer loading by normal springs only. This generates higher normal spring force and wider spread in facet normal stress distribution.

These lattices also take small amount of shear stress as well. According to the polar diagram on $\sigma^n$ in 4.13a, the normal springs oriented along loading direction take most stress and the magnitude increases with $\alpha$. For $\alpha = 1.0$, lattices orientated along z-direction take about 0.65$p_L$ of normal stress and then increase to 1.3$p_L$ for $\alpha = 0.0$ lattice models. For $\alpha = 1.0$ models, the unfavourably oriented lattices can still share the loading by mobilising shear springs.

Shear springs are most efficient when lattices are orientated at 45° to the loading direction. The maximum $\sigma_n^f$ is limited to 0.6$p_L$ for $\alpha = 1.0$ and 0.4$p_L$ for $\alpha = 0.3$. The distinct peak in $\sigma_n^f$ distributions comes from 45° lattices as shown in Figure 4.13.

From Figure 4.13, $\sigma_n^f$ is independent of $n$. When $\alpha$ is small, it has slight effect on $\sigma_s^f$ which explains the slight change in macroscopic Possion ratio $\nu$ as shown in Figure 4.10c.
Fig. 4.13 Normalised facet stress distributions and their polar diagrams of lattice models under uni-axial loading with different $\alpha$ and $n$. (a) Polar diagram of averaged normalised facet normal stress $\frac{\sigma_f}{p_L}$ projected on xy-plane, xz-plane and yz-plane, (b) Polar diagram of averaged normalised facet shear stress $\frac{\sigma_f}{p_L}$ projected on xy-plane, xz-plane and yz-plane, (c) distribution of $\sigma_f/n$/p_L and (d) distribution of $\sigma_f/s$/p_L.
Nodal stresses

Fig. 4.14 Nodal stresses distributions of lattice models under uniaxial loading $p_L$ with different $\alpha$ and $n$. (a) $\sigma_{xx}/p_L$ with $n = 0.5$, (b) $\sigma_{zz}/p_L$ with $n = 0.5$, (c) $\sigma_{xx}/p_L$, (d) $\sigma_{zz}/p_L$, (e) $3p^n/p_L$ and (f) $q^n/p_L$. 
The normalised normal nodal stress distributions along \((\sigma_{zz}^n)\) and perpendicular to \((\sigma_{xx}^n, \sigma_{yy}^n)\) the load direction of D50 models with different values of \(\alpha\) are plotted in Figures 4.14a,b. For \(\alpha = 1.0\), the lattice model is said to be elastically homogeneous under uniform axial loading and no normal stress in the lateral direction is produced (Bolander and Saito, 1998; Bolander and Sukumar, 2005). This is reflected by a very narrow PDF curve of nodal lateral stress \(\sigma_{xx}^n\). There is spread of nodal longitudinal normal stress \(\sigma_{zz}^n\) distribution. If different values of \(\alpha\) are applied, there is stress heterogeneity but the mean values of \(\sigma_{zz}^n\) and \(\sigma_{xx}^n\) (and \(\sigma_{yy}^n\) ) are close to the macroscopic values of 1.0\(p_L\) and 0.0 respectively. The spread of nodal normal stress distribution increases with decreasing \(\alpha\).

There is no stress heterogeneity when regular lattice network is used because of the symmetry of cells. When a disordered lattice model is subjected to loading, nodes have to move to achieve equilibrium, resulting in a non-uniform local stress field. Extra stress is also resulted in a non-uniform displacement field as well (Wang et al., 2009b).

Figures 4.14c and d plot the nodal normal stresses \(\sigma_{xx}^n\) and \(\sigma_{zz}^n\) under different values of \(\alpha\) and \(n\). For distribution of \(\sigma_{xx}^n\), the spread increases with \(\alpha\) but it is insensitive to \(n\). In contrast, under isotropic load, normal nodal stress distribution varies with \(n\). For \(\sigma_{zz}^n\) distribution, the spread increases by decreasing \(\alpha\) and \(n\). The nodal normal stress distribution changes with \(\alpha\) because shear springs are mobilised in uniaxial loading, whereas shear springs are not mobilised under isotropic loading. Stress is more uniform when \(n\) increases. Since cells tend to be regular and symmetric for larger value of \(n\), less additional stress is induced for nodes to remain in equilibrium.

For nodal stress invariants, the distributions of nodal mean stress \(p^n\) and nodal deviator stress \(q^n\) are plotted in Figures 4.14e and f respectively. Macroscopically, \(p = 1/3p_L\) and \(q = p_L\). At nodal level, \(<p^n> = 1/3p_L\) and \(<q^n> = p_L\). The distributions of both \(p^n\) and \(q^n\) increase with decreasing \(\alpha\) and decreasing \(n\). This means that nodal stresses becomes more heterogeneous for smaller \(\alpha\) and \(n\) values and cells are more likely to dilate (volumetric expansion) more and to distort more.
4.6 Applying statistical distribution on lattice parameters

Rock is heterogeneous in different scales. The heterogeneity comes from fractures (joints, fissures, faults), voids, bedding planes and the presence of different minerals. So the properties of lattice in LEM model should not be uniform. One of the ways to introduce heterogeneity is varying lattice parameters by PDFs.

In this thesis, three types of PDF are applied, namely normal, lognormal and Weibull distributions. Normal distribution is the most commonly used in all disciplines. Lognormal and Weibull are commonly used PDFs in rock mechanics and fracture mechanics. A random factor $x$ is produced by pseudo random number generator following specified PDFs are applied on $E_{micro}$ that controls spring stiffness and $f_{st}$ and $f_{ss}$ that control lattice breaking threshold. The PDFs of the three probability distributions are given below

Normal : $N(x : \mu, \sigma) = \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{1}{2} \left( \frac{x-\mu}{\sigma} \right)^2}$

Lognormal : $LN(x : \mu, \sigma) = N(\ln x : \mu, \sigma) = \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{1}{2} \left( \frac{\ln x-\mu}{\sigma} \right)^2}$

Weibull : $W(x : \lambda, k) = \begin{cases} \frac{k}{\lambda} \left( \frac{x}{\lambda} \right)^{k-1} e^{-(x/\lambda)^k}, & x \geq 0 \\ 0, & x < 0 \end{cases}$

The means of these PDFs are all set to 1 such that $\mu = 1$ for normal, $\mu = 0$ for lognormal and $\lambda = 1.0$ for the Weibull distribution. The only parameter that controls the degree of heterogeneity is given by $\sigma$ for normal and lognormal distributions and $k$ (shape factor) for Weibull distribution.

If $x$ generated is smaller than a threshold $x_0$, it will be discarded to avoid negative values and unrealistically small values. Throughout the simulation presented in this thesis, $x_0 = 0.2$ is used. Such truncation modifies the mean of $x$ and other statistics parameters such as standard deviation $\sigma$ and skewness $\gamma_1$. A linear transformation $x' = ax + b$ is carried out to ensure the transformed values $x'$ have a mean of 1 so that the distribution does not affect the homogenised macroscopic values of lattice under study. Nine different PDFs listed below are studied in this thesis and they are plotted in Figure 4.15. The nine PDFs are named as follow throughout this thesis:

- Normal distributions: N(0.25), N(0.5), N(0.75)
- Lognormal distributions: LN(0.25), LN(0.5), LN(0.75)
- Weibull distributions: W(3.0), W(2.5), W(2.0)
The values in brackets for normal and lognormal distributions mean the values of \( \sigma \) of respective probability distribution before truncation. For Weibull distribution, the values in brackets mean the value \( k \) before truncation. Because of such truncation, the PDF is slightly altered. For example, truncated normal distribution is skewed instead of symmetrical non-truncated one.

### 4.6.1 Macroscopic behaviour

Figure 4.16 shows the effects of applied heterogeneity on macroscopic parameters \( E, G, K \) and \( \nu \). Modifying the spring stiffness by a PDF shows a reduction of the macroscopic stiffness of \( E, G \) and \( K \) and the reduction increases with the applied heterogeneity even the mean of spring stiffness remains unchanged when applying heterogeneity. This means the spring stiffness obtained by RBSN from geometry of cell and facets is optimal. The macroscopic Possion ratio is insensitive to the applied heterogeneity.

### 4.6.2 Facet stress

Figure 4.17 shows how different PDFs applied on \( E_{\text{micro}} \) affect facet stresses \( \sigma_n^f \) and \( \sigma_s^f \) under isotropic load and uni-axial load. The standard deviation \( \sigma \), skewness \( \gamma_1 \) and excess kurtosis \( \gamma_2 \) (measures of stress heterogeneity) of \( \sigma_n^f \) and \( \sigma_s^f \) increases with heterogeneity applied in \( E_{\text{micro}} \). It has much significant effects under isotropic load than under uni-axial load. In general, applying lognormal distribution has much distinct effects than normal and Weibull distributions because of its high standard deviation and skewness.

Under isotropic loading, applying heterogeneity on \( E_{\text{micro}} \) only slightly changes \( <\sigma_n^f> \) (Figure 4.17a) but it increases \( <\sigma_s^f> \) substantially. \( <\sigma_s^f> \) changes from \( 0.0177p_L \) for no distribution case to \( 0.104p_L \) for LN(0.75) case, as shown in Figure 4.17b. The PDFs of both \( \sigma_n^f \) and \( \sigma_s^f \) give a positive skew and the skewness increases with the applied heterogeneity. This is because the PDFs applied on \( E_{\text{micro}} \) are also positively skewed and skewness increases with its variance.

Under uni-axial loading, the PDF of \( \sigma_n^f \) has a very sharp peak on the left with a bumped tail on the right (Figure 4.17c) if no distribution is applied. The applied heterogeneity on \( E_{\text{micro}} \) does little effect on \( <\sigma_n^f> \) and the sharp peak, it mainly makes the bumped tail smoother. From Figure 4.17d, \( <\sigma_s^f> \) is insensitive with the increase in applied heterogeneity on \( E_{\text{micro}} \). Without applied heterogeneity on \( E_{\text{micro}} \), the PDF shows a very short bumped tail toward zero and the peak located on the right and \( \sigma_s^f < 0.4p_L \). With applied heterogeneity, PDFs are skewed and the degree of skewness increases with the degree of heterogeneity.
4.6 Applying statistical distribution on lattice parameters

Fig. 4.15 PDF applied in lattice models
Fig. 4.16 Effect of applied heterogeneity [LN(0.75), LN(0.5), and LN(0.25)] on macroscopic behaviour of lattice model. (a) Normalised Young's modulus \( \frac{E}{E_{\text{micro}}} \), (b) Normalised shear modulus \( \frac{G}{G_{\text{micro}}} \), (c) Normalised bulk modulus \( \frac{K}{K_{\text{micro}}} \), and (d) Poisson's ratio \( \nu \).
Therefore, applying heterogeneity affects mainly on $\sigma_s^f$, meaning that shear springs are mobilised more in heterogeneous models.

Figure 4.18 shows the breakdown of PDFs according to lattices orientation. Under isotropic load, the orientation of lattices does not affect the distribution in both $\sigma_p^f$ and $\sigma_s^f$ as shown in Figure 4.18a,b. Under uni-axial loading, the applied heterogeneity on $E_{\text{micro}}$ does little effect on unfavourable oriented lattices which contributes mostly by the negative $\sigma_n^f$ lattices. For favourably oriented lattices, the distribution becomes more uniform with wider spread. This gives a smoother tail for the overall PDF. For shear, different orientations of lattice contribute differently but skewness increases when heterogeneity on $E_{\text{micro}}$ is applied.

### 4.6.3 Nodal stress

Figure 4.19 shows the nodal mean stress $p^n$ and nodal deviatoric stress $q^n$ with different PDFs applied on $E_{\text{micro}}$ under isotropic and uni-axial loading. Under isotropic load, the heterogeneity on $E_{\text{micro}}$ increases, the variance of $p^n$ increases significantly and inverts the negative skewness to positive. For $q^n$, the mean, variance, skewness and kurtosis all increases with increasing heterogeneity on $E_{\text{micro}}$. It is similar to the effect of decreasing $\alpha$ and $n$ as shown in Figure 4.12d.

Under uni-axial load, applying PDFs on $E_{\text{micro}}$ has less effects compared to decreasing $\alpha$ and $n$ as shown in Figure 4.14. $<p^n> \approx 1/3p_L$ and $<q^n> \approx 1.0p_L$ for all PDFs applied.

The effect of applied heterogeneity is small on nodal stress than facet stress because nodal stress is the homogenisation of facet stress. The effect of introducing PDFs on $E_{\text{micro}}$ is averaged out.
PDF applied on $E_{micro}$. Under isotropic load $p$ and different $\mu$ and different $\mu E_{micro}$. Under uni-axial load and isotropic load with different $\mu$ and different $\mu E_{micro}$. Under uni-axial load $p$ and different $\mu$ and different $\mu E_{micro}$. Under uni-axial load $p$ and different $\mu$ and different $\mu E_{micro}$.
Fig. 4.18 Distribution of nodal stress invariant $p^n/p_L$ and $p^n/p_L$ under uni-axial load and isotropic load with different $n$ and different PDF applied on $E_{micro}$. Under isotropic load $p_L$: (a) $p^n/p_L$, (b) $q^n/p_L$. Under uniaxial load $p_L$: (c) $p^n/p_L$, (d) $q^n/p_L$. 
Fig. 4.19 Distribution of nodal stress invariant $p_n/p_L$ and $p_n/p_L$ under uni-axial load and isotropic load with different $n$ and different PDF applied on $E_{\mu}$. Under isotropic load $p_L$: (a) $p_n/p_L$, (b) $q_n/p_L$. Under uniaxial load and isotropic load $p_L$: (c) $p_n/p_L$, (d) $q_n/p_L$. Under uniaxial load and different $n$ and different PDF on $E_{\mu}$. Under isotropic load $p_L$: (a) $p_n/p_L$, (b) $q_n/p_L$. Under uniaxial load and different $n$ and different PDF on $E_{\mu}$.
4.7 Conclusion

This section provides the generation of disordered lattice network that minimizes the effect of mesh dependency. The geometric heterogeneity of lattice model is characterised by node density \( n \). Statistical analysis on different geometrical properties such as length of lattice \( l_{lattice} \), area of facet \( A_{lattice} \), volume \( V_{cell} \) and sphericity \( \Psi_{cell} \) of cells and coordination number \( n_{coord} \) are carried out on different \( n \) values.

This Chapter also provides the formulation of RBSN for lattice constitutive relationship. A C++ code, LEM3D, is written for the implementation and the code is validated by uni-axial loading of a cubic lattice and a cantilever beam under lateral load. The model requires three parameters: \( E_{micro} \), \( \alpha \) and \( \beta \). \( E_{micro} \) is the overall scaling factor for macroscopic lattice stiffness. \( \alpha \) specifies the stiffness ratio of shear spring \( k_s \) to normal spring \( k_n \) and \( \beta \) scales the three rotational spring stiffness. \( \beta \) is found to have negligible effects on macroscopic properties of lattice.

For macroscopic behaviour, \( \alpha \) can be used to specify Possion ratio \( \nu \). It affects macroscopic Young’s modulus \( E \) and macroscopic shear modulus \( G \) but it does not affect macroscopic bulk modulus \( K \). Node density \( n \) also affects the macroscopic behaviour, but its effect is smaller than varying \( \alpha \).

LEM shows stress heterogeneity in microscopic level which is one of its major characteristic and has been studied at facet level and nodal level. In general, decrease in \( \alpha \) increases stress heterogeneity except nodal mean stress \( p^n \) under isotropic load. Decrease in \( n \) also increases stress heterogeneity in a lesser extent. \( n \) is insensitive to both facet normal stress \( \sigma_{f n} \) and shear stress \( \sigma_{fs} \) under uni-axial load.

Facet normal stress \( \sigma_{f n} \) and shear stress \( \sigma_{fs} \) are independent to lattice orientation under isotropic load but it affects significantly under uni-axial load. \( \sigma_{fs} \) is very small in isotropic load but it contributes significantly in uni-axial load. Shear springs are mobilised by macroscopic stress anisotropy.

Additional heterogeneity can be introduced by applying PDFs to \( E_{micro} \). Lognormal distribution is most effective to increase stress heterogeneity. Applied heterogeneity shows substantial increase in stress heterogeneity in isotropic load than uni-axial load, particular in facet stress.
Chapter 5
Fracturing simulation using LEM

This Chapter explores the capacity of LEM to simulate fracturing process. Constitutive model for the post-peak behaviour of lattice is proposed. Relationships between LFEM and microscopic parameters of LEM are established. Uniaxial tensile tests and uniaxial compression tests with different lattice parameters are simulated. Relationship between microscopic model parameters with macroscopic response of lattice models such as macroscopic tensile strength, microscopic compression strength and ductility. Simulation result on fracture pattern, stress-strain curves, statistics on fracture and stress at microscopic levels are analysed. These results are linked with model parameters that give the macro-micro relationship. The LEM simulation results are also compared with experimental data available in the literature.

5.1 Proposed fracture model

In RBSN, lattice can resist axial force, shear and rotation. Since the contribution of rotation is very small, the failure criterion considers only the contribution from facet axial stress $\sigma_{n}^f$ and facet shear stress $\sigma_{s}^f$. Lattice element is assumed to be elastic before meeting two failure criteria below:

\[ \sigma_{n}^f \geq f_{st} \] tensile criterion \hspace{1cm} (5.1)

\[ \sigma_{s}^f \geq f_{ss} \] shear criterion \hspace{1cm} (5.2)

where $f_{st}$ Microscopic tensile strength

$f_{ss}$ Microscopic shear strength
Lattice fails when one of the above criteria is met. Two criteria are studied for shear failure criterion: constant shear strength $f_{ss}$ in which a lattice acts like a bond and Mohr-Coulomb failure criterion in which lattices model a frictional material.

Fracture can only be initialised and propagate along the pre-defined facets. Existing fracture or the potential fracture facet can be constructed according to Section 4.1.2.

5.1.1 Adaptive load step

Since the system is linearly elastic given no lattice breakage within a load step or changing of fracture state from closed to open or vice versa, load step can be adaptively determined after calculation of each load step. This highly increases the computational efficiency as load step varies greatly from the beginning to approaching failure. The size of load step is adaptively adjusted to a smaller value when the model is sensitive to load change. Also, it can capture the snap-back post-peak behaviour by applying negative load step which cannot be captured by strictly increasing load step.

In each load step, lattice forces are calculated to check whether their failure criteria are met. In theory, load step should be chosen small enough such that only one lattice fails within one load step. However, this requires a large number of load steps. To reduce computation time, load step is chosen large enough to allow multiple lattices to be failed within one load step. At the same time, the number of failure lattice cannot be too large that the simulation may not accurately capture some phenomenons in fracture. The maximum number of failure lattices $N_{f,max}$ can be specified to control the number of lattice breakage. If the number of failure lattice is smaller than $N_{f,max}$, all of them are removed for the subsequent calculation. Otherwise, only the most critical $N_{f,max}$ lattices are removed.

To begin with LEM stimulation on fracturing, a small initial load $p_0$ is applied on the model. After lattice force calculation, the load capacity ratio $\rho_l$ of each lattice is calculated.

$$\rho_l = \max \left\{ \frac{\sigma_f^l}{\sigma_{st}}, \frac{\sigma_f^l}{\sigma_{ss}} \right\}$$

(5.3)

Whether new loading $p_{n+1}$ increases or decreases depends on $\rho_{l,max}$ (the greatest $\rho$ among all lattices) which is obtained by

$$p_{n+1} = \begin{cases} \frac{\alpha^+}{\rho_{l,max}^{N_{f,max}}} \min (\alpha^-), & \text{if } \rho_{l,max} < 1.0 \\ \min (\rho_{l,max}^{N_{f,max}} \alpha^-), & \text{if } \rho_{l,max} \geq 1.0 \end{cases}$$

(5.4)
5.1 Proposed fracture model

where \(<\rho_{l,max}>_{N_{f,max}} is the average \rho_l of the most critical \ N_{f,max} lattices. When there is no lattice breakage (i.e. \rho_{max} < 1.0), loading increases and the parameter \alpha^+ > 1.0 controls the number of lattice to be broken in the next load step. For a load step that involves lattice removal (i.e. \rho_{max} \geq 1.0), the applied force decreases (i.e. negative load steps). The parameter \alpha^- < 1.0 controls the possibility of lattice breakage in the next load step. Since \(<\rho_{max}>_{N_{f,max}} may be greater than 1.0 while \rho_{max} \geq 1.0, the loading is capped by \alpha^- p_n to ensure loading always decreases after lattice breakage.

5.1.2 Calculation of fracture aperture

Fracture may be either open or closed after it is formed. The aperture of fracture \(\delta\) corresponding to a lattice formed by node 1 and node 2 is given by

\[
\delta = (u_2 - u_1) \cdot (d_2 - d_1) \quad (5.5)
\]

where

\[
u_i \quad \text{displacement vector of node } i = 1, 2
\]

\[
d_i \quad \text{position vector of node } i = 1, 2
\]

Fracture is regarded as closed if the fracture aperture \(\delta\) is smaller than the residual aperture \(\delta_0\) arisen from asperities.

When \(\delta > \delta_0\), fracture is regarded as open and all the spring stiffness in lattice is set to zero. Figure 5.1 shows the constitutive models for open and closed fracture. Brittle behaviour is shown if fracture is opened. For closed fracture, lattice can be re-established to transfer forces between cells through their asperities but its original stiffness cannot be fully restored.

5.1.3 Reconnecting lattice

\(\gamma\) reduction method

A lattice reconnection factor \(\gamma \leq 1.0\) is applied to all translation and rotation springs of a reconnected lattice. The material matrix \(D\) in Eq. 4.10 becomes

\[
D = \text{diag}[\gamma k_n, \gamma' k_s, \gamma' k_a, \gamma k_{\phi n}, \gamma k_{\phi s}, \gamma k_{\phi t}] \quad (5.6)
\]

where \(\gamma' < \gamma\) is determined iteratively such that shear springs follow plastic behaviour (shear stress remain \(\gamma' f_{as}\) as strain increases). \(\gamma\) accounts for the reduction on stiffness by reduced contact area during shear deformation and dilation. It also models the inter-locking by asperity of a closed fracture. Barton and Choubey (1977) suggested that the contact area...
could vary from 0.1 to 0.001 of the gross area. Such area may be increased due to the plastic
deformation of asperity. Also, \( \gamma \) should be greater than the contact area to gross area ratio as
contact stiffness must be greater than \( E_{\text{micro}} \). Also, inter-locking effects also enhance load
transfer between closed fracture. In this Chapter, \( \gamma \) in the range of 0.01 - 0.4 is studied.

From Figure 5.1 the post-peak behaviour of normal spring and shear spring are modelled
differently for closed fracture. For a closed fracture, normal springs continue to behave
elastically with reduced stiffness \( \gamma k_n \) due to the reduction on contact area. For a shear spring,
it behaves perfectly plastic with shear stress fixed at \( \gamma f_{ss} \).

**Comparison with rock joint model in literature**

There is plenty of literature studying the modelling of rock joint behaviour assuming fractures
are pre-existing (Barton, 2013; Cai and Horii, 1992; Leichnitz, 1985; Saeb and Amadei, 1992;
Yoshinaka and Yamabe, 1986). Figure 5.2 shows a commonly adopted rock joint constitutive
model under normal and shear stresses. Joint under normal stress and shear stress behaves
differently. Also, rock joint demonstrates dilation under shear, meaning normal and shear
joint deformations are coupled. However, there are no literature on modelling of stiffness
degradation from intact rock to fracture. A pre-existing fracture has an initial mis-match of
asperity such that it shows highly non-linear behaviour at small initial normal stress (Figure
5.2a). For shear stress, the drop from peak stress to residual stress at non-dilating part in
conventional model is small (Figure 5.2b). The proposed \( \gamma \) reduction method ignores the
initial non-linearity of closed fracture under normal compression. But it mimics constant
dilation part of a closed fracture under shear stress. There should be separate but correlated \( \gamma \).
5.1 Proposed fracture model

Fig. 5.2 Rock joint constitutive models in literature (a) under normal stress (after Saeb and Amadei, 1992), (b) under shear stress (after Barton, 1973)

for normal springs and shear springs. With the lack of available laboratory data, same γ is applied for both springs in this study.
5.2 Relationship between LEFM and microscopic parameters in LEM

5.2.1 Stress approach

The hydraulic fracturing of a penny shape crack under hydrostatic pressure $p$ is equivalent to applying same tensile stress on the boundary of an infinite domain. The macroscopic tensile strength can be viewed as the maximum pressure $p$ that the material can sustain with an initial crack. For a continuum, the stress at crack tip is infinite and the singular stress near crack tip is described as the stress intensity factor.

There is no concept of microscopic strength in LEFM. In LEM, each lattice represents the interaction between adjacent cells with a finite size. The input strength parameter is the breaking stress at cell level, or the microscopic tensile strength $f_{st}$ for a given facet. By the presence of a penny shape crack that induces stress concentration, the macroscopic tensile strength is smaller than the microscopic one. This section establishes the relationship between the macroscopic tensile strength and the microscopic tensile strength for LEM.

Stress around a penny shape crack is given by Irwin (1957). Assuming that mode I fracturing is dominant, from Eq (2.8),

$$\sigma_{ij} = \frac{K_I}{\sqrt{2\pi r}} f_{ij}(\theta)$$

where intensity factor $K_I = pY\sqrt{\pi R}$, $R$ is the crack radius and the geometry factor $Y = 2/\pi$ for a penny shape crack. Therefore $K_I = 2p\sqrt{R/\pi}$. Consider the crack only propagates on the same horizontal plane of the penny shape crack, $f_{ij}(\theta) = 1$. The vertical stress $\sigma_{zz}$ is reduced to

$$\sigma_{zz} = \frac{p}{\pi} \sqrt{\frac{2R}{r}}$$

(5.8)

For the lattice adjacent to the crack, the average microscopic tensile stress $\sigma_{st}$ for the lattice immediately adjacent to the crack is given by integrating vertical stress $\sigma_{zz}$ across the facet (the geometry as sketched in Figure 5.3) that the lattice represents

$$\sigma_{st} = \frac{\int \sigma_{zz} dA}{A}$$

(5.9)

where $A$ is the area of facet. The tensile force on facet $F_s$ is given by the integral for a new rectangular fracture facet of width $l_w$ along the circumferential direction and length $l_r$ along the radial direction adjacent to the penny shape crack.
5.2 Relationship between LEFM and microscopic parameters in LEM

![Diagram of a facet adjacent to the penny shape crack](image)

**Fig. 5.3 Geometry of a facet adjacent to the penny shape crack**

\[
F_s = \int \sigma_{zz} dA = \int_0^{\ell_w} \int_0^{\ell_r} \frac{K_I}{\sqrt{2\pi r}} dr dw = \frac{\sigma_{st}\ell_w\sqrt{2R}}{\pi} \int_0^{\ell_r} r^{-1/2} dr = \frac{2\sigma_{st}\ell_w\sqrt{2R\ell_r}}{\pi} \tag{5.10}
\]

Note that the stress along the circumferential direction does not vary. Since \( \sigma_{st} = F_s / (\ell_r\ell_w) \), the relationship between the microscopic tensile stress \( \sigma_{st} \) and the macroscopic tensile stress \( \sigma_t \) is given by

\[
\frac{\sigma_t}{\sigma_{st}} = \pi \sqrt{\frac{\ell_r}{8R}} \tag{5.11}
\]

The macro-micro relationship \( \sigma_t / \sigma_{st} \) is now established. It depends on the radius of penny shape crack \( R \) which is expected. It also varies with the size of lattice facet \( \ell_r \).

When fracture propagates, the stress intensity factor reaches the fracture toughness \( K_{Ic} \) and material reaches it macroscopic tensile strength \( f_t \). Eq (5.7) now becomes

\[
K_{Ic} = 2f_t\sqrt{\frac{R}{\pi}} \tag{5.12}
\]

Using the macro-micro relationship from Eq. (5.11), \( K_{Ic} \) is related to the microscopic tensile strength \( f_t \) and a length scale of lattice facet \( \ell_r \).

\[
K_{Ic} = f_{st}\sqrt{\frac{\pi\ell_r}{2}} \tag{5.13}
\]

Hence, \( K_{Ic} \) depends on \( f_{st} \) and \( \ell_r \). If \( K_{Ic} \) and \( f_t \) (that is governed by the microscopic tensile strength \( f_{st} \)) are two independent parameters, \( \ell_r \) that governs the fineness of lattice model cannot be chosen freely.
5.2.2 Energy approach

Wong et al. (2014) provided a lattice failure criterion of Hookean spring in LEM using the energy approach. Here the failure criterion is extended to RBSN model. The elastic energy stored in the normal spring, shear springs and rotation springs of a lattice is given by

\[ E_{\text{elastic}} = \frac{k_n}{2} d_n^2 + \frac{\alpha k_n}{2} (d_s^2 + d_t^2) + \frac{\beta k_\phi}{2} (\theta_{\phi_n}^2 + \theta_{\phi_s}^2 + \theta_{\phi_t}^2) \] (5.14)

where \( d \) and \( \theta \) are the translational displacement and rotation of springs and the subscripts \( n, s \) and \( t \) denote normal direction and 2 transverse directions. Since the contribution of rotational springs \( k_{\phi_n}, k_{\phi_s} \) and \( k_{\phi_t} \) is negligible as demonstrated in Section 4.4.1, \( \beta \) is taken as zero.

Define \( \kappa \) as

\[ \kappa = \frac{d_{s1}^2 + d_{s2}^2}{d_n^2} \] (5.15)

Eq (5.14) becomes

\[ E_{\text{elastic}} = \frac{k_n d_n^2}{2} (1 + \alpha \kappa) \] (5.16)

According to the LEFM (Griffith, 1921), the surface energy \( G_c \) stored in a lattice \( E_{\text{surface}} \) is given by

\[ E_{\text{surface}} = G_c A_f \] (5.17)

where \( A_f \) is the area of facet. If the surface energy solely comes from the elastic energy of lattice \( E_{\text{elastic}} \), Eq. (5.16) and \( E_{\text{surface}} \), Eq. (5.17) can be equated. Rearranging,

\[ d_n = \sqrt{\frac{2G_c A_f}{k_n (1 + \alpha \kappa)}} \] (5.18)

Since the lattice normal force \( F_n = k_n d_n \) and \( k_n = E_{\text{micro}} A_f / l_l \) where \( l_l \) is the lattice length, Eq(5.18) can be written as

\[ F_n = A_f \sqrt{\frac{2G_c E_{\text{micro}}}{l_l (1 + \alpha \kappa)}} \] (5.19)

Introducing the microscopic tensile strength \( f_{st} = F_n / A_l \). Consider the Mode I failure of lattice (i.e. \( G_c = G_{Ic} \)), Eq (5.19) is now expressed as

\[ f_{st}^2 = \frac{2G_{Ic} E_{\text{micro}}}{l_l (1 + \alpha \kappa)} \] (5.20)
Another length scale of a lattice model $l_l$ as illustrated in Figure 5.4 now becomes

$$l_l = \frac{2G_{lc}E_{micro}}{f_{st}^2(1 + \alpha \kappa)} \quad (5.21)$$

(Fig. 5.4 Relationship between the length scales $l_r$ and $l_l$)

The length scale $l_l$ is now expressed into two material parameters, the microscopic tensile strength $f_{st}$ and the critical energy release rate $G_{lc}$. In other words, the lattice length $l_l$ that governs the fineness of a lattice model cannot be arbitrarily specified. However, using this relationship to specify the aspect ratio of cell may introduce anisotropy in a lattice model. This will create a preferred fracture orientation.

### 5.2.3 Stress-Energy Relationship

The stress-energy relationship in LEFM is given by the elasticity solution

$$G_{lc}E_{micro} = K_{lc}^2 \quad (5.22)$$

Noting that the microscopic Possion’s ratio $\nu_s = 0$ as the normal spring and shear springs are not coupled. The energy release rate $G_{lc}$ is given by rearranging Eq. (5.20)

$$G_{lc} = \frac{f_{st}^2(1 + \alpha \kappa)l_l}{2E_{micro}} \quad (5.23)$$
The fracture toughness $K_{lc}$ is given by

$$K_{lc} = f_{st} \sqrt{\frac{\pi l_r}{2}}$$

(5.24)

Therefore,

$$\frac{l_l}{l_r} = \frac{\pi}{(1 + \alpha\kappa)}$$

(5.25)

The stress-energy relationship in LEFM removes the microscopic parameters $E_{micro}$ and $f_{st}$. Since $G_{lc}$ is not easily be determined by experiments, Eq. (5.25) can be used to specify $l_l$ as $l_r$ can be determined by $K_{lc}$ and $f_{st}$ using Eq. (5.13). However, using this relationship to determine the aspect ratio of cells may introduce unwanted anisotropy in a lattice model.

### 5.2.4 Mode II and Mode III fracturing

Similarly, for Mode II (and Mode III) fracture, the length scales $l_r$ and $l_l$ becomes

$$l_r = \frac{2K_{IIc}^2}{\pi f_{ss}^2}$$

(5.26)

$$l_l = \frac{2G_{IIc}E_{micro}}{f_{ss}^2 \alpha (1 + \kappa')}$$

(5.27)

$$\frac{l_l}{l_r} = \frac{\pi}{\alpha (1 + \kappa')}$$

(5.28)

where $\kappa'$ is defined as

$$\kappa' = \frac{\alpha d_t^2 + d_n^2}{\alpha d_n^2}$$

(5.29)

### 5.2.5 Relationship between length scales from geometry of lattice models and from LEFM

In a lattice model, $l_l$ and $l_r$ vary from cell to cell which is generated by the Voronoi tessellation from disordered nodes. Also, $l_l/l_r$ derived from LEFM [Eq. (5.25)] depends on $\kappa$ that depends on the relative displacement of the traverse deformations $d_{s1}$ and $d_{s2}$ to the longitudinal displacement $d_n$ [Eq. (5.15)]. Because of the stress heterogeneity giving disorder in the nodal displacements, $l_l/l_r$ also varies among lattices. So, there are heterogeneities in $K_{lc}$ and $G_{lc}$ at local levels. The following explores the relationship of $\langle l_l/l_r \rangle$ obtained from lattice geometry and LEFM.
From Eq. (5.15)

$$\kappa = \frac{d_{s1}^2 + d_{s2}^2}{d_{n}^2} = \left( \frac{d_s}{d_n} \right)^2$$  \hspace{1cm} (5.30)

where $d_s$ is the total nodal shear displacement. $\kappa$ can be expressed in a more meaningful form. Given that $d_s = F_s/k_s = \sigma_{fs}^f A_f/k_s = \sigma_{fs}^f A_f/(\alpha k_n)$ and $d_n = F_n/k_n = \sigma_{fn}^f A_f/k_n$,

$$\kappa = \left( \frac{\sigma_{fs}^f A_f/(\alpha k_n)}{\sigma_{fn}^f A_f/k_n} \right)^2 = \frac{1}{\alpha^2} \left( \frac{\sigma_{fs}^f}{\sigma_{fn}^f} \right)^2 , \hspace{0.5cm} \kappa = 0 \hspace{0.5cm} \text{for} \hspace{0.5cm} \alpha = 0$$  \hspace{1cm} (5.31)

Now, $\kappa$ is expressed as the ratio of facet shear stress $\sigma_{fs}^f$ to facet normal stress $\sigma_{fn}^f$. $\kappa$ varies among lattices and $<\kappa>$ is related to $\alpha$ and the ratio $\sigma_{fs}^f/\sigma_{fn}^f$ that depends on the loading condition.

Table 5.1 lists the statistics of $l_l$, $l_r$ and $l_l/l_r$ in lattice models of D50, M50 and S50. $<l_l/l_r>$ varies from 1.563 to 1.694 and increases slightly with decreasing $n$. For the lattice models under isotropic stress, shear springs are not mobilised (i.e. $\sigma_{fs}^f = 0$) as demonstrated in Section 4.5.2. This gives $\kappa = 0$ and $l_l/l_r = \pi$. This gives as much as 100% difference in the calculations of $<l_l/l_r>$.

Under uni-axial load, the mobilisation of shear springs depends on their orientation such that $\kappa$ also depends on the lattice orientations. Table 5.2 lists $<l_l/l_r>$ computed from Eq (5.25), $\kappa$ is obtained from Eq (5.31) and the LEM simulation results. $<l_l/l_r>$ varies from 1.440 to 1.534 with different $\alpha$ and $n$. $<l_l/l_r>$ given by the geometry of lattice models is slightly larger than the computed values from Eq. (5.25) and their difference lies between 2% and 16%.

In order to comply with LFEM, the length scales have to be chosen for a particular loading condition. This is because LFEM is derived based on the assumption of continuum mechanics in which there is no length scale except the fracture itself. LEM has intrinsic length scales that characterises the heterogeneity of material. It also gives the local variation of fracture toughness $K_{Ic}$ and critical energy release rate $G_c$ that deviated from the assumptions of continuum mechanics. So continuum based numerical methods are more suitable in modelling homogeneous material that complies with LFEM.

<table>
<thead>
<tr>
<th>Lattice model</th>
<th>$l_l$(m)</th>
<th>S.D.</th>
<th>$l_r$(m)</th>
<th>S.D.</th>
<th>$l_l/l_r$</th>
<th>S.D.</th>
</tr>
</thead>
<tbody>
<tr>
<td>D50</td>
<td>2.709</td>
<td>0.473</td>
<td>1.460</td>
<td>1.157</td>
<td>1.563</td>
<td>1.053</td>
</tr>
<tr>
<td>M50</td>
<td>2.737</td>
<td>0.624</td>
<td>1.461</td>
<td>1.256</td>
<td>1.644</td>
<td>1.144</td>
</tr>
<tr>
<td>S50</td>
<td>2.757</td>
<td>0.781</td>
<td>1.471</td>
<td>1.327</td>
<td>1.694</td>
<td>1.200</td>
</tr>
</tbody>
</table>

Table 5.1 Statistics of length scales $<l_l>$ and $l_r$ and their ratio $l_l/l_r$ of lattice models
Fracturing simulation using LEM

<table>
<thead>
<tr>
<th>Lattice model</th>
<th>( \alpha )</th>
<th>( \sigma_f^L / \sigma_f^L ) Mean</th>
<th>( \sigma_f^L / \sigma_f^L ) S.D.</th>
<th>( \sigma_f^F / \sigma_f^F ) Mean</th>
<th>( \sigma_f^F / \sigma_f^F ) S.D.</th>
<th>( \kappa )</th>
<th>( l_l / l_r )</th>
</tr>
</thead>
<tbody>
<tr>
<td>D50</td>
<td>0.3</td>
<td>0.2020</td>
<td>0.1627</td>
<td>0.3463</td>
<td>0.6579</td>
<td>3.781</td>
<td>1.472</td>
</tr>
<tr>
<td>M50</td>
<td>0.5</td>
<td>0.2672</td>
<td>0.2115</td>
<td>0.3476</td>
<td>0.5630</td>
<td>2.364</td>
<td>1.440</td>
</tr>
<tr>
<td>S50</td>
<td>0.5</td>
<td>0.2716</td>
<td>0.2170</td>
<td>0.3476</td>
<td>0.5578</td>
<td>2.442</td>
<td>1.414</td>
</tr>
</tbody>
</table>

\*\( \sigma_f^L / \sigma_f^L \) is approximated by \( \sigma_f^L / \sigma_f^L \) since it is strongly affected by small values of \( \sigma_f^L \).

Table 5.2 Ratio of length scales \( l_l \) and \( l_r \) as determined by LEFM and the LEM simulation results of lattice models under uni-axial stress.

5.3 Flow of fracturing simulation

![Flow chart of fracture simulation in LEM3D](image)

Fig. 5.5 Flow chart of fracture simulation in LEM3D
Figure 5.5 shows the flow of LEM3D in fracture simulation. To proceed to the next load step, there should be no lattice reconnection or disconnection. Iterations are carried out to reconnect and to disconnect lattices until there are no such lattice or the total number of them is smaller than an allowable number $N_{rd}$ or the iteration number is larger than $i_{rd}$. These relaxation criteria are introduced because some fractures may oscillate between connected and disconnected states under tiny load change, particular in highly heterogeneous models and models close to failure.

The statistics of the lattice models used for simulations in this Chapter are listed in Table 5.3.

<table>
<thead>
<tr>
<th>Lattice model</th>
<th>Dimensions (m)</th>
<th>$l_{min}$ (m)</th>
<th>$&lt;l&gt;$ (m)</th>
<th>n</th>
<th>$N_{node}$</th>
<th>$N_{lattice}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2D D80</td>
<td>40 × 3 × 80</td>
<td>1.0</td>
<td>1.454</td>
<td>0.5</td>
<td>6,788</td>
<td>41,392</td>
</tr>
<tr>
<td></td>
<td>40 × 3 × 80</td>
<td>0.585</td>
<td>1.392</td>
<td>0.1</td>
<td>6,788</td>
<td>41,415</td>
</tr>
<tr>
<td>3D D50</td>
<td>100×100×100</td>
<td>2.0</td>
<td>2.716</td>
<td>0.5</td>
<td>88,388</td>
<td>631,147</td>
</tr>
<tr>
<td></td>
<td>40 × 40 × 80</td>
<td>1.0</td>
<td>1.358</td>
<td>0.5</td>
<td>90,509</td>
<td>645,094</td>
</tr>
</tbody>
</table>

Table 5.3 Details of lattice models used for simulations on fracturing in uni-axial tension and compression load.
5.4 Simulation of fracturing due to uniaxial tension

To start with, the lattice models under uniaxial tension are simulated with different $\alpha$ and $n$. Both 2D and 3D simulations are carried out to study the 3D effects in fracturing simulation. Afterwards, heterogeneities are applied to both the spring stiffness $E_{\text{micro}}$ and the microscopic strengths, $f_{st}$ for tensile and $f_{ss}$ for shear to study the effects of heterogeneity on fracturing.

A series of 3D lattice models with different $n$ (D50, M50 and S50 models) under uni-axial tensile loading by applying uniform strain on boundaries along z-direction. Figure 5.7 shows the stress-strain curves from 9 simulations with different $n$ and $\alpha$. The macroscopic tensile strength $f_t$ (peak stress) is largely governed by $\alpha$. When $\alpha = 1.0$, $f_t \approx f_{st}$ ($f_t / f_{st} = 0.975$ for $n = 0.5$). However, it shows extremely brittle behaviour. $f_t$ decreases with $\alpha$. $f_t / f_{st} \approx 0.65$ for $\alpha = 0.3$ and $f_t / f_{st} \approx 0.29 - 0.34$ for $\alpha = 0.0$. With decreasing $\alpha$ the lattice model becomes more ductile, but it is considered very brittle for rock even $\alpha = 0.0$ is used.

5.4.1 Effect of mesh fineness

Fig. 5.6 Stress strain curve of cubic lattice model with different mesh fineness (D100,D50,D25)
Figure 5.6 compares the strain-strain curves of 3 different mesh fineness (D100, D50 and D25) under uni-axial tension when $\alpha$ is fixed at 0.3. Mesh fineness has negligible effect on both $f_t$ and the residual tensile stress after the peak $f_{t,r}$. The distinct difference lies on the degree of snap back. A finer model (e.g. D50 and D100 models) gives higher degree of snap-back and hence higher brittleness. D25 models shows negligible snap-back.

A finer model corresponds to the material with fine grains. They have lower toughness as size of facet is smaller according to Eq. (5.13). However, the macroscopic strength $f_t$ remain almost constant because the initiation of isolated fracture is not affected by the fineness of the model.

### 5.4.2 Effect of node density $n$

From the stress-strain curves shown in Figure 5.7 for different $\alpha$, the effect of $n$ is negligible for $\alpha = 1.0$ and $\alpha = 0.3$ cases. For $\alpha = 0$, smaller $n$ gives slightly smaller $f_t$ but more ductility. $n$ affects more when $\alpha = 0.0$. Local heterogeneity given by irregularity of cell has a greater effect on the macroscopic behaviour provided by smaller $\alpha$.

### 5.4.3 Stage of fracturing

Figure 5.8 shows the snapshots of fracture development at different stages in 3D simulations (D50 models). Tensile fracturing can be roughly classified into three stages according to their stress strain curves in Table 5.4:

<table>
<thead>
<tr>
<th>Demarcation in stress-strain curve</th>
<th>Region</th>
</tr>
</thead>
<tbody>
<tr>
<td>‘o’ - ‘a’</td>
<td>Pre-peak</td>
</tr>
<tr>
<td>‘a’ - ‘b’</td>
<td>Linear</td>
</tr>
<tr>
<td>‘b’ - ‘d’</td>
<td>Non-linear</td>
</tr>
<tr>
<td></td>
<td>Post-peak</td>
</tr>
</tbody>
</table>

Table 5.4 Stages of fracturing as delineated by stress strain curves

Point ‘o’ is the starting point and point ‘a’ is the location where a lattice model starts to undergo non-linear behaviour. Point ‘b’ is well defined which is the peak stress. Point ‘d’ is the point of the sudden change of stress-strain curve after peak, usually the lowest point of the curve. Point ‘c’ is the point between ‘b’ and ‘d’ for visualisation of fracturing in the post-peak region in Figure 5.8 and other figures in this Chapter. Points ‘a’ and ‘d’ are not well-defined. Numerous isolated and distributed fractures appear in regions ‘o-b’ for $\alpha = 0.3$ and $\alpha = 0.0$. For $\alpha = 1.0$, only a few distributed microcracks formed and the fractures are rapidly localised as a single horizontal fracture. The curve beyond ‘d’ is considered as the completely collapse. The behaviour beyond point ‘d’ is not well captured by LEM3D.
Fracturing simulation using LEM

Fig. 5.7 Stress strain curve of cubic lattice model with different mesh fineness, \( n \) for D50, M50 and S50 models, and effect of \( \alpha \) when \( \alpha = 1.0 \), (a) \( \alpha = 0.3 \) and (c) \( \alpha = 0.0 \) under uniaxial tension. Effect of \( n \) when (a) \( \alpha = 1.0 \), (b) \( \alpha = 0.3 \) and (c) \( \alpha = 0.0 \) for D50, M50 and S50 models.
Fig. 5.8 Snapshots of fracture evolution at point ‘a’ to ‘d’ (in stress strain curves defined in Figure 5.7) of D50 lattice model with different $\alpha$ under uniaxial tension. Fracture colour indicates time of formation (blue-early, red-late).
simulations because it involves large deformation and detachment of fragments which are not considered in LEM.

The non-linear region is contributed by isolated and distributed microcracks formed before the peak load. They are spatially uncorrelated. Their formation is related to the stress heterogeneity which is also spatially uncorrelated. For $\alpha = 0.3$, fractures coalescence and localise immediately after peak load is reached. For $\alpha = 0.0$, the stress heterogeneity is high enough that fracture coalescence happens in several locations simultaneously after peak stress and competing with one another before forming into a single fracture. This results in a rougher fracture surface.

### 5.4.4 Post-peak behavior: Snap back

All the stress-strain curves show a snap back after peak (from point ‘b’ to ‘d’). The significant decrement in axial strain $\varepsilon_{zz}$ is observed for $\alpha = 0.3, 1.0$ and slight decrement is observed for $\alpha = 0.0$. This is called Class II behaviour as first observed in laboratory tests of brittle rock by Wawersik and Fairhurst (1970). They pointed out that this was an unstable fracture propagation that the fracture growth was self-sustaining without any work done from external load. In other words, after the peak, the strain energy stored in lattice network is sufficient to sustain fracture growth until collapse. Energy must be extracted from the system to capture such unstable propagation. In LEM simulation, this is done by unloading of model when breaking of lattice is detected as described in Section 5.1.1.

The area under a stress-strain curve indicates the strain energy stored in lattice network. The snap-back part of the stress strain curve indicates energy release during fracturing. The area under the stress-strain curve denotes energy dissipated by the entire fracturing process and the curve under the snap-back part means negative contribution. The smaller the energy dissipated is, the higher the brittleness of a lattice model becomes. As the energy dissipation of models decreases with increasing $\alpha$, the brittleness increases with $\alpha$.

The residual tensile stress after unstable fracturing comes from unfavourably orientated lattices (i.e. sub-horizontal). They still connect two cells that are separated by the main fracture, as shown in Figure 5.9. These springs are difficult to be mobilised under loading.
5.5 Applying heterogeneity - Uni-axial tension

To simulate more ductile fracture failure of rock, additional heterogeneity has to be applied on both microscopic stiffness $E_{\text{micro}}$ and microscopic strengths $f_{st}$ and $f_{ss}$. There should be a correlation between them. In this study, it is assumed that they are fully correlated by applying the same modification factor to both parameters. Simulations are carried out in 2D models (D80p models) with 9 different PDFs applied, 3 of each normal, lognormal and Weibull distributions with different variances as detailed in Section 4.6.

Figure 5.10 shows the stress-strain curves of D80p models with and without applied heterogeneity. The macroscopic tensile strength $f_t$ significantly decreases with the applied heterogeneity. On the contrary, the residual tensile strength increases. Some models show Class II snap back behaviour but the degree of snap back reduces with heterogeneity. Lattice model becomes more ductile as heterogeneity increases.

As shown in Figure 5.10a, there is a linear correlation between $f_t$ and standard deviation $\sigma$ of PDFs applied, irrespective of the type of distribution. The graph also shows strong correlation between strength and brittleness. Models with higher strength are more brittle. Ductility can be enhanced by introducing heterogeneity at the expense of reducing strength. At low stress stage, weak lattices break that weaken the model macroscopically. At higher stress and post peak stages, strong lattices survive to hold the model that provides higher residual strength and ductility.
Fracturing simulation using LEM

Fig. 5.10 Stress-strain curves of D80p plain strain model ($\alpha = 0.3$) with different PDFs applied on stiffness and strength of lattices under uni-axial tension. (a) Relationship between standard deviation $\sigma$ with $f_t$ and residual macroscopic residual tensile strength $f_{t,r}$. (b) Applying normal distribution with $\sigma = 0.25$, 0.5, and 0.75. (c) Applying lognormal distribution with $\sigma = 0.25$, 0.5, and 0.75. (d) Applying Weibull distribution with $k = 3.0$, 2.5, and 2.0. The insert figure shows the PDF curves being applied.
5.5 Applying heterogeneity - Uni-axial tension

5.5.1 Fracture evolution

Fracture evolution can be roughly classified into 2 stages, (1) isolated and distributed fracturing and (2) fracture localisation.

Figure 5.11 shows the snapshots of fracture evolution of the D80p models (2D) with and without PDFs applied on the lattice strength and stiffness. Without applying heterogeneity, the dominant fracture is horizontal except $\alpha = 0.0$.

For the extremely brittle models with $\alpha = 1.0$, a micro-crack rapidly localises and develops into a dominant fracture without transition stages. For models with $\alpha = 0.3$, there are only one fracture clusters that localises and grows rapidly without coalescence with other fractures. The rest of fracture clusters are too small to compete and interfere with the main one so a relatively horizontal fracture is formed.

When a higher heterogeneity model is used for $\alpha = 0.0$, more distributed micro-cracks are formed and they grow before developing a dominant fracture. The density of micro-cracks increases with the heterogeneity of lattice models. The dominant fracture becomes more tortuous and formed a ‘fracture band’ with certain width instead of a distinct fracture. As the result of complex interaction among competing fracture clusters, the fracture propagation orientation changes constantly to search for a path of least resistance. Coalescence of larger fracture clusters results in a rapid change of fracture path and a thicker fracture band.

5.5.2 Comparison between 2D and 3D models

Figure 5.12 compares the stress-strain curves of the 2D (D80p models) and 3D (D50 models) lattice models under uniaxial tension. Without applied heterogeneity, the macroscopic behaviours between 2D and 3D lattice models are very similar.

With PDFs applied on lattice stiffness and strength, $f_t$ in 3D case is larger and the difference increases with increasing the applied heterogeneity. 2D models are more brittle compared with 3D models and the difference increases with the applied heterogeneity as well.

For 3D models, the extra dimension increases the node coordination number $n_{\text{coord}}$. There are more neighbouring lattices to share loading after lattice breakage. This deters coalescence of fracture, resulting in the lengthening of the non-linear region ‘a’ to ‘b’ as well. The increase in residual strength also results in more unfavourably orientated lattices which gives higher $n_{\text{coord}}$. 
Fracturing simulation using LEM

Fig. 5.11 Snapshots of fracture geometry evolution of D80p plain strain model under uni-axial tension with different $\alpha$ (0.0, 0.3 and 1.0) and 9 different PDFs [normal N(0.25), N(0.50), N(0.75), lognormal LN(0.25), LN(0.50), LN(0.75) and Weibull W(3.0), W(2.5), W(2.0)] applied on stiffness and strength of lattices. Point 'b' and 'd' are marked in relevant stress-strain curves ('b' - peak load, 'd' - end of unstable propagation (may absent for some cases) and 'j' - end of simulation). Fracture colour indicates time of formation (blue early, red late).
5.5 Applying heterogeneity - Uni-axial tension

Fig. 5.12 Comparison of stress-strain curves fracture simulation under uni-axial tension in 2D (D80p models) and 3D (D50 models). (a) Uniform model, $\alpha = 0.0, 0.3$ or $1.0$, (b) with applied heterogeneity, $\alpha$ is fixed at 0.3.

5.5.3 Stages of fracture development

Figure 5.13 shows the snapshots of fracture evolution under uni-axial tension in the 3D cases. Similar to the 2D cases, more isolated and distributed fractures are formed during the linear region when the applied heterogeneity increases. At the peak load (point ‘b’), large fracture clusters have already formed in the 3D cases with large applied heterogeneity such as LN(0.50), LN(0.75), W(2.0) cases but not in the 2D simulations (Figure 5.11). For these 3D simulations, multiple horizontal fracture clusters are formed but only one horizontal fracture is formed for their corresponding 2D simulations.

By in-depth investigation of the uni-axial tension simulation in 3D, the fracture development can be further divided into the following 5 stages:

Figure 5.14 compares the snapshots of tensile fracturing simulations at different stages among D50 models of various applied heterogeneity [Uniform, LN(0.25), LN(0.50) and LN(0.75)] with demarcation of 5 stages of fracture development. For uniform lattice model, there is no stage III and IV of fracturing. Growth of microcracks localises rapidly and develops into a dominant fracture when the macroscopic tensile stress approaches its peak value. Because of the minimal interference with other large fracture clusters, the dominant fracture is less rough compared with the models with larger applied heterogeneity.

For LN(0.25) model, there is no stage IV fracturing. There is localisation of microcracks forming small fracture clusters at multiple locations. It is interesting to note that the dominant fracture developed after peak loading is not formed by coalescence of these small fracture clusters. It is formed at the location where there are several strong lattices which
Fig. 5.13 Snapshots of fracture evolution at point ‘a’ to ‘d’ of D50 lattice model with different applied heterogeneity [No PDF applied, LN(0.25), LN(0.50), LN(0.75), N(0.50), W(2.0)] under uniaxial tension. $\alpha$ is fixed at 0.3. Fracture colour indicates time of formation (blue-early, red-late).
### 5.5 Applying heterogeneity - Uni-axial tension

<table>
<thead>
<tr>
<th>Stage</th>
<th>Descriptions</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td><strong>Distributed formation of micro-cracks</strong></td>
</tr>
<tr>
<td></td>
<td>Formation of micro-crack is spatially uncorrelated and individual fracture cluster growth is non-continuous during loading</td>
</tr>
<tr>
<td>II</td>
<td><strong>Distributed growth of micro-cracks</strong></td>
</tr>
<tr>
<td></td>
<td>Microcracks grow slowly alongside with formation of new microcracks. Both processes are spatially uncorrelated and micro-crack growth is non-continuous and its size remains small.</td>
</tr>
<tr>
<td>III</td>
<td><strong>Localised and non-competing fracture grow</strong></td>
</tr>
<tr>
<td></td>
<td>Majority of fracture growth happens in one or several large fracture clusters (or ‘fracture band’) and fracture growth is continuous during loading. Fracture coalescence start to take place among small fractures. They are separated far enough from one another such that their growth are not interfered.</td>
</tr>
<tr>
<td>IV</td>
<td><strong>Localised and competing fracture grow</strong></td>
</tr>
<tr>
<td></td>
<td>Fracture clusters interact with one another, either reinforcing their growth or hindering their growth (stress shadowing). For the former case, large fracture clusters start to coalesce.</td>
</tr>
<tr>
<td>V</td>
<td><strong>Dominant fracture growth</strong></td>
</tr>
<tr>
<td></td>
<td>Fracture growth happens predominantly in a single large fracture with minor interference with other fracture clusters.</td>
</tr>
</tbody>
</table>

Table 5.5 Five stages of fracture development
Fracturing simulation using LEM

Fig. 5.14 Snapshots of fracture cluster evolution (from 0.7 to 0.75, where 0.7 corresponds to calculation step at Point b of stress-strain curve) of D50 lattice model with different applied heterogeneity [No applied, LN(0.25), LN(0.5) and LN(0.75)] under uniaxial tension showing five stages of fracture development. Fracture clusters are distinguished by different colours.
are equally critical. When one of them fails, the adjacent lattices fail simultaneously and fracture propagates very fast to form a dominant fracture. It is also a characteristic of the brittle failure.

For LN(0.50) model, the growth of multiple fracture clusters can sustain longer, forming larger clusters. As they grow, the separation between clusters reduces and they may interact with one another, either the growth is suppressed or reinforced and coalesce to a large cluster. When a dominant fracture is formed, it may coalesce with smaller fracture clusters or is interfered by them. Therefore, the fracture surface becomes very bumpy.

For even more heterogeneous models like LN(0.75) model, multiple fracture growth sustains longer and forms larger clusters before a dominant one is formed. The model may consists of several horizontal main fractures.

For more quantitative analysis, Figure 5.15 shows the growth of isolated fractures and fracture clusters with (lognormal distributions in this case) and without applying PDFs (uniform) on lattice strength and stiffness during fracturing. The demarcation of the five stages of fracture development are shown in the figure.

All the fracturing starts from stage I. Stage II fracturing starts when the curve of isolated fractures and that of the total facet starts to diverge in Figure 5.15, meaning that there is growth of micro-fractures. Stage III starts when the curve of isolated fracture stops increasing, indicating the growth of microcracking stops and fracture growth happens mainly in fracture clusters. There are fracture coalescence among small fractures. Stage IV is not easily be demarcated in Figure 5.15. It is determined by snapshots in Figure 5.15 showing that fracture clusters are close to one another. In Stage V, the curve shows the dominant growth of the largest fracture cluster.

Apart from the uniform model, the dominant fracture forms shortly after reaching the peak load in Stage V. The majority of fracture growth happens in the dominant fracture and the growth of other fracture clusters virtually stops.

Homogeneous models are characterised by predominantly stage I and II fracturing before peak. In this two stages, cracks formed are mainly isolated as indicated by small difference between the curves of the number of isolated fracture facets and the total number of fracture facets in Figures 5.15a,b. The size of fracture cluster remains small as indicated by slow increase of the curve of total number of fracture facets of the first 10 fracture cluster in the same figure. Stages III and IV may be absent or cannot sustain for a long time before the formation of the dominant fracture. Once a dominant fracture forms, it grows rapidly and freezes the growth of the rest of fracture clusters in the homogeneous models.

For heterogeneous models, isolated and distributed fractures are easier to grow into clusters before the peak load as indicated by the steadily increasing of the curve of total
Fracture colour indicates time of formation (blue-early, red-late).

Fig. 5.15 Snapshots of fracture evolution of D80p/S80p lattice model ($\alpha = 0.3$) under uniaxial compression and failure type of fracture.
number of fracture facets in the first 10 fracture clusters as shown in Figure 5.15c,d. This gives a relatively short stage I fracturing. Instead, these models demonstrate longer stage III and IV fracturing which gives the macroscopic non-linear softening in the stress-strain curves as shown in Figure 5.10.

5.5.4 Evolution of fracture cluster size

Fig. 5.16 Evolution of fracture cluster of D80p plain strain model under uni-axial tension with and different applied heterogeneity [LN(0.25), LN(0.5), LN(0.75)]. Step number n is normalised by step number at peak \( n_{\text{peak}} \).

Figure 5.16 shows the evolution of (i) the ratios of the total number facets of isolated fracture, (ii) that of the largest five fracture clusters and (iii) that of the largest fracture cluster to the total number of fracture facets among models with different heterogeneities. The growth of micro-cracks starts earlier for the heterogeneous models as indicated by the onset of decreasing of the ratio of the number of facets of isolated fractures to the total number of fracture facets. For example, the microcrack growth starts at \( \approx 0.1 n_{\text{peak}} \) for LN(0.75) model compared with \( \approx 0.35 n_{\text{peak}} \) for LN(0.25) model, where \( n_{\text{peak}} \) is the step number at the peak load.
After that, larger fracture clusters start to develop which is indicated by the onset of the growth of the ratio of total number of fracture facets of the largest 5 fracture clusters to the total number of fracture facets as shown in Figure 5.16. For the homogeneous models, large fracture clusters develop later \( \approx 0.6n_{\text{peak}} \) for LN(0.25) model as compared with the heterogeneous models \( \approx 0.2n_{\text{peak}} \) for LN(0.75) model and \( \approx 0.3n_{\text{peak}} \) for LN(0.5) model.

In more homogeneous model [LN(0.25)], the percentage of isolated fracture facets is very high (>95%) before the peak load and the largest fracture cluster remains very small (<2%). This means that there is only the formation of microcracks (Stage I) and the distributed growth of microcracks (Stage II) before the peak stress.

Before the peak stress in the heterogeneous models, the percentage of the number of fracture facets of the largest 5 clusters increases slowly (<10%) while the percentage of the isolated fracture facets decrease steadily [from 100% to 45% LN(0.75) or 55% LN(0.5)] as shown in Figure 5.16. The large difference in percentage shows that the growth of fracture clusters happens at multiple locations. Also, among the largest 5 fracture clusters, they are of similar sizes and grow at similar rates which is reflected by the difference between curves of largest 5 clusters and the largest cluster as shown in Figure 5.16. This shows the steady growth of fracture clusters (Stage III or Stage IV).

For all three simulations, the onset of dominant fracture growth (Stage V) happens at the peak load when the rapid growth of the largest fracture cluster happens as shown in Figure 5.16. The growth of other fracture clusters virtually stop.
5.6 Microscopic stress evolution during tensile fracturing

5.6.1 Facet normal stress $\sigma_{fn}^f$

Facet normal stress reflects the mobilisation of normal springs in a lattice model. Figure 5.17 shows the evolution of the PDF curves of facet normal stress $\sigma_{fn}^f$ among four D50 lattice models with different degrees of applied heterogeneity under uni-axial tension. The PDF curves also show contributions from different lattice orientations.

For the homogeneous models, the change of PDFs is small during the pre-peak stage but significant changes are observed in the post-peak stage. The mean of the facet normal stress $<\sigma_{fn}^f>$ remains roughly unchanged during the entire fracturing process among all lattice orientations. For sub-vertical lattices (80°-90° to horizontal), $<\sigma_{fn}^f>$ changes from 0.894$p_L$ to 0.853$p_L$ for the uniform model and 0.896$p_L$ to 0.948$p_L$ for LN(0.25) model in the entire fracture process. As discussed in Sections 5.5.3 and 5.5.4, there are small amount of distributed microcracks form in the pre-peak stage so changes in the PDFs are small.

In the post-peak stage, both the standard deviation (SD) and the kurtosis significantly increase. For sub-vertical lattices in the uniform model, the SD changes from 0.675$p_L$ to 1.243$p_L$ and the kurtosis changes from 1.074$p_L$ to 10.26$p_L$. This means that $\sigma_{fn}^f$ are spread towards both ends. At one end, there are substantial releases of tensile stress or even the development of compressive stress among some lattices. At the another end, some lattices experience substantial increase in tensile stress. These two distinctive behaviours are created by the formation of the dominant fracture in the post-peak stage. Lattices behind the dominant fracture are unloaded and the remaining lattices in front of the dominant fracture need to take extra load.

For the heterogeneous models, the trend is the opposite. There are significant changes in the PDF curves in the pre-peak stage and small changes in the post-peak stage. For the sub-vertical lattices in LN(0.75) model, the SD changes from 0.851$p_L$ to 1.702$p_L$. Referring to Figure 5.14, there are many fracture clusters formed in the heterogeneous models. This creates a lot of loading and unloading of lattices locally. Another interesting observation is that there are increases in tensile stress among vertical lattices and compressive stress among horizontal lattices. A plausible explanation is that the fracture clusters formed are rough and slightly inclined. They also interact with one another. So the load transfer between lattices has to take a tortuous path. More stresses are induced for this inefficient path as compared with a more direct load path.

In the post-peak stage, there are less changes in PDF curves compared with the pre-peak stage. From Figure 5.15, the growth of the largest fracture cluster (dominant fracture) after
Fig. 5.17 Evolution of facet normal stress $\sigma_{fn}/p_L$ ($p_L$ is applied pressure) of uni-axial tension test of D50 models with different applied heterogeneity. The PDF curves are decomposed into 9 components according to lattice orientation to horizontal ($1: 0^\circ - 10^\circ$, $9: 80^\circ - 90^\circ$), only 5 curves are shown for clarity. [(a),(b) No distribution, (c),(d) LN(0.25), (e),(f) LN(0.5) and (g),(h) LN(0.75)]. The failed lattices are excluded in calculation.
5.6 Microscopic stress evolution during tensile fracturing

the post-peak stage is smaller in the heterogeneous models. The dominant fracture is formed
by coalescence of other fracture clusters so fewer lattices are affected.

5.6.2 Facet shear stress $\sigma_s^f$

Figure 5.18 shows the PDF curves of facet shear stress $\sigma_s^f$ among four D50 lattice models
with different degrees of applied heterogeneity under uni-axial tension. The PDF curves
show contributions from different lattice orientations. In general, inclined lattices which
orientated between $40^\circ$ and $50^\circ$ from horizontal take more shear than the rest of them.

Shear stress in lattice increases along the fracturing process for all four models but the
rates of increase among them are different. The rates are smaller among the homogeneous
models. For example, among lattices orientated between $40^\circ$ and $50^\circ$ in the uniform model,
$<\sigma_s^f>/p_L$ increases from 0.241 to 0.260 and finally 0.294 at point ‘o’, point ‘b’ and point
‘d’ respectively, where $p_L$ is applied macroscopic tensile stress. The corresponding values for
LN(0.75) model are 0.254, 0.461 and 0.533. Point ‘o’ to ‘b’ is the pre-peak stage and point
‘b’ to point ‘d’ is the post-peak stage. Lattices oriented in other directions also show this
trend. So one of the characteristics of the heterogeneous models is the increased mobilisation
of shear springs in fracturing.

For the homogeneous models, the changes in the PDF curves mostly happen in the
post-peak stage while most changes happen in the pre-peak stage for the heterogeneous
models. This is similar to the findings in Section 5.6.1 about facet normal stress $\sigma_n^f$.

5.6.3 Nodal stress invariant

Figure 5.19 shows the evolution of the PDFs of the nodal mean stress $p^n$ and the nodal
deviator stress $q^n$ among D50 lattice models with different applied heterogeneities. $p^n$ and
$q^n$ are regarded as the homogenised stresses of the facet normal stress $\sigma_n^f$ and the facet shear
stress $\sigma_s^f$ of facets (lattices) in different orientations. $p^n$ is a measure of bulk deformation of
cell while $q^n$ is a measure of cell distortion.

During the whole fracturing process, $<p^n> \approx 1/3p_L$ for both homogeneous and hetero-
genous models. This is the value for the macroscopic mean stress $p$ as well. The SDs of $p^n$
increase with the applied heterogeneity. At the peak load, the SDs of $p^n/p_L$ among uniform,
LN(0.25), LN(0.5) and LN(0.75) models are 0.187, 0.336, 0.554 and 0.754 respectively.
These trends are similar for $\sigma_n^f$ as mentioned in Section 5.6.1.

$<q^n>$ increases with the fracturing process. At the peak load, $<q^n>/p_L$ are 1.120,
1.184, 1.226 and 1.370 for uniform, LN(0.25), LN(0.5) and LN(0.75) models respectively.
The SDs also increase with the heterogeneity of the models from 0.144 (uniform model) to
Fig. 5.18 Evolution of facet shear stress $\sigma_f^d/p_L$ ($p_L$ is applied pressure) of uni-axial tension test of D50 models with different applied heterogeneity [(a), (b) No PDF applied, (c), (d) LN(0.25), (e), (f) LN(0.5) and (g), (h) LN(0.75)]. The PDF curves are decomposed into 9 components according to lattice orientation to horizontal (1: $0^\circ - 10^\circ$, 9: $80^\circ - 90^\circ$), only 5 curves are shown for clarity. The failed lattices are excluded in calculation.
Fig. 5.19 Evolution of nodal stress of uni-axial tension test of D50 models with different applied heterogeneity (No distribution, LN(0.25), LN(0.50), LN(0.75)).

(Con’t) (a,b) normalised nodal mean stress $3p^n/p_L$ ($p_L$ is applied pressure) and (c,d) normalised nodal deviator stress $q^n/p_L$.
0.534 [LN(0.75) model]. Again, this trend is similar to facet shear stress $<\sigma_s^f>$ mentioned in Section 5.6.1.

## 5.6.4 Summary

In the homogeneous models, the changes in the PDFs of the facet microscopic stresses $\sigma_n^f$, $\sigma_f^f$ are small during the pre-peak stage but their changes are large during the post-peak stage. The small changes in the pre-peak stage are due to small amount of distributed macro-cracks in the pre-peak stage. The large changes in the post-peak stage are due to the formation of the dominant fracture causing large amount of loading and unloading of lattices.

In the heterogeneous models, the trend is the opposite. The changes in the PDFs of the facet microscopic stresses $\sigma_n^f$ and $\sigma_f^f$ are large during the pre-peak stage but their changes are smaller during the post-peak stage. The large changes in the pre-peak stage is due to formation of multiple fracture clusters causing a lot of loading and unloading of lattices locally. At the post-peak stage, dominant fracture is formed by coalescence of these fracture clusters so fewer lattices are affected.

For the nodal mean stress $p^n$, the SDs increase with increasing heterogeneity of models while the means $<p^n>$ remain roughly unchanged. The mean and SDs of the nodal deviator stress $q^n$ increase with heterogeneity of models.
5.7 Experiment comparison

There are several model parameters defining microscopic behaviour of lattice and the micro-macro relationship has been explored in Chapter 4 and this Chapter. This section compares the experimental results from a literature with LEM simulation results to gain an understanding on obtaining realistic model parameters.

The laboratory test results of a direct tension test reported from Labuz et al. (1985) is used for comparison. The rock sample is called Charocal black which is a medium to fine grained granite.

The laboratory setup is illustrated in Figure 5.20a. The crack mouth displacement was measured by linear variable differential transformer (LVDT). The dimensions of the sample were $280 \times 75 \times 13$ mm and the nominal notch length was 13mm. Wedge-type friction grips were used to apply tension. The test was displacement-controlled. Figure 5.20b shows the LEM model for simulations. Only 75mm length of the sample is modelled. The base of the model is constrained in the vertical direction only and uniform displacement is applied on top.

Five simulations are carried out to compare with the experimental results. 4 of them use D75 model with different PDFs [uniform, LN(0.5), LN(0.75) and LN (1.0)]. To test the sensitivity of mesh finesss, another simulation is carried out in a finer model D115. The model parameters of LEM simulation are summarised in Table 5.6.
Fig. 5.21 Snapshot of last step of LEM simulation on double notch rock sample under direct tension test with different PDF applied on lattice parameters. D75 model: (a) Without PDF applied (b) lognormal LN(0.5), (c) lognormal LN(0.75) and (d) lognormal LN(1.0). D115 model: (e) lognormal LN(0.75). Red indicates distributed fracture, blue indicate main fracture.
Table 5.6 Parameters of LEM simulation for double notch rock sample under direct tension test

<table>
<thead>
<tr>
<th>Lattice model</th>
<th>( E_{\text{micro}} ) (GPa)</th>
<th>( \alpha )</th>
<th>( f_{st} ) (MPa)</th>
<th>( f_{ss}/f_{st} )</th>
<th>( n )</th>
<th>( l_{\text{min}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>D75</td>
<td>71.42</td>
<td>0.3</td>
<td>19.53</td>
<td>1.0</td>
<td>0.5</td>
<td>1.0</td>
</tr>
<tr>
<td>D115</td>
<td>71.42</td>
<td>0.3</td>
<td>19.53</td>
<td>1.0</td>
<td>0.5</td>
<td>0.65</td>
</tr>
</tbody>
</table>

Figure 5.21 shows the snapshots of the LEM simulations on the double notch sample. When no PDF is applied to lattice parameters, the main fracture formed is planar with little asperities as shown in Figure 5.21a. There are only few isolated fractures near the main fracture. When heterogeneity is applied, distributed microcracks are formed and the amount increases with increasing heterogeneity of sample. Also, the main fracture shows higher asperity and tortuosity when the heterogeneity of model increases. Apart from distributed microcracking, crack band fracture (Bazant, 1984) as illustrated in Figure 5.22 can be observed in the heterogeneous models. Clusters of microcracks develop ahead of the fracture tip and form a crack band. The width of the band increases with the heterogeneity of the model. The formation of crack band is originated by the reduction of stress concentration because of load sharing mechanism near the fracture tip. So, stress at fracture tip is more distributed instead of concentrated at the fracture tip. The more heterogeneous the sample is, the more widespread of stress distributed that gives a thicker fracture band.

Figure 5.23 compares the experimental result and five simulation results. Without applying PDF on lattice parameters, the curve shows elastic behavior before reaching its peak strength. It shows slightly snap back behaviour in the softening curve. This deviates from the experimental result.
Fig. 5.23 Comparison of experimental result and LEM simulation on double notch rock sample under direct tension test
When a PDF is applied, it shows better match with the experimental result. As shown in Figure 5.23, simulation results show a non-linear part before peak which is a better match with the experimental result. This non-linear part is caused by distributed micro-cracking.

The D75 model of LN(0.5) gives the best match with the experimental result. After the peak, it shows a transition before the sudden drop of stress. With higher heterogeneity applied, the peak is less abrupt and the model sustains higher stress after the peak.

Mesh fineness is found to be insensitive by comparing D75 and D115 models. As there are only two simulations for comparison, more studies should be carried out for verification.

This study shows applying PDF on lattice parameter can model more realistically the rock behaviour. Different rock types can be modelled by applying different PDFs.
5.8 Simulation of fracturing under uni-axial compression

Simulations of lattice models under uni-axial compression is studied in this section. The mechanism of failure under uni-axial compression is much more complicated compared to the uni-axial tension case. While the pre-dominant lattice failure is tensile when a lattice model is subjected to uni-axial tension, macroscopic response in uni-axial compression depends on the interaction between both the tensile and shear failure of lattice. Tensile fractures can be formed either by sliding crack model or by force chain model as shown in Figure 5.24. By sliding of a crack inclined from loading direction, tension is induced at both ends of the crack and generates a pair of wing cracks. Simulations of wing cracks are presented in Section 5.8.5. For the force chain model, force transmission between cells (force chain) may deviate from loading direction. A tensile component is induced perpendicular to the loading direction to maintain the equilibrium of the deviated force chain.

Fracture may be open or closed in different loading stages. Majority of fractures are closed during uni-axial compression. The load transfer between closed fractures plays an significant role in both the microscopic and the macroscopic levels. This is modelled by elastic perfectly plastic model detailed in Section 5.1.3 and $\gamma$ is the parameter governing the behaviour of a closed fracture.

In this section, $f_{ss}/f_{st}$, $\gamma$ and variance of PDFs applied are studied in 2D LEM simulations (D80p models, $n = 0.5$). The effect of $n$ is studied briefly by the comparison of two simulation results on S80p model ($n = 0.1$) and D80p model ($n = 0.1$). Three 3D simulations (D80 model) are carried out. For all the simulations, $\alpha$ is set to be 0.3. Table 5.7 provides a summary of the uni-axial compression simulation configurations.

In Figure 5.25, Evans et al. (2013) summarised the phenomenology of brittle-ductile transition of rock under uniaxial compression of low porosity crystalline rocks. For the
5.8 Simulation of fracturing under uni-axial compression

Table 5.7 Parametric study for uni-axial compression strength of lattice models

<table>
<thead>
<tr>
<th>$\gamma$</th>
<th>$f_{ss}/f_{st}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1.0</td>
</tr>
<tr>
<td>0.01</td>
<td>$\bigcirc$</td>
</tr>
<tr>
<td>0.025</td>
<td>$\bigcirc$</td>
</tr>
<tr>
<td>0.05</td>
<td>$\bigcirc$</td>
</tr>
<tr>
<td>0.1</td>
<td>$\bigcirc$</td>
</tr>
<tr>
<td>0.2</td>
<td>$\bigcirc$</td>
</tr>
<tr>
<td>0.3</td>
<td>$\bigcirc$</td>
</tr>
<tr>
<td>0.4</td>
<td>$\bigcirc$</td>
</tr>
</tbody>
</table>

$\alpha = 0.3$ for all simulations.

- $\bigcirc$ - D80p model (2D), $\bigtriangleup$ - D50 model (3D), $\Box$ - S80p model ($n = 0.1$), $\bigstar$ - D80p model, MC criterion
- $\bigdiamond$ - D80p model, with lognormal distribution applied on lattice stiffness and strength

A possible relationship between microscopic (model) and macroscopic parameters is explored in this section. Figure 5.26a shows the relationships among $f_c/f_{st}$, $f_{ss}/f_{st}$ and $\gamma$ where $f_c$ is the macroscopic compressive strength. $f_c$ is found to be insensitive to $\gamma$ but highly correlated to $f_{ss}/f_{st}$. For models without applying PDFs to lattice parameters, the following linear relationship can be obtained

\[
f_c/f_{st} = 1.925 f_{ss}/f_{st} + 0.542 \quad \text{for} \quad f_{ss}/f_{st} > 1.0 \tag{5.32}
\]

Applying PDFs to lattice parameters also affects $f_c$ to a less extent compared with $f_{ss}/f_{st}$.

Figure 5.26b plots the ratio between macroscopic compressive to tensile strength $f_c/f_t$ against macroscopic $f_{ss}/f_{st}$. $f_c/f_t$ is referred to brittle index $B$ in rock mechanics. Again, there is a linear relationship between these two variables

\[
f_c/f_t = 2.94 f_{ss}/f_{st} + 0.99 \quad \text{for} \quad f_{ss}/f_{st} > 1.0 \tag{5.33}
\]
Fig. 5.25 Schematic diagram illustrating the phenomenology of the brittle-ductile transition (after Evans et al., 2013).
5.8 Simulation of fracturing under uni-axial compression

Fig. 5.26 Macro-micro relationship of uniaxial compression simulation. (a) Relationship among normalized macroscopic compressive strength $f_c/f_{st}$, normalized microscopic shear strength $f_{ss}/f_{st}$ and $\gamma$. (b) Relationship among ratio of macroscopic compressive strength $f_c$ to macroscopic tensile strength $f_t$, ratio of microscopic shear strength to microscopic tensile strength $f_{ss}/f_{st}$ and $\gamma$. (c) Relationship between normalized macroscopic compressive strength $f_c/\langle f_{ss} \rangle$ and standard deviation $\sigma$ of applied PDF on lattice parameters.
Fracturing simulation using LEM

For practical applications on rock mechanics, $B$ is often assumed to be 10 (Bieniawski, 1974), corresponding to $f_{ss}/f_{st} \approx 3$ from Eq. (5.33).

As introducing PDFs on lattice stiffness and strength affects the macroscopic behaviour, Figure 5.26c plots the relationship between $f_c/\langle f_{ss} \rangle$ with the standard deviations $\sigma$ of PDFs applied. $\gamma$ has a slight effect on the relationship. The following linear relationships are found.

\[
f_c/\langle f_{ss} \rangle = -0.810\sigma + 2.14 \quad \text{for } \gamma = 0.05 \quad (5.34)
\]
\[
f_c/\langle f_{ss} \rangle = -0.620\sigma + 2.24 \quad \text{for } \gamma = 0.2 \quad (5.35)
\]

### 5.8.2 Stress-strain curves

Figures 5.27 shows the snapshots of fracture evolution and failure mode (tension or shear) for all 2D simulations. Before the peak load, only distributed micro-cracks are formed and they are all tensile cracks. The amount of distributed micro-cracking increases with the ratio $f_{ss}/f_{st}$. It is because higher $f_{ss}$ can sustain higher $f_c$ so more lattices meeting $f_{st}$. Given $f_{st}$ stays constant, the microscopic tensile stress increases and more lattices reach $f_{st}$ and produce tensile microcracks.

For very low $\gamma$ (0.01), cone and spilt failure model is observed. Shear bands are observed when $\gamma$ increases to 0.2. For higher $\gamma$ value (0.3-0.4), the failure is more ductile and multiple shear bands are formed. When a fracture forms but remains closed, high $\gamma$ value gives higher residual spring stiffness. Less loading is transferred to their adjacent lattices. This minimises progressive failure which is the source of brittleness.

The effect of heterogeneity is investigated using lattices with $\gamma = 0.2$, $f_{ss}/f_{st} = 2.0$ case and $\gamma = 0.05$, $f_{ss}/f_{st} = 2.0$ case. Lognormal distributions LN(0.25), LN(0.5) and LN(0.75) are applied. Shear band is less distinctive when heterogeneity increases and the model becomes more ductile.

Figures 5.30a-f show the normalised stress-stain curves (both longitudinal and lateral) of the uni-axial compression simulations. The stress is normalised by $f_{ss}$ as it is found to be roughly proportional to $f_{ss}$ in the above section so the effects of other parameters can be studied. For all simulations, the pre-peak stage is linear for longitudinal stress-strain curves and it shows non-linearity for the transverse stress-strain curves. It is because only longitudinal tensile microcracks are formed by the force-chain model before the peak. The force chains for compressive force transmission is mostly undistributed by the formation of
these longitudinal microcracks. But the microcracks affects the force chain in lateral stiffness which gives the non-linearity in transverse stress-strain curves.

Other model parameters such as $\gamma$ and variance of PDFs on lattice are found to be less sensitive to $f_c$. From Figure 5.30a and 5.30b, increasing $\gamma$ increases $f_c$ slightly. $\gamma$ governs the brittleness of a lattice model, as indicated by the difference between the peak strength (point ‘b’ in the figures) and the residual strength (point ‘d’ in the figure). Smaller $\gamma$ gives a smaller residual strength. Figure 5.30e compares UCS simulations with different PDFs [LN(0.25), LN(0.5) and LN(0.75)] applied. Introducing heterogeneity in lattices decreases the peak strength but increases the ductility of the model. Figure 5.30f compares 2D models and 3D models. 3D effects slightly increase $f_c$ and give similar ductility.

### 5.8.3 Shear fracture evolution

Figure 5.31 shows the evolution of fracture failed by shear in LEM simulations of uni-axial compression test. From Figure 5.31a and Figure 5.31b, fractures start to fail by shear after the peak load, except for the case of low microscopic shear strength $f_{ss}/f_{st} = 1$.

Figure 5.31c shows the effect of $\gamma$ on shear fracture evolution in the $f_{ss}/f_{st} = 2.0$ case. The formation of shear fracture starts only after the peak load for the Dense model (node density $n = 0.5$). The evolution of the number of shear fractures are very similar when $\gamma$ varies from 0.01 to 0.2. For the Sparse model ($n = 0.1$), shear fracture starts before peak for $\gamma = 0.2$ and number of shear failure is more than that of the Dense models. However, for brittle models (for example $\gamma = 0.01$), shear fracture appears after the peak load in the Sparse model and the number of shear failure is similar to that of the Dense models.

Figure 5.31d compares the models with different heterogeneities applied to lattices for the cases of $\gamma = 0.05$ and $\gamma = 0.2$. When the heterogeneity increases, the number of shear failure increases. Also, shear fracture starts to form before the peak load and it starts earlier when the degree of heterogeneity increases.

Figure 5.31e compares 2D and 3D simulations. There is insignificant difference between shear fracture evolution except for $f_{ss}/f_{st} = 1$ case due to low shear strength. Shear fractures are easier to form and localise.
Fracturing simulation using LEM

Fig. 5.27 Snapshots of fracture evolution of D80p/S80p plain strain lattice model ($\alpha = 0.3$) under uniaxial compression and failure type of fracture. For first three rows, fracture colour indicates time of formation (blue-early, red-late). In the last row, red lattice indicates shear failure and blue tensile failure.
5.8 Simulation of fracturing under uni-axial compression

(Cont’d) Snapshots of fracture evolution of D80p/S80p lattice model ($\alpha = 0.3$) under uni-axial compression and failure type of fracture. Fracture colour indicates time of formation (blue-early, red-late).
Fig. 5.29 Snapshots of fracture evolution of D80 3D lattice model ($\alpha = 0.3$) under uni-axial compression. Left - snapshots of fracture evolution and failure type of fracture. Right - deformation contour at the end of simulation.
5.8 Simulation of fracturing under uni-axial compression

Fig. 5.30 Strain-strain curve of LEM simulation on uni-axial compression test. Both longitudinal strain and lateral strain are plotted. Stress is normalised by microscopic shear strength $f_{ss}$ and strain is normalised by $E/<E_{micro}>$ and $f_{ss}/f_{st}$.
Fig. 5.31 The evolution of fracture failed by shear in LEM simulation of uni-axial compression test. X-axis: ratio of number of fracture failed by shear to total number of fracture, y-axis: step number normalised by step number at peak load.
5.8 Simulation of fracturing under uni-axial compression

Fig. 5.32 Unaxial compression simulation of D80p models using Mohr-Coulomb failure criterion with 4 different frictional angles ($\phi = 0^\circ, 15^\circ, 20^\circ, 30^\circ$) for the case of $f_{ss}/f_{st} = 2.0$ and $\gamma = 0.025$. (a) Snapshots of simulation, (b) stress strain curve (axial and lateral), (c) evolution of the share of fracture failed by shear, and (d) evolution of the share of fracture cluster statistics.
5.8.4 Mohr-Coulomb failure criterion

The lattice shear failure criterion in this section is changed to Mohr-Coulomb instead of a constant value. The failure microscopic shear stress \( \tau_f \) is related to the microscopic axial stress \( \sigma_{fn} \)

\[
\tau_f = f_{ss} + \sigma_{fn} \sin \phi
\]  

(5.36)

Four simulations with \( \phi = 0^\circ, 15^\circ, 20^\circ \) and \( 30^\circ \) are carried out for \( f_{ss}/f_{st} = 2.0 \) and \( \gamma = 0.025 \). It is a brittle model when \( \gamma = 0.025 \) as discussed in the previous section. Figure 5.32a shows the snapshots of these simulations. Shear band appears for \( \phi = 0^\circ, 15^\circ \) and \( 20^\circ \). Shear band is not so distinct for \( \phi = 20^\circ \). There is no shear band formed for \( \phi = 30^\circ \) and its failure model is more ductile without the formation of shear band. The number of distributed tensile microcracks increases with \( \phi \). Shear microcracks are mostly formed along shear band for lower \( \phi \). For \( \phi = 30^\circ \) shear microcracks are distributed.

Figures 5.32b and 5.32c show the stress strain curves and the shear fracture evolution respectively with \( \phi = 0^\circ, 15^\circ, 20^\circ \) and \( 30^\circ \). The peak stress decreases with \( \phi \). This is due to more shear failure formed before the peak stress for higher \( \phi \) as shown in Figure 5.32c. Also, model becomes more ductile when \( \phi \) increases.

Figure 5.32c shows the fracture cluster evolution. Fractures start to cluster, almost the same time as shear failure starts to occur. For \( \phi = 0^\circ \) and \( 15^\circ \), a dominant shear band forms only after the peak load. For \( \phi = 20^\circ \) and \( 30^\circ \), fracture coalescence starts before the peak load.

The study here is preliminary and more work is needed in the future.

5.8.5 Simulation of inclined crack under uni-axial compression

This section presents simulations of the compression of lattice models with a pre-existing inclined crack. This study tries to figure out how a pre-existing fracture propagates in a heterogeneous material. Figure 5.33a illustrates the model often referred in the literature from the field of rock mechanics. Wing crack is initiated at right angle to the inclined crack. It is a tensile crack formed by sliding of the inclined crack. Figure 5.33b shows the experimental result of different inclination angles \( \theta = 30^\circ, 45^\circ \) and \( 60^\circ \) of the pre-existing inclined crack. Fracture propagates along the initial crack orientation for \( \theta = 30^\circ \) case. It is a shear failure and there is no wing crack formed. For \( \theta = 45^\circ \) and \( \theta = 60^\circ \) cases, wing cracks are formed.

Four LEM simulations are carried out to simulate the formation of wing cracks under uni-axial compression. The pre-existing crack is inclined at \( 30^\circ, 45^\circ \) and \( 60^\circ \) from the vertical. For \( \theta = 30^\circ \), fracture propagation aligns with the pre-existing crack. Fractures formed are
5.8 Simulation of fracturing under uni-axial compression

Fig. 5.33 (a) Simplified crack pattern observed in pre-crack specimens of rock in uniaxial compression (Bobet and Einstein, 1998) and (b) experiment of inclined pre-crack specimens at different angles (Yang et al., 2012)

Fig. 5.34 LEM simulation of rock sample with pre-existing inclined crack at different angle ($30^\circ$, $45^\circ$ and $60^\circ$) under uniaxial compression. Blue fracture indicates tensile failure and red fracture indicates shear fracture.
mainly shear. For $45^\circ$ case, two simulations are carried out. For $f_{ss}/f_{st} = 2.0$, wing cracks are formed and fractures are failed by tension. The case of $f_{ss}/f_{st} = 1.0$ is more interesting. Both the tensile wing cracks and the shear cracks are formed. Shear cracks are formed more easily as $f_{ss}/f_{st}$ reduces. There is a competition between them and another crack is formed between them. For $\theta = 60^\circ$, tensile wing cracks are formed. There are a short secondary cracks formed which matches the model illustrated in Figure 5.33a.

In summary, LEM simulation results match the trend suggested by the well-established model and the experimental results. The results presented here are preliminary and more work is needed.

5.9 Guidance on selection of model parameters

This section gives some guidance on the selection of model parameters (microscopic parameters) in LEM to relate the macroscopic parameters of rock that can be determined by laboratory experiments and in-situ measurements.

The elastic model parameters $E_{\text{micro}}$ and $\alpha$ should be first determined according to macroscopic Young modulus $E$ and Poisson ratio $\nu$. The mode parameters, microscopic tensile strength $f_{st}$, microscopic shear strength $f_{ss}$ and reconnection parameter $\gamma$, are determined by macroscopic tensile strength $f_t$, macroscopic compressive strength $f_c$ and the ductility of rock from stress-strain curve.

Finally, the length scale of lattice model is determined by fracture toughness $K_{Ic}$.

5.9.1 Elastic properties of rock

The macroscopic parameters governing the elastic deformation of an isotropic material are macroscopic Young modulus $E$ and Poisson ratio $\nu$. There can be related by four model parameters $E_{\text{micro}}$, $\alpha$, $\beta$ and node density $n$.

$\beta$ is found to be negligible to both the microscopic and macroscopic parameters as demonstrated in Figure 4.10b. It is recommended that $\beta$ is taken as 1.

$n$ does not affect the macroscopic parameters. It mainly affects the stress heterogeneity. It also slightly affects $\nu$ and other macroscopic parameters. The maximum attainable value of $n$ is about 0.533 but the time required to generate a lattice model towards this value is very long. It is recommended to adopt $n$ to be 0.5 as a starting point. Stress heterogeneity can be controlled by other parameters.

$\alpha$ should be first determined using Figure 4.10c that relates $\alpha$ and $\nu$. $\alpha$ also varies slightly with $n$. The maximum $\nu$ attainable in a lattice model is approximately 0.32 which is sufficient
to model the majority of rock type. For instance, $\nu$ of carbonate rock is about 0.3 and that of sandstone is about 0.2. The corresponding values of $\alpha$ are 0.0 and 0.22 respectively when $n$ is taken as 0.5. In this thesis, $\alpha = 0.3$ (corresponds to $\nu \approx 0.17$) is adopted for most of the simulations presented.

$E_{\text{micro}}$ is the overall scaling parameter for the stiffness of lattice model. After specifying $\alpha$, $E_{\text{micro}}$ can be determined by $E$ using Figure 4.10a.

### 5.9.2 Microscopic strength parameters

The macroscopic strength parameters are macroscopic tensile strength $f_c$ and macroscopic shear strength $f_t$. The relevant model parameters are microscopic tensile strength $f_{st}$, microscopic shear strength $f_{ss}$ and reconnection parameter $\gamma$.

The selection of $\alpha$ and applied heterogeneity also affects $f_t$. Both the ductility and the macroscopic strengths of material can be specified by a combination of the above model parameters. As a general rule, the increase in the ductility of the material leads to the decrease in the macroscopic strengths.

The relationship between $f_t$ and $f_{st}$ varies with $\alpha$ and the applied heterogeneity (assigning PDFs to model parameters $E_{\text{micro}}$, $f_{st}$ and $f_{ss}$). $\alpha$ can be solely determined by $\nu$. The ductility of material can be controlled by applied heterogeneity. $f_t$ decreases with standard deviation of applied heterogeneity and their relationship can be found in Figure 5.10a. The relationship between $f_t$ and $f_{st}$ can be found in Figure 5.7.

$f_{ss}$ is proportional to $f_c$ as demonstrated in Figure 5.26a. It also slightly varies with the standard deviation of applied heterogeneity. $f_{ss}$ is required to be adjusted by using Figure 5.26c. $\gamma$ governs the ductility of rock under uni-axial compression. $f_c$ increases slightly with $\gamma$. For brittle rock that shows a snap back in stress strain curve, $\gamma$ should be less than 0.2. For rock that exhibits nearly fully plastic behaviour after reaching its peak load, $\gamma$ should be taken as 0.4 or greater. Another parameter governing the ductility of model is the ratio $f_{ss}/f_{st}$. It is directly proportional to $f_c/f_t$ and their relationship is established in Figure 5.26b. A ductile material has a smaller ratio $f_c/f_t$. The typical range of $f_{ss}/f_{st}$ is between 2.0 to 4.0 corresponding to $f_c/f_t$ of 7.0 and 13.0 respectively.

### 5.9.3 Strength and toughness

The relationship between macroscopic strength and fracture toughness $K_{Ic}$ is discussed in Section 5.2. $K_{Ic}$ is proportional to $f_{st}$ and a length scale (average width of facet $<l_r>$) of the lattice model according to Eq. (5.13). After determination of $f_{st}$, the length scale $<l_r>$ can be determined.
5.10 Conclusions

This Chapter has explored fracturing process simulated by LEM. Lattice fails by either tension or shear in which a lattice act like a bond between two cells. Fractures can be either open and closed. For closed fractures, a reconnection ratio $\gamma$ is introduced to model the reduced stiffness of a lattice from its unfractured stage.

Relationships are established between material properties in LEFM of fracture toughness $K_{Ic}$, critical energy release rate $G_{Ic}$, and microscopic (model) parameters in LEM which are microscopic tensile strength $f_{st}$, microscopic shear strength $f_{ss}$, microscopic Young Modulus $E_{\text{micro}}$, ratio of normal spring stiffness to shear spring stiffness $\alpha$. It also related to two length scales, length of facet $l_r$ and lattice length $l_l$. So, the size of cell has to be specified to model a material given both its macroscopic strength and toughness.

Simulations are carried out for fracturing by uni-axial tension. Shear fracture only happens in the post-peak stage. Macroscopic tensile strength $f_t$ is governed by $\alpha$. Brittleness reduces with $\alpha$. Applying heterogeneity by introducing PDFs on lattice stiffness and strength makes the lattice model more ductile. There is negligible difference between 2D and 3D lattice models under uni-axial tension. Five stages of fracturing are identified: distributed formation of micro-cracks, distributed growth of micro-cracks, localised and non-competing fracture growth, localised and competing fracture growth and dominant fracture growth. They are related to the heterogeneity of models. Some stages may be absent for homogeneous models. For heterogeneous models, multiple fracture clusters are formed before the formation of a dominant fracture after the peak stress.

Fracturing by uni-axial tension is studied microscopically. The SDs of facet normal stress $\sigma_n$ and nodal mean stress $p^n$ increase with the fracturing process while the changes in their mean values are negligible. Both the means and the SDs of facet shear stress $\sigma_s$ and nodal deviatoric stress $q^n$ increase during fracturing. This indicates the increased mobilisation of shear springs to carry load during fracturing. The homogeneous models show different trends in the pre-peak stage and the post-peak stage on microscopic stresses. Most changes happen in the pre-peak stage for heterogeneous models while most changes happen in the post-peak stage for homogeneous models.

An experiment from a literature is simulated by LEM and applied heterogeneity is required to match their stress-strain curves.

Simulations of the fracturing by uni-axial compression is are presented. Load transfer through a closed fracture is modelled by a reconnection factor $\gamma$. It governs the brittleness of the model. Higher value of $\gamma$ gives a more ductile model. The ductility can also be enhanced by applying heterogeneity. Macroscopic compressive strength $f_c$ increases linearly with $f_{ss}/f_{st}$, the ratio of microscopic shear strength to microscopic tensile strength. $f_c$ also
increases with $\gamma$ and SD of applied heterogeneity, but their effects are smaller compared with $f_{ss}/f_{st}$.

Simulation results of fracturing under uni-axial compression using Mohr-Coulomb failure criterion for lattices are presented. It is found that internal frictional angle $\phi$ increases with the ductility of a lattice model.

Simulations of lattice model with a pre-existing inclined crack under uni-axial compression are carried out. Two fracturing models, shear crack and wing crack are simulated depending on the angle of inclined crack. The simulation agrees with both the trend of the well-established model in rock mechanics and the experimental results from a literature. Further work is required.
Chapter 6

Dual lattice model for hydraulic fracturing simulation

For modelling hydraulic fracturing which involves the interplay between solid part and fluid part, a novel technique called Dual Lattice Model (DLM) is proposed by coupling a solid lattice model with a fluid lattice model. LEM for solid lattice model has been covered in the previous two Chapters. Fluid lattice model is called pipe network model in this Chapter. A C++ code, DualLattice3D has been developed to implement hydraulic fracture simulations. The coupling scheme of the solid-fluid dual lattice system and the numerical technique for solution searching are formulated.

Simulations are carried out using the classical penny shape crack problem under hydrostatic pressure for validation by comparing the simulation results to the analytical solution. Further hydrostatic simulations are carried out to investigate the effects of asperity and applied heterogeneity.

A semi-analytical approximate solution for the penny shape fracture flow under viscous flow is derived. The solution gives two asymptotic solutions applied for the regions near borehole region and crack tip region. DLM simulations of planar penny shape fracture are carried out and compared with the approximate solution. Several DLM simulations of planar and rough penny shape crack are carried out and the results are discussed in detail. The transition of regimes during the hydraulic fracturing region is identified.

6.1 Pipe Network Model

In order to simulate hydraulic fracturing, a novel technique DLM is proposed which is composed of solid lattice model and fluid lattice model as illustrated in Figure 6.1.
Fig. 6.1 Illustration of Dual Lattice Model which combines a solid lattice model and a fluid lattice model
Fig. 6.2 Illustration of pipe network representing fluid flow in fracture and the lattice network representing rock
Figure 6.2 illustrates the fluid lattice model (pipe flow network) overlapping a LEM model (in 2D for visualization purpose only). Flow in fracture is simplified as a pipe network flow. Pipe network model is comprised of three basic elements: fracture, fluid node and pipe. It is the analogy of a fluid lattice model for flow in fracture, but in 2D. Fluid node, fracture and pipe correspond to solid node, cell and lattice for solid lattice model respectively. One of the fluid nodes is the injection node where fluid is injected and where the fluid flow starts. A fluid node is created when a fracture forms and there exists a path connecting to the injection node. This means that no fluid node is formed for isolated and distributed fractures which are not connected to the main fracture. Two fluid nodes are connected by a pipe if their corresponding fractures (cells) share an edge. The fluid node is located at the centroid of a fracture surface (facet) corresponding to the broken lattice. It stores the information about the fracture like fracture area, aperture and fluid storage.

Flow between fractures is modelled by pipes. This idealises a 2D fluid flow between fractures to a 1D pipe flow problem. The only parameter of pipe is permeability but it changes with the fracture apertures of two connecting fracture surface. This couples a solid lattice model with a fluid lattice model.
As mentioned above, a pipe network model is also a lattice model, so pipe network model can be regarded as lattice model for fluid part of the entire hydraulic fracturing model. In other words, it is a dual lattice model for a two phase material. Both lattice models are built by 1D lattice elements in a 3D space.

Figure 6.3 shows the interdependence between the geometry of fracture and the fluid lattice model. The fracture facets are formed from the solid lattice model. They are the 2D cells of the fluid lattice model in 3D space. The fluid nodes are located at the centroid of fracture facets. The connectivity of fluid lattices (pipes) also depends on the topology of the fracture facets.

However, there are several differences between lattice models for solid part and fluid part (i.e. pipe network model). A cell represented by a node is 3D in solid model but 2D in fluid model. A lattice model for solid solves the three dimensional deformation problem while a pipe network model solves the two dimensional fluid flow problem. The solid lattice model is a vector model as the fluid lattice model is a scalar model. A solid node has 6 DOFs to describe its displacement and rotation. A fluid node has 1 DOF as the only variable is fluid storage in fracture. During fracturing, the numbers of node and lattice are fixed for the solid lattice model while the numbers of node and lattice are increasing during fracturing for the fluid lattice model.
6.1.1 DLM for penny shape problem

To simulate the hydraulic fracturing of the penny shape crack problem, a lattice model with a 50m diameter penny shape crack at the center is constructed as shown in Figure 6.4. This model is used throughout this Chapter.

Fluid pressure is assumed to be hydrostatic, implying the viscosity of fracturing fluid to be zero and permeability of pipes to be very large. Leak off is assumed to be negligible. This is applicable to hydraulic pressure of low viscosity, high fracture toughness and high confining pressure. These conditions apply to later stage of hydraulic fracturing and hydraulic fracturing in deep ground of impermeable rock. For these conditions, most of the pressure changes happen at a very small crack tip region which has negligible effect on the overall process.

The overall size of model is $200 \times 200 \times 200\text{m}^3$ and all 6 faces are fixed in all directions to mimic the infinity boundary condition of the penny shape problem. No confining pressure is applied at boundaries. A horizontal penny shape crack of diameter 50m is located at the centre of model and fluid is injected at the centre of the crack. To simulate the penny shape crack problem, fracture propagation is restricted in the horizontal direction by generating a weak plane. Fracture is not allowed to happen elsewhere.

To reduce the computation time while maintaining high accuracy of modelling, 3 different lattice fineness is applied at different regions. The finest lattice is constructed adjacent to penny shape fracture and potential fracture path. Lattice is coarser further away from the
penny shape fracture. The inner $100 \times 100 \times 100 \text{m}^3$ region has a coarser lattice and outer $200 \times 200 \times 200 \text{m}^3$ region has even coarser lattice.

Three lattice models of different fineness are used for the penny shape crack simulation. They are D100, D75 and D50 models and the details are shown in Table 6.1. Unless otherwise specified, Table 6.2 lists the model parameters for all the simulations presented in this thesis. The parameters used in the DLM refer to stiff brittle rock from the simulation results in Section 5.8.

<table>
<thead>
<tr>
<th>Lattice model</th>
<th>$l_{\text{min}}$ (m)</th>
<th>$n$</th>
<th>$N_{\text{node}}$</th>
<th>$N_{\text{lattice}}$</th>
<th>Initial $N_{\text{fluid node}}$</th>
<th>Initial $N_{\text{pipe}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>D100</td>
<td>1.0</td>
<td>0.5</td>
<td>153,094</td>
<td>1,080,275</td>
<td>1,324</td>
<td>3,840</td>
</tr>
<tr>
<td>D75</td>
<td>1.333</td>
<td>0.5</td>
<td>64,946</td>
<td>450,246</td>
<td>745</td>
<td>2,137</td>
</tr>
<tr>
<td>D50</td>
<td>2.0</td>
<td>0.5</td>
<td>20,499</td>
<td>137,719</td>
<td>329</td>
<td>920</td>
</tr>
</tbody>
</table>

Table 6.1 Details of lattice models used for simulations on penny shape problem

<table>
<thead>
<tr>
<th>$E_{\text{micro}}$ (kPa)</th>
<th>$\alpha$</th>
<th>$\beta$</th>
<th>$\gamma$</th>
<th>$f_{\text{st}}$ (kPa)</th>
<th>$f_{\text{ss}}$ (kPa)</th>
<th>$q$ ($\text{m}^3/\text{s}$)</th>
<th>$R$ (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2 \times 10^7$</td>
<td>0.3</td>
<td>0.0</td>
<td>0.1</td>
<td>2,000</td>
<td>8,000</td>
<td>0.25</td>
<td>25</td>
</tr>
</tbody>
</table>

Table 6.2 Parameters for hydraulic simulation of dual lattice model
6.2 Solving coupled solid-fluid dual lattice system

6.2.1 Coupling scheme between pipe network and solid lattice network

Figure 6.5 shows the flow chart of solving coupled system of DLM. The simulation is divided into two phases; fracture propagation phase and fluid flow phase. Fracture is assumed to form spontaneously and its time-scale is much shorter than that of fluid flow. So, during the fracture propagation stage, the solid model and the fluid model are decoupled. This means that the fluid pressure and the fluid network do not change. This simplification reduces one loop of solution searching in the coupled fluid flow stage. The solution in the coupled stage is more stable. The stability of solution can also reduce the number of iterations required to search for solution and hence the computation time is controlled in a manageable manner. Small amount of fracture may be very sensitive to the change in loading and fall into an open-closed oscillation. The number of cycle is capped to a specified value.

In the fluid flow phase, it involves the coupling between the pipe network and the lattice network. There is no new fracture formed but fracture closure and re-opening are checked. Such checking is necessary because the closed fracture has negative aperture which constitutes to unrealistic negative fluid storage. The pipe network is updated to ensure the connectivity of every active node with an injection node. The injection pressure is assumed and the pressure on the fracture is converted to nodal forces for solving solid lattice network. After solving solid part, the fracture aperture is updated and the system of fluid flow equations are solved.

As the coupled system is non-linear and the pipe network may change due to open or closure of fracture, iterations are required until the pipe network is stable while the injection pressure converges. The pipe network is stable when the change of total fluid storage is smaller than a tolerance. The continuity equation Eq (6.15) is then checked. The residual (difference between fluid storage in fracture and fluid injected) is used to search for the next injection pressure, which is discussed later. The injection pressure is updated and the above process repeated. The solution is found when the pipe network is stable and the global continuity equation is fulfilled.

The coupled solid-fluid system is then solved for one time-step. The simulation proceeds to the next time-step and starts again at the fracture propagation stage and then the fluid flow stage.
6.2 Solving coupled solid-fluid dual lattice system

Fig. 6.5 Flow chart of coupled solid lattice network – pipe network simulation
6.2.2 Calculation of pipe permeability

![Diagram of pipe permeability calculation]

Fig. 6.6 Calculation of equivalent pipe permeability. The pipe $ij$ crosses cell $i$ and cell $j$. The pipe $ij$ is sub-divided into sub-pipe $i$ and sub-pipe $j$.

This section provides the details on the calculation of the permeability of a pipe. Figure 6.6 shows a pipe connecting two fluid nodes (fluid node $i$ and fluid node $j$) crossing fracture $i$ and fracture $j$. The pipe is divided into sub-pipe $i$ and sub-pipe $j$ at the interface between cell $i$ and cell $j$. Each sub-pipe has its own aperture $\delta_i$ and $\delta_j$. Thus two sub-pipes have different permeabilities. These sub-pipes are in series. Consider a flow $q_{ij}$ passing through fluid node $i$ or $j$ along pipe $ij$. 
6.2 Solving coupled solid-fluid dual lattice system

Using Dracy’s law for sub-pipe $i$

$$q_{ij} = k_i A_i \frac{\Delta P_i}{l_i}$$  \hspace{1cm} (6.1)

where $A_i$ is the area of the cross section of the sub-pipe, $A_i = \delta_i w_{ij}$. $k_i$ is given by cubic law

$$k_i = \frac{\delta_i^2}{12\mu}$$  \hspace{1cm} (6.2)

$\delta_i$ is determined by Eq. (5.5). Rearranging Eq. (6.1) and Eq. (6.2),

$$\Delta P_i = \frac{q_{ij} l_i}{A_i k_i \delta_i w_{ij}} = \frac{12\mu q_{ij} l_i}{\delta_i^3 w_{ij}}$$  \hspace{1cm} (6.3)

Similar equation follows for sub-pipe $j$.

$$\Delta P_j = \frac{12\mu q_{ij} l_j}{\delta_j^3 w_{ij}}$$  \hspace{1cm} (6.4)

Two sub-pipes $i$ and $j$ are in series, so

$$\Delta P_{ij} = \Delta P_i + \Delta P_j$$  \hspace{1cm} (6.5)

Define permeability of pipe $ij$ to be $K_{ij}$, by Dracy’s law,

$$q_{ij} = K_{ij} \Delta P_{ij}$$  \hspace{1cm} (6.6)

Put Eq. (6.6), (6.3) and (6.4) into Eq. (6.5)

$$\frac{1}{K_{ij}} = \frac{12\mu}{w_{ij}} \left( \frac{l_i}{\delta_i^3} + \frac{l_j}{\delta_j^3} \right)$$  \hspace{1cm} (6.7)

So,

$$K_{ij} = \frac{w_{ij}}{12\mu \left( \frac{l_i}{\delta_i^3} + \frac{l_j}{\delta_j^3} \right)}$$  \hspace{1cm} (6.8)
6.2.3 Assemble system of equations

Figure 6.3a shows a regular grid of pipe network. Fluid can flow between neighbourhood. A pipe is used to connect two neighbourhood fluid nodes.

For each pipe connecting fluid node $i$ and $j$, the pipe flow equation in matrix form is given by

$$
\begin{bmatrix}
q_{ij} \\
-q_{ij}
\end{bmatrix} = K_{ij} \begin{bmatrix}
1 & -1 \\
-1 & 1
\end{bmatrix} \begin{bmatrix}
p_i \\
p_j
\end{bmatrix}
$$

(6.9)

where $q_{ij}$ is an unknown in the above equation. After assembling all the pipes in the pipe network, the following system of equations are formed

$$\{q\} = [K]\{p\}$$

(6.10)

where $q_i$ is the sum of discharge from fluid node $i$ from its neighbour $j$. From mass balance of node $i$,

$$q_i = \sum_{j=1}^{n} q_{ij} = a_i + s_i + c_i$$

(6.11)

where $a_i$ and $s_i$ and $c_i$ are source term, fluid storage rate and leak off rate at fluid node $i$ respectively. $n$ is the number of neighbour of node $i$. The source term has a non-zero value only at the injection node. The fluid storage rate is given by

$$s_i = -\frac{A_i \delta_i}{t}$$

(6.12)

where $A_i$ is fracture facet area and $\delta_i$ is fracture aperture and $t$ is time. The negative sign represents a discharge of fluid from the pipe network.

The leak off term can be obtained using Carter equation.

$$c_i = -\frac{C_L}{\sqrt{t - t_{exp}}}$$

(6.13)

where $C_L$ is leak-off coefficient and $t_{exp}$ is fracture aperture and $t$ is time. Again, the negative sign represents a discharge from the system. In this Chapter, leak off is not considered. $C_L$ is taken as zero.

So, the system of equations (6.10) becomes

$$\{q\} = \{a\} + \{s\} + \{c\} = [K]\{p\}$$

(6.14)
The vectors \( \{a\} \), \( \{s\} \) and \( \{c\} \) are known. The pressure vector \( \{p\} \) has to be solved. The permeability matrix \( [K] \) is singular. Additional equation given by the global mass balance serves as a restraint:

\[
\sum (a_i + s_i + c_i) = 0 \tag{6.15}
\]

Since the DOFs for a pipe network problem is much fewer than a solid lattice model as the dimension of problem is reduced by one, solving system of equations for fluid lattice model is a lot faster.

### 6.2.4 Solution searching technique

The only variable in the hydraulic fracturing simulation is pressure \( P_o \) at the injection node. The pipe network is non-linear because of the non-linearity of pipe permeability calculated by cubic law. The permeability of pipe and its fracture aperture are related to the cubic law. Also, small changes in pressure can cause fractures to change from open or closed or vice versa. The pipe network is then changed constantly. Searching for a solution may require several hundred iterations.

#### Convergence of pressure profile

In the viscous regime when the aperture is small, the change of pressure profile is very sensitive with the aperture, in particular in determination the extent of fluid lag where most change of aperture happens. A controlled iteration technique is used to obtain a converged pressure profile.

\[
\alpha_i^n = \frac{|p_i^n - p_i^{n-1}|}{p_i^n + p_i^{n-1}} \tag{6.16}
\]

\[
\beta_i^n = (1 - \beta_{\text{min}})(1 - \alpha_i^n)^\chi + \beta_{\text{min}} \tag{6.17}
\]

where \( \chi \geq 0 \) is the sensitivity factor to reduce the rate of change of pressure profile. \( \alpha_i^n \) can be regarded as residual. \( \chi = 0 \) which gives \( \beta_i = 1 \) corresponding to the traditional iteration technique.

\[
p_{i}^{n+1} = \beta_i^n p_i^n + (1 - \beta_i^n) p_i^{n-1} \tag{6.18}
\]

\( \chi \) varies according to the average residual \( \alpha_{\text{avg}} = \langle \alpha_i^n \rangle \) according to Figure 6.4. \( \chi_{\text{base}} \) is chosen according to the degree of non-linearity of the problem. In this thesis, \( \chi_{\text{base}} = 0.8 \)
is found to be sufficient for DLM simulations in the viscosity regime. For the elastic deformation region or the mixture of elastic deformation and toughness regime, $\chi_{\text{base}} = 0$ as the changes in each iteration is small and conventional iteration technique is sufficient to converge.

\[
\chi = \begin{cases} 
\chi = \sqrt{\chi_{\text{base}}} & \text{if } \chi_{\text{base}} \geq 1.0 \\
\chi = \chi_{\text{base}}^2 & \text{if } \chi_{\text{base}} < 1.0 \\
\chi = 0 & \text{if } r_i > 100\alpha_{\text{avg}}^n
\end{cases}
\]

\[
\chi = \begin{cases} 
\chi = \sqrt{\chi_{\text{base}}} & 10\varepsilon_r < \alpha_{\text{avg}}^n \leq 100\varepsilon_r \\
\chi = \chi_{\text{base}}^2 & \alpha_{\text{avg}}^n \leq 10\varepsilon_r
\end{cases}
\]

Table 6.3 Sensitivity factor $\chi$ according to the residual $r_i$

There are two criteria for the convergence of pressure profile as shown in Table 6.4. The solution converges if either criterion is achieved. The global convergence is achieved if the average residual $\alpha_{\text{avg}}^n$ is smaller than a tolerance $\varepsilon_r$. The global convergence criterion is first checked. The local convergence criterion is specified to converge the solution if there are few $\sqrt{N}$, where $N$ is fluid node number, fluid nodes that their pressures are oscillating, particular for highly disordered fluid lattice. $\varepsilon_r$ is set as $10^{-4}$ for the DLM simulations presented in this thesis.

<table>
<thead>
<tr>
<th>Local convergence</th>
<th>$\alpha_{\text{avg}}^n &lt; \sqrt{N}\varepsilon_r$ for $\sqrt{N}$ or fewer than nodes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Global convergence</td>
<td>$\alpha_{\text{avg}}^n &lt; \varepsilon_r$</td>
</tr>
</tbody>
</table>

Table 6.4 Fluid pressure profile convergence criteria

Convergence of injection pressure

For a given injection rate, the pressure at injection node $P_0$ is first guessed and the coupled solid-fluid systems are solved. The initial guess of $P_0$ is the solution of the previous time step. If the global continuity equation, Eq (6.15), does not converge to a given tolerance, the residual $R_i$ is calculated as below

\[
R_i^n = \frac{\sum q_i + \sum s_i}{|\sum q_i| + |\sum s_i|}
\]
Two iteration formula of successive higher convergence rate are used to interpolate new injection pressure $P_{0}^{n+1}$. The simplest one is the method of bisection

$$P_{0}^{n+1} = \begin{cases} \frac{P_{0}^{n} + P_{0}^{n,\text{max}}}{2} & \text{if } R^n > 0 \\ \frac{P_{0}^{n} + P_{0}^{n,\text{min}}}{2} & \text{if } R^n < 0 \end{cases} \tag{6.20}$$

The next iteration formula is the secant method which is given by below

$$P_{0}^{n+1} = P_{0}^{n} - \frac{R^n (P_{0}^{n} - P_{0}^{n+1})}{R^n - R_{n-1}^{n}} \tag{6.21}$$

In some cases, the gradient of $P_{0}^{n}$ changes rapidly because of the highly non-linearity of the problem. So different formula are tried to obtain $P_{0}^{n+1}$. The upper bound $P_{0}^{n,\text{max}}$ and the lower bound $P_{0}^{n,\text{min}}$ are first searched. The secant method is first used. If secant method fails to find $P_{0}^{n+1}$ within the bounds, the method of bisection is used which guarantees $P_{0}^{n+1}$ to be bounded.

<table>
<thead>
<tr>
<th>Criterion 1</th>
<th>$R_{0}^{n} &lt; \varepsilon_R$</th>
</tr>
</thead>
<tbody>
<tr>
<td>If criterion 1 fails, check criterion 2</td>
<td>$\frac{(P_{0}^{n,\text{max}} - P_{0}^{n,\text{min}})}{P_{0}^{n}} &lt; \varepsilon_P$</td>
</tr>
</tbody>
</table>

Table 6.5 Convergence criteria of pipe network flow calculation

Table 6.5 lists the convergence criteria of $P_{0}^{n}$. The problem is solved when the residual is small enough. There is possibility that the residual does not converge as it oscillates. So, another convergence criterion is introduced that the difference in two bound is small enough. In this thesis, $\varepsilon_R = 10^{-4}$ is adopted in the DLM simulations presented in this thesis.

### 6.2.5 Validation of pipe network model

For the validation of the pipe network model, a constant discharge flow of a rectangular fracture is simulated using a square grid of pipe network as illustrated in Figure 6.7.

The dimensions of the rectangular fracture is $40 \times 10$ m. The aperture of the fracture is $\delta = 5 \times 10^{-4}$ m. The aperture is constant along the entire fracture. Two longer sides of the fracture are impermeable. A constant discharge rate of $q = 0.0025$ m$^3$/s at 1500 kPa is imposed along the shorter side. Fluid of viscosity $\mu = 10^{-6}$ kPa.s flows from left to right.

The fracture is sub-divided into $20 \times 5$ sub-fractures. Each sub-fracture is a $2 \times 2$ m square. The flow within fracture is modelled by a square grid of pipe network.

The permeability of the fracture is given by Eq (6.8),

$$K = \frac{w \delta^3}{12} \tag{6.22}$$
where the width of the fracture is taken as 1m, the length of fracture is taken as \( l = 40 \). The permeability of fracture \( K = 2.604 \times 10^{-6} \text{m}^2/\text{kN} \).

From Dracy’s law, i.e Eq (6.6),

\[
q = K \Delta p 
\]  

(6.23)

The pressure gradient \( \Delta p \) is 960kPa. The fluid pressure at discharge end is 540kPa.

Figure 6.8 shows the comparison of the analytical solution and the simulation result of the pipe network model. They show good agreement.
6.3 Modelling of hydraulic fracturing under uniform pressure inside a fracture

In order to validate the DLM simulation in hydrostatic condition, an analytical solution is first derived for the planar penny shape crack problem. Several DLM simulations are carried out and validated against the analytical solution.

6.3.1 Analytical solution to penny-shape crack problem under hydrostatic pressure

Sneddon (1946) and Sneddon and Elliot (1946) developed the solutions for the stress field and pressure related to a static pressurized crack. Using linear elasticity, the aperture $\delta(r)$ of a statically pressurised penny-shaped crack (a circular crack) under net injection pressure $P_o$ is given by

$$\delta(r) = \frac{8P_o R}{\pi E'} \sqrt{1 - \left(\frac{r}{R}\right)^2}$$

(6.24)

where

- $E'$ Plain strain Young’s Modulus, $E' = E/(1 - \nu^2)$, $\nu$ is the Poission’s ratio
- $r$ Distance from source
- $R$ Radius of crack

And the volume of ellipsoid $V$ formed by the crack is given by

$$V = 4\pi \int_0^R r\delta(r) dr = \frac{16R^3}{3E'}P_o$$

(6.25)

Sack (1946) expressed the injection pressure $P_o$ using LEFM

$$P_o = \sqrt{\frac{\pi \gamma_f E'}{2R}}$$

(6.26)

where $\gamma_f$ is fracture surface energy per unit area. This equation tells us the energy required to create a fracture surface has to be equal to the work done by the pressure from fluid.

Perkins and Kern (1961) showed that, by combining Equation (6.24) and (6.26) and replacing the pressure $P_o$ by the injection rate $q$, assuming it is constant with time $t$, then

$$R = \left(\frac{9E'q^2t^2}{128\pi \gamma_f}\right)^{1/5}$$

(6.27)
Eliminating $R$ using Eq (6.26) and Eq (6.27), the injection pressure $P_0$ can be expressed as

$$P_0 = \left( \frac{2\pi^3 \gamma^3 E^2}{3q t} \right)^{1/5}$$

(6.28)

### 6.3.2 DLM simulation results

Six simulations are carried out for D100, D75 and D50 lattice models for each $\alpha = 0.3$ and $\alpha = 1.0$ where $\alpha$ is the ratio of shear spring stiffness to normal spring stiffness.

![Pressure histories of lattice model simulation on penny shape crack hydraulic fracture problem.](image)

Fig. 6.9 Pressure histories of lattice model simulation on penny shape crack hydraulic fracture problem. (a) $\alpha = 0.3$ and (b) $\alpha = 1.0$.

Figure 6.9 shows the pressure histories of all six simulations. Two stages can be identified in the time histories. The first stage is the linear part of the pressure history curve which represents the elastic deformation of the penny shape crack. Fluid pressure is insufficient to initiate fracture. Since the solid lattice model is elastic, the pressure building is linear with time. When the fluid pressure reaches a critical value, it is sufficient to start fracturing. This is the demarcation of the second stage in which pressure starts decreasing steadily. The pressure drops because new fracturing provides the room to accommodate the injected fluid.

A coarser model gives a higher injection pressure and the peak pressure happens later.

**Comparison with analytical solution**

The analytical solution for the penny shape hydraulic fracture problem is derived as below. Using the macro-micro relationship of the penny shape problem in Eq. (5.11), the critical
6.3 Modelling of hydraulic fracturing under uniform pressure inside a fracture

Pressure $p_{cr}$ at which fracture starts to propagate is given by

$$p_{cr} = \pi f_{st} \sqrt{\frac{<l_r>}{8R}} \tag{6.29}$$

where $<l_r>$ is the average length of fracture given by the square root of average area of the fracture facet $<A_f>$. $R$ is the radius of the penny shape crack.

At critical time $t_{cr}$ when the fracture starts to propagate, the volume of fluid in the penny shape crack $V_{cr}$ is simply

$$V_{cr} = qt_{cr} \tag{6.30}$$

From Eq (6.25), the volume of penny shape crack is given by

$$V_{cr} = \frac{16R^3p_{cr}}{3E'} \tag{6.31}$$

where $E'$ is the macroscopic plain strain Young modulus. Combining Eq (6.30) and (6.31), $t_{cr}$ is given by

$$t_{cr} = \frac{16R^3p_{cr}}{3qE'} \tag{6.32}$$

<table>
<thead>
<tr>
<th>Lattice model</th>
<th>$&lt;l_r&gt;$</th>
<th>$p_{cr}$</th>
<th>$t_{cr}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>D100</td>
<td>1.157</td>
<td>489.8</td>
<td>7.77</td>
</tr>
<tr>
<td>D75</td>
<td>1.543</td>
<td>565.5</td>
<td>8.98</td>
</tr>
<tr>
<td>D50</td>
<td>2.315</td>
<td>676.0</td>
<td>10.94</td>
</tr>
</tbody>
</table>

Table 6.6 Pressure and time at the initiation of fracturing for lattice simulation of penny shape problem

Table 6.6 lists the critical pressure its corresponding time of different lattice models. Finer model gives a smaller $p_{cr}$ at a shorter time $t_{cr}$. It is because for the same microscopic tensile strength $f_{st}$, finer model gives a fracture facet smaller $l_r$, giving a smaller $l_r/R$ and stress is more concentrate at the facet adjacent to penny shape crack.

Figure 6.10 shows the pressure histories of the six simulations normalised by $p_{cr}$ and $t_{cr}$ and compare with the analytical solution. Figure 6.10a shows the simulation of the three models (D100, D75 and D50) when $\alpha = 0.3$. All three models overestimates the injection pressure. Finer model gives a better match with the analytical solution. For $\alpha = 1.0$ as shown in Figure 6.10b, D50 model overestimates the injection pressure while the D75 and D100 models underestimates the injection pressure. The pressure histories of the D75 and D100 models are similar and closer to the analytical solution compared with the D50 model.
Fig. 6.10 Comparison of analytical solution and lattice model simulation on penny shape crack hydraulic fracture problem. Normalised injection pressure $p/p_{cr}$ verse normalised time $t/t_{cr}$ normalised at the initialisation of fracture. (a) $\alpha = 0.3$ and (b) $\alpha = 1.0$.

The small fluctuation of the pressure histories is due to the deviation of slightly uneven growth of discretised fracture facets from the perfect growing of circular crack assumed in the analytical solution.
6.4 Further DLM simulations assuming hydrostatic pressure

In this section, two types of DLM simulation under hydrostatic pressure are presented: hydraulic fracturing in a rough crack in homogeneous material and a planar crack in heterogeneous material.

6.4.1 Rough crack

Fig. 6.11 Geometry of initial rough crack formed by facets of Voronoi cell for hydraulic fracturing simulation
Geometry of rough crack

Planar fracturing is the idealisation of a natural fracture because it has asperity and its fracture path is tortuous. The natural asperity increases the resistant against hydraulic fracturing. Hydraulic fracturing simulation of the initial rough crack has been carried out. Figure 6.11 shows the geometry of rough crack. The asperity of fracture comes from an irregular facets of Voronoi cells. The fracture asperity modelled in this simulation is much tortuous than the natural fracture. The length scale (correlation length) of the asperity is small relative to fracture size. Also, the orientation of the adjacent facets can change rapidly which is impractical in the natural fractures. There are large amount of facets that are orientated sub-vertically.

Figure 6.12 compares the statistics of pipe network coordination number $n_{coord}$ of a planar crack and a rough crack. The theoretical value of $<n_{coord}>$ is 6 (Puschmann et al., 2015). $<n_{coord}>$ for a planar crack and a rough crack are 5.41 and 5.76 respectively. They are slightly smaller than the theoretical value because of the edge fluid nodes which have fewer $n_{coord}$. The standard deviation of $n_{coord}$ for a rough crack pipe network (5.33) is much higher than that of a planar crack (3.14). The skewness of a rough crack is also higher. The common edge of neighbour fracture facets has a greater variation in length so it is likely to give higher variation of $n_{coord}$ of fluid node.
6.4 Further DLM simulations assuming hydrostatic pressure

Model parameters

Three simulations of models D50, D75 and D100 of different fineness are carried out. The lattice model is similar to the planar penny shape problem as shown in Figure 6.4, except the initial penny shape crack has a rough surface. Also, fractures in all orientation are allowed.

![Fig. 6.13 Pressure histories of hydraulic fracturing simulation of rough crack. (a) before normalisation and (b) after normalisation.](image)

Pressure histories comparison

Figure 6.13 shows the pressure histories of these simulations. The trend is similar to the planar shape crack simulation. The pressure histories can also be divided into two stages: elastic deformation of fracture and fracture propagation. In the fracture propagation stage, fluid pressure remains roughly constant with some fluctuations. For the finer models, smaller fluid pressure is required to initiate fracture according to Eq (6.29). When the pressure histories graph is normalised using $p_{cr}$ and $t_{cr}$ to adjust the effect of the fineness of lattice model, three curves converge. $p_{cr}$ is the critical pressure required to start fracture propagation in planar penny shape problem at critical time $t_{cr}$. Compared with the planar penny shape case, the pressure required to initiate fracture is much higher, about $5.5 - 6p_{cr}$. The time when fracture initiates is also longer, about $5.5 - 6t_{cr}$.

The much higher fluid pressure for fracture initiation and propagation is contributed by highly tortuous fracture path with very short correlation length. Orientation of the fracture surfaces deviates from the horizontal plane. These fractures are less effective in contributing the stress intensity at the fracture tip. Also, the facets along the circumference of the penny shape crack do not align along the horizontal plane, particularly for sub-vertical one. Higher
fluid pressure is needed so that the resolved pressure component perpendicular to these facets can meet their tensile strength to fracture.

**Fracture aperture and fluid storage**

Figure 6.14 compares the aperture of the planar and rough penny shape fractures. The apertures are normalised by their maximum values at the centre of the crack. The injection volume of the both fractures are similar. The aperture of the planar crack follows nicely with the analytical profile. For the rough fracture, the apertures of fracture facets scatter but they are bounded by the normalised aperture profile of the planar crack. The scatteredness is due to variation of fracture facet orientation. This means that the fluid storage for the rough case is highly uneven among fractures, even among fractures in their vicinity. Also, fractures which are horizontal have larger aperture and store more fluid.

![Comparison of fracture aperture of plane crack and rough crack of D50 model.](image)

Fig. 6.14 Comparison of fracture aperture of plane crack and rough crack of D50 model. (a) planar crack and (b) rough crack.

Figure 6.15 compares the fracture apertures just before the fracture initiation and towards the end of simulation. The diameter of the fracture at the end of simulation is almost doubled
Fig. 6.15 Fracture aperture comparison of hydraulic fracturing of rough crack (D50 model) just before fracture initiation and the end of simulation.
as compared with that of before fracture initiation. The maximum aperture of fracture is also doubled. However, the ability of the fluid storage near the fracture tip has reduced. This is because as fracture propagates, its path gradually deviates from horizontal. The tortuosity of fracture increases and fluid pressure at central part has reduced influence in opening up fracture.

6.4.2 Planar crack with applied heterogeneity

Three D50 model simulations with different applied heterogeneity, LN(0.25), LN(0.5) and LN(0.75), are carried out to investigate the effect of heterogeneity on hydraulic fracturing. Figure 6.16 shows the snapshots of the simulations. For the homogeneous model, the majority of fracture facets are formed adjacent to the main fracture. For the heterogeneous model, fracture facets formed not only along the circumference of fracture, but also some isolated fracture facets are formed away from the main fracture. The spread increases when heterogeneity increases. For the heterogeneous model, weak lattices break under lower stress even away from the main fracture.

When fracture propagates, some strong lattices within the main fracture do not break. The main fracture becomes 'porous'. These lattices share fluid loading and reduce the stress near the fracture tip. The growth of the main fracture is restrained. When fracture continues to propagate, some strong lattices in the fracture break. For the highly heterogeneous model, there are strong lattices inside the main fracture that do not break easily as they have higher strength and more of such lattices are present to share loading.

Figure 6.17 plots the time histories of the three models. All three models are stronger in resisting fluid pressure compared with the uniform model. The curves are similar to the rough crack fracture; they do not show a declining part after fracturing initiates. The pressure history of LN(0.25) model starts to level off at $p \approx 1.4p_{cr}$ when $t \approx 2.5t_{cr}$. For LN(0.5) and LN(0.75), their pressure histories are similar and the fluid pressure increases steadily and reaches $2.0p_{cr}$. It may indicate that there is a limit on the increase of apparent toughness by applied heterogeneity. Further studies are suggested.

Applying heterogeneity increases the apparent toughness against fracturing but the effect is smaller than the increase in toughness ($\approx 5.5 - 6.0p_{cr}$) by asperity of crack.
6.4 Further DLM simulations assuming hydrostatic pressure

Fig. 6.16 Snapshots of fracture evolution of planar crack hydraulic fracturing under solid lattice model with three different applied heterogeneity: LN(0.25), LN(0.5) and LN(0.75).
Fig. 6.17 Injection pressure histories of planar crack hydraulic fracturing with three different applied heterogeneity, LN(0.25), LN(0.5) and LN(0.75), of solid lattice model.
6.5 Modelling of viscous flow during pre-fracture stage

For the validation of DLM simulation of fluid injection of viscous fluid into a planar penny shape crack (pre-fracture stage), a semi-analytical approximation solution is derived in this section. Simulation of hydraulic fracturing by viscous fluid is presented in the next section.

The viscosity regime solution of fluid flow in a penny shape crack assuming no fluid lag is provided by (Spence and Sharp, 1985) and the asymptotic solution is given by (Detournay, 2004). A semi-analytical approximation solution presented here is intuitive and simple to manipulate. It also takes into account the effect of fluid lag. However, this solution assumed that the crack radius is given. This means that this solution does not account for the growth of crack radius by fracture propagation.

The fluid flow in a penny shape crack is similar to pump out test in geotechnical engineering for the determination of in-situ permeability. The pump out well is replaced by an injection well and the permeability along fracture follows the cubic law instead of constant permeability assumed in pump out test.

This section also provides two asymptotic solutions and some sensitivity analysis.

6.5.1 Formulation

Assuming a thin ring of distance \( r \) from the center of well of length \( dr \). The permeability across this ring is assumed constant and Dracy’s law applies.

\[
q = -k(r)A \frac{dp}{dr}
\]  

(6.33)

The negative sign means the pressure gradient \( dp/dr \) is negative for increasing \( r \). The area of the ring is given by

\[
A = 2\pi r \delta(r)
\]  

(6.34)

The aperture of crack \( \delta \) is given by Eq (6.24), i.e.

\[
\delta(r) = \frac{8P_s R_s}{\pi E'} \sqrt{1 - \left( \frac{r}{R_s} \right)^2}
\]  

(6.35)

where \( P_s \) is the effective hydrostatic pressure acting on fracture. This assumes that the variation of fluid pressure across most of the crack is small except at the crack tip region and near the borehole region. This corresponds to high toughness, high confining pressure regime. This also applies to late time solution in the viscosity regime. \( R_s \) is the effective
Fig. 6.18 Derivation of approximate solution of penny shape crack problem under assuming cubic law for flow
radius of crack. By the cubic law, the permeability at the ring is given by

\[ k(r) = \frac{\delta^2(r)}{12\mu} \]  

(6.36)

Putting Eq. (6.34) and (6.35) into Eq. (6.33) and substitute \( \delta(r) \) by Eq (6.35),

\[ q_i = \frac{-256P^3R^3_r}{3\pi^2E^3\mu} \left( 1 - \left( \frac{r}{R_s} \right)^2 \right)^{3/2} \frac{dp}{dr} \]  

(6.37)

Denote dimensionless parameters \( \rho = r/R_s \) and \( \rho_o = R_o/R \), the following integration equation is obtained

\[ \int_{\rho_o}^{\rho} \frac{d\xi}{\xi(1 - \xi^2)^{3/2}} = -\frac{256P^3R^3_s}{3\pi^2q\mu E^3} \int_{P_o}^{P} dp \]  

(6.38)

where \( \xi \) is the integration variable. The pressure profile is given by

\[ p = P_o - \frac{3\pi^2q\mu E^3}{256P^3_sR^3_s} \int_{\rho_o}^{\rho} \frac{d\xi}{\xi(1 - \xi^2)^{3/2}} \]  

(6.39)

\[ \int_{\rho_o}^{\rho} \frac{d\xi}{\xi(1 - \xi^2)^{3/2}} = \left( \frac{1}{2} \ln \left( \frac{1 - \sqrt{1 - \xi^2}}{1 + \sqrt{1 - \xi^2}} \right) + \frac{1}{\sqrt{1 - \xi^2}} \right) \Big|_{\rho_o}^{\rho} \]  

(6.40)

### 6.5.2 Solving \( R_s \) and \( P_s \)

There are two parameters \( R_s \) (effective radius) and \( P_s \) (radius of the effective hydrostatic pressure) to be determined and their relationship is sketched in Figure 6.19. \( R_o, R_w \) are the radii of the injection well and the wetted part of the penny shape crack. There are three calibration parameters introduced, \( \eta, \omega \) and \( \lambda \), for the adjustment of \( P_s \) and \( R_s \). They are calibrated to match the DLM simulation results.

\[ R_s = (1 - \eta)R_w + \eta R \]  

(6.41)

where \( 0 \geq \eta \geq 1 \) which indicates the contribution of the dry part of the fracture in deformation of crack. \( \eta = 0 \) corresponds to the upper bound solution as it assumes that the dry part of fracture is completely closed. \( \eta = 1 \) corresponds to the lower bound solution because this assumes zero lag condition. \( \eta \) decreases with \( \rho_w \), where \( \rho_w = R_w/R \). For the elastic
Fig. 6.19 Relationship between $P_*$, $P_o$, $R_*$, $R_w$ and $R$ in approximation solution of viscous flow in penny shape problem

depression regime where fluid lag is small $\eta \to 1$ and $R_* \to R$. For a rough estimation, the following relationship is suggested

$$\eta = 1 - 0.2\rho_w \quad \text{for} \quad \rho_w > 0.7 \quad (6.42)$$

The value of $P_*$ ($< P_o$) is given by integrating over the positive part of the pressure profile

$$P_* = \frac{\int_{\rho_o}^{\rho_w} \omega(\rho) p \, d\rho}{(\rho_w - \rho_o) \int_{\rho_o}^{\rho_w} \omega(\rho) \, d\rho} \quad (6.43)$$

a weighting function $\omega(\rho)$ is introduced to recognise that the pressure near $\rho_o$ is more effective to open the fracture as compared to the same pressure near fluid front $\rho_w$. It is suggested that

$$\omega(\rho) = 1 - \left( \frac{\rho}{\rho_w - \rho_o} \right)^\chi \quad (6.44)$$

where $\chi$ is approximately 0.9 to 0.95 for $\rho_w > 0.7$.

Recall that $P_*$ and $R_*$ are related by Eq. (6.25) to conserve mass balance.

$$\lambda P_* R_*^3 = \frac{3E'qt}{16} \quad (6.45)$$
which gives \( P_* \propto 1/R_w^3 \). \( P_* \) has to be decreases when \( R_w \) increases due to the growth of fluid lag. \( \lambda(\rho_w) \geq 1 \) is introduced to adjust the fluid volume which is underestimated by using \( R_w \) in the above equation. For \( \rho_w \to 1 \), \( \lambda(\rho_w) \to 1 \). There is not much study for \( \rho_w \), based on the information on several DLM simulations, \( \lambda \approx 1/\rho_w \) for \( \rho > 0.7 \).

Under the constraint by Eq. (6.45), \( P_* \) and \( R_* \) in Eq. (6.38) can be determined. After solving, \( P_o \) can be obtained by Eq. (6.43).

The three calibration parameters, \( \eta, \omega \) and \( \lambda \) are not thoroughly calibrated for the whole range of \( \rho_w \). Also, the approximate solution starts to deviate from the simulation result for \( \rho_w \lesssim 0.7 \). It is because the approximate solution is derived for the elastic deformation regime which gives large \( \rho_w \) (i.e. small fluid lag). The problem becomes the viscosity dominant so the assumed hydrostatic aperture profile and the aperture profile deviate too much with their actual profiles. Another model should be derived for \( \rho_w \lesssim 0.7 \).

The calibration parameters and their relationships proposed in this section are based on only several DLM simulation results. More simulations should be done to to establish a more precise relationship.

### 6.5.3 Asymptotic solutions

There are two asymptotic solutions for the cubic flow of the penny shape crack solution. Inspecting the integral,

\[
\int_{\rho_o}^{\rho} \frac{d\xi}{\xi(1-\xi^2)^{3/2}} \tag{6.46}
\]

There are two parts of the denominator which give two asymptotes at both ends of the integrating limit. They are \( 1/\xi \) when \( \rho_o \to 0 \) and \( 1/(1-\xi^2)^{3/2} \) when \( \rho \to 1 \). Near the injection point where \( \rho_0 \to 0 \), the asymptotic solution in Eq (6.46) becomes

\[
\int_{\rho_o}^{\rho} \frac{d\xi}{\xi} = \ln \frac{\rho}{\rho_o} \tag{6.47}
\]

The change in fracture aperture is small so the permeability along the fracture is close to a constant. So the radial flow obeys Dracy’s law for constant permeability along the entire fracture and the solution reduces to a radial flow problem. The asymptotic near the injection point is given by very high fluid velocity across a small flow area \( r \) (\( v = q_i/A = q_i/(2\pi r \delta) \)).

Towards the fracture tip \( \rho \to 1 \), the asymptotic solution in Eq (6.46) becomes

\[
\int_{\rho_o}^{\rho} \frac{d\xi}{(1-\xi^2)^{3/2}} \bigg|_{\rho_o}^{\rho} = \frac{\xi}{\sqrt{1-\xi^2}} \bigg|_{\rho_o}^{\rho} \tag{6.48}
\]
The curvature of fracture profile changes rapidly. The permeability of fracture decreases even more rapidly due to the cubic law. The asymptotic solution applies for small crack tip region and small fluid lag, i.e. the problem is in the toughness regime or the confining pressure is high.

![Asymptote of penny shape problem under cubic flow and its asymptotes](image)

**Fig. 6.20 Solution of penny shape problem under cubic flow and its asymptotes**

Figure 6.20 plots the profiles of the integration part of the approximate solution in Eq. (6.40) and profiles of the integration parts of its two asymptotes. The radial flow asymptotic solution governs a longer range of solution ($\rho_o \leq \rho \lesssim 0.5$) from the injection point and the crack tip asymptotic solution governs a shorter range near the tip region ($0.95 \leq \rho \leq 1.0$). Between them, it is the interaction region of two asymptotic solutions. However, the rate of convergence to the asymptote at the fracture trip end is much faster with an order of convergence of 3, compare with a convergence order of 1 of the radial flow asymptote near the injection point.

### 6.5.4 Sensitivity analysis

Figure 6.21 illustrates the typical pressure profiles and the interplay between different mechanisms for the viscosity regime and the elastic deformation regime. The viscosity regime is characterised by the steep pressure gradient along the fracture, large fluid lag, large
6.5 Modelling of viscous flow during pre-fracture stage

Fig. 6.21 Sketch showing typical pressure profiles and mechanisms of the viscosity regime and elastic deformation regime
drag pressure by fluid viscosity and small aperture. On the other hand, the elastic deformation regime is characterised by mostly small pressure gradient, small fluid lag, small drag pressure by fluid viscosity and large aperture.

Figure 6.22 shows the parametric studies of five parameters $q, t, E', \mu, R$ and $\rho_o$ to the pressure profiles along the fracture.

For the injection rate $q$ shown in Figure 6.22a, the problem becomes the elastic deformation dominant by increasing $q$. This is because the aperture has to be increased to store more fluid. The permeability increases that gives higher permeability of the fracture. The drag pressure by fluid viscosity decreases. For the same reasons, increasing time $t$ increases the volume of fluid injection as shown in Figures 6.22b. The problem becomes elastic deformation with sufficient time.

Figure 6.22c shows the parametric study on $E'$. It shows that the problem becomes the viscosity dominant for small $E'$. It is because for the same injection rate, smaller pressure is required to open the crack. For smaller injection pressure while the drag pressure remains unchanged, the pressure gradient becomes large.

The effects on $\mu$ is shown in Figure 6.22d. Obviously, increasing $\mu$ gives the viscous flow to be viscosity dominant as the drag pressure increases with $\mu$.

From Figure 6.22e, it shows that increasing $R$ makes the problem to be viscosity dominant. To inject the same amount of fluid, large $R$ gives smaller aperture. This reduces the permeability of the penny shape crack. Also, large $R$ means larger fluid lag. Since the volume of the penny shape crack is proportional to $R^2$ but it only increases linearly with aperture. $R$ is a sensitive parameter for the change of regimes.
6.5 Modelling of viscous flow during pre-fracture stage

Fig. 6.22 Sensitivity analysis of approximate solution of penny shape crack under cubic flow. (a) Discharge rate $q$, (b) injection time $t$, (c) plain strain Young Modulus $E'$, (d) viscosity $\mu$ and (e) penny shape crack radius $R$
6.6 DLM simulations on hydraulic fracturing by viscous fluid

This section presents some DLM simulations of hydraulic fracturing by viscous fluid with a pre-existing planar penny shape crack. First, the DLM simulations before fracture propagation are studied and compared with the semi-analytical solution presented in Section 6.5. Two regimes are identified: viscosity regime and elastic deformation regime. The evolution of pressure profiles are studied to identify the evolving regimes in different stages of hydraulic fracturing. The regimes are viscosity regime, elastic deformation regime and mixture of elastic deformation and toughness regime. The injection fluid pressures profiles of hydraulic fracturing by fluid of different viscosities are compared to study their evolving regimes of hydraulic fracturing.

The simulation results are compared with the planar crack case.

6.6.1 Comparison of simulation results with approximate solution before fracture propagation

Figure 6.23 presents 4 cases to compare the pressure profile obtained by the approximate solution as presented in Section 6.5 and the DLM simulations of viscous flow in an existing penny shape crack. The crack tip is assumed to be stationary in this case, meaning that the penny shape crack does not propagate. By this assumption, two regimes of energy dissipation mechanism are investigated. One is viscosity regime in which energy is dissipated by drag pressure induced by fluid viscosity. Another one is elastic deformation regime in which majority of energy is used for work done in opening the crack. There is no energy dissipated by toughness before the propagation of fracture. So, Figure 6.23 compares the pressure profiles and the aperture profiles in penny shape crack from the viscous regime to the elastic deformation regime.

In the viscous regime as shown in the first two cases (Figures 6.23a-d) where fluid lag and pressure gradient are large, the pressure profiles before the fluid lag show a good match between the approximate solution and the DLM simulations as shown in Figures 6.23a and c. The simulation does not show smooth transition toward the fluid front. The pressure suddenly drops to zero from \( \approx 0.5P^* \) (case 1) and \( \approx 0.75P^* \) (case 2). This is likely due to the coarse mesh of D50 DLM that cannot model the sensitive change in permeability from the small fracture aperture. The aperture profile assumed in the approximate solution underestimates the aperture near the injection point and overestimates far away from it. This is the compromise of using hydrostatic aperture profile to estimate the aperture profile due to
6.6 DLM simulations on hydraulic fracturing by viscous fluid

Fig. 6.23 Comparison of the approximate solution of viscous flow in the penny shape crack with the DLM simulations. Left: pressure profile normalised by $P^*$ (the equivalent hydrostatic pressure in the approximate solution), right: aperture profile normalised by the maximum aperture $\delta^*$, derived from the equivalent hydrostatic pressure and the equivalent radius in the approximate solution.
pressure induced by the viscous flow of fluid in which steep pressure gradient happens at both ends of the fracture.

The last two cases (Figure 6.23e-h) illustrate the viscous flow in the elastic deformation regime where the fluid front is close to the crack tip and the pressure gradient along fracture is small. The pressure profiles show good agreement between the DLM simulations and the approximate solution up to \( \rho \approx 0.6 \), beyond which the steep pressure gradient happens because of the rapid decrement of the aperture near the crack tip. The pressure profiles from the DLM simulations follow the radial flow asymptote but do not show the pressure drop near the pressure profile as predicted by the approximate solution. It is because the DLM mesh is not fine enough to simulate the near tip behaviour where rapid changes of aperture and steep fluid pressure gradient happen. For the aperture profiles, the DLM simulation results match the approximate solution from \( 0.4\rho \) to \( 1.0\rho \). Near the injection point, the approximate solution underestimates the aperture profile from the simulation because of steep pressure gradient from the radial flow asymptote. This does not affect much of the pressure profile near the injection point as the flow is insensitive to the permeability change arising from the change in fracture aperture.

\[ 6.6.2 \text{ Fluid pressure profile evolution} \]

![Fracture starts to propagate](image)

Fig. 6.24 Injection pressure history of hydraulic fracture of penny shape crack by viscous fluid simulated by DLM.
A DLM simulation is presented to study the evolution of pressure profiles in the hydraulic fracturing of the penny shape crack. Figure 6.24 plots the injection pressure history. The simulation starts with the injection of fluid in a dry penny shape crack. At the beginning, the injection pressure drops quickly with time when the fluid flow along the fracture to displace the fluid lag. When the fracture propagation starts, the injection pressure continues to drop, but the rate drops steadily. The pressure drop after fracture propagation is similar to that of the hydrostatic case as discussed in Figure 6.10 and Eq. (6.28). The pressure profile is further discussed in Section 6.6.3 and Figure 6.26.

Figure 6.25 plots the pressure profiles along the fracture at different time points. Before the fracture propagation as shown in Figure 6.25a, at early time that little fluid is injected, large injection pressure is required to open the existing crack. Pressure gradient is steep along the fracture because of the small fracture aperture that gives low permeability. This is the viscosity regime because steep pressure gradient means high energy loss by fluid viscosity. Before $t = 110s$, the fluid front advances to displace the fluid lag and the pressure gradient drops with time. At $t = 140s$, the fluid front reaches the crack tip. As $t$ increases further, the pressure near injection point drops at a slower rate but the pressure gradient decreases. The pressure profiles in general increase. Without advancing the fluid front, the aperture profile has to be raised to store the injected fluid. The decline in pressure gradient means the pressure loss by drag pressure due to viscosity reduces. The energy dissipation by the fluid viscosity decrease and more energy is used for the work done in increasing fracture aperture. Energy dissipation transits from the viscosity regime to the elastic deformation regime.

When the fracture starts to propagate from $t = 190s$, the pressure profiles along the fracture are plotted in Figure 6.25b. Both the injection the pressure and the pressure along the fracture drops but the fluid front advances with the crack tip. Also, the pressure gradient decreases and approaches to the hydrostatic pressure. Energy dissipated by the viscosity reduces and more energy is consumed for the elastic deformation of rock and toughness. Hydraulic fracturing continues to approach the toughness regime. It should be noted that literatures often use the term toughness regime but actually two energy dissipation mechanisms are included.

### 6.6.3 Comparison of injection pressure histories

Figure 6.26 plots the injection pressure histories of hydraulic fracturing of the planar penny shape crack under viscous fluid of different viscosities.

For hydraulic fracturing by fluid of low viscosity $\mu \leq 10^{-6}$kPa, the curves can be divided into 3 stages as delineated in Figure 6.26. The first stage is the decrement of the injection pressure. In this stage, fluid flow is in the viscosity regime and large injection pressure is
Fig. 6.25 Pressure profile evolution of hydraulic fracture of penny shape crack by viscous fluid simulated by DLM. (a) Before fracture propagation, (b) after fracture propagation.
Fig. 6.26 Injection pressure histories of hydraulic fracturing of planar penny shape crack by fluid of different viscosities from DLM simulation. Different stages of hydraulic fracturing is demarcated.
required initially. In the second stage where the injection pressure starts to increase, the fluid front reaches the crack tip and the pressure gradient decreases. This means that the influence of the viscosity decreases. The injection pressure has to be increased to increase the overall aperture to accommodate the injected fluid, as if the hydrostatic case before fracture initiates. The fluid pressure is used for the work done to open the crack (the elastic deformation regime). The third stage starts when the fracture starts to propagate at $1.0 - 1.1 t_c r$, irrespective the viscosity of fluid. Injection pressure curves converge to the hydrostatic case and follow the declining curve by Eq (6.28). Energy is consumed to propagate the crack (toughness) and to increase its aperture (elastic deformation).

For hydraulic fracturing by high viscosity fluid ($\mu \geq 5 \times 10^{-6}$kPa), the injection pressure curve is smooth and strictly decreases at a reducing rate. Fluid flow gradually transits from the viscosity regime to the elastic deformation regime (i.e. energy stored in fluid is transferred to the elastic energy of the surrounding rock for increasing fracture aperture) before fracture propagation. During fracture propagation, the problem transits to the mixture of the elastic deformation and toughness regimes. The difference between the curves of different viscosities reduces as the fracture propagates. It is because of the reducing influence of viscosity when the problem is evolved away from the viscosity regime. For sufficient long time, injection pressure curve converges to the hydrostatic case and the fluid flow approaches further to the mixture of the elastic deformation and toughness regime.

### 6.6.4 Hydraulic fracturing of rough fracture

This section explores hydraulic fracturing of rough fracture under viscous fluid. The simulation cannot be completed because of the convergence of solution could not be achieved. Further work is need on the convergence issues. However, the partial results give some insight of viscous flow in rough crack and fracturing.

Figure 6.27 plots the injection pressure histories of hydraulic fracturing by three fluid of different viscosities: $\mu = 0$Pa.s (hydrostatic), $\mu = 10^{-6}$kPa.s and $\mu = 10^{-5}$kPa.s. There are three stages of pressure histories for the $\mu = 10^{-6}$kPa.s case, which is similar to the planar penny fracture case as discussed in Section 6.6.3. The pressure histories of the injection pressure remain roughly constant when the fracture propagates. For the $\mu = 10^{-6}$kPa.s and the hydrostatic cases, the injection pressures stay at $\approx 5.5 p_{cr}$. For the $\mu = 10^{-5}$kPa.s case, the injection pressure remains roughly constant at $7 p_{cr}$ before and after the fracture propagation.

Figure 6.28 shows the snapshots of the pressure distribution of a fluid lattice of the planar and a rough penny shape crack. The pressure drops near the injection point is smaller in
6.6 DLM simulations on hydraulic fracturing by viscous fluid

Fig. 6.27 Injection pressure histories comparison of hydraulic fracturing of rough fracture by fluid of different viscosities from DLM simulation.
the rough crack case compared with the planar crack case. At the edge of the rough crack, pressure dissipation is large because of the tortuosity of fluid path.

Figure 6.29 plots the evolution of the pressure distribution along the fracture. Initially, the pressure scatters because different fracture facets oriented differently, causing the variation of permeability of pipes. The scatteredness increases further away from the injection point. The overall scatteredness reduces with time as the pressure increases. The variability of permeability by the change in aperture has less effect on fluid pressure.
Fig. 6.28 Comparison of pressure distribution of rough and planar penny shaped crack under viscous fluid flow of different viscosities simulated by DLM.
Fig. 6.29 Evolution of pressure profiles of fracturing of rough penny shape crack by viscous fluid simulated by DLM. (a) Viscosity $\mu = 10^{-6}$ kPa.s, (b) Viscosity $\mu = 10^{-5}$ kPa.s
6.7 Conclusions

Dual Lattice Model (DLM) is proposed that couples a solid lattice and a fluid lattice for hydraulic fracturing simulation. Both the solid part and the fluid part are simplified into a network of 1D lattice elements. Solid lattice and fluid lattice are geometrically interdependent. Solution techniques are presented to solve pressure distribution of flow in a fracture surface and to search for the injection pressure. A C++ code, DualLattice3D was written for DLM simulations presented in this Chapter. The code is validated by the analytical solution of the classical penny shape crack problem under hydrostatic pressure.

DLM simulations of hydraulic fracturing of a rough crack and a planar crack with applied heterogeneity under hydrostatic pressure are carried out. The fluid pressure required for fracture propagation of a rough crack substantially increases compared with the planar crack case. This means that there is an increase in the apparent toughness by the asperity of fracture. Applied heterogeneity also increases the apparent toughness, but to a lesser extent.

A simple semi-analytical approximate solution is derived for the viscous flow in an existing planar penny shape crack. Two asymptotes are identified. One is the radial flow near the injection point governing the steep pressure gradient for the far field (relative to the crack tip). Another one is the near field which governs a much smaller region where steep pressure gradient happens.

Several DLM simulations are compared with the approximate solution. They show good agreement for the fluid pressure near the injection point but the pressure profile deviates near the crack tip. The mesh near the crack tip is not fine enough to model the large pressure gradient which happens there.

For hydraulic fracturing simulation by DLM, the injection pressure profiles simulated decrease before and after fracture propagation for high viscosity fluid. For low viscosity fluid, there are three stages in hydraulic fracturing. They are viscosity dominant, elastic deformation dominant and the mixture of elastic dominant and toughness dominant. In the viscosity regime, the injection pressure drops initially. In the elastic dominant regime, the injection pressure increases. After the fracture propagates, the injection pressure decreases again in the mixture of elastic deformation and toughness regime.
Chapter 7

Conclusions and future work

7.1 Conclusions

This thesis examines the mechanisms of hydraulic fracturing. It is a complicated process because of its multi-physics and multi-scale nature. Many numerical studies focus on the multi-physics nature of the problem. The aim is to propose a new numerical method for multi-physics multi-scale simulation of hydraulic fracturing.

Lattice Element Method (LEM) is proposed to model heterogeneous material. LEM simplifies material model into a network of 1D lattice elements. The computational cost of a LEM simulation is low, making three-dimensional multi-scale modelling feasible in desktop computers. Modelling of fracturing process is straightforward by removing lattices meeting a threshold. Complicated fracturing process can be modelled. Failure mode of a lattice model does not require to be specified as a priori. It fails at its most critical mode.

Dual Lattice Model (DLM) couples a solid lattice model and a fluid lattice model. DLM is highly efficient in hydraulic fracturing simulation. It allows three-dimensional multi-scale hydraulic fracturing simulation in desktop computers.

7.1.1 Relationships between model parameters and macroscopic response

From LEM simulations, the relationships between model parameters and macroscopic response are identified. Model parameters govern the microscopic response.

The microscopic parameters studied in this thesis are the ratio of shear spring to normal spring stiffness $\alpha$, node density $n$ and applied heterogeneity (by assigning PDFs on the lattice parameters).

The normal spring stiffness governs the bulk deformation of the model while the shear spring stiffness governs the distortion of the model.
Stress heterogeneity is found to be one of the features in LEM. Under macroscopic isotropic stress, both the facet normal $\sigma_n^f$ and the shear stresses $\sigma_s^f$ do not show any stress heterogeneity, by either changing $\alpha$ or $n$. Interestingly, it shows stress heterogeneity at nodal level by changing $n$ but not $\alpha$. It is because shear springs are not mobilised under isotropic loading, so $\alpha$ that governs the shear spring stiffness does not affect the nodal heterogeneity.

The nodal stress calculation depends on the geometry of cell which is governed by $n$. So different $n$ gives different nodal stress heterogeneity. Also, the mean of nodal deviatoric stress $<q^n>$ increases with decreasing $n$.

Under macroscopic uni-axial stress, both $\alpha$ and $n$ contribute to stress heterogeneity. Decreasing $\alpha$ and $n$ increases the degree of stress heterogeneity. However, $<q^n>$ does not change as in the macroscopic isotropic stress case. For the applied heterogeneity, even the mean of the lattice parameters does not change, the model becomes less stiff in terms of both the macroscopic bulk modulus $K$ and the macroscopic shear modulus $G$. This implies that the spring stiffness as determined by the RBSN is the optimal in providing macroscopic stiffness.

### 7.1.2 Relationships between microscopic parameters with LEFM

LEM is capable to model complex fracturing process in heterogeneous material by simply changing lattices properties once they reach their microscopic strengths. The analytical relationships between fracture toughness $K_{Ic}$ and microscopic parameters of microscopic tensile strength $f_{st}$, microscopic Young modulus $E_{micro}$ and $\alpha$ is established. $K_{Ic}$ also relates to a length scale of the lattice models. This means that cell size and fineness of the lattice model have to be specified to match both the macroscopic strengths and $K_{Ic}$ of a material. LFEM can be complied only by selecting the appropriate length scales and under the specific loading configuration.

### 7.1.3 Fracturing simulations by LEM

Fracturing under uni-axial tension and compression are simulated by LEM to investigate the evolution of microscopic fracturing process and how it relates to the macroscopic response. The model parameters mainly related to fracturing are microscopic tensile strength $f_{st}$, microscopic tensile strength $f_{ss}$ and reconnection ratio $\gamma$. The macroscopic responses studied are macroscopic shear strength $f_t$, macroscopic compressive strength $f_c$ and ductility. Their relationship with the model parameters are studied by uni-axial tension and uni-axial compression simulations.
The macroscopic tensile strength $f_t$ increases with $\alpha$ but the ductility decreases or vice versa. $n$ has negligible effects on $f_t$.

By inspecting the statistics of fracture facets, the evolution of different fracturing stages before and after peak load are identified where heterogeneity plays a significant role. In heterogeneous models, multiple fracture clusters are formed before reaching their peak loads. This is the origin of the ductility in heterogeneous models. In homogeneous models, a few microcracks are formed at higher load but one of them propagates rapidly. This gives the brittleness of the homogeneous models.

From LEM simulations of uni-axial compression, the macroscopic compressive strength $f_c$ has a linear relationship with the ratio of microscopic shear strength to microscopic tensile strength, $f_{ss}/f_{st}$. Ductility depends mainly on the reconnection ratio $\gamma$ which is the ratio of the stiffness of a closed fracture as compared that of the unfractured one.

Applying heterogeneity increases the ductility of the model in both uni-axial tension and compression simulations at the expense of decreasing macroscopic strengths ($f_t$ and $f_c$). This trend also applies for increasing heterogeneity by decreasing $\alpha$.

Comparisons are made between the LEM simulations and the experimental results on the uni-axial tension test results reported in a literature. Their stress-strain curves can be matched by applying heterogeneity on the lattice models.

### 7.1.4 DLM simulations

For coupled solid-fluid simulation of hydraulic fracture, a novel technique called Dual Lattice Model (DLM) is presented. DLM couples a solid lattice model with a fluid lattice model. Fluid lattice model is called pipe network model in this thesis. Fluid flow in fractures is simulated by a pipe network, which is a lattice model for fluid.

DLM is validated by the hydraulic fracturing of the classical penny shape problem under hydrostatic pressure. From DLM simulations, both the asperity of the fracture and the applied heterogeneity increase the apparent fracture toughness.

A semi-analytical approximate solution for the viscous flow in the penny shape crack is derived to understand how different parameters such as injection rate, viscosity and elastic modulus of solid affect the pressure profile along the fracture.

From both the semi-analytical solution and the DLM simulations, the pressure profiles show two asymptotes governing the regions near the injection point and near the fracture tip. These two regions give steep pressure gradient, but the latter gives a steeper gradient as compared with the former. For hydraulic fracturing by viscous fluid, three evolving regimes for energy dissipation mechanisms in fluid are identified: starting from viscosity dominant, elastic deformation dominant and mixture of toughness and elastic deformation.
7.2 Proposed future work

This thesis shows that LEM is a promising numerical method in modelling heterogeneous material, in particular for fracturing process modelling. However, there are very limited research on LEM for engineering applications. DLM is a novel technique developed in this doctorate research which is suitable for multi-scale simulation of hydraulic fracturing. The research work presented in this thesis lays a foundation for the development of these two numerical schemes and paves a way for the understanding on how natural material behaves when it is modelled as a heterogeneous medium. The following are proposed to extend the work presented in this thesis.

7.2.1 Model generation

Currently the geometry of cells are controlled by a single parameter - node density $n$. Size of cells that can be varied by specifying the ‘diameter’ of nodes that follows a statistical distribution to mimic the variation of grain size in material. Anisotropy is one of the properties in geomaterial and can be modelled by elongated cells or by assigning different lattice parameters according to their orientations. Different node generation techniques can be explored, such as loose and dense packing from DEM. For the above models, statistical analysis on the microscopic response under isotropic load, uniaxial load and triaxial load are suggested to give an insight into the effects on different shape of cells, its packing and the anisotropy. Pre-existing microscopic cracks and voids can be modelled by removing lattices and nodes. Fractures and joint sets can be modelled but handling intersections of fractures is a challenge.

7.2.2 Fracturing simulation

LEM demonstrated in this thesis is an promising numerical tool for the simulation of fracture evolution and the complex interactions between fractures. Using different lattice models suggested in Section 7.2.1, it was expected to produce some interesting fracturing phenomena. Behaviour of rock joints has been researched extensively in rock mechanics. Different constitutive relationships can be applied to the normal springs and the shear springs to model the post-peak behaviour of springs. For example, modelling cohesive crack by a linear softening law for the normal springs. Mohr-Coulomb frictional law can be applied for shear response of closed fracture. Dilatation of a closed fracture can be studied and modelled. The challenge lies on the selection of parameters. Simulation on fracturing under triaxial stress is highly recommended to mimic the stress condition underground. Effects of pore water
pressure can be included by the poroelasticity theory. Beside the cubic, rectangular or thin slice models, simulations of models of other geometries can be carried out such as cylindrical models for the Brazilian test which is a standard test to determine the tensile strength of rock. The above simulations should be compared with experimental results reported in the literature for calibration of microscopic parameters such as $\alpha$, $f_{st}$, $f_{ss}$ and PDFs applied on these parameters. LEM can be a numerical tool to analyse acoustic emissions during loading of rock which are observed in experiments.

Different analyses on LEM simulation results are suggested, especially quantitative one on the micromechanics and establishing the micro-macro relationships. Some examples are the spatial and temporal relationships between fracture formation, growth and coalescence, the correlation length of rough fracture and it multi-scale nature. Analysis commonly carried out in DEM can be referenced such as fabric tensor evolution during fracturing process and the characteristic of force chain network.

### 7.2.3 Hydraulic fracturing

Hydraulic fracturing is the most complicated process studied in this thesis that involves mechanical deformation, fracturing and viscous flow in heterogeneity material. Studies on DLM simulations assuming hydrostatic fluid pressure is applicable for high toughness, high confining pressure and late time response of flow which is initially in viscosity regime. DLM simulations assuming hydrostatic pressure can be extended to study more cases in different kind of heterogeneity, particular the geometric heterogeneity. It can also extend to study the interaction between hydraulic fracture with natural fractures. The effects on leak off can be substantial and should be modelled and studied.

Considering the viscosity of fluid, more fluid models, such as the power law fluid models usually used to model fracturing fluid by the oil and gas industry can be included. The semi-analytical approximate solution is useful to give an insight before simulation but it is suggested for further calibrations. The solution provides a simple framework without much mathematical and numerical manipulation so it can easily be extended for more complicated cases. For the penny shape crack problem, the modelling of crack tip behaviour and fluid lag at the start of simulation need further investigation. It seems that mesh used for the simulations presented in this thesis is too coarse to model such behaviour. Also, it is recommended for complex cases to study simulations under hydrostatic pressure before going into modelling fracturing by viscous fluid.
Conclusions and future work

7.2.4 Computation

Given the simplicity of LEM and DLM, they have the advantage of low computation cost that allows three-dimensional multi-scale and multi-physics simulations involving large amount of nodes and lattices. To extend their capacity for simulations to even larger and complicated models suggested above, more computing resources can be sought, thanking to the advancement of computing technology. Current codes utilise multiple cores in a single CPU for computation. The code can be modified to run on High Performance Computer (HPC) with multiple CPUs. The use of GPU can also be explored. The parallelisation of the current code is done manually in a serial linear algebra library. The scalability of the code can be improved by using parallel linear algebra library. Also, the algorithm can be further optimised. For example, during formation of micro-cracks which are spatially uncorrelated, more lattices can be removed in one step.
7.3 Future vision on numerical modelling

The lack of geological details is a major hurdle for the use of modelling in rock mechanics and reservoir engineering. The attempt to include too much detail to fully describe the problem in rock mechanics is often impractical. Bigger and more sophisticated models need more data from field measurements and laboratory testing (Starfield and Cundall, 1988).

Current modelling processes are laborious. Field data is first collected by monitoring, site loggings and in-situ testings. Data is then processed and model parameters interpreted. Idealised numerical models are built and executed. The output are interpreted and compared with new data obtained. This process repeats again to improve the model. It also involves a lot of intervention from engineers.

By the advancement of monitoring techniques, large amount of data can be collected remotely and automatically. Microseismicity monitoring now becomes the common practice in hydraulic fracturing in the oil and gas industry. However, the monitoring data cannot be interpreted by engineers easily because of the huge amount of data involved and very limited understanding on the microseismic events from the heterogeneous ground. The use of over-simplified models without utilising most of the monitoring data available is the only choice. This limits the predictive ability of numerical modelling. Very ofte, models become a back-analysis tool.

Recently, there is significant advancement of artificial intelligence (AI) in handling big data set for applications such as sales analysis, image and speech recognition, automatic stock trade algorithm. AI can evolve itself by self learning in mastering complicated tasks such as playing Go (Silver et al., 2016) by processing massive amount of data using high performance computing power available.

Future numerical models will be simple models that are sufficient to mimic the essential mechanisms, but big models that accept large amount of data as input. As illustrated in Figure 7.1, monitoring data can serve as training data that modifies microscopic parameters and their PDFs. Simulation results can predict the response in field and the response can validate models. Statistical analysis can be carried out for output such as ground responses (microseismic events for example) and simulation results and comparison can be made from their statistical behaviours.

Such models evolve and optimise themselves for better predictive power. They allow engineers to comprehend large amount of monitoring data in real time from simple but big models. For researchers, it pushes the boundary of our understanding in geomechanics and broader field in engineering by analysing the big data.

LEM and DLM are promising numerical methods for building such simple and big models because of the simplicity and the ability for multi-scale modelling.
Fig. 7.1 Future vision of Dual Lattice Model application using Machine Learning technique
References


References


References


