Effect of clumping and clustering on more realistic behaviour of Bonded-Particle Model

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ABSTRACT
Distinct Element Method has been used by researchers as a means to overcome the shortfall of fracture mechanics in assessing the accumulation of microcracks in rocks, but in this method researchers have been faced by some restrictions. The Bonded-Particle Model (BPM), which has Distinct Element Method implemented in it, has some difficulties in the simulation of unstable propagation of cracks after initiation. In this paper challenges and a possible solution in the Bonded-Particle Model approach will be discussed.

RÉSUMÉ
La mèthode d'éléments distincts (Distinct Element Method) a été utilisé par les rechercheurs comme un moyen de surmonter le manque de compréhension de l'accumulation de microfissures dans les roches. Cependent, certains limitations ont eté identifiées. Le modèle de particules-attachées (Bonded-Particle Model), utilisé dans la mèthode d'éléments distincts, a certaines difficultés dans la simulation de la propagation instable des fissures. Ce papier discute les défis et propose une solution pour utiliser le modèle de particules-attachées.

1 INTRODUCTION

The inability of fracture mechanics in prediction of correct crack propagation and accumulation in rocks has lead the researchers to move toward the application of Distinct Element Method (DEM) in their research. The Distinct Element Method enables researchers to study different damage threshold levels in rock that are not possible to simulate using other methods such as Finite element or Boundary element. Study of damage thresholds and crack accumulation in rocks helps to better understand the behaviour of brittle rocks in the field and to better predict short or long term behaviour of structures in highly stressed environments. However, fundamental limitations for fracture modelling still exist and must be addressed.

2 BONDED-PARTICLE METHOD

Particle Flow Code (PFC) as a Bonded-Particle analogue has been chosen for the purpose of simulating Brazilian, direct tensile, unconfined compressive strength (UCS) and confined tests in crystalline rocks. PFC has been developed by Itasca consulting group and is available in both 2 and 3 dimensions. The ability of this code in simulating the initiation and propagation of cracks and also tracking the number and position of the cracks which is comparable with Acoustic Emission (AE) monitoring of rock tests in laboratory (Hazzard and Young 2000) have made PFC a suitable code for simulation of brittle rocks under high stress. Many underground rock structures has been successfully simulated using PFC, for instance simulation of spalling and notch formation in the URL Mine-by-Test at Pinawa, Manitoba, Canada (Potyondy and Cundall 1998).

In PFC, damage is represented directly by the formation of cracks (Potyondy and Cundall 2004). Computational modelling of rocks can be classified into direct and indirect methods. In direct method, such as Bonded-Particle method, damage is being represented by simulating the cracks initiation and propagation therefore it provides a suitable means for better understanding of the rock behaviour and study of the progressive damage development in rocks. In indirect approach, which most computational models use for describing the mechanical behaviour of rocks for engineering purposes, the material is being idealized as a continuum and the weakness will be distributed over the material using the constitutive relations. Cracks in PFC are being represented by bond breakage. After breaking a bond, the broken bond stress will be distributed over the neighbour bonds. This prevents the expected stress concentration on tip of the crack. Because of this stress redistribution, unstable crack propagation does not occur in PFC.

Previous modelling works with PFC have shown some inaccuracy in the slope of the confinement-strength curve (internal angle of friction) and in the relationship between tensile strength and compressive strength of the synthesised sample (Diederichs 2000,2003). Calibration to UCS resulted in inaccurate tensile strength and vice versa. In addition, the full dilational peak strength (hardening after initial yield) observed in actual samples could not be reproduced. These inaccuracies in simulations can be the result of mathematical and kinematic formulation of the Bonded-Particle Model which restricts the unstable propagation of initiated

cracks. As said before in PFC cracks are simulated by bond rupture and so a crack can initiate but does not extend beyond a single bond. A new approach in Bonded-Particle Modelling is needed for more accurate results in simulations.

PFC code lends itself to experimentation due to the inclusion of a user scripting language FISH (Itasca 2008). Fish is a programming language being embedded in PFC. Using Fish, user can define new variables and functions. Also using Fish user can access different objects in a PFC model for instance, walls, balls, contact bonds, parallel bonds, clumps etc. These objects can be removed, new ones can be added or their properties can be changed while the model is running.

2.1 Contact Model

The main two contact models in PFC are contact bond and parallel bond. There are several other contact models and new contact models can be written using C++ programming language. Nevertheless, parallel and contact bonds are the most common. The overall model behaviour produces "measureable" macro-properties and are equivalent to the measurements in the laboratory. These are the result of micro-properties or contact properties such as normal and shear strength, normal and shear stiffness, ball friction etc.. These properties which define the ball-ball or ball-wall interaction characteristics are called micro-properties. Contact bond is the simplest form of contact for calibration available in PFC and acts like glue between two spheres, connecting them together. Parallel bond can be assumed as a cylinder connecting the centre of two neighbouring spheres. Parallel bond acts like a cementing material acting over a finite area at the contact between two spheres, (Itasca 2008). Both parallel and contact bonds can transfer force. Parallel bond can also transfer moment while contact bond is unable of transferring the moment which allows rotation of spheres that can cause some deviation in behaviour (Cho et al 2007).

2.2 Clumping and Clustering

In PFC, there is a possibility of attaching a group of spheres together to make a rigid body, called a Clump. Clumping is a useful feature for the study of the effects of grain shape and grain size distribution in rocks. Each clump can represent a grain in the model. Clump has a rougher surface rather than a single sphere and therefore it can increase the macro-mechanical angle of friction. The interactions between clumps are governed by the defined micro-properties of spheres making the clumps. There already exists a method for clumping in PFC and clumps are supported by Fish.

Cluster is another terminology being used in PFC that corresponds to an assembly of spheres being packed together and form a cluster (Itasca 2008). Cluster properties can be the same or different from the neighbour clusters. Clusters can be used in simulating blocky rock systems or here they can be used to represent grains. The difference between a clump and a cluster is that clumps are rigid while clusters are not and clusters can break apart. Cluster is merely a terminology in PFC-3D and there is no Command or Fish support for it at present.

2.3 Ball Size

Ball size or resolution of the model is an important parameter in a PFC model. Balls must be small enough to let the crack propagate through its desired path and not to create a tortuous path as cracks can only propagate across the balls and not through them (It is a fundamental assumption in PFC that spheres are rigid). On the other hand the computation time must be kept in mind. A slight difference in D_{min}, which is the diameter of the smallest ball in the assembly of balls, can significantly change the computation time.

When a model has been calibrated to a certain D_{min} and D_{max}/D_{min} ratio, it should not be changed or the model must be calibrated again. As it is shown in Figure 1, although in PFC2D the grain modulus is independent of the grain size but in PFC3D the grain modulus must be scaled with the particle radii. Parallel bond moduli in both 2 and 3 dimensions are dependent upon the particle size and correct modulus must be calibrated to the particle size (Diederichs 2000).

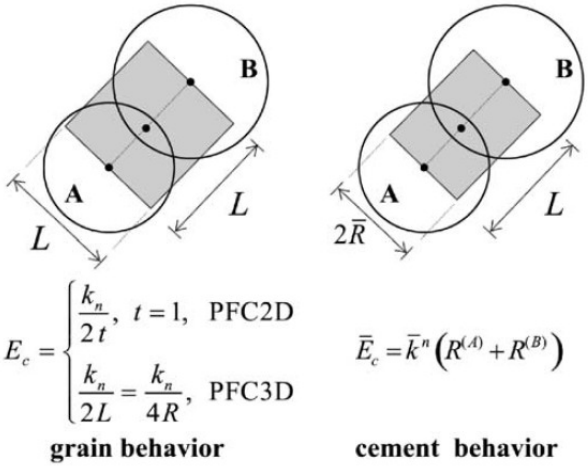

Figure 1. Formulation of grain and cement elastic constants in PFC, (from Potyondy and Cundall 2004).

3 CONTACT BONDED MODEL

3.1 2D Simulations

Many researchers (Diederichs 2003, Potyondy and Cundall 2004, Cho et al 2007) have simulated rock engineering laboratory tests in PFC2D and they have shown their concern regarding the accuracy of the result. Diederichs (2000, 2003) could simulate the progressive damage accumulation within brittle rocks, benefiting from the restrictive internal geometry of PFC that inhibits the

unstable propagation of cracks once initiated. PFC is able to simulate crack initiation in a continuum and transition from continuum to discontinuum. After initiation of the first cracks the stress concentration on tip of the cracks dissipates due to the stress redistribution amongst the neighbour contacts. In a UCS test or axisymmetric compression test, due to the stress state and test geometry, shear failure or axial fracture happens through the crack coalescence and accumulation rather than splitting due to single-crack propagation. Diederichs et al (2004) could identify the onset of different damage levels by using accumulative cracks which can be recorded in PFC and is equal to acoustic emission (AE) monitoring in laboratory. In Figure 2 it can be seen that systematic cracking is the onset of damage in the sample and crack coalescence is the starting point for localization and yielding limit of the rock.

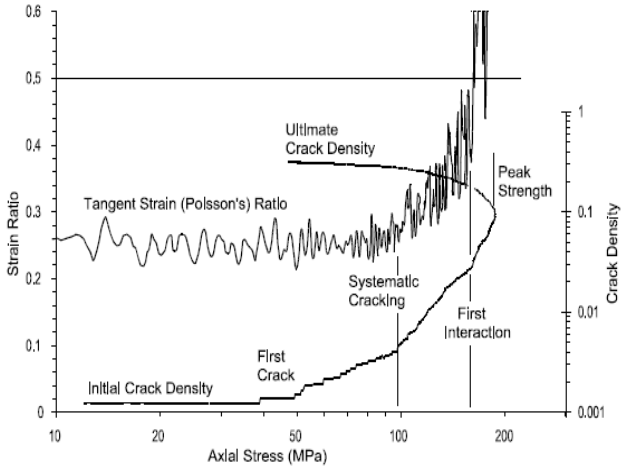

Figure 2. Detection of different damage levels using accumulative cracks recorded in PFC2D (from Diederichs et al 2004).

Diederichs (2000), based on his simulations in PFC2D using contact bond for Lac du Bonnet granite reported that the peak strength envelope does not coincide with the actual strength envelope of rock and better represents the yielding limit. The internal angle of friction for the numerical sample was lower than for actual rock while the tensile strength of the model was much higher than the actual tensile strength (Figure 3).

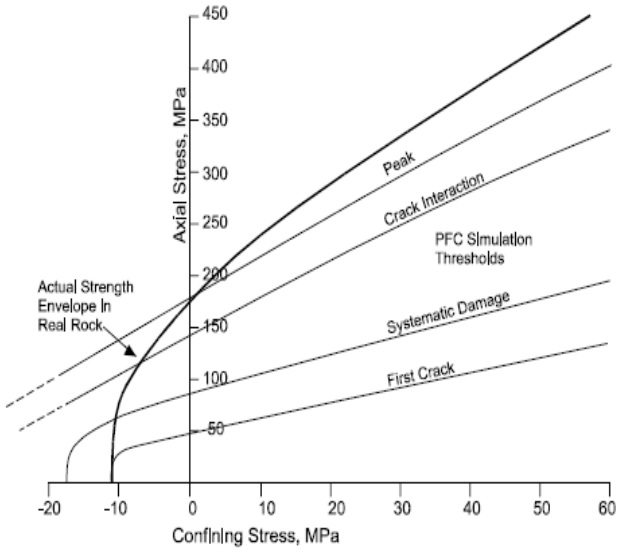

Figure 3. Comparison between PFC2D simulation and real rock behaviour (from Diederichs, 2003)

The difference between simulation and laboratory results is much greater in tension. In reality any initiating crack will immediately progress in an unstable fashion to failure due to stress field around the crack tip. But in PFC, after initiation of the first crack still accumulation of cracks are required for rupture (Figure 4). Diederichs (2003) suggested that the use of parallel bonding, 3D simulation, clumping, clustering and maybe combination of these may improve the tensile/compression strength ratio. This suggestion is tested here.

Bonds in PFC act as truss elements in a truss structure. As it is shown in Figure 4, ruptured tensile bonds cannot cross active compressive bonds. There is the same situation in the Brazilian test. The centre of Brazilian disc is not in a pure unconfined tension ($\sigma 1 = -3\sigma 3$). Therefore, the disc does not split after initiation of the first crack. As shown in Figure 4, in Brazilian test there is a difference between First-Crack stress and peak strength. For reaching the localization and peak strength cracks must be accumulated. The process is similar in direct tension. The point of first crack initiation correlates with true tensile strength values while the ultimate failure stress is unrealistic (Diederichs 2000,2003).

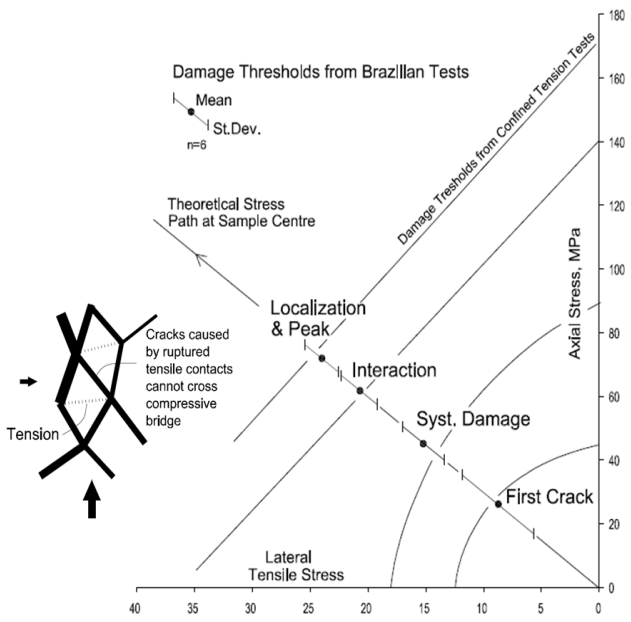

Figure 4. Difference between stresses associated with the first-crack and rupture due to confining stress (from Diederichs 2000).

3.2 3D Simulations

To evaluate the consistency of the result inaccuracy in 3 dimensions, a series of laboratory tests simulated in PFC3D using contact bond. Brazilian, direct tensile, UCS and confined compressive tests have been simulated (Figure 5). Specimen dimensions and geometries have been chosen based on the International Society for Rock Mechanics (ISRM) Suggested Methods (SM) (ISRM 1978 and 1999) and Hoek (1964) for direct tensile test geometry.

The models have been calibrated to Lac du Bonnet granite. The target properties (Diederichs, 2003) for calibration and calibrated micro-properties are shown in tables 1 and 2.

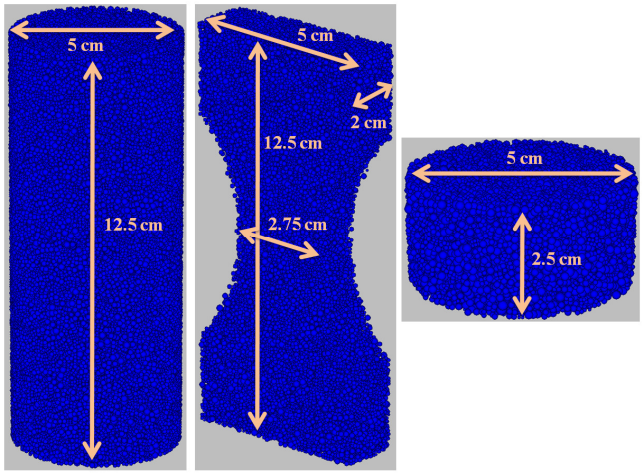

Figure 5. Simulated laboratory test specimen geometries.

Table 1. Target properties for calibration of the models.

Unconfined Compressive Strength, UCS	180 MPa
Damage Initiation Threshold	60 to 100 MPa
Young's Modulus	55 to 60 GPa
Poisson's Ratio	0.25
Residual Friction Coefficient	1 = tan(45 deg.)

Table 2. Calibrated micro-properties for contact bonded model.

R_{min}	0.75 mm	k_n/k_s	4.7
R_{max}/R_{min}	1.66	$\bar{\sigma}_n$	87±17.4 MPa
μ	1	$\bar{\sigma}_s$	350±70 MPa
E_c	104 GPa		

In Table 2, R_{min} is the radius of smallest ball. R_{max}/R_{min} is the ratio of largest to smallest ball radii. μ is the ball friction coefficient. E_c is the ball modulus. k_n/k_s is the normal to shear stiffness ratio for balls. $\bar{\sigma}_n$ is the normal strength of contact bonds. $\bar{\sigma}_s$ is the shear strength.

Figure 6 shows the damage threshold levels for 3D contact bonded model. Damage thresholds have been detected for each test using the previously mentioned method in Figure 2. It can be seen in Figure 6 that peak strength and first interaction are almost linear. Result of the 3D simulation using contact bond, like 2D simulation is not satisfactory.

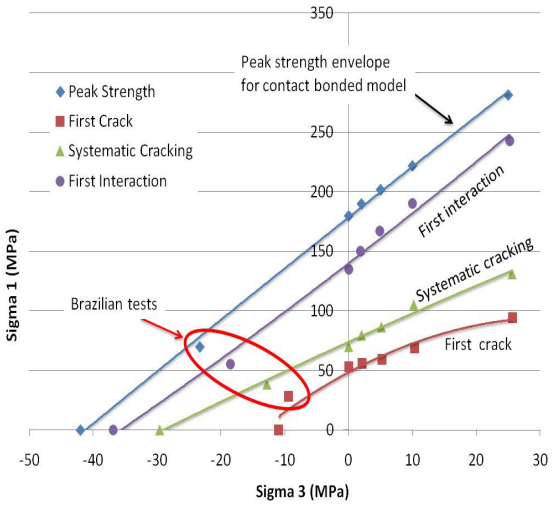

Figure 6. Damage thresholds for contact bonded model.

4 CLUMPED MODEL USING IMPLEMENTED METHOD OF CLUMPING IN PFC3D

Another set of models has been created using clumping method in PFC3D. This method, which has been implemented into PFC3D, replaces each single fabricating sphere of a model with a clump with the same volume. These clumps can be defined by the number, centre position and radius of each of the constructing spheres. Different clump shapes can be defined and used in a model. This type of clumping by replacement creates composites that have a rougher surface rather than a single ball but do not have high interlocks with other clumps.

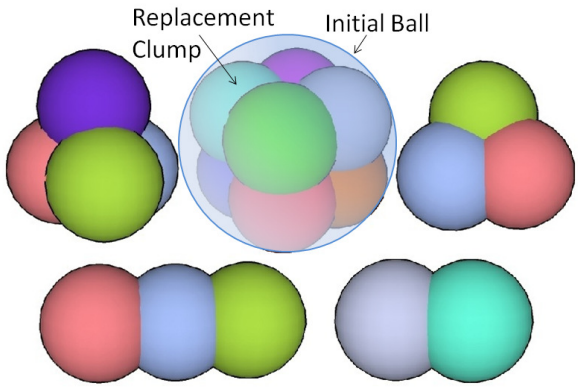

Figure 7. Defined clump shapes for replacement with balls in the model (from Ghazvinian and Diederichs 2010).

In this study five different clump shapes have been defined. Clump geometries can be seen in Figure 7. All clump shapes have been used equally in number, comprising 20% of original number of spheres in the sample. Parallel bond is used as the contact model in this set of simulations and the calibrated micro-properties for the clumped model are shown in Table 3.

Table 3. Calibrated micro-properties for clumped model with parallel bond.

R_{min}	0.8 mm	$\overline{\sigma}_n$	129±25.8 MPa
R_{max}/R_{min}	1.66	$\overline{\sigma}_s$	516±103 MPa
μ	1	$\overline{\lambda}$	1
E_c	51.5 GPa	$\overline{E}_c$	51.5 GPa
k_n/k_s	4.6	$\overline{k}_n/\overline{k}_s$	4.6

In this table, R_{min} is the radius of smallest sphere before clumping. R_{min} will decrease significantly after clumping as the total number of spheres jumps from 33100 to 132400. R_{max}/R_{min} is the ratio of largest to smallest sphere radii before clumping. μ is the ball friction coefficient. E_c is the ball modulus. k_n/k_s and $\overline{k}_n/\overline{k}_s$ are the normal to shear stiffness ratios for ball and parallel bond respectively. $\overline{\sigma}_n$ is the normal strength of parallel bonds. $\overline{\sigma}_s$ is the shear strength. $\overline{\lambda}$ is the parallel bond radius multiplier. $\overline{E}_c$ is the parallel bond modulus.

Different damage level thresholds for clumped model with parallel bond have been presented in Figure 8. It can be seen that clumping using PFC3D clumping method, could help to decrease the predicted tensile strength and increase the curvature but still the result is not satisfactory as the peak envelope does not line up with Hoek-Brown criterion. For the sake of comparison, Hoek-Brown criterion with standardized “s” (equal to 1) and “a” (equal to 0.5) for intact Lac du Bonnet granite has been drawn in Figure 8.

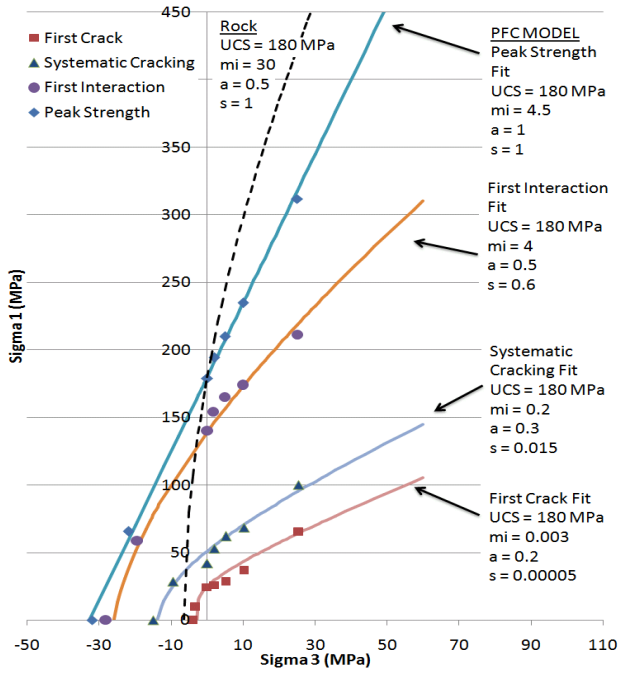

Figure 8. Damage thresholds for clumped model using implemented method of clumping in PFC3D along with best Hoek-Brown envelope fitted (from Ghazvinian and Diederichs 2010).

The principal stress result for Brazilian test in Figure 8 has been calculated based on the relation $\sigma_1 = -3\sigma_3$, but it should be mentioned that interestingly the ratio of the major to minor principal stress in the centre of the disk was measured to be around 4.

As a reason for the unsatisfactory result of clumped model combined with parallel bonding, the clumping method itself can be questioned. In this method, replacing a ball with a clump that has the same volume leads to a colony of clumps with very wide variety of sizes sitting beside each other. This arrangement does not introduce any interlocking resistance to normal or shear loading. Interlock is the key behind the apparent success of the clumping algorithm in PFC2D introduced by Cho et al (2007). Interlocks between the clumps can bear some the load, letting the bonds being calibrated with a lower strength that helps to decrease the predicted tensile strength of the model to a more realistic value.

5 DEVELOPING A NEW METHOD FOR CLUMPING IN PFC

Based on the poor result of implemented method of clumping in PFC, the authors decided to develop a new method for clumping that suits their needs. The authors are of the opinion that with 3D clumps of random shape, interlocks will increase (as seen in the 2D studies of Cho et al. 2007). Interlocks bear some of the applied load in compression and would let the bonds to be calibrated to a lower strength comparing to the time that no clump exist. Low strength bonds can lead to a lower predicted value for the ratio of tensile/compressive strength.

In this method of clumping, the code traverses through all balls in the model which are randomly distributed in the model. For each ball, the code finds the other balls that are surrounding this ball and do not belong to other clumps. If the count of found balls is equal or greater than the specified clump size, then sufficient number of them will be clumped together to make a clump of specified size. If found balls are less than the specified clump size then the code jumps to a ball adjacent to the original ball and finds the balls surrounding this second ball that do not belong to other clumps and again compares the total number of found balls with specified clump size. This will continue for a third adjacent ball in case of not enough balls found. After that, even if the number of found balls is not reaching the desired number, PFC clumps them together. These smaller clumps fill the gaps between bigger clumps. A detailed procedure employed for this method can be seen in Figure 9.

An example for a clumped model using the new method with the maximum clump size of 10 balls has been shown in Figure 10. It can be seen that comparing to the PFC clumping method; how interlocks between the clumps have been increased. In this method each clump has its own random shape rather than a predefined geometry.

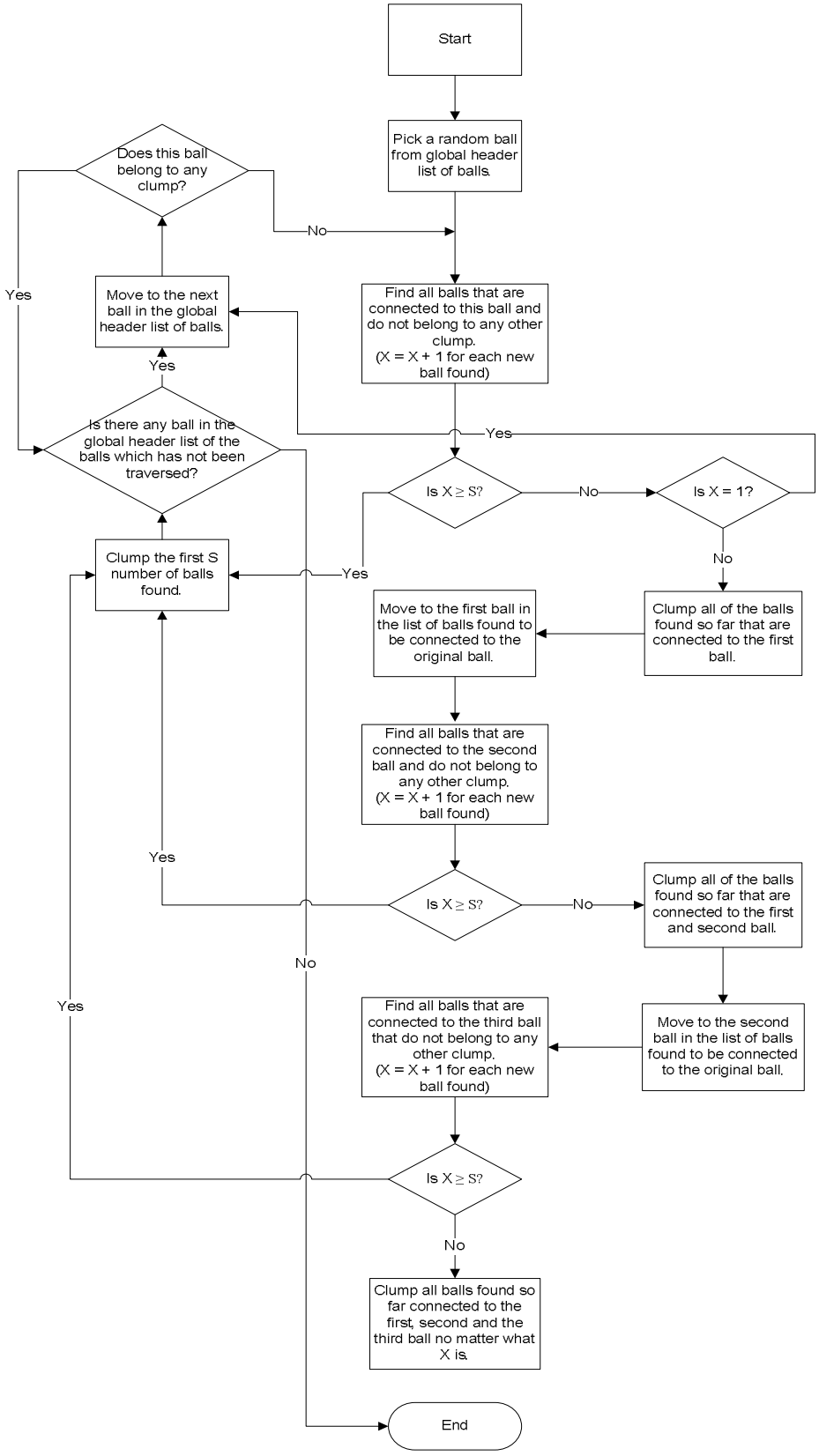

Figure 9. Algorithm showing the procedure of the developed clumping method, (S is the clump size).

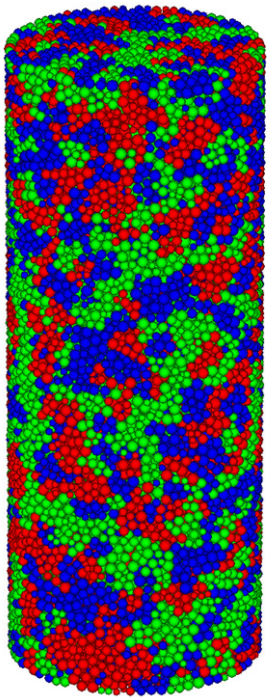

Figure 10. Clumped UCS model using the new developed clumping method shows how interlocks between clumps have been greatly increased.

In Figure 11, distribution of balls for each clump size for the model shown in Figure 10 has been shown. It shows the efficiency of the method in producing the largest number of clumps for the specified size. When the developed code is unable of finding enough number of balls for the desired clump size then it starts of making smaller clumps. As it can be seen this method is producing a uniform distribution of the clumps all over the model. Currently authors are working on other Fish codes that are able to produce different kind of grain size distribution such as bell shape (standard) or bimodal distributions.

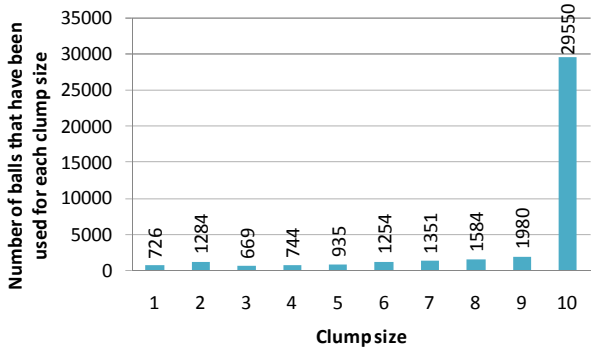

Figure 11. Different clump size distribution in the model.

The Poisson's ratio generated within this model is unrealistically high for the micro-parameter suite selected. It is possible to reduce the Poisson's ratio to 0.25 by decreasing the K_n/K_s ratio for both ball and parallel bond to 0.25. But in this case not a satisfactory result will be achieved in triaxial simulations because, the K_n/K_s ratio of less than one is not fundamentally correct. High Poisson's ratio for this model could have been predicted beforehand as clumps are rigid bodies that are not breakable. So due to axial loading they can only slip and rotate. Slipping and rotation cause empty spaces to form between the clumps and increase the specimen diameter which means an increase in the Poisson's ratio.

6 CLUSTERED MODEL USING THE DEVELOPED METHOD FOR CLUMPING

Authors were of the opinion that clustering can solve the problems associated with clumping due to the rigid bodies. Therefore they came up with the idea of replacing clumps with clusters that are not rigid and cracks can propagate through them. To simulate the weaker intergranular and stronger intragranular bonding, normal and shear strength of bonds within clusters have approximately been set to three times of the magnitude of the shear and normal strength of the bonds between clusters. A schematic view of clustering concept can be seen in Figure 12. In this Figure black bonds are intragrangular and approximately three times stronger than red intergranular bonds.

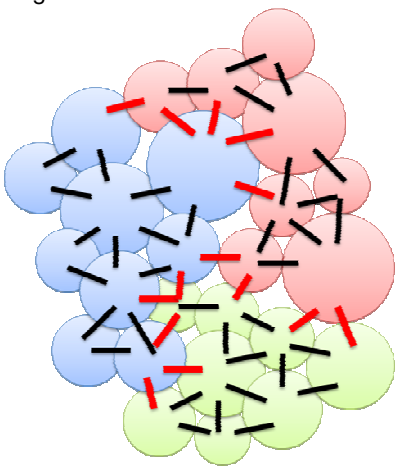

Figure 12. Schematic of clustering in which red bonds are intergranular and black ones are stronger intragranular bonds.

Clustering has been done by developing a Fish code that is traversing through all parallel bonds. If two balls on each end of the bond are in the same clump then the normal and shear strength of the parallel bond will be multiplied by three. This can even be extended for simulating multi-grain samples that bonds in different clumps can be multiplied by different constants. After assigning the new bond properties, balls will be released from clumps constraints. Calibrated parameters for clustered model can be seen in Table 4.

The result of simulations using clustering method can be seen in Figure 13. It can be seen that however the tensile strength of the specimen has been slightly decreased still the peak envelope is not coinciding with

the Hoek-Brown criterion for intact rock. More work is needed to correct this fundamental problem.

Table 4. Calibrated micro-properties for the clustered model using the developed method for clumping.

R_{min}	0.75 mm	$\overline{\sigma}_n$	109.5±27.375 MPa
R_{max}/R_{min}	1.66	$\overline{\sigma}_s$	438±43.8 MPa
μ	1	$\overline{\lambda}$	1
E_c	62 GPa	$\overline{E}_c$	62 GPa
k_n/k_s	3.9	$\overline{k}_n/\overline{k}_s$	3.9

Although there are some other parameters in this method that potentially are able to change the model behaviour. For instance clump size and the ratio of intergranular/intragranular bond strength can be mentioned and authors are working to better calibrate the model behaviour with more emphasis on these key parameters. The authors were unable to replicate in 3D the 2D work of Cho et al (2007).

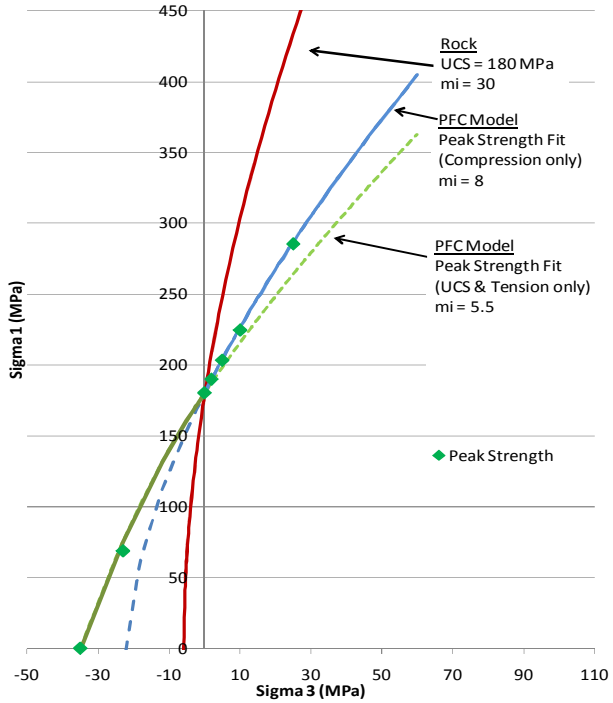

Figure 13. Peak strength envelope for clustered model with best Hoek-Brown envelope fitted.

7 CONCLUSION

Bonded-Particle Model, which works based on Distinct Element Method (DEM), has been developed for direct simulation of crack initiation and propagation in material. This method can be a very helpful means for better understanding of the behaviour of brittle rocks; however still there are some limitations in the application of this method. Particle Flow Code (PFC), available in 2 and 3 dimensions, has been developed based on bonded-particle method. PFC, because of its ability in initiation and propagation of cracks, provides a good opportunity for the study of damage accumulation in brittle rocks. However due to some internal mechanics it lacks the ability of unstable propagation of cracks after initiation. Different methods have been examined in this study for solving the issues associated with PFC3D results by simulating UCS, confined compressive, direct tensile and Brazilian tests.

Authors duplicated Diederichs (2000) work in PFC3D using contact bond. Then PFC method of clumping by replacement has been used with parallel bond. Due to some shortfalls in PFC method of clumping, authors developed their own method for clumping which is able to construct clumps with random geometry. This new method for clumping then has been used for making realistic clustered models with breakable grains. Clustered model seems to be able to provide the desired behaviour but calibrating the clump size and intergranular/intragranular bond strength ratio is pre-requirement.

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