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Title	An overview on advances in computational fracture mechanics of rock
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Citation	Geosystem Engineering, 24(4), 206-229 https://doi.org/10.1080/12269328.2018.1448006
Issue Date	2021-07-04
Doc URL	https://hdl.handle.net/2115/86193
Rights	This is an Accepted Manuscript of an article published by Taylor & Francis in Geosystem Engineering on [date of publication], available online: http://www.tandfonline.com/10.1080/12269328.2018.1448006.
Type	journal article
File Information	Manuscript (accepted).pdf

An overview on advances in computational fracture mechanics of rock

Due to its complexities, rock fracturing process still poses many pressing challenges despite intense research efforts. With the rapid development of computational mechanics, numerical techniques have gradually become robust tools for the investigation of rock fracture. Nevertheless, not all of the devised methods are capable of adequately modelling the rock fracture process. For an accurate simulation of the process, a numerical method needs to be capable of modelling crack initiation, propagation, bifurcation, coalescence and separation. This paper provided a review of recent advances in computational analysis of the rock fracture process, which is built upon a number of literature on numerical modelling of mechanics of failure in rock and other brittle materials. After briefly discussing the fundamentals of rock fracture mechanisms, the basic structure of the existing and recently developed numerical techniques such as Finite Element Method, Boundary Element Method, Discrete Element Method, Combined methods and Multiscale coupled method are illustrated. Finally, the strengths and weaknesses of these numerical techniques are discussed and the most promising methods are highlighted.

Keywords: Rock Fracture; Numerical techniques; Finite Element Method; Boundary Element Method; Discrete Element Method; Combined Methods

1. Introduction

Brittle and semi-brittle rock is very likely to experience observable crack growth at some stage of its life cycle under severe loading. Since the pioneering work by Griffith (1921), for many years, the mechanisms of the crack growth in brittle materials have been studied extensively under the assumptions of linear elastic fracture mechanics (LEFM). However, it was not until the mid-seventies that the fracture of ductile materials was first explored using elasto-plastic fracture mechanics (EPFM) principles. The complexity of the fracture process is even more complicated in a naturally heterogeneous brittle material such as rock and concrete. There are basically three types of investigation techniques in fracture mechanics, namely experimental, analytical and

numerical. Computational fracture mechanics has long been used for determination of the stress intensity factors, and later has been expanded into the simulation of crack nucleation and propagation. Generally, rock fracture is essentially a dynamic process, at least in the final stage (Cox et al., 2005; Zhou et al., 1996b), and not all of the numerical methods are capable of correctly capturing the cracking process, due to difficulties posed by time dependency of crack onset and rate dependency of crack velocity (Owen et al., 2007). For a realistic simulation of the fracture process, numerical techniques are required to model crack onset and arbitrary crack growth, the correct crack length within a given time interval as well as the propagating directions. Recent advances in computational mechanics have facilitated a much better understanding of complex process, and accordingly numerical simulation of the fracture process has been the object of massive interests. Generally, computational mechanics can be classified mainly into continuum and discontinuum formulations. Continuum-based methods discretise the domain into elements and the domain is treated as a single continuous body using a mathematical formulation involving a constitutive law, balance principles, boundary conditions and initial conditions (Munjiza, 2004). The main continuum methods are Finite Element Method (FEM), Finite Difference Method (FDM), Boundary Element Method (BEM), Scaled Boundary Finite Element Method (SBFEM), Extended Finite Element Method (XFEM) and Mesh-less Methods. Discontinuum-based methods are relatively new, and they model the domain as a collection of discrete bodies that can move, rotate and interact. Accordingly, their mathematical formulation includes the law between particles and balance principles (Munjiza, 2004). Discrete Element Method (DEM), Lattice Model (LM), and Molecular Dynamics (MD) are the common discontinuum methods in the field of fracture analysis. In recent years, increasing attention has been paid on these techniques, which can bring together the

advantages of the continuum-based and discontinuum-based methods. Attempts in this direction lead to the development of Coupled Methods, Combined Methods and Multi-scale Coupled Methods.

Until now, a number of publications has reviewed the numerical techniques and their application in the field of rock engineering, rock fracture and fragmentation modelling. Jing and Hudson (2002) and Jing (2003) reviewed numerical methods and their application in rock mechanics engineering. Their state of art review has been recently updated by Nikolic et al. (2016) and Zhao et al. (2011a). Meanwhile, Ingraffea (2007) reviewed different computational fracture mechanics codes. Song et al. (2008) compared the capability of different FEMs in dealing with dynamic fracture in brittle materials. More specifically, Bobet et al. (2009) reviewed the discontinuous numerical methods in the field of rock mechanics and Lisjak and Grasselli (2014) also presented a review on discrete element techniques for modelling of rock fracturing process. Additionally, Rabczuk (2013) reviewed the computational methods for simulation of fracture in brittle and quasi-brittle solids. Although past works provide valuable information, none of them has addressed specifically computational rock fracture analysis. Therefore, this paper aims to review recent advances in numerical techniques for simulation of dynamic rock fracture and fragmentation, and discusses their principles, weakness and strengths. The paper first explains the mechanism of rock fracture and then briefly reviews the previously and recently developed numerical techniques as well as their key characteristics and applications mostly based on the published articles over the past two decades. The organization of this paper is as follow. Section 2 explains the mechanics of rock fracture and its principles. The continuum and discontinuum methods are discussed in section 3 and section 4, respectively. Section 5

reviews the hybrid method and their recent improvements, while the multi-scale methods are the subject of the section 6.

2. Mechanics of fracture in rock

Understanding the mechanism of the crack initiation and propagation in intact rocks is extremely important in rock engineering. Crack propagation in rock has been explored theoretically by modifying the Griffith (1921) theory and also based on laboratory tests by Hoek (1968), Bieniawski (1967), Jaeger (1969), Fairhurst (2004), Kemeny and Cook (1987) as well as Paterson and Wong (2005). The basic theory of fracture mechanics and its related modifications for rock materials have been discussed extensively in many publications and will not be repeated here. Generally, rock fracture can be investigated at three distinct levels i.e. micro-, meso- and macro scales (Figure 1).The micro-crack refers to very small cracks, which are not visible to the naked eye. At the micro scale, individual grains can be distinguished. The micro cracks which propagate along the boundary between grains are known as intergranular cracks which can propagate or die out within the length scale of a single grain (Rutter et al., 2001). A meso scale crack extends further than micro cracks and appears when a number of micro cracks connect with each other. At the macro scale, no internal material structure is recognised and explicit cracks span to several decimetres. Studies mostly focused on meso and macro scale in rock fracture mechanics. In rock mechanics, the micro and meso scales are mainly employed to understand the physical mechanisms of rock fracture, while the macro scale crack corresponds to the study of crack growth and failure mechanism.

Figure 1: Different scales of observations in rock fracture analysis (modified after Van Mier (1996))

Due to the heterogeneity, non-linearity and rate-dependency behaviour of rock, LEFM is not a satisfactory theory to describe the fracture process of rock after initiation. Sub critical crack growth and microcracking at the crack tip are two important phenomena, which cannot be explained by the LEFM principles (Carpinteri, 1985). The sub critical crack growth occurs when cracks extend at a stress intensity factor less than the critical value (Ko and Kemeny, 2011). Furthermore rock does not realistically behave linearly elastically up to fracture. As shown in Figure 2, micro-cracks first arise in vicinity of crack tips and develop gradually into dominant meso and macro-scale discrete cracks. Thus, the fracture process can be subdivided in general into two stages: 1) creation of narrow deformation regions, and 2) initiation and propagation of discrete cracks (Tejchman and Bobiński, 2012). The region in front of the crack tip, namely Fracture Process Zone (FPZ), is the region of micro crack initiation and coalescence. This region can play a dual role in the rock fracture. While it mitigates the effect of the acting load by softening the rock material around the tip, it reduces the resistance to fracture (Ortiz, 1988). The FPZ can occur as tensile zones (mode I), shear zones (mode II) or mixed tensile-shear zones.

Figure 2: Schematic shape of FPZ development ahead of a crack tip (modified after (Bažant, 1992))

A comprehensive study on FPZ was conducted by (Brooks, 2013), which can be referred to by interested readers. The FPZ zone undergoes progressive softening damage due to micro cracking (Bažant, 1992). It means that the rock material inside the fracture process zone softens and acquires different properties from the unaffected parts. The softening behaviour of the rock material plays a very important role in the rock failure process. Therefore, the prediction of rock damage requires a mathematically

correct and physically realistic description of the strain softening behaviour (Bažant and Pijaudier-Cabot, 1988).

3. Conventional Continuum methods

3.1 Finite Element Method

FEM is one of the most popular numerical methods in rock engineering field which resolves the problems by approximating the solutions of partial differential. FEM is capable of modelling complex geometries, loading conditions and heterogeneous material distributions (Mohammadi, 2008; Semblat, 2011). Nevertheless, the classical displacement based FEM is not able to describe the strain localization properly since the differential motion equations change type and lead to an ill-posed boundary value problem (Tejchman and Bobiński, 2012). To avoid the emerged difficulties, regularization techniques are developed within different theories such as higher order continuum models, gradient based models, polar theories, nonlocal models, viscous models and cohesive zone models (CZM) (Rabczuk, 2013). These techniques are explained in detail in literature (Bažant and Jirásek, 2002; Hillerborg et al., 1976; Ortiz, 1988; Tejchman and Bobiński, 2012). The softening behaviour can be also modelled using continuum damage mechanics based approaches by merely degrading the stiffness of the rock. For further information about these approaches, reader can refer to the following literatures (de Borst, 2002; Öchsner, 2016; Pellet and Selvadurai, 2017).

A number of techniques have been implemented into the standard FEM to facilitate the computational simulation of crack propagation problems, namely the inter-element crack methods, element erosion methods, embedded element methods and extended finite element methods (Mohammadi, 2008; Song, 2012). Among them the inter-element crack method, element erosion method and XFEM have been employed

much extensively to model brittle fracture which are discussed further through the following sections.

In inter-element methods, cracks propagate along the finite element edges. Since the crack propagates along an inter-element boundary, these methods suffer from mesh size and mesh bias dependency. These approaches are developed on basis of CZM fracture modelling technique. The main concept of the CZM model for fracture mode I is shown in Figure 3-A. In this model, when the maximum principal stress reaches the cohesive strength of the material (stage I), cracking process initiates and two crack faces starts to separate. The cohesive traction falls to zero when the separation reaches a critical value (Stage II). Two general approaches have been developed based on the inter-element crack technique and CZM. Xu and Needleman (1994) developed a technique in which the domain is discretised into individual elements which are bonded based on cohesive law (Figure 3-A). In the purposed model, the traction force increases firstly and reaches the cohesive strength of the material and then decreases, reaching zero at the critical separation. This technique is referred to as Intrinsic CZM (ICZM) (Zhang et al., 2007). In this formulation, since the stiffness of the block is dependent on both cohesive properties and volumetric constitutive relation, the cohesive surface controls the wave speeds. In this technique, the cohesive surfaces are assigned to all applicable surfaces (Figure 3-b). This technique may result in reduction of the stiffness, especially in dynamic problems. Camacho and Ortiz (1996) proposed a new formulation that treats the problem by considering a criterion prior to activation of any cohesive surfaces and accordingly the cohesive zone is only placed in front of the crack tip by adoptive re-meshing technique (Figure 3-c). In this formulation, as shown in Figure 3-a, the onset of crack nucleation is different than ICZM and is referred as Extrinsic CZM (ECZM) (Zhang, et al., 2007).

Figure 3: (a)The concept of the cohesive zone model, ICZM and ECZM (Adapted from Zhang, et al. (2007)); (b) Sketch of the developed inter-element crack by Xu and Needleman (1994); and (c) by Camacho and Ortiz (1996)

In addition to mesh dependency, this approach does not have time continuity in the cohesive zone formation. In terms of application in rock engineering, Cho et al. (2003) employed the ECZM technique to investigate the loading effect of fracture process in rock. Cho and Kaneko (2004) simulated fracture process of rock around a borehole using inter-element technique. These approaches have been extended to heterogeneous materials (Chen et al., 2009). In a relatively similar way, a class of combined finite/discrete element formulations have been successfully developed in the past decades for simulation of progressive fracturing process and post-cracking interactions. This method will be explained and discussed further in the section of combined methods.

3.1.1 Element Erosion method

This method is considered as one of the simplest methods in dealing with discrete nature of fracturing process within the framework of the standard FEM (Beissel et al., 1998; Rabczuk, 2013; Song, 2012). According to the element erosion (deletion) algorithms, there is no need to represent the topology of cracks, and the fracturing process can be modelled by a set of deactivated elements. As shown in Figure 4, the elements, which contain the crack, are deactivated and have no material resistance or stress for the rest of the simulation process. A removed element represents a meso/macro crack. The deactivation of elements in this method can be achieved through two approaches: 1) complete element deletion technique, in which the deleted elements are replaced by rigid masses and 2) setting the stress of the deactivated elements to zero (Rabczuk, 2013; Song, et al., 2008).

Figure 4: Schematic illustration of crack simulation by element erosion method

This method has been widely used to simulate the fracture process of rock, particularly due to impact and blasting loads. Ma and An (2008) investigated rock fracturing due to blasting operation by implementing Johnson–Holmquist (J–H) material model into LS-DYNA. Similar investigations were conducted using different material models and software packages (Changping, 2013; Saharan and Mitri, 2008; Sjöberg et al., 2012; Wang et al., 2008; Wei et al., 2009). Despite such developments, the element dependency of this method makes it not well suited for brittle fracture analysis. In addition, it suffers from the inability of modelling crack propagation and fragmentation and being computationally expensive.

3.1.2 Extended Finite Element Method (XFEM)

Belytschko and Black (1999) developed an enriched FEM technique to model elastic crack growth. Improved by Moës et al. (1999) and Dolbow (1999), the technique was later called the extended finite element method (XFEM). Theoretically, the basic idea of XFEM is to include discontinuities via shape functions within the finite elements to prevent sticking of the mesh to the discontinuous surfaces (Pommier et al., 2013) (Figure 5). Generally the XFEM displacement approximation for any element comprising an arbitrary crack can be defined as (Moës, et al., 1999; Mohammadi, 2008):

$$U^h = \sum_{i \in I}^{n} U_i \, \emptyset_i + \sum_{j \in J}^{m} b_j \, \emptyset_j H(X) + \sum_{k \in K}^{mf} \emptyset_k \left(\sum_{l=1}^{4} \boldsymbol{C}_k^{l2} F_l^2(X) \right) \tag{1}$$

In Eq. 1 , U is the enriched displacement, Ø is the FEM conventional shape functions, H is the Heaviside function, F is the front enrichment functions, b_j and $\boldsymbol{C}_k^{l2}$ are additional degrees of freedom.

Figure 5: Arbitrary crack growth in XFEM; circles are nodes enriched by front enrichment functions and squares are enriched nodes by Heaviside enrichment (Adapted from Moës, et al. (1999))

The XFEM has been employed successfully in simulation of rock fracturing (Dolbow, 1999; Eftekhari et al., 2015, 2016; Mohammadnejad and Andrade, 2016; Weber et al., 2013). These investigations were mainly focused on simple static rock failure and hydraulic fracturing simulations, i.e. the problems involving growth of a single or multiple cracks. The formulation of the XFEM becomes more complicated and time-consuming with multiple crack initiation and propagation (Rabczuk, 2013). Additionally, because of the lack of reliable crack branching criterion (Rabczuk, 2013), it cannot automatically follow propagation of the crack (Song, et al., 2008) to model the resultant separation and fragmentation (Sukumar et al., 2015). In spite of these drawbacks, XFEM is still a fast-growing numerical technique, which has attracted a lot of attentions in geomechanics field and may become one of the powerful tools in simulation of rock fracture process.

The generalized finite element method (GFEM) is similar to XFEM (Rabczuk, 2013), and uses a technique with the same concept as XFEM. However, it uses an element enrichment scheme instead of the nodal enrichment. This technique is known as the embedded finite element method (EFEM). Saksala (2015) successfully simulated rock fracture using EFEM incorporating rock heterogeneity. Generally, the applicability of this technique in the field of rock fracture needs to be explored more in the future.

3.1.3 Other Finite Element based methods
In addition to the above techniques, several other methods have been developed based on FEM to simulate the failure process of brittle materials; some examples are as follows. Tang et al. (1998) introduced a two dimensional FEM code, namely Realistic Failure

Process Analysis (RFPA) code, on the basis of continuum damage mechanics, and employed it to simulate failure mechanism of rock. Zhu et al. (2015) was proved the capability of the code in simulating rock fracturing process subjected to impact/dynamic loading (Zhu, et al., 2015), which was followed by introducing a dynamic version of code named as RFPA2D-Dynamic (Tang and Yang, 2011; Zhang et al., 2012). Another extension of this method developed by Liu (2004) known as R-T2D which was focused in simulation of static (Liu et al., 2008) and dynamic (Wang et al., 2011) mechanical rock fragmentation. FRANC 2D (FRacture ANalysis Code) is an interactive finite element code which developed firstly based on the LEFM principles and then expanded into EPFM and three dimensional modelling (Wawrzynek and Ingraffea, 1994). Different rock fracture mechanisms have been investigated using this code (Carter et al., 1995; Erarslan, 2017). Despite all the achievements of these codes, they suffer from basic difficulties of continuum-based methods such as mesh dependency and being untrustworthy in modelling of the transition from a continuum to discontinuum domain.

3.2 Finite Difference Method (FDM)

FDM is a continuum-based method similar to FEM that differs in using a grid of nodes instead of elements for approximating. However, the conventional FDM suffers from the use of regular grid system for the description of material heterogeneity, complex boundary conditions and fractures (Elmo, 2006; Jing and Hudson, 2002). To overcome these shortcomings, the general FDM has been improved particularly thanks to the development of finite volume methods, which make it capable of using irregular quadrilateral, triangular and Voronoi grids (Figure 6) (Nikolic, et al., 2016). The commercial FLAC code is the most common FDM tool for stress analysis in geomechanics problems. Konietzky et al. (2009) developed and implemented an algorithm based on linear elastic fracture mechanical approach in FLAC 2D code.

According to the algorithm, each element comprises a micro crack with a random length that propagates when the critical value is satisfied by the stress intensity factors. Based on this method, two new crack propagation schemes were proposed by Li and Konietzky (2015). Venticinque and Nemcik (2014) developed a new constitutive model based on FDM to simulate dynamic fracturing in coal. Li and Konietzky (2015) studied time-dependent crack growth in brittle rock utilizing the FDM. Li et al. (2015) investigated three dimensional crack propagation in brittle rock mass using FLAC 3D.

Figure 6: crack simulation via Voronoi grid

Despite all these improvements, FDM still suffers from inability to model fracture propagation appropriately due to its continuum nature where the entire domain is employed for calculation. Therefore, based on current knowledge, this method will not be considered as a robust numerical technique for the simulation of rock fracture process.

3.3 Boundary Element Method

In comparison with standard FEM, the BEM treats crack propagation problems relatively simpler due to its dimension reduction technique and also its ability to accurately evaluate the SIF (Aliabadi, 1997; Rabczuk, 2013). This method has been successfully employed to investigate crack growth in elasto-dynamics domain (Dominguez, 1993). The difficulties of the standard direct BEM in dealing with fracture problems such as the coincidence of crack nodes, gave rise to new techniques such as Subregion Boundary Element Method (SBEM), Displacement Discontinuity Methods (DDM), Dual Boundary Element Method (DBEM) and Dual Reciprocity Boundary Element Method. The SBEM and DBEM are direct BEMs while the DDM is an indirect BEM. As shown in Figure 7-A, this method divides medium into subregions. By introducing new artificial boundaries to connect the fractures to the boundary, the subregion method creates regions containing cracks. The regions remain connected until the equilibrium of tractions and compatibility

of displacements are satisfied, and then fractures grow along the interfaces. Different formulations of this method have been developed. Nevertheless, it still suffers from inability to model crack path autonomously and to take into account the growth rate. Additionally, the method needs to derive a relatively larger system of equations than those normally required. Originally developed by Crouch (1976) to treat stress analysis problems, different formulations of the DDM have been extensively employed in fracture mechanics problems. This method considers each crack as an element (Shen et al., 2014) instead of two separating surfaces like other BEMs (Figure 7-B), and basically it is defined as the relative displacements between two sides of the element via Eq. (2), where D_n and D_s are normal and shear relative displacements, respectively.

$$D_s = u_x^- - U_x^+$$

$$D_n = u_n^- - U_n^+ \tag{2}$$

When the relative displacement at the fracture tip exceeds defined critical threshold, a certain length of fracture will develop without any need for a re-meshing process. Stress intensity factor, in this method, controls the fracture propagation at the crack tip. In comparison with mesh-based methods, the DDM is more accurate and efficient, which are important factors in dynamic fracture analysis. At the same time, the DDM suffers from incapability to model rock heterogeneity and its nonlinear behaviours. By implementing different fracture criteria, DDM was used relatively widely by researchers in simulation of rock fracture process. For example, Shen (1993) investigated hard rock fracture mechanism by developing a modified version of the energy based fracture propagation criterion into DDM formulation, and later converted it to become a commercial code namely FRACOD (Shen, et al., 2014). FROCK is another code which was developed based on DDM and originally used stress-based criterion proposed by Bobet (1998). Bobet and Einstein (1998), Vásárhelyi and Bobet (2000), Bobet (2001) and

Bobet and García Marín (2014) demonstrated modelling of crack propagation in a rock material using FROCK. Meanwhile, the DDM has been widely employed to simulate hydraulic fracture problems (Wu and Olson, 2015; Zhang and Li, 2016). Despite all progress made, there are more needs to be done to male this method able to model post-cracking phenomenon or detachment processes. Portela et al. (1992,164) introduced a two dimension DBEM as an indirect BEM for modelling of crack growth, which was extended to three dimensional by Mi and Aliabadi (1992). In this method, displacement and traction equations are applied on the both crack surfaces simultaneously. Despite all of the improvement and development of different formulations, yet no successful application of this method in simulation of rock fracture has been reported.

Figure 7: Three Boundary element techniques in fracture analysis: (a) Subregion method, (b) DDM, (c) DBEM

3.4 Meshfree methods

Different formulations in the concept of meshfree technique have been developed to remove limitations of continuum-based methods (Zhang et al., 2000). Their flexibilities in dealing with fracturing problems make them suitable for rock mechanics application (Jing and Hudson, 2002). They are also much advantageous when dealing with modelling of crack growth. The meshfree methods employ a system of interacting nodes and sets of internal and external boundaries and interfaces to model material. The character of the nodes is provided by three functions: i) approximation function, ii) weight function and iii) compact support of weight functions (Chen et al., 2006b). In the domain of support the weight function is non-zero and outside the domain it is set be zero. Based on this principle, pioneered by Gingold and Monaghan (1977) for development of the Smoothed Particle Hydrodynamics Method (SPH), different formulations of the meshfree method have been established. These can be classified into

two categories: the methods based on global weak form requiring background mesh for integration; and the methods based on local weak form requiring predefinition of particles for their mass. Among the popular meshfree methods, the element-free Galerkin (EFG) method belongs to the first group while others such as the point interpolation method (PIM), the meshfree local-Petrov Galerkin method (MLPG) and SPH belong to the second group. A complete explanation of developed methods and their specifics and classifications can be found via the studies conducted by Belytschko et al. (1996), Fries and Matthies (2004a), Nguyen et al. (2008), (Liu and Gu, 2005) and Zhuang et al. (2012). The fracture of brittle materials has been simulated using different formulations of this technique. As the oldest meshfree method, the SPH widely employed in simulation of rock fracture and fragmentation process (Das and Cleary, 2010; Deb and Pramanik, 2013; Lu et al., 2016; Pramanik and Deb, 2015; Wang and Ma, 2006). Despite all of the developments and application of meshfree methods in fracture analysis of rock and brittle materials, this method suffers from inconsistency and relatively high computational cost (Augarde and Heaney, 2009; Fries and Matthies, 2004b). Moreover, other drawbacks are the need of the development of appropriate constitutive model to trace fracture, calibration process, contact detection and boundary conditions difficulties.

Material Point Method (MPM) is another recently developed meshfree method which can be categorized as a meshfree particle method similar to SPH. The MPM is developed based on the standard DEM formulation, where the technique discretises the domain into the Lagrangian particles (Junior et al., 2013). Unlike the SPH, boundary condition can be assigned easily, and it does not suffer from tensile instability (Ma et al., 2009b). Kakouris and Triantafyllou (2017) developed a new formulation of MPM to simulate brittle fracture in anisotropic media and concluded that the MPM can be

considered as an efficient and promising technique for these applications. It seems there is good potential for application of this technique in rock fracture simulation. The applicability in simulation of the rock cracking is an open area of research.

3.5 Recently developed continuum based methods

During the past years, two continuum based techniques, i.e. Peridynamics (PD) and Phase Field (PF) approaches, have emerged as a promising approach to simulate brittle fracture. These methods have been developed to deal with the problem of the other continuum based methods in three dimensional simulation of multi-crack initiation and propagation. The PD incorporates a new continuum mechanics theory and can be solved by either FEM or meshfree methods. The main advantage of the PD concept is the non-locality. In fact it uses integration instead of spatial differentiation in computation of forces, which can solve the stress singularity problem at the crack tip. The original PD method, i.e. bond-based PD, was introduced by Silling (2000) and can be considered as an extension of the MD to the macro scale level (Lai et al., 2015). Different formulations of this numerical technique have been employed in simulation of rock fracture (Gu and Wu, 2016; Lai, et al., 2015; Ouchi et al., 2015; Panchadhara et al., 2017; Zhou and Shou, 2017). The ordinary and non-ordinary state-based PD are two common formulations in solid mechanics, since they facilitate the implementation of the continuum constitutive models. Reviewing the recent developments Rabczuk and Ren (2017) proposed a formulation for simulation of quasi-static fracture in rock. Whilst PD seems to be a powerful technique for simulation of rock fracture as it can easily simulate the transition from continuum to discontimuum while does not require defining crack topology and cracking criterion into the mode. However, it is a newly developed technique and mostly is used for dynamic fracture analysis and its capabilities in rock fracture analysis need to be explored much deeply in future.

The Phase Field (PF) is another recently developed phenomenological continuum algorithm, which has been successfully applied to simulate complex 3-D microstructural kinetics evolution of material at the meso-scale. This method is based on the thermodynamics equations (Li et al., 2017). PF treats fracture problems based on energy minimization principles (Sargado et al., 2017) and does not model a crack as a geometric feature with a physical discontinuity (Klinsmann et al., 2015). Instead, PF differentiates fractured field using order parameter. The order parameter is a variable representing the state of the structure, and is coupled to elastic properties of the material using degradation function (Kuhn et al., 2015). The detailed explanation about the theory of a PF model for fracture analysis can be find in Kuhn and Müller (2008), Ulmer et al. (2013), Vignollet et al. (2014), Klinsmann, et al. (2015), Kuhn and Müller (2016). Although, the PF models have been becoming popular technique in fracture simulation, unlike the PD, it suffers from inability to model detachment and separation. Therefore, its application in rock fracture analysis is currently limited to crack initiation and propagation problems.

4. Discontinuum Methods

Discontinuum method can be considered as the one of the mostly employed numerical technique in the field of rock mechanics. Distinct Element Method (DEM), Discontinuous Deformation Analysis (DDA) and Bonded Particle Method (BPM) are the most common discontinuum methods in rock fracture analysis, and comprehensive explanations of these methods from theory to application can be found in the studies by Hart (1988), Bobet, et al. (2009), Jing (2003) and Jing and Stephansson (2007). The Lattice Model and Molecular Dynamics (MD) are relatively recent developments of the discontinuum methods, which have been growing for simulation of fracture problems.

4.1 Distinct Element Method (DEM)

Proposed by Cundall (1971), DEM, is an explicit discrete element method, implemented in computer codes such as UDEC and 3DEC (Itasca, 2009). It has been employed widely to investigate rock fracture and resultant fragmentation process. This method divides discontinuous medium into rigid discrete bodies that can move, slip, rotate, interact and separate based on defined contact mechanism (Bobet, et al., 2009; Itasca, 2009; Lee, 2007). The ability of new contact detection during simulation process is known as the main advantage of DEM over other methods. In this method, cracks initiate and grow along the boundaries of blocks when the maximum stress exceeds tensile or shear strength thresholds (Figure 8-a), represented in Eq. (3).

$$F_n = k_n u_n$$

$$\Delta F_s = k_s \Delta u_s$$

$$|F_s| \leq c + F_n tan\phi \tag{3}$$

where F_n is normal force, k_n is normal stiffness, u_n is normal displacement, ΔF_s is change in shear force, k_s is shear stiffness, Δu_s is incremental shear displacement, and c and ϕ are cohesion and joint friction angle, respectively. To facilitate the simulation of the progressive fracture and fragmentation process, Lorig and Cundall (1989) developed Voronoi discretization model into DEM, and employed improved method to model fracture process and fragmentation in rock and concrete. This method enjoys the advantage of using the tensile strength of Voronoi contact to evaluate the tensile strength of the rock but meanwhile it can cause kinematic freedom limitation.

Figure 8: Comparison between (a) Fracture constitutive behaviour in DEM (after Kazerani and Zhao (2010)) and (b) Fracture constitutive behaviour in FEM

Detailed explanation in regards to this technique can be found in the studies by Lorig and Cundall (1989), and Itasca (2009). Figure 8-B schematically illustrates a

typical fracture constitutive model based on fracture mechanics principals for continuum methods where the softening behaviour of rock material is taken into account. Some efforts have been made to incorporate fracture mechanics principles into the UDEC formulation. Kemeny (2005) implemented a first-order differential equation for joint cohesion into the UDEC and validated it against few simple examples such as direct shear test. Jiang et al. (2009) introduced expanded distinct element method (EDEM) based on UDEC and simulated crack initiation and propagation (Yang et al., 2012). Kazerani (2013) took into account the effect of FPZ developing a Cohesive Fragment Model into UDEC to model rock fracture. By introducing the concept of bonded block models (BBM) into 3DEC, this code become much compatible with fracture simulation problems, where rock strength dependency can be modelled parallel to crack initiation and propagation simulation (Itasca, 2017; Turichshev and Hadjigeorgiou, 2017). Generally, the DEM is a widely used technique in investigation of rock fracturing and failure process (Kazerani and Zhao, 2010; Li et al., 2016; Mayer and Stead, 2017).

4.2 Bonded Particle Method

The BPM is one of the widely used particle based Discrete Element Methods used in study of fracturing process of rock. This method divides the domain into circular (2D) and spherical (3D) rigid elements that are distributed non-uniformly and bounded by cohesive force, obeying Newton's second law. The technique was first introduced by Cundall and Strack (1979) to model dynamics of granular materials, and later improved and implemented as a commercial computer code named as Particle Flow Code (PFC). The interaction of particles can be modelled by different methods, but the simplest model is the contact bond model as shown in Figure 9-A. When tension or shear stress exceed their limits, crack initiates and propagates along the boundary of rigid elements.

This inter-particle model, however, does not resist particle rotation compared to the parallel bond model as shown in Figure 9-B. Compared with the contact bond model (Figure 9-A), after the parallel bond is broken under shear stress, the shear strength falls down from peak value to its residual value and remains constant. The residual shear strength is a function of the normal force and the friction coefficient of discrete particles. Further development on contact models in this method came from Potyondy and Cundall (2002) and Fakhimi et al. (2005). Further details of this method and its recent developments can be found in literatures (Bobet, et al., 2009; Fakhimi, et al., 2005; Potyondy, 2012; Potyondy and Cundall, 2004). The BPM is confirmed to be an appropriate method to model fracture mechanism and be a good alternative to UDEC or 3DEC, but not without drawbacks. The main drawbacks includes particle size dependency in both stages of simulation and calibration, overestimation of tensile strength, relying on linear failure envelope, considering low friction angle and difficulties in modelling of complex geometries. Since aforementioned parameters are used to evaluate normal and shear bonds, the calibration and running of model would be very time consuming, especially for large models of fracture process simulation. Despite of these weaknesses, this method was employed successfully by researches to investigate rock fracture and crack propagation (Fakhimi and Villegas, 2006; Hazzard et al., 2000; Konietzky et al., 2002; Lee and Jeon, 2011; Poulsen and Adhikary, 2013; Yue et al., 2017).

Figure 9: The implemented bond models PFC a) Normal contact bond model (after (Turichshev and Hadjigeorgiou, 2017)) b) the parallel bond model (after (Lisjak and Grasselli, 2014))

Kozicki and Donzé (2008) introduced an open source code, YADE, developed based on relatively similar principles as PFC proposed by Frédéric and Magnier (1995) and Donzé and Magnier (1997). In comparison with PFC formulation, YADE employs

a softening factor and an interaction detection coefficient which improves its capabilities in control of the released energy and nonlinear failure (Lisjak and Grasselli, 2014). This code was employed to model fracture initiation and propagation in both soft and hard rocks (Scholtès and Donzé, 2013) and for three dimensional simulation of crack nucleation and propagation (Scholtès and Donzé, 2012). This technique, however, suffers from similar drawbacks as PFC.

4.3 Discontinuous Deformation Analysis (DDA)

Firstly introduced by Shi and Goodman (1985) as an implicit formulation of DEM, DDA has been developed rapidly in the field of rock mechanics and accordingly rock fracture analysis. This method shares some procedures with the FEM, but it is a discontinuum method satisfying the definition by (Cundall and Hart, 1992). Similar to FEM, in order to find a solution, the DDA minimises the total potential energy of model (Π), while the domain comprises rigid blocks. The original DDA assumes stress and strain to be constant within the block which results in the limitation of block deformation. Fundamental of the DDA was explained in detail by (Shi, 1988, 1992) and its application in the field of rock engineering was presented later (Shi, 1999).

A wide range of DDA application and its validation in different fields of engineering is demonstrated by MacLaughlin and Doolin (2006). However, the assumption of constant stress results in an inaccurate evaluation of contact pressures between blocks. This is where the contact mechanism plays an important role in fracture and fragmentation simulation. The original DDA was not able to model failure occurring along the block boundaries and block fragmentation. To address the drawback and also to enhance the capability of the technique in modelling the continuous-discontinuous transition, a sub-block technique is developed employing artificial block interfaces within each block. Lin et al. (1996) improved sub-blocking technique by

implementing a new contact algorithm and two block-fracturing algorithms, based on Mohr-Coulomb criterion. Further developments were made by Ke (1997) who employed the sub-block technique in combination with a Mohr-Coulomb based tension criterion. In addition, Koo and Chern (1997) investigated the capability of a fracture criterion that, at each step, compared the principal stress of each block centroid with compressive and shear strengths of the block. This algorithm allowed fractures to initiate and propagate arbitrarily where the stress criterion was satisfied. Cheng and Zhang (2000) improved the sub-block technique by developing an automatic triangular sub-block generation approach, which could be considered as a technique similar to Voronoi tessellation technique. Later Zhang and Jiao (2008) and Jiao and Zhang (2012) improved the method by introducing many more modifications such as the ability of modelling material heterogeneity and taking into account the linear fracture mechanics concept.

As shown in Figure 10, although three types of contacts can be employed in two dimensional DDA as angle-to-angle contacts, angle-to-edge contacts, and edge-to-edge contacts (Shi, 1988), all fracturing process can be modelled by edge-to-edge contact forces (Ning et al., 2011). Block size sensitivity and being computationally expensive, due to having a larger number of time steps, are much striking weaknesses of this method in dealing with fracture and fragmentation problems. With all of the improvements implemented in the method, the DDA has been employed widely by researchers to simulate fracture and fragmentation process of rock (Ben et al., 2013; Morgan and Aral, 2015; Ning and Gu, 2013; Ning et al., 2010; Zhang and Jiao, 2008). Despite all of these efforts and validation reports of DDA application in rock engineering, it is relatively new and its performance, particularly for dynamic rock fracture and fragmentation analysis, is not fully developed and verified. Besides, it is

still computationally expensive for highly dynamic and practical-scale simulations such as dynamic rock fragmentation.

Figure 10: The contact types in two-dimensional DDA: (a) angle to angle contact; (b) angle to edge contact; (c) edge to edge contact

4.4 Lattice Model Techniques

Lattice models, which are also known as dynamic lattice network models, are relatively simpler, modern techniques among other discontinuum methods. The basic concept is similar to BPM, where material can be represented as a collection of interacting discrete masses. As illustrated in Figure 11, the medium compromises of a set of either regular or irregular distributed point masses, which interact through simple zero-size spring/beam with ability to transfer forces. Although the technique is not new, its application in dynamic fracture modelling is a recent development. This method enjoys two main advantages of continuum and discontinuum methods in terms of being flexible and computationally efficient (Cundall, 2011). Different types of cells can be developed into the lattice model, allowing for model heterogeneity. In this technique, fracturing is simulated based on a linear elastic analysis with spring deletion when the force exceeds a threshold. A comprehensive explanation of this technique and its application in fracture mechanics can be found through the studies conducted by Schlangen (1995), Schlangen and Garboczi (1997), Bolander and Sukumar (2005), Slepyan (2005), Grassl et al. (2006) and Quintana-Alonso and Fleck (2009). Different formulations of this technique were employed by researchers to investigate rock fracturing process. Song and Kim (1994) developed a Dynamic Lattice Network Model (DLNM) and simulated fracturing process due to blasting. In the proposed model, the rock heterogeneity was assigned as a random stiffness of springs and the system was considered to follow linear elastic model. Zhao (2010) developed a Distinct Lattice

Spring Model (DLSM) in which material was modelled through an un-uniform distribution of masses interacting via distributed bonds. A new algorithm based on the lattice model was also introduced into PFC by Cundall (2011) to improve the flexibility and efficiency of the method by removing the contact detection process. In the proposed method, the material is modelled by a series of springs which link masses. This method was successfully employed to simulate rock failure and rock fracturing from blasting (Cundall, 2011; Onederra et al., 2009; Poulsen et al., 2015). Despite all merits of the lattice models, they suffer from difficulties in model calibration and practical-scale modelling.

Figure 11: (a) Square lattice cell; (b) Hexagonal lattice cell; (c) Triangular lattice cell

4.5 Molecular Dynamics (MD)

Because of the exponential growth of computing power, large scale atomic simulations are being developed rapidly to study the failure mechanisms of materials (Zhang and Ghosh, 2013). Molecular Dynamics is a time-dependent numerical solution of Newton's equation of motion for all particles in atomic-scale (Poschel and Schwager, 2005). The model in MD is composed of a collection of interacting spherical atoms under assumed interaction potential (Ravi-Chandar, 2004). The interaction are descried using potential functions, i.e. Hooke's law, Lennard-Jones potential, embedded atom method potential and the reactive force-field interatomic potential (Adcock and McCammon, 2006). Several studies have investigated the different aspects of crack initiation and propagation mechanism, such as the plastic deformation process at the crack, cohesive zone model parameters and dynamic crack processes using MD (Zhou et al., 1996a). Generally, the MD simulation is a very useful tool of studying the change in the microstructure (Ma and Garofalini, 2006) and, therefore, it is a suitable technique for investigating crack nucleation and propagation at the micro-scale. However, the small

computational system sizes and short time scales are two major limitations of this technique (Zhou, et al., 1996a). Additionally, the nano/micro structures of rock materials are too complicated to model due to there being a multi-phase material.

5. Combined methods

The use of combined models has been increased rapidly in rock engineering owing to their unique advantages such as the ability to model both rigid and deformable objects and discontinuous features (Owen et al., 2003), strain/stress problems, and moving from continuum to discontinuum medium. In fact, unlike coupled methods which use physical coupling of two different methods, the combined (hybrid) models combine the advantages of both continuum and discontinuum methods (Eberhardt et al., 2003). The main types of combined models which have been used in rock mechanics are the combined BEM/FEM, DEM/FEM, BEM/DDM, DEM/BEM, BEM/DEM and recently developed NMM (Jing and Hudson, 2002; Zhao, et al., 2011a). Not all of hybrid models are suitable for fracture mechanics problems. An appropriate combined models for fracture simulation are the ones that can model pre-failure and the post-failure process of material (Darve et al., 2004). Following is a brief explanation of combined methods, which have been developed and employed successfully to model transition from continuum to discontinuum in fracturing process.

5. 1 Combined finite/discrete element method (FEM /DEM)

Over the past two decades a class of combined finite/discrete element procedures have been successfully developed for simulation of progressive fracture process in brittle materials. The basic FEM/DEM has been employed successfully to model problems dealing with transition process from continuum to discontinuum such as rock fracturing and fragmentation (Liu et al., 2015; Mahabadi et al., 2016; Munjiza, 2004; Owen et al.,

2000; Rockfield, 2005). Overall a hybrid FEM/DEM method is considered as a robust approach for modelling of fracture process in brittle/semi-brittle materials, and different formulations of this method have been proposed. ELFEN (Rockfield, 2005) and Y (Munjiza, 2004) are the two most common implementations of hybrid DEM/FEM (Lisjak and Grasselli, 2014). Since these methods are being developed extensively for modelling rock fracture problems, their principles are discussed in relative detail hereafter.

5.1.1 ELFEN

ELFEN is a combined continuum–discrete element code that was firstly introduced in the early 1990s to simulate brittle material behaviour under impact loading. The basic idea behind ELFEN is the transition from continuum to discontinuum through discrete fracture insertion. In ELFEN, the medium is formulated using an explicit finite element model (Klerck et al., 2004). Continuum based failure and fracture mechanisms associated with material softening are obtained by developing a modified Mohr-Coulomb elastoplastic model, which can deal with both tension and compression states. Taking into account the fracture mechanics principles, strain localization can also be obtained. In order to model tensile fractures, the Rankine rotating crack model is implemented into the code. Additionally, to deal with combined compressive and tensile stress field, a combination of Rankine rotating crack model with isotropic non-associative Mohr-Coulomb yield surface, known as compressive fracture model, is employed. . A nodal fracture scheme is responsible for the transition from continuum to discontinuum by transferring the virtual smeared crack into a physical fracture in the finite element mesh. The scheme includes three stages: 1) creating failure map for the whole domain by defining a failure factor defined as the ratio of the inelastic fracturing strain to the critical fracturing strain via Eq. (4); 2) identifying the direction of fractures

with respect to the magnitude of failure indicator; and 3) inserting the discrete cracks and remeshing:

$$F_k = \left(\frac{\varepsilon^f}{\varepsilon_c^f}\right)$$

$$\varepsilon_c^f = \frac{2G_f}{h_c f_t} \tag{4}$$

where F_k is failure indicator, G_f is specific fracture energy, h_c is element dimention, f_t is tensile strength, and ε^f and ε_c^f are inelastic fracturing strain and critical fracturing energy, respectively

As shown in Figure 12, both intra-element and inter-element insertion algorithms can be employed to insert discrete elements into the model. The fracture insertion procedure follows detecting and defining contacts between continuous regions and/or the resulted discrete parts using either penalty or Lagrangian multiplier method. The principles of this method can be found in detail in studies by Klerck (2000) and Owen et al. (2004).

Figure 12: Crack indentation techniques in ELFEN (a) initial model; (b) inter-element crack insertion; (c) intra-element crack insertion (after Klerck (2000))

Compared with the continuous and discontinues methods, ELFEN is relatively more capable in modelling the post failure behaviour and fragmentation of brittle material, and yet, it is computationally expensive where ill-posed conditions may occur in the case of inter-element crack insertion. The application of ELFEN in different fields of rock engineering was reviewed by Lisjak and Grasselli (2014).

5.1.2 Y-Code
The Y-code can be considered as the most common implementation of combined finite/discrete element method, which has been employed extensively in geomechanics

problems. The computational algorithm of Y-code was originally developed as an open source code by Munjiza (2004). The general feature of Y-code is relatively similar to DEM, particularly BPM, where rigid bodies are replaced by deformable elements. In fact, the Y-code considers the model as a formation of interacting discrete bodies, which are discretised into finite elements to be able to analyse deformability, fracture and fragmentation of even complex geometries. A constant strain triangle elements was employed by the original code to simulate both linear and non-linear two-dimensional problems. Similar to the developed techniques implemented into the standard FEM, the combined model employs ICZM to implement strain-hardening behaviour, where strain-softening part is addressed by fracture mechanics (energy failure criterion) and damage mechanics principles. In this method, fracture initiates and grows by separation of cohesive finite elements, which are bonded together using a defined bonding stress as a function of damage index and both peak tensile and shear strengths (Figure 13). A four-node joint element bonds the elements together. When the magnitude of separation (δ_c) exceeds a critical value, this element is damaged and fractured. This magnitude (δ_c) at any point on fracture surface and bonding stress for separation can be derived via Eq. (5).

$$\delta = \delta_n n + \delta_s t \tag{5}$$

where, δ is separation and $\boldsymbol{n}$ and $\boldsymbol{s}$ are unit normal and tangential vectors, respectively (Munjiza, 2004). By the same assumption the traction vector p during fracture can be written as Eq. (6)

$$p = \sigma_n n + \tau t \tag{6}$$

where, σ_n and τ are the normal and tangential stresses, respectively. Without any separation, the bond stress is in its maximum value equal to either peak tensile strength (f_{tp}) or peak shear stress (f_{sp}). By increasing the degree of separation of the elements, $0 < \delta_n \leq \delta_{tp}$ or $0 < \delta_s \leq \delta_{sp}$, the bonding stress starts decreasing as a function of damage index D and a peak strength σ_{tp} according to the Eq. (7).

$$\sigma = g(D)\sigma_{tp}$$

$$\tau = h(D)\sigma_{sp} \tag{7}$$

In these equations σ and τ define bonding stresses, σ_{tp} and σ_{sp} are peak tensile and shear strengths, respectively. Element separation occurs when the $\delta_n > \delta_{tp}$ or $\delta_s > \delta_{su}$ is satisfied, which means the bonding stress is zero and so the crack can initiate and propagate along the boundary of the elements. This concept of the model is shown in Figure 13. The values of δ_{tp} and δ_{su} are function of joint element strength (tensile and shear) and fracture energy (G_{IC} and G_{IIC}).

Figure 13: Fracture modes in combined FEM/DEM

Because of the capabilities of this code, especially in modelling of fracture and fragmentation mechanism, the Y-code has been developing rapidly in the field of rock mechanics. However, the Y-code suffers from difficulties such as modelling shearing fracture and mixed-mode fracture, and taking into account loading rate effect and heterogeneity (An et al., 2017). The Y-code has been modified by researches to address such shortcomings and also to make it more compatible and applicable to rock engineering problems, particularly when dealing with rock fracturing problems.

After the development of a two-dimensional code named Y2D by Munjiza (2004), Xiang et al. (2009) employed ten-noded tetrahedral element to extend the

application of Y-code into three-dimensional problems. Further development was made by Munjiza et al. (2010), introducing a virtual geoscience workbench (VGW) to simplify the use of Y-code. Later, Mahabadi et al. (2012) introduced Y-Geo, based on the original Y-code, improving some of its features for more compatibility with rock engineering problems. Y-Geo was later improved to include three dimensional application, commercially named as Irazu (Mahabadi, et al., 2016). Another improvement of Y-code was presented by Rougier et al. (2011) in a software package known as MUNROU. Similar work was produced by Liu, et al. (2015) where an integrated development environment (IDE) was generated for a combined FEM/DEM on basis of enriched FEM-based codes known as Y2D/3D IDE. The Y-code and its extensions have been employed in different areas of rock fracture analysis (An et al., 2017; Fukuda et al., 2017; Mahabadi et al., 2010; Munjiza et al., 2000; Munjiza et al., 2013; Rougier, et al., 2011).

5.2 Numerical Manifold Method (NMM)

The NMM is a hybrid DDA/FEM which was firstly introduced by Shi (1991). Two types of covers are employed in NMM: mathematical and physical covers. The mathematical cover defines domain approximations and is independent of the problem domain; whereas the physical cover defines the integration fields and is the intersection of mathematical cover and the physical domain. The physical domain comprises problem domain as well as all physical features such as cracks, interfaces and joints. Additionally, cover based element is another basic concept of NMM which is known as the common region of several physical covers (Ma et al., 2009a). Through the NMM's algorithm, the physical block with sub-block system are rebuilt using mathematical covers. Then the manifold element system is constructed through the second stage where the geometric information is defined into mathematical covers by sub-block

systems (Figure 14). Since two covers are independent, mathematical covers can be defined freely and therefore their size and shape are not abstract. Discontinuities are simulated by dividing mathematical covers into several physical covers attached with independent cover functions. Detailed explanation in this regard can be found through Ma, et al. (2009a) and Ma et al. (2010) studies. Eliminating meshing task and combining continuum and discontinuum problems into one framework are two advantages of the NMM; whereas instability due to using small elements, being computationally expensive and being awkward to model rigid body rotation are main drawbacks of the method. It seems this method needs further development to be considered as a robust technique in the field of dynamic analysis of discontinuous medium (Zhao et al., 2011b). A number of improvements have been made to address these weaknesses which can be found in the study conducted by (Ma, et al., 2010). Several studies have reported the successfully application of NMM in simulation of rock fracture and fragmentation process (Chen et al., 2006a; Wu and Wong, 2014; Zhang et al., 2015). Relatively similar technique was introduced by Tang and Lü (2013) as DDD which is a hybrid RFPA/DDA method. Miki et al. (2010) developed a hybrid NMM/DDA method to deal with dynamic problems.

Figure 14: (a) physical domain; (b) mathematical domain; (c) mathematical cover; (d) physical covers; (e) manifold elements (after (Ma, et al., 2009a))

5.3 Other combined methods

There are also other formulations of a combined FEM/DEM, which are developed and used in the field of rock fracture analysis. The Livermore Distinct Element Code (LDEC), which was originally developed as a DEM method, extended to a combined FEM/DEM by incorporating the finite element capability into the model (Morris et al., 2006). This hybrid FEM/DEM uses a nodal cohesive element formulation, allowing

finite element to fracture and fragment (Block et al., 2007). The capability of this method in the field of rock mechanics and fragmentation was presented by Morris and Johnson (2009). Similar efforts were made by Mohammadi and Pooladi (2012) by developing other combined FEM/DEM formulations to simulate rock blasting and resultant fragmentation. Paluszny et al. (2013) introduced an impulse-based discrete element method, which uses stress intensity factors to simulate fracture and fragmentation. In this method the interaction and movement of elements is controlled by the impulse dynamics instead of the penalty-based method (Paluszny, et al., 2013). The Scaled Boundary Finite Element Method (SBFEM) is another recently developed numerical technique for fracture analysis, which combines the advantages of the FEM and BEM. Pioneered by Song and Wolf (1997), this technique only discretises the boundary while standard finite element interpolation is employed on the boundary(Li et al., 2013). Song et al. (2017) reviewed the application of the SBFEM technique in linear elastic fracture mechanics, which was further developed by introducing principles of combined FEM/DEM (Luo et al., 2017). The combined SBFEM and DEM method offers the possibility of convex polygons to be used but, because of the use of semi-analytical method, the use of plasticity criteria still requires further research. Therefore while the combined SBFEM-DEM method seems to be a promising numerical technique for the rock fracture simulation, its feasibility is still need to be explored.

6. Multiscale coupled methods

Multiscale methods are regarded as a promising method to solve the significant computational power requirement of micro-scale methods, such as MD. The purpose of multi scale method is to efficiently derive materials' response at a micro scale from micro mechanical interactions (Sansoz and Molinari, 2007). As explained earlier, macro scale fracturing in rock materials is the result of microscale cracking and therefore the

multiscale approaches can be useful techniques in the study of rock fracture mechanism. In fact the multiscale techniques facilitate modelling the effect of micro-cracking in the micro-scale on macro-scale fractures (Sfantos and Aliabadi, 2007). For example, the microscale region can be employed to model crack tips in crack propagation. Different multiscale approaches have been developed, e.g. hierarchical, semi-concurrent and concurrent methods. A comprehensive review on multiscale methods for fracture study has been conducted by Budarapu and Rabczuk (2017), in which recent achievements in simulation of quasi-brittle fracture have been discussed.

7. Summary

This paper provides an overview of common numerical techniques which have been capable of modelling rock fracture processes. Unlike other review articles, where either focus on general application of numerical methods in rock engineering problems or are limited to some special classes of numerical methods such as discrete element methods, this paper aimed to explore the capabilities of newly developed techniques as well as exiting methods in dealing with rock fracture problems. Generally, not all of numerical techniques are capable of properly simulating the rock fracture process. This is mainly due to the complex nature of rock fracture processes, which requires consideration of the effect of heterogeneity, softening behaviour and rate-dependency behaviour of rock, transition mechanism from continuum to discontinuum, and the time and cost considerations. The general trend of the development of the numerical techniques shows that the study of rock fractures started from macro scale and then extended to meso and micro scales and finally a combination of the micro and macro scales. A schematic sketch of the mostly developed techniques for simulation of rock fracture are depicted in Figure 15.

Figure 15: Schematic of common numerical techniques in rock fracture simulation

Despite all of the improvements, standard continuous numerical methods such as FEM and FDM can only deal with the fracture process of rock up to a certain extent. Mesh-erosion and XFEM are the most developed FEM techniques in the field of rock fracture analysis. These techniques have the general advantages of the FEM such as flexibility in dealing with complex geometries and boundary conditions, well-developed constitutive models for pre-failure behaviour of rock and ability to model explicit crack initiation and propagation. Meanwhile the mesh-erosion method suffers from mesh-size dependency, using complex damage models and the persistence effects of the eroded elements. The XFEM is awkward in dealing with multi crack propagation and interaction, and is not capable of modelling fragmentation process. Although it is relatively simple and fast, the main weaknesses of FDM are the inability of modelling explicit cracks, separation and fragmentation, and having trouble in dealing with complex boundary conditions, material heterogeneity and post-failure behaviour of rock. The BEM is capable of modelling explicit crack initiation and propagation and is also computationally efficient, while it is limited to the analysis of elastic homogenous materials and is unable to model crack separation and rock fragmentation. The meshless methods can model explicit crack initiation, propagation and separation process properly, especially when subjected to dynamic loading, while they suffer from instability in solutions, difficulty in defining boundary conditions and being computationally expensive. The capabilities of DEM in modelling of block movements, explicit crack initiation and propagation, dynamic problems make them a robust technique. At the same time, apart from the lattice method, the remainder of DEM techniques are particle or block size dependent in both simulation and calibration stages. Moreover, the drawbacks of DEM include relying on linear failure envelope, considering low friction angle and difficulties in modelling of pre-failure behaviour of

rock. The hybrid methods such as combined FEM/DEM methods and NMM have been developed to relieve the limitations of both continuum and discontinuum methods. They enjoy the advantages of both techniques with the ability of modelling pre-failure and post-failure behaviours of rock, explicit crack initiation and propagation and transition from continuum to discontinuum. However, the NMM is awkward in modelling of rigid bodies, contact detection and is computationally expensive while the combined FEM /DEM suffers from mesh dependency and being computationally expensive in three-dimensional simulation. The multi–scale coupled methods seems to be a robust technique in modelling fracture process and have received a good deal of attention in the field of fracture analysis; however they are still computationally expensive and their performance need to be explored further.

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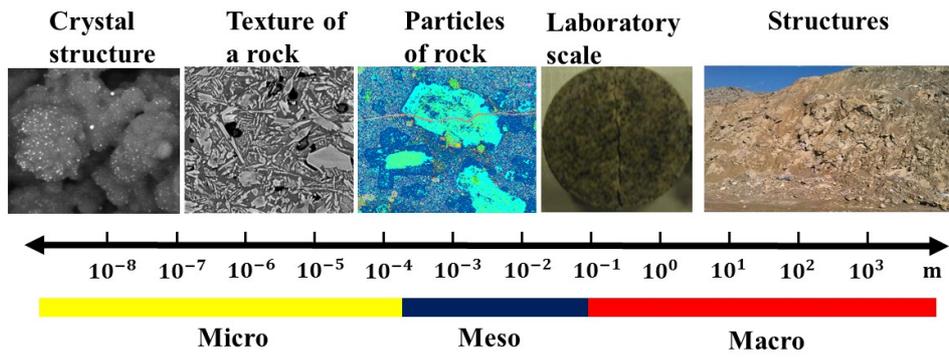
Figure 1: Different scales of observations in rock fracture analysis (modified after Van Mier (1996))
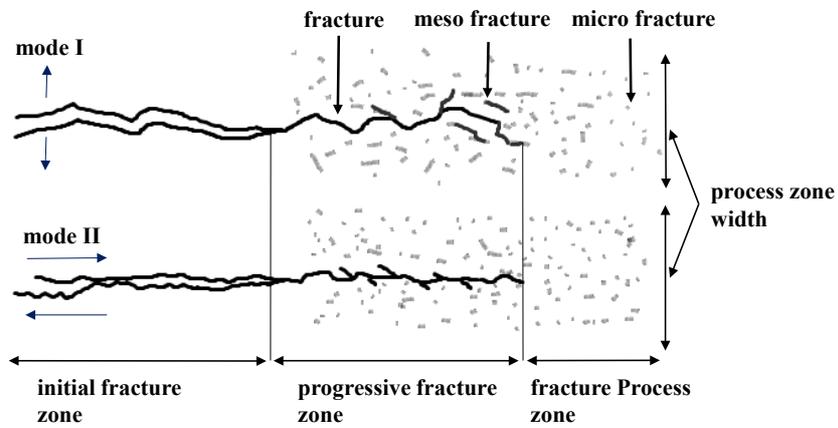

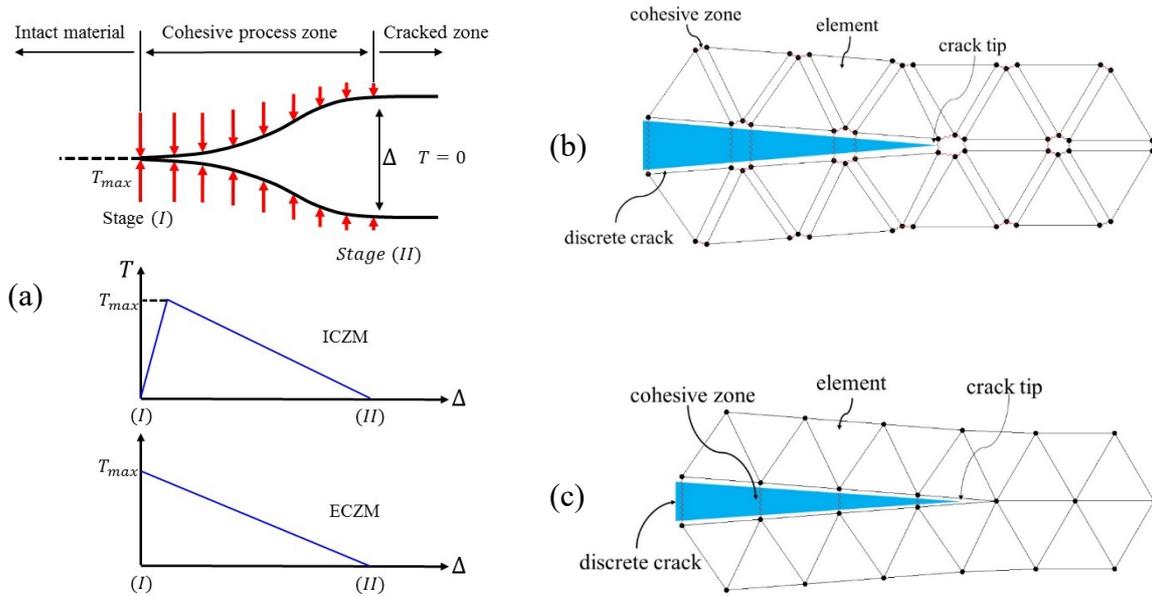Figure 2: Schematic shape of FPZ development ahead of a crack tip (modified after (Bazant, 1992))

Figure 3: (a)The concept of the cohesive zone model, ICZM and ECZM (Adapted from Zhang, Paulino, & Celes (2007)); (b) Sketch of the developed inter-element crack by Xu and Needleman (1994); and (c) by Camacho and Ortiz (1996)
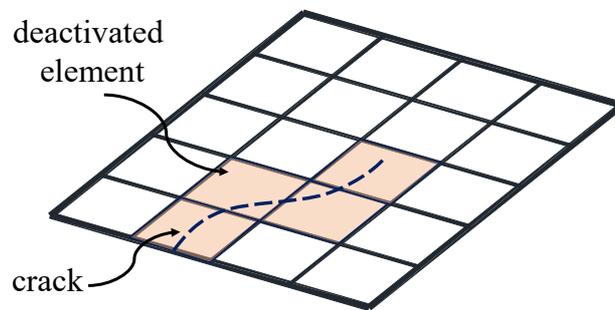

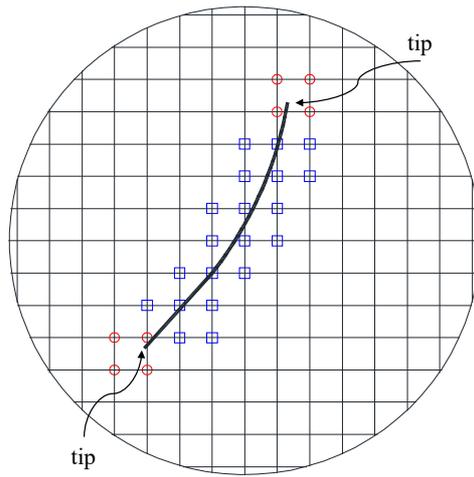Figure 4: Schematic illustration of crack simulation by element erosion method

Figure 5: Arbitrary crack growth in XFEM; circles are nodes enriched by front enrichment functions and squares are enriched nodes by Heaviside enrichment (Adapted from Moës et al. (1999))
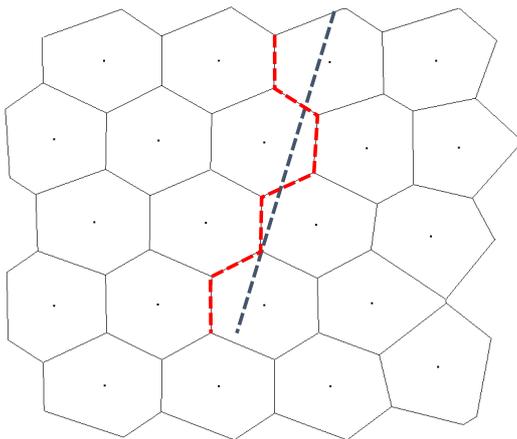

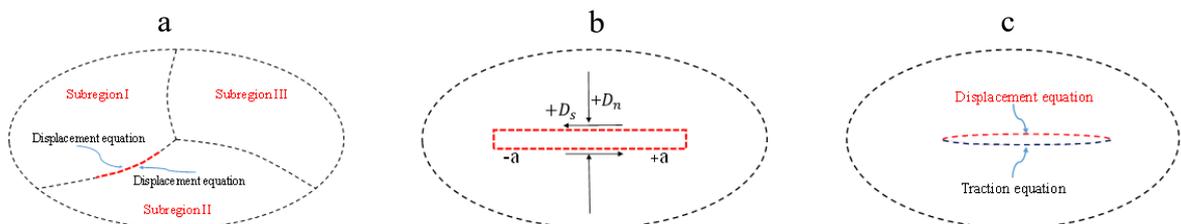Figure 6: crack simulation via Voronoi grid

Figure 7: Three Boundary element techniques in fracture analysis: (a) Subregion method, (b) DDM, (c) DBEM

F_n, F_s- Normal/shear force
F_n^{max}, F_s^{max} - Peak Normal/shear strength
k_n, k_s- Normal/shear stiffness
u_n, u_s- Normal/shear displacement

F_t, F_s- Tensile/shear force
F_t^{max}, F_s^{max} - Peak tensile/shear strength
G_I, G_{II}- Mode I/Mode II fracture energy release rate
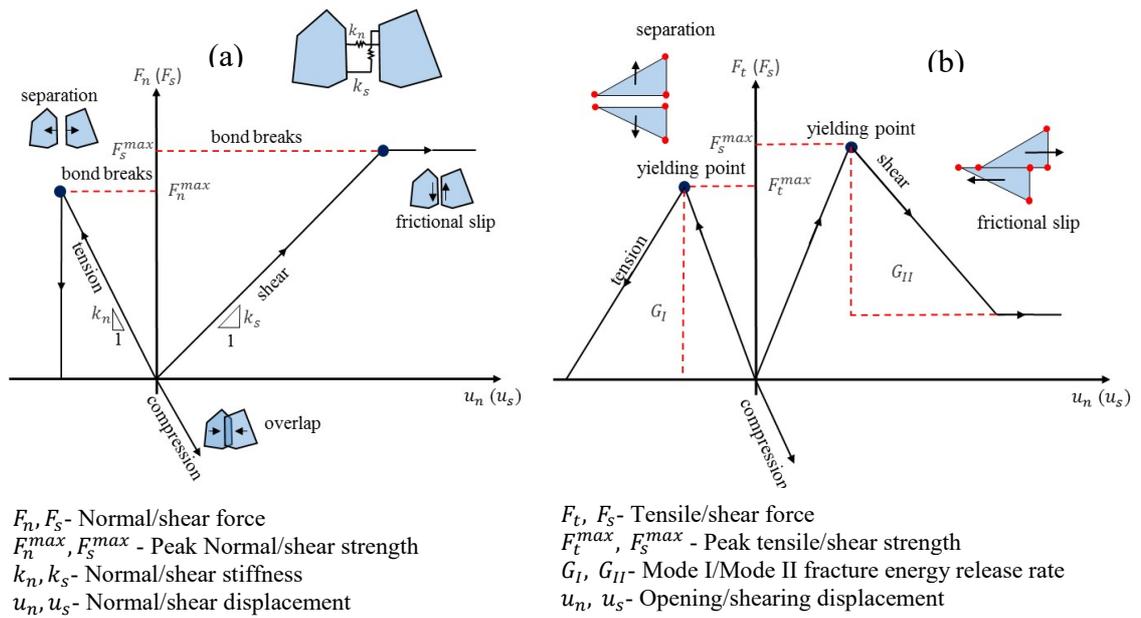u_n, u_s- Opening/shearing displacement

Figure 8: Comparison between (a) Fracture constitutive behaviour in DEM (after Kazerani and Zhao (2010)) and (b) Fracture constitutive behaviour in FEM
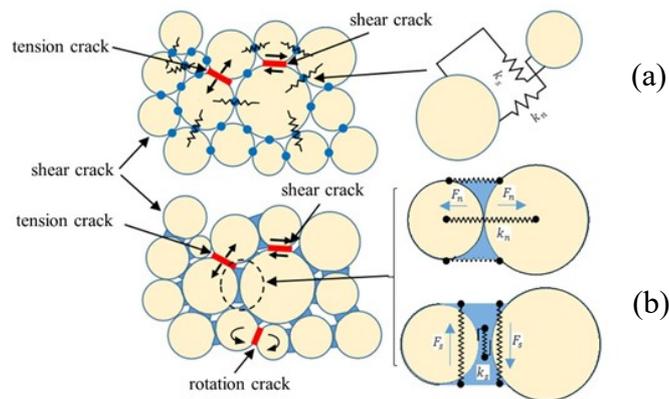

Figure 9: The implemented bond models PFC a) Normal contact bond model (after (Turichshev and Hadjigeorgiou, 2017)) b) the parallel bond model (after (Lisjak and Grasselli, 2014))
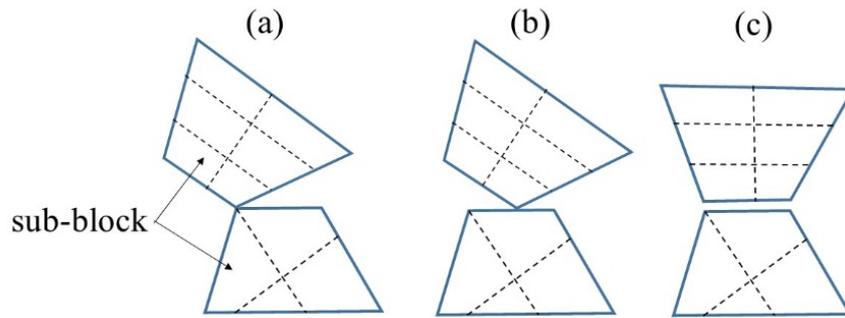
Figure 10: The contact types in two-dimensional DDA: (a) angle to angle contact; (b) angle to edge contact; (c) edge to edge contact
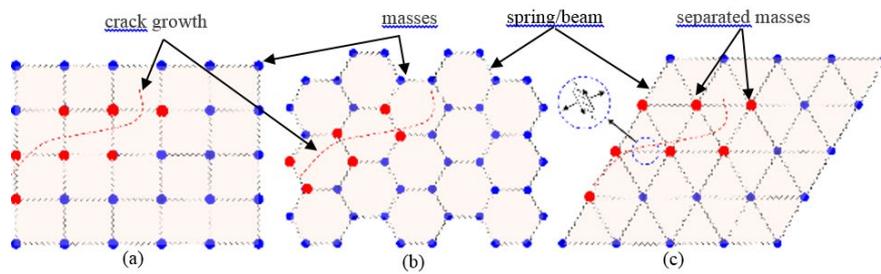

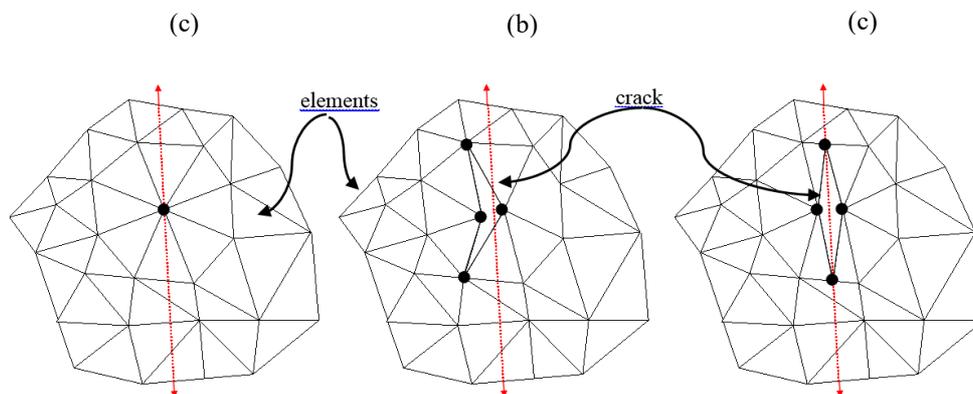Figure 11: (a) Square lattice cell; (b) Hexagonal lattice cell; (c) Triangular lattice cell

Figure 12: Crack indentation techniques in ELFEN (a) initial model; (b) inter-element crack insertion; (c) intra-element crack insertion (after Klerck (2000))

Mode-I Fracture

elastic elements

δ_t

joint element

$$\sigma = \begin{cases} \left[2\dfrac{\delta_t}{\delta_{tp}} - \left(\dfrac{\delta_t}{\delta_{tp}}\right)^2\right]\cdot\sigma_t & if \quad 0 \le \delta_t \le \delta_{tp} \\ f(D)\cdot\sigma_t & if \quad \delta_{tp} \le \delta_t \le \delta_{tu} \\ 0 & if \quad \delta_t \ge \delta_{tu} \end{cases}$$

σ_t

$G_{IC} = \int_{\delta_{tp}}^{\delta_{tu}} \sigma(\delta)d\delta_t$

G_{IC}

δ

δ_{tp} δ_{tu}

Mode-II Fracture

elastic elements

joint element

δ_s

$$\sigma = \begin{cases} \left[2\dfrac{\delta_s}{\delta_{sp}} - \left(\dfrac{\delta_s}{\delta_{sp}}\right)^2\right]\cdot\sigma_s & if \quad 0 \le \delta_s \le \delta_{sp} \\ g(D)\cdot\sigma_s & if \quad \delta_{sp} \le \delta_s \le \delta_{su} \\ \tau_r = \sigma_n \tan\phi & if \quad \delta_s \ge \delta_{su} \end{cases}$$

σ

σ_s

$G_{IIC} = \int_{\delta_{sp}}^{\delta_{su}} [\tau(\delta) - \tau_r]d\delta_s$

G_{IIC}

δ

δ_{sp} δ_{su}

Mixed-mode Fracture

δ_t elastic elements

joint element

δ_s

$$\left(\frac{\delta_t - \delta_{tp}}{\delta_{tu} - \delta_{tp}}\right)^2 - \left(\frac{\delta_s - \delta_p}{\delta_{su} - \delta p}\right)^2 \ge 1$$

δ_s

δ_{su}

δ_{sp}

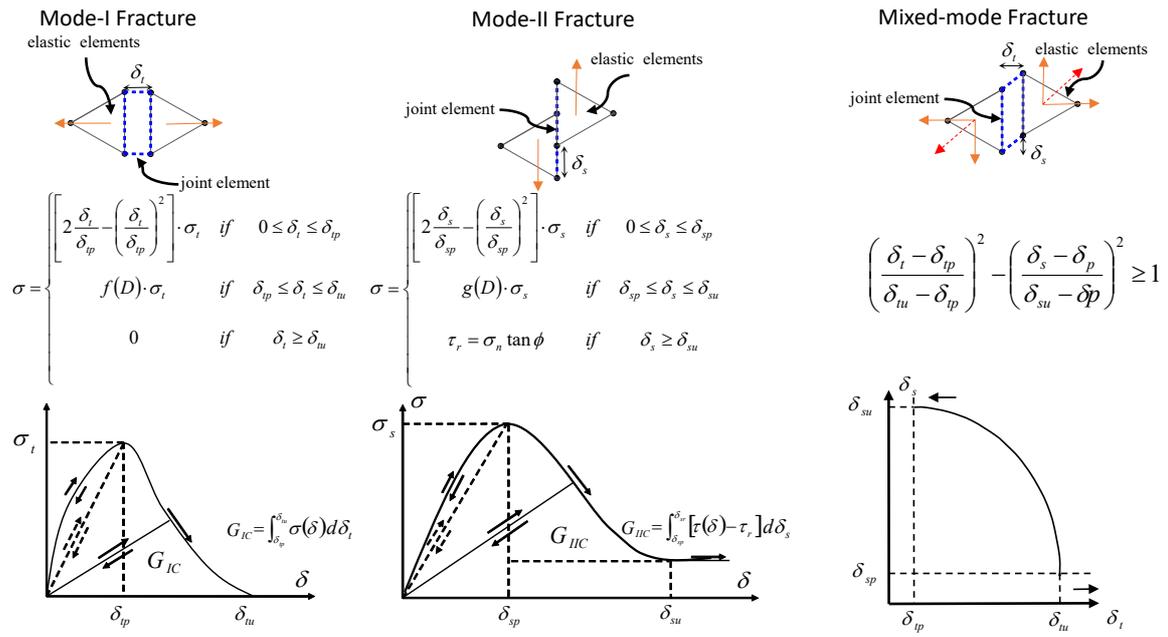δ_{tp} δ_{tu} δ_t

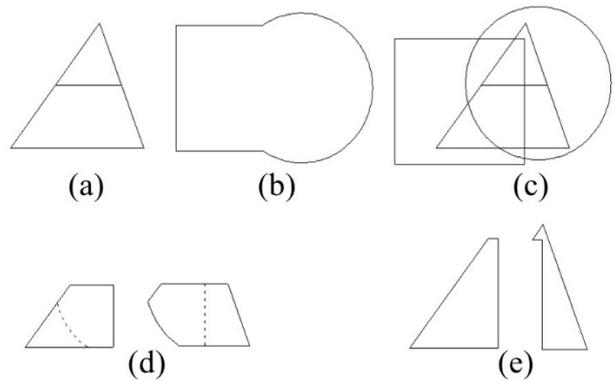Figure 13: Fracture modes in combined FEM/DEM

Figure 14: (a) physical domain; (b) mathematical domain; (c) mathematical cover; (d) physical covers; (e) manifold elements (after (Ma, An, Zhang, & Li, 2009))

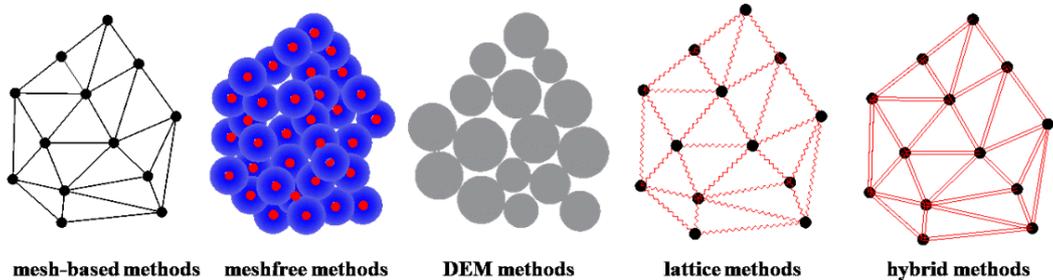mesh-based methods   meshfree methods   DEM methods   lattice methods   hybrid methods

Figure 15: Schematic of common numerical techniques in rock fracture simulation

Despite all of the improvements, standard continuous numerical methods such as