EFFECT OF THE REPRESENTATION OF GRAIN STRUCTURE ON THE PREDICTION OF BRITTLE ROCK MECHANICAL BEHAVIOR USING BONDED BLOCK MODELS

by

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A thesis submitted to the Faculty and the Board of Trustees of the Colorado School of Mines in partial fulfillment of the requirements for the degree of Master of Science (Mining and Earth Systems Engineering).

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During the last few decades, many studies have been focused on the understanding of brittle failure mechanisms in hard rocks where the intact rock strength controls the rock mass strength. Discrete element methods have been used to study fracture development processes in intact rocks through laboratory-scale simulations. The simulations represent the grain structure of a rock as an assembly of Voronoi blocks, where each block represents a mineral grain, and a set of parameters that represents the micro-properties of the grains and the contacts between them is calibrated to numerically replicate the macro-mechanical behavior of the rock. Although Voronoi grain assemblies provide reasonable approximations of actual grain structures, the random nature of such assemblies increases the uncertainty of the calibrated contact micro-properties, potentially leading to incorrect estimations of the rock strength. This study investigated whether a more realistic depiction of the grain structure can be used in combination with previously calibrated sets of micro-properties to predict brittle rock mechanical behavior with a reasonable degree of accuracy and minimal micro-property calibration. A series of 3D Voronoi and 2D deterministic models were developed to assess the effects of grain size, shape, and arrangement on the simulated rock strength. The modeling results show that it is possible to predict the strength of a rock with a high degree of accuracy using reasonably simplified representations of the grain structure in Voronoi models. In addition, the results of the comparative analysis can be used as guidelines to simplify the process of representation of grain structures.
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<tr>
<td>ASTM</td>
<td>American Society for Testing and Materials</td>
</tr>
<tr>
<td>BBM</td>
<td>Bonded Block Model</td>
</tr>
<tr>
<td>BPM</td>
<td>Bonded Particle Model</td>
</tr>
<tr>
<td>BTS</td>
<td>Brazilian Tensile Strength</td>
</tr>
<tr>
<td>CD</td>
<td>Crack Damage Stress</td>
</tr>
<tr>
<td>CI</td>
<td>Crack Initiation Stress</td>
</tr>
<tr>
<td>ISRM</td>
<td>International Society for Rock Mechanics</td>
</tr>
<tr>
<td>SEM</td>
<td>Scanning Electron Microscopy</td>
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<tr>
<td>UCS</td>
<td>Uniaxial Compressive Strength</td>
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LIST OF SYMBOLS

Block Bulk modulus ...................................................................................................................... \( K \)
Block Density............................................................................................................................ \( \rho \)
Block Poisson’s ratio .................................................................................................................. \( \nu \)
Block Shear modulus .................................................................................................................. \( G \)
Block Young’s modulus .............................................................................................................. \( E \)
Contact Dilation Angle ........................................................................................................... \( \psi_c \)
Contact Normal Stiffness .......................................................................................................... \( k_{nc} \)
Contact Peak Cohesion ............................................................................................................. \( c_{pc} \)
Contact Peak Friction Angle .................................................................................................... \( \phi_{pc} \)
Contact Peak Tensile Strength ................................................................................................. \( \sigma_{tpc} \)
Contact Residual Cohesion ....................................................................................................... \( c_{rc} \)
Contact Residual Friction Angle .............................................................................................. \( \phi_{rc} \)
Contact Residual Tensile Strength .......................................................................................... \( \sigma_{trc} \)
Contact Shear Stiffness ........................................................................................................... \( k_{sc} \)
Crack Damage Stress ............................................................................................................... \( \text{CD} \)
Crack Initiation Stress ............................................................................................................. \( \text{CI} \)
Macroscopic Density ................................................................................................................ \( \rho_m \)
Macroscopic Poisson’s ratio ..................................................................................................... \( \nu_m \)
Macroscopic Young’s modulus ...........................................................................................................\( E_m \)

Brazilian Tensile Strength.............................................................................................................\( BTS \)

Uniaxial Compressive Strength ......................................................................................................\( UCS \)
ACKNOWLEDGEMENTS

I would like to express my deepest appreciation to my advisors, Dr. Elizabeth Holley and Dr. Gabriel Walton, for their guidance along the whole research process. Also, I would like to thank Dr. Jurgen Brune and Dr. Ahmadreza Hedayat for providing very useful suggestions and for being part of the thesis committee.

Also, I would like to acknowledge the personnel of the different laboratories of the Colorado School of Mines where different parts of this study were conducted: Omid Frough, Bruce Yoshioka, Brent Duncan, and Muthu Vinayak of the Earth Mechanics Institute; Jae Erickson of the thin-section preparation laboratory; and Dr. Katharina Pfaff of the automated mineralogy laboratory for their help during diverse tests and analyses.

Finally, I would like to thank all the friends and student fellows who helped me with his comments and opinions, particularly, Sankhaneel Sinha, Rami Abousleiman, David Hernandez, and Isaac Simon.
DEDICATION

To my parents.
CHAPTER 1

INTRODUCTION

1.1 Background

In massive rock masses, where the strength of the intact rock controls the strength of the rock mass, ultimate shear strength criteria (e.g., Hoek-Brown) do not represent the multiple stages of rock damage and fracturing processes that are relevant to their brittle behavior in-situ. This can lead to an incorrect estimation of the in-situ rock strength. In recent years, numerical modeling has been used to predict brittle failure mechanisms, first through continuum models that use constitutive models based on failure criteria, and more recently through discontinuum models, which can explicitly represent fracturing processes in brittle rock.

Considerable research has been conducted to understand brittle failure mechanisms using discontinuum numerical models for laboratory-scale simulations (Potyondy and Cundall, 2004; Kazerani and Zhao, 2010; Lan et al., 2010; Kazerani et al., 2012; Chen and Konietzky, 2014; Gao and Stead, 2014; Ghazvinian et al., 2014; Nicksiar and Martin, 2014; Farahmand and Diederichs, 2015; Chen et al., 2016; Mayer and Stead, 2017; Sinha and Walton, 2018; Wang and Cai, 2018; Li et al., 2019; Wang and Cai, 2019; Zhu et al., 2019). A common approach involves replicating the fracture processes occurring in Uniaxial Compressive Strength (UCS) tests and Brazilian Tensile Strength (BTS) tests. The internal grain structure of intact rock specimens is approximated by an assembly of particles, which represent mineral grains that interact at their interfaces. Potyondy and Cundall (2004) developed Bonded Particle Models (BPM) that represent the grains as disks whereas other authors used non-spherical Bonded Block Models (BBM), which represent the grains as triangles (Kazerani et al., 2012), or as polygons (Nicksiar and Martin, 2014)
assembled in a Voronoi structure. In both cases, the BPM and BBM “grains” are always randomly generated.

The results of simulations using different approaches (Lan et al., 2010; Nicksiar and Martin, 2014; Mayer and Stead, 2017; Sinha and Walton, 2018; Liu et al., 2018; Wang and Cai, 2018) show the impact of the grain geometry and grain arrangement within the grain structure on the micro-mechanical behavior of the rock, as well as on the macroscopic response of the specimen. Whereas disk-shaped and triangular grains favor shear failure, due to the lack of interlocking among grains, polygonal grains favor tensile failure as expected in brittle rocks (Mayer and Stead, 2017). Also, the degree of interlocking among grains is controlled by the grain heterogeneity of the rock’s internal structure.

A realistic representation of the grain structure would depict the geometry (i.e., shape and size) of the grains with high accuracy. For our purposes, we would consider a realistic representation to only neglect or approximate minor sub-millimetric details. The differences between the actual grain structure and a realistic representation would not be expected to have a significant effect on the associated representation of the rock’s micro-mechanical characteristics. Although there is no absolute or quantitative measure of “realism” for grain structures, it can generally be acknowledged that the more attributes of a real grain structure that are accurately reproduced in a simulated grain structure, the more realistic that simulated grain structure is.

So far, Voronoi blocks have achieved the most realistic representations of the geometrical heterogeneity of the grain structure within an intact rock (Lan et al., 2010; Gao et al., 2016; De-Fu et al., 2017; Li et al., 2017; Wang and Cai, 2018; Zhang et al., 2018; Wang and Cai, 2019). Voronoi blocks resemble the shape of polygonal/polyhedral grains more accurately compared to other block shapes (i.e., triangles or tetrahedrons). Also, conventional Voronoi blocks can depict the mineral
composition and average grain size of the rock’s internal structure (Lan et al., 2010; Gao et al., 2016), allowing for a reasonable representation of the grain structure that can replicate commonly measured rock mechanical attributes. Nevertheless, such conventional Voronoi structures have limitations to account for the wide variability of grain sizes and grain shapes within a grain structure. The geometrical representation provided by conventional Voronoi models can be considered an intermediate degree of realism, which offers a basic representation of the average grain shape, average grain size, and average mineral composition. Therefore, Voronoi models allow for a reasonable approximation of the rock’s micro-mechanical characteristics to be developed, but predictions of macro-properties made with these models have uncertain accuracy. Conversely, reasonably accurate predictions of macro-properties (i.e., UCS, tensile strength, crack initiation stress, crack damage stress, Young’s modulus, and Poisson’s ratio) would be expected to display results within the variability range of measurements made in actual rock specimens. For example, if an intact rock presents UCS with an average value of 200 MPa and variability of ± 20 MPa (i.e., variability of ± 10%), reasonably accurate predictions would show results between 180 MPa and 220 MPa.

To numerically replicate the macroscopic response of the rock specimen, the parameters that represent the micro-mechanical properties of mineral grain and grain-to-grain contacts undergo an iterative calibration process. Accordingly, the values of the micro-mechanical properties are adjusted until the macro-response of the model reproduces the actual macro-mechanical behavior of the intact rock (Farahmand and Diederichs, 2015; Li et al., 2017). The random nature of Voronoi block assemblies adds uncertainty to the contact micro-properties obtained from the calibration process. Therefore, it is not possible to obtain a fully calibrated system with definitive micro-
properties to be employed in the prediction of rock mechanical behavior (Mayer and Stead, 2017) due to the randomness of the Voronoi grain structure.

Increasing the realism of the grain structure representation would minimize the uncertainty of the set of calibrated micro-properties. Consequently, the prediction of rock mechanical behavior using a set of calibrated micro-properties obtained from a model with the actual grain structure of a rock specimen could achieve reasonable accuracy when used for forward predictions.

1.2 Problem Statement

The realistic simulation of brittle fracture using calibrated numerical models is important for rock engineering purposes, particularly if the goal is to predict the mechanical behavior of brittle rocks with reasonable accuracy (i.e., accuracy on the order of the natural variability between rock specimens). The application of Voronoi blocks in Bonded Block Models (BBM), has improved the representation of the grain structure of a rock by allowing a depiction of the microstructure that approximates the actual average grain shape and grain size. However, the random nature of the Voronoi block assemblages prevents the complete calibration of the micro-properties of the model, since, for every set of Voronoi blocks, a different set of micro-properties is obtained from the calibration.

With that said, a properly conducted calibration process that produces a match of the rock’s macro-properties in agreement with the micro-mechanical behavior of the rock can generate a set of micro-properties that allows for the approximate prediction of rock mechanical behavior. However, considering the great variability of the values of calibrated micro-properties obtained by diverse authors (Lan et al., 2010; Chen and Konietzky, 2014; Farahmand and Diederichs, 2015;
Chen et al., 2016), it is difficult to determine which of the previously established sets of micro-properties results is the most accurate for prediction of rock mechanical behavior. Since each set of micro-properties was calibrated using a different Voronoi model, the values of the calibrated properties are not universal due to the random nature and degree of realism represented in each Voronoi structure.

With all this in mind, a model that implements a realistic grain structure in terms of grain size, shape, and arrangement can be used in combination with those various sets of micro-properties to test which set can most reasonably replicate the macro-properties of a given rock. Consequently, the identified set of micro-properties can be used to run numerical simulations that allow for more realistic predictions of rock strength.

1.3 Thesis Objectives

The general goal of this research is to assess whether the use of a more realistic representation of the grain structure (i.e., detailed representation of the geometry of each grain, and the distribution of grains) in a BBM can improve the accuracy of the prediction of brittle mechanical behavior of brittle rocks. A more realistic grain structure representation would prevent or minimize the effort required for the calibration of micro-properties, as the same (or similar) micro-properties could be used for the same mineral or mineral-to-mineral contact properties between different rocks.

The specific objectives of this study are to:

- Characterize, the mineral composition, and texture (i.e., grain size, shape, and arrangement) of specimens cut from one core sample of Wausau granite
• Digitize the grain arrangement of the previously characterized disk-shaped specimens of Wausau granite, representing the actual mineral type, shape, size, and distribution of the mineral grains

• Develop 2D deterministic BBMs, based on the digitized grain arrangements of disk-shaped specimens, to comparatively analyze them against conventional Voronoi BBMs

• Generate 3D and 2D Voronoi BBMs of the rock core specimens with different grain arrangements, grain sizes, and grain shapes to conduct a comparative analysis of the effect of each geometric parameter on rock mechanical attribute predictions

• Run 3D and 2D simulations of UCS and BTS tests using four previously established sets of contact micro-properties to assess whether the macro-mechanical behavior of the rock can be predicted

• Compare the results of 3D simulations against those from 2D simulations to analyze whether the four sets of contact micro-properties are useful to predict the rock’s mechanical behavior in 3D and 2D

• Document the limitations of BBMs as a tool to predict intact rock mechanical behavior

1.4 Thesis Outline

This thesis is structured as a paper-based thesis, where the main chapter will be submitted as a journal manuscript. In total, the thesis includes three chapters, which are outlined below. All references are provided at the end of the thesis.

Chapter 1 introduces the context for this thesis with respect to the depiction of the grain structure of rocks in numerical simulations to model failure mechanisms of intact brittle rock. The objectives and contributions of this research are also explained in this chapter. Finally, this chapter
provides a literature review of brittle failure mechanisms, testing procedures for describing the mechanical behavior of the rock, techniques for the characterization of the internal structure of rocks, and numerical modeling methods used to simulate rock damage.

Chapter 2 presents the approach developed to assess the impact of the representation of the grain structure of intact rocks on the behavior of numerical models for the prediction of rock damage. This chapter, in its first sections, describes the methodology followed for generating two-dimensional deterministic BBMs of the Wausau granite, and three-dimensional Voronoi BBMs with different grain assemblies. Following, this chapter describes the rock mechanics tests run on specimens of Wausau granite, as well as the setup of 3D and 2D laboratory-scale simulations with varied micro-mechanical properties. The final section provides a comparative analysis of the results of the simulations.

Chapter 3 provides a discussion of the results and findings of this research work, a summary of the conclusions of this study, and recommendations for future work.

1.5 Literature Review

1.5.1 Brittle Failure Mechanisms

For underground excavations, failure modes are mainly a function of the intact rock strength, the geometry and strength of pre-existing discontinuities, and the in-situ stress conditions affecting the rock mass (Martin et al., 1999). The failure mechanisms that take place in an excavation are the result of the combinations of these factors. Rock mass classification systems are the typical means to quantify the rock mass quality, taking into account the previously mentioned factors that
control the failure mechanism of the rock mass. Classification systems like RMR (Bieniawski, 1973) and GSI (Marinos and Hoek, 2002) are employed to estimate support requirements, and, in combination with the Hoek-Brown strength criterion (Hoek et al., 2002), to estimate the overall strength of the rock mass.

As described by Carter et al. (2008), classification-based strength criteria are effective in representing rock masses at the mid-range of the competence scale, where failure is controlled by the inter-block shear strength rather than intact rock strength. On the other hand, this approach is not accurate for rock masses at both ends of the same competence scale, for example, where pre-existing discontinuities are sparse enough such that they are not highly relevant to the failure mechanism. The strength of the rock masses at the low end of the scale, with very low Unconfined Compressive Strength (UCS) or an intensely fractured structure, is controlled by the weakest component of the system. Similarly, the strength of massive hard rocks at the high end of the scale is defined by the intact rock strength.

Martin et al. (2001) explained the occurrence of two primary rock failure modes: structurally-controlled failure and stress-controlled failure. Figure 1.1 summarizes the possible mechanisms in terms of the degree of fracturing (expressed as a GSI value), and the magnitude of the in-situ stress. Structurally-controlled failures occur in moderately to highly fractured rock masses under low in-situ stresses. The main failure mechanism is the falling or sliding of rock wedges under the force of gravity. The susceptibility to failure is controlled by the shear strength of the discontinuities.

Stress-controlled failures or brittle failures are typical of massive to sparsely fractured rock masses in environments of intermediate to high in-situ stresses. Brittle failures are controlled by the micromechanical properties of the rock, in combination with the changing stresses around the excavation (Diederichs, 2007). In an underground opening, the high induced compressive stresses
around the excavation lead to the initiation and propagation of stress-induced fractures parallel to the excavation boundary, which is parallel to the direction of maximum principal stress (Ghazvinian, 2010; Azocar, 2016). In the absence of any confining pressure, the high induced stresses tangent to the excavation periphery lead to the extension of the fractures parallel to the excavation wall. This kind of failure occurs, depending on the stress magnitude, in the form of localized spalling under intermediate in-situ stress levels, or as slabbing or even strain-bursting under high in-situ stress levels.

Multiple authors have used Uniaxial Compressive Strength (UCS) tests to interpret brittle failure mechanisms in hard rock (Martin et al., 2001; Cai et al., 2004; Diederichs et al., 2004). Analysis of several laboratory UCS tests (Diederichs et al., 2004; Hoek and Martin, 2014) shows that there are various stages of brittle rock damage development: a) Initial closure of pre-existing flaws due to increasing axial stress applied on the rock specimen. b) Crack initiation (CI) at a stress level of 30% to 50% of the UCS, which indicates the beginning of stable crack growth. c) Unstable crack growth initiates at the crack damage (CD) threshold at a stress level of 70% to 80% of the UCS, showing a characteristic reversal in the volumetric strain slope (under uniaxial loading conditions). d) Finally, the coalescence of the cracks results in the formation of macro-scale shear bands at the peak strength (Martin et al., 2001). The crack initiation (CI) threshold and crack damage (CD) threshold are the values commonly used to denote the main transitions among those stages. Figure 1.2 shows the stages of damage development in laboratory tests of brittle rock, and the relationship between the strength thresholds and the peak strength of the rock.
Figure 1.1: Modes of failure in hard rock tunnels (modified after Martin et al., 2001).
1.5.2 Rock Mechanics Laboratory Testing

In order to understand fracture mechanisms in rocks, it is necessary to measure the strength and elastic properties of rocks, which govern the mechanical behavior of the rock. Unconfined compressive, confined compressive, direct tensile, and indirect tensile tests are the usual methods to measure such rock properties. These tests are designed to simulate the stress state that affects a rock in the field and to monitor the resulting rock mechanical behavior. While conducting these tests, the development of the different stages of rock damage can be detected using techniques.
such as acoustic emission monitoring, strain gauge measurements, or other less common methods like electrical resistivity, photo-elastics, or ultrasonic probing (Eberhardt et al., 1998). This section reviews the most commonly used rock mechanics laboratory tests and crack development detection techniques.

1.5.2.1 Laboratory Test Monitoring Methods

a) Strain Measurements

This method records slight changes in the rock sample deformation in both the axial and radial directions and allows for quantitative description of the associated strains and analysis of stress-strain data for indications of crack development (Eberhardt et al., 1998).

In this method, deformations are often measured by attaching electric resistance strain gauges to the surface of the rock specimen using glue or cement. The electric resistance strain gauges function under a principle discovered by Lord Kelvin, where the resistance of a wire changes in proportion with the strain (Brady and Brown, 2004). Changes in the resistance of the strain gauges are recorded, while stresses are induced on a rock specimen during a test. Such resistance changes are proportional to the rock specimen strains. Wire and foil strain gauges are commonly used in rock mechanics testing. These materials are able to show more sensitivity to strain thanks to their high resistance and high impedance, which makes them optimal for strain gauges (Ghazvinian, 2010). The use of electric resistance strain gauges has some limitations that may affect the readings, such as the difficulty in having a good contact bond between the rock and the gauge, the fact that only the area covered by the gauge is monitored rather than the entire specimen, and the fact that temperature cannot be eliminated (Brady and Brown, 2004).
Linear variable displacement transformer (LVDT) gauges and extensometers are used as an alternative to electric resistance strain gauges. LVDTs work on a mutual inductance principle and monitor the voltage changes. The linear displacement of the core along the axis of the instrument is directly proportional to the voltage changes. These sensors consist of a cylindrical ferromagnetic core within a tube surrounded by three solenoidal coils, which is attached to the object to be measured. The movement of the core produces an electrical output that is recorded by the sensor (Dunnicliff, 1982).

b) Acoustic Emission Monitoring

Acoustic Emission (AE) monitoring allows for the detection and location of the cracks that form in a rock specimen during a rock mechanics test, as well as their propagation in real-time. The method consists of the detection of self-generated acoustic signals within the rock specimen during loading. The AEs occur as a result of the induced stresses throughout the specimen (Koerner et al., 1981), while mineral grains slide past each other, causing crack development. The sudden release of stored elastic strain energy is turned into an elastic strain wave, which travels throughout the specimen and then can be detected as an AE signal when it reaches the specimen surface (Ghazvinian, 2010). The AE monitoring system uses high-frequency emission sensor transducers attached to the specimen surface to detect cracking propagation (Wang et al., 1989). The emission sensors detect the mechanical energy associated with AE events and convert them into an electrical signal (Dunnicliff, 1998). The frequency of the electrical signal usually ranges from 50 to 500 kHz. Depending on the expected frequency, a different type of sensor can be used. The differences in arrival times of different AE signals allows one to locate the source of an AE, and subsequently to interpret the processes of crack initiation or propagation.
1.5.2.2 Laboratory testing

a) Compression Tests

There are two commonly applied types of compression tests in rock mechanics: The Uniaxial Compressive Strength (UCS) test, and the triaxial compressive strength test.

The UCS test is the most common test for rock mechanics purposes, where the primary goal is often to measure the peak strength of the rock specimen. The ideal result of a UCS test is a complete stress-strain curve for a specimen, which is obtained if the axial and lateral strains are recorded. The Young’s modulus and the Poisson’s ratio can be estimated from these data. Also, a complete stress-strain curve allows for analysis of how the deformations take place in relation to the crack development during the different stages of rock damage; thus, the CI and CD damage thresholds can be determined (Martin et al., 2001). Following the recommendations of the International Society for Rock Mechanics (ISRM, 1999) and the American Society for Testing and Materials (ASTM, 2008), the UCS test should be performed on a cylindrical rock specimen with a height to diameter ratio of 2 to 3, preferably with a diameter greater than 50 mm. Moreover, the diameter of the specimen should be at least 20 times the average grain size of the specimen (Ghazvinian, 2010). The testing apparatus for a UCS test should be capable of applying and measuring the axial load to the specimen (see figure 1.3). The loading frame should have a stiffness greater than 5 MN/m. During the test, load should be applied at a constant stress rate in such a way that failure occurs within 5-10 minutes of loading (ISRM, 1979).
The triaxial compressive strength test measures the strength of a rock specimen under confined conditions, which is an approximation of three-dimensional stress conditions. The triaxial test is performed on cylindrical rock specimens prepared in the same way as the ones for UCS tests. As shown in Figure 1.4, the testing equipment consists of a pressure vessel or triaxial cell, where the rock specimen is confined, a loading device to apply axial load, a device to apply confining pressure, and equipment to monitor the loading and strains (ISRM, 1978). When the rock specimen is placed inside the triaxial cell, a rubber jacket surrounds and isolates the specimen from the
confining fluid (Brady and Brown, 2004). During the test, an initial uniform hydraulic pressure, \( \sigma_3 \), is applied to the surface of the specimen, and then axial compressive stress, \( \sigma_1 \), is increased at the top of the sample (Mishra and Janecek, 2017). The results of the triaxial tests are stress-strain curves, where the different stages of crack development under different confining pressures can be analyzed.

Figure 1.4: Two triaxial test designs: (a) Hoek cell; (b) cell used by Elliot and Brown (after Elliot, 1993).

b) Tensile tests

Tensile testing of rocks is commonly conducted following two methods, the direct tensile strength test and the indirect Brazilian Tensile Strength (BTS) test. The direct tensile test is considered the most valid method for determining the tensile strength of rocks, when the test is
conducted properly (Perras and Diederichs, 2014). The basic test arrangement consists of pulling a rock specimen from both ends using a pull frame until tensile failure occurs. A direct tensile test is considered valid when tensional failure occurs at the midpoint of the specimen. Commonly, the rock specimen has a dog-bone shape that allows to grip the ends of the specimen to the testing apparatus through special caps as designed by Hoek (1964) or a cylindrical shape in which case metal caps should be glued or cemented to the ends of the specimen and then attached to the testing machine (ISRM, 1978). Also, as referred by Perras and Diederichs (2014), Brace (1964) and Gorski (1993) introduced variations of this test named biaxial extension and compression load converter tests, respectively, which use axial compression to induce tensional failure on bone-shaped rock specimens (see Figure 1.5).

The BTS test is the most used method to measure the tensile strength of rock, given the difficulty of executing direct tensile tests on rock. The stress state in a BTS test is not purely tensional, and it is comparable with confined direct tensile tests (Diederichs, 1999). For this test, a disk-shaped specimen with flat and parallel faces is loaded diametrically by two opposed curved steel jaws that have a contact surface with the rock specimen over an arc of approximately 10 degrees at failure. However, there are other loading platen arrangements also used for this test (Perras and Diederichs, 2014), as shown in Figure 1.6. The disk diameter should be at least 50 mm and the diameter to thickness ratio about 2:1. According to the ISRM (1978) and ASTM (2001) standards, the tensile stress at failure is a function of the applied load, the diameter, and the thickness of the rock specimen. The BTS test has been found to give tensile strengths higher than those of direct tension tests. Nevertheless, it is commonly assumed that they provide a good approximation of tensile strength of rock, and an empirical correction can be applied to estimate direct tensile strength from BTS test results (Perras & Diederichs, 2014). Although strains are
usually not monitored in BTS tests, for studies focused on fracture processes, strain monitoring is common.

Figure 1.5: Direct tension testing arrangements. (a) Split grips for dog-bone shaped specimens. (b) Glued end caps for cylindrical specimens. (c) Biaxial extension. (d) Compression to tension load converter (after Perras and Diederichs, 2014).
1.5.3 Grain Structure and Fracture Characterization Techniques

To fully understand fracturing processes in brittle rock, it is necessary to have a comprehensive description of the intact rock’s grain structure, which controls fracture propagation together with the micro-mechanical properties of the rock. The characterization of the grain structure of a rock specimen involves conducting petrographic and mineralogical analyses to determine its mineral composition and texture (Haldar and Tisljar, 2014). This kind of analysis is commonly performed in thin sections using microscopes, but also in hand specimens, and includes qualitative and quantitative descriptions (Haldar and Tisljar, 2014).

The description of the mineral composition consists of the identification of the different types of minerals and the estimation of their abundance within the rock. This information is fundamental
for the classification of the rock. The texture of a rock describes the size, shape, and arrangement of the grains (Hughes, 1982; Haldar and Tisljar, 2014). Usually, the texture qualitatively describes the grain size, shape, and distribution within the rock (e.g., phaneritic, equigranular, porphyritic). In addition, the size and shape are commonly characterized based on the measured grain size per type of mineral (i.e., mean diameter, and corresponding standard deviation) and the roundness/sphericity of the grains, respectively. The identification and description of fractures and micro-fractures are also part of the petrographic characterization. Micro-cracks are usually described depending on their relationship with the mineral grains (i.e., trans-granular, intergranular, or intragranular; Kranz, 1979), as well as geometric characteristics (i.e., aperture and length).

The basic technique for the petrographic and mineralogical analyses is the thin-section optical microscopy, which is commonly conducted using a transmitted light polarizing microscope (Hughes, 1982). Other more sophisticated techniques for the characterization of mineral content based on microscopy are the Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), and SEM coupled with Energy Dispersive Analysis of X-rays (SEM-EDAX), among others (Hawkes and Spence, 2007). Imaging techniques such as confocal microscopy, Nuclear Magnetic Resonance (NMR), and X-ray Computerized Tomography (CT) have been proved useful to analyze the spatial distribution of cracks, and in the case of the latter method can also provide some mineralogical information. However, no single technique is able to perform a complete characterization of the internal structure of the rock. Therefore, a combination of different methods is required.

The thin-section optical microscopy, SEM, and X-ray CT are some of the most employed methods for the study of fracturing processes in rock (Mohan and Poobal, 2018, Nicco et al., 2018).
These techniques are described in more detail in this section. A detailed description of other methods can be found in the literature (Hawkes and Spence, 2007; Griffiths et al., 2017; Nicco et al., 2018).

1.5.3.1 Optical Microscopy

Thin-section optical microscopy is the traditional technique employed in petrography to determine the mineralogy of a rock specimen, as well as to detect and describe crack characteristics. This technique uses properties of light absorption and propagation for identification of the different mineral phases (Nesse, 1986).

For this analysis, a thin section of the rock is prepared. The standard thin section is a slice of rock with a thickness of 30 μm mounted with epoxy onto a 27 x 46 mm glass slide. A polarized light microscope is a usual tool employed with this technique. This kind of microscope filters (polarizes) light and constrains it to vibrate along one specific plane, changing the way light interacts with materials (McDonald, 2011). Such polarized light is useful for the study of minerals with anisotropic crystals by varying the vibration direction of light to specific directions within the crystals (Gribble and Hall, 1992). The observations made before and after the light beam is polarized provide information concerning the optical characteristics of the minerals within a rock sample. Commonly, thin-section optical microscopy is conducted using transmitted-light. Non-opaque minerals (e.g., quartz, feldspar) that allow significant light transmission through them can be easily identified with this technique, as opposed to opaque minerals (e.g., sulfides, oxides) that reflect or absorb light. For the latter group of minerals, reflected-light microscopy is recommended.
In order to ease the process of crack identification, it can be helpful to prepare the specimen using passive impregnation of colored or fluorescent epoxy (Nicco et al., 2018). Fractures in the thin sections can be described qualitatively and quantitatively. Features such as length and aperture are usually described (Griffiths et al., 2017). One approach to quantitatively characterize cracks consists of defining a grid over a microscope image and counting the number of intersections between the cracks and the grid to quantify the crack density (Wu et al., 2000; Griffiths et al., 2017). The process of fracture characterization using thin-section optical microscopy is a time-consuming task due to the intrinsic effort required for the qualitative mineralogical description and the quantification of crack density, as well as because of the difficulty of identifying some grain boundaries. This manual approach to quantify cracks is open to subjectivity (Griffiths et al., 2017). However, it is an easily applied tool for the initial description of the grain structure and grain contacts.

1.5.3.2 Scanning Electron Microscopy

The electron microscope was developed when the light wavelength used in optical microscopes became a limiting factor for the study of materials (Van der Biest and Thomas, 1976). Electron microscopy uses an electron gun that shoots an electron beam at the study sample. As a result of the interaction between the electron beam and the sample, different signals (i.e., backscattered electrons and x-rays) are produced (Van der Biest and Thomas, 1976; Hawkes and Spence, 2007). These signals are collected to generate information about the surface topography and composition of the sample. The main advantage of the electron microscope is its superior resolution resulting from the very small wavelengths of electrons, as opposed to other forms of radiation used by
optical microscopic systems (Van der Biest and Thomas, 1976). Also, the use of the small wavelength of electrons allows a large depth of focus (Goldstein et al., 2003).

Scanning Electron Microscopy (SEM) is a method that allows for qualitative mineralogical analysis of a sample. As its name indicates, SEM uses an electron microscope that scans the position of the electron beam over the surface of the sample. Therefore, data on determined areas of the sample can be collected. Depending on the composition of the surface of the sample, different absorption/reflection indexes are collected and registered by the microscope (Hawkes and Spence, 2007). These data are then used to generate an image representing a compositional map of the sample surface. However, these reported data do not make distinctions between mineral species or mineral grains of similar composition (Hawkes and Spence, 2007).

SEM also allows for crack detection in a rock sample using compositional data. In a thin section, the basic approach for crack detection depends on the epoxy used to impregnate the sample. Crack detection is possible thanks to the compositional difference between the minerals and the epoxy that backfilled the voids (i.e., cracks and other pores) within the sample. Further processing of the compositional images enables the spatial quantification and statistical analysis of some crack characteristics (Arena et al., 2014). Although SEM is preferred over optical microscopy for the study of microfractures, it is more expensive, technically demanding, and time-consuming (Griffiths et al., 2017).

Automated mineralogy based on SEM mechanizes and makes more efficient the process of compositional characterization, as well as quantitative measurement of mineral abundance and cracks within a sample (Scott et al., 2008). However, SEM-based automated mineralogy carries the limitations previously described concerning the differentiation between mineral grains/phases of similar composition.
1.5.3.3 Computerized Tomography

This method has a broad spectrum of applications from the medical sciences to engineering and geosciences. As opposed to the previously described techniques, the X-ray computerized tomography (CT) is classified as a nondestructive image technique (Johns et al., 1993). A CT scanner irradiates x-rays through a rock sample to obtain one- or two-dimensional radiographs for different positions of the sample. Further processing of the images allows for reconstruction of a three-dimensional image of the rock specimen. CT scanning allows characterization of the microstructure of a rock specimen by detecting changes in x-ray attenuation, a quantity that depends on the density and atomic number (Jia et al., 2014). These changes in attenuation translate into different mineralogical phases and porosity (Siddiqui and Khamees, 2004). The sensitivity of this technique to detect different mineral phases is limited by attenuation contrasts between mineral grains, which must be sufficiently high in order to obtain satisfactory results.

Similarly, for the study of induced fractures, the differences in x-ray absorption between fractures (or voids) and mineral grains are crucial to obtain CT-images with a satisfactory contrast (Jia et al., 2014). Several experiments have been conducted for the characterization of the induced fractures, and the study of fracturing processes in rocks (Johns et al., 1993; Nasseri et al., 2011; Weerakone et al., 2012; Jia et al., 2014; Martinez-Martinez et al., 2016). Usually, this technique is employed to visualize the distribution and measure the aperture of fractures. The success of the measurements depends on different factors such as the artefactual noise, calibration curves for interpretation, CT scan resolution, sample size, and the fracture aperture (Johns et al., 1993; Vandersteen et al., 2003; Weerakone et al., 2012).
1.5.4 Numerical Modeling of Fracturing Processes in Rock

During recent decades, several researchers have developed diverse approaches to model rock engineering problems at both the field and laboratory scales. Broadly speaking, there are three groups of numerical methods commonly applied to rock mechanics problems (Jing, 2003): continuum, discontinuum, and hybrid methods. The decision on which method should be used will depend on the specific characteristics of the rock mass, the scale, circumstances of the problem that is to be modeled, and the goals of the analysis.

The continuum approach considers materials as continuous bodies, implying that the materials cannot be broken into pieces (Jing, 2003). This method is recommended to represent rock masses with few fractures, or highly fractured rock masses that behave like an equivalent continuum. This method is useful in cases where fracture opening and block detachment are not significant factors (Jing and Hudson, 2002). The finite element method (FEM), finite difference method (FDM), and boundary element method (BEM) are considered in this group.

The discontinuum method treats materials as assemblages of distinct rigid or deformable blocks able to interact and separate during the rock damage process (Jing and Stephansson, 2007). This approach is most appropriate to represent moderately fractured rock masses, where relative large-scale displacements of individual blocks are possible (Jing and Hudson, 2002). The Discrete Element Method (DEM) and the Discrete Fracture Network (DFN) methods are part of this group. Hybrid methods can combine the advantages of both the continuum and discontinuum methods. Commonly, in a hybrid model, the simulation starts with a continuous representation of the
domain; then, as the simulation progresses, new discontinuities are created, leading to the formation of new discrete bodies (Lisjak and Grasselli, 2014).

Given the intrinsic characteristics of the different modeling approaches described above, some of them are able to realistically simulate fracturing processes in rock masses and intact rock, whereas others are not. Continuum models lack the ability to simulate fracture processes since they are based on continuum mechanics and cannot explicitly represent the slip, rotations, and separation induced by fractures (Hammah et al., 2008). Conversely, discontinuum and hybrid models allow the explicit representation of fractures and subsequent simulation of fracture processes in rock masses and intact rock (Jing, 2003; Lisjak and Grasselli, 2017). Thus, fracturing processes are often studied using Distinct Element Methods (DEM) that employ Bonded Particle Models (BPM), Bonded Block Models (BBM), or hybrid Finite/Distinct Element Methods (FDEM).

1.5.4.1 Bonded Particle Models

Although particle models were originally developed to simulate the micro-mechanical behavior of non-cohesive materials such as soils, BPMs are also useful to simulate the micro- and macro-mechanical behavior of rocks. This approach is appropriate to model intact rocks with a structure that includes both grains and cement, like a sandstone. The rock structure is modeled as an assembly of circular (2D) or spherical (3D) particles, which represents both grains and cement within the intact rock (Potyondy and Cundall, 2004). The particles within the structure are assigned a broad distribution of diameters to account for the heterogeneity in the distribution of the actual sizes of the grains of the rock.
The evolution of rock damage in a BPM is simulated in two steps: first, crack initiation is represented through the breaking of internal bonds, whereas fracture propagation is represented by coalescence of various bond breakages. BPM uses two types of bonds: the contact bond and the parallel bond. The contact bond models the adhesion of two particles over a very small area of contact. It is represented by an elastic spring, with constant normal and shear stiffnesses, that acts at the contact point between particles. The parallel bond model reproduces the behavior of the cement that bonds adjacent particles together, where the moment induced by particle rotation is resisted by a set of elastic springs lying on the contact plane at the contact point (Lisjak et al., 2014). Figure 1.7 shows the implementation of the parallel bond model in the commercially available code PFC (Itasca, 2012), and the constitutive behavior of the model in shear and tension.

Figure 1.7: Implementation of the parallel bond in PFC. (a) Normal and shear stiffness between particles. (b) Constitutive behavior in shear and tension. (after Lisjak and Grasselli, 2014).
The micro-properties of both the grains and cement applied in the model have to be calibrated using laboratory test data. Those micro-properties are as follows (Potyondy and Cundall, 2004):

**Grain micro-properties**

- Normal stiffness ($k_n$)
- Shear stiffness ($k_s$)
- Young’s modulus of grain ($E_c$)
- Coefficient of friction ($\mu$)

**Cement micro-properties**

- Normal stiffness ($k_n$)
- Shear stiffness ($k_s$)
- Young’s modulus of cement ($\bar{E}_c$)
- Radius multiplier ($\lambda$)
- Tensile strength ($\tau_c$)
- Shear strength ($\sigma_c$)

Early BPMs had some limitations given that the circular or spherical shape of the particles cannot fully represent the behavior of the interlocked grain structure of some rocks. Thus, those BPMs modeled unrealistically low ratios of unconfined compressive strength to indirect tensile strength, resulting in very low effective friction angles. Improvements for BPMs by Cho et al. (2007) and Potyondy (2012) using the clumping function or a flat-joined model, respectively, have helped to overcome those issues partially. The clumping function clusters particles together and
the resulting irregular particle shape helps to obtain a more realistic macroscopic friction angle (Potyondy and Cundall, 2004). The flat-joint logic allows the direct tensile and the unconfined compressive strength of hard rocks to be matched using a single common set of micro-properties (Fakhimi et al., 2002).

1.5.4.2 Bonded Block Models

BBMs were primarily developed to generate a grain-based structure that simulates the microstructure of low-porosity brittle rocks. As opposed to BPMs, BBMs use non-spherical blocks to represent the mineral grains in a rock (Lan et al., 2010). The grains can be represented using trigons (triangles in 2D and tetrahedrons in 3D) or Voronoi blocks (polygons in 2D and polyhedrons in 3D). A BBM represents an assembly of discrete blocks with assigned constitutive relations for both the continuous blocks and the contacts. The grains can be modeled as rigid or deformable. When the grains are modeled as rigid, failure is governed by the behavior of the contacts. When grains are modeled as deformable, a constitutive model can be assigned to the blocks, and both intergranular and intragranular fractures can be simulated, although depending on the approach, intragranular fractures can be implicitly or explicitly represented.

The mechanical interaction between blocks is defined by yielding contacts with a finite stiffness and a tensile strength criterion in the normal direction, whereas in the tangential direction to the contact surface is defined with a tangential stiffness in combination with a shear strength criterion (Lisjak and Grasselli, 2014). According to this relationship, a crack is created when the strength at the contact between blocks is exceeded. Figure 1.8 shows the fracture model as implemented in UDEC (Itasca, 2016). According to the contact constitutive relationship, a crack
is created when the tensile strength at the contact between blocks is exceeded, and then the tensile strength is set to zero.

Similarly to BPMs, in order to match the macro-response of the rock specimen recorded during rock mechanics tests, it is necessary to calibrate the contact micro-properties, which govern the micromechanical behavior of the rock. BBMs with elastic blocks require the following micro-properties to be defined (Ghazvinian et al., 2014; Nicksiar and Martin, 2014):

**Grain (block) micro-properties**

- Young’s modulus (E)
- Poisson’s ratio (ν)
- Density (ρ)

**Contact micro-properties**

- Normal stiffness (kₙ)
- Shear stiffness (kₛ)
- Peak cohesion (cₚ)
- Residual cohesion (cᵣ)
- Peak tensile strength (Tₚ)
- Residual tensile strength (Tᵣ)
- Peak friction angle (φₚ)
- Residual friction angle (φᵣ)
- Dilation angle (ψ)
Figure 1.8: Modeling of fracture propagation as implemented in UDEC. (a) Normal and shear stiffness between blocks. (b) Constitutive behavior in shear and tension (after Lisjak and Grasselli, 2014).

1.5.4.3 Hybrid Finite/Distinct Element Models

This technique, also known as FDEM, takes advantage of its DEM component to simulate fracturing processes. Typically, FDEM consists of a progressive simulation that starts as a continuous domain, which in turn allows for the formation of new discontinuities or fractures as the simulation progresses (Lisjak and Grasselli, 2014). There is a finite element mesh associated with each discrete block. The continuum part of the model is solved using FEM, whereas the discontinuum part is solved through DEM (Munjiza and John, 2002). Three of the most well-known FDEM codes are ELFEN (Rockfield Software Ltd., 2007), Y-Geo (Munjiza, 2004), and Irazu (Mahabadi et al., 2016) which represent different implementations of the same principles.

ELFEN’s domain is initially modeled as a continuum using the explicit finite element method, with a triangular mesh. The material constitutive behavior is implemented using a non-associative Mohr-Coulomb elastoplastic model, with shear strength parameters defined as a function of effective plastic strain (Lisjak and Grasselli, 2014). Fracturing is simulated in
compression through a Mohr-Coulomb model combined with an anisotropic smeared crack model, whereas in tension, anisotropic rotating crack models can be used (Lisjak and Grasselli, 2014). Every time an intra-element fracture is created, a dynamic re-meshing function updates the initial mesh topology.

Y-Geo and Irazu discretize the model domain into three-noded triangular elements together with four-noded cohesive crack elements between the triangular element edges (Lisjak et al., 2016; Mahabadi et al., 2016). As opposed to ELFEN, the mesh topology in Y-Geo and Irazu is never updated. The continuum part of the model is assigned a linear elastic constitutive model. Fracture initiation within the continuum is simulated by the breakage of the cohesive crack elements. The crack elements are distributed over the original mesh, so when the cracks are developed, their trajectory will depend on the mesh topology (Mahabadi et al., 2012). The crack elements are assigned a constitutive behavior that incorporates principles of non-elastic fracture mechanics. Figure 1.9 shows the continuum representation and the constitutive behavior of crack elements implemented in Y-Geo. In particular, the material starts to yield in tension or shear once it reaches a displacement value corresponding to the peak cohesive strength. Coulomb-type friction is applied along every new crack. As the simulation progresses, the created discrete bodies are able to displace and rotate, and the new contacts are automatically recognized (Munjiza and John, 2002). In addition, Irazu includes a fully-coupled hydro-mechanical formulation where hydraulic calculations are solved using a flow network developed from the same triangular mesh utilized for the mechanical calculations (Lisjak et al., 2016).
1.5.5 Calibration of Micro-properties in Bonded Block Models

The calibration of a BBM is an iterative multi-step process that consists of modifying the grain and contact micro-properties until a set of micro-properties is identified that replicates the rock’s macro-properties obtained in an actual laboratory test. The set of calibrated micro-properties should allow for properties such as Young’s modulus ($E_m$), Poisson’s ratio ($\nu_m$), crack initiation (CI) and crack damage (CD) thresholds, uniaxial compressive strength (UCS), tensile strength ($\sigma_{t,m}$), cohesion ($c_m$), friction angle ($\varphi_m$), and triaxial compressive strength to be replicated (Kazerani and Zhao, 2010). The calibration procedure should ideally involve running a series of BTS, UCS, and triaxial compressive strength test simulations.

Given the difficulties or lack of physical means to directly measure grain and contact micro-properties, most of these micro-properties must be calibrated. The approach employed for the calibration of grain micro-properties varies depending on whether the blocks are modeled as rigid,
elastic, or inelastic. In the case of rigid blocks, only the grain density is directly assigned to the grains. Similarly, when blocks are modeled as elastic, properties measured in experimental tests (i.e., density, \( \rho \); Young’s modulus, \( E \); and Poisson’s ratio, \( \nu \)) are assigned to the mineral grains. If blocks are modeled as inelastic, the micro-properties of the grains (tensile strength, cohesion, and friction angle, besides the previously mentioned grain micro-properties) need calibration (Li et al., 2017; Wang and Cai, 2018; Li et al., 2019). All the contact micro-properties (i.e., normal stiffness, \( k_{nc} \); shear stiffness, \( k_{sc} \); peak cohesion, \( c_{pc} \); peak tensile strength, \( \sigma_{tpc} \); peak friction angle, \( \phi_{pc} \); residual friction angle, \( \phi_{rc} \)) require calibration. To simplify the calibration process, the contact residual cohesion (\( c_{rc} \)) and residual tensile strength (\( \sigma_{trc} \)) are commonly assumed to be zero (Gao et al., 2014; Ghazvinian et al., 2014; Wang and Cai, 2018).

Potyondy and Cundall (2004), Kazerani and Zhao (2010), Gao and Stead (2014), Ghazvinian et al. (2014), Fabjan et al. (2015), Farahmand and Diederichs (2015), Li et al. (2017), and Wang and Cai (2018) among other authors, have developed procedures for the calibration of those micro-properties based on the relations between micro- and macro-properties found in their studies. Therefore, the values of the micro-properties cannot be selected randomly; rather, they should be estimated based on reasonable simplifications that follow the micro- to macro-properties relations (Wang and Cai, 2018). In general terms, the calibration procedure for a BBM with elastic blocks is as follows:

- Select a grain size that is representative of the rock specimen. Ideally, block sizes should be similar to the grain size of the actual rock
- Calibration of deformability micro-properties
  - Assign the grain micro-properties (density, \( \rho \); Young’s modulus, \( E \); Poisson’s ratio, \( \nu \)) measured in laboratory tests under the assumption that they are real
The contact shear stiffness to normal stiffness ratios ($k_s/k_n$) governs the macroscopic Poisson’s ratio ($\nu_m$). Adjust $k_s/k_n$ until $\nu_m$ is matched. In turn, $k_s/k_n$ can be approximated using the equivalent macroscopic shear modulus ($G_m$) to Young’s modulus ($E_m$) ratio.

The contact normal stiffness ($k_n$) directly relates to the macroscopic Young’s modulus ($E_m$). Correct $k_n$ to obtain $E_m$ while maintaining the calibrated $k_s/k_n$ value.

- Calibration of strength micro-properties
  - The contact tensile strength ($\sigma_t$) has a direct influence on the macroscopic tensile strength ($\sigma_{t,m}$) and crack initiation stress (CI). Change $\sigma_t$ values until $\sigma_{t,m}$ and CI are obtained.
  - The contact cohesion ($c$) affects the uniaxial compressive strength (UCS) directly, and crack damage stress (CD). Vary $c$ together with the calibrated $\sigma_t$ to obtain a range of $c$ that matches UCS and CD.
  - The contact peak and residual friction angles ($\varphi_{pc}$ and $\varphi_{rc}$), together with the contact cohesions ($c$), control the macroscopic cohesion ($c_m$) and friction angle ($\varphi_m$). Adjust $\varphi_{pc}$, $\varphi_{rc}$, and the previously calibrated ranges of $c$ to match $c_m$ and $\varphi_m$.

Lan et al. (2010), Chen and Konietzky (2014), Farahmand and Diederichs (2015), and Chen et al. (2016), among others, have calibrated the micro-properties specific to mineral types and mineral-to-mineral contacts, but have obtained a wide range of results. Table 1.1 summarizes the grain micro-properties reported by different sources, measured in the laboratory (i.e., micro-indentation in the case of elastic parameters), estimated from the literature or calibrated in numerical simulations. Tables 1.2 to 1.5 show the contact micro-properties calibrated for the Lac
du Bonnet granite (Lan et al., 2010; Chen and Konietzky, 2014; Farahmand and Diederichs, 2015) and the Kirchberg-II granite (Chen et al., 2016).

Table 1.1: Summary of grain micro-properties.

<table>
<thead>
<tr>
<th>Mineral</th>
<th>ρ (g/cc)</th>
<th>E (GPa)</th>
<th>K (GPa)</th>
<th>G (GPa)</th>
<th>ν</th>
<th>Source</th>
</tr>
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<tbody>
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<td>K-feldspar - Hyalophane</td>
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<td>a</td>
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<td>29.3</td>
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<td>a</td>
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<td></td>
<td>a</td>
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<td>a</td>
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<tr>
<td>K-Feldspar - Orthoclase67 Albite29</td>
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<td></td>
<td></td>
<td>a</td>
</tr>
<tr>
<td>K-Feldspar - Orthoclase54 Albite35</td>
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<td>24.2</td>
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<td>a</td>
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<tr>
<td>K-Feldspar - Orthoclase65 Albite27</td>
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<td></td>
<td></td>
<td>a</td>
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<td>24.9</td>
<td></td>
<td></td>
<td>a</td>
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<tr>
<td>Plagioclase - Albite</td>
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<td>56.9</td>
<td>28.6</td>
<td></td>
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<td>a</td>
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<td>Plagioclase - Anorthite</td>
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<td>39.9</td>
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<td>a</td>
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<td>Plagioclase - Labradorite</td>
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<td>33.7</td>
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<td>a</td>
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<td>a</td>
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<td>Plagioclase - Anorthite29</td>
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<td>Plagioclase - Anorthite53</td>
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<td>a</td>
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<td>Plagioclase - Anorthite56</td>
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<td>a</td>
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<td>0.35</td>
<td></td>
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<td>Feldspar</td>
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<td>73.0-89.0</td>
<td>50.0-63.0</td>
<td>29.0-35.0</td>
<td>0.20</td>
<td>d</td>
</tr>
</tbody>
</table>

(a) Bass, 1995 (micro-indentation testing); (b) Mavko et al., 2003 (micro-indentation testing); (c) Bewick et al., 2003 (compilation from different sources); (d) Chen et al., 2004 (source not specified); (e) Chen and Konietzky, 2014 (average from different sources); (f) Chen et al., 2016 (calibrated from simulations); (g) Zhou et al., 2019 (compilation from different sources).
Table 1.1: Continued.

<table>
<thead>
<tr>
<th>Mineral</th>
<th>( \rho ) (g/cc)</th>
<th>( E ) (GPa)</th>
<th>( K ) (GPa)</th>
<th>( G ) (GPa)</th>
<th>( v )</th>
<th>Source</th>
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<td>0.27</td>
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<td>44.4</td>
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<td>45.6</td>
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<td>37.9</td>
<td>44.3</td>
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<td>72.0-98.0</td>
<td>36.0-38.0</td>
<td>44.0-46.0</td>
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<td>65.0-95.0</td>
<td>g</td>
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<td>12.4</td>
<td>0.36</td>
<td>b</td>
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<td></td>
<td>40.0</td>
<td>0.20</td>
<td>d</td>
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<tr>
<td></td>
<td>35.0</td>
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<td>e</td>
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(a) Bass, 1995 (micro-indentation testing); (b) Mavko et al., 2003 (micro-indentation testing); (c) Bewick et al., 2003 (compilation from different sources); (d) Chen et al., 2004 (source not specified); (e) Chen and Konietzky, 2014 (average from different sources); (f) Chen et al., 2016 (calibrated from simulations); (g) Zhou et al., 2019 (compilation from different sources).
Table 1.2: Summary of calibrated grain contact micro-properties for Lac du Bonnet granite by Lan et al., 2010.

<table>
<thead>
<tr>
<th>Contact</th>
<th>$K_n$ (Pa/m)</th>
<th>$K_s/K_n$</th>
<th>$C$ (MPa)</th>
<th>$\varphi$ (°)</th>
<th>$\varphi_r$ (°)</th>
<th>$\sigma_t$ (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>K-feldspar / K-feldspar</td>
<td>9.20E+13</td>
<td>0.67</td>
<td>40.0</td>
<td>27.0</td>
<td>27.0</td>
<td>14.4</td>
</tr>
<tr>
<td>K-feldspar / Plagioclase</td>
<td>8.56E+13</td>
<td>0.67</td>
<td>40.0</td>
<td>27.0</td>
<td>27.0</td>
<td>14.4</td>
</tr>
<tr>
<td>K-feldspar / Quartz</td>
<td>1.29E+14</td>
<td>0.67</td>
<td>40.0</td>
<td>27.0</td>
<td>27.0</td>
<td>14.4</td>
</tr>
<tr>
<td>K-feldspar / Biotite</td>
<td>1.51E+14</td>
<td>0.67</td>
<td>40.0</td>
<td>27.0</td>
<td>27.0</td>
<td>14.4</td>
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<td>27.0</td>
<td>27.0</td>
<td>14.4</td>
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<tr>
<td>Biotite / Biotite</td>
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<td>27.0</td>
<td>27.0</td>
<td>14.4</td>
</tr>
</tbody>
</table>

Table 1.3: Summary of calibrated grain contact micro-properties for Lac du Bonnet granite by Chen and Konietzky, 2014.

<table>
<thead>
<tr>
<th>Contact</th>
<th>$K_n$ (Pa/m)</th>
<th>$K_s/K_n$</th>
<th>$C$ (MPa)</th>
<th>$\varphi$ (°)</th>
<th>$\varphi_r$ (°)</th>
<th>$\sigma_t$ (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>K-feldspar / K-feldspar</td>
<td>7.75E+14</td>
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<td>55.0</td>
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<td>59.0</td>
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<td>24.0</td>
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<td>60.5</td>
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<tr>
<td>Plagioclase / Biotite</td>
<td>6.10E+14</td>
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<td>47.0</td>
<td>53.5</td>
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<td>62.0</td>
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<td>22.5</td>
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<td>Biotite / Biotite</td>
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<td>37.0</td>
<td>48.0</td>
<td>24.0</td>
<td>19.0</td>
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</table>
Table 1.4: Summary of calibrated grain contact micro-properties for Lac du Bonnet granite by Farahmand and Diederichs, 2015.

<table>
<thead>
<tr>
<th>Contact</th>
<th>$K_n$ (Pa/m)</th>
<th>$K_s/K_n$</th>
<th>$C$ (MPa)</th>
<th>$\phi$ (°)</th>
<th>$\phi_r$ (°)</th>
<th>$\sigma_t$ (MPa)</th>
</tr>
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<tbody>
<tr>
<td>K-feldspar / K-feldspar</td>
<td>2.30E+14</td>
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<td>5.0</td>
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<tr>
<td>K-feldspar / Plagioclase</td>
<td>2.10E+14</td>
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<td>108.0</td>
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<td>5.0</td>
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</tr>
<tr>
<td>K-feldspar / Biotite</td>
<td>2.30E+14</td>
<td>0.65</td>
<td>60.0</td>
<td>48.0</td>
<td>5.0</td>
<td>11.4</td>
</tr>
<tr>
<td>Plagioclase / Plagioclase</td>
<td>2.50E+14</td>
<td>0.65</td>
<td>112.0</td>
<td>63.0</td>
<td>5.0</td>
<td>37.0</td>
</tr>
<tr>
<td>Plagioclase / Quartz</td>
<td>2.30E+14</td>
<td>0.65</td>
<td>80.0</td>
<td>49.0</td>
<td>5.0</td>
<td>28.2</td>
</tr>
<tr>
<td>Quartz / Quartz</td>
<td>2.80E+14</td>
<td>0.65</td>
<td>130.0</td>
<td>65.0</td>
<td>5.0</td>
<td>35.0</td>
</tr>
<tr>
<td>Quartz / Biotite</td>
<td>2.30E+14</td>
<td>0.65</td>
<td>57.0</td>
<td>52.0</td>
<td>5.0</td>
<td>23.4</td>
</tr>
<tr>
<td>Biotite / Biotite</td>
<td>1.30E+14</td>
<td>0.65</td>
<td>88.0</td>
<td>5.0</td>
<td>5.0</td>
<td>25.3</td>
</tr>
</tbody>
</table>

Table 1.5: Summary of calibrated grain contact micro-properties for Kirchberg-II granite by Chen et al., 2016.

<table>
<thead>
<tr>
<th>Contact</th>
<th>$K_n$ (Pa/m)</th>
<th>$K_s/K_n$</th>
<th>$C$ (MPa)</th>
<th>$\phi$ (°)</th>
<th>$\phi_r$ (°)</th>
<th>$\sigma_t$ (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feldspar / Feldspar</td>
<td>5.71E+14</td>
<td>1.00</td>
<td>52.0</td>
<td>48.0</td>
<td>0.48</td>
<td>23.0</td>
</tr>
<tr>
<td>Feldspar / Quartz</td>
<td>7.17E+14</td>
<td>1.00</td>
<td>57.0</td>
<td>53.0</td>
<td>0.53</td>
<td>24.5</td>
</tr>
<tr>
<td>Feldspar / Biotite</td>
<td>4.28E+14</td>
<td>1.00</td>
<td>44.5</td>
<td>43.0</td>
<td>0.43</td>
<td>21.0</td>
</tr>
<tr>
<td>Quartz / Quartz</td>
<td>8.63E+14</td>
<td>1.00</td>
<td>62.0</td>
<td>58.0</td>
<td>0.58</td>
<td>26.0</td>
</tr>
<tr>
<td>Quartz / Biotite</td>
<td>5.74E+14</td>
<td>1.00</td>
<td>49.5</td>
<td>48.0</td>
<td>0.48</td>
<td>22.5</td>
</tr>
<tr>
<td>Biotite / Biotite</td>
<td>2.85E+14</td>
<td>1.00</td>
<td>37.0</td>
<td>38.0</td>
<td>0.38</td>
<td>19.0</td>
</tr>
</tbody>
</table>
1.5.6 Uncertainties Related to Bonded Block Models

It is known that the grain structure of a rock has a great influence on fracture initiation and fracture propagation in brittle rock (Jing and Hudson, 2002; Lan et al., 2010). Therefore, the generation of a realistic grain-scale model geometry is a crucial aspect for the numerical simulation of brittle failure in rock. However, it is not currently known which specific attributes of the grain structure are most critical to BBM behavior.

At the grain-scale, intact crystalline rocks such as phaneritic igneous rocks consist of a variety of mineral grains of varying types, shapes, and sizes, each with different elastic and strength properties. Such heterogeneity of the rock’s microstructure, in turn, introduces a heterogeneous grain-scale stress distribution (Van de Steen et al., 2003). Lan et al. (2010) mentioned that both mineral grains and grain contacts influence several types of microscopic heterogeneity:

- Geometric heterogeneity (grain size and shape)
- Elastic heterogeneity (stiffness contrast between grains)
- Contact heterogeneity (anisotropy of contact distribution and differences in stiffness or strength)

Lately, some researchers have focused their attention on the study of heterogeneity in the process of brittle rock damage (Lan et al., 2010; Chen and Konietzky, 2014; Gao et al., 2016; Mayer and Stead, 2017; Wang and Cai, 2018). Two different approaches have been taken to represent the microstructure of brittle rock in BBMs, with different results. BBMs built using trigonal blocks (Kazerani et al., 2012; Gao et al., 2016; Mayer and Stead, 2017) show how trigons favor the development of shear failure over tensile failure. As opposed to BBMs with trigons, BBMs that use Voronoi blocks mainly develop tensile damage, as is expected in brittle rocks. That
is a direct result of the more realistic representation of the grain heterogeneity that, in turn, creates a higher degree of interlocking among the grains, similar to the interlocking of an actual grain assembly in crystalline rocks (Kazerani et al., 2012; Azocar, 2015; Mayer and Stead, 2017).

As mentioned in the previous section, BBMs are used as a tool to obtain the values of the contact micro-properties through a calibration process that consists of matching the macro-responses of the rock observed in the laboratory by varying the micro-properties (Kazerani and Zhao, 2010; Kazerani et al., 2012; Gao and Stead, 2014; Ghazvinian et al., 2014). In the case of the calibration process for a specific rock specimen, although the grain structure generated using conventional Voronoi tessellations achieves a first-order approximation of the microstructure of the rock, the stochastic nature of the grain assemblies has an effect on the calibration process of the micro-properties of the grain blocks and contacts. Thus, since every attempt of calibration aims to match the same macroscopic response, but different grain structures with different micromechanical behavior are used each time, the calibrated micro-properties will always be different. This means that as long as a simulation incorporates a randomly generated grain structure, with a particular grain arrangement, grain sizes, and grain shapes, an exact calibration of the system is not possible (Mayer and Stead, 2017).

Lan et al. (2010), Chen and Konietzky (2014), and Farahmand and Diederichs (2015), among others, have calibrated the micro-properties for models of diverse specimens of granite and diorite, obtaining different calibrated micro-properties for the various components of the grain structure (grain and contact types). Due to the complexity of the calibration process, diverse assumptions have been applied to simplify the process. Nevertheless, some assumptions are open to criticism due to their effects on the calibration results. This is noticeable in the study of Lan et al. (2010), where BBMs of the Lac du Bonnet Granite and the Aspo Diorite were developed. In that study,
given the mineralogical similarity of both rocks, it was assumed that most of their micro-properties were the same. Thus, identical elastic parameters were applied to the grains of the same mineralogy in both BBMs. Also, the strength parameters, as well as the normal to shear stiffness ratio, were assumed to be the same for all the contacts, leaving the normal stiffness as the only variable per type of contact. Although the assumptions made for the grain micro-properties are quite logical, the assumptions for the contact micro-properties are not. Apparently, they were made only to simplify the calibration process, and there may not be a physical explanation to support that kind of assumption.

Other studies (Kazerani and Zhao, 2010; Chen and Konietzky, 2014; Farahmand and Diederichs, 2015) considered a progressive calibration procedure that relies on previously established correlations between the micro- and macro-properties of the rock allowing for a more reliable adjustment of the micro-properties. Nevertheless, there is an intrinsic degree of uncertainty linked to the sensitivity analyses within the calibration process that cannot be avoided. Also, considering that those calibrated micro-properties were estimated for different rock specimens with different grain structures, the obtained sets of micro-properties could not be expected to have the same values. However, there is a chance that one or more of the mentioned studies generated a reasonably accurate representation of the grain structures using random Voronoi grains, which led to contact micro-properties that realistically approximate the micro-mechanical behavior of the rock. Considering that the specimens tested in those studies have similar macro-properties, the sets of micro-properties that realistically represent the micro-mechanical behavior of the rock could be used to reasonably predict the brittle mechanical behavior of other similar rock specimens.
2.1 Abstract

Previously published laboratory-scale simulations have demonstrated that grain structure impacts the micro-mechanical behavior and macroscopic response of intact rock under loading. A commonly applied approach for such simulations approximates the grain structure through an assembly of bonded polyhedral Voronoi blocks. To numerically replicate the specimen-scale behavior of the rock, a set of properties that represents the micro-mechanical properties of grains and grain contacts is calibrated. Voronoi block assemblies provide reasonable approximations of actual grain structures, but the random nature of the Voronoi assemblies increases the uncertainty of the contact micro-properties obtained from the calibration process, potentially leading to incorrect estimations of the rock strength when used for predictive modeling. This study evaluates how different representations of the grain structure influence predictions of brittle rock mechanical behavior. Three-dimensional (3D) Voronoi and two-dimensional (2D) deterministic Bonded Block Models of Wausau granite specimens were generated and used as a basis for 3D and 2D simulations of UCS and BTS tests. The quality of agreement between the strength of actual granite specimens and the strength predicted using Bonded Block Models was tested through a comparative analysis. The modeling results show that great influence of the model dimensionality and the grain shape, and also prove that it is possible to predict with reasonable accuracy within
10% of variability the strength of a rock using reasonably simplified representations of the grain structure in Voronoi models.

2.2 Introduction

It is well known that the grain structure of a rock controls the micro-mechanical behavior of the grains, and consequently, the macro-mechanical behavior of a rock (Gao et al., 2016; Wang and Cai, 2018). The mechanical behavior and strength of rocks are usually characterized using laboratory tests such as uniaxial compression, triaxial compression, and tensile tests. Laboratory studies show how individual rock specimens can show different fracturing behavior as well as different strength even when they are the same rock type (Liu et al., 2018). The reason for such differences is the heterogeneous nature of rocks.

Rocks show a noticeable grain structure heterogeneity as a result of their complex formation processes. At the grain-scale, rocks are composed of diverse minerals (i.e., mineral grains) in different shapes and sizes and are also affected by different defects (e.g., micro-cracks). That micro-structural heterogeneity governs a complex micro-mechanical behavior that generates intricate localized stress concentrations within a rock specimen and results in fracture development (Gao et al., 2016; Wang and Cai, 2018).

The sources of heterogeneity of intact rock are: (i) grain-geometry heterogeneity associated with the variability of size and shape of the grain structure; (ii) grain-scale deformability heterogeneity related to the contrasts in density and elastic properties of different mineral phases; and (iii) grain-grain contact heterogeneity connected to the variation of contact distribution and stiffness anisotropy (Lan et al., 2010; Farahmand and Diederichs, 2015; Wang and Cai, 2018).
In recent decades, thanks to significant developments in computer power, numerical modeling has become a useful means to quantitatively investigate fracturing processes in brittle rock.

Continuum, discontinuum, and hybrid continuum-discontinuum methods can be used to conduct brittle rock failure modeling (Potyondy and Cundall, 2004), with different results. The continuum approach represents rock damage with a constitutive relation with a failure criterion in the form of elastic-plastic, elastic-brittle, or strain-softening models. One disadvantage of the continuum approach is its inability to explicitly represent progressive failure in rocks (Wang and Cai, 2018).

The discontinuum and hybrid continuum-discontinuum approaches, on the other hand, depict rocks as assemblies of discrete particles or blocks and model fracturing processes in an explicit manner without the need for pre-defined constitutive models (Wang and Cai, 2018). These two last methods are widely used to model brittle rock mechanical behavior under different loading conditions, such as unconfined and confined compression, or direct and indirect tension. The Discrete Element Method (DEM) and the hybrid Finite Discrete Element Method (FDEM), are the most commonly applied discontinuum and hybrid approaches, respectively.

In numerical modeling, different approaches have been developed to address intact rock heterogeneity from the point of view of grain geometry, and specifically grain shape. Among DEM models, Bonded Particle Models (BPM) and Bonded Bock Models (BBM) are the most popular representations of the grain structure. BPMs represent the grain heterogeneity using disks and spheres in two-dimensional (2D) and three-dimensional (3D) models, respectively (Potyondy and Cundall, 2004). In contrast, BBMs depict grain structures using triangular or polygonal shapes in 2D, and tetrahedral or polyhedral shapes in 3D (Jing and Hudson, 2003; Ghazvinian et al., 2014; Lisjak and Grasselli, 2014). The polygonal and polyhedral grain structures, compared with other
grain shape assemblies, have achieved the most realistic depiction of the rock’s microstructure from the grain-geometry perspective (Wang and Cai, 2018). Voronoi tessellation is a popular technique to generate polygonal and polyhedral grain structures for BBMs and has been widely applied (Ghazvinian et al., 2014; Farahmand and Diederichs, 2015; Quey and Renversade, 2018).

Generally speaking, the macroscopic mechanical response to loading of a BBM depends on three different factors: numerical model physics, micro-properties, and grain structure attributes, as summarized in Figure 2.1. The numerical model physics includes the various fundamental properties of the solution approach used (e.g., explicit time-stepping DEM) as well as any relevant boundary conditions. The micro-properties are highly relevant in numerical simulations since they represent both the grain and grain-to-grain contact elastic and strength properties and define the way grains interact with each other within a rock structure. Finally, the grain structure attributes include all the geometric features that define the geometry of grains within a rock, and consequently, the local loading conditions. “Conventional” Voronoi models only consider basic features of the grain structure to represent the grain structure, whereas more complex BBMs can include even small-scale features that add complexity and realism to the models.
Figure 2.1: Summary of the elements required for the proper prediction of rock strength.
Simplifications to the grain structure in conventional Voronoi models have consequences for the micro-properties that are derived from the calibration of BBMs to macroscopic laboratory test data. For example, individual grain boundaries, in reality, can have a great deal of small-scale roughness and interlocking but are typically represented as straight lines in BBMs. Accordingly, a conventional BBM calibrated to rock with significant grain-grain contact roughness at scales smaller than what can be represented using a Voronoi geometry might end up with a higher friction angle than the true mineral-mineral contact friction. The further a true grain structure deviates from the Voronoi representation in a BBM, the more the microparameters derived from matching model attributes to laboratory test data represent pure calibration parameters as opposed to fundamental material properties. The degree to which BBM microparameters do approximate fundamental material properties and the corresponding degree to which the Voronoi grain structure approximates true grain structures has not been studied in the literature.

The main objective of the present study is to assess the influence of the grain structure heterogeneity on the macro-mechanical response for prediction of brittle rock mechanical behavior. The first part of the study used a baseline 3D Voronoi BBM that represents the grain structure of Wausau granite in terms of mineral composition and average grain size to analyze different aspects of the representation of the grain structure. A first assessment analyzes the influence of model dimensionality through comparisons of UCS test simulation results using 3D and 2D representations of the same microstructure. The second assessment examined whether the 3D Voronoi model can be used in combination with previously published sets of micro-properties to predict brittle rock strength in Uniaxial Compressive Strength (UCS) and Brazilian Tensile Strength (BTS) test simulations. Another evaluation analyzed the effect of the characterization and representation of feldspars in Wausau granite in the results of the simulations. Additional
assessments compared the baseline BBM against a series of Voronoi BBMs with diverse grain size, grain shape, and grain arrangement to individually evaluate the impact of these grain-geometric parameters in UCS and BTS test simulations. For the second part of the study, different 2D deterministic BBMs were developed based on the detailed characterization of the grain arrangement, grain shape, and grain size of specimens of Wausau granite. BTS test simulations were run to compare the deterministic models against conventional Voronoi models with equivalent mineralogical composition and grain size. Comparative analyses were performed to assess the combined effect of the grain structure geometric parameters on the macro-properties of the rock and identify the critical aspects of grain structure representation needed to ensure a proper prediction of rock strength.

2.3 Overview of the Study Methods

This study involved the development of a series of 2D and 3D BBMs, where different grain structure geometric parameters are represented. The BBMs are the basis for UCS and BTS test simulations that attempt to replicate the macroscopic behavior of actual specimens of Wausau granite. UCS and BTS tests were conducted on core and disk-shaped specimens of Wausau granite, respectively, to characterize its macro-mechanical behavior (i.e., UCS, Young’s modulus, Poisson’s ratio, tensile strength, crack initiation stress, and crack damage stress). The numerical simulations attempt to replicate the macroscopic behavior of Wausau granite using different sets of micro-properties previously established by four separate studies: Lan et al. (2010), Chen and Konietzky (2014), Farahmand and Diederichs (2015), and Chen et al. (2016).
The first part of the study includes four different types of assessments: (1) evaluation of the model dimensionality; (2) evaluation of published micro-properties; (3) evaluation of feldspar representation; and (4) evaluation of grain-geometric parameters. The first assessment analyzes the impact of 3D and 2D representations of the same grain structure in the results of laboratory-scale test simulations. The second section analyzes whether a Voronoi BBM that represents the grain structure of Wausau granite could be used in combination with previously calibrated sets of micro-properties to reasonably replicate the macroscopic behavior of the rock specimen. The third assessment analyzes the effects of the representation of feldspar grains within Wausau granite as two separate mineral phases and as one single group. Then, the final assessment analyzes the individual influence of different grain-geometric parameters (i.e., grain size, shape, and arrangement) on the representation of BBMs and subsequent laboratory-scale simulation results.

For the simulations of the first part of the study, a baseline 3D Voronoi BBM developed in the software Neper (Quey, 2019) was used in combination with previously calibrated sets of micro-properties to replicate the macroscopic behavior of Wausau granite. Three cross-sections (two axial and one diametral) were then cut from the 3D Voronoi structure. UCS test simulations were run on the 3D BBM, and the 2D BBMs generated from the axial sections, whereas BTS test simulations were performed on the 2D BBMs built based on the diametral sections. The third assessment required developing various 3D Voronoi BBMs with different grain size, grain shape, and grain arrangement to be compared against the baseline model. The software Neper was employed for this task. Similarly to the previous cases, three sections, two axial and one diametral, were cut from the 3D BBMs to generate 2D BBMs. In this case, only 2D UCS and BTS test simulations were run and compared.
The second part of the study evaluates how two different representations of the same grain structure developed under different approaches influence the results of laboratory-scale simulation by comparing deterministic and Voronoi-based representations of the same microstructure. A sub-group of the BBMs was developed in a deterministic manner to depict the actual grain structure of disk-shaped specimens of the Wausau granite, based on petrographic characterization and detailed representation of the grain geometry within the specimens. The other sub-group of BBMs was developed using the Voronoi tessellation approach in the software Neper. All the BBMs of this section of the study were used to simulate BTS tests.

2.4 Wausau Granite

For the prediction of brittle rock mechanical behavior, this study uses BBMs in combination with different sets of micro-properties selected from the literature. All those sets of micro-properties were calibrated to reflect the micro-mechanical behavior and macro-response of certain rocks. Therefore, to obtain comparable results, the rock for this research should have a similar grain structure and macro-response to those with calibrated micro-properties. The Wausau granite was selected as the subject of this study because of its similarities with Lac du Bonnet granite (Lan et al., 2010) and Kirchberg-II granite (Chen et al., 2016), the micro-properties of which are used in the simulations. The three granites present similar mineral composition, average grain size, and UCS.

The Wausau granite is a dark red alkali-feldspar granite from Marathon County, Wisconsin (Sims et al., 1993). For this study, specimens of Wausau granite were obtained directly from a quarry. Specimens of Wausau granite were characterized through macroscopic petrography, thin-
section microscopy, and automated mineralogy based on Scanning Electron Microscopy (SEM). Three standard thin-sections were prepared for the microscopy analyses, all of them taken from different sections of a single core specimen. The automated mineralogy analyses were conducted on a TESCAN-VEGA-3 Integrated Mineral Analyzer (TIMA) model LMU VP-SEM. Spectral data were acquired using four energy dispersive X-ray (EDX) spectrometers with a beam stepping interval (i.e., spacing between acquisition points) of 15 μm, acceleration voltage of 24 keV, and beam intensity of 14. The EDX spectra records were compared with spectra held in a look-up table, allowing a phase assignment to be made at each acquisition point.

According to SEM-based automated mineralogy analyses conducted on the three thin-sections, the mineral composition of the Wausau granite averages 24% K-feldspar, 41% plagioclase (albite), 32% quartz, and 3% mafic and accessory minerals (mainly biotite). Macroscopically, K-feldspar and plagioclase in Wausau granite were described as a single group of feldspars due to the lack of contrast between them. The studies of La Berge and Myers (1983), and Sims et al. (1993) identified microperthite as the dominant feldspar in this rock. Microperthite is described as exsolution or irregular intergrowth of sodic and potassic feldspars. Such feldspar intergrowth was identified in this study’s Wausau granite specimens through thin-section microscopy and automated mineralogy analyses. Figure 2.2 shows the feldspar intergrowth identified in a compositional map of thin-section sample WG-08-21 generated with automated mineralogy.

For the construction of deterministic models, three disk-shaped specimens of Wausau granite were petrographically characterized. In these specimens, the proportion of K-feldspar to plagioclase (approximately 3:5) was determined based on the results of the automated mineralogy. Table 2.1 summarizes the mineral composition determined for each disk specimen. Also, the grain
size distribution of Wausau granite was estimated based on digitized grain structure data from these three disk-shaped specimens of Wausau granite. The apparent grain size ranges from 0.1 mm to 7 mm, with mean grain sizes of 2.5 mm for feldspars, 4 mm for quartz, and 0.5 mm for biotite.

Figure 2.2: Compositional map of specimen WG-08-21 generated with automated mineralogy.
Table 2.1: Summary of the mineralogical composition of specimens WG-08-01, WG-08-21, and WG-08-41.

<table>
<thead>
<tr>
<th>Specimen</th>
<th>K-feldspar</th>
<th>Plagioclase</th>
<th>Quartz</th>
<th>Biotite</th>
<th>Number of grains</th>
</tr>
</thead>
<tbody>
<tr>
<td>WG-08-01</td>
<td>26%</td>
<td>44%</td>
<td>28%</td>
<td>2%</td>
<td>821</td>
</tr>
<tr>
<td>WG-08-21</td>
<td>21%</td>
<td>37%</td>
<td>41%</td>
<td>1%</td>
<td>782</td>
</tr>
<tr>
<td>WG-08-41</td>
<td>22%</td>
<td>37%</td>
<td>39%</td>
<td>2%</td>
<td>744</td>
</tr>
</tbody>
</table>

2.4.1 Macro-Properties

The Wausau granite was geomechanically characterized for this study through UCS and BTS tests. The UCS tests were executed on cylindrical specimens of approximately 51 mm in diameter and length-to-diameter ratio of 2.5:1. According to the results of eleven UCS tests, the peak strength ranges from 204 MPa to 260 MPa. The indirect tensile strength was estimated based on three BTS tests performed on specimens of approximately 51 mm in diameter and 25 mm in thickness. Reported indirect tensile strengths vary between 11 MPa and 12 MPa. Complete stress-strain information was registered in three UCS tests. The Young’s modulus (E), and Poisson’s ratio (ν), crack initiation stress (CI) and crack damage stress (CD) were determined from the strain-stress curves of those three tests. The CD was calculated using the volumetric strain ($\varepsilon_v$) method (Martin and Chandler, 1994), whereas the CI was estimated using the crack volumetric strain ($\varepsilon_{v,c}$) method (Nicksiar and Martin, 2012). Table 2.1 summarizes the average macro-mechanical properties of Wausau granite based on three UCS tests with complete strain-strain information and three BTS tests.
Table 2.2: Experimental macro-mechanical properties of Wausau granite, expressed in terms of arithmetic mean and two standard deviations (i.e., $\mu \pm 2\sigma$).

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density, $\rho_M$ (kg/m³)</td>
<td>2600 ± 20</td>
</tr>
<tr>
<td>Uniaxial Compressive Strength, UCS (MPa)</td>
<td>209 ± 18</td>
</tr>
<tr>
<td>Crack initiation threshold, CI (MPa)</td>
<td>91 ± 29 (~ 44% UCS)</td>
</tr>
<tr>
<td>Crack damage threshold, CD (MPa)</td>
<td>196 ± 19 (~ 94% UCS)</td>
</tr>
<tr>
<td>Young’s Modulus, $E_M$ (GPa)</td>
<td>69.6 ± 2.8</td>
</tr>
<tr>
<td>Poisson’s Ratio, $\nu_M$</td>
<td>0.24 ± 0.06</td>
</tr>
<tr>
<td>Brazilian tensile strength, BTS (MPa)</td>
<td>11.7 ± 1.0</td>
</tr>
</tbody>
</table>

2.4.2 Block and Contact Constitutive Models

Experimental observations indicate that the failure process of brittle rocks under compression consists of several stages: (i) crack closure, (ii) linear elastic deformation, (iii) stable crack growth after crack initiation, (iv) unstable crack growth after crack coalescence, and (v) post-peak deformation (Bieniawski, 1967). These stages are bounded by four characteristic stress thresholds: crack closure (CC), crack initiation (CI), crack damage (CD), and peak failure strength (Martin and Chandler, 1994).

During the deformation process, both grains and grain contacts can fail within a rock’s grain structure. Therefore, intergranular cracks (i.e., cracks along the grain boundaries) and intragranular cracks can be found (Wang and Cai, 2018; Li et al., 2019). Most of fracturing in rocks prior to peak strength under unconfined loading conditions occurs along the grain boundaries (Lim et al., 2012). Results of simulations using discontinuum models show that under unconfined...
compression, intergranular cracks initiate at the CI stress threshold, whereas intragranular cracks initiate at the CD stress threshold (Bahrani et al., 2014; Gao et al., 2016; Li et al., 2019).

The micromechanical behavior of BBMs is controlled by the mechanical micro-properties of the grains (or blocks), and contacts between grains. A common practice of model simplification consists of modeling the mineral grains within the BBMs as elastic materials, allowing failure to occur only along the grain contacts (Nicksiar and Martin, 2014). Although in reality grain failure (i.e., grain crushing) can also occur, models that represent grains as elastic materials are able to appropriately replicate the pre-peak deformational response, dominant tensile failure mechanism, and macroscopic strength parameters (i.e., UCS, CI, CD, $\sigma_{tm}$, $c_m$, $\phi_m$), and volumetric strain of a specimen under unconfined compression. However, the brittleness of the axial stress-strain curve and the post-peak deformational response are not properly captured (Wang and Cai, 2018; Wang and Cai, 2019).

In this study, the mineral grains within the BBMs are modeled as unbreakable elastic blocks. Considering that this study is focused on the prediction of the pre-peak macro-mechanical properties (i.e., UCS, CI, CD, $E_m$, $\nu_m$, $\sigma_{tm}$) of rock specimens, such a simplification is expected to have a negligible effect on the results of the numerical simulations. Previous studies use a similar simplification criterion for their BBMs (Kazerani and Zhao, 2010; Lan et al., 2010; Chen and Konietzky, 2014; Ghazvinian et al., 2014; Nicksiar and Martin, 2014; Farahmand and Diederichs, 2015; Chen et al., 2016). This simplification helps to save computational time, particularly during 3D simulations. Appendix A provides information concerning the computational cost of this study.

The block micro-properties applied in this study correspond to an elastic constitutive model with specific density, Young’s modulus, and Poisson’s ratio for each mineral type. The grain contacts are modeled following a Coulomb slip-joint constitutive model with residual strength
properties. As failure progresses in the simulations, the contacts are assumed to transition their cohesion, friction, and tensile strength to their residual values (Nicksiar and Martin, 2014).

2.4.3 Micro-Properties

The grain and contact micro-properties applied to the BBMs are taken from the literature. Lan et al. (2010), Chen and Konietzky (2014), Farahmand and Diederichs (2015), and Chen et al. (2016) published the results of their micro-properties calibration using BBMs to investigate Lac du Bonnet granite (three first studies) and Kirchberg II granite (last study). Given the similarities in terms of mineral composition and macro-mechanical response of Wausau granite with Lac du Bonnet granite (i.e., UCS = 200 ± 22 MPa, E = 69.0 ± 5.8 GPa, v = 0.26 ± 0.04, σt = 9.3 ± 1.3 MPa; Farahmand and Diederichs, 2015; Chen and Konietzky, 2014) and Kirchberg II granite (i.e., UCS = 193 MPa, E = 62.6 GPa, v = 0.22, σt = 12.5 MPa; Chen et al., 2016), it is expected that such calibrated parameters in combination with the BBMs should be able to deliver a reasonable estimation of the strength of Wausau granite; this, of course, assumes that the physics of the models (including the influence of grain structure) is a close approximation of reality.

A rock’s mineral composition determines the number of grain types to be included in a model. In the case of Wausau granite, although K-feldspar and plagioclase can be identified within the rock, both varieties of feldspar a part of exsolved grains with different proportions of sodium and potassium feldspar. Such exsolved grains are difficult to differentiate into K-feldspar and plagioclase to be represented in a block model. This difficulty in identifying the types of feldspars could bias the results of the numerical simulation if some grains are incorrectly identified. Thus, to assess the effect of the characterization of feldspar grains, Wausau granite is modeled in two ways: the first case considers a total of four types of grains (K-feldspar, plagioclase, quartz, and
biotite) with ten corresponding types of grain-to-grain contacts, whereas the second case considers three types of grains (feldspar, quartz, and biotite) with six types of contacts.

In the case of BBMs with four types of grains, the calibrated micro-properties from the studies of Lan et al. (2010), Chen and Konietzky (2014), and Farahmand and Diederichs (2015) were directly applied to the models. For the models with three grain types, the micro-properties calibrated in the studies of Chen et al. (2016) were applied to the BBMs. For analysis of BBMs with three types of grains, “average-feldspar” sets of contact micro-properties were established using weighted averages of the original K-feldspar and plagioclase micro-properties from the three previously mentioned studies.

Table 2.2 summarizes the grain micro-properties used by the authors mentioned above. The “average-feldspar” contact micro-properties calculated from Lan et al. (2010), Chen and Konietzky (2014), and Farahmand and Diederichs (2015) are summarized in tables 2.3 to 2.5. As in previous studies, the residual values of tensile strength and cohesion are assumed to be zero (Ghazvinian et al., 2014; Nicksiar and Martin, 2014; Farahmand and Diederichs, 2015).
Table 2.3: Summary of grain micro-properties.

<table>
<thead>
<tr>
<th>Mineral</th>
<th>$\rho$ (g/cc)</th>
<th>$E$ (GPa)</th>
<th>$\nu$</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>K-Feldspar</td>
<td>2.56</td>
<td>69.8</td>
<td>0.28</td>
<td>Lan et al., 2010; Farahmand and Diederichs, 2015</td>
</tr>
<tr>
<td></td>
<td>62.0</td>
<td>2.7</td>
<td></td>
<td>Chen and Konietzky, 2014</td>
</tr>
<tr>
<td>Plagioclase</td>
<td>2.63</td>
<td>88.1</td>
<td>0.26</td>
<td>Lan et al., 2010; Farahmand and Diederichs, 2015</td>
</tr>
<tr>
<td></td>
<td>69.0</td>
<td>0.23</td>
<td></td>
<td>Chen and Konietzky, 2014</td>
</tr>
<tr>
<td>Feldspar</td>
<td>52.0</td>
<td>0.19</td>
<td></td>
<td>Chen et al., 2016</td>
</tr>
<tr>
<td>Quartz</td>
<td>2.65</td>
<td>94.5</td>
<td>0.08</td>
<td>Lan et al., 2010; Farahmand and Diederichs, 2015</td>
</tr>
<tr>
<td></td>
<td>91.0</td>
<td>0.20</td>
<td></td>
<td>Chen and Konietzky, 2014</td>
</tr>
<tr>
<td></td>
<td>81.0</td>
<td>0.16</td>
<td></td>
<td>Chen et al., 2016</td>
</tr>
<tr>
<td>Biotite</td>
<td>3.05</td>
<td>33.8</td>
<td>0.36</td>
<td>Lan et al., 2010; Farahmand and Diederichs, 2015</td>
</tr>
<tr>
<td></td>
<td>35.0</td>
<td>0.25</td>
<td></td>
<td>Chen and Konietzky, 2014</td>
</tr>
<tr>
<td></td>
<td>25.0</td>
<td>0.22</td>
<td></td>
<td>Chen et al., 2016</td>
</tr>
</tbody>
</table>

Table 2.4: Summary of “average-feldspar” contact micro-properties calculated from Lan et al., 2010.

<table>
<thead>
<tr>
<th>Contact</th>
<th>$K_n$ (Pa/m)</th>
<th>$K_s/K_n$</th>
<th>$C$ (Mpa)</th>
<th>$\phi$ (°)</th>
<th>$\phi_r$ (°)</th>
<th>$\sigma_t$ (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feldspar / Feldspar</td>
<td>9.03E+13</td>
<td>0.67</td>
<td>40.0</td>
<td>27.0</td>
<td>27.0</td>
<td>14.4</td>
</tr>
<tr>
<td>Feldspar / Quartz</td>
<td>1.27E+13</td>
<td>0.67</td>
<td>40.0</td>
<td>27.0</td>
<td>27.0</td>
<td>14.4</td>
</tr>
<tr>
<td>Feldspar / Biotite</td>
<td>1.50E+14</td>
<td>0.67</td>
<td>40.0</td>
<td>27.0</td>
<td>27.0</td>
<td>14.4</td>
</tr>
<tr>
<td>Quartz / Quartz</td>
<td>2.55E+14</td>
<td>0.67</td>
<td>40.0</td>
<td>27.0</td>
<td>27.0</td>
<td>14.4</td>
</tr>
<tr>
<td>Quartz / Biotite</td>
<td>3.13E+14</td>
<td>0.67</td>
<td>40.0</td>
<td>27.0</td>
<td>27.0</td>
<td>14.4</td>
</tr>
<tr>
<td>Biotite / Biotite</td>
<td>4.70E+14</td>
<td>0.67</td>
<td>40.0</td>
<td>27.0</td>
<td>27.0</td>
<td>14.4</td>
</tr>
</tbody>
</table>

Table 2.5: Summary of “average-feldspar” contact micro-properties calculated from Chen and Konietzky, 2014.

<table>
<thead>
<tr>
<th>Contact</th>
<th>$K_n$ (Pa/m)</th>
<th>$K_s/K_n$</th>
<th>$C$ (Mpa)</th>
<th>$\phi$ (°)</th>
<th>$\phi_r$ (°)</th>
<th>$\sigma_t$ (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feldspar / Feldspar</td>
<td>7.78E+14</td>
<td>1.00</td>
<td>52.5</td>
<td>55.4</td>
<td>27.7</td>
<td>23.1</td>
</tr>
<tr>
<td>Feldspar / Quartz</td>
<td>8.95E+14</td>
<td>1.00</td>
<td>57.4</td>
<td>58.8</td>
<td>29.4</td>
<td>24.6</td>
</tr>
<tr>
<td>Feldspar / Biotite</td>
<td>6.01E+14</td>
<td>1.00</td>
<td>45.3</td>
<td>52.2</td>
<td>26.1</td>
<td>21.2</td>
</tr>
<tr>
<td>Quartz / Quartz</td>
<td>1.01E+15</td>
<td>1.00</td>
<td>62.0</td>
<td>62.0</td>
<td>31.0</td>
<td>26.0</td>
</tr>
<tr>
<td>Quartz / Biotite</td>
<td>7.16E+14</td>
<td>1.00</td>
<td>49.5</td>
<td>55.0</td>
<td>27.5</td>
<td>22.5</td>
</tr>
<tr>
<td>Biotite / Biotite</td>
<td>4.20E+14</td>
<td>1.00</td>
<td>37.0</td>
<td>48.0</td>
<td>24.0</td>
<td>19.0</td>
</tr>
</tbody>
</table>
Table 2.6: Summary of “average-feldspar” contact micro-properties calculated from Farahmand and Diederichs, 2015.

<table>
<thead>
<tr>
<th>Contact</th>
<th>$K_n$ (Pa/m)</th>
<th>$K_s/K_n$</th>
<th>$C$ (Mpa)</th>
<th>$\phi$ (°)</th>
<th>$\phi_r$ (°)</th>
<th>$\sigma_t$ (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feldspar / Feldspar</td>
<td>2.27E+14</td>
<td>0.65</td>
<td>110.0</td>
<td>61.9</td>
<td>5.0</td>
<td>34.6</td>
</tr>
<tr>
<td>Feldspar / Quartz</td>
<td>2.56E+14</td>
<td>0.65</td>
<td>77.4</td>
<td>51.6</td>
<td>5.0</td>
<td>28.2</td>
</tr>
<tr>
<td>Feldspar / Biotite</td>
<td>2.30E+14</td>
<td>0.65</td>
<td>58.0</td>
<td>58.0</td>
<td>5.0</td>
<td>15.1</td>
</tr>
<tr>
<td>Quartz / Quartz</td>
<td>2.80E+14</td>
<td>0.65</td>
<td>130</td>
<td>65.0</td>
<td>5.0</td>
<td>35.0</td>
</tr>
<tr>
<td>Quartz / Biotite</td>
<td>2.30E+14</td>
<td>0.65</td>
<td>57.0</td>
<td>52.0</td>
<td>5.0</td>
<td>23.4</td>
</tr>
<tr>
<td>Biotite / Biotite</td>
<td>1.30E+14</td>
<td>0.65</td>
<td>88.0</td>
<td>5.0</td>
<td>5.0</td>
<td>25.3</td>
</tr>
</tbody>
</table>

2.5 Generation of Bonded Block Models

Two approaches were applied to generate the BBM grain structures for this study. On the one hand, deterministic grain structures were built based on images and petrographic descriptions of actual specimens of Wausau granite, whereas, on the other hand, random grain structures were generated using the Voronoi tessellation technique.

2.5.1 Deterministic Bonded Block Models

Two-dimensional deterministic BBMs were developed based on the petrographic characterization of actual specimens of Wausau granite. For the process of characterization, a cylindrical core specimen (51 mm in diameter and 128 mm high) of Wausau granite was cut into thin disk-shaped slices, around 1 mm thick. Three of those disks (WG-08-01, WG-08-21, and WG-08-41) taken from both ends and mid-section of the core specimen were selected for macroscopic inspection to determine the mineralogical composition and identify the grain boundaries.

The macroscopic petrographic characterization was validated by using thin-section petrography and SEM-based automated mineralogy to assure the accurate determination of the
mineralogy of the granite specimens. The macroscopic petrography and the modal analyses reported by the TIMA were the basis for defining the mineral proportions of the block models.

Photographs of the disk-shaped specimens were the basis for the block models. In the photographs, the boundaries of each mineral grain were identified and digitized using AutoCAD (AutoDesk, 2019). Broadly speaking, the mineral grains were represented as convex or concave polygons with multiple edges and vertices. Although the idea of a deterministic model implies an exact representation of the geometry of a grain structure, some simplifications were applied during the digitization process. The simplifications were focused on small-scale geometric features, omission of which has little impact on the simulations. Thus, as a general rule for the digitization, grains with an equivalent diameter below 0.10 mm were not represented. Also, grain boundaries with a serrated shape and small concavities were represented as straight lines. Such simplifications prevent the inclusion of excess of details within the model that could result in misrepresentations of the interactions among grains and associated shear or tensile failure mechanisms.

The digitized grain boundaries were then imported into UDEC (Itasca Consulting, 2014), where different micro-properties were assigned depending on the type of grain or contact. As explained in a previous section, Wausau granite is represented as a grain structure with four types of grains, but also as a grain structure with three types of grains. In the models with four types of minerals, the feldspar grains were randomly assigned K-feldspar or plagioclase micro-properties. That decision was made given the difficulties of identifying a dominant sodic or potassic proportion within the grains of the feldspar group. Such random assignment complies with the mineral proportions determined on each of the granite disks, but also with the approximate 3:5 K-feldspar to plagioclase ratio determined based on automated mineralogy analyses. Table 2.1 summarizes the mineral composition determined for each disk specimen.
On the other hand, models with three types of minerals considered all feldspar grains in a single group under the general denomination “average-feldspar,” independently of their potassium or sodium content. These models followed the mineral proportion described for each disk-shaped specimen. Figure 2.3 shows the photographs of Wausau granite disk-shaped specimens and their corresponding deterministic BBMs.

Figure 2.3: Photographs and corresponding deterministic BBM grain structures for Wausau granite specimens (a) WG-08-01, (b) WG-08-21, and (c) WG-08-41.
2.5.2 Voronoi Bonded Block Models

The randomly generated grain structures used for this study were generated using Neper, which is an open-source software package for polycrystal generation and meshing in 2D and 3D (Quey, 2019) that consists of three modules for generation, meshing, and visualization of tessellations. Neper generates grain assemblies using Voronoi tessellations with convex-shaped cells within space domains of different configurations (e.g., prismatic, cylindrical, and circular shapes).

Neper allows the definition of cell morphological properties using statistical distributions, specifically cell size (or equivalent diameter) and sphericity, to be employed in the generation of Voronoi tessellations. If the centroids of the cells are known, this aspect can also be defined in Neper as a basis for the tessellations. Neper also offers an option for the generation of two-scale Voronoi tessellations, which involves partitioning every cell of a “primary” Voronoi tessellation into “secondary” Voronoi tessellation cells (Ghazvinian et al., 2014; Wang and Cai, 2018). Neper is able to generate files containing the 3D grain structure model information that can be directly imported into 3DEC (Itasca Consulting, 2017).

Two types of Voronoi BBMs were developed for this research using Neper: (a) 3D BBMs representing cylindrical core specimens with a diameter of 51.4 mm and a length of 128.8 mm, each one with different morphological properties (i.e., grain size, and shape); and (b) 2D BBMs representing disk-shaped specimens with a diameter of 51.4 mm, and fixed numbers of grains.

A 3D baseline Voronoi BBM was defined to represent the average mineral composition, average grain size, equivalent number of grains, and approximate average grain shape of Wausau granite. The mineralogical composition was based on the results of the automated mineralogy
analyses. Cases with three grain types and four grain types were developed. Measurements of the apparent grain size made on disk-shaped specimens of Wausau granite were used to define the average grain size of the baseline model (2.3 mm) and the corresponding equivalent number of grains (39000 grains). An average grain shape was defined to represent an intermediate degree of sphericity that qualitatively resembles the average shape of a real mineral grain.

Additionally, another six 3D BBMs were constructed. Two of them with the same characteristics of the baseline model, but different grain arrangement. Another two BBMs have the same mineral composition, average grain size, and equivalent number of grains as the baseline BBM, but different grain shape (i.e., degree of sphericity). Finally, another two BBMs were developed with the same mineral composition and average grain shape as the baseline model, but different average grain sizes.

From each of the 3D BBMs, three 2D BBMs were derived as 2D representations of the same grain structure. The 2D BBMs were built based on sections cut from the 3D models using 3DEC: two axial sections orthogonal between each other, and one diametral section orthogonal to the other two sections (See Figure 2.4). The sections generated in 3DEC were later imported into UDEC (Itasca Consulting, 2016) to execute the 2D simulations.

The 2D Voronoi BBMs developed in Neper were set to replicate the number of grains and mineral composition identified in specimens WG-08-01, WG-08-21, and WG-08-41. Both the number of grains and mineral composition for each specimen were determined to develop the deterministic models and are described in the previous section. The models were developed under a “conventional” Voronoi tessellation approach that considers uniform shape and size parameters for the grains, similar in geometry to the grain structures used in previous studies (Kazerami and Zhao, 2010; Lan et al., 2010; Nicksiar and Martin, 2014; Sinha and Walton, 2018).
Figure 2.4: Baseline BBM generated in Neper and the three BBMs derived from it. (a) 3D BBM; (b) first axial 2D BBM section, “XZ”; (c) second axial 2D BBM section, “YZ”; and (d) diametral 2D BBM section, “XY”.

2.6 Numerical Tests Set-up

In this study, UCS tests are simulated in 3D and 2D, whereas BTS tests are simulated only in 2D. For the UCS test simulations, axial loading is applied via a constant vertical velocity directly to the top and bottom surfaces of the model (-v/2 and v/2, respectively) to produce an effective loading velocity, v. Given the great influence of the loading velocity on the modeling results, a sensitivity analysis of the loading velocity was performed to determine a proper loading rate that ensures quasi-static equilibrium conditions for the model. A constant velocity of 0.1 m/s was established as a loading velocity, below which changes in velocity have limited influence (< 4%)
on the model results. For the BTS test simulations, compressive loading is applied via two rigid platens. In a similar manner to the UCS tests, a constant vertical velocity is applied to the top and bottom platens, \(-v/2\) and \(v/2\), respectively, for a total effective loading velocity, \(v\). The effective loading velocity, \(v\), for the BTS tests was set to be 0.05 m/s. Although these loading velocities are much larger than those used in laboratory tests, what is more relevant in numerical simulations is the velocity in units of displacement per solution step. For a loading rate of 0.1 m/s, the equivalent rate of \(10^{-5}\) mm/step implies that over 100,000 steps are required to produce a displacement of 1 mm (Lisjak et al., 2014; Gao et al., 2016; Wang and Cai, 2018).

The axial and lateral strains are tracked through multiple pairs of control grid points. In both cases, the strain is calculated by averaging the displacements between the pairs of control points using a FISH script. As shown in Figure 2.5, for the two-dimensional UCS tests, five pairs are arranged for tracking the axial strains, and eleven pairs for tracking the lateral strains. The control grid points are located 2 mm away from the boundaries of the model to prevent any influence of the boundary conditions on the displacement measurements. For the three-dimensional UCS tests, nine and twenty-two pairs of points are set for tracking the axial and lateral strains, respectively. A similar arrangement is used for the BTS tests where five and nine pairs of grid points are set for tracking the axial and lateral strains, respectively.

The axial stress is tracked and calculated by averaging the axial stresses (\(\sigma_{zz}\)) measured in the zones of the blocks inside the core specimen through a FISH script. All the zones within the model are considered for this calculation.
Figure 2.5: Test configuration for (a) UCS, and (b) BTS test simulations.
2.7 Comparative Analyses

The goal of this study is to compare the results of laboratory-scale simulations run on BBMs with different representations of the same Wausau granite grain structure, in combination with various sets of grain/contact micro-properties. First is a comparison of 3D and 2D representations of the same grain structure in the results of UCS test simulations. This assessment was run using a baseline Voronoi BBM that achieves a fair approximation of Wausau granite internal structure (see Figure 2.4). The baseline Voronoi BBM represents the average mineral composition estimated using automated mineralogy analyses, as well as the average grain size, the equivalent number of grains, and approximate grain shape determined by petrographic characterization of Wausau granite specimens. For this analysis, the 3D baseline Voronoi BBM is compared with two equivalent 2D models, which are derived from the original 3D baseline BBM.

Then, using the same baseline model, the study focuses on evaluating which sets of micro-properties calibrated by four selected authors (Lan et al., 2010; Chen and Konietzky, 2014; Farahmand and Diederichs, 2015; and Chen et al., 2016) can best replicate the UCS, Young’s modulus, Poisson’s ratio, CI, CD, and indirect tensile strength of Wausau granite in UCS and BTS tests. Next, the influence of the representation of feldspar grains on the results of UCS and BTS tests is analyzed. In this analysis, feldspar grains are represented as two different types of grains (i.e., K-feldspar and plagioclase), but also as one single feldspar group. A fourth section of the comparative analyses focuses on the impact of certain grain-geometry parameters using diverse BBMs where such parameters were individually varied. In such an analysis, the following parameters were analyzed in both UCS and BTS test simulations: (a) grain size, (b) grain shape, and (c) grain arrangement. Finally, the results of BTS test simulations using deterministic 2D
BBMs were compared with the results of “conventional” Voronoi BBMs, with randomly generated grain structures.

2.7.1 Evaluation of the Effect of Model Dimensionality

The baseline Voronoi BBM (see Figure 2.4) employed for this analysis represents the internal structure of Wausau granite in terms of mineral composition (24% K-feldspar, 41% plagioclase, 32% quartz, and 3% biotite), and average grain size (2.3 mm). Additionally, the model attempts to replicate a common average grain shape observed in Wausau granite specimens. According to thin-section microscopy and macroscopic observations, grains tend to show a prismatic shape, rather than uniform rounded shapes like the ones used in many previous studies (Chen and Konietzky, 2014; Fabjan et al., 2015; Chen et al., 2016). In all the analyzed cases in this section, the grain arrangement was not varied. Four different sets of calibrated micro-properties were used for this group of simulations (Lan et al., 2010; Chen and Konietzky, 2014; Farahmand and Diederichs, 2015; and Chen et al., 2016).

To assess the influence of model dimensionality, one 3D and two 2D UCS test simulations were run with each set of micro-properties. The 2D BBMs were derived from the baseline 3D BBM. Therefore, all the models represent the same grain structure with the same grain arrangement and geometry, but from different perspectives. Figures 2.6 to 2.9 show the stress-strain curves obtained from 3D and 2D simulations using different sets of micro-properties.

Independently of the resulting macro-property values, simulations run using the same set of micro-properties show a clear contrast between 2D and 3D results. On the one hand, the results of both 2D simulations present the same Young’s modulus (E) and Poisson’s ratio (ν) values,
whereas the UCS, crack initiation stress (CI), and crack damage stress (CD) values show differences around 10% between each other. On the other hand, the 3D simulations compared to the 2D simulations present in most cases greater equivalent axial strains ($\varepsilon_a$) and lower equivalent lateral strain ($\varepsilon_l$), which translates into lower $E$ and $\nu$ values. Also, the predicted UCS values are between 5% and 50% lower than the predicted in 2D simulations. The CI and CD values, expressed as a percentage of the UCS values, are quite consistent among most 3D and 2D simulations (i.e., CI $\approx$ 39% UCS; CD $\approx$ 90% UCS) with differences below 10%.

Figure 2.6: Stress-strain curves obtained from two 2D and one 3D UCS test simulations using Lan et al. (2010) micro-properties.
Figure 2.7: Stress-strain curves obtained from two 2D and one 3D UCS test simulations using Chen and Konietzky (2014) micro-properties.

Figure 2.8: Stress-strain curves obtained from two 2D and one 3D UCS test simulations using Farahmand and Diederichs (2015) micro-properties.
2.7.2 Evaluation of the Effect of Micro-properties

The simulations run on the baseline BBMs in the previous analysis were also used for this evaluation. Additionally, 2D BTS simulations were run to predict the indirect tensile strength of Wausau granite using the same four sets of micro-properties.

According to the 2D simulation results, the micro-properties from Farahmand and Diederichs (2015) and Chen and Konietzky (2014) are the sets that result in emergent peak strength that is most similar to the UCS of the rock specimen, reaching just above 86% of the actual peak strength of Wausau granite. Conversely, in the 3D simulations, the models reach less than 74% of Wausau granite’s UCS; again, the parameters from Farahmand and Diederichs (2015) predicted the highest peak strength (closest to the actual peak strength).
Similarly to the UCS, the micro-properties from Farahmand and Diederichs (2015) and Chen and Konietzky (2014) provided the best approximations of CD and CI. Predicted CD values are below the actual CD stress value (201.7 MPa) and are up to 18% lower. The predicted values for the CI stress are up to 32% lower than the real value (91 MPa). The 3D simulations show similar behavior with the same two sets of micro-properties providing the best predictions. The values predicted using those sets are 23% below the actual values of CD stress, and up to 43% below CI stress actual values.

In the case of the Young’s modulus, all the results from 2D simulations are similar to the laboratory specimen’s actual value (E = 69.6 GPa), with the micro-properties from Chen and Konietzky (2014), and Farahmand and Diederichs (2015) providing values slightly above (up to 7% greater than) the actual E value of Wausau granite. The other sets of micro-properties result in values of Young’s modulus around 18% below the real value. In the case of the 3D simulations, the macro-properties of Farahmand and Diederichs (2015) provided a very close approximation of the real E value (less than 4% difference), whereas the properties of Lan et al. (2010), Chen and Konietzky (2014), and Chen et al. (2016) predict values 14%, 8% and 25% below the real Young’s modulus value, respectively.

The micro-properties of Farahmand and Diederichs (2015) very closely approximated the actual ν value (0.24) in the 2D simulations. The micro-properties of Chen and Konietzky (2014) produced values 18% above, whereas the micro-properties of Lan et al. (2010), and Chen et al. (2016) produced values more than 6% below the ν. All the 3D simulations predicted values of ν over 20% below the actual 0.24 value.

The simulations of UCS tests properly captured the evolution of crack distribution under different stress levels. Figure 2.10 shows the distribution of cracks within the 2D baseline model
obtained using the micro-properties of Farahmand and Diederichs (2015). At the CI stress (around 40% of UCS), almost no cracks can be observed. Once the CD stress (around 90% of UCS) is reached, fracturing accelerates into the peak and post-peak stress levels.

UCS test simulations also achieve to replicate the fracture patterns obtained in the laboratory (see Figure 2.11). The failed laboratory specimens show dominant tensile fractures, but also some minor shear fractures and areas of crushed grains. The simulations replicated shorter tensile macro-fractures and shear macro-fractures product of the coalescence of various smaller tensile and shear fractures. Although the blocks within the models cannot break, areas of crushed grains are approximated by areas of intense cracking around the grains.

Figure 2.10: Evolution of crack distributions under different stress levels during UCS test. (a) CI stress, (b) CD stress, (c) peak stress, and (d) post-peak stress at 0.5% of axial stress.
The results of the BTS tests simulations show that the micro-properties of Chen and Konietzky (2014) provide the best prediction of the indirect tensile strength with a 6% difference compared to the actual value (11.7 MPa). The micro-properties of Farahmand and Diederichs (2015) and Chen et al. (2016) predicted values with a 19% difference, whereas the micro-properties of Lan et al. resulted in a 52% difference below the actual value.

Figures 2.10 to 2.15 show the results of the various models, for UCS, CD stress, CI stress, Young’s modulus, Poisson’s ratio, and tensile strength respectively, compared to the average values reported for Lac du Bonne (LDB) granite (Farahmand and Diederichs, 2015), Kirchberg II (KII) granite (Chen et al., 2016), and Wausau (WAU) granite. In these figures, the “Upper Bound”
and “Lower Bound” represent the mean values for Wausau granite plus or minus two standard deviations, respectively. Table 2.7 summarizes the results.

Figure 2.12: Comparison of predicted UCS using different sets of micro-properties.

Figure 2.13: Comparison of predicted CD stress using different sets of micro-properties.
Figure 2.14: Comparison of predicted CI stress using different sets of micro-properties.

Figure 2.15: Comparison of predicted Young’s modulus using different sets of micro-properties.
Figure 2.16: Comparison of predicted Poisson’s ratio using different sets of micro-properties.

Figure 2.17: Comparison of predicted BTS using different sets of micro-properties.
Table 2.7: Summary of results, evaluation of the effect of micro-properties.

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* Difference compared to real macro-property value.
2.7.3 Evaluation of the Effect of Feldspar Representation

Two-dimensional UCS and BTS test simulations were performed for this section of the study using the baseline grain structure. The two modeled cases compare two different ways to represent feldspars described in Wausau granite. The first BBM populates the baseline grain structure with four types of grains: quartz, biotite, and two separate phases of feldspar (K-feldspar and plagioclase). The second block model populates the baseline grain structure with three types of minerals: quartz, biotite, and one single group of feldspar (i.e., microperthite, an intergrowth between K-felspar and plagioclase). The micro-properties of Lan et al. (2010), Chen and Konietzky (2014), and Farahmand and Diederichs (2015) were applied to the model with four types of minerals, whereas the “average-feldspar” sets of micro-properties (created from the mentioned studies) were applied to the models with three types of minerals.

The results of the simulations (see Table 2.8) reflect the connection between the original sets of micro-properties and the “average-feldspar” sets of micro-properties derived from them. In both cases, the results for predicted UCS, CD stress, CI stress, E, and ν are very similar. The difference between the results of both cases is below 10% for all the macro-properties mentioned above. In the case of σt, although the results using “average-feldspar” properties are consistent with those obtained using the original micro-properties, the dispersion of the results is more prominent. The similarity of the results of both models indicates that the micro-properties of two mineral grains with similar composition, or as in this case, exsolved mineral grains, can be successfully represented with one single set of micro-properties. Figures 2.16 to 2.21 show the comparison of the results of both types of models.
Figure 2.18: Comparison of predicted UCS using “average-feldspar” vs. original micro-properties.

Figure 2.19: Comparison of predicted CD stress using “average-feldspar” vs. original micro-properties.
Figure 2.20: Comparison of predicted CI stress using “average-feldspar” vs. original micro-properties.

Figure 2.21: Comparison of predicted Young’s modulus using “average-feldspar” vs. original micro-properties.
Figure 2.22: Comparison of predicted Poisson’s ratio using “average-feldspar” vs. original micro-properties.

Figure 2.23: Comparison of predicted BTS using “average-feldspar” vs. original micro-properties.
Table 2.8: Summary of results, evaluation of the effect of feldspar representation.

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* Difference compared to real macro-property value.

2.7.4 Evaluation of the Effect of Grain Arrangement

In order to simulate the influence of grain arrangement variations, three different grain distributions (i.e., positions of individual minerals) were randomly assigned to the same baseline Voronoi grain structure, while maintaining Wausau granite’s volumetric mineral composition. Thus, the baseline 3D BBM used in previous sections was established as the first case of the analysis (“A”), whereas the other two cases are duplicates of the baseline grain structure but with different grain arrangements (“B” and “C”). Figure 2.22 presents the three 2D block models generated from each of the 3D BBMs to execute two-dimensional UCS and BTS test simulations. Considering that the sets of micro-properties of Chen and Konietzky (2014), and Farahmand and Diederichs (2015) provide the best predictions of the different macro-properties of Wausau granite, only those sets of micro-properties are used in the simulations of this and the following sections of the study.
Figures 2.23 to 2.28 present comparisons of the predicted macro-properties obtained with each of the three different grain distributions. Grain arrangements “A” (baseline, “BL”), “B,” and “C” show different results, and even when comparing each pair of “XZ” and “YZ” 2D BBMs that correspond to a single 3D BBM, they do not provide the same result. The obvious grain arrangement variations can explain such differences among all the 2D BBMs. Nevertheless, the results obtained using the same set of micro-properties tend to vary around a single value by less than 14%. For example, in the case of UCS, the values predicted using Farahmand and Diederichs (2015), properties vary around 205 MPa. With the properties of Chen and Konietzky (2014), the predicted values vary around 195 MPa. In both cases, the differences between the results obtained using different grain arrangements are less than 14%. The same behavior was identified in the results of other macro-properties. Table 2.9 summarizes the results.
Figure 2.24: BBMs with different grain arrangement but equal volumetric mineral composition. (a) Arrangement “A” (baseline), (b) Arrangement “B”, and (c) Arrangement “C”. For each arrangement, from left to right: 3D BBM, 2d BBM "XZ", 2D BBM "YZ", and 2D BBM "XY".
Figure 2.25: Comparison of predicted UCS using BBMs with different grain arrangement.

Figure 2.26: Comparison of predicted CD stress using BBMs with different grain arrangement.
Figure 2.27: Comparison of predicted CI stress using BBMs with different grain arrangement.

Figure 2.28: Comparison of predicted Young’s modulus using BBMs with different grain arrangement.
Figure 2.29: Comparison of predicted Poisson’s ratio using BBMs with different grain arrangement.

Figure 2.30: Comparison of predicted BTS using BBMs with different grain arrangement.
Table 2.9: Summary of results, evaluation of the effect of grain arrangement.

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* Difference compared to real macro-property value. BL = Baseline BBM.
Table 2.9: Continued.

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* Difference compared to real macro-property value. BL = Baseline BBM.

2.7.5 Evaluation of the Effect of Grain Shape

Different 3D BBMs, with the same volumetric mineral composition and number of grains as the baseline block model, but different grain shapes were used for this part of the study. The grain shape was expressed as a function of sphericity in Neper (Quey, 2019) and represented in three different BBMs. The sphericity is defined as the ratio between the surface area of the sphere of equivalent volume and the surface area of the polyhedral grain. Sphericity takes a maximum value of 1 for a spherical grain (Quey and Renversade, 2018; Quey, 2019).

The first model depicts grains with high sphericity (i.e., sphericity = 0.85) similar to the regular rounded shape usually employed in BBMs. The second model represents grains with an intermediate degree of sphericity (i.e., sphericity = 0.80) that resembles the average shape of actual
mineral grains within Wausau granite. This intermediate degree of sphericity is as used in the baseline BBM. The third model denotes an assembly of grains with low sphericity (i.e., sphericity = 0.75), exaggerated angularity, and slightly elongated shapes. Figure 2.29 shows the three BBMs employed in this analysis.

The results of the simulations (see Figure 2.10) show a vague correlation between the predicted UCS values and the degree of sphericity represented in some of the models (see Figure 2.30). Representations of low sphericity of the grains predicted higher values of UCS. This correlation can be explained by the degree of interlocking among grains, which increases when the grains are more irregular (i.e., low sphericity), and directly influences the peak strength of the rock.

The predictions of CD stress, CI stress, E, ν, and tensile strength do not show any apparent direct correlation with the shape of the grains. Figures 2.31 to 2.35 show the predicted values for the macro-properties mentioned above.
Figure 2.31: BBMs with different grain shape, but equal volumetric mineral composition. (a) “High sphericity” (b) “Intermediate sphericity” (baseline), and (c) “Low sphericity.” For each model, from left to right: 3D BBM, 2D BBM “XZ”, 2D BBM “YZ”, and 2D BBM “XY”.
Figure 2.32: Comparison of predicted UCS using BBMs with different grain shapes.

Figure 2.33: Comparison of predicted CD stress using BBMs with different grain shapes.
Figure 2.34: Comparison of predicted CI stress using BBMs with different grain shapes.

Figure 2.35: Comparison of predicted Young’s modulus using BBMs with different grain shapes.
Figure 2.36: Comparison of predicted Poisson’s ratio using BBMs with different grain shapes.

Figure 2.37: Comparison of predicted BTS using BBMs with different grain shapes.
Table 2.10: Summary of results, evaluation of the effect of grain shape.

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* Difference compared to real macro-property value. BL = Baseline BBM.
### 2.7.6 Evaluation of the Effect of Grain Size

This part of the study used three BBMs with different average grain size, but the same volumetric mineral composition. The first BBM (baseline model) represents an average grain diameter of 2.3 mm, with a total of 39000 grains. The second model has an average equivalent diameter of 2.6 mm, and 27000 grains in total. The third BBM contains 15000 grains with an average diameter of 3.1 mm.

The results obtained in this analysis do not show a clear influence of the grain size on the prediction of macro-properties. However, a rough correlation was detected in Young’s modulus prediction, where an increase of the grain size appears to lead to a slight increase in the value of elastic modulus (see Figure 2.40). Such an increase in elastic modulus is probably related to elastic
behavior assigned to the grains within the BBMs. Larger elastic grains add stiffness to the whole system, as the number of soft grain-boundary elements is decreased. Figures 2.36 to 2.42 show all the results of this analysis, and Table 2.11 shows a summary of the results.
Figure 2.38: BBMs with different grain size, but equal volumetric mineral composition. (a) 2.3 mm in diameter (baseline model), (b) 2.6 mm in diameter, and (c) 3.1 mm in diameter. For each arrangement, from left to right: 3D BBM, 2D BBM “XZ”, 2D BBM “YZ”, and 2D BBM “XY”.
Figure 2.39: Comparison of predicted UCS using BBMs with different grain sizes.

Figure 2.40: Comparison of predicted CD stress using BBMs with different grain sizes.
Figure 2.41: Comparison of predicted CI stress using BBMs with different grain sizes.

Figure 2.42: Comparison of predicted Young’s modulus using BBMs with different grain sizes.
Figure 2.43: Comparison of predicted Poisson’s ratio using BBMs with different grain sizes.

Figure 2.44: Comparison of predicted BTS using BBMs with different grain sizes.
Table 2.11: Summary of results, evaluation of the effect of grain size.

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<th>CD (MPa)</th>
<th>CI (MPa)</th>
<th>BTS (MPa)</th>
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<td>74.6</td>
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<td>D (%)</td>
<td></td>
<td></td>
<td></td>
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<td>18.3</td>
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</tbody>
</table>

* Difference compared to real macro-property value. BL = Baseline BBM.
Table 2.11: Continued.

<table>
<thead>
<tr>
<th>Micro-properties</th>
<th>Grain Size (mm)</th>
<th>Model</th>
<th>UCS (Mpa)</th>
<th>E (Gpa)</th>
<th>ν</th>
<th>CD (Mpa)</th>
<th>CI (Mpa)</th>
<th>BTS (Mpa)</th>
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<td>D (%)*</td>
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<td>8.3</td>
<td>2.7</td>
<td>-7.9</td>
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<tr>
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<td>105</td>
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<td>D (%)*</td>
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<td>8.8</td>
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<td>-0.3</td>
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<td></td>
</tr>
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<td></td>
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<tr>
<td></td>
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<td>D (%)*</td>
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<td></td>
<td></td>
<td></td>
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<tr>
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<td>0.25</td>
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<td>94.0</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>D (%)*</td>
<td>-3.6</td>
<td>13.6</td>
<td>2.9</td>
<td>-7.1</td>
<td>3.6</td>
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</tr>
<tr>
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<td></td>
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<td>0.25</td>
<td>208</td>
<td>99.0</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>D (%)*</td>
<td>1.8</td>
<td>12.6</td>
<td>5.6</td>
<td>3.8</td>
<td>8.8</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>XY</td>
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<td></td>
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<td>15.2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>D (%)*</td>
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<td></td>
<td></td>
<td></td>
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<td>29.7</td>
</tr>
</tbody>
</table>

* Difference compared to real macro-property value. BL = Baseline BBM.

2.7.7 Comparison Between Deterministic BBMs and Voronoi BBMs

This part of the study was designed to show the difference between a deterministic model that represents a grain structure with a high degree of realism, against a “conventional” (randomly generated) Voronoi model.

Three different disk-shaped specimens of Wausau granite (WG-08-01, WG-08-21, and WG-08-41) were characterized and deterministically modeled. Although all three disk specimens come from a single granite core sample, their mineralogical composition and number of grains slightly differ from each other. Also, as expected, the grain arrangement is unique for each specimen, as well as the grain shape and grain size. Table 2.6 summarizes the composition and number of grains described in each specimen. This information is the basis for the deterministic
models, which reproduce the mineralogical composition, grain arrangement, and number of grains on each specimen, as well as the shape and size of each individual grain.

To generate the group of Voronoi BBMs, Neper was set to replicate the specific number of grains in each granite specimen, and randomly generate grains with a homogeneous shape and size, in the way “conventional” Voronoi models are usually created and used in previous studies (Chen and Konietzky, 2014; Fabjan et al., 2015; Chan et al., 2016). Figure 2.43 shows the deterministic and Voronoi models generated for each granite disk specimen for comparison.

Figure 2.45: Deterministic and Voronoi BBMs generated for specimens (a) WG-08-01, (b) WG-08-21, and (c) WG-08-41.
As a premise for this assessment, the deterministic models are supposed to deliver the “actual” macro-mechanical response in BTS test simulations, thanks to their very realistic representation of the grain structures that control the micro-mechanical behavior within specimens WG-08-01, WG-08-21, and WG-08-41. The micro-properties of Chen and Konietzky (2014) were used in the simulations, given that they provide the best approximations of indirect tensile strength.

As expected, the results of the deterministic BBMs (WG-01, WG-21, and WG-41) are different from the results of the conventional Voronoi BBMs (VO-01, VO-21, and VO-41) as shown in Figure 2.44 and Table 2.12. Such differences in the predicted indirect tensile strength are directly related to the geometry of the grain structures. Each pair of Voronoi and deterministic models is the representation of the same areal mineralogical composition and number of grains, but the arrangement, shape, and size of the grains are completely different. Even though using an average grain size provides certain realism to the Voronoi representation, the lack of a detailed depiction for each mineral grain lowers the chances of representing the actual degree of interlocking among grains, which is closely related to the micro-mechanical behavior of the rock. Nevertheless, the prediction of indirect tensile strength with Voronoi models is quite close to the predictions provided by deterministic models (differences of 6%, 10%, and 5% for the WG-08-01, WG-08-21, and WG-08-41 cases, respectively).
Figure 2.46: Comparison of BTS test simulation results between deterministic and Voronoi BBMs.

Table 2.12: Comparison between deterministic and Voronoi models.

<table>
<thead>
<tr>
<th>Model</th>
<th>Axial strain (%)</th>
<th>Diff. (%)</th>
<th>Lateral strain (%)</th>
<th>Diff. (%)</th>
<th>Brazilian Tensile Strength (MPa)</th>
<th>Diff. (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>WG-01</td>
<td>0.0004</td>
<td>8.4</td>
<td>-0.0167</td>
<td>-5.8</td>
<td>8.8</td>
<td>6.3</td>
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<tr>
<td>VO-01</td>
<td>0.0004</td>
<td></td>
<td>-0.0157</td>
<td></td>
<td>9.3</td>
<td></td>
</tr>
<tr>
<td>WG-21</td>
<td>0.0005</td>
<td>23.0</td>
<td>-0.0044</td>
<td>234.9</td>
<td>13.3</td>
<td>-10.5</td>
</tr>
<tr>
<td>VO-21</td>
<td>0.0007</td>
<td></td>
<td>-0.0146</td>
<td></td>
<td>11.9</td>
<td></td>
</tr>
<tr>
<td>WG-41</td>
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<td>-0.0075</td>
<td>114.1</td>
<td>10.9</td>
<td>4.7</td>
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<td>VO-41</td>
<td>0.0005</td>
<td></td>
<td>-0.0162</td>
<td></td>
<td>11.4</td>
<td></td>
</tr>
</tbody>
</table>
2.8 Discussion

The results of the simulations in this study show that slight changes in the representation of certain geometric parameters of the grain structure can make a great impact on the prediction of rock mechanical behavior. Table 2.13 summarizes the degree of influence of the representation of different factors expressed in terms of predicted UCS, compared to the values obtained using the baseline BBM in combination with Farahmand and Diederichs (2015) micro-properties.

Table 2.13: Influence of different representations on the predicted UCS.

<table>
<thead>
<tr>
<th>CASE</th>
<th>UCS (Mpa)</th>
<th>Difference (%)</th>
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</thead>
<tbody>
<tr>
<td>Baseline BBM (2D, four mineral types, intermediate sphericity, average diameter of 2.3 mm)</td>
<td>207</td>
<td></td>
</tr>
<tr>
<td>BBM in 3D (4 mineral types, intermediate sphericity, average diameter of 2.3 mm)</td>
<td>155</td>
<td>-25.0</td>
</tr>
<tr>
<td>BBM with low sphericity (2D, four mineral types, average diameter of 2.3 mm)</td>
<td>231</td>
<td>11.5</td>
</tr>
<tr>
<td>BBM with high sphericity (2D, four mineral types, average diameter of 2.3 mm)</td>
<td>219</td>
<td>5.6</td>
</tr>
<tr>
<td>BBM with three mineral types (2D, intermediate sphericity, average diameter of 2.3 mm)</td>
<td>201</td>
<td>-2.8</td>
</tr>
<tr>
<td>BBM with different grain arrangement (2D, four mineral types, intermediate sphericity, average diameter of 2.3 mm)</td>
<td>213</td>
<td>2.8</td>
</tr>
<tr>
<td>BBM with average diameter of 2.6 mm (2D, four mineral types, intermediate sphericity)</td>
<td>210</td>
<td>1.3</td>
</tr>
<tr>
<td>BBM with average diameter of 3.1 mm (2D, four mineral types, intermediate sphericity)</td>
<td>207</td>
<td>0.1</td>
</tr>
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</table>

Model dimensionality has, by far, the most significant impact on the numerical simulations. The results of the simulations showed a difference of 25% between the estimation of UCS in 3D and 2D. Besides the obvious effect of grain arrangement, these results can be explained by the
origin of the micro-properties used in the analysis, which were calibrated to satisfy the micro-
mechanical behavior of 2D models. Also, the difference between 2D and 3D results can be
explained by the way UDEC (2D) and 3DEC (3D) represent the interaction and movement of
elastic blocks within the grain structure. UDEC (Itasca, 2014) uses polygonal blocks with rounded
corners; so, blocks can smoothly slide on one another when two opposing corners interact. This
representation allows us to account for the crushing effect of two corners interacting in a real grain
structure and prevents these blocks from becoming numerically locked (Itasca, 2014). Conversely,
3DEC (Itasca, 2016) represents the grains as polyhedral blocks with sharp corners and sharp edges.
The interaction between sharp corners (or edges) of two neighbor blocks could cause stress peaks
and subsequently could lead to unrealistic representations of high damage within the grain
structure.

Grain shape variations also had a great influence on the results of the simulations, particularly
affecting the degree of interlocking among grains and, consequently, the simulated peak strength.
Such an effect is especially noticeable when the grains have lower than typical sphericity, resulting
in UCS values up to 11.5% higher. The representation of grains with high sphericity produced a
lower degree of variability with predicted UCS values 5.6% higher. Having into account that actual
specimens of Wausau granite present lower UCS variability (i.e., ±8.6% for UCS), the predictions
made using BBMs with inadequate representations of model dimensionality or grain shape could
be considered of low accuracy.

The effect of grain arrangement is not as noticeable as the previous two factors; however, it
produces variations on the predicted UCS in the order of 2.8%. Although grain arrangement
heterogeneity is an expected issue when dealing with geo-materials such as rocks and its effect
cannot be prevented, it is necessary to control and minimize its uncertainty in order to predict the
rock’s mechanical behavior with reasonable accuracy. The representation of feldspars within Wausau granite also affects the results of the simulations, producing a variation of 2.8% on the predicted UCS. Taking into consideration this small variation, it appears that relative to other factors, the explicit separation of different mineral phases with similar mechanical parameters in BBMs is not a major control of simulated stress-strain behavior. As opposed to the other factors, the simulations show a minor influence of the grain size representation in the model’s predicted UCS, producing variations below 1.3%.

The influences of the grain and contact micro-properties on the prediction of rock strength were assessed by comparing estimated values of macro-properties using four different sets of micro-properties taken from the literature. Two of these sets of micro-properties lead to a reasonable agreement between model predictions and test results on actual specimens of Wausau granite. A quick comparison between the two sets of micro properties that predicted the rock strength with fair accuracy (Chen and Konietzky, 2014; and Farahmand and Diederichs, 2015) against the other sets used in this study (Lan et al., 2010; Chen et al., 2016) shows some clear differences. In particular, the contact tensile strength (which directly influences the macroscopic tensile strength), and the friction angle and cohesion (which have a direct effect in the UCS) are notably different. The sets of properties that provided a reasonably accurate prediction of tensile strength present average contact tensile strengths around 23 MPa, whereas the other sets have very different tensile strength values. Concerning the contact friction angle and cohesion values, these are also higher in the sets that accurately predicted UCS as opposed to the values in the other sets, which are 15% to 50% lower.

The comparison between a deterministic BBM and a conventional Voronoi BBM attempted to contrast the benefits of a detailed depiction of the grain structure against a basic approximation
through Voronoi tessellations. The premise of this analysis was that a deterministic model provides the “actual” macro-mechanical response of the rock in BTS test simulations thanks to its very realistic representation of the grain structure. The results of the analysis showed that even though the predictions of BTS using Voronoi BBMs were different than the ones obtained from the deterministic models, the predictions were quite similar, with differences between 4.7% and 10.5%. Such differences are similar to the range of variability of the actual Wausau granite BTS (i.e., ± 8.5%). These results suggest that whereas it may be possible to obtain more accurate estimations of rock mechanical behavior using a deterministic BBM grain structure representation, for practical purposes, the conventional Voronoi approach provides a good approximation.

2.9 Conclusions

A BBM that properly represents the grain size, grain shape, and relative mineral proportions of a rock can be used in combination with previously published calibrated micro-properties to predict rock strength, as was done with the Wausau granite. The procedure of using different sets of published micro-properties to reproduce the macroscopic behavior of rock proved to be useful to easily identify what the optimum combination of micro-properties that would provide accurate estimations of the macro-mechanical behavior of rock is. The results of the numerical simulations show that the effects of grain size and grain shape can be approximated to provide a reasonable representation of the grain structure using a Voronoi approach; such a grain structure can then be used for the prediction of rock strength in combination with properly calibrated micro-properties.

With that said, there is a complex interaction between approximations made in the Voronoi BBM grain structure used for micro-property calibration and the resulting influences on the micro-
properties. If a set of micro-properties was derived using an inappropriate grain structure, they will likely not be useful for predictive modeling. Alternatively, it may not be possible to predict the laboratory-scale stress-strain behavior of a given rock using previously determined micro-properties if the rock in question has a grain structure that deviates significantly from what can be approximated using a Voronoi representation.

2.10 Acknowledgments

The author would like to thank the personnel of the Colorado School of Mines Earth Mechanics Institute, particularly Omid Frough, Bruce Yoshioka, and Muthu Vinayak, for their help with the rock mechanics tests. Also, the author would like to thank Jae Erickson and Dr. Katharina Pfaff of the Colorado School of Mines Department of Geology and Geological Engineering for their support with thin-section preparation and automated mineralogy analysis, respectively. The author also thanks Itasca Consulting for providing the software licenses required to perform the numerical simulations in this study. Finally, the author would like to thank Dr. Romain Quey, developer of Neper for his support during the generation of Voronoi assemblies.
CHAPTER 3

DISCUSSION AND CONCLUSIONS

3.1 Discussion and Conclusions

In this study, the combined influence of the grain size and grain shape on Voronoi BBMs was identified. Every attempt to individually vary one of those two parameters also resulted in the change of the other parameter. For example, if the shape of the grains varies from a lower degree of sphericity to a higher degree of sphericity, the grains must change their size distribution in order to maintain themselves as an assembly of blocks without porosity. Thus, to obtain a faithful representation of grain heterogeneity, both grain shape and grain size should be characterized for each mineral type, instead of defining a general shape or size for all grains. As a result, the uncertainty related to the heterogeneity of the grain structure is minimized.

Grain arrangement heterogeneity is another factor that adds uncertainty to the prediction of the mechanical behavior of the rock. This factor is particularly important when a 3D rock specimen is simulated in 2D, as in the present study. If multiple axial sections are cut from a 3D cylindrical BBM, each of them will show a unique grain distribution. Even though all the sections are derived from the same 3D BBM, it is unlikely that the mechanical behavior that they predict will match a single set of micro-properties will match. Grain arrangement heterogeneity is always going to be present in the representation of grain structure, and the only way to minimize its influence is by representing it as realistically as possible.

The results of the simulations showed a great disparity between the rock strength obtained from 3D simulations and 2D simulations, although both scenarios were supposed to depict the
same rock. That discrepancy is probably related to the origin of the calibrated micro-properties, which were obtained from 2D simulations. Although the properties calibrated in 2D simulations entirely comply with the micro-mechanics of the BBM, that might not be the case in 3D. This raises questions about the broader validity of the micro-properties calibrated in the literature, given that the vast majority of laboratory-scale BBM studies have been conducted in 2D.

The analysis of the two representations of the feldspar grains within Wausau granite compared models where the only difference was the micro-properties applied to the grains of feldspar. The mechanical properties obtained from both cases are similar, and this suggests that explicit consideration of different mineral phases with similar mechanical properties is not as important as the use of a reasonable geometric approximation of the simulated rock’s grain structure.

The mechanical behavior of brittle rocks cannot be predicted with reasonable accuracy if the calibrated micro-properties do not follow the mechanical principals that guide the relationship between the micro and macro-mechanics of the rock, even if a BBM accurately represents the grain structure. The procedure of combining different sets of calibrated micro-properties with a conventional Voronoi BBM has proven to be an easy and fast way to determine what parameters should be calibrated for a more realistic simulation of the rock’s mechanical behavior. Lan et al. (2010), Chen and Konietzky (2014), Farahmand and Diederichs (2015), and Chen et al. (2016) calibrated the contact micro-properties of rocks with similar characteristics (or in some cases the same type of rock), and yet the values of the parameters they obtained are quite different. Parameters from two of these studies fail to predict the rock unconfined peak strength by more than 50%. In one of the cases (Lan et al., 2010), the lack of a proper procedure to calibrate the parameters and the use of excessive simplification lead to the derivation of mechanical micro-properties that do not reflect the micro-mechanical state of the rock. Specifically, a reduced-scale
model was used for the calibration of elastic parameters, whereas strength parameters were calibrated using a full-scale model. Moreover, properties such as friction angle were adjusted only to match the rock’s macro-response without any apparent physical basis. In the other case (Chen et al., 2016), although a comprehensive calibration procedure was followed to match the macroscopic response recorded in triaxial tests, the procedure did not include UCS or BTS data, leading to a set of micro-properties that only provides realistic predictions of mechanical behavior under confined compression conditions. On the other hand, Chen and Konietzky (2014), and Farahmand and Diederichs (2015), follow an iterative process to adjust the micro-properties to match the corresponding macro-properties of the rock. However, Chen and Konietzky (2014) calibrated the micro-properties based only on UCS and BTS data, so the use of such parameters is restricted to unconfined or low-stress environments.

The advantage of BBMs that deterministically represent the grain structure of rock relative to conventional Voronoi BBMs is that they minimize the extra uncertainty associated with the aleatory nature of Voronoi tessellations. Deterministic, semi-deterministic, or even Voronoi-based BBMs that incorporate grain-geometric parameters have advantages over the conventional method and help to achieve more realistic predictions of the rock mechanical behavior. The more realistic the representation of the grain structure, the better the resultant rock strength prediction. However, the effort required to model a highly realistic BBM is likely to be impractical in most cases.

3.2 Future Research

A logical next step to follow from the current study would involve completing the mechanical characterization of Wausau granite. So far, only UCS and BTS tests have been run on this rock.
Ideally, triaxial compressive tests should also be performed on this rock. Some future tests could include the use of AE sensors as well to identify the rock damage thresholds together with the data gathered with strain gauges.

Once the geomechanical characterization of Wausau granite is completed, additional efforts could be directed to the full calibration of BBMs representing Wausau granite’s grain structure. Such calibration should use UCS, BTS, and triaxial compressive strength information. There are very few published papers that reference the use of triaxial test data for the calibration of BBMs (Farahmand and Diederichs, 2015; Chen et al., 2016; Mayer and Stead, 2017; Li et al., 2017; Wang and Cai, 2018; Li et al., 2019; Wang and Cai, 2019). Therefore, the process of calibration referred to in most studies is incomplete, and those calibrated properties may not be able to replicate the mechanical behavior of the rock under different stress conditions.

The BBMs to be calibrated should represent in detail the grain structure of Wausau granite specimens to properly capture the micro-mechanical behavior of the rock. Thus, to complement the process initiated in this study with 2D models of disk-shaped specimens, other 2D deterministic models of core specimens could be developed to execute the calibration under compressive uniaxial and biaxial states. Also, to obtain calibrated BBM micro-properties in 3D, the development of semi-deterministic models should be pursued. One of the approaches for the development of semi-deterministic models consists of cutting rock specimens into closely spaced slices. Each slice of rock is characterized and interpreted for the reconstruction of the 3D structure within the rock specimen. Semi-deterministic models should work in 3D, in a similar way as deterministic models work in 2D, by providing a detailed representation of the geometry of the grains within the grain structure.
Lastly, the option of using X-ray Diffraction Contrast Tomography (DCT) to capture a more detailed three-dimensional depiction of the internal structure of rocks should be evaluated. This technique is becoming more popular, particularly in the material science and petroleum sectors, and has been successfully used to record the grain structure of alloys and rocks (Bargmann et al., 2018; Quey and Renversade, 2018). This tomographic technique collects a series of 2D projection images of the microstructure from different angles. Such 2D images are computationally combined to reconstruct the 3D grain structure. DCT uses a beam of X-ray to measure the absorption contrast to identify different mineral phases within the grain structure. Also, the diffraction contrast is measured to identify grain orientation. However, this method can be expensive. Thanks to the measurement of diffraction contrast, DCT has partially overcome the issue of other X-ray tomography techniques that were ineffective in differentiating minerals with similar absorption properties within a rock.
REFERENCES


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APPENDIX A

COMPUTATIONAL COST

The computational cost required to complete a numerical simulation using discontinuum models varies in function of different model parameters, such as the number of blocks (i.e., number of grains), mesh density (i.e., discretization grid or mesh), and timestep (Itasca, 2014; Sirois and Grilli, 2015; Itasca 2016). In this study, a sensitivity analysis was performed to identify the proper loading velocity rate (i.e., loading velocity rate equivalent to the timestep) that ensures quasi-static equilibrium conditions for the models and optimizes the computational time in the laboratory-scale simulations. Neither the number of blocks nor the mesh density was adjusted to save computational time.

For the sensitivity analysis a personal computer with Intel Xeon CPU E5-2630 v3 @2.4 GHz processor, 64-bit operating system, and 32 GB of RAM was used for the simulations. Three different velocity rates were analyzed in UDEC (Itasca, 2014) using the same bonded block model in uniaxial compressive test simulations: 0.005 m/s, which is the loading velocity usually employed in similar studies (Fabjan et al., 2015; Sinha and Walton, 2018), and two higher velocity rates 0.02 m/s, and 0.1 m/s. According to the results, the computational cost is inversely proportional to the loading rate. Specifically, the computational cost decreases quadratically as a function of increasing loading rate. A velocity of 0.1 m/s was identified as the loading velocity rate below which changes in velocity have limited influence on the model results. Figure A.1 shows the computational times obtained in 2D UCS test simulations corresponding to each loading velocity rate. Both the 2D and 3D UCS simulations were run using a loading velocity rate of 0.1 m/s for the UCS test simulations, whereas BTS test simulations were run using 0.05 m/s. The
runtime for the 2D UCS test simulations reached up to 12 hours, whereas for the 3D UCS test simulations reached up to 720 hours. The computational time for the BTS test simulations reached up to 5 hours. Table A.1 summarizes the runtimes per each type of simulation.

Figure A.1: Computational time and predicted UCS obtained from 2D UCS test simulations using loading velocity rates of 0.005 m/s, 0.02 m/s, and 0.1 m/s.

Table A.1: Summary of runtimes per type of simulation.

<table>
<thead>
<tr>
<th>Type of simulation</th>
<th>Loading velocity (m/s)</th>
<th>Runtime (hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3D UCS</td>
<td>0.1</td>
<td>720</td>
</tr>
<tr>
<td>2D UCS</td>
<td>0.1</td>
<td>12</td>
</tr>
<tr>
<td>2D BTS</td>
<td>0.05</td>
<td>5</td>
</tr>
</tbody>
</table>
APPENDIX B

FISH CODE FOR UCS TEST SIMULATION IN 3DEC

;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;
;;SET MODEL GEOMETRY
new
set atol 5E-10
set edge 1E-04
set random 10000

;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;
;; IMPORT GEOMETRY FROM NEPER
call model.3dec ;;Neper file

;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;
;;BUILD MESH
group block 'CORE' range z -0.0644 0.0644
gen edge 1E-03 alt range group 'CORE'

;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;
;;DEFINE PROPERTIES - Lan et al. (2010)
def input_properties_2010

;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;
;;BLOCK PROPERTIES
;;K-feldspar
K_dens=2560.0
K_young=69.8E+9
K_poisson=0.28
K_{bulk}=K_{young}/(3*(1-2*K_{poisson}))
K_{shear}=K_{young}/(2*(1+K_{poisson}))

;;Plagioclase
P_{dens}=2630.0
P_{young}=88.1E+9
P_{poisson}=0.26
P_{bulk}=P_{young}/(3*(1-2*P_{poisson}))
P_{shear}=P_{young}/(2*(1+P_{poisson}))

;;Quartz
Q_{dens}=2650.0
Q_{young}=94.5E+9
Q_{poisson}=0.08
Q_{bulk}=Q_{young}/(3*(1-2*Q_{poisson}))
Q_{shear}=Q_{young}/(2*(1+Q_{poisson}))

;;Biotite
B_{dens}=3050.0
B_{young}=33.8E+9
B_{poisson}=0.36
B_{bulk}=B_{young}/(3*(1-2*B_{poisson}))
B_{shear}=B_{young}/(2*(1+B_{poisson}))

;base CONTACT PROPERTIES

;;K-K
KK_{jkn}=9.20E+13
KK_{jks}=6.13E+13
KK_{jc}=40.0E+06
KK_{jfr}=27.0
KK_{jt}=14.4E+06
KK_{jresc}=0.0
KK_{jrf}=27.0
KK_jrt=0.0
KK_dil=5.0
;;K-P
KP_jkn=8.56E+13
KP_jks=5.71E+13
KP_jc=40.0E+06
KP_jfr=27.0
KP_jt=14.4E+06
KP_jresc=0.0
KP_jrf=27.0
KP_jrt=0.0
KP_dil=5.0
;;K-Q
KQ_jkn=1.29E+14
KQ_jks=8.60E+13
KQ_jc=40.0E+06
KQ_jfr=27.0
KQ_jt=14.4E+06
KQ_jresc=0.0
KQ_jrf=27.0
KQ_jrt=0.0
KQ_dil=5.0
;;K-B
KB_jkn=1.51E+14
KB_jks=1.01E+14
KB_jc=40.0E+06
KB_jfr=27.0
KB_jt=14.4E+06
KB_jresc=0.0
KB_jrf=27.0
KB_jrt=0.0
KB_dil=5.0
;;P-P
PP_jkn=9.28E+13
PP_jks=6.19E+13
PP_jc=40.0E+06
PP_jfr=27.0
PP_jt=14.4E+06
PP_jresc=0.0
PP_jrf=27.0
PP_jrt=0.0
PP_dil=5.0
;;P-Q
PQ_jkn=1.24E+14
PQ_jks=8.27E+13
PQ_jc=40.0E+06
PQ_jfr=27.0
PQ_jt=14.4E+06
PQ_jresc=0.0
PQ_jrf=27.0
PQ_jrt=0.0
PQ_dil=5.0
;;P-B
PB_jkn=1.49E+14
PB_jks=9.93E+13
PB_jc=40.0E+06
PB_jfr=27.0
PB_jt=14.4E+06
PB_jresc=0.0
PB_jrf=27.0
PB\_jrt=0.0
PB\_dil=5.0
::Q-Q
QQ\_jkn=2.55E+14
QQ\_jks=1.70E+14
QQ\_jc=40.0E+06
QQ\_jfr=27.0
QQ\_jt=14.4E+06
QQ\_jresc=0.0
QQ\_jrf=27.0
QQ\_jrt=0.0
QQ\_dil=5.0
::Q-B
QB\_jkn=3.13E+14
QB\_jks=2.09E+14
QB\_jc=40.0E+06
QB\_jfr=27.0
QB\_jt=14.4E+06
QB\_jresc=0.0
QB\_jrf=27.0
QB\_jrt=0.0
QB\_dil=5.0
::B-B
BB\_jkn=4.70E+14
BB\_jks=3.13E+14
BB\_jc=40.0E+06
BB\_jfr=27.0
BB\_jt=14.4E+06
BB\_jresc=0.0
BB\_jrf=27.0
BB_jrt=0.0
BB_dil=5.0
end
@input_properties_2010

;;-----------------------------------------------------------------------------------
;;: ASSIGN GROUPS TO GRAINS AND CONTACTS
;;-----------------------------------------------------------------------------------
;;:COUNT BLOCKS
def count_blocks
b_count=0
i=block_head
loop while i#0
    b_count=b_count+1
    i=b_next(i)
end_loop
end
@count_blocks
;;-----------------------------------------------------------------------------------
;;:DEFINE BLOCK VOLUME
def def_block_volume
j=0
array b_infoo(b_count,3)
k=block_head
loop while k#0
    j=j+1
    b_infoo(j,1)=k
    b_infoo(j,2)=b_vol(k)
    b_infoo(j,3)=0
    k=b_next(k)
end_loop
end
@def_block_volume

;;--------------------------------------------------------------------------------------

;; ASSIGN GRAIN MAT AND GROUPS
;;Calculation of the volumes per type of grains
def sum_vol
tot_b_vol=0
loop i (1,b_count)
  tot_b_vol=tot_b_vol+b_infoo(i,2)
end_loop
vol_B=(tot_b_vol)*0.03
vol_Q=(tot_b_vol)*0.32
vol_P=(tot_b_vol)*0.41
vol_K=(tot_b_vol)*0.24
end
@sum_vol

;;----------------------------------------------------------------------

;; Biotite (mat 4)
def bl_Bio
check_vol=0
loop while check_vol<vol_B
  aa=round(urand*b_count)
  if b_infoo(aa,3)=0 then
    check_vol=check_vol+b_infoo(aa,2)
    b_mat(b_infoo(aa,1))=4
    pp=b_zone(b_infoo(aa,1))
    loop while pp#0
      z_group(pp)='Biotite'
      pp=z_next(pp)
end_loop
    b_infoo(aa,3)=1
    end_if
end_loop
end
@bl_Bio

;;-----------------------------------------------

;; Quartz (mat 3)
def bl_Qtz
  check_vol=0
  loop while check_vol<vol_Q
    aa=round(urand*b_count)
    if b_infoo(aa,3)=0 then
      check_vol=check_vol+b_infoo(aa,2)
      b_mat(b_infoo(aa,1))=3
      pp=b_zone(b_infoo(aa,1))
      loop while pp#0
        z_group(pp)='Quartz'
        pp=z_next(pp)
      end_loop
      b_infoo(aa,3)=1
    end_if
  end_loop
end
@bl_Qtz

;;-----------------------------------------------

;; Plagioclase (mat 2)
def bl_Plag
  check_vol=0
  loop while check_vol<vol_P
aa=round(urand*b_count)
if b_infoo(aa,3)=0 then
    check_vol=check_vol+b_infoo(aa,2)
    b_mat(b_infoo(aa,1))=2
    pp=b_zone(b_infoo(aa,1))
    loop while pp#0
        z_group(pp)=’Plagioclase’
        pp=z_next(pp)
    end_loop
    b_infoo(aa,3)=1
end_if
end_loop
end
@bl_Plag

;;---------------------------------------------------------------------------
;; K-feldspar (mat 1)
def bl_Kspar
loop i (1,b_count)
    if b_infoo(i,3)=0 then
        b_mat(b_infoo(i,1))=1
        pp=b_zone(b_infoo(i,1))
        loop while pp#0
            z_group(pp)=’K-feldspar’
            pp=z_next(pp)
        end_loop
        b_infoo(i,3)=1
    end_if
end_loop
end
@bl_Kspar
ASSIGN CONTACT JMAT AND GROUPS

def assign_contact_groups
i=contact_head
loop while i#0
bi1=c_b1(i)
bi2=c_b2(i)

;----------
; K-K (11)
if b_mat(bi1)=1 then
if b_mat(bi2)=1 then
  c_cons(i)=1
  c_mat(i)=11
  c_group(i)='K-K'
end_if
end_if

;----------
; K-P (12)
if b_mat(bi1)=1 then
if b_mat(bi2)=2 then
  c_cons(i)=1
  c_mat(i)=12
  c_group(i)='K-P'
end_if
end_if
if b_mat(bi1)=2 then
if b_mat(bi2)=1 then
  c_cons(i)=1
  c_mat(i)=12
end_if
c_group(i)='K- P'
end_if
end_if

;j:---------------------------------------------------------------
;j:K-Q (13)
;j:---------------------------------------------------------------
;if b_mat(bi1)=1 then
if b_mat(bi2)=3 then
    c_cons(i)=1
    c_mat(i)=13
    c_group(i)='K-Q'
end_if
end_if
if b_mat(bi1)=3 then
if b_mat(bi2)=1 then
    c_cons(i)=1
    c_mat(i)=13
    c_group(i)='K-Q'
end_if
end_if

;j:---------------------------------------------------------------
;j:K-B (14)
;j:---------------------------------------------------------------
;if b_mat(bi1)=1 then
if b_mat(bi2)=4 then
    c_cons(i)=1
    c_mat(i)=14
    c_group(i)='K-B'
end_if
end_if
if b_mat(bi1)=4 then
if b_mat(bi2)=1 then

\[c_{\text{cons}}(i)=1\]
\[c_{\text{mat}}(i)=14\]
\[c_{\text{group}}(i)='K-B'\]
\end_if
\end_if

;;-----------------------------------------------------------
;;P-P (22)
if b_{\text{mat}}(bi1)=2 then
if b_{\text{mat}}(bi2)=2 then
  \[c_{\text{cons}}(i)=1\]
  \[c_{\text{mat}}(i)=22\]
  \[c_{\text{group}}(i)='P-P'\]
end_if
end_if

;;------------------------------------------------------------
;;P-Q (23)
if b_{\text{mat}}(bi1)=2 then
if b_{\text{mat}}(bi2)=3 then
  \[c_{\text{cons}}(i)=1\]
  \[c_{\text{mat}}(i)=23\]
  \[c_{\text{group}}(i)='P-Q'\]
end_if
end_if
if b_{\text{mat}}(bi1)=3 then
if b_{\text{mat}}(bi2)=2 then
  \[c_{\text{cons}}(i)=1\]
  \[c_{\text{mat}}(i)=23\]
  \[c_{\text{group}}(i)='P-Q'\]
end_if
end_if
end_if
if \text{b_mat(bi1)} = 2 \text{ then}
\text{if b_mat(bi2)} = 4 \text{ then}
  \text{c_cons}(i) = 1
  \text{c_mat}(i) = 24
  \text{c_group}(i) = 'P-B'
\text{end_if}
\text{end_if}
\text{if b_mat(bi1)} = 4 \text{ then}
\text{if b_mat(bi2)} = 2 \text{ then}
  \text{c_cons}(i) = 1
  \text{c_mat}(i) = 24
  \text{c_group}(i) = 'P-B'
\text{end_if}
\text{end_if}
\text{if b_mat(bi1)} = 3 \text{ then}
\text{if b_mat(bi2)} = 3 \text{ then}
  \text{c_cons}(i) = 1
  \text{c_mat}(i) = 33
  \text{c_group}(i) = 'Q-Q'
\text{end_if}
\text{end_if}
\text{if b_mat(bi1)} = 3 \text{ then}
\text{if b_mat(bi2)} = 4 \text{ then}
  \text{c_cons}(i) = 1
\text{end_if}
if b_mat(bi1)=4 then
if b_mat(bi2)=3 then
    c_cons(i)=1
    c_mat(i)=34
    c_group(i)='Q-B'
end_if
end_if

if b_mat(bi1)=4 then
if b_mat(bi2)=4 then
    c_cons(i)=1
    c_mat(i)=44
    c_group(i)='B-B'
end_if
end_if

i=c_next(i)
end_loop
end

@assign_contact_groups

;; ASSIGN PROPERTIES
call Assign_Props_4.3ddat

;; ASSIGN PROPERTIES TO GRAINS AND CONTACTS

set jcondf 1
set jmatdf 10

prop jmat 10 jks 4E+14 jkn 4E+14 jfri 5 jco 0 jte 0 jdi 5 res_co 0 res_te 0 res_fri 5

;; Grain micro-properties

zone model elastic dens @K_dens shear @K_shear bulk @K_bulk range group 'K-feldspar'
zone model elastic dens @P_dens shear @P_shear bulk @P_bulk range group 'Plagioclase'
zone model elastic dens @Q_dens shear @Q_shear bulk @Q_bulk range group 'Quartz'
zone model elastic dens @B_dens shear @B_shear bulk @B_bulk range group 'Biotite'

;; Contact micro-properties

prop jmat 11 jks @KK_jks jkn @KK_jkn jfri @KK_jfr jco @KK_jc jte @KK_jt res_co @KK_jresc res_te @KK_jrt res_fri @KK_jrf jdi @KK_dil
change jmat 11 range group 'K-K'

prop jmat 12 jks @KP_jks jkn @KP_jkn jfri @KP_jfr jco @KP_jc jte @KP_jt res_co @KP_jresc res_te @KP_jrt res_fri @KP_jrf jdi @KP_dil
change jmat 12 range group 'K-P'

prop jmat 13 jks @KQ_jks jkn @KQ_jkn jfri @KQ_jfr jco @KQ_jc jte @KQ_jt res_co @KQ_jresc res_te @KQ_jrt res_fri @KQ_jrf jdi @KQ_dil
change jmat 13 range group 'K-Q'

prop jmat 14 jks @KB_jks jkn @KB_jkn jfri @KB_jfr jco @KB_jc jte @KB_jt res_co @KB_jresc res_te @KB_jrt res_fri @KB_jrf jdi @KB_dil
change jmat 14 range group 'K-B'

prop jmat 22 jks @PP_jks jkn @PP_jkn jfri @PP_jfr jco @PP_jc jte @PP_jt res_co @PP_jresc res_te @PP_jrt res_fri @PP_jrf jdi @PP_dil
change jmat 22 range group 'P-P'

prop jmat 23 jks @PQ_jks jkn @PQ_jkn jfri @PQ_jfr jco @PQ_jc jte @PQ_jt res_co @PQ_jresc res_te @PQ_jrt res_fri @PQ_jrf jdi @PQ_dil
change jmat 23 range group 'P-Q'
prop jmat 24 jks @PB_jks jkn @PB_jkn jfri @PB_jfr jco @PB_jc jte @PB_jt res_co @PB_jresc res_te @PB_jrt res_fri @PB_jrf jdi @PB_dil

change jmat 24 range group 'P-B'

prop jmat 33 jks @QQ_jks jkn @QQ_jkn jfri @QQ_jfr jco @QQ_jc jte @QQ_jt res_co @QQ_jresc res_te @QQ_jrt res_fri @QQ_jrf jdi @QQ_dil

change jmat 33 range group 'Q-Q'

prop jmat 34 jks @QB_jks jkn @QB_jkn jfri @QB_jfr jco @QB_jc jte @QB_jt res_co @QB_jresc res_te @QB_jrt res_fri @QB_jrf jdi @QB_dil

change jmat 34 range group 'Q-B'

prop jmat 44 jks @BB_jks jkn @BB_jkn jfri @BB_jfr jco @BB_jc jte @BB_jt res_co @BB_jresc res_te @BB_jrt res_fri @BB_jrf jdi @BB_dil

change jmat 44 range group 'B-B'

;;-------------------------------------------------------------------------------------------------

;; BOUNDARY CONDITIONS + FIELD STRESSES

;; BOUNDARY CONDITIONS

;;Applying constant velocity to the top and bottom surfaces of the model
boundary zvel -0.05 range z 0.0644
boundary zvel 0.05 range z -0.0644

;; APPLY GRAVITY
gravity 0 0 -9.81

;;-------------------------------------------------------------------------------------------------

;; RECORD HISTORY

;;-------------------------------------------------------------------------------------------------

;; AXIAL STRAIN

def ax_strain
whilestepping
;;top
zt_1=gp_near(-0.02,0.0,0.0624)
zt_2=gp_near(-0.01,0.0,0.0624)
zt_3=gp_near(0.0,0.0,0.0624)
zt_4=gp_near(0.01,0.0,0.0624)
zt_5=gp_near(0.02,0.0,0.0624)
zt_6=gp_near(0.0,-0.02,0.0624)
zt_7=gp_near(0.0,-0.01,0.0624)
zt_8=gp_near(0.0,0.01,0.0624)
zt_9=gp_near(0.0,0.02,0.0624)

; bottom
zb_1=gp_near(-0.02,0.0,-0.0624)
zb_2=gp_near(-0.01,0.0,-0.0624)
zb_3=gp_near(0.0,0.0,-0.0624)
zb_4=gp_near(0.01,0.0,-0.0624)
zb_5=gp_near(0.02,0.0,-0.0624)
zb_6=gp_near(0.0,-0.02,-0.0624)
zb_7=gp_near(0.0,-0.01,-0.0624)
zb_8=gp_near(0.0,0.01,-0.0624)
zb_9=gp_near(0.0,0.02,-0.0624)

; axial displacement
ax_1=(gp_zdis(zb_1)-gp_zdis(zt_1))
ax_2=(gp_zdis(zb_2)-gp_zdis(zt_2))
ax_3=(gp_zdis(zb_3)-gp_zdis(zt_3))
ax_4=(gp_zdis(zb_4)-gp_zdis(zt_4))
ax_5=(gp_zdis(zb_5)-gp_zdis(zt_5))
ax_6=(gp_zdis(zb_6)-gp_zdis(zt_6))
ax_7=(gp_zdis(zb_7)-gp_zdis(zt_7))
ax_8=(gp_zdis(zb_8)-gp_zdis(zt_8))
ax_9=(gp_zdis(zb_9)-gp_zdis(zt_9))
ax_disp=(ax_1+ax_2+ax_3+ax_4+ax_5)/9

; axial strain
ax_strain=ax_disp/0.1248
end

;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;

;; LATERAL STRAIN
def lat_strain
while stepping
;; X-axis
;; X-axis
xp_1=gp_near(0.0237,0,-0.05)
xp_2=gp_near(0.0237,0,-0.04)
xp_3=gp_near(0.0237,0,-0.03)
xp_4=gp_near(0.0237,0,-0.02)
xp_5=gp_near(0.0237,0,-0.01)
xp_6=gp_near(0.0237,0,0.00)
xp_7=gp_near(0.0237,0,0.01)
xp_8=gp_near(0.0237,0,0.02)
xp_9=gp_near(0.0237,0,0.03)
xp_10=gp_near(0.0237,0,0.04)
xp_11=gp_near(0.0237,0,0.05)
xn_1=gp_near(-0.0237,0,-0.05)
xn_2=gp_near(-0.0237,0,-0.04)
xn_3=gp_near(-0.0237,0,-0.03)
xn_4=gp_near(-0.0237,0,-0.02)
xn_5=gp_near(-0.0237,0,-0.01)
xn_6=gp_near(-0.0237,0,0.00)
xn_7=gp_near(-0.0237,0,0.01)
xn_8=gp_near(-0.0237,0,0.02)
xn_9=gp_near(-0.0237,0,0.03)
xn_10=gp_near(-0.0237,0,0.04)
xn_11=gp_near(-0.0237,0,0.05)
Y-axis

yp_1=gp_near(0,0.0237,-0.05)
yp_2=gp_near(0,0.0237,-0.04)
yp_3=gp_near(0,0.0237,-0.03)
yp_4=gp_near(0,0.0237,-0.02)
yp_5=gp_near(0,0.0237,-0.01)
yp_6=gp_near(0,0.0237,0.00)
yp_7=gp_near(0,0.0237,0.01)
yp_8=gp_near(0,0.0237,0.02)
yp_9=gp_near(0,0.0237,0.03)
yp_10=gp_near(0,0.0237,0.04)
yp_11=gp_near(0,0.0237,0.05)

yn_1=gp_near(0,-0.0237,-0.05)
yn_2=gp_near(0,-0.0237,-0.04)
yn_3=gp_near(0,-0.0237,-0.03)
yn_4=gp_near(0,-0.0237,-0.02)
yn_5=gp_near(0,-0.0237,-0.01)
yn_6=gp_near(0,-0.0237,0.00)
yn_7=gp_near(0,-0.0237,0.01)
yn_8=gp_near(0,-0.0237,0.02)
yn_9=gp_near(0,-0.0237,0.03)
yn_10=gp_near(0,-0.0237,0.04)
yn_11=gp_near(0,-0.0237,0.05)

Lateral Displacement

latx_1=(gp_xdis(xp_1)-gp_xdis(xn_1))
latx_2=(gp_xdis(xp_2)-gp_xdis(xn_2))
latx_3=(gp_xdis(xp_3)-gp_xdis(xn_3))
latx_4=(gp_xdis(xp_4)-gp_xdis(xn_4))
latx_5=(gp_xdis(xp_5)-gp_xdis(xn_5))
latx_6=(gp_xdis(xp_6)-gp_xdis(xn_6))
latx_7=(gp_xdis(xp_7)-gp_xdis(xn_7))
latx_8=(gp_xdis(xp_8)-gp_xdis(xn_8))
latx_9=(gp_xdis(xp_9)-gp_xdis(xn_9))
latx_10=(gp_xdis(xp_10)-gp_xdis(xn_10))
latx_11=(gp_xdis(xp_11)-gp_xdis(xn_11))
laty_1=(gp_ydis(yp_1)-gp_ydis(yn_1))
laty_2=(gp_ydis(yp_2)-gp_ydis(yn_2))
laty_3=(gp_ydis(yp_3)-gp_ydis(yn_3))
laty_4=(gp_ydis(yp_4)-gp_ydis(yn_4))
laty_5=(gp_ydis(yp_5)-gp_ydis(yn_5))
laty_6=(gp_ydis(yp_6)-gp_ydis(yn_6))
laty_7=(gp_ydis(yp_7)-gp_ydis(yn_7))
laty_8=(gp_ydis(yp_8)-gp_ydis(yn_8))
laty_9=(gp_ydis(yp_9)-gp_ydis(yn_9))
laty_10=(gp_ydis(yp_10)-gp_ydis(yn_10))
laty_11=(gp_ydis(yp_11)-gp_ydis(yn_11))
latx_disp=(latx_1+latx_2+latx_3+latx_4+latx_5+latx_6+latx_7+latx_8+latx_9+latx_10+latx_11)
laty_disp=(laty_1+laty_2+laty_3+laty_4+laty_5+laty_6+laty_7+laty_8+laty_9+laty_10+laty_11)
lat_disp=(latx_disp+laty_disp)/22
lateral strain
lat_strain=-lat_disp/0.0474
end

; AXIAL STRESS ; summ of zz stress in zones

def ax_stress
whilestepping
sum_stress=0
b_count=0
i=block_head
loop while i#0
    j=b_zone(i)
    loop while j#0
        sum_stress=sum_stress+z_szz(j)
        j=z_next(j)
        b_count=b_count+1
    end_loop
    i=b_next(i)
end_loop
;;axial stress
ax_stress=-sum_stress/b_count
end

;;-------------------------------------------------------------------------------

;; SOLUTION

damp

;;-------------------------------------------------------------------------------

;; HISTORIES
hist ncyc 10 @ax_strain
hist ncyc 10 @lat_strain
hist ncyc 10 @ax_stress
hist ncyc 10 unbal
hist ncyc 10 ratio

;;-------------------------------------------------------------------------------

;; STEPPING
def step_n_save
    nstepps=500000
    loop n(1,(nstepps/5000))
        fname1="results_{n}.3dsav"
        fname2="data_{n}.his"
        command
            step 5000
            save @fname1
            hist write 1 2 3 4 5 file @fname2
        endcommand
    endloop
end
@step_n_save