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Development and Testing of a Discrete Element Model of Crushing Sand

by

Matthew Steven Jurgens, B.S.

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Approved by

Supervising Committee:

Kenneth E. Gray

Eric Becker
Dedication

To my family
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Without the love and support of my parents, Ken and Peggy, I could not have possibly accomplished nearly as much. You have taught me the value of hard work, dedication, and believing in myself. I have learned everything I need to be successful in life from both of you.

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Abstract

Development and Testing of a Discrete Element Model of
Crushing Sand

Matthew Steven Jurgens, M.S.E.
The University of Texas at Austin, 2007

Supervisor: Kenneth E. Gray

Crushing sands play a significant role in many oilfield phenomena and applications such as subsidence and compaction, permeability reduction, sand production, and drill bit efficiency. Numerical methods can help to better understand the process of crushing and tailor engineering decisions in which crushing is involved.

This thesis describes the development and testing of a discrete element model of crushing sand. Sand grains are represented by networks of bonded, rigid particles that behave according to simple spring theory at their contacts, and this material is calibrated to the elasticity and statistical strength of quartz grains. Groups of these agglomerates are then inserted into testing cells where they are stressed to observe the macroscopic and grain scale evolution of crushing in hydrostatic and biaxial compression.
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1. INTRODUCTION

Granular crushing is the process of particles in a material breaking into multiple pieces due to an applied load, and is commonly observed in rocks and unconsolidated sands. Studies show that granular crushing is associated with various fundamental granular material behaviors, such as the yield strength in compression (Nakata et al., 2001a), friction and dilation (Bolton, 1986), plasticity (Robertson et al., 2001), and porosity and permeability reduction (Valdes et al., 2006). For these reasons, the need to understand the mechanism of granular crushing is internal to many engineering applications, such as crushing grains for powder (Tsongui et al., 1999), dam settlement (Hoelestit et al., 1965; Sowers et al., 1965), building pile design (Lobo-Guerrero et al., 2005a), oilfield subsidence (Roberts, 1965), estimating permeability reduction of stressed, porous media (Penny, 1986; Penny, 1988; Papamichos et al., 1993), drill bit design, and wellbore stability. To accentuate this importance, it is noted that Tsongui et al. (1999) estimated crushing grains for powder consumes nearly 2% of world energy production.

Naturally, there are inherent difficulties in understanding granular crushing often encountered during studies. First and foremost, the properties and behavior of individual grains in a granular material are difficult to quantify due to their small size, complexity, and geologic variation (Shipway and Hutchings, 1993a; Shipway and Hutchings, 1993b; Takei et al., 2001; Nakata et al., 2001b). The limited number of known relationships are often generalized with statistics due to these unknowns and because large number of grains are usually involved in typical problems (Nakata et al., 2001b; Takei et al., 2001). Second, the relationship between grain scale and sample scale mechanics is unknown,
and it is rarely, if ever, entirely possible to observe the behavior of both scales at the same time within any laboratory experiment. As a result, numerical methods, such as the discrete element model, are commonly used to circumvent these problems by synthesizing large numbers of grain scale bodies into sample scale simulations where behavior can be more thoroughly investigated (Potyondy et al., 2004; Lobo-Guerrero et al., 2005b; Robertson et al., 2001; Tsongui et al., 1999). And furthermore, even though numerical methods are useful in relating grain to rock scale behavior, simulating “grains” with real material properties is often complicated since simplified behavior laws, such as linear spring contacts, must often be used for computational efficiency.

This thesis describes the development and testing of a numerical crushing model developed in PFC$^{3D}$ which can be used to better understand the behavior of soft sediment systems researched by the “Life-of-Well: Rock, Fluid, and Stress Systems” group at the University of Texas at Austin. It is intended that this model be versatile and serve as the foundation for future research on granular crushing in petroleum engineering applications such as sand production, proppant permeability reduction, formation compaction, perforation damage, and drill bit development. In this thesis, a review of particle scale mechanics and several previously proposed numerical crushing models lays the foundation for the development of a version of the agglomerate model, which was first proposed by Robertson et al. (2001). The agglomerate model represents each grain in a rock simulation by a set of bonded, rigid particles in PFC$^{3D}$ that have the same observed material behavior as the rock grain, as defined by calibration tests. These crushable agglomerates can be implemented in any rock simulation by the use of the general extraction and replacement code illustrated in this thesis, which replaces general rigid particles in PFC$^{3D}$ with a crushable agglomerate of desired size, statistical strength, and
elasticity. In essence, the model uses a reductionism approach to move calibration procedures, which are almost always necessary in discrete element modeling, from a rock scale to grain scale.

The agglomerate model in this thesis differs from previously proposed models (Robertson et al., 2001; McDowell et al., 2002; Cheng et al., 2003) since a method of generating and calibrating agglomerates is used that is believed to be more accurate and versatile. This improved method allows for the modeling of grains of different shapes and sizes, which has not been previously accomplished, and still retains all of the useful behaviors of the previously proposed models, such as Weibull statistical distribution of agglomerate strength and correct failure mode. Additionally, it is shown that the new agglomerate modeling method can relatively accurately represent the elastic behavior of a grain, through a comparison to a finite element model of a grain with equivalent elastic properties. No previous author has validated their model’s agglomerate elastic behavior as completely as shown in this thesis. The proposed model is only slightly more complicated than previous models, and it is believed that the gained accuracy outweighs these complications.

The remainder of this thesis is organized as follows:

- **Chapter 2** presents an overview of previous works related to granular crushing that largely focuses on grain scale mechanics and statistics integral to the development of the agglomerate unit cell model, and previous numerical crushing models proposed by authors, such as previous versions of the agglomerate model.

- **Chapter 3** details the contact, slip, and bonding models utilized in the numerical model, PFC\textsuperscript{3D}, to model the interactions of large numbers of individual particles.

- **Chapter 4** presents a new method for modeling a grain in PFC\textsuperscript{3D} by bonding
together sets of PFC particles, which has been termed by other authors as the agglomerate model for a grain.

- **Chapter 5** presents visual and graphical data from hydrostatic and biaxial tests on breakable agglomerates and compares this data to laboratory tests in the literature.

- **Chapter 6** offers a conclusion based on the work of this thesis and direction for future work.

- **Appendices** provide supporting information and algorithms related to the theory and development of the agglomerate model.
2. PREVIOUS WORK

2.1. Three Modes of Crushing

2.1.1. OVERVIEW

Before undertaking a literature review exploring the details of granular crushing, it is advantageous to very quickly review why and how grains tend to break. Therefore, the following three sections broadly define the three accepted modes of grain failure and common causal conditions.

2.1.2. TENSILE FAILURE MODE

Tensile fracture of grains occurs when the tensile strength of the material is exceeded by the tensile stress along a plane and a crack develops perpendicular to the tensile stress (Shipway and Hutchings, 1993b; Shipway and Hutchings, 1993c). It is undeniably the most understood and researched mode of grain failure for geologic grains largely because it is the only mode having an accepted laboratory testing method for a geologic grain (Shipways and Hutchings, 1999a; Shipway and Hutchings, 1993b; Shipway and Hutchings, 1993c; Takei et al., 2001; Nakata et al., 2001b).

Tensile failure is often linked to the coupled conditions of high local grain stresses and poor grain confinement. As Lobo-Guerrero et al. (2005a) points out, this situation simulates a pseudo-Brazilian loading condition (Figure 2.1), which laboratory tests have shown to largely produce vertical tensile failure of grains (Takei et al., 2001). Obviously, any location within a rock or sand sample can produce these conditions;
however, certain locations tend to be more prone to high stresses and poor confinement. For example, grains near walls of loading platens (Lobo-Guerrero et al., 2005b; Valdes et al., 2006; Yamamuro et al., 2005), next to building piles (Lobo-Guerrero et al., 2005a), or within granular force chains, or chains of grains absorbing a greater proportion of the rock sample’s loading stress (Karner et al., 2006), tend to experience more crushing, and particularly tensile crushing.

The first condition of high stresses on a grain, high defined by material tensile strength, is a necessary condition for tensile grain failure, whereas poor confinement tends to be more of a sufficient condition, since confinement only serves to counteract the tensile stresses developing in the grain (Tsongui et al., 1999). So for tensile crushing to occur, it seems that the grain should be in a compromised geometric location, such that the grain is absorbing a greater proportion of the total load in the rock sample (Lobo-Guerrero et al., 2005a; Karner et al., 2006), or there must be high global stresses within the rock sample so that most grains are experiencing high stresses. Therefore, we expect localized tensile crushing in the former case and large amounts of tensile crushing in the latter case, since it seems very possible that many grains in the latter case would, at some point, also satisfy the sufficient condition of poor confinement and break under our simplified model. Nakata et al. (2001a) clearly illustrates this effect with one-dimensional compactions tests of samples of silica sand that had embedded colored grains. They note that a small, localized amount of major tensile splitting occurs at vertical stress levels lower than 10 MPa, and probably not until closer to 20 MPa, and at these lower stress levels crushing is found to be isolated to the edges of the grains and potentially occurs due to other failure modes, such as shear or abrasion. At higher stresses, more tensile crushing occurs and is more widespread in the sample.
Consequently, it seems necessary to generate high stresses throughout the rock sample in order to view large amounts of tensile crushing. Yet, Li and Holt (2002) point out that high stress laboratory tests, where high stress could be thought of as a vertical loading stress on a rock sample, can only be performed under confined conditions, such as hydrostatic or one-dimension compaction tests. Without confinement, shear failure occurs prematurely, as evidenced by formation of shear bands (Li and Holt, 2002), and stresses will not reach the “high” level necessary for large amounts of tensile crushing. In essence, shearing acts as an alternate stress release mechanism and prevents large amounts of tensile failure from ever occurring.

![Illustration of tensile failure](image)

Figure 2.1. Illustration of tensile failure: the orange particle is poorly confined and subjected to a pseudo-Brazilian load located along the tensile crack axis. The blue particle is well-confined and therefore is less likely to crush in the tensile mode even though it may be under high grain stress.

### 2.1.3. Shear Failure Mode

Likewise, shear fracture in grains occurs when the shear strength is exceeded by
the shear stress along a plane causing translation in the direction of the shear stress (Shipway and Hutchings, 1993a; Shipway and Hutchings, 1993b). Unfortunately, the number of shear strength studies on geologic grains pales in comparison to number of tensile strength studies, and there isn’t a widely accepted testing method for measuring the shear strength of geologic particles. As a result, the geologic particle shear strength information in this thesis is incomplete.

Nevertheless, it is quite obvious that more shear failure will occur in particles with higher internal shear stresses, as can be evidence by observing the basis of any empirical shear failure criterion for materials, such as the Tresca (Shipway and Hutchings, 1993a) or Mohr-Coulomb failure criterions (Terzaghi, 1948). The distinct difference between various shear failure criterions is the extent to which the normal stress acting on the plane is considered, which increases the frictional resistance to sliding and the apparent shear strength.

Therefore, it is reasonable to believe that testing conditions producing large offset, parallel loads will cause more shear crushing. This condition can occur locally within a rock for any number of geometric reasons. For example, experiments on quartz sands show large amounts of asperity and edge breakage throughout the sample (Takei et al., 2001). Although the failure method in these experiments is not specifically indicated, it seems possible that this breakage could be associated with shear (Figure 2.2). This is the most common type of failure observed in quartz grains (Takei et al., 2001), and is possible to attribute this to the non-spherical geometry of the quartz grains tested. Larger shear stresses can also be induced due to controllable testing conditions. For example, if a rock sample is subjected to large, macroscopic deviatoric stresses, which would produce large shear stresses in a theoretically continuous material, it is expected that
larger shear stresses will also occur on a grain scale level and cause increased crushing. Li and Holt (2002) note that shear bands occur in laboratory tests with high deviatoric stresses, and it is likely that these bands are associated with shear, rather than tensile, crushing.

In the lone particle shear strength study found for this thesis, high velocity particle impact tests are shown to produce “cone cracking” along the boundary of particles, and is attributed to shear failure as the theoretical maximum shear stress is calculated to be relatively constant in all tests (Shipway and Hutchings, 1993b). Unfortunately, this only proves that shear stress is correlated to shear failure, but does not validate or disprove any shear failure criterion or give accurate values for shear strength. Under different loading conditions, such as confined loading, it is very possible that the maximum observed shear stress would be much different than that observed for impact tests due to a varying contribution to strength from Coulomb friction.

Instead of defining an absolute value for shear strength of geologic particles, it is more advantageous to simply try and ascertain if the shear strength of a material is higher or lower than the tensile strength. By comparing compressive strength data for rock grade quartz to fused quartz, for which the shear strength is known, the author believes that the shear strength of rock grade quartz will be at least as large as its tensile strength (Sosman, 1926; Goodfellow, 2007), and it is possibly closer to 1.5 times as great.
Figure 2.2. Illustration of shear failure: the orange particle’s corner is failing in shear mode due to the application of a transverse load across its protruding edge. This type of failure does not usually result in catastrophic grain damage.

2.1.4. ABRASIVE FAILURE MODE

Unlike the tensile and shear failure modes, abrasive failure tends to correlate to work performed on the particle surface rather than a stress function surpassing a limit. Difficulties in measuring such a parameter in a laboratory experiment confine grain abrasion studies to numerical methods.

Jensen et al. (2001) illustrates a model for granular shear tests using clusters of bonded particles that can break from each cluster after a prescribed amount of work is performed on its surface. The defining amount of work characterizing the particle release point is calibrated until the simulation obtains similar results as laboratory shear tests. The general graphical trends produced by this model appear valid and pinpoint abrasion as a significant factor in the development of shear zones in granular materials.

In light of the correlation to work, it is reasonable to assume that abrasion would be more common in large displacement processes, such as in pile driving or shear tests.
(Figure 2.3). Nevertheless, it is difficult to quantify abrasion, or even to completely separate the mechanism of abrasion from tensile and shear cracking.

![Illustration of abrasive damage](image)

Figure 2.3. Illustration of abrasive damage: the particles along the moving boundary are subject to larger amounts of sliding work as the platen grinds the top surface and causes them to roll. Grain movement decreases further from the boundary.

### 2.2. Quantifying Grain Scale Behavior

#### 2.2.1. Overview

The list of variables that have been used to quantify grain scale mechanics is lengthy. Fundamentally, crushing is a function of grain stress, strength, and stress path (Lade et al., 1996); however, due to complexities in defining these variables many other empirical variables are often used. The goals of Section 2.2 are to provide a basis in theoretical grain scale mechanics and illustrate how empirical variables are often
incorporated to compensate for unknowns. The theories from Section 2.2 lay the groundwork for the development of the unit cell agglomerate model in Chapter 4.

It is noted that there are other theories and variables related to quantifying rock scale crushing in laboratory tests; however, these theories are not directly covered in this thesis because the discrete element model is used to bypass the grain scale to rock scale relationship.

### 2.2.2.** GRAIN STRESS DISTRIBUTION**

As emphasized in Section 2.1, internal grain stress is important in predicting the moment and mode of failure (Tsongui et al., 1999; Khanal et al., 2005). It is well known that grain stress is a function of the grain’s material properties and the way in which the grain is loaded. However, defining this relationship is not trivial, and our current understanding of grain stress distribution is largely derived from the simplifying law of linear elastic mechanics (Shipway and Hutchings, 1993a; Tsongui et al., 1999; Timoshenko and Goodier, 1970).

The most common way of calculating a material’s elastic properties is to stress the material in some fashion, observe the response, and then calculate the material properties that cause such a response using the law of linear elasticity (Timoshenko and Goodier, 1970). Two common assumptions of homogeneity and isotropy are often invoked in order to simplify the measurements and calculations, and ultimately reduce the number of unique material properties to two. The first assumption of homogeneity states that material properties do not vary with position, and the second assumption of isotropy states that material properties are non-directional. Based on these assumptions, the most commonly calculated material properties are known as Young’s modulus and Poisson’s ratio, although there could be other sets.
It is immediately apparent that there are problems with this method of property measurement and the commonly invoked assumptions. For example, some grains are composed of multiple minerals and therefore it is likely that the properties vary from point to point, resulting in a non-homogeneous material (Takei et al., 2001; Nakata et al., 2001b). Additionally, it is certain that imperfections exist in geologic materials (Shipway and Hutchings, 1993a) and this can cause properties to vary directionally. Furthermore, it is obvious that designing an apparatus to deform a grain and measure its elastic properties is problematic. For example, it is often necessary to cut grains into specific shapes for testing (Levien et al., 1980), and it is possible that this cutting modifies the properties of the material or that the cut section is not representative of the entire sample. Nevertheless, this elasticity measurement technique and associated assumptions is often the best method practical.

Table 2.1 summarizes some of the data collected on elastic properties of quartz for this study.

Table 2.1. Values of Young's modulus and Poisson's ratio of quartz from various authors.

<table>
<thead>
<tr>
<th>E (GPa)</th>
<th>ν</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>89.5 – 101.5</td>
<td>0.041 – 0.112</td>
<td>Simmons and Wang (1971)</td>
</tr>
<tr>
<td>78.5 - 102.8</td>
<td>not available</td>
<td>Sosman (1927)</td>
</tr>
<tr>
<td>103 (Graph)</td>
<td>0.119 – 0.13</td>
<td>Cady (1946)</td>
</tr>
</tbody>
</table>

In the absence of more precise data, simple uniaxial compressive tests of grains, illustrated in Figure 2.4, can provide insight into the stiffness of different materials through the calculation of the uniaxial compression modulus, $E_p$ (Takei et al., 2001):
\[ E_p = \frac{\sigma_p}{\varepsilon_a} \] ...........................................................(Eq. 2.1)

where:
\[
\sigma_p = \frac{F}{\frac{1}{4}\pi d^2} \] ...........................................................(Eq. 2.2)
\[
\varepsilon_a = \frac{d - L_f}{d} \] ...........................................................(Eq. 2.3)

where \( F \) is the force acting on the grain of initial diameter, \( d \), that has deformed to a new height of \( L_f \), which is in the direction of loading.

The uniaxial compressive modulus can be thought of as being related to Young’s modulus, but only valid for the uniaxial compressive test since it also depends upon geometry of the material and loading condition. The benefit of knowing this simple parameter is that it can be used for quick, or additional, calibration. Although quite variable, values for the uniaxial compressive modulus for quartz are on the order of \( 1e9 \) Pa (Takei et al., 2001; Nakata et al., 2001b).

Once suitable material properties are determined, it is possible to calculate the theoretical stress distribution for various loading conditions, such as for the simple uniaxial compression test of a grain (Shipway and Hutchings, 1993a). Figure 2.4, Figure 2.5, and Figure 2.6 show the axisymmetric, elastic solution calculated by ABAQUS, a commercially available finite element model, for a sphere subjected to a vertical load. It can be seen from these figures that the maximum tensile and shear stresses occur at the center and near the platens, respectively. This justifies the visual observation of vertical tensile failure through the center of the grain in uniaxial compression (Takei et al., 2001; Nakata et al., 2001b; Shipway and Hutchings, 1993c) with occasional cone cracking, due to shearing, near the platens.
Figure 2.4. Stress in the theta direction (hoop stress) for the Hertzian solution of a sphere subjected to uniaxial compression: the colored areas signify tension with the maximum tension in the center and reducing toward the horizontal edges. The top and bottom of the sphere is in compression.
Figure 2.5. Stress in the radial direction for the Hertzian solution of a sphere subject to uniaxial compression: the tensile stress is maximum at the center and moves to compression along the boundaries. Maximum tensile stresses in the radial and theta directions are the same.
Figure 2.6. Shear stresses for Hertzian solution of a sphere subject to uniaxial compression: maximum shear stress is near the platens in the red and blue colored regions.

The previous stress distribution figures are helpful for understanding grain failure in laboratory tests, but do not help understand grain failure within a rock. In a rock, the loading configuration on a grain is much different than in uniaxial compression and it is imprudent to expect a similar grain failure method. Therefore, several empirical variables will be illustrated that take into account different loading conditions, and can be calibrated based on laboratory experience.

The simplest empirical stress parameter is the coordination number (Figure 2.7), which is the number of grains that are in contact with any grain of interest (Nakata et al.,
Although use of this parameter is often restricted to numerical methods since it is usually difficult to define how many grains are touching any particular grain, Nakata et al. (2001b) provides an estimate of coordination number in a granular sample based on void ratio defined as:

\[
C = \frac{12}{1 + e}
\]  

(Eq. 2.4)

where \( C \) is the coordination number and \( e \) is the void ratio of the granular sample.

It is believed that the coordination number should increase confinement of a particle, resulting in a decreased internal tensile stress (Tsongui et al., 1999) and shear stress as the loading condition approaches hydrostatic. The downfall of the coordination number is that it doesn’t take into account the magnitude of loading provided by each confining grain. Consider a confinement grain that is not in a critical geometric location or has a low level of contact force with the grain of interest; it is obvious that it will not contribute significantly to confinement.

Figure 2.7. Coordination number: defined as the number of particles that are touching any given particle. In this case, the coordination number is 4 for the central particle.

Instead, the average stress tensor for the grain subjected to an arbitrary number of loads, \( N \), is a more accurate method of quantifying confinement, and is defined as
(Tsongui et al., 1999; Itasca, 2005a):

\[ \bar{\sigma}_{y} = \frac{R}{V_p} \sum_{c=1}^{n_i} n_i^{(c)} F_j^{(c)} \]  

(Eq. 2.5)

where \( \bar{\sigma}_{y} \) is the average stress tensor, \( R \) is the radius of the grain, \( V_p \) is the volume of the grain, \( n_i \) is the unit normal vector directed from the grain center to contact point, and \( F_j \) is the force vector acting at the contact point (Figure 2.8).

![Diagram](Figure 2.8. Orientations of vectors for average stress tensor calculations: unit normal is directed from particle center to contact of interest.)

It is emphasized that this tensor is the average tensor for the grain, accurate to the first order, and not the actual tensor at any point within the grain.

It is apparent that there are many possible ways to use this tensor for comparison of relative stress levels within the grain under different loading conditions. One particular method uses the average stress tensor to approximate the maximum tensile stress that is occurring within the center of the grain (Tsongui et al., 1999). First, the eigenvalues of the stress tensor in 2-D yield the principle stresses as:

\[ \bar{\sigma}_{\text{max, min}} = \frac{\sigma_{xx} + \sigma_{yy}}{2} \pm \sqrt{\left( \frac{\sigma_{xx} - \sigma_{yy}}{2} \right)^2 + \sigma_{xy}^2} \]  

(Eq. 2.6)

where \( \bar{\sigma}_{\text{max, min}} \) are the average maximum and minimum principal stresses, and \( \bar{\sigma}_{xx}, \bar{\sigma}_{yy}, \) and \( \bar{\sigma}_{xy} \) are the average stresses from the average stress tensor.

With the principle stresses known, it is possible to approximate the tensile stress in the
center of the grain by summing the contribution of each principle stress (superposition).
This tensile stress is only an estimate, since the central stress in the grain induced by each
principle stress will be slightly non-linear due to the spherical geometry. For the two
dimension problem, Tsongui et al. (1999) estimates the tensile stress, $\sigma_{xx}$, as:
$$\sigma_{xx} = \frac{\sigma_{\text{max}} - 3\sigma_{\text{min}}}{2}$$
(Eq. 2.7)
This equation illustrates that confinement, introduced by the $\sigma_{\text{min}}$ term, reduces the tensile
stress in the center of the grain.

The previous discussion on stress distribution has been limited to the assumption
of spherical grains, but it is well known that spherical grains rarely, if ever, exist in rocks.
Therefore, it is advantageous to quantify the extent that the physical shape of the grain
will affect the stress distribution. This is difficult since there are infinite numbers of
possible grain shapes, and simple geometric variables are often used to simplify
quantification. The most common geometric variable is angularity, which describes the
relative roundness of a grain when compared to a perfect sphere (Nakata et al., 2001b):
$$R = \frac{P^2}{4\pi A}$$
(Eq. 2.8)
where $R$ is the measure of roundness, $P$ is the perimeter of the grain, and $A$ is the 2-D
measured area of the grain.
This measure is simply the ratio of the true perimeter of the grain to the perimeter of a
perfect sphere. Noting this, it is apparent that other measures of angularity could also be
used, for example the ratio of the maximum principal radius to the average radius.

In general, increasing angularity causes an increase in the amount of crushing.
For example, angular quartz grains are observed to have more edge collapse than more
spherical grains in 2-D compaction tests observed through a clear testing apparatus
(Takei et al., 2001) and pre and post-crushing sieve samples of sand reveal more fines
production from more angular particles (Lee and Farhoomand, 1967; Figure 2.9). Additionally, Nakata et al. (2001b) shows that more angular grains have higher variability in crushing strength. All of these observations are likely due to variations in loading conditions induced by the angularity of the grains.
Figure 2.9. Affect of angularity on crushing evolution: larger amount of crushing observed in angular particle versus subrounded particle samples (Modified from Lee and Farhoomand, 1967).
2.2.3. **GRAIN STRENGTH**

As stated in Section 2.1.2, the uniaxial compressive test is the only widely accepted test for measuring grain strength. In this test, the grain generally fails vertically through the central, maximum tensile stress region, with this tensile stress given as (Nakata et al., 2001b; Shipway and Hutchings, 1993b; Takei et al., 2001):

\[
\sigma_p = \frac{F_p}{\frac{1}{4} \pi d_c^2}
\]

...(Eq. 2.9)

\[
d_c = \frac{d_1 + d_2 + d_3}{3}
\]

...(Eq. 2.10)

where \(\sigma_p\) is the characteristic tensile stress on the grain, \(F_p\) is the force applied through the opposed platens crushing the grain, and \(d_c\) is the characteristic grain diameter often defined by averaging the maximum, \(d_1\), intermediate, \(d_2\), and minimum diameter, \(d_3\), of the grain.

It is recognized that there are many issues that can cause Eq. 2.9 to be inaccurate. For example, variations in loading due to grain angularity (Nakata et al., 2001b), platen stiffness (Shipway and Hutchings, 1993b), varying material properties (Takei et al., 2001), or flaws in the material (Shipway and Hutchings, 1993a) render the assumptions of spherical grain, rigid platens, homogeneity, isotropy, and linear elasticity invalid. In these situations, the true maximum tensile stress and distribution is likely different than predicted. Even so, it is generally accepted that this test provides reasonably consistent measurements as long as the failure mode is primarily tensile (Shipway and Hutchings, 1993c; Takei et al., 2001; Nakata et al., 2001b).

Many authors have concluded that the characteristic tensile strength for large numbers of similar particles is generally described by Weibull probability distribution (Takei et al., 2001; Nakata et al., 2001b; Robertson et al., 2001; McDowell et al, 2002;
Harireche and McDowell, 2003; Cheng et al., 2003). The Weibull probability distribution is a statistical survival function that relates the probability of a grain surviving a stress characteristic of failure (Takei et al., 2001):

\[
P(d) = \exp \left( -\frac{d}{d_0} \frac{\sigma}{\sigma_o}^m \right) \text{……………………………………………………} \text{(Eq. 2.11)}
\]

where \( P(d) \) is the probability of a grain of diameter \( d \) survives the characteristic stress of \( \sigma \), \( d_0 \) is the characteristic diameter of the sample of grains such that 37% survive the characteristic stress of \( \sigma_o \).

Several key points are helpful in understanding the Weibull probability distribution. First, the base set parameters, \( d_0 \) and \( \sigma_o \), are approximately equal to the strength and diameter of the grain that has the mean strength of the sample (McDowell et al., 2002). Second, the Weibull modulus, \( m \), is a measure of material variation in strength. For example, manufactured granular materials with little variation in strengths have a high Weibull modulus, possibly near 10, whereas geologic materials with large variation in strength have a low Weibull modulus, such as 3-5 (Takei et al., 2001; Nakata et al., 2001b). Lastly, the size weighting term, \( d/d_0 \), specifies that smaller grains have a larger mean strength compared to larger grains, which is commonly accepted (Takei et al., 2001; Nakata et al., 2001b).

Figure 2.10 illustrates the shape of the Weibull probability distribution and Table 2.2 lists typical Weibull variables for several materials.
Figure 2.10. The Weibull probability density function: models the variation of strength in grains. Note how the higher Weibull modulus has less variability in strength.
Table 2.2. Weibull variables from the literature for several materials.

<table>
<thead>
<tr>
<th>Material</th>
<th>m</th>
<th>$\sigma_0$ (MPa)</th>
<th>$d_o$ (mm)</th>
<th>diameters tested (mm)</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chalk Bars</td>
<td>7.5</td>
<td>0.68</td>
<td>Not given</td>
<td>0.85 - 2.0</td>
<td>Takei et al. (2001)</td>
</tr>
<tr>
<td>Tale Bars</td>
<td>4.5</td>
<td>0.917</td>
<td>Not Given</td>
<td>0.85 - 2.0</td>
<td>Takei et al. (2001)</td>
</tr>
<tr>
<td>Glass Beads</td>
<td>8</td>
<td>330</td>
<td>Not Given</td>
<td>0.85 - 2.0</td>
<td>Takei et al. (2001)</td>
</tr>
<tr>
<td>Quartz Grain</td>
<td>3</td>
<td>31</td>
<td>Not given</td>
<td>1.3 - 1.9</td>
<td>Takei et al. (2001)</td>
</tr>
<tr>
<td>Quartz Grain</td>
<td>2</td>
<td>18</td>
<td>Not given</td>
<td>2.7 - 3.3</td>
<td>Takei et al. (2001)</td>
</tr>
<tr>
<td>Silica</td>
<td>3.04</td>
<td>30.96</td>
<td>Not given</td>
<td>1.4 - 1.7</td>
<td>Nakata et al. (2001b)</td>
</tr>
<tr>
<td>Silica</td>
<td>2.17</td>
<td>72.87</td>
<td>Not given</td>
<td>0.6 - 0.71</td>
<td>Nakata et al. (2001b)</td>
</tr>
<tr>
<td>Silica</td>
<td>1.82</td>
<td>110.87</td>
<td>Not given</td>
<td>0.25 - 0.30</td>
<td>Nakata et al. (2001b)</td>
</tr>
<tr>
<td>Glass</td>
<td>5.90</td>
<td>365.80</td>
<td>Not given</td>
<td>0.85 - 1.0</td>
<td>Nakata et al. (2001b)</td>
</tr>
</tbody>
</table>

2.2.4. **GRAIN STRESS PATH**

Even if stress distribution and strength of a grain for general loading conditions can be described, further complications arise due to changes in the stress path and time dependency of crushing (Takei et al., 2001). DEM models of fracturing agglomerates indicate that micro-fractures and asperity damage are generated at various locations in the grain body throughout loading before coalescing and forming a large fracture (Robertson et al., 2001; Khanal et al., 2005). This micro-cracking causes repeated loading/unloading which changes the stress path, loading, and causes fatigue. Additionally,
loading/unloading behavior also occurs in granular samples as particles move and reposition. Repositioning is probably responsible for observation of continued strain (Terzaghi and Peck, 1948) and “popping of grains” (Lee and Farhoomand, 1967) without additional load in sand. Therefore, it is likely that the stress path is very rarely linear in most cases of grain loading. Analytically modeling non-linear stress paths in granular samples is difficult, and therefore we can only be aware that they exist and use numerical methods to overcome their difficulties.

2.3. Previous Numerical Crushing Models

2.3.1. Overview

Numerical methods are well equipped for handling crushing problems. Numerical crushing models predefine the crushing behavior of small elements or regions empirically and then utilize the numerical model to synthesize these elementary units into larger, full-scale simulations. Through this reductionism method, reasonably accurate simulations of driven piles (Lobo-Guerrero et al., 2005a), laboratory shear tests (Lobo-Guerrero et al., 2005b; Jensen et al., 2001), laboratory hydrostatic tests (Cheng et al., 2003), and isotropic, cyclic loading in laboratory tests (Harireche and McDowell, 2003) in granular media has been performed. Nevertheless, the exact methods of each crushing model vary and have considerable differences in capabilities, accuracy, and computational speed, though no available study has directly compared any two sets of models. Several of these models will be discussed in the remainder of Chapter 2.
2.3.2. Lade’s Method

A model by Lade et al. (1996) incorporates an empirical relationship for crushability of sand samples into finite element simulations. Their study of Cambria sand compaction illustrates that a parameter termed “breakage factor” varies predictably with increasing energy input regardless of the materials initial packing arrangement (Figure 2.11).

![Figure 2.11. Correlation of breakage factor to input energy: best fit curve of data is shown to be hyperbolic (modified from Lade et al. 1996).](image)

The breakage factor, which generally describes the size distribution of grains in the laboratory sample, is defined as:

\[ B_{10} = 1 - \frac{D_{10f}}{D_{10i}} \]  

(Eq. 2.12)

where the \( D_{10} \) value is the grain size such that 10% of particles are finer and it is measured at the initial, i, and final, f, parts of the test.
Permeability can then estimated from this breakage factor since the $D_{10}$ grain size is related to permeability, $k$, in empirical equations such as (Lade et al., 1996):

$$k \approx 100D_{10}^2$$

(Eq. 2.13)

This relationship can be incorporated into finite element simulations in order to modify the permeability at each element according to energy input. Lade’s method is computationally inexpensive and realistically applicable to large scale problems; however, it largely relies upon laboratory data that is relatively unavailable in the literature for most materials and time consuming to measure.

2.3.3. DEM AGGLOMERATE MODEL

Other models attempt to reproduce the behavior of individual grains. One such model, the agglomerate model (Robertson et al., 2001; Cheng et al., 2003; McDowell et al., 2002) models the grain by a set of particles held together by bonds (Figure 2.12).

![Figure 2.12. Model of agglomerate: balls interact based on springs and are bonded together at the contacts with bonds of finite strength (from Cheng et al., 2003)](image)

In the model, the contacts between balls behave as linear springs and the bonds have a finite value of strength (discussed in further detail in Chapter 3). Obviously, there is no direct relationship between the material properties of the real grain and this simplified model (Potyondy, 2004), so the spring properties are calibrated through a
series of tests to quantify agglomerate behavior. This modeling method is essentially like modeling material behavior with an artificial, yet similarly behaving material.

It is apparent that more calibration results in a better agglomerate model. In the aforementioned author’s models, the agglomerate is calibrated to the uniaxial compressive strength and elastic modulus of laboratory tests (Eq. 2.1, Eq. 2.2). Additionally, a method of removing elemental particles in the agglomerate is utilized to induce a Weibull statistical distribution of strength.

This model is particularly useful because it allows for the direct study of grain scale mechanics, including all three modes of fracture, and the potential development of better material models. Additionally, sets of agglomerates can be modeled together and simulate granular materials. There are significant drawbacks; however, such as failure to conserve mass, permeability of agglomerates, and unrealistically rough agglomerate boundaries. Other specific issues with the previous agglomerate models are the failure to verify the accuracy of agglomerate elastic behavior, and inability to model sets of agglomerates with varying size.

2.3.4. DEM REPLACEMENT MODEL

In an aim at increased computational efficiency over the agglomerate model, other authors use failure criterions to determine when a grain should break within a discrete element simulation and then modify the grain to account for damage. Three proposed failure criterions will be discussed in more detail.

The first failure criterion predicts tensile failure by approximating the stress in poorly confined grains by a pseudo-Brazilian condition (Lobo-Guerrero et al., 2005a; Lobo-Guerrero et al., 2005b). Specifically, if the coordination number of the grain, C, is less than 3 and the stress defined by Eq. 2.9, $\sigma_{\text{max}} (r)$, exceeds the strength, $\sigma_{\text{critical}} (1\text{mm})$, 30
of an arbitrary sized grain, in this case 1 mm, the grain breaks:

\[
\text{If } C < 3 \\
\text{If } \sigma_{\text{max}}(r) > \frac{\sigma_{\text{critical}}(1\text{mm})}{r} \\
\text{then break particle} \quad \text{.................................................................(Eq. 2.14)}
\]

End If
End If

where \( r \) is the radius of the grain under consideration.

The second failure criterion utilizes the average stress tensor of a grain (Eq. 2.5) to approximate the tensile stress within the grain, \( \sigma_{xx} \) (Eq. 2.7) (Tsongui et al., 1999). The failure strength of the particle, \( \sigma_{\text{critical}}(R) \), is then calculated through the Weibull function based on predetermined data and the grain radius, \( R \), and if this value is exceeded by the value from Eq. 2.7, the grain breaks:

\[
\text{If } \sigma_{xx} \text{ (Eq. 4.2)} > \sigma_{\text{critical}}(r) \\
\text{then break particle} \quad \text{.................................................................(Eq. 2.15)}
\]

End If

The third failure criterion relates work input/volume, \( W_i \), and volume, \( V_i \), of a grain number, \( i \), to a work failure limit, \( W_i^{\text{max}} \) at which an elemental particle within an agglomerate should break from the main agglomerate body (Jensen et al., 2001):

\[
\text{If } W_i V_i > W_i^{\text{max}} \\
\text{then break particle} \quad \text{.................................................................(Eq. 2.16)}
\]

End If

Unlike the agglomerates in Section 2.3.3., the agglomerates in Jensen’s model are bonded together with infinite strength and only release individual particles upon exceeding the failure criterion described by Eq. 2.16.

All DEM replacement models require some sort of replacement scheme for the grain once it has reached the failure criterion. One particular 2-dimensional replacement scheme is shown in Figure 2.13.
Figure 2.13. Replacement scheme for Lobo-Guerrero et al. (2005a), Lobo-Guerrero et al. (2005b), and Tsongui et al. (1999): the 2-D grain is replaced with 8 fragment particles.

It is apparent that DEM replacement models are computationally less expensive and conserve mass better than the agglomerate models of Section 2.3.3, since not all particles will break in the simulation. However, the failure criterions are largely empirical and only model one mode of failure.
3. DISCRETE ELEMENT METHOD

3.1. Overview

The discrete element method models the interaction of individual particles based upon a simplified contact and bonding criterion at the point of contact. Fundamentally, the overall behavior of the discrete element artificial-material is comparable to the real material because the micro-mechanisms, rather than micro-properties, mimic that of the real material (Itasca, 2005b). It is apparent that the uses of such a model in geomechanics are varied in both type and size (Park, 2006): ranging from modeling earthquakes to the fracture toughness of materials. In this thesis, PFC\textsuperscript{3D} (Itasca, 2005a), a commercially available discrete element code, is used. The proprietary particle tracking routine and utilization of explicit time stepping allow PFC to model the interactions of a large number of particles relatively efficiently, with additional efficiency gained through simplifying assumptions, such as simple contact criterions and rigid particles.

A basic knowledge of PFC\textsuperscript{3D} theory is useful in understanding many of the details within Chapters 4 and 5. Therefore, the contact, slip, and bonding model physics are discussed in brevity in the remaining sections of this chapter to aid in further discussion. Additionally, more detailed information is available in Appendix A: Additional Information Regarding PFC Physics, or in Potyondy (2004) or Itasca (2005a).
3.2. Contact Model

The contact model describes the interaction of two particles (particle is an element in PFC) or particle and wall (wall is a flat surface in PFC) that come into contact and are not bonded together. In PFC, the contact model is based upon spring theory where the interaction of two particles, or a particle and a wall (walls do not interact with each other), is modeled by the interaction of two springs that can generate normal and shear forces depending on the amount of normal and shear compression that has occurred at the contact, respectively (Figures 3.1, 3.2, and 3.3). Two springs in series comprise each contact, and the resultant contact stiffness, $K_R$, is given by the series stiffness law as:

$$K_R = \frac{K_1 K_2}{K_1 + K_2}$$

(Eq. 3.1)

where $K_1$ and $K_2$ are the stiffnesses assigned to each particle or wall in the contact.

Figure 3.1. Total contact model: normal resultant spring acts in the direction of the normal unit vector, $N$, directed in the line connecting the particle centers while shear resultant spring acts in the direction of shear unit vector, $S$, perpendicular to the normal unit vector.
Figure 3.2. Normal contact model: each particle contributes a spring at the contact, and the two springs act in series. The amount of compression is defined by the overlap, $U$, of the particles.

Figure 3.3. Shear contact model: each particle contributes a spring in the shear direction at the contact, and the two springs act in series. The amount of compression of the series springs is defined by $\Delta U_s$, which is the movement in the shear direction over the last calculation cycle.

The normal and shear springs at a contact behave in the exact same manner as described through the simple spring law, $F = Kx$, where $F$ is the force developed in a spring with stiffness, $K$, that is compressed a distance $x$. The main difference in
calculation of the normal and shear spring’s forces is method in which the apparent compression distance, x, is calculated. For the normal spring, the compressed distance is equal to the distance that the particles overlap (Figure 3.2). This overlap, \( U \), can be calculated based upon geometry alone at each calculation cycle according to the formula:

\[
U = 2R - d ~ \text{.................................................................(Eq. 3.2)}
\]

where \( R \) is the radius of two particles and \( d \) is the distance between the particle centers. Alternatively, the shear springs compressed distance is calculated by tracking the cumulative distance moved in the shear direction (perpendicular to the normal direction) throughout the history of the contact (Figure 3.3). Unfortunately, this cannot be calculated by geometry alone, as in the normal spring case, since it depends on the history of movement.

It is often helpful to use simple examples to aid in understanding the contact model and how it relates to macroscopic properties, which are generally of interest. For example, consider the example of an infinite cubic pack which could be representing some arbitrary material of interest (Figure 3.4). It is possible to examine a unit cell of this material, defined by the rectangular area containing 4 springs in Figure 3.4, and calculate the resultant spring stiffness, \( K_R \), using simple series and parallel spring laws as:

\[
K_R = \frac{1}{\frac{1}{K} + \frac{1}{K} + \frac{1}{K} + \frac{1}{K}} = K ~ \text{.................................................................(Eq. 3.3)}
\]

where \( K \) is the resultant series stiffness at any contact between any two balls. It is apparent that the resultant stiffness of the infinite pack is equal to the stiffness at any contact. Conveniently, this greatly simplifies the problem conceptually – instead of looking at the material as a large set of particles, it is possible to generalize the pack behavior from one contact.
Figure 3.4. Cubic pack of material: each contact can be representing by a single spring with stiffness equal to the resultant stiffness of the series contact of the two particles.

Now imagine that the cubic packed PFC material is actually representing a continuous material. It can therefore be said that the contact between any two given particles is representing a square section of the continuous material (Figure 3.5), and considering this square section, Young’s modulus, \( E_{\text{cubic}} \), for the material is simply calculated as:

\[
E_{\text{cubic}} = \frac{\sigma}{\varepsilon} = \frac{K_{\text{RN}} U}{(2R)^2} = \frac{K_{\text{RN}}}{2R}
\]  

(Eq. 3.4)

Figure 3.5. Particle representation of continuous material: particle contact is representing continuous material defined by the shaded area.
where $K_{RN}$ is the resultant normal stiffness at the contact, $U$ is the overlap of the particles, $\sigma$ is axial stress on the square section, $\varepsilon$ is axial strain of the square section, and $R$ is the radius of the balls, which are equal in this case. This simplification provides an easy way of approximating the Young’s modulus of a pack of particles that have average resultant contact stiffness equal to $K_R$. Although calculated using the cubic packing assumption, it is interesting to note that this equation also provides a reasonable initial guess for calibrating non-cubic granular packs.

For the cubic pack considered above, it is apparent that the material will not expand when compressed vertically – no Poisson’s effect – since the particles are rigid. This is unrealistic, and severely limits the usefulness of the cubic packed material. Fortunately, expansion does occur in random packings as the particles slide past one another. Consider the particles in Figure 3.3 – imagine that the lower particle is fixed, possibly by surrounding balls, and the upper particle is moving from left to right by an outside force. In this case, it is apparent that the shear spring will resist horizontal movement while the normal spring will cause movement in the vertical direction. This is strikingly similar to Poisson’s effect, and therefore it is not surprising that the ratio of the normal to shear spring stiffness values largely controls Poisson’s ratio in PFC materials (Itasca, 2005b):

$$\nu = f\left(\frac{K_{RN}}{K_{RS}}\right)$$

(Eq. 3.5)

Finally, a graphical illustration of the contact model (Itasca, 2005a) is shown in Figure 3.6 and Figure 3.7 to help conceptualize the previously described information.
Figure 3.6. Normal compression at contact: the normal force is linear with overlap, $U$, for constant resultant normal spring stiffness, $K_{RN}$.

Figure 3.7. Shear compression at contact: the shear force developed at the contact is linear with cumulative shear displacement for constant resultant shear stiffness, $K_{RS}$. If the contact has infinite frictional resistance, the shear force will continue to increase with increasing displacement.
3.3. Slip Model

After close examination of Figure 3.7, it is apparent that the shear force continues to increase with shear displacement, and therefore it is difficult for the particles to slide past each other. To account for sliding, the slip model limits the shear force at the contact based upon frictional resistance calculated using Coulomb sliding friction law. Specifically, each particle is assigned a frictional coefficient, $\mu$, thereby limiting the maximum shear force allowed at a contact, $F_{\text{max}}$, to:

$$F_{\text{max}} = \mu |F_i^n|$$

(Eq. 3.6)

where $F_i^n$ is the normal force at the contact. If the current value of shear force at the contact is greater than this maximum value, slip is allowed to occur at the contact, and the value of shear force is set to the maximum value. This is illustrated graphically in Figure 3.8:
Figure 3.8. Modification of shear force for sliding: if the shear force meets the frictional resistance at the contact, the shear force value of at the contact is set equal to the frictional resistance, and sliding is permitted.

3.4. Bonding Model

Finally, two general bonding models, contact and parallel, are available in PFC, since it is obviously sometimes useful to bond particles together to simulate cementation or solid materials. In general, the contact bond only provides strength while the parallel bond provides both strength and additional stiffness at each contact where it exists. In other words, the contact bond is similar to a spot weld while the parallel bond acts like a column of cementitious glue (Figure 3.9). Nevertheless, the exact behavior of each bond is still sometimes ambiguous, so each will be discussed in more detail (Figure 3.4).
Figure 3.9. Simplified illustration of bonding models: contact bond acts as a spot weld, and the parallel bond acts like a column of glue.
Figure 3.10. Normal bonding model analogy: the parallel bond adds compressive and tensile stiffness while the contact bond only prevents separation of the particles. The parallel bond does not prevent separation of the particles (Jurgens and Gray, 2007b).
First, a discussion of the parallel bond analogy, which is shown on the left of Figure 3.10: As the name suggest, the parallel bond adds an additional spring in parallel to the normal and shear springs of the contact model. This bond can be installed at any point of compression of the springs in the contact model, and upon installation, the forces and moments acting on the parallel bond are initialized to zero values. In other words, even though the contact model springs are compressed, the parallel bond springs are initially relaxed. At this point, if the contact undergoes additional compression, resistance is provided by both the contact model and parallel bond springs. Conversely, if the particles pull apart from the initial parallel bond position, the bond moves into tension since it is imagined as being hooked to the particle centers. The bond continues to pull on each particle and provide resistance even when the particles are no longer overlapping and the contact model is inactive. The fact that the particles can separate while parallel bonded is extremely significant as the stress in the bond is related not only to its elastic properties, but also to its length through beam theory. Additionally, since it acts like a beam, the parallel bond also contributes an additional bending and rotational moment to the contact.

Alternatively, the contact bond (right side of Figure 3.10) acts like a rigid wall preventing separation of the two particles beyond the zero overlap point. This resistance continues until a specified amount of tensile force is exerted on the contact bond and it breaks. When contact bonded, the two particles are prevented from sliding at the contact by inactivating the slip model. Therefore, shear force can continue to increase until reaching the shear strength of the bond, at which point the bond breaks.
4. UNIT CELL MODEL DEVELOPMENT

4.1. Overview

The goal of this chapter is to briefly describe and test a new method of generating a bonded set of particles in PFC$^{3D}$ (agglomerate) that could serve to model a grain within a rock. In general, the agglomerate generation procedure consists of 2 parts: generating a material with the elastic and strength properties of the grain material and cutting a grain of desired size from this material and setting the strength. It is quite apparent after examining the brief PFC physics discussion in Chapter 3 that there are many numbers of ways to generate such a model. Specifically, choosing packing arrangements, particle sizes comprising the agglomerate, type of bonding model, as well as other variables seems somewhat illogical and ambiguous, but nevertheless important. Therefore the method described in this chapter is largely derived from many trial models; however, the final result, not the iteration, is discussed. In order to validate the procedure and methods used, it is necessary to show that the agglomerate model is capable of reproducing the stress, strength, and stress path variables identified as important in Chapter 2.

As a note: Sections 4.3 and 4.4.1, which are the first two sections after Assumptions, describe the procedures for generating the agglomerate material, cutting the agglomerate from the material, and the design of the uniaxial compressive test, which is use for further calibration. Although these procedures are important to the modeler trying to reproduce the agglomerate described in this thesis, they are not entirely necessary for understanding the concept of the model, and certain readers may elect to avoid these
4.2. Assumptions

There are several notable assumptions within this model beyond the assumptions inherent to PFC$^{3D}$ (Potyondy and Cundall, 2004). They are generally listed here and, if necessary, explained in more detail in later sections.

1. A rock grain and its broken fragments are described by a network of equal sized particles bonded together by parallel bonds.

2. The resulting agglomerate is permeable since there are gaps between the particles composing it.

3. The agglomerate has limited fragmenting size, which is the smallest particle size in the agglomerate.

4. The agglomerate boundary is not smooth since it is defined by particles.

5. Assumptions 2, 3, and 4 are affected by the particle size composing the agglomerate; however, due to computational limitations, elemental particle size is primarily used as a scaling factor. It is accepted that particle size will affect fracture toughness, but this effect is not be quantified.

4.3. Agglomerate Generation Procedure

A PFC material is initially created with elastic properties of the desired grain material. First, elastic microproperties for a parallel-bonded PFC material are estimated
from the desired grain material elastic properties (Appendix B: Initial Agglomerate Microproperty Selection). Then, the expansion algorithm (Itasca, 2005b, Appendix C: Expansion Algorithm) is used to place bonded particles with these elastic microproperties within a container such that the material is at a suitable initial stress level (Appendix D: Choosing Pack Porosity for Initial Target Stress). This results in a container full of parallel bonded particles of desired elastic microproperties and extremely high strength (Figure 4.1).

Figure 4.1. Agglomerate material packed within cylindrical container (blue walls): particles (yellow) and parallel bonds (red) have the desired elastic microproperties based on a desired Young’s modulus and Poisson’s ratio guess.

The newly generated PFC material must then be tested and, if necessary, recalibrated to
determine whether the properties chosen truly represent the elastic behavior desired. Therefore, a biaxial test (Itasca, 2005b – Appendix E: Information Regarding the Biaxial Test in PFC) is conducted on this agglomerate material as the first calibration test in order to provide information regarding the true elastic response of the material and iterate to the desired elastic properties of Young’s modulus and Poisson’s ratio. This iterative procedure is relatively rapid and smooth, as can be seen from Table 4.1. In the example in the table, the variables $E_{\text{guess}}$ and $\lambda$ are successively changed in order to calculate different microproperties, as shown in Appendix B, and approach the desired material properties of $E = 4.7e9$ and $v = 0.10$.

Table 4.1. Relationship Between Macro and Micro Properties

<table>
<thead>
<tr>
<th>$\lambda$</th>
<th>$E_{\text{guess}}$</th>
<th>$E_{\text{Actual}}$</th>
<th>Poisson Ratio ($v$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>8.50E+09</td>
<td>6.56E+09</td>
<td>0.061</td>
</tr>
<tr>
<td>0.9</td>
<td>7.50E+09</td>
<td>5.69E+09</td>
<td>0.069</td>
</tr>
<tr>
<td>0.7</td>
<td>6.50E+09</td>
<td>4.70E+09</td>
<td>0.096</td>
</tr>
<tr>
<td>0.7</td>
<td>6.30E+09</td>
<td>4.68E+09</td>
<td>0.095</td>
</tr>
</tbody>
</table>

Then, once the correct elastic material properties are obtained through iteration, an agglomerate can be cut from the container (Figure 4.2) (Appendix F: Agglomerate Cutting and Angularity Algorithm and Equations). If desired, additional modification of the cutting program makes it possible to generate angular particles of specific angularity (Figure 4.3) (Appendix F: Agglomerate Cutting and Angularity Algorithm and Equations).
Figure 4.2. Cut agglomerate from cell: particles are deleted that fall outside the desired cut radius so that a spherical agglomerate is created.

Figure 4.3. Angular agglomerate generation: agglomerates are generated with desired angularity and maximum radius. This set of agglomerates shows that the agglomerate can represent the wide variety of grain shapes present within sand.

Finally, an equilibration routine is called in order to reduce the locked in stresses within the agglomerate (Appendix G: Agglomerate Equilibration Routine) that occur due to the previous loading from surrounding particles. Upon removal of these confinement particles, the tendency of the agglomerate is to expand as internal contacts separate. Although this expansion is necessary to reduce internal stress in the agglomerate, it is crucial to prevent complete separation of the particles, and uncontrollable lengthening of the bond, since this destroys model predictability.
The initial development and calibration results in an agglomerate cut from a PFC material calibrated to specific elastic properties; however, the resulting elastic and strength behavior of the grain is still largely unknown. Therefore, additional tests must be performed to provide further insight into the elastic and strength behavior of the agglomerate and to calibrate its strength for modeling granular material. This is described in the next sections.

4.4. Agglomerate Testing

4.4.1. Uniaxial Compression Testing Procedure

Due to availability of grain uniaxial compressive data (Shipway and Hutchings, 1993c; Takei et al., 2001; Nakata et al., 2001b), a PFC code for a uniaxial compressive test is used to further calibrate the agglomerate to grain behavior.

A uniaxial testing routine is first created. At this point, the agglomerate is within the container and no walls are touching it, therefore an initialization routine (Appendix H: Uniaxial Compression Initialization Routine) is used move the walls into position immediately above and below the agglomerate (infinite strength to avoid damage). The final state of the initialization routine is defined by the agglomerate static between the walls, which are now exerting a predefined force on its exterior (Figure 4.4). As a note, the initialization routine is necessary because the agglomerate wants to inevitably roll when PFC walls begin to push on its exterior, and this rolling causes inefficiencies in calculation time and large amounts of noise in the stress-strain graphs at the beginning of the test.
Figure 4.4. Agglomerate static between two platens: testing apparatus for uniaxial compressive test. Red lines represent contact forces (Jurgens and Gray, 2007b)

A few more steps are required to finish prepping and test the agglomerate. First, the parallel bond strengths in the agglomerate are set to the desired testing values, and variables are created to track pertinent agglomerate parameters, such as tensile stress and strain, according to Eq. 2.2 and Eq. 2.3, respectively. Then, a velocity is prescribed for the two walls above and below the agglomerate and loading occurs until failure, which is usually identified by a nearly vertical split in the particle (Figure 4.5). Note that the velocity must be chosen carefully to avoid damage due to dynamic loading, and it is helpful to ramp wall velocities incrementally to a final velocity target to reduce accelerations.
Figure 4.5. Typical vertical failure of agglomerate: left picture shows a side view and right picture shows an aerial view of the agglomerate uniaxial compressive test. Particles of similar shade of grey are bonded within the same group, while black particles are not bonded to anything else (Jurgens and Gray, 2007b).

4.4.2. Testing the Elastic Behavior of the Agglomerate

A fine resolution uniaxial compression test is then performed to visualize the Hertzian stress distribution and validate the biaxial test calibration and cutting procedures (Figure 4.6; Jurgens et al., 2007a). Since the model is very fine, the average stress values at each particle (Eq. 2.5) within the agglomerate are comparable to values calculated at similarly positioned elements in a finite element model with the same properties. Although numerical errors arise are present, the finite element model can be considered relatively close to the true solution.

The results of two trial agglomerate models are shown below (Jurgens et al., 2007a); the first model uses parallel bonds to bond the particles together, while the second model uses contact bonds. The input values for both models and a comparison finite element model are shown in Table 4.2. As an aid in understanding the data, it is re-stated that $E$ is the observed Young’s modulus for the PFC material obtained from a
biaxial compression test, $E_{\text{cubic}}$ is the Young’s modulus calculated from the value of $k_n$ for a cubic pack, $v$ is Poisson’s ratio, $k_s/k_n$ is the ratio of shear to normal stiffness in the model, Agglom Radius is the radius of the agglomerate, and Particle radius is the radius of a particle composing the agglomerate.

Table 4.2. Properties in elastic comparison models (from Jurgens et al., 2007a)

<table>
<thead>
<tr>
<th>Finite Element Model</th>
<th>Parallel Bond Model</th>
<th>Contact Bond Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model Radius (mm)</td>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td>E (Pa)</td>
<td>4.8e9</td>
<td>4.8e9</td>
</tr>
<tr>
<td>v</td>
<td>0.10</td>
<td>0.10</td>
</tr>
<tr>
<td>$E_{\text{cubic}}$ (Pa)</td>
<td>6.7e9</td>
<td>7.8e9</td>
</tr>
<tr>
<td>Particle radius (mm)</td>
<td>0.02</td>
<td>0.02</td>
</tr>
<tr>
<td>$k_s/k_n$</td>
<td>0.8</td>
<td>1.7</td>
</tr>
</tbody>
</table>

Figure 4.6. Elastic solution test on agglomerate model: model is composed of 8300 particles to obtain fine resolution (Jurgens et al., 2007a).
Two specific comparisons are made of the three models. First, each model is loaded to a prescribed force level (defined by walls) and the characteristic stress at each element or particle is calculated, plotted (Figure 4.7), and compared (Figure 4.8, Figure 4.9, and Figure 4.10). Second, the average tensile stress in the radial direction is calculated and plotted throughout loading (Figure 4.11). Examples of the results are shown in the following figures below.

Figure 4.7. Agglomerate center exposure (aerial view): agglomerate is cut vertically to expose the center for plotting stress tensor values. Left picture is from before the cut, right picture is after the cut was made (Jurgens et al., 2007a).
Figure 4.8. Stress in Pascals in the radial direction for finite element solution at 35

Newtons platen force: maximum tensile stress is in the center of the particle and reduces to compression toward the edges (Jurgens et al., 2007a).
Figure 4.9. Stress in Pascals in the radial direction for parallel bond solution at 35
Newton platen force: tensile stress is maximum in center and reduces to
compression toward edges (Jurgens et al., 2007a)

Figure 4.10. Stress in Pascals in radial direction for contact bond solution at 35 Newtons
platen force: tensile stress is maximum in center and reduces to compression
toward edges (Jurgens et al., 2007a)
Figure 4.11. Comparison of average tensile stress in the radial direction: the parallel bond model closely approximates the solution of the finite element model (Jurgens et al., 2007a)

The results indicate that the parallel bonded material most closely models grain material, which is theoretically represented by the finite element model. By a comparison of the magnitudes and distributions of Figure 4.8 and 4.9, it is apparent that the stress distributions of the parallel bond and finite element models are very similar. This similarity is further emphasized by the overlay of the parallel bond and finite element model average tensile stress values in Figure 4.11. It is also apparent that a contact bonded model does not provide as accurate of a solution as the parallel bonded model, and this is significant since other researchers have used contact bonds for agglomerate modeling (Cheng et al., 2003; Robertson et al., 2001; McDowell et al., 2002) and not tested the ability to model the spatial elastic solution. The results of Jurgens et al. (2007a) prove that a randomly packed, parallel bonded agglomerate model can accurately model the elastic behavior of a continuous material and provides greater
confidence in the method of agglomerate generation illustrated in this thesis.

A note on this method: There are some differences in the finite element and DEM models arise from averaging procedures, such as estimating slopes of the axial stress vs. axial strain and volumetric strain vs. axial strain graphs for the biaxial compression calibration test. To ensure the best possible results, multiple sizes of the biaxial calibration sample should be tested to ensure convergence is met.

4.4.3. Testing the Strength Behavior of an Agglomerate

A quick summary of what has been accomplished thus far: It has been shown that a PFC material can be calibrated to specific elastic properties using a biaxial compression test, and that an agglomerate (or group of bonded balls) cut from this material retains these elastic properties. However, information regarding agglomerate strength is still absent. Consider again that the use of a PFC agglomerate to model a grain is comparable to modeling a real material with an artificial, yet similar material. Therefore, before it is possible to prescribe strength to the agglomerate, the failure behavior and its relationship to bond strengths must be characterized. This strength information can be obtained using additional uniaxial compressive test and elementary statistics.

The results of 347 uniaxial compressive tests on agglomerates of different shapes, sizes, and strengths are shown below (Jurgens and Gray, 2007b). Of these 347 tests, 225 of the tests are strength tests of various sized agglomerates cut from the same PFC material with the identical bond strengths. The remaining 122 tests are strength tests on randomly sized agglomerates with varying bond strengths. Note that all tests have slightly different particle packing arrangements since the particles were randomly placed using a random number generator for each test. From these tests, it is possible to
additionally quantify the behavior of the agglomerate, such as visual failure behavior, relationship between agglomerate compressive strength and internal bond strength, and the effect of agglomerate size on the overall measured strength.

Jurgens and Gray (2007b) describe the general behavior of failing agglomerates (Figure 4.12 – Figure 4.15). Similarly to sand (Nakata et al., 2001; Takei et al., 2001), agglomerates display abrasion (Figure 4.12), cone cracking, and tensile failure (Figure 4.13, Figure 4.14) throughout loading in uniaxial compression. Abrasion commonly occurs near the platen walls as asperities, simulating by largely protruding particles, are broken from the body. Under additional loading, shear cracking begins to form underneath the platen in the high shear stress regions illustrated in Chapter 2. And finally, the agglomerate fails vertically in tension through one or more failure planes. As note for viewing the figures: same colored particles are bonded to other particles of the same color while black colored particles are not bonded to any other particle (Appendix J: Broken Pieces Algorithm).

Figure 4.12. Abrasion of agglomerate: particle in black is sheared from the wall-agglomerate contact (Jurgens and Gray, 2007b).
Figure 4.13. Tensile failure of agglomerate: near vertical crack forms and main agglomerate pieces (light and dark gray) move at high velocity to the side, simulating brittle failure. Additionally, the agglomerate has smaller pieces that have broken free from the two main broken pieces (medium gray) (Jurgens and Gray, 2007b).

Figure 4.14. Plan view of agglomerate failure: multiple vertical fractures form as agglomerate is reloaded. Additional particles are abraded from edges near platen boundary (Jurgens and Gray, 2007b).
Figure 4.15. Example of particle stress vs. particle strain: Graphs shows failure consistent with Takei (2001) and Nakata (2001) failure curves for quartz particles (Jurgens and Gray, 2007b).

The statistical results of the agglomerate uniaxial compressive tests are shown in Figure 4.16 through Figure 4.18 (Jurgens and Gray, 2007b) to relate overall strength to relevant material input properties. From Figure 4.16, it is apparent that the strengths of different sized agglomerates are approximately the same within a reasonable amount of error, which is somewhat contradictory to behavior shown by other researchers (Potyondy and Cundall, 2004). Although it is noticed that the standard deviation of the agglomerate strength is inversely related to the number of particles, this is relatively insignificant when dealing with the much larger level of uncertainty present in crushing models. Additionally, Figure 4.17 indicates that the entire strength distribution of agglomerates of any size cut from the same material is normally distributed about a mean.
with an insignificantly small standard deviation, further indicating that the strengths of various sized agglomerates are approximately the same. Finally, Figure 4.18 shows that the agglomerate strength is linearly related to parallel bond strength. From viewing these figures, the main conclusion to draw is that it is possible to prescribe an approximate strength to any agglomerate in statistical sense.

Figure 4.16. Strength of varying sized agglomerates: all agglomerates cut from material with same bond strength have approximately same tensile strength (Jurgens and Gray, 2007b).
Figure 4.17. Failure strength distribution: agglomerate tensile strength is normally distributed (Jurgens and Gray, 2007b).

Figure 4.18. Agglomerate tensile strength vs. bond strength: relationship is approximately linear over averages (Jurgens and Gray, 2007b).
4.5. Weibull Probabilistic Strength of Groups of Agglomerates

The preceding sections show that the agglomerate model does a reasonably good job modeling a grain’s elasticity and strength behavior, and that the model is predictable within statistical limits. It is now possible to take advantage of these insights in order to reproduce a Weibull strength distribution for a sample of agglomerates (Jurgens and Gray, 2007b). This method will be useful when using groups of agglomerates to model granular material where it is well known that the strength of each grain will not be the same, but will vary statistically, such as in sand (Nakata et al., 2001b; Takei et al., 2001).

First, the Weibull probability distribution equation (Eq. 2.11) is solved for tensile strength of a particle of diameter, d:

\[
\sigma(d) = \sigma_o \exp \left( \frac{1}{m} \ln \left( \frac{d}{d_o} \ln \left( \frac{1}{P_s} \right) \right) \right)
\]

(Eq. 4.1)

where \(P_s\) is the probability of survival of a grain of diameter, d, subject to a tensile stress of \(\sigma\), where the diameter, \(d_o\), is the particle size such that 37% of particles survive its tensile strength of \(\sigma_o\), and \(m\) is the Weibull modulus describing strength variability.

If the number of grains to be simulated is known, each grain can be assigned a successive probability of survival according to the following equation:

\[
P_s = \frac{i}{n+1}
\]

(Eq. 4.2)

where \(P_s\) is the probability of survival, \(i\) is the \(i_{th}\) agglomerate tested or inserted into a model, and \(n\) is the total number of agglomerates to be modeled.

Then, the based on this probability of survival, the necessary parallel bond strength is calculated using the strength calibration graph (Figure 4.18):

\[
\sigma_{pb}(\sigma(d)) = \frac{\sigma(d) - b}{m}
\]

(Eq. 4.3)
where $\sigma_{pb}$ is the parallel bond tensile strength, and $b$ and $m$ are the y-intercept and slope of the strength calibration graph, respectively.

This method of assigning strength variation is convenient since it incorporates the size of the agglomerate directly into the bond strength calculation.

The overall goal of the preceding method is to produce a sample of agglomerates with a Weibull modulus close to the input value in Eq. 4.3, and therefore model the statistical strength of a group of varying sized grains. Jurgens and Gray (2007) validate this method with data from a set of uniaxial compressive tests on a sample of randomly sized agglomerates (Table 4.3, Figure 4.19). As a note for viewing Figure 4.19, rearranging Eq. 4.13 yields:

$$\ln\left(\frac{d_o}{d} \ln\left(\frac{1}{P_s}\right)\right) = m \ln\left(\frac{\sigma}{\sigma_0}\right) \quad \text{...(Eq. 4.4)}$$

and therefore the slope of the graph is $m$, the Weibull modulus, when the x and y variables $P1$ and $P2$ are defined as:

$$P1 = \ln\left(\frac{\sigma}{\sigma_0}\right) \quad \text{...(Eq. 4.5)}$$

$$P2 = \ln\left(\frac{d_o}{d} \ln\left(\frac{1}{P_s}\right)\right) \quad \text{...(Eq. 4.6)}$$

Figure 4.19 indicates that this method of assigning statistical strength is relatively accurate. The reproduced Weibull modulus of the test data is 2.8, obtained from an input value of 3.0, and is excellent when considering that the Weibull modulus of silica sand for one set of tests ranged from 1.82 – 3.04 (Nakata et al., 2001b).

At first glance, it appears that this method of adjusting bond strengths is not representative of real grain material. However, it is noted that adjusting bond strengths can be thought of as incorporating flaws at the bond level, and seems valid since it is generally accepted that flaws within the grain material are responsible for controlling the
distribution of strengths and the resulting Weibull modulus of real grains (Cheng et al., 2003; McDowell et al., 2002; Robertson et al., 2001).

Table 4.3. Agglomerate strength test results (Jurgens and Gray, 2007b).

<table>
<thead>
<tr>
<th>Assigned probability of survival</th>
<th>Probability of Survival</th>
<th>Particle Radius (m)</th>
<th>bond normal strength (Pa)</th>
<th>bond shear strength (Pa)</th>
<th>Tensile strength (Pa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0625</td>
<td>0.0625</td>
<td>4.09E-04</td>
<td>1.60E+08</td>
<td>2.34E+08</td>
<td>8.50E+07</td>
</tr>
<tr>
<td>0.125</td>
<td>0.125</td>
<td>4.32E-04</td>
<td>1.46E+08</td>
<td>2.12E+08</td>
<td>6.10E+07</td>
</tr>
<tr>
<td>0.3125</td>
<td>0.1875</td>
<td>3.75E-04</td>
<td>1.40E+08</td>
<td>2.03E+08</td>
<td>5.26E+07</td>
</tr>
<tr>
<td>0.1875</td>
<td>0.25</td>
<td>4.16E-04</td>
<td>1.28E+08</td>
<td>1.85E+08</td>
<td>4.82E+07</td>
</tr>
<tr>
<td>0.25</td>
<td>0.3125</td>
<td>4.88E-04</td>
<td>1.32E+08</td>
<td>1.91E+08</td>
<td>4.81E+07</td>
</tr>
<tr>
<td>0.375</td>
<td>0.375</td>
<td>4.24E-04</td>
<td>1.23E+08</td>
<td>1.78E+08</td>
<td>4.70E+07</td>
</tr>
<tr>
<td>0.5625</td>
<td>0.4375</td>
<td>4.32E-04</td>
<td>1.13E+08</td>
<td>1.64E+08</td>
<td>4.17E+07</td>
</tr>
<tr>
<td>0.625</td>
<td>0.5</td>
<td>4.58E-04</td>
<td>1.09E+08</td>
<td>1.58E+08</td>
<td>4.16E+07</td>
</tr>
<tr>
<td>0.8125</td>
<td>0.5625</td>
<td>3.93E-04</td>
<td>1.09E+08</td>
<td>1.58E+08</td>
<td>3.91E+07</td>
</tr>
<tr>
<td>0.75</td>
<td>0.625</td>
<td>3.57E-04</td>
<td>1.03E+08</td>
<td>1.50E+08</td>
<td>3.77E+07</td>
</tr>
<tr>
<td>0.5</td>
<td>0.6875</td>
<td>4.95E-04</td>
<td>9.87E+07</td>
<td>1.43E+08</td>
<td>3.38E+07</td>
</tr>
<tr>
<td>0.4375</td>
<td>0.75</td>
<td>4.95E-04</td>
<td>1.02E+08</td>
<td>1.48E+08</td>
<td>3.17E+07</td>
</tr>
<tr>
<td>0.875</td>
<td>0.8125</td>
<td>4.06E-04</td>
<td>9.57E+07</td>
<td>1.39E+08</td>
<td>3.02E+07</td>
</tr>
<tr>
<td>0.6875</td>
<td>0.875</td>
<td>4.74E-04</td>
<td>9.06E+07</td>
<td>1.31E+08</td>
<td>2.14E+07</td>
</tr>
<tr>
<td>0.9375</td>
<td>0.9375</td>
<td>3.86E-04</td>
<td>8.74E+07</td>
<td>1.27E+08</td>
<td>2.03E+07</td>
</tr>
</tbody>
</table>
Figure 4.19. Calculation of Weibull modulus: the slope of the data trend is 2.8 from an input value of 3.0 (Jurgens and Gray, 2007b).
5. COMPRESSION OF UNCONSOLIDATED SAND

5.1. Overview

Chapter 4 demonstrated that the agglomerate model seemingly accurately models the stress and strength solution of a single grain. Additionally, it was illustrated that it is possible to statistically prescribe the strength to any agglomerate, and therefore model the statistical strength of a set of grains. It is now of interest to determine how accurately this modeling method can predict the behavior of sets of grains, such as in laboratory compression tests of unconsolidated sand. This chapter documents several such tests: biaxial compression of unbreakable agglomerates, hydrostatic compression of breakable agglomerates, and biaxial compression of breakable agglomerates.

Note: the method of incorporating the agglomerates into the tests in this chapter was accomplished using a programming routine to extract data from single agglomerates and use said data to replace the default, rigid PFC particles in each model (Figure 5.1). This routine is described in Appendix K: Agglomerate Extraction and Replacement Algorithm.

Figure 5.1. Agglomerate replacement scheme and compaction model of Chapter 5.
5.2. Characterizing the Elastic Solution of Unbreakable Agglomerate Packs

Tests on packs of high strength agglomerates can validate the elastic behavior of agglomerate packs prior to significant crushing. The results of two such tests at varying confining pressures are shown in Figures 5.2 and 5.3 for the input data of Table 5.1. For comparison, data from a similarly packed model using the Hertzian contact model is also shown. Since the particles in the Hertzian model have the same elastic properties as calibrated to the agglomerates, the behavior of both models should be similar when the agglomerates are extremely strong and do not crush.
Table 5.1. Properties for unbreakable agglomerate tests.

<table>
<thead>
<tr>
<th>Input Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Agglomerate diameter (mm)</td>
<td>0.5</td>
</tr>
<tr>
<td>Diameter of particle in agglomerate (mm)</td>
<td>0.04</td>
</tr>
<tr>
<td>Young’s modulus of cubic pack, $E_{\text{cubic}}$ (Pa)</td>
<td>$1.4 \times 10^9$</td>
</tr>
<tr>
<td>Young's modulus, $E$ (Pa) (through triaxial test)</td>
<td>$7.7 \times 10^9$</td>
</tr>
<tr>
<td>Poisson ratio of agglomerate, $\nu$</td>
<td>0.10</td>
</tr>
<tr>
<td>$K_s/K_n$ ratio, $\lambda$</td>
<td>0.7</td>
</tr>
<tr>
<td>Porosity of agglomerate, $\varphi$</td>
<td>0.42</td>
</tr>
<tr>
<td>Ball normal stiffness (N/m)</td>
<td>$1.29 \times 10^7$</td>
</tr>
<tr>
<td>Ball shear stiffness (N/m)</td>
<td>$9.04 \times 10^6$</td>
</tr>
<tr>
<td>Density of PFC particle ($\text{kg/m}^3$)</td>
<td>2650</td>
</tr>
<tr>
<td>Parallel bond normal stiffness (Pa/m)</td>
<td>$1.82 \times 10^{15}$</td>
</tr>
<tr>
<td>Parallel bond shear stiffness (Pa/m)</td>
<td>$1.28 \times 10^{15}$</td>
</tr>
<tr>
<td>Parallel bond radius multiplier</td>
<td>1.0</td>
</tr>
<tr>
<td>Friction coefficient between particles</td>
<td>0.4</td>
</tr>
</tbody>
</table>

The results indicate that agglomerate packs have the correct expected elastic behavior. By comparing the slopes of Figures 5.2 and 5.3, it is apparent that the agglomerate packs display similar values of Young’s modulus and Poisson’s ratio as the Hertzian pack. Additionally, the calculated Young’s modulus and Poisson’s ratio for the agglomerate packs, which are calibrated to properties of quartz, ranged from $2 \times 10^9$-$4 \times 10^9$ Pa and 0.20-0.30, respectively, and are thus consistent with values observed in laboratory
tests for unconsolidated sands (Cheng et al., 2003; Budhu, 2007). This provides further assurance that the method of agglomerate development is valid.

It is obvious that plasticity is not modeled by the unbreakable agglomerate pack since the rough agglomerate surface prevents sliding. As a potential fix for this problem, the particle size in the agglomerates can be decreased, producing a smoother boundary, and possibly lowering the internal friction angle. Although difficult to define real values for rough, arbitrary shaped materials, it is hypothesized that real quartz particles have a frictional angle somewhere between the values of the perfect Hertzian sphere and agglomerate.

![Figure 5.2. Deviatoric stress vs. strain: note that the Young’s moduli for the Hertzian and agglomerate test cases are quite similar.](image)

Figure 5.2. Deviatoric stress vs. strain: note that the Young’s moduli for the Hertzian and agglomerate test cases are quite similar.
Figure 5.3. Volumetric strain vs. deviatoric strain: all cases are similar showing a consistent value of Poisson’s ratio.

5.3. Characterizing Hydrostatic Compaction of Breakable Agglomerate Packs

Additionally, hydrostatic tests on breakable agglomerate packs can quantify to model’s ability to characterize fracturing development in granular material, often highlighted in the laboratory by porosity reduction with pressure. For this reason, the data from several tests with the properties of

Table 5.2 (same elasticity as Table 5.1) are shown below. The strength values in Table 5.2 are generally representative of quartz sand grains and based upon data from
McDowell et al. (2002) and Table 2.1, but also similar to data by Cheng et al. (2003) and Nakata et al. (2001b). As well, the size and size distribution is representative of loose, fine to medium grained, well sorted sand (No. 35 – No. 50 sieve) (Budhu, 2007). However, these strength values, agglomerate sizes, and the packing arrangement and porosity are not representative of any laboratory test that the author has specifically conducted.

Table 5.2. Sample Input Parameters for Hydrostatic Tests

<table>
<thead>
<tr>
<th>Input Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Agglomerate Size Distribution</td>
<td>Uniform between max and min</td>
</tr>
<tr>
<td>Maximum Agglomerate Diameter</td>
<td>0.5 mm</td>
</tr>
<tr>
<td>Minimum Agglomerate Diameter</td>
<td>0.3 mm</td>
</tr>
<tr>
<td>Characteristic Strength, $\sigma_0$ (Pa)</td>
<td>147e6</td>
</tr>
<tr>
<td>Characteristic Size, $d_0$ (mm)</td>
<td>0.5 mm</td>
</tr>
<tr>
<td>Weibull Modulus, m</td>
<td>3.0</td>
</tr>
</tbody>
</table>
Figure 5.4. Mean stress vs. volumetric strain: the sample elastically compresses, followed by crushing induced plasticity, and then finally hardens as the crushed particles begin to interlock.

Figure 5.5. Theoretical hydrostatic compaction curve (modified from Goodman, 1989).
Figure 5.6. Total void ratio vs. mean stress: total void ratio is the volume of voids per volume of solids, where the volume of voids includes the volume of porosity inside each agglomerate.
Figure 5.7. Effective void ratio vs. mean stress: effective void ratio is the volume of voids per volume of solids, where the volume of voids only includes the volume initially present between the agglomerates and does not include agglomerate porosity.

Figure 5.8. Comparison of total and effective void ratio reduction to laboratory data.
Figure 5.9. Broken bonds vs. mean stress: the curve has a striking resemblance to the normally consolidated sand curve marking void ratio reduction vs. stress.
Figure 5.10. Volumetric strain vs. axial strain for agglomerates: as expected the relationship between volumetric strain and axial strain is linear for a hydrostatic test. Volumetric strain is overestimated by the agglomerate model; however, it is not entirely apparent in this graph since there is no comparison data available.

Before discussing the results, it is important to discuss the roughness seen in the graphs (example in Figure 5.4). This roughness is quite common in discrete element simulations of crushable agglomerates (Cheng et al., 2003; Harireche et al., 2002) and is attributed to limitations in the number of agglomerates usually present in these simulations. Consider when an agglomerate fractures in these small simulations; large changes to the stress levels on the walls occurs due to associated reorientation and large stress redistribution due to the limited number of agglomerates. It is possible to reduce the size of these stress changes by allowing larger velocity increases on the walls, so that the walls can rebuild the required stress level faster; however, increasing the wall velocities also increases the risk of inducing further crushing due to dynamic forces.
The general elastic and plastic behavior of hydrostatic compaction is similar to real sand. Figure 5.4 illustrates that three of the four main elastic and plastic regions of real sand (Figure 5.5) are present during loading. First, the behavior is initially elastic as since little movement and crushing is occurring in the pack. In this initial region, the Young’s modulus and Poisson’s ratio are similar to the values shown in the unbreakable agglomerate tests of Section 5.2. Then, once large amounts of crushing and rearrangement occur, plastic behavior develops in the material. This plastic behavior continues until particle locking and hardening eventually occur as the sample becomes more packed and solid. It is apparent that fissure closing is not demonstrated by the material since the lower data limit is 1 MPa, and probably beyond fissure closing.

Before discussing the void ratio reductions graphs, it is advantageous to understand definition of void ratio used in this thesis and how it relates to agglomerate packs. Since void ratio is the volume of voids in the pore space per volume of solids, the inherent porosity of the agglomerate makes it difficult to define a meaningful value of void ratio for the pack at any given moment. For example, under low amounts of crushing, the internal voids exert little influence on the shape of the compaction curve, since these voids are still representing solid material within the agglomerate. In this small strain situation, it is most meaningful to observe the change in effective void ratio, or the ratio calculated only using voids outside the agglomerate bodies. But as fracturing commences, voids present within the agglomerates become additional pore space and can compact. Once all bonds are broken, it is most useful to view the total void ratio, which includes agglomerate and pore space voids. Note that the 100% bond break limit is never reached in these simulations (Figure 5.9, Figure 5.9), and therefore behavior is usually defined by some median case.
Nevertheless, and under this relatively significant limitation, the agglomerate pack behaves similarly to a normally consolidated soil (Figure 5.8), or a soil never previously compressed (Budhu, 2007). Normally consolidated soils behave elastoplastically (Budhu, 2007); the plastic strain is attributed to agglomerate rearrangement, fracturing, and particle rearrangement, and the elastic strain is due to bond and contact spring compression, and is recoverable as particles push apart upon unloading. The slope transitions on Figure 5.8 mark the change from strongly elastic to strongly plastic behavior, and are also evidenced by the increase in the slope on the bond graph of Figure 5.9. At this transition point, any increases in strain cause larger amounts of rearrangement or continued fracturing rather than spring compression. While the total void ratio vs. stress curve begins to approach the curves approximated from data by Valdes and Caban (2006) and Cheng et al. (2003), the resulting reduction in both total and effective void ratio is considerably larger than observed in laboratory tests. This is reasonable, since it can be seen that the new voids contributed by fractured agglomerates are quickly compacted with additional strain (Figure 5.12- Figure 5.22), and cause larger inaccuracies with increasing stress. Although it may be possible to modify the normal consolidation curve by accounting for the number of fractured agglomerates, the exact relationship is not apparent and non-linear. Nevertheless, even with this downfall, it is encouraging that the void ratio vs. stress curve shows similar behavior as laboratory data with the general properties chosen.

It is hypothesized that this void problem can be fixed by considering agglomerate packing arrangements with lower porosities, such as regular packs or packs of larger and smaller particles. However, it is noted that previous hexagonal close packing models have shown similar problems (Cheng et al., 2003), even with lower porosities. And
additionally, in order to obtain the correct failure mode in regular packings it is necessary to install defects (Robertson et al., 2001; McDowell et al., 2002; Cheng et al., 2003) by removing balls and subsequently increasing porosity. If defects are not introduced, all bonds tend to break catastrophically, simulating glass-type brittle failure. In summary, it is apparent that any lower porosity packing arrangement may solve the void problem, but may also have its own set of unique problems and therefore has to be extensively studied to quantify behavior.

The visual evolution of crushing shown in Figure 5.12- Figure 5.22 provides interesting information into the mechanism of hydrostatic crushing. Most significantly, it is observed that abrasion of the agglomerate boundaries, largely simulated by the black particles, plays the dominant role in damage and repacking of the sample. Comparing to the unbreakable tests in Section 5.2 with little plasticity, abrasion is recognized as the main plasticity mechanism, and this result infers that abrasion and asperity damage also control plasticity in sand, with Coulomb sliding and large fracturing being less important. In other cases, particles fracture with a clearly defined break, simulating tensile or shear fracture, and continue to fracture until a stable, local hydrostatic state is reached near the agglomerate. These observations of crushing development in the agglomerate model are in general accordance with laboratory experiments and observations. For example, Takei (2001) indicates that the dominant failure mechanism in quartz grain crushing is edge collapse and abrasion, while increasing confinement is significant in reducing crushing on a local scale (Lobo-Guerrero et al., 2005a; Tsongui et al., 1999).
Figure 5.11. Illustrating location of cross-sections: shows approximate locations of
where cross-sections were plotted throughout the hydrostatic simulation.
Figure 5.12. Cross-section #1 – stress = 5e6 Pa: colored particles are bonded together and black particles are not bonded to any other particle. During this initial elastic phase, relatively little damage occurs and any damage that does occur is due to small amounts of abrasion between agglomerates.
Figure 5.13. Cross-section #2 - stress = 1e7 Pa: continued elastic compression with additional abrasion. One large fracture is apparent at the top right of the figure. Comparing this figure to the previous figure illustrates that relatively little pore collapse has occurred.
Figure 5.14. Cross-section #3 – stress level = 1.5e7 Pa: this is the first figure illustrating the plastic behavior of the pack. The agglomerate in the upper right has continued to fracture and repack. As well, several other agglomerates have fractured, and pore space has been reduced considerably. More abrasion has occurred.
Figure 5.15. Cross-section #4 – stress = 2.0e7 Pa: continued fracturing has occurred near the upper-right, bottom-right, and left-center. Abrasion also seems to be concentrated to certain areas where there appeared to be poor confinement at the beginning of the test (cross-section #1). Pore space has almost complete disappeared, except for pore space between particles (not agglomerates).
Figure 5.16. Cross-section #5 – stress = 2.5e7 Pa: continued abrasion is occurring, primarily near original fractures, which are probably defining high stress areas. Compression is starting to become elastic again as the pack is beginning to stiffen due to reduced crushing.
Figure 5.17. Cross-section #6 – stress = 3.0e7 Pa: continued abrasion is occurring as before. Compression is largely elastic as pack has hardened.
Figure 5.18. Cross-section #7 – stress = 3.5e7 Pa: relatively little change can be seen from this cross-section forward as the pack has hardened, crushing has slowed, and compression is largely elastic.
Figure 5.19. Cross-section #8 – stress = 4.0e7 Pa: undamaged agglomerates continue to become more confined as abraded particles from other agglomerates reposition.
Figure 5.20. Cross-section #9 – stress = $4.5 \times 10^7$ Pa: small amounts of damage continue in form of abrasion.
Figure 5.21. Cross-section # 10 – stress = 5.0e7 Pa: continued damage due to abrasion.
Figure 5.22. Cross – section # 11 – stress = 5.5e7 Pa: pack is well compacted with a distinct compaction band forming across center of sample in a top-left to bottom-right fashion.

5.4. Characterizing Biaxial Compression of Breakable Agglomerate Packs

Biaxial tests provide further information into the shear behavior of agglomerate packs. To test this behavior, the hydrostatic tests in the preceding section were saved at various hydrostatic stress states for conducting biaxial tests. In these biaxial tests, the stress on the horizontal walls (confinement) is held constant and the vertical walls are
used to load the sample axially at constant strain rate. The results are shown in Figure 5.23 – Figure 5.33.

Figure 5.23. Biaxial axial stress-axial strain test data for agglomerate model: notice that the results for two simulations are compared to real laboratory data from Cheng et al. (2003).
Figure 5.24. Volumetric strain vs. axial strain for the agglomerate model: the data is compared to results from Cheng et al. (2003) for real laboratory data from sand. Notice how the agglomerate model largely overestimates volumetric strain due to internal voids within the agglomerate.
Figure 5.25. Failure envelope for agglomerate material: the angle of internal friction is approximately 44 degrees and reduces to approximately 25 degrees upon additional shearing, indicating that the material is dilating.

The biaxial compression stress-strain behavior is largely similar to real sand. Figure 5.23 shows that the deviatoric stress, which is proportional to the amount of shearing, initially increases linearly with increasing strain and then begins to display plastic behavior as the agglomerate material begins to crush and provide less resistance to shearing. As well, increased confining stress causes a more rapid transition between elastic, strain softening, and plastic behavior since the additional confinement increases the frictional resistance of the material and causes more drastic failure. This type of behavior is consistent with the elastic behavior of Type I soils, such as loose sand or lightly overconsolidated clay (Budhu, 2007).

Recalling the discussion of internal agglomerate voids, it is no surprise that Figure 5.24 indicates agglomerate model is overestimating strains, particularly volumetric strain. It is encouraging that the shape of the curve is similar; however, and this provides evidence indicating that the agglomerate model could more accurately simulate the
behavior of sand if packing porosity is reduced.

The frictional strength of the material is modeled closely by Mohr-Coulomb or Drucker-Prager failure criterions, which is in accordance with real sand. As shown in Figure 5.25, the fall in frictional strength with increasing confinement indicates that the material is displaying dilational behavior, similar to sand (Budhu, 2007), due to the abrasion of the rough boundary of the agglomerates during sliding. The lower limit of frictional strength is again controlled by the properties of the unbonded material at the point when all bonds are broken within the shear zone. From the graph, it is calculated that the peak effective friction angle is approximately 44 degrees and reduces to around 25 degrees for higher confining stresses, where nearly all particles are unbonded in the shear zone.

As briefly mentioned above, the increasing numbers of black particles, which are particles that are no longer bonded to anything else, within the center of the sample define shear zone development (Figures 5.27-Figure 5.33). As loading is continued, this shear region becomes increasingly crushed and the resulting frictional strength is reduced to that of a region of unbonded balls, which can more easily slide than bonded agglomerates. It is apparent that this crushed zone is different from the hydrostatic test crushed zone in that it is oriented diagonally rather than horizontally, and is largely indicative of shearing.
Figure 5.26. Locations of cross-sections for biaxial test at 2e7 Pa confining stress.
Figure 5.27. Cross-section #1 – axial strain = 0: marks beginning of biaxial test. It can be seen that there are two to three regions that have experienced crushing from the hydrostatic loading. As well there is small amounts of abrasion throughout the sample.
Figure 5.28. Cross-section #2 – axial strain = 1.2e-1: this cross-section marks the beginning of the plastic portion of the stress-strain curve. It is observed that a few agglomerates have been crushed and abrasion is beginning to occur in a top-left to bottom-right trend.
Figure 5.29. Cross-section #3 – axial strain = 1.94e-1: continued abrasion is occurring near regions of initial crushing defined by the beginning of plastic behavior. A distinct shear band is beginning to form.
Figure 5.30. Cross-section #4 – axial strain = 2.28e-1: continued abrasion and crushing can be seen with two rows of black particles in a top-left to bottom-right trend defining the shear band formation.
Figure 5.31. Cross-section #5 – axial strain = 3.24e-1: since the sample has already failed along the shear band, continued abrasion occurs in this region and more distinctly defines this shear band formation.
Figure 5.32. Cross-section #6 – axial strain = 4.33e-1 axial strain: this cross-section marks even more distinct crushing with another failure region seemingly occurring in the upper-right corner.
Figure 5.33. Crushing during biaxial loading at 5.87e-1 axial strain: this last cross-section is not shown on the graph, but illustrates how increased abrasion occurs in the shear zones due large strain. The shear bands are more distinct than compaction bands observed in the hydrostatic test.
6. CONCLUSIONS

This thesis provides additional investigation into the effectiveness of modeling sand grains by agglomerates, or a collection of rigid particles connected by bonds that interact based on simple spring laws. It is shown that the generated agglomerate grain can represent the elastic and statistical strength solutions of varying sized grains, and by synthesizing a collection of these agglomerates into a model it is possible to directly relate behavior observed at a macroscopic scale to the properties associated with the grains. This model could theoretically be used to perform sensitivity studies on the effects of crushing in applications such as hydraulic fracture proppant sizing.

The agglomerate model can reproduce many of the macroscopic behaviors seen in unconsolidated sands. Specifically, from unbreakable agglomerate simulations, it is observed that the bulk elastic constants of agglomerate packs (Young’s modulus and Poisson’s ratio) are in agreement with data from unconsolidated sand tests and simulations using Hertzian particles. As well, hydrostatic tests on breakable agglomerates illustrate three distinct regions of elasticity, softening, and finally hardening behavior, similar to unconsolidated sand tests, and the normal consolidation curve shows typical characteristics of a Type I soil, as would be expected. Additionally, biaxial tests on crushable agglomerates show strikingly similar behavior to that of real sand tests. Shearing of the agglomerates during sliding is largely associated with abrasion and induces changes in the frictional angle of the material, with significant dilation occurring over increasing stress. Increased shear strength develops with increased confinement, as well as a more rapid transition from elastic to purely plastic behavior, similar to that seen
in unconsolidated sand tests. Visual observation of crushing indicates that abrasion and asperity damage are the most significant factors in damage accumulation of individual grains, and this is in agreement with laboratory results on quartz grains. This observation questions the validity of DEM grain replacement models that use a failure criterion based solely upon the tensile strength of particles. Finally, definitive shear zones develop in agglomerate biaxial tests, and this is representative of real sand behavior.

There are several model assumptions that limit the validity of the model. First, the sole use of a uniaxial compressive test to calibrate strength behavior of grains completely ignores the shear strength of the agglomerate. It would be useful to have an additional shear strength calibration test; however, no reliable test is available for real grains and therefore no data is available. It is possible that the shear strength of artificial materials is more readily available, such as for artificial proppants, and therefore a simple shear calibration test could be incorporated if modeling this material. Second, elemental particle size of the agglomerates is used as a scaling factor; however, this size affects fracture toughness and therefore will effect the fracturing behavior of the agglomerate. As computer calculation capabilities increase, a fracture toughness calibration test can be incorporated into the agglomerate calibration routine. Third, mass of the grain represented by the agglomerate is not conserved, and this causes increasing compaction rates as the agglomerates fractures. The effect of these internal voids can be reduced by using lower porosity packing algorithms, such as packing routines with multiple particle sizes; however, any packing routine has to be extensively tested and can potentially have other difficulties associated with it. Finally, since the agglomerate is porous, estimates of permeability reduction with compaction cannot be simulated at this time. Decreases in agglomerate porosity and agglomerate particle size can reduce the permeability of the
agglomerate, simulating a solid material, and potentially solve this problem.

Most of the assumptions behind the agglomerate model can be eliminated or reduced upon increases in computer calculation speed. Therefore, it is possible that agglomerate modeling will become more accurate in the near future. However, it is still unclear whether it will play a strong role in the modeling of granular materials for field applications due to the large number of uncertainties in calibration for such problems. Instead, it seems that agglomerate models are primarily suited for modeling laboratory testing, and understanding the mechanisms of granular crushing.

At this time, the author believes that the agglomerate model may be well suited to further refine the replacement models of Chapter 2, which have better computational efficiency and mass conservation. For example, confined loading tests can be simulated on agglomerates and used to predict or validate failure criterions for grains in a rock to be used in replacement models. As well, agglomerates can be used as a more accurate particle replacement scheme for the DEM replacement models. In this case, the failure criterion would not define failure, but rather would be used to screen grains in high stress regions that should be replaced by breakable agglomerates. It may be most advantageous to consider a combination of agglomerate and replacement models to most accurately model grains in rock.
APPENDICES

A. Additional Information Regarding PFC Physics

Additional information regarding the contact models and bonding models in this thesis is provided in this Appendix (information modified from Itasca, 2005a)

CONTACT MODEL

There are two commonly used contact models available in PFC$^{3D}$: linear and Hertzian. The linear model is used in the development of the agglomerate model in this thesis, and the Hertzian model is used for an elasticity comparison test in Chapter 5.

In the linear model, each particle’s stiffness is constant throughout the simulation, whereas in the Hertzian model the resultant spring stiffness increases for increasing compression of the contacts series spring in order to approximate the Hertzian contact of two spheres. The properties of the Hertzian model are therefore specified by assigning a shear modulus, $G$, and Poisson ratio, $\nu$, of a representative material yielding the relationship to the secant normal stiffness, $K_n$, as:

$$
K_n = \left( \frac{2\langle G \rangle \sqrt{2R}}{3(1-\nu)} \right) \sqrt{U} \quad \text{(Eq. A. 1)}
$$

and shear stiffness, $K_{rs}$, as:

$$
K_{rs} = \left( \frac{2\langle G \rangle^2 (1-\nu) \sqrt{R}}{2-\nu} \right) \left| \frac{F_i}{\pi \rho^2} \right|^{1/3} \quad \text{(Eq. A. 2)}
$$

where:

$$
\langle G \rangle = 0.5(G^{[A]} + G^{[B]}) \quad \text{(Eq. A. 3)}
$$
\[ \{v\} = 0.5(v^{A} + v^{B}) \] \hspace{1cm} \text{..................................................................(Eq. A. 4)}

\[ \overline{R} = \frac{2R^{A}R^{B}}{R^{A} + R^{B}} \] \hspace{1cm} \text{..................................................................(Eq. A. 5)}

where \( G, v, \) and \( R \) are the shear modulus, Poisson’s ratio, and radius of particles \( A \) and \( B \).

Ultimately, it is the contact forces in the normal and shear directions that are of interest since they control movement at the contact in the next calculation cycle. The amount of force in the normal direction, \( F_{n}^{\text{new}} \), is calculated based on the amount of overlap, \( U \), between the two rigid particles according the following formula:

\[ F_{n}^{\text{new}} = K_{n}U \] \hspace{1cm} \text{..................................................................(Eq. A. 6)}

where \( K_{m} \) is the resultant stiffness calculated at the contact between two particles or a particle and wall.

Similarly, the incremental shear force is calculated based on the amount of displacement in the shear direction, \( \Delta U \), yielding an incremental shear force, \( \Delta F_{s} \), given as:

\[ \Delta F_{s} = -K_{s}\Delta U \] \hspace{1cm} \text{..................................................................(Eq. A. 7)}

It is extremely important to note that the shear force increment calculated is an incremental force, unlike the normal force, which was absolute and given on geometry alone in each step. This incremental force must be added to the previous shear force at each calculation cycle. Therefore, the new shear force is given as:

\[ F_{s}^{\text{new}} = F_{s}^{\text{old}} + \Delta F_{s} \] \hspace{1cm} \text{..................................................................(Eq. A. 8)}

This shear force will continue to increment at the contact until the frictional slip resistance is exceeded at which point the shear force is constant for additional calculations.
PARALLEL BONDING MODEL

The parallel bonding model is used in the development of the agglomerate model of this thesis. The parallel bonding model is based on cylindrical beam theory and is illustrated in the remainder of this Appendix.

The force and moment vectors for the parallel bond are composed of normal and shear components as follows:

$$F_i = F_i^n + F_i^s$$

$$M_i = M_i^n + M_i^s$$

(Eq. A. 9, Eq. A. 10)

All components of force and moment are calculated in increments over each time step. The incremental normal component of the force, $\Delta F_i^n$, is given as:

$$\Delta F_i^n = (-k^n A \Delta U_i^n) n_i$$

(Eq. A. 11)

where $k^n$ is the normal spring stiffness, defined in stress/displacement units, $A$ is the area of the bond, and $\Delta U_i^n$ is the incremental normal movement over the last calculation, and $n_i$ is the unit normal vector.

The incremental shear component of the force, $\Delta F_i^s$, is given as:

$$\Delta F_i^s = -k^s A \Delta U_i^s = -k^s A V_i \Delta t$$

(Eq. A. 12)

where $k^s$ is the shear spring stiffness, defined in stress/displacement units, $A$ is the area of the bond, $V_i$ is the velocity vector, and $\Delta t$ is the incremental time.

The incremental normal component of the moment, $\Delta M_i^n$, is given as:

$$\Delta M_i^n = (-k^s J \Delta \theta^n) n_i$$

(Eq. A. 13)

where $k^s$ is the shear stiffness, $J$ is the polar moment of inertia, $\Delta \theta^n$ is incremental relative rotation, in radians, that the particles have rotated relative to one another, and $n_i$ is the unit vector.

The incremental shear component of the moment, $\Delta M_i^s$, is given as:

$$\Delta M_i^s = (-k^s J \Delta \theta^n) n_i$$
\[ \Delta M_{i}^{\sigma} = -k^\sigma I \Delta \theta_{i}^{\sigma} \]  
……………………………………………………………………..(Eq. A. 14)

where \( k^\sigma \) is the normal stiffness, \( I \) is the moment of inertia of the disc cross section, and \( \Delta \theta_{i}^{\sigma} \) is the incremental relative rotation of the particles, in radians.

The incremental rotation of the particles, \( \Delta \theta_{i} \), in these formulas is given as:
\[ \Delta \theta_{i} = (\omega_{i}^{[B]} - \omega_{i}^{[A]}) \Delta t \]  
……………………………………………………………………..(Eq. A. 15)

where \( \omega_{i} \) is the angular velocity, in radians/time, of the particles A and B.

As well, the polar, J, and area, I, moments of inertia are given as:
\[ J = 0.5 \pi R^4 \]  
……………………………………………………………………..(Eq. A. 16)
\[ I = 0.25 \pi R^4 \]  
……………………………………………………………………..(Eq. A. 17)

where \( R \) is the radius of the parallel bond.

These incremental force and moment components are added to the values of the previous calculation. By beam theory, the maximum tensile, \( \sigma_{\text{max}} \), and shear stress, \( \tau_{\text{max}} \), of the parallel bond are given as:
\[ \sigma_{\text{max}} = \frac{-F_{\sigma}^{\sigma}}{A} + \frac{M_{i}^{\sigma}}{I} R \]  
……………………………………………………………………..(Eq. A. 18)
\[ \tau_{\text{max}} = \frac{F_{i}^{\sigma}}{A} + \frac{M_{\sigma}^{\sigma}}{J} R \]  
……………………………………………………………………..(Eq. A. 19)

If these values exceed the tensile or shear strength of the parallel bond, it breaks.
B. Initial Agglomerate Microproperty Selection

The first step in generating a PFC$^{3D}$ material capable of representing a continuous material composing a grain, such as quartz, is to choose suitable elastic micro-properties that will give the desired macroscopic behavior. As mentioned in Chapter 3, this is an iterative process since the packing arrangement is variable and will also affect behavior of the material. However, it is shown in Section 3.2 that it is at least possible to estimate our stiffness values from Young’s modulus by considering a cubic pack, and that Poisson’s ratio will vary depending on the ratio of the normal to shear stiffness. This estimation procedure can also be used effectively to prescribe bonding properties to a randomly packed model, as used in this thesis.

Again, a cubic packing model is used to estimate microproperties for a bonded model. Section 3.2 shows that the stiffness at a contact for a cubic pack is representative of the stiffness for the entire model; however, for the parallel bonded case, the stiffness at a contact is the result of the contact model, or stiffness due to the contacting particles, as well as the parallel bond. Therefore, for a solid material it is reasonable to invoke the additional constraint that the stiffness contribution of the parallel bond is proportional to the percentage of void space in the granular pack, since that is the area the bond is representing:

\[ k_{pm} = \phi k_{rn} \]  
\[ k_{bn} = (1 - \phi)k_{rn} \]

where $k_{pm}$ is the stiffness of the parallel bond (Force/distance), $k_{bn}$ is the stiffness of each contacting ball (Force/distance), $\phi$ is the porosity (percentage of voids per volume), and $k_{rn}$ is the required resultant contact stiffness necessary at the contact (Force/distance). As
shown in Section 2.2, the non-series resultant stiffness, \( k_m \), can be calculated using Young’s modulus, \( E \), in the equation relating stiffness to Young’s modulus for a cubic pack of particles:

\[
k_m = 2K_{\text{result}} = 2(2Er)\]

where \( K_{\text{result}} \) is the series stiffness for the contact and \( r \) is the radius of the particles in the pack.

Since Poisson’s ratio is controlled by the ratio of shear to normal stiffness, \( \lambda \), the ball and parallel bond shear stiffness, \( k_{bs} \) (Force/distance) and \( k_{ps} \) (Force/distance), are calculated as:

\[
k_{ps} = \lambda k_{pn} \]

\[
k_{bs} = \lambda k_{bn} \]

Finally, since the parallel bond stiffness values are defined in terms of stress/distance, \( k_{pn} \) and \( k_{ps} \) are divided by the factor \( \Pi r^2 \) to calculate the PFC input values.

It is noted that the strength parameters of friction coefficient and parallel bond normal and shear strength are initially set high to avoid material damage during elastic calibration.
C. Expansion Algorithm

1. Create a container using walls that can hold the PFC material (Figure C.1).

![Figure C.1. Container for holding particles during expansion algorithm.](image)

2. Specify the porosity, $\phi$, and average particle radius, $r$, for the particles that will be placed within this container and calculate the number of particles necessary, $m$, based on the volume of the container, $V_b$:

$$m = \frac{(1 - \phi)V_b}{\frac{4}{3} \pi r^3}$$

(Eq. B1.1)

3. Shrink each calculated particle’s radius by a constant, arbitrary factor, $s$, such that the particles placed are smaller than the final desired sizes. This allows for placement of the particles within the container without overlapping.

4. Place the reduced size particles in the container (Figure C.2). Calculate the new porosity, $\phi_r$, of the reduced size particles in the container.

$$\phi_r = 1 - \frac{\sum_{i=1}^{m} \frac{4}{3} \pi r_i}{V_b}$$

(Eq. B1.2)
5. Calculate the expansion factor, $\lambda$, to achieve the initial, desired porosity $\phi$ as:

$$\lambda = \left(\frac{1 - \phi}{1 - \phi_r}\right)^{1/3}$$

…………………. (Eq. B1. 3)

6. Expand the particles by the expansion factor and let equilibrate (Figure C.3).

7. Bond particles with parallel bonds.

Figure C. 2. Reduced sized particles in container.

Figure C. 3. Particles packed in container at final, desired porosity.
D. Choosing Pack Porosity for Initial Target Stress

The value used for porosity in the expansion procedure is particularly sensitive. Consider the idea of modeling a solid material; it is necessary that the majority of particles be touching the other particles around them so that the contact distribution is continuous. If the contacts are not touching, the material behaves as a collection of loose particles that initially flow and do not build resistance to stress. Additionally, it is useful and time saving if this densely packed state is reached upon the initial packing of particles, in this case performed by the expansion algorithm of Appendix C. Therefore, it is necessary to choose a low enough porosity for the expansion algorithm in order to obtain a packed sample, but at the same time, not too low of a porosity so that extremely high stresses are generated within the sample, as too many particles are packed within too small of a space. Observe the graph in Figure D. 1:
Figure D. 1. Change in stress of a packed sample with varying porosity: it can be seen that the stress in a packed sample is highly sensitive to the porosity or number of balls in the container.

It can be seen that the average stress on each particle within the rectangular container (Itasca, 2005a – measurement circle logic) is highly sensitive to the porosity, or number of particles in the container. This sensitivity indicates there is generally a small range of suitable porosity values, or number of balls, suitable for any sized container before the stress after packing becomes incredibly large. Again, the chosen value of stress, although arbitrary, should be high enough to provide a tight pack, but does not exceed a set limit of stress, generally 1-5% of the maximum testing stress that the PFC pack will see during modeling.
E. Information Regarding the Biaxial Test in PFC

The biaxial test is referenced several times in this thesis during calibration procedures. A biaxial test is a stress test on a sample of material where the stress in the horizontal direction is held constant while the stress in the vertical direction is increased (Figure E. 1)

![Biaxial Test Diagram]

Figure E. 1. Illustration of biaxial test: the horizontal stress is held constant while the sample is loaded in the vertical direction.

Young’s modulus, $E$, and Poisson’s ratio, $\nu$, are calculated from a biaxial test as:

$$E = \frac{\Delta \sigma_z}{\Delta \varepsilon_z} \quad \text{.................................................................(Eq. E. 1)}$$
\( \nu = 0.5 \left( 1 - \frac{\Delta \varepsilon_v}{\Delta \varepsilon_a} \right) \) 

(Eq. E. 2)

where \( \frac{\Delta \sigma}{\Delta \varepsilon} \) and \( \frac{\Delta \varepsilon_v}{\Delta \varepsilon_a} \) are the slope of the axial stress vs. axial strain and volumetric strain vs. axial strain graphs (Figure E. 2 and Figure E. 3).

Figure E. 2. Graphical calculation of Young’s modulus: Young’s modulus is the slope of the axial stress vs. axial strain graph.

Figure E. 3. Graphical relationship to Poisson’s ratio: The slope of the volumetric vs. axial strain graph is the value of \((1-2v)\), where \(v\) is Poisson’s ratio of the material.
The routine for conducting a biaxial test in PFC$^{3D}$ is extensively covered in the PFC$^{3D}$ User’s Guide (Itasca, 2005c) and should be consulted for additional information regarding implementing the stresses using a wall servo mechanism and plotting the stress and strain graphs.
F. Agglomerate Cutting and Angularity Algorithm and Equations

A programming algorithm is used to cut an agglomerate of an average radius from a container and add angularity, as described in Chapter 4. The general equations and procedures are briefly summarized here.

First, the center for the agglomerate is chosen with the coordinates x0, y0, and z0. Then all particles in the container are traversed and a maximum distance, di, from the center of the agglomerate is calculated for each particle, i, according to:

\[ d_i = \sqrt{(x_i - x0)^2 + (y_i - y0)^2 + (z_i - z0)^2 + r_i} \]  

(Eq. F. 1)

where \( x_i, y_i, \) and \( z_i \) are the coordinates of the particle and \( r_i \) is the particle radius.

If this distance is greater than the desired cut radius, the particle is deleted leaving an agglomerate in the cell as shown in Figure F. 1.

![Figure F. 1. Agglomerate in cell after cutting: Particles outside the desired cut radius are deleted to leave the remaining agglomerate.](image)

Each coordinate for the centroid of the agglomerate is then calculated according to:
\[ x = \frac{1}{n} \sum_{i=1}^{n} x_i \] \hspace{1cm} \text{(Eq. F. 2)}

where \( x = \{x, y, z\} \) and \( n \) is the number of particles.

In order to measure the average size of the rough agglomerate, it is necessary to measure its size in several directions and average. The distance of any given particle, \( d_i \), from the centroid in the \( j^{th} \) direction defined by the angles \( \theta_j \) and \( \phi_j \), is calculated by the following formula:

\[
d_i = (x_i - x) \sin(\phi_j) \cos(\theta_j) + (y_i - y) \sin(\phi_j) \sin(\theta_j) + (z_i - z) \cos(\phi_j) + r_i \hspace{1cm} \text{(Eq. F. 3)}
\]

where \( \theta \) is the rotation angle, \( \phi \) is the declination angle, \( x_i, y_i, \) and \( z_i \) are the coordinates of the particle, and \( r_i \) is the radius of the particle.

The maximum radius, \( R_j^{\max} \), in the \( j^{th} \) direction is then given as:

\[
R_j^{\max} = \max(d_i) \hspace{1cm} \text{(Eq. F. 4)}
\]

The average radius, \( R_{\text{avg}} \), is then found by summing the maximum radius over a finite number of rotations, \( N \):

\[
R_{\text{avg}} = \frac{1}{N} \sum_{j=1}^{N} R_j^{\max} \hspace{1cm} \text{(Eq. F. 5)}
\]

Figure F. 2 and Figure F. 3 illustrate the relationship between the cut radius and the average radius of the agglomerate. This relationship is variable depending on the size of the particles used for developing the agglomerate.
Figure F. 2. Average radius measurement: black line highlights agglomerate average radius.

![Graph showing relationship between average radius and cut radius](image)

Figure F. 3. Average radius vs. cut radius: the average radius is slightly smaller than the cut radius and approximately linearly related.

Additionally, it is possible to introduce angularity into the particle geometry by making selective cuts to approximate a rough surface. First, a random number of cuts are
chosen to be performed on the particle. For each cut, a new random cut radius for the particle, \( T \), is calculated as:

\[
T = (1 - \lambda)R_{\text{avg}} \tag{Eq. F. 6}
\]

where \( \lambda \) is the percentage of the radius desired to trim.

A random rotational direction is then chosen and the distance of each particle in that particular direction is calculated using Eq. F. 3. If the distance of the particle is greater than the trim radius, \( T \), the particle is deleted. This generates a smooth cut perpendicular to the rotational direction and angular agglomerates can be created as shown in Figure F. 4.

![Figure F. 4. Angular agglomerate generation: all agglomerates are the same maximum size but of different random angularity.](image)

The roundness of any agglomerate, \( \psi \), generated using this algorithm is calculated according to the following equation:

\[
\psi = \sqrt[3]{\frac{V_p}{V_{\text{max}}}} = \sqrt[3]{\frac{(4/3)\pi R_{\text{avg}}^3}{(4/3)\pi R_{\text{max}}^3}} \tag{Eq. F. 7}
\]

where \( R_{\text{avg}} \) is the average radius of the agglomerate, and \( R_{\text{max}} \) is the maximum radius of the agglomerate in any direction. An agglomerate of desired roundness is calculated by performing successive cuts until the desired angularity is reached.
G. Agglomerate Equilibration Routine

As noted in Chapter 4, the agglomerate is cut from an initially compressed material, and therefore the natural tendency is for the agglomerate to expand after calculations continue. This expansion is desirable since the initial internal stress within the agglomerate should be approximately zero, as would be expected in a true unloaded material; however, overexpansion causes the parallel bonds to extend to unreasonable levels and render their behavior unpredictable (Figure G. 1). This Appendix describes this process and a method for eliminating overexpansion and retaining the models reproducibility.

Figure G. 1. Overexpansion of parallel bond: parallel bond is represented by three brown lines at the edges and center of the balls. Bond can extend to unreasonable levels without breaking upon equilibration due to stored energy within the contact springs.
In order to counteract overextension shown in Figure G.1, contact bonds of infinite strength are added to the agglomerate, and then calculations are performed until equilibrium is reached and stored energy is removed. The contact bonds prevent the bonded particles from extending past the point of zero overlap (Figure G. 2). This generates a stable model with all particles overlapping by small amounts with negligible locked-in forces, which is desirable (Potyondy and Cundall, 2004). The agglomerate average radius is essentially unchanged after equilibration, indicating that large amounts of extension do not occur. After equilibrium is reached, the contact bonds can be deleted. Then, agglomerates of smaller sizes can be cut from the pre-existing agglomerate at a later time without the additional installation of contact bonds since stored bond energy at equilibrium is negligible.

Figure G. 2. Overexpansion inhibition using contact bond: contact bonds (thicker, orange line in center of particles) prevent particles from separating and are a good method to removed stored potential energy in contact springs. Parallel bond (three thin lines) does not overextend as in Figure G. 1.
H. Uniaxial Compression Initialization Routine

The initialization routine is used to bring walls in for testing and find a static position under a desired external force, as highlighted in Chapter 4. This appendix outlines this procedure.

First, the strengths of the parallel bonds are multiplied by a factor to achieve extremely high levels and avoid any bond breakage during the loading procedure. Then, all particle degrees of freedom are fixed and the top and bottom walls are brought into position by prescribing a translational velocity and cycling until the walls fully touch the particle (Figure H. 1, Figure H. 2). The distance between the walls and the agglomerate can be calculated and used to prescribe an appropriate velocity to yield touching in a desired number of calculations.

---

Figure H. 1. Initializing agglomerate: walls are being brought closer to the agglomerate by prescribing a velocity (red arrows).
Figure H.2. Initialization of agglomerate: Agglomerate is held static between the two walls.

Then, an iterative programming routine, where the forces on each wall are successively increased, stopped, and increased again, is used to find a stable position on the agglomerate boundary (Figure H.3). This routine is needed since the agglomerate will inevitably roll until a static position is found between the walls. After finding the static position, the force is reduced to a suitable start level for testing, usually 5-10% of the maximum predicted load.
Figure H.3. Graph of iterative procedure for finding a stable testing position on agglomerate: Walls are successively compressed and relaxed until a stable, static position is held on agglomerate.
I. Discussion of Assumptions in Agglomerate Strength

The discrete element method differs from other modeling methods, such as finite element, in that the strength behavior is not completely prescribed. For example, in finite element models it is possible to prescribe elastic, plastic, and brittle failure points for the model and the exact behavior that occurs throughout those regions. However, in the discrete element method, bonds are only prescribed strength in pure tension or shear, and the full behavior of the material is greatly dependent upon other material properties, such as elemental particle size, packing arrangement, and type of bonding model used.

For example, Potyondy (2004) indicates that the fracture toughness of a material in PFC$^{2D}$ can be calculated for the simple case of a cubic packing arrangement of rigid discs. In this case, the mode-I fracture toughness, $K_I$, for contact bonded material is given as:

$$K_I = \sigma \sqrt{\pi R}$$

(Eq. I. 1)

where $\sigma$ is the tensile strength of the material and $R$ is the radius of a single disc.

Similarly, Potyondy and Cundall (2004) hypothesizes that the fracture toughness for a parallel bonded material is given as:

$$K_I = \beta \sigma \sqrt{\pi \alpha R}$$

(Eq. I. 2)

where the new parameters $\beta$ and $\alpha$ are coefficients to account for added brittleness provided by the parallel bond bending moment and packing irregularity, respectively.

It is apparent that the fracture toughness for a parallel bonded material is dependent upon the parallel bond radius, packing arrangement, and the radius of the particles. Nevertheless, it is often necessary to use elemental particle size as a scaling parameter in models and the packing arrangement is limited to arrangements that can be
generated relatively easily with a programmed algorithm. At typical computing
capabilities, the maximum number of particles that can be modeled in any discrete
element simulation is 100,000 (Itasca, 2005c). If each agglomerate is composed of 100
particles, this limits the number of agglomerates that can be modeled to 1000. By using
elemental particle size as a scaling parameter and using an expansion algorithm, as
described previously, we are accepting the fact that there may be inherent errors in the
plastic behavior on a granular scale. This potentially affects the speed of failure, as well
as the overall distribution of broken fragments that are generated within the model.

Under all of these inherent assumptions in model generation, it is only necessary
to calibrate the tensile and shear strength of the elemental bonds to the ultimate strength
of the true material. In this project, this strength calibration is achieved by calibrating the
ultimate strength of the discrete element material to the strength of the real particle under
the uniaxial compressive test.

There are also inherent assumptions in the strength calibration performed since
the uniaxial compressive test only defines the tensile strength of the material (Shipway
and Hutchings, 1993a). In this thesis, a ratio of the pure shear to pure tensile strength is
specified, and this ratio is chosen based upon data found for the pure shear and pure
tensile strength of fused quartz at one manufacturer’s website (Goodfellow, 2007). Fused
quartz is melted quartz, and therefore does not have a crystalline form; however, many of
the properties of fused and natural quartz are quite similar (Sosman, 1926), and it is in
this hope that this strength ratio somewhat approximates the true shear strength of the
material. A ratio of shear to tensile strength of 1.45 is used in this thesis.

Other researchers use similar empirical and approximating methods to calibrate
the strength behavior of agglomerates. Cheng et al. (2003), McDowell et al. (2002), and
Robertson et al. (2001) choose a ratio of shear to tensile strength of 1.0, and McDowell et al. (2002) indicates that this is because the bonding material should fracture under the same stress in pure tension and pure shear if the material contains a wide distribution of flaws. Additionally, Khanal et al. (2005) uses other methods to calibrate their agglomerate model of concrete, such as comparing crack patterns, particle distributions, and the degree of liberation between the discrete element model and laboratory tests.

In summary, the accuracy of the strength solution of the agglomerate is extremely difficult to quantify and is largely dependent upon the number of calibration tests available for comparison. Nevertheless, it is possible to run mechanistic simulations with relatively few calibration tests. If it is desired to perform predictive simulations of very specific field situations, more calibration than is performed in this thesis will ultimately be necessary.
J. Broken Pieces Algorithm

This algorithm describes a programming code developed in this thesis for grouping networks of bonded particles in PFC. This code makes it possible to observe fragmentation of models and perform statistics on the sizes, shapes, etc., of broken pieces (Figure J. 1, Figure J. 2).

Figure J. 1. Illustration of broken pieces code: the code separates groups of bonded balls and colors them in order to visualize fragmentation and perform fragmentation statistics, such as in the case of an agglomerate.

1. Define a two column vector with at least as many rows as the number of particles within the model. The first column is used for the particle id number, and the second column is used to store the group number that the particle belongs.

2. Use a programming code to loop through each particle in the model. At each particle (bp), first determine whether it has been assigned a group.

3. If bp is not in a group, check the group numbers of the surrounding particles to which particle bp is bonded and obtain the minimum group number value. Do not look past the initial surrounding contacts. Assign bp and all its bonded contacts into the minimum group number obtained.

4. If particle bp is not bonded to any other particles and does not have a group
assigned to it, assign it a new group number that is 1 greater than the maximum group number in the model.

5. After all particles have been assigned a group, re-loop through all particles and check to make sure that each particle, bp, is in the same group as all of the particles to which it is bonded. If not, change the group number of bp, and all its contacts to the minimum group number in this set. (continued below figure)

Figure J. 2. Illustration of broken pieces code: the code recognizes which groups of particles are interconnected and groups all networks of particles into vectors so that they can be colored. In this case the contact bonds are represented by red lines, and the colored particles are within a distinct group. The black particles are not bonded to anything else.

6. Sort the array by group number.
7. This array can then be used to assign plotting colors or perform statistics on groups.
K. Agglomerate Extraction and Replacement Algorithm

DESCRIPTION OF ALGORITHM

This routine is used in Chapter 5 to replace the rigid PFC particles by breakable agglomerates. The general algorithm for the modeling scheme is as follows:

1. Create an agglomerate with properties and an average radius of the largest grain which will be modeled.
2. Extract all position, bond, force, and contact data for this agglomerate to binary data files and normalize this data based on the center of mass and order of extraction of the particle data.
3. Generate the model in which it is desirable to use breakable agglomerates. Initially use rigid, PFC particles (exospheres, Robertson et al., 2001) at the positions where each agglomerate will be located.
4. Replace each exo-sphere with an agglomerate.

FURTHER DESCRIPTION

First, an agglomerate is created with the desired elastic properties. It is not necessary to prescribe strength properties at this time, since these properties can be modified later. This agglomerate is equal to the largest size grain that will be modeled in the simulation, since other smaller agglomerates can be cut from this base agglomerate. It is noted that when additional particles are removed from this base agglomerate, insignificant expansion of the agglomerate is seen due to stored energy release upon removing the surrounding particles (as was emphasized as being important in Appendix
The extraction point of all micro and state properties is immediately after cutting the particle from the cell and allowing the bonds to equilibrate (Appendix G: Agglomerate Equilibration Routine), and prior to the point of the walls touching the agglomerate before the uniaxial compression test (Appendix H: Uniaxial Compression Initialization Routine). At this point, the agglomerate is static and floating within the triaxial cell with no external forces (Figure K. 1). In this figure, it can be seen that the maximum force acting on the bonds within the agglomerate is 1.239e-2 N, and the maximum velocity of any particle is 1.338e-17 m/s. From these two values, it is reasonable to say that the agglomerate is static and has relatively small amounts of locked in forces; however, the network of contact forces indicates that all particles are still in contact and therefore simulating a continuous material. It is now useful to extract the data from this static agglomerate so that it can be used in other simulations.

To accomplish this data extraction, a programming routine is used to extract all properties into binary data files while looping through the particle and contact information headers in the PFC memory. The exact position, properties, and state of the agglomerate in this static position are stored. Position variables are normalized by the centroid of the agglomerate and particle id numbers are normalized based on the order in which the particle data is extracted. Contact information is then referenced and sorted relative to this extraction order, which makes it possible to quickly locate data when obtaining the data from the extraction files. Each data variable is then written to its own binary source file with the value referenced to the particle extraction number of particle ids, with the lowest value of extraction number associated with the contact information. It is now possible to use this extracted data to replace the default particles, or exospheres,
in PFC with breakable agglomerates.

---

**PFC3D 3.10**

Settings: Model/Perspective

<table>
<thead>
<tr>
<th>Center:</th>
<th>Rotation</th>
</tr>
</thead>
<tbody>
<tr>
<td>X: 0.000e+000</td>
<td>X: 0.000</td>
</tr>
<tr>
<td>Y: 0.000e+000</td>
<td>Y: 0.000</td>
</tr>
<tr>
<td>Z: 6.250e+004</td>
<td>Z: 0.000</td>
</tr>
<tr>
<td>Dist: 4.490e-003</td>
<td>Mag.: 1</td>
</tr>
<tr>
<td>Angle: 22.500</td>
<td></td>
</tr>
</tbody>
</table>

**Wall**

**Ball**

**Velocity**

| Maximum = 1.338e-017 |

**Linestyle**

**CForce Chains**

- Compression
- Tension

| Maximum = 1.239e-002 |

---

**Figure K.1.** Static state of agglomerate: contact force lines (Newtons) indicate that locked-in forces are small and that majority of particles are touching, simulating a continuous material. Additionally, small velocities (meters/second) indicate the agglomerate is static.

A separate replacement code is used to replace the exospheres by agglomerates. This code used a loop routine to traverse each exosphere’s memory data. At each exosphere, the x, y, and z coordinates and radius are stored and the particle is deleted from the simulation. Then a cut radius is calculated based on the exosphere radius and a size calibration curve (Figure F. 3) and particles in the data file that fall within the distance of the cut radius around centroid of the original exosphere are created and assigned predefined id numbers. Then, a separate programming loop is performed
through each contact in the newly created agglomerate particles. Each contact id is normalized so that it can be compared to the data files, and then its location is determined in the data files. If this contact exists within the new agglomerate (i.e. is not a contact between a particle in the agglomerate and another particle outside the agglomerate, or between two particles that do not exist because they fall outside the cut radius) it is given properties and bonded based on the properties and bond data in the binary file data.

It is necessary to obtain the orientation of the contacting particles, since the convention of the forces and moments in PFC is that they act upon particle B (Figure K.3), which is the second particle given in the contact memory within the header loop. It is possible that the PFC code will switch the order of the particles in the contact from the agglomerate extraction simulation to the replacement simulation, since the header is automatically created in each simulation and is not controlled by the user. If this occurs, it is necessary to reverse the sign convention of certain extracted data values, such as shear force and moment values.

Using this routine, a pack of agglomerates is generated within the original positions of the exospheres as shown in Figure K.4. For example, a pack of particles, or exospheres is shown for the biaxial test (Figure K.2). The properties of the exo-spheres and walls, as well as the initial hydrostatic stress, in this initial phase are relatively arbitrary, since all values change when each exosphere is replaced by an agglomerate; however, it is desirable that when the exospheres are replaced by agglomerates the pack still remains tight. This tight pack is desirable since it is computationally less expensive to reduce stress in a tight pack rather than move walls together to compress a loose pack. The tight pack performs less rearrangement upon unloading than a loose pack during loading. This tightly packed initial condition is obtained iteratively by changing the
initial stress level of the exosphere pack, replacing the exospheres with agglomerates, cycling to equilibrium, checking the stress level, and repeating if necessary. Small changes in exosphere properties generally produce large changes in the agglomerate pack stress.
Table K. 1. Information extracted to agglomerate binary data files to be used for replacement.

<table>
<thead>
<tr>
<th>Extracted Information</th>
<th>PFC Function</th>
<th>Modification to Original Data</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>General Information</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td># of balls in agglomerate</td>
<td></td>
<td></td>
</tr>
<tr>
<td># of contacts in agglomerate</td>
<td></td>
<td></td>
</tr>
<tr>
<td>porosity of agglomerate</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Ball Information</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>PFC ball id #</td>
<td>b_id(bp)</td>
<td>Order in which ball is extracted</td>
</tr>
<tr>
<td>normalized ball id #</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ball radius</td>
<td>b_rad(bp)</td>
<td></td>
</tr>
<tr>
<td>local damping coefficient</td>
<td>b_damp(bp)</td>
<td></td>
</tr>
<tr>
<td>ball density</td>
<td>b_dens(bp)</td>
<td></td>
</tr>
<tr>
<td>ball friction</td>
<td>b_fric(bp)</td>
<td></td>
</tr>
<tr>
<td>ball normal stiffness</td>
<td>b_kn(bp)</td>
<td></td>
</tr>
<tr>
<td>ball shear stiffness</td>
<td>b_ks(bp)</td>
<td></td>
</tr>
<tr>
<td><strong>Ball State Information</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>x+translation fix flag</td>
<td>b_xfix(bp)</td>
<td></td>
</tr>
<tr>
<td>y+translation fix flag</td>
<td>b_yfix(bp)</td>
<td></td>
</tr>
<tr>
<td>z+translation fix flag</td>
<td>b_zfix(bp)</td>
<td></td>
</tr>
<tr>
<td>x+rotation fix flag</td>
<td>b_rxfix(bp)</td>
<td></td>
</tr>
<tr>
<td>y+rotation fix flag</td>
<td>b_ryfix(bp)</td>
<td></td>
</tr>
<tr>
<td>z+rotation fix flag</td>
<td>b_rzfix(bp)</td>
<td></td>
</tr>
<tr>
<td>x position</td>
<td>b_x(bp)</td>
<td></td>
</tr>
<tr>
<td>y position</td>
<td>b_y(bp)</td>
<td></td>
</tr>
<tr>
<td>z position</td>
<td>b_z(bp)</td>
<td></td>
</tr>
<tr>
<td>accumulated x displacement</td>
<td>b_xdisp(bp)</td>
<td></td>
</tr>
<tr>
<td>accumulated y displacement</td>
<td>b_ydisp(bp)</td>
<td></td>
</tr>
<tr>
<td>accumulated z displacement</td>
<td>b_zdisp(bp)</td>
<td></td>
</tr>
<tr>
<td>x-translational velocity</td>
<td>b_xvel(bp)</td>
<td></td>
</tr>
<tr>
<td>y-translational velocity</td>
<td>b_yvel(bp)</td>
<td></td>
</tr>
<tr>
<td>z-translational velocity</td>
<td>b_zvel(bp)</td>
<td></td>
</tr>
<tr>
<td>x-rotational velocity</td>
<td>b_rxvel(bp)</td>
<td></td>
</tr>
<tr>
<td>y-rotational velocity</td>
<td>b_ryvel(bp)</td>
<td></td>
</tr>
<tr>
<td>z-rotational velocity</td>
<td>b_rzvel(bp)</td>
<td></td>
</tr>
<tr>
<td><strong>Contact General Information</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1st ball in contact</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2nd ball in contact</td>
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<td></td>
</tr>
<tr>
<td>Bonding Information</td>
<td>c_pb(cp)</td>
<td></td>
</tr>
<tr>
<td>Bonding Information</td>
<td></td>
<td></td>
</tr>
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</table>

*CONTINUED NEXT PAGE*
<table>
<thead>
<tr>
<th><em>Contact State Information</em></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>normal force</td>
<td>c_nforce(cp)</td>
</tr>
<tr>
<td>x shear force</td>
<td>c_xsforce(cp)</td>
</tr>
<tr>
<td><em>Table continued</em></td>
<td></td>
</tr>
<tr>
<td>y shear force</td>
<td>c_ysforce(cp)</td>
</tr>
<tr>
<td>z shear force</td>
<td>c_zsforce(cp)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><em>Parallel Bond Properties</em></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>normal stiffness</td>
<td>pb_kn(pbp)</td>
</tr>
<tr>
<td>shear stiffness</td>
<td>pb_ks(pbp)</td>
</tr>
<tr>
<td>normal strength</td>
<td>pb_nstrength(pbp)</td>
</tr>
<tr>
<td>shear strength</td>
<td>pb_sstrength(pbp)</td>
</tr>
<tr>
<td>bond radius multiplier</td>
<td>pb_rad(pbp)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><em>Parallel Bond State Information</em></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>normal force</td>
<td>pb_nforce(pbp)</td>
</tr>
<tr>
<td>x-shear force</td>
<td>pb_xsforce(pbp)</td>
</tr>
<tr>
<td>y-shear force</td>
<td>pb_ysforce(pbp)</td>
</tr>
<tr>
<td>z-shear force</td>
<td>pb_zsforce(pbp)</td>
</tr>
<tr>
<td>twisting moment</td>
<td>pb_tmom(pbp)</td>
</tr>
<tr>
<td>x-bending moment</td>
<td>pb_xbmom(pbp)</td>
</tr>
<tr>
<td>y-bending moment</td>
<td>pb_ybmom(pbp)</td>
</tr>
<tr>
<td>z-bending moment</td>
<td>pb_zbmom(pbp)</td>
</tr>
<tr>
<td>current normal bending stress</td>
<td>pb_nstress(pbp)</td>
</tr>
<tr>
<td>current shear bending stress</td>
<td>pb_sstress(pbp)</td>
</tr>
</tbody>
</table>

Figure K. 2. Example of biaxial test apparatus filled with exospheres that will be replaced by agglomerates.
Figure K. 3. Sign convention in PFC: normal vector is from A to B, with forces and
moment convention that they act upon B (modified from Itasca (2005a)).

Figure K. 4. Results of replacement scheme: each exo-sphere is replaced with an
agglomerate of equivalent radius.

Upon placement of the agglomerates, the strength values of all bonds bonding the
agglomerates are scaled by a large, arbitrary multiplication factor, such as 1e6, so that no
bonds break during the equilibration process. After scaling the bond strengths,
calculations continue until equilibrium, and then the PFC walls are moved until a small
level of hydrostatic stress is achieved. The bond strength is then reduced by the same
multiplication factor of 1e6, so that the original, correct value of bond strengths are
present at each bond preserving any distribution of strengths. A small, arbitrary number
of bonds usually broke during this initialization procedure.
**TESTING OF REPLACEMENT CODE**

The previously described replacement scheme was tested using the uniaxial compressive test.

First, an agglomerate was created and tested as highlighted in Chapter 4 to obtain a baseline stress-strain curve. If the extraction and replacement scheme works properly, it is possible to extract the data from this agglomerate, delete it, replace it, and still obtain the same stress-strain curve as the baseline curve. The graph in Figure K.5. illustrates that the replacement code developed in this thesis is therefore accurate.

![Graph showing stress-strain curve](image)

Figure K. 5. Replacement scheme verification.
REFERENCES


Penny, G.S., 1988, *An Investigation of the Effects of Fracturing Fluids Upon the Conductivity of Proppants*, Final Report STIM-LAB, Duncan, OK.


