Up-Scaling DEM Simulations LaTeX

by

Mike Yetisir

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I hereby declare that I am the sole author of this thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

I understand that my thesis may be made electronically available to the public.

Abstract

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Acknowledgements

I would like to thank all the little people who made this possible.

Dedication

This is dedicated to the one I love.

Table of Contents

List of Tables

List of Figures

Chapter 1

Introduction

Traditional modelling approaches tend to focus only on one scale. For example, when considering the macroscale response of a system, the effect of the microscale mechanics are described implicitly by macroscale phenomenological constitutive relations. Conversely, when interested in the microscale behaviour, macroscale features are assumed to be homogeneous and irrelevant to the microscale response.

These macroscale constitutive relationships are obtained empirically based on simple methods such as linearization, Taylor series expansion, and symmetry Weinan [2011]. For simple systems, this approach can yield sufficiently accurate approximations of the overall behaviour. However, this approach is often insufficient to capture an accurate constitutive response of complex systems with materials containing key physical behaviour over multiple length scales (multi-scale material).

Alternatively, one can model the microscale behaviour explicitly throughout the system in order to accommodate complex systems and multi-scale materials. This approach is far more accurate, however the degree of complexity is orders of magnitudes higher, making solutions difficult to find and often becoming computationally prohibitive.

To overcome these limitations of single-scale models, multi-scale approaches have been developed. Multi-scale methods attempt to model a system at both the microscale an the macroscale in such a means that shares the computational efficiency of the macroscale models and the accuracy of the microscale models.

The most common types of multiscale methods are hierarchical and concurrent [Gracie and Belytschko, 2011]. In concurrent multiscale models, different scales are used in different regions of the domain; the solution of the coupled model proceeds by solving both scales simultaneously. This approach is computationally expensive since the time step of the entire simulation is controlled by requirements of the fine-scale model; however, the solution is often more accurate. In hierarchical multiscale methods, the constitutive behavior at the coarser scale is determined by exercising a finer scale Representative Elementary Volume (REV) [Li et al., 2014]. The finer scale models vary from relatively simple models, as in micromechanics, to complex nonlinear models such as FE^2 models [Feyel, 2003]. This approach is much more efficient, but can be less accurate, and furthermore presents challenges when the REV loses stability [Belytschko et al., 2008]. Up-scaling in this investigation can be considered to be a hierarchical multiscale method using computational homogenization.

Many homogenization techniques have been developed and proposed in the past, but none have presented algorithms for homogenizing DEM simulations with deformable blocks. The homogenization algorithms presented here are based on the work of D'Addetta et al. [2004] and Wellmann et al. [2008] in which homogenization is applied to rigid body DEM simulations and focused on the computation of the homogenized stress and strain.

1.1 Context and Research Motivation

Naturally Fractured Rock (NFR) is often modeled as a multiscale material because of the vastly different length and time scales involved in the deformation process [Zhou et al., 2003]. At the fracture scale (10^{-2} m), the physics is dominated by brittle fracture propagation and fracture-to-fracture contact force interaction. However, one is normally interested in the reservoir scale (10^3 m) response as a result of the spatial extension of the fractures. Because these length scales of interest span approximately five orders of magnitude, multiscale methods may aid in assessing the overall response, as models with natural fracture scale resolution at the reservoir scale becomes computationally prohibitive.

When dealing with reservoir scale geomechanics problems, the complex behaviour of pre-existing fractures become influential upon and indeed may dominate the constitutive response of the rock mass because of strain localization, stress redistribution, and damage-induced anisotropy [Petracca et al., 2015]. However, attempting to capture the constitutive response of the NFR in a laboratory context becomes impractical because of the prohibitively large samples required to obtain a representative response. Since natural fracture spacing in a stiff sedimentary rock can be between 0.1 m to 1m [Nelson, 2001], samples required to obtain a response representative of the macroscale could be as large as $1000m^3$, an impossible scale for testing.

There exist methods to estimate constitutive parameters of rock masses, but their validity can be tenuous and methods exist only to estimate some of the parameters. These methods can either be based directly from in-situ geophysical measurements, or deduced indirectly through small scale laboratory testing and empirical correlations. A common way to estimate the elastic properties is through the use of seismic methods by comparing the seismic wave velocities measured in-situ to the seismic velocities of the intact rock mass [Sjogren et al., 1979]. These in-situ methods however, do not have the capacity to estimate the plastic parameters very well, and it is well-known that seismically deduced elastic parameters invariably over-estimate the system stiffness exhibited in response to static stress changes [Barton, 2006]. Attempts to estimate the plastic properties of the rock mass through small scale lab testing and qualitative assessments of the rock mass have been presented such as the Geological Strength Index (GSI) proposed by Hoek and Brown [1997]. These methods are limited by the necessarily qualitative aspect of the rock mass classification systems employed. More recently, others [Min and Jing, 2003, Chen et al., 2012, Bidgoli et al., 2013] have used numerical methods to estimate the elastic properties of the rock mass using prescribed fracture networks. These methods are again limited by the lack of plastic behaviour characterization.

To address this limitation of continuum models, Discrete Element Method (DEM) models are used commonly in geomechanics to explicitly model the mechanics of Naturally Fractured Rock (NFR) masses to capture the constitutive response of the rock mass indirectly [Jing, 2003].

DEM models, unlike standard continuum models, consider the fractures within the rock mass as a Discrete Fracture Network (DFN) which explicitly defines the geometry of the rock blocks. The physics of block interaction is then governed by the motion, contact forces and traction-separation laws between the rock blocks and the fractures [Thallak et al., 1990]. Because NFR behavior is complex, even sophisticated phenomenological constitutive relationships may be inadequate to describe the complete rock mass behavior. The DEM approach aims to address this deficiency by requiring only constitutive relations for the block interactions and the intact rock [Barbosa and Ghaboussi, 1990]. In this paper, deformable DEM blocks are considered which require the constitutive parameters of the intact rock to be specified, but these parameters are more easily acquired from lab testing.

However, the main issue with DEM models is primarily the computational demands. Because of the large number of degrees of freedom in the models and the requirement for very small time steps — because of the constant need for contact detection between blocks — running reservoir-scale models is computationally prohibitive. The intent of this article is to develop a framework that incorporates the response of DEM models while harnessing the computational speed of continuum models. The general goal of up-scaling is to formulate simplified coarse-scale governing equations that approximate the fine-scale behavior of a material [Geers et al., 2010]. In the case of the DEM simulations in this investigation, the aim of up-scaling is to identify the parameters of a continuum model that best mimic the response of the DEM model. Up-scaling is accomplished in this paper by 'calibrating' a continuum model with DEM virtual experimental data using a combination of a heuristic optimization algorithm and an iterative least squares regression algorithm.

The general goal of up-scaling is to formulate simplified coarse-scale governing equations that approximate the fine-scale behavior of a material [Geers et al., 2010]. In the case of the DEM simulations in this investigation, the aim of up-scaling is to identify the parameters of a continuum model that best mimic the response of the DEM model.

1.2 Research Objectives

In this thesis, a multi-scale up-scaling framework is developed to address the computational demands of simulating microscale phenomenon in a macroscale domain in the context of NFR. The primary research objectives of this research revolve around developing and validating aspects of the proposed up-scaling framework. Here, four key research objective have been identified:

1. the application of homogenization to DEM models with deformable blocks.
2. the presentation of a methodology to parameterize complex nonlinear continuum constitutive models based on the DEM homogenized stress and strain curves.
3. the demonstration that the performance of the up-scaled continuum FEA models are accurate and significantly more computationally efficient.
4. the development and implementation of a modular software framework for up-scaling DEM simulations.

Homogenizing DEM simulations with deformable blocks

***Algorithms to assess the homogenized stress and strain tensors of DEM simulations with deformable blocks are to be developed. As part of the homogenization algorithm, a method to automatically assess the RVE of the given rock mass is also necessary.

Macroscale Constitutive Relationship

***A macroscale constitutive relationship that represents the homogenized DEM response is to be identified. The constitutive relationship must be able to capture all the salient features of the discrete system. Furthermore, this constitutive relationship is to be parameterized by as few scalar parameters as possible while representing the rock mass accurately.

Parameter Estimation Algorithms

***An appropriate parameter estimation algorithm is to be identified that converges to the optimal solution most of the time, while minimizing the required number of iterations.

Up-Scaling Framework

***More specifically, an automated framework for up-scaling DEM simulations is to be developed. It is required that the key aspects of the framework remain modular, so as to facilitate extensibility for future applications. Furthermore, the framework must have the flexibility to drive the different modules individually, based on saved states in order to modify the results without having to redo the entire analysis.

1.3 Scope of Study and Research Limitations

The scope of this research is to present an up-scaling framework and a simple implementation as a proof of concept. Here, the goal is to provide all the necessary pieces using in-house and third-party software to show the up-scaling process from DEM simulations to optimal macroscale parameter set.

For simplicity, the DEM simulations considered here are isotropic, two-dimensional, and purely mechanical (not thermo-hydro-mechanically coupled). These simplifications reduce the complexity of the implementation significantly. As a result, the homogenization algorithms presented are designed for two-dimensional DEM simulations, though they can easily be adapted for three-dimensional problems.

The macroscale constitutive models that are used are also following an isotropic medium assumption and do not account for any thermal or hydraulic coupling effects. These macroscale models used are pre-implemented materials, but custom material subroutines are required for more sophisticated constitutive responses.

There are countless different optimization algorithms to investigate along with their respective optimization parameters. Exhaustively searching for the most efficient and accurate algorithm for this particular application in a quantitative capacity was not a focus of this thesis. As such, a couple different algorithms are presented and compared in their capacity to accurately and efficiently converge to the optimal parameter set.

Ultimately, the research presented in this thesis aims to show the efficacy of a modular upscaling framework for DEM simulations that can facilitate installation of upgraded modules in the future to account for more sophisticated physics.

Chapter 2

Background in Geomechanics

In a general sense, the study of geomechanics aims to understand (in theory and in practice) the behavioural response of a geological system subjected to an applied disturbance. These disturbances can either be anthropogenic or naturogenic. Though the mechanics of these two types of loads should be the same, the difference in magnitude between the disturbance that can be applied manually, and that which is applied tectonically span several order of magnitude. The presence of scale effect, combined with the uncertainty of geosystems, results in necessarily different approaches to understanding the expected behaviour of the systems.

Geomechanics can be considered to consist of two subdisciplines: rock mechanics and soil mechanics. Where rock mechanics is concerned with the study of intact rock, soil mechanics is concerned with the behaviour of unconsolidated material. The difference between what constitutes soil and rock is arbitrary and can be highly nuanced in some cases (e.g. a highly weathered/fractured rock or a partially lithified soil). The transition from rock to soil (and *vice versa*) can be considered to be a continuous process whereby unfractured intact rock is at one end of the spectrum and fine grained unconsolidated soil is at the other. Whether or not one uses rock mechanics or soil mechanics for a particular engineering application is decided in a discretionary manner depending on which system features are more dominant.

In the context of this thesis, the focus of geomechanics considered here is rock mechanics subjected to anthropogenic loading. That being said, the up-scaling methodology may be applicable to soil mechanics and naturogenic loading as well. Rock mechanics is a special discipline of mechanics which presents a unique set of challenges. Challenges such as uncertainty, fractures, scale effects and heterogeneities can quickly lead to very complex engineering problems.

Uncertainty is probably the most challenging aspect of engineering rock mechanics. etc..

Complexities such as fracture and scale effects are important challenged to consider as well. etc...

2.1 Geomechanics of Naturally Fractured Rock

2.1.1 Intact Rock

To understand the behaviour of naturally fractured rock masses, it is first necessary to understand how the rock behaves without fractures. Unfractured rock can be referred to in this context as intact rock.

2.1.2 Rock Fractures and Discontinuities

2.1.3 In-Situ Stress

2.1.4 Pore Pressure and Fluid Flow

2.2 Computational Geomechanics

Numerical modelling of naturally fractured geomechanical systems can be approached in two ways: by considering the constitutive relationship of the rock mass to be either continuous or discontinuous. The difference between these methods is a function of how one decides to conceptualize the rock mass. In a rock mass modelled as a continuum, the average macroscale response is considered while a rock mass modelled as a discontinuum is modelled by explicitly representing the natural fractures.

2.2.1 Continuum Modelling

2.2.2 Discontinuum Modelling

2.3 Slope Stability Analysis

Slope stability analysis is an important aspect of geotechnical engineering as it allows one to determine how susceptible a given engineered or natural slope is to failure. The primary purpose of slope stability analysis is often to contribute to the safe and economic design of slopes. There are a number of parameters that affect the stability of a slope. When assessing the stability of a slope, one needs to be aware of the impact that these parameters have on the overall system stability and how to account for them in the model (ref):

- Geological discontinuities such as joints, faults, and bedding planes
- Groundwater, drainage patterns, and rainfall events
- Strength parameters of the material comprising the slope
- Slope construction method
- Applied forces such as structures on top, or seismic events
- Geometry of the slope

As such, a thorough understanding of geology, hydrogeology, and geotechnical engineering principles are required in order to apply slope stability principles properly. Even with a working knowledge of all the required areas of expertise, there is always a certain level of uncertainty with respect to these parameters such that any slope stability model will always be insufficient to accurately model the real system. However, very good approximations can be made with properly conducted slope stability analysis.

The determination of the stability of a slope is by no means a trivial task. To accurately and effectively determine the stability of a given slope, one must identify and understand the impact of the various factors that affect slope stability as outlined in Section 1.0. In addition, one must recognize that there exists multiple mechanisms of failure such that even if the slope is stable with respect to one failure mechanism, there is still a possibility of the slope failing through a different mechanism. Due to the complexity of the analysis, many assumptions are often made to simplify the solution.

In practice, there are two main approaches to assessing the stability of a given slope: the limit equilibrium method (LEM), and the shear strength reduction method (SSRM).

The former can be achieved analytically, and therefore much faster, but also has to make assumptions about the nature of the failure surface a priori and can only address one failure mechanism at a time, which limits its applicability and efficacy. The SSRM addresses these issues, but is more difficult to implement and more costly in terms of computational time.

2.3.1 Mechanisms of Slope Failure

2.3.2 Factor of Safety for Slope Stability

In slope stability analysis, the factor of safety (FOS) is the primary metric used to assess the slope stability. Fundamentally, the FOS is a system parameter which describes the capacity of a static system to perform under a given load. By definition, a FOS above 1.0 would describe a slope with a low susceptibility to failure such that it is stable under greater loads. Conversely, a FOS below 1.0 would describe a slope in a state of failure, while a FOS of 1.0 would indicate a slope on the verge of failure. In general, a FOS of at least 1.5 under maximum expected load is required for slopes in order to be considered sufficiently stable [Das, 2009].

Assessing the FOS for a slope is not a trivial task and functions on numerous parameters. Conventional analysis methods are based on limit equilibrium methods (LEM) which require several *a priori* assumptions which, if not correctly chosen, can result in inaccurate solutions. The main drawback of these methods is the requirement to assume a failure surface, which quite often does not accurately represent the actual failure surface. Alternatively, with the advent of FEA, it becomes possible to conduct slope stability analysis of these systems in such a way that the weakest failure surface or failure mechanism will prevail inherently.

2.3.3 Limit Equilibrium Methods (LEM)

2.3.4 Shear Strength Reduction Methods (SSRM)

Chapter 3

Up-Scaling Methodology

The goal of the up-scaling methodology is to identify the parameters of a continuum constitutive model (macroscale model) that best emulates the average response in the DEM REV (microscale model). Let the displacement, strain and stress of the DEM REV (microscale) model be denoted by $\mathbf{u}^m$, $\boldsymbol{\epsilon}^m$, and $\boldsymbol{\sigma}^m$, respectively. Let the homogenized (averaged) strain and stress in the DEM REV model be denoted by $\langle\boldsymbol{\epsilon}\rangle$ and $\langle\boldsymbol{\sigma}\rangle$, respectively. Finally, let the strain and stress from the continuum (macroscale) constitutive model be denoted as $\boldsymbol{\epsilon}^M$ and $\boldsymbol{\sigma}^M$, respectively. The rate of macroscale stress, $\dot{\boldsymbol{\sigma}}^M = \dot{\boldsymbol{\sigma}}^M\left(\dot{\boldsymbol{\epsilon}}^M, \boldsymbol{\chi}, \mathbf{h}\right)$, is defined in terms of the rate of macroscale strain, $\dot{\boldsymbol{\epsilon}}^M$, a set of material parameters $\boldsymbol{\chi}$ and a set of internal history variables $\mathbf{h}$.

The up-scaling methodology has five steps:

1. Identify the DEM REV for the NFR.
2. Exercise the DEM REV using multiple load paths. Store $\mathbf{u}^m$, $\boldsymbol{\epsilon}^m$, and $\boldsymbol{\sigma}^m$ for each load path.
3. Apply homogenization algorithms to the microscale results ($\mathbf{u}^m$, $\boldsymbol{\epsilon}^m$, and $\boldsymbol{\sigma}^m$) to determine the average stress-strain response of the REV, i.e., $\langle\boldsymbol{\sigma}\rangle$-$\langle\boldsymbol{\epsilon}\rangle$, for each load path.
4. Identify a continuum constitutive model, $\dot{\boldsymbol{\sigma}}^M = \dot{\boldsymbol{\sigma}}^M\left(\dot{\boldsymbol{\epsilon}}^M, \boldsymbol{\chi}, \mathbf{h}\right)$, that captures the salient features of NFR mechanics.
5. Run parameter estimation algorithms to identify the parameters, $\boldsymbol{\chi}$, that minimize the difference between $\langle\boldsymbol{\sigma}\rangle$-$\langle\boldsymbol{\epsilon}\rangle$ and $\boldsymbol{\sigma}^M$-$\boldsymbol{\epsilon}^M$ over all load paths.

Once an optimal parameter set, $\boldsymbol{\chi}$, for the desired model, $\dot{\boldsymbol{\sigma}}^M = \dot{\boldsymbol{\sigma}}^M\left(\dot{\boldsymbol{\epsilon}}^M, \boldsymbol{\chi}, \mathbf{h}\right)$, has been identified, the newly established constitutive model can be used in Finite Element Method (FEM) models or with other suitable numerical or analytical simulations.

3.1 Up-Scaling Implementation Overview

The up-scaling framework that is presented here consists of four main software components (Figure 3.1): a DEM simulator, a homogenization module, a FEM simulator, and a parameter estimation module. In procedural order, the first software component involved is a DEM simulation package, which is used to directly model the NFR. The DEM software accepts as inputs the geometry of the DFN, the material properties of the rock and the natural fractures, and the load paths. The DEM REV is exercised for different load-paths in a way that is akin to conducting multiple triaxial tests on physical specimens to characterize the full range of material behaviour. The DEM software outputs the microscale displacement, $\mathbf{u}^m$, and stress-strain, $\boldsymbol{\sigma}^m$-$\boldsymbol{\epsilon}^m$, responses for each load path. This microscale data is subsequently fed into the homogenization module to compute the average stress-strain response, $\langle\boldsymbol{\sigma}\rangle$-$\langle\boldsymbol{\epsilon}\rangle$, for each load path. Next, the homogenized stress-strain data, $\langle\boldsymbol{\sigma}\rangle$-$\langle\boldsymbol{\epsilon}\rangle$, is used by the parameter estimation software as observation data (i.e., laboratory/field data). The parameter estimation module iteratively executes a constitutive model, $\dot{\boldsymbol{\sigma}}^M = \dot{\boldsymbol{\sigma}}^M\left(\dot{\boldsymbol{\epsilon}}^M, \boldsymbol{\chi}, \mathbf{h}\right)$, embedded in the FEM simulator for each load path using different parameter sets, $\boldsymbol{\chi}^i$, while attempting to minimize the error between the homogenized microscale, $\langle\boldsymbol{\sigma}\rangle$-$\langle\boldsymbol{\epsilon}\rangle$, and macroscale, $\boldsymbol{\sigma}^M$-$\boldsymbol{\epsilon}^M$, stress-strain curves. Eventually, the algorithm converges to a near-optimal parameter set, $\boldsymbol{\chi}$, that can be viewed to be the best estimate of the NFR responses by the given continuum model. In our implementation, UDEC$^{\mathrm{TM}}$ was used as the DEM simulator and ABAQUS$^{\mathrm{TM}}$ was used as the FEM simulator. In ABAQUS$^{\mathrm{TM}}$, single element simulations were performed with a strain-history prescribed through displacement boundary conditions for a given set of material parameters and the stress is obtained as the output. There is nothing particularly special about the DEM or FEM simulators chosen; each could easily be replaced to overcome any inherent limitations. Moreover, a FEM simulator is not actually needed, since its inclusion in this framework is simply to gain access to the constitutive models within. The FEM simulator could easily be replaced by a FDM simulator or simply by a material subroutine. OSTRICH$^{\mathrm{TM}}$, a model-independent optimization package [Matott, 2016], is used for the parameter estimation module. The homogenization module was written in-house in Python$^{\mathrm{TM}}$. Python$^{\mathrm{TM}}$ was also used to interface and drive the various components of the up-scaling framework.

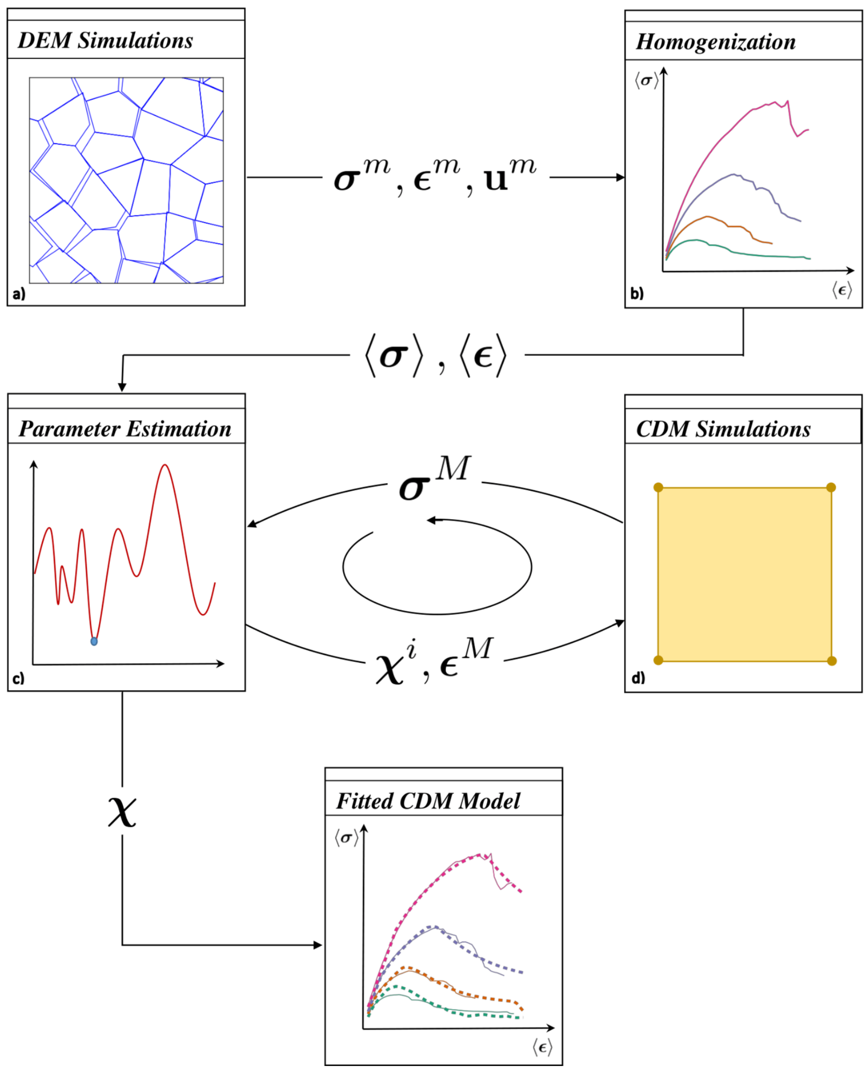

Figure 3.1: Up-scaling workflow used to estimate the optimal continuum model parameter set. The DEM software (a) produces a data set which is run through homogenization software (b) which in turn produces another dataset that is fed into the parameter estimation program (c). This parameter estimation program drives the CDM simulations (d) iteratively in order to find an optimal parameter set for the fitted model.

3.2 Distinct Element Method

Discontinuous systems are characterized by the existence of discontinuities that separate discrete domains within the system. In order to effectively model a discontinuous system, it is necessary to represent two distinct types of mechanical behaviour: the behaviour of the discontinuities and the behaviour of the solid material.

There exists a set of methods, referred to as discrete element methods, which provide the capacity to explicitly represent the behaviour of multiple intersecting discontinuities. The methods allow for the modelling of finite displacements and rotations of discrete bodies, including contact detachment as well as automatic detection of new contacts. Within the set of Discrete Element Methods, there are four subsets [Cundall and Hart, 1992]: Modal Methods, Discontinuous Deformation Analysis Methods, Momentum Exchange Methods, and Distinct Element Methods (DEM). In this paper, the discrete element method used is DEM.

With DEM methods, the discontinuous system is represented as an assembly of deformable blocks such that the interfaces between the blocks represent the discontinuities. With respect to NFR, the blocks can be used to represent the intact rock while the discontinuities represent the joints in the rock mass.

Consider an arbitrary deformable domain, Ω, with a boundary, Γ, that is subdivided by prescribed discontinuities into i number of subdomains, each denoted by Ω_i (Figure 3.2). Let $\Gamma_{ij} = \Gamma_{ji}$ represent the boundary between Ω_i and Ω_j. The motion of these subdomains (discrete elements) is governed by the conservation of momentum which relates the divergence of the stress field within the element, $\nabla \boldsymbol{\sigma}^m$, to the element acceleration, $\ddot{\mathbf{u}}^m$, and density, ρ:

$$\rho \ddot{\mathbf{u}}^m = \nabla \cdot \boldsymbol{\sigma}^m \tag{3.1}$$

The interaction between Ω_i and Ω_j along Γ_{ij} is the distinguishing feature in the DEM formulation, and is comprised of two main components: contact detection and the constitutive relationship. The contact detection algorithms are responsible for ensuring that Ω_i and Ω_j do not penetrate each other and ensuring that the appropriate contact forces are transferred between elements. These contact forces are governed by constitutive models of Γ_{ij} which can be described in general by a shear stiffness, k_s, in a direction parallel to the Γ_{ij}, and a normal stiffness, k_n, in a direction normal to Γ_i. The normal stress over any Γ_{ij}, σ^n, can be expressed as a function of the normal elastic displacement, u^n, up until the tensile strength, T, is exceeded:

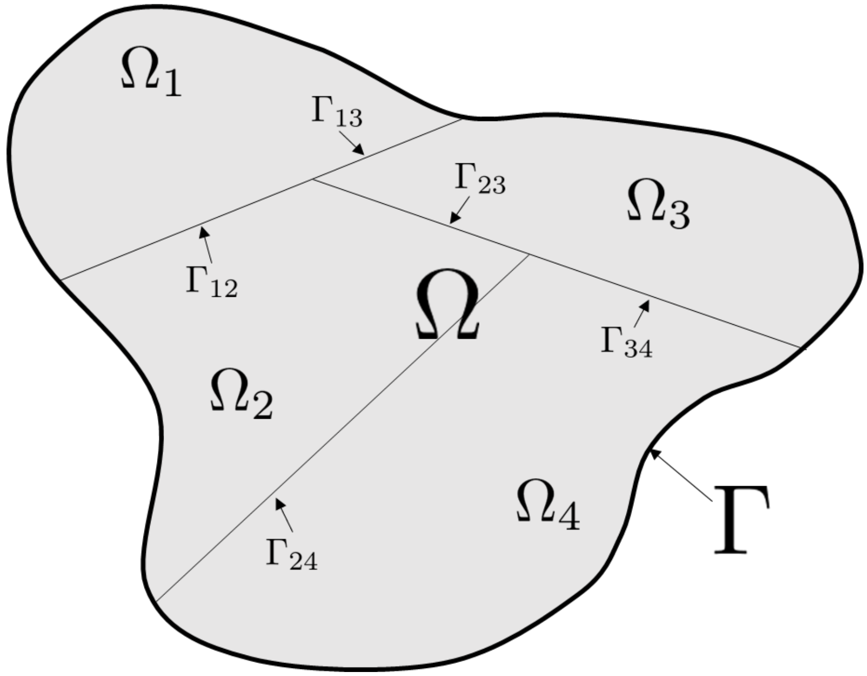

Figure 3.2: DEM block formulation for an arbitrary domain, Ω, with a set of subdomains, Ω_i.

$$\sigma^n = \begin{cases} \sigma^n\left(k^n, u^n\right) & if \quad \sigma^n \geq -T \\ 0 & if \quad \sigma^n < -T \end{cases} \tag{3.2}$$

Futhermore, the shear stress, τ, over any Γ_{ij} can be written in terms of the elastic shear displacement, u^s, until the maximum shear strength, τ^{max} is reached. The point when the shear stress at a point on Γ_{ij} exceeds the prescribed maximum shear stress, the discontinuity experiences plastic shear displacements in order not to exceed the maximum shear stress:

$$\tau = \begin{cases} \tau\left(k^s, u^s, \sigma^n\right) & if \quad |\tau| < \tau^{max} \\ \frac{u^s}{|u^s|}\tau^{max} & if \quad |\tau| \geq \tau^{max} \end{cases} \tag{3.3}$$

The microscale stress field, $\boldsymbol{\sigma}^m$, within Ω_i is described by standard continuum constitutive relationships. With the constitutive behaviour of the discontinuities and the constitutive behaviour of the continuum blocks, the overall behaviour of the rock mass can be characterized through material properties of the rock discontinuities and the intact rock.

3.2.1 Block Model

3.2.2 Joint Model

3.3 Homogenization Approach

The main objective of up-scaling DEM simulations is to be able to describe the behavior of the discontinuous medium in terms of a more computationally efficient continuum model. The homogenization algorithms used herein to determine the average stress-strain behaviour, $\langle \boldsymbol{\sigma} \rangle$-$\langle \boldsymbol{\epsilon} \rangle$, of the REV from the microscale displacements $\mathbf{u}^m$, strain $\boldsymbol{\epsilon}^m$, and stresses $\boldsymbol{\sigma}^m$ are based on the methods developed by D'Addetta et al. [2004] and Wellmann et al. [2008]. In this homogenization process, the resultant inter-block contact forces and block displacement from the DEM simulations are converted to average stresses and strains.

For the homogenization procedure to yield meaningful results, it should be applied to a Representative Elementary Volume (REV). The exact size of the REV depends on the geometry and mechanical properties of the DEM model. For the homogenization approach to hold, the REV of size d within a system with a characteristic length D and consisting of blocks with a characteristic diameter δ, must satisfy scale separation: $D \gg d \gg \delta$ [Wellmann et al., 2008].

In the following sections, all deformations are assumed to be small, such that there is no need to differentiate between the deformed and undeformed configurations.

We begin by defining a $L \times L$ square DEM simulation domain over which mixed-boundary conditions will be applied. The REV is taken as a circular domain of radius R, $2R < L$. The REV is taken to be a subdomain of the actual DEM simulation domain to eliminate any boundary effects. As will be seen below, it is convenient to take the boundary of the domain used for homogenization as a slightly larger domain encompassing the REV boundary. The boundary of the homogenization domain, denoted as Γ_h, is defined by the outer edges of the deformable blocks, i.e., the cohesive/contact surfaces between deformable blocks, which intersect a circle of radius R located in the center of the DEM simulation domain. Let the homogenization domain, the domain bounded by Γ_h, be denoted by Ω_h. These definitions are illustrated in Figure 3.3 for a 10m $\times$ 10m DEM domain, where the deformable blocks are defined through a Voronoi tessellation. The radius of the REV domain is 2.5m. It can be seen that the actual domain used for homogenization is non-circular and larger than the REV domain.

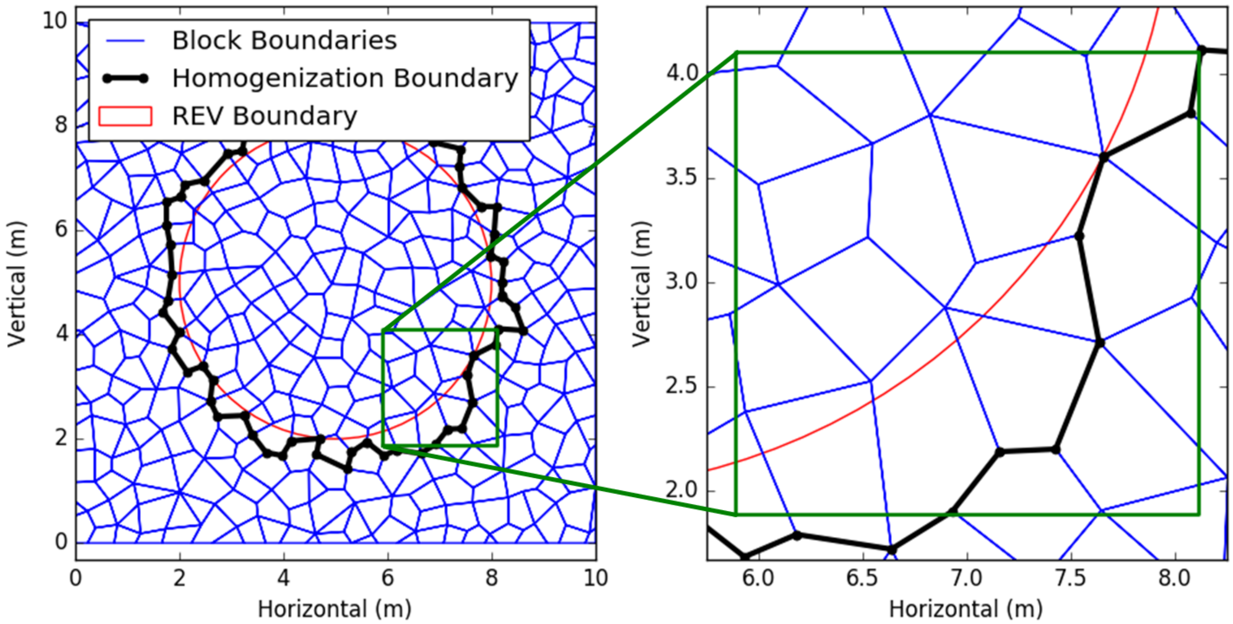

Figure 3.3: Assessment of the homogenization boundary given a circular REV.

The homogenization boundary, Γ_h, can be described in terms of n ordered boundary vertices, $V_i^h = (x_i^h, y_i^h)$, representing the i-th set of vertex coordinates along the boundary, such that the area of the homogenization domain, A^h, can be calculated using the following formulation for the area of an arbitrary, non-self-intersecting polygon [Zwillinger, 1995]:

$$A^h = \frac{1}{2} \sum_{i=1}^{n} x_i^h (y_{i+1}^h - y_{i-1}^h) \tag{3.4}$$

3.3.1 Stress Homogenization

The homogenized Cauchy stress, $\langle \boldsymbol{\sigma} \rangle$, is derived from the definition of the spatial average of the microscale stress of the deformable blocks of the DEM simulation, $\boldsymbol{\sigma}^m$, over the homogenization domain Ω^h.

$$\langle \boldsymbol{\sigma} \rangle = \frac{1}{A^h} \int_{\Omega^h} \boldsymbol{\sigma}^m dA \tag{3.5}$$

When each deformable block is discretized by constant stress triangles (elements/zones), the integration of the stress over each deformable block subdomain can be written as a summation in the form of a spatially weighted average of the zone stresses. Let $\boldsymbol{\sigma}^m_{IJ}$ denote the stress in zone J of deformable block I, N^z_I denote the number of zones within block I, A_{IJ} denote area of zone J in block I, and N^b denote the number of deformable blocks. The homogenized stress is then defined as

$$\langle \boldsymbol{\sigma} \rangle = \frac{1}{A^h} \sum_{I=1}^{N^b} \sum_{J=1}^{N^z_I} \boldsymbol{\sigma}^m_{IJ} A_{IJ} \tag{3.6}$$

In our implementation, (3.6) is incorporated into the homogenization module.

3.3.2 Strain Homogenization

The derivation for the homogenized strain tensor, $\langle \boldsymbol{\epsilon} \rangle$, begins in a similar manner to the homogenized stress tensor derivation with the familiar definition of the spatial average:

$$\langle \boldsymbol{\epsilon} \rangle = \frac{1}{A^h} \int_{\Omega^h} \boldsymbol{\epsilon}^m dA \tag{3.7}$$

At this point, it becomes convenient to assume a small displacement formulation of strain. This displacement assumption limits the applicability of the strain homogenization, but in the context of large scale geomechanics, this assumption remains reasonable. As such, the linear infinitesimal strain tensor can be written in terms of the displacement vector, $\mathbf{u}^m$:

$$\boldsymbol{\epsilon}^m = \frac{1}{2} \left[\nabla \mathbf{u}^m + \left(\nabla^\top \mathbf{u}^m \right) \right] \tag{3.8}$$

The above integral can be converted to the following boundary integral using the divergence theorem:

$$\langle \boldsymbol{\epsilon} \rangle = \frac{1}{2A^h} \oint_{\Gamma^h} \left[\mathbf{u}^m \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{u}^m \right] d\Gamma \tag{3.9}$$

where $\mathbf{n}$ is the outward pointing normal to Γ_h.

When Γ_h is defined by a set of line segments over which the displacement is also linear, the boundary integral can be rewritten as a summation over each of the N boundary segments. Let $\bar{\mathbf{u}}^m_I$ denote the average displacement along the I^{th} boundary segment of the homogenization boundary, which is calculated as the average of the two nodal displacements defining the boundary of each segment. Let $\mathbf{n}_I$ represent the outward pointing normal to the I^{th} boundary segment on the homogenization boundary. Let the length of boundary segment I be denoted by L_I. The homogenized strain can be rewritten as

$$\langle \boldsymbol{\epsilon} \rangle = \frac{1}{2A^h} \sum_{I=1}^{N} \left[\bar{\mathbf{u}}_I^m \otimes \mathbf{n}_I + \mathbf{n}_I \otimes \bar{\mathbf{u}}_I^m \right] L_I \tag{3.10}$$

3.4 Assessment of the REV Size

Homogenizing DEM simulations requires the existence and determination of the REV for that medium. Generally, the REV of a given domain can be described as the smallest subdomain that is statistically representative of the entire domain [Kanit et al., 2003, Gitman et al., 2007]. This qualitative definition is insufficient to rigorously define an REV as it is subjective with respect to what "statistically representative" means. Hence, the assessment of the REV can be a contentious issue, fraught with ambiguity.

One can conceptualize an REV to be "statistically representative" in two primarily different ways [Drugan and Willis, 1996]. The classically cited means for characterizing an REV suggests that the micro-scale heterogeneities (e.g. fractures, voids, grains, etc.) should be statistically representative within the REV such that the REV should contain a sufficiently large sample of these heterogeneities. This characterization of the REV is potentially problematic when attempting to quantify the REV as the descriptions of these heterogeneities tend to be nominally qualitative, and at best, quasi-quantitative.

The alternative means of conceptualizing "statistically representative", and arguably a more pragmatic way, proposes that the constitutive response of the REV should be statistically representative of the domain. In other words, as one increases the size of a sample domain, the point at which the constitutive response within the domain becomes sensibly constant can be referred to as the REV. Thus, the subdomain constitutive response is quantifiable through resultant model properties and parameters. This REV interpretation has been widely used because of its quantifiability [Kanit et al., 2003, Gitman et al., 2005, Gusev, 1997, Müller et al., 2010], and is adopted for this work.

3.4.1 Spatial Variance of RVE

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3.4.2 RVE Size Convergence

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3.5 Macroscale Constitutive Model

In this section we describe two macroscale stress-strain relationships, $\dot{\boldsymbol{\sigma}}^M = \dot{\boldsymbol{\sigma}}^M\left(\dot{\boldsymbol{\epsilon}}^M, \boldsymbol{\chi}, \mathbf{h}\right)$, used in the validation examples. The models are chosen to be complex enough to make the validation of the framework meaningful; however, we do not claim that these are the "best" macroscale models. The framework presented is general and the macroscale constitutive models described here can be replaced in particular applications by different ones. To simplify the discussion and notation in this section, the superscript "M" is omitted since all quantities defined describe macroscale behaviour.

Continuum Damage Mechanics (CDM) constitutive models are chosen to represent the NFR at the macroscale. CDM is a branch of continuum mechanics that is concerned with modeling the progressive failure and stiffness degradation in solid materials. CDM in this investigation is used to help describe the micro-mechanical degradation of the rock mass due to the nucleation and growth of cracks and voids. This micro-mechanical degradation is represented in a CDM model by using macroscopic state variables to represent a spatial average of the effects of this degradation. These state variables used in this context with respect to CDM are known as damage variables.

The damage variables in a CDM model can be described in different capacities. Often, for mathematical and physical simplicity, a single scalar damage variable is used to characterize the state of damage in the material. In this case, the damage variable, D, takes a value between 0 and 1 to represent the degree of damage to the material, where $D = 0$ represents a completely undamaged material (original stiffness) and $D = 1$ represents a completely damaged material with no stiffness. A scalar damage description limits the applicability of the CDM model to an isotropically damaged state, which may not be appropriate in some circumstances. More sophisticated CDM models use 2^{nd} and 4^{th} order tensorial representations of the damage variables as well as distinguishing between compressive damage and tensile damage states in order to more accurately characterize anisotropic damage evolution.

Consider the standard elastic relationship described by Hooke's law which relates the stress, $\boldsymbol{\sigma}$, and the elastic strain, $\boldsymbol{\epsilon}^{el}$ through an elastic stiffness tensor, $\mathbf{E}$:

$$\boldsymbol{\sigma} = \mathbf{E} : \left(\boldsymbol{\epsilon}^{el}\right) \tag{3.11}$$

Applying a scalar damage variable, D, to Hookes law using CDM to describe the stiffness degredation of the material can be shown as:

$$\boldsymbol{\sigma} = (1 - D)\,\mathbf{E} : \left(\boldsymbol{\epsilon}^{el}\right) \tag{3.12}$$

Here, the damaged stiffness of the material, $\mathbf{E}^d$, is described as folows:

$$\mathbf{E}^d = (1 - D)\,\mathbf{E} \tag{3.13}$$

Allowing the constitutive elastic CDM relationship to be written as:

$$\boldsymbol{\sigma} = \mathbf{E}^d : \boldsymbol{\epsilon}^{el} \tag{3.14}$$

In addition to damage, the elasto-plastic behaviour of the rock is also considered. Models that incorporate theories of plasticity and damage mechanics in a unified approach to damage evolution and constitutive relationships are often referred to as damage-plasticity models [Zhang and Cai, 2010]. In general, the constitutive relation for these damage-plasticity models describes the relationship between the stress, $\boldsymbol{\sigma}$, and the strain, $\boldsymbol{\epsilon}$ as a function of the damage variable, the original elastic stiffness tensor, $\mathbf{E}$, and the plastic strain, $\boldsymbol{\epsilon}^{pl}$:

$$\boldsymbol{\sigma} = \mathbf{E}^d : \left(\boldsymbol{\epsilon} - \boldsymbol{\epsilon}^{pl}\right) \tag{3.15}$$

Here, an additive decomposition of the elastic and plastic strain is assumed:

$$\boldsymbol{\epsilon} = \boldsymbol{\epsilon}^{el} + \boldsymbol{\epsilon}^{pl} \tag{3.16}$$

In CDM, the notion of effective stress, $\bar{\boldsymbol{\sigma}}$, becomes useful to describe the mechanics of the system as it refers to the stress that the system would be experiencing without damage. This effective stress can be related to the actual Cauchy stress through the scalar damage variable:

$$\boldsymbol{\sigma} = (1 - D)\,\bar{\boldsymbol{\sigma}} \tag{3.17}$$

3.5.1 General Formulation and Assumptions

The plasticity models used here are assumed to comprise of three key components: The yield function, the flow rule and the hardening rule. The yield function, $F\left(\bar{\boldsymbol{\sigma}}, \bar{\epsilon}^{pl}\right)$ indicates whether or not the material has experienced yield given a particular stress state. The yield function varies between the two models but can be written in general as a function of the effective stress, $\bar{\boldsymbol{\sigma}}$, and equivalent plastic strain, $\dot{\bar{\epsilon}}^{pl}$, expressed through three stress invariants: the Von-Mises equivalent stress, $p\left(\bar{\boldsymbol{\sigma}}\right)$, the hydrostatic stress, $q\left(\bar{\boldsymbol{\sigma}}\right)$, and the third invariant of deviatoric stress, $r\left(\bar{\boldsymbol{\sigma}}\right)$:

$$F = F\left(p\left(\bar{\boldsymbol{\sigma}}\right), q\left(\bar{\boldsymbol{\sigma}}\right), r\left(\bar{\boldsymbol{\sigma}}\right), \bar{\epsilon}^{pl}\right) \tag{3.18}$$

The Von Mises equivalent stress is written as:

$$p\left(\bar{\boldsymbol{\sigma}}\right) = \frac{1}{3}\,\mathrm{trace}\left[\boldsymbol{\sigma}\right] \tag{3.19}$$

The hydrostatic stress is written as:

$$q\left(\bar{\boldsymbol{\sigma}}\right) = \sqrt{\frac{3}{2}}\left[\mathbf{S} : \mathbf{S}\right] \tag{3.20}$$

Where $\mathbf{S}$ is known as the stress deviator with $\mathbf{I}$ being the identity matrix:

$$\mathbf{S} = \boldsymbol{\sigma} + p\left(\bar{\boldsymbol{\sigma}}\right)\mathbf{I} \tag{3.21}$$

The third invariant of the deviatoric stress is written as:

$$q\left(\bar{\boldsymbol{\sigma}}\right) = \tag{3.22}$$

In addition, the flow rule describes the amount of plastic deformation that the material should exhibit given an applied stress. The flow rule in these models is assumed to be of the following form:

$$\dot{\boldsymbol{\epsilon}}^{pl} = \dot{\lambda}\frac{\partial G\left(\bar{\boldsymbol{\sigma}}\right)}{\partial \bar{\boldsymbol{\sigma}}} \tag{3.23}$$

Where $\dot{\boldsymbol{\epsilon}}^{pl}$ is the plastic strain rate, $\dot{\lambda}$ is referred to as the plastic consistency parameter, and $G\left(\bar{\boldsymbol{\sigma}}\right)$ is the flow potential function. In addition to the yield function and the flow rule, the hardening rule is prescribed to govern the increase/decrease in yield stress as the plastic strain increases. More specifically, the hardening function, $\boldsymbol{h}\left(\bar{\boldsymbol{\sigma}}, \bar{\epsilon}^{pl}\right)$, in these models is used to relate the equivalent plastic strain, $\bar{\epsilon}^{pl}$, to the plastic strain in rate form:

$$\dot{\bar{\epsilon}}^{pl} = \boldsymbol{h}\left(\bar{\boldsymbol{\sigma}}, \bar{\epsilon}^{pl}\right) : \dot{\boldsymbol{\epsilon}}^{pl} \tag{3.24}$$

For the damage models, the damage initiation criteria and evolution equations are different for each material model. In general though, the damage initiation criteria for both material models is strain based and the nature of the damage evolution is assumed to be a function of the effective stress, and the equivalent plastic strain:

$$D = D\left(\bar{\boldsymbol{\sigma}}, \bar{\epsilon}^{pl}\right) \tag{3.25}$$

3.5.2 Drucker-Prager Plasticity Model with Ductile Damage

In this constitutive model, a ductile isotropic damage formulation is prescribed using a modified Johnson-Cook damage initiation criterion and a linear stiffness degradation model. In addition to damage, the elasto-plastic behaviour of the rock is also considered using an extended Drucker-Prager model with a linear yield criterion and a Barcelona hardening function.

The Drucker-Prager plasticity model was developed by Drucker [1950] for modelling frictional materials like granular soils and rock. An important aspect of this plasticity model is the use of a pressure dependent yield criterion to account for the increase in yield stress of geomaterials as the in-situ stresses increase. Specifically, the Drucker-Prager material model is formulated and used for materials with compressive yield strength much greater than the tensile yield strength such as one finds in soils and rocks. However, this material model is intended to simulate the material response under essentially monotonic loading which limits the capacity for modeling cyclic loading.

In addition, the Drucker-Prager model is suitable for using in conjunction with progressive damage and failure models. In this formulation, the Johnson-Cook Damage model is used to model the damage evolution of the rock mass [Johnson and Cook, 1985a]. At a sufficiently large scale, the damage response of NFR can be thought of as behaving in a ductile capacity.

Here, for the extended Drucker-Prager plasticity model, a linear yield function, $F\left(\bar{\boldsymbol{\sigma}}, \bar{\epsilon}^{pl}\right)$, is assumed to be a function of three stress invariants: the Von-Mises equivalent stress,

$p(\bar{\boldsymbol{\sigma}})$, the hydrostatic stress, $q(\bar{\boldsymbol{\sigma}})$, and the third invariant of deviatoric stress, $r(\bar{\boldsymbol{\sigma}})$. In addition, the yield function is written in terms of the compressive yield stress, $\sigma_c^y\left(\bar{\epsilon}^{pl}\right)$, which is defined by the hardening function and two material parameters: the friction angle, ϕ, and a parameter K, defined as the ratio of the yield stress in triaxial tension to the yield stress in triaxial compression:

$$F\left(\bar{\boldsymbol{\sigma}}, \bar{\epsilon}^{pl}\right) = \frac{1}{2} q(\bar{\boldsymbol{\sigma}}) \left[1 + \frac{1}{K} - \left(1 - \frac{1}{K} |\right) \left(\frac{r(\bar{\boldsymbol{\sigma}})}{q(\bar{\boldsymbol{\sigma}})}\right)^3\right] - p(\bar{\boldsymbol{\sigma}}) \tan\phi - \left[1 - \frac{1}{3}\tan\phi\right] \sigma_c^y\left(\bar{\epsilon}^{pl}\right) \quad (3.26)$$

The flow rule in this formulation is non-associated but the flow potential function, $G(\bar{\boldsymbol{\sigma}})$, is written in a very similar form as the yield function with dilation angle, ψ, in place of the friction angle. As with the yield function, the flow potential function is written in terms of three stress invariants and two material parameters, dilation angle, and K:

$$G(\bar{\boldsymbol{\sigma}}) = \frac{1}{2} q(\bar{\boldsymbol{\sigma}}) \left[1 + \frac{1}{K} - \left(1 - \frac{1}{K}\right) \left(\frac{r(\bar{\boldsymbol{\sigma}})}{q(\bar{\boldsymbol{\sigma}})}\right)^3\right] - p(\bar{\boldsymbol{\sigma}}) \tan\psi \quad (3.27)$$

In addition to the yield function and the flow rule, the hardening rule is assumed to take the form of the Barcelona model [Lubliner et al., 1989]. The Barcelona model allows for material hardening before softening and approaches a yield stress of 0 as the plastic strain increases. This form of the hardening function can be written in terms of three material parameters, initial compressive yield strength σ_c^{iy}, α and β:

$$\sigma_c = \sigma_c^{iy}\left[(1+\alpha) e^{-\beta\bar{\epsilon}^{pl}} - \alpha e^{-2\beta\bar{\epsilon}^{pl}}\right] \quad (3.28)$$

The damage initiation criterion for this material model is based on the Johnson-Cook model of ductile damage initiation [Johnson and Cook, 1985a]. The standard Johnson-Cook model assumes the equivalent plastic strain when damage is initiated, $\bar{\epsilon}_f^{pl}(\eta)$, is a function of triaxiality, η, and is written in terms of five material parameters. However, assuming isothermal conditions, neglecting rate effects, and assuming a simplified form of the exponential relationship, the initiation criterion can be reduced to two material parameters, D_2 and D_3:

$$\bar{\epsilon}_f^{pl}(\eta) = D_2 e^{D_3 \eta} \tag{3.29}$$

After the material has experienced yield and material damage has occurred, the stress-strain relationship becomes strongly mesh-dependent because of strain localization due to the energy dissipation decreasing as the mesh is refined. As such, Hillerborg et al. [1976] proposed a stress-displacement response based on fracture energy after damage initiation assuming that evolving damage is a linear degradation of the material stiffness in compression. Assuming a linear form, the effective plastic displacement when the material is completely damaged, $\bar{u}_f^{pl}$, can be specified, and the damage evolution can then be written in terms of the effective plastic displacement, $\bar{u}^{pl}$:

$$\dot{D} = \frac{\dot{\bar{u}}^{pl}}{\bar{u}_f^{pl}} \tag{3.30}$$

3.5.3 Damage-Plasticity Model for Quasi-Brittle Materials

In this constitutive model, a quasi-brittle isotropic damage formulation is prescribed using a linear stiffness degradation model that accounts for cyclic loading. In addition to damage, the elasto-plastic behaviour of the rock is also considered using Lubliner's plasticity model with a linear yield criterion and a Barcelona hardening function [Lubliner et al., 1989].

This damage-plasticity model was developed by Lubliner et al. [1989] as a plasticity based damage model for non-linear analysis of concrete failure. Subsequently, Lee and Fenves [1998] further developed the model to facilitate cyclic loading by adding a second damage variable and introducing a new yield function to account for the additional damage variable.

This model was specifically formulated for modeling quasi-brittle materials under low confining stresses subject to cyclic loading. In addition to the separate damage variables governing the stiffness degradation, the stiffness recovery and material hardening/softening is also treated separately in both compression and tension. Because the formulation does not consider the effects of large hydrostatic stresses, the applicability of this plastic to in-situ geomechanics at depth may not be sufficiently accurate. As such, this model is more appropriate for shallow geological models that require cyclic loading paths to be considered.

The yield function for this model is based on the yield function proposed by Lee and Fenves [1998] which was developed to allow for differential hardening under tension and compression. The resultant yield function, $F\left(\bar{\boldsymbol{\sigma}}, \bar{\epsilon}^{pl}\right)$, can be expressed in terms of two stress invariants: the Von-Mises equivalent stress, $p\left(\bar{\boldsymbol{\sigma}}\right)$, the hydrostatic stress, $q\left(\bar{\boldsymbol{\sigma}}\right)$:

$$F\left(\bar{\boldsymbol{\sigma}}, \bar{\epsilon}^{pl}\right) = \frac{1}{1-A}\left(q\left(\bar{\boldsymbol{\sigma}}\right) - 3Ap\left(\bar{\boldsymbol{\sigma}}\right) + B\left(\bar{\epsilon}^{pl}\right)\left\langle\hat{\bar{\boldsymbol{\sigma}}}\right\rangle - \gamma\left\langle-\hat{\bar{\boldsymbol{\sigma}}}\right\rangle\right) - \bar{\sigma}_c\left(\bar{\epsilon_c}^{pl}\right) \tag{3.31}$$

Where A and γ are dimensionless material constants. Experimental testing has yielded values of A between 0.08 and 0.12, as well as a typical γ value of approximately 3 Lubliner et al. [1989]. Additionally, the hat notation $\hat{\bar{\boldsymbol{\sigma}}}$ for an arbitrary stress tensor, $\bar{\boldsymbol{\sigma}}$, represents the algebraically maximum eigenvalue, or, the maximum principle stress.

The flow rule in this formulation is non-associated which means that the flow potential function, $G\left(\bar{\boldsymbol{\sigma}}\right)$, follows a different form than the yield function. Like with the yield function, the flow potential function, is written in terms of two stress invariants, $p\left(\bar{\boldsymbol{\sigma}}\right)$ and $q\left(\bar{\boldsymbol{\sigma}}\right)$, and two material parameters, dilation angle, ψ, and eccentricity ε:

$$G\left(\bar{\boldsymbol{\sigma}}\right) = \sqrt{\left[\varepsilon\sigma^{iy}\tan\psi\right]^2 + q\left(\bar{\boldsymbol{\sigma}}\right)^2} - p\left(\bar{\boldsymbol{\sigma}}\right)\tan\psi \tag{3.32}$$

In this formulation of damage-plasticity, the brittle nature of rock necessitates separate characterization of tensile and compressive damage. With quasi-brittle materials such as rock, it has been found that compressive stiffness can be recovered upon crack closure. Conversely, in these materials, tensile stiffness is not recovered after compressive cracks have developed. This behaviour implies that two separate scalar damage values should exist for the given system to account for both the compressive stiffness degradation and the tensile stiffness degradation. As such, the equivalent plastic strain is also considered separately for tension ($\bar{\epsilon}_t^{pl}$) and compression ($\bar{\epsilon}_c^{pl}$) and is represented as follows:

$$\bar{\epsilon}^{pl} = \begin{bmatrix} \bar{\epsilon}_t^{pl} \\ \bar{\epsilon}_c^{pl} \end{bmatrix} \tag{3.33}$$

The hardening rule for this model is slightly modified from equation 3.24 to accommodate two hardening variables (equivalent plastic strains) for tension and compression. The hardening rule can thus be written in matrix form:

$$\mathbf{h}\left(\bar{\boldsymbol{\sigma}}, \bar{\epsilon}^{pl}\right) = \begin{bmatrix} r\left(\hat{\bar{\sigma}}_{ij}\right)\frac{\sigma_t\left(\bar{\epsilon}_t^{pl}\right)}{g_t} & 0 & 0 \\ 0 & 0 & -\left(r\left(\hat{\bar{\sigma}}_{ij}\right) - 1\right)\frac{\sigma_c\left(\bar{\epsilon}_c^{pl}\right)}{g_c} \end{bmatrix} \tag{3.34}$$

Where σ_t and σ_c are the yield stresses in tension and compression as specified by the hardening curves which describe the evolution of the equivalent plastic strains. The compressive hardening rule is approximated here using the Barcelona model in a similar capacity as was done for the Drucker-Prager model in the previous section. The only difference here being that the hardening is defined in terms of the inelastic strain, $\bar{\epsilon}^{in}$, rather than the plastic strain before:

$$\sigma_c = \sigma_c^{iy} \left[(1+\alpha) e^{-\beta \bar{\epsilon}^{in}} - \alpha e^{-2\beta \bar{\epsilon}^{in}} \right] \tag{3.35}$$

There exists a subtle but important distinction between these two strain measurements when considering CDM. The plastic strain refers to all the strain that is non-elastic (i.e. the remaining strain after the applied stress is unloaded in the damaged state), while the inelastic strain refers to the theoretical plastic strain that would remain if the material was unloaded with the original material stiffness (i.e. in an undamaged state).

The tensile hardening function has a fundamentally different behavior than the compressive hardening function, and is therefore approximated using an exponential function. This function is described by the initial tensile yield stress, σ_t^{iy}, and a decay parameter, λ. These parameters describe the relationship between the tensile yield stress, σ_t, and the cracking strain, $\bar{\epsilon}^{ck}$ which is the tensile portion of inelastic strain:

$$\sigma_t \left(\bar{\epsilon}^{ck} \right) = \sigma_t^{iy} e^{\lambda \bar{\epsilon}^{ck}} \tag{3.36}$$

In addition, g_t and g_c from (3.34) represent the dissipated fracture energy density during micro-cracking. The use of the dissipated fracture energy density over fracture energy (a material property) stems from the fact that the strain softening part of the stress-strain curve cannot represent a local physical property of the material in addition to being highly mesh sensitive. The dissipated fracture energy densities are defined in terms of a characteristic length, l, associated with the mesh size and the fracture energy in tension, G_t, and compression, G_c:

$$g_t = \frac{G_t}{l} \tag{3.37}$$

$$g_c = \frac{G_c}{l} \tag{3.38}$$

Furthermore, the weighting function, $r\left(\hat{\bar{\sigma}}\right)$, weights the hardening functions depending on the degree of tension or compression that the model is experiencing:

$$r\left(\hat{\bar{\sigma}}\right) = \frac{\sum_{i=1}^{3}\left\langle \hat{\bar{\sigma}}_i \right\rangle}{\sum_{i=1}^{3}\left| \hat{\bar{\sigma}}_i \right|}, \qquad 0 \leq r\left(\hat{\bar{\sigma}}\right) \leq 1 \tag{3.39}$$

Loading a quasi-brittle in compression or tension causes damage in the material, which reduces the effective stiffness, weakening the unloading response. This damage is characterized by two damage variables, one of which represents the damage due to tensile loading, D_t, the other represents damage due to compressive loading, D_c.

$$D_t = D_t\left(\bar{\epsilon}_t^{pl}\right), \qquad 0 \leq D_t \leq 1 \tag{3.40}$$

$$D_c = D_c\left(\bar{\epsilon}_c^{pl}\right), \qquad 0 \leq D_c \leq 1 \tag{3.41}$$

The damage in both compression and tension is a necessarily increasing function of the equivalent plastic strains. For cyclic loading, both the compressive and tensile damage need to be considered. Two stiffness recovery factors are introduced, s_t and s_c, which represent the stiffness recovery effects associated with stress reversals. The damage can be said to take the form of:

$$[1 - D] = [1 - s_t D_c]\,[1 - s_c D_t]\,, \qquad 0 \leq s_t, s_c \leq 1 \tag{3.42}$$

3.6 Parameter Estimation Algorithms

Parameter estimation involves a process of obtaining a parameter set $\boldsymbol{\chi}$ of a CDM model that minimizes the difference between $\boldsymbol{\sigma}^M$-$\boldsymbol{\epsilon}^M$ and $\langle\boldsymbol{\sigma}\rangle$-$\langle\boldsymbol{\epsilon}\rangle$ for all load paths. Herein, the parameter estimation was conducted using calibration algorithms, a subset of optimization which attempts to minimize a least-squares objective function [Matott, 2008]. Optimization algorithms are often described as either deterministic, which find the local optimum precisely, or heuristic, which find the global optimum approximately.

Deterministic optimization algorithms primarily focus on searching for the optima within the local parameter space by iteratively converging towards a solution. Heuristic optimization algorithms explore the entire parameter space approximately and provide an estimate of the global optima. Heuristic techniques are useful for highly non-linear problems, where there are numerous local optima within the prescribed parameter space. When searching the global parameter-space deterministically becomes too computationally demanding, heuristic methods are used, at the cost of completeness and accuracy. A compromise between speed and accuracy can be obtained by strategically using both types of algorithms.

A combination of two optimization algorithms is used to assess the optimal parameter set. An initial heuristic algorithm is applied to search for the approximate global optima, followed by a deterministic algorithm as a local refinement of the optimal parameter set. Particle Swarm Optimization (PSO) is used for the global heuristic search, whereas the Levenberg-Marquardt Algorithm (LMA) is used for the local deterministic search.

Consider a j^{th} arbitrary homogenized stress measurement at any given time, $\langle s \rangle_j$, which acts as the target solution for the macroscale model. The same stress measurement in the macroscale model, $s_j^M(\boldsymbol{\chi}, \langle e \rangle)$, can be expressed as a function of the parameter set for the continuum constitutive model, $\boldsymbol{\chi}$, containing n number of parameters, and the homogenized strain at the given load step, $\langle e \rangle$. Here, the weighted least-squares objective function to be minimized, Ψ, can be written in terms of a weighting parameter, w_j, for m number of stress measurements:

$$\Psi = \sum_{j=1}^{m} \left[w_j \left[\langle s \rangle_j - s_j^M(\boldsymbol{\chi}, \langle e \rangle) \right] \right]^2 \tag{3.43}$$

The aim of the following optimization algorithms can be described as an attempt to minimize Ψ by varying $\boldsymbol{\chi}$, subject to the constraint that all parameters values within $\boldsymbol{\chi}$ represent physically realistic values and fall within specified bounds.

The parameter estimation works by iteratively running a single element CDM model, subject to boundary conditions provided by the homogenized DEM simulations, with successive parameter sets that intelligently adapt in order to converge to the DEM data. The approach used here is similar in aim to the Least Squares method that was briefly described in Marquardt [1963].

3.6.1 Heuristic vs. Deterministic Search Algorithms

3.6.2 Particle Swarm Optimization (PSO)

The PSO algorithm was developed by Kennedy and Eberhart [1995] as a byproduct of modeling the cooperative-competitive nature of social behaviour in birds as they flocked searching for food. The PSO algorithm, in a conceptual sense, consists of a series of 'particles' (birds) which 'swarm' through the entire parameter space (sky) searching for the global optima (food) using a combination of individual 'particle' knowledge and global 'swarm' (flock) knowledge.

etc...

Consider a particle in an n dimensional parameter space with an arbitrary velocity, $\vec{v}_i$, and position, $\vec{x}_i$. At each position in this parameter space, Ψ can be evaluated with an attempt to find the position that minimizes Ψ. The motion of this particle allows the the exploration of the parameter space to find a minimum value of Ψ and the corresponding position. After a period of time Δt, the new position of the particle, $\vec{x}_{i+1}$ can be written as a combination of the old position and the new velocity, $\vec{v}_{i+1}$.

$$\vec{x}_{i+1} = \vec{x}_i + \vec{v}_{i+1}\Delta t \tag{3.44}$$

Here, $\vec{v}_{i+1}$, is considered to be influenced by $\vec{v}_i$, the position of the current local optimum, p_l, and the position of the current global optimum, p_g. The local optimum refers to the minimum value of Ψ observed by the particle, while the global optimum refers to the minimum value of Ψ observed by all particles. As such, $\vec{v}_{i+1}$ is written as a linear combination of $\vec{v}_i$, the velocity required to move the particle back to the local optimum and the velocity required to move the particle back to global optimum. In order to prevent the algorithm from oscillating indefinitely in a predictable manner, a randomization vector, $\vec{U}(\phi)$, of length n is introduced to provide coefficients between 0 and ϕ to the velocity vectors. The operator $\odot$ refers to the Hadamard product (element-wise multiplication):

$$\vec{v}_{i+1} = \vec{v}_i + \frac{\vec{U}_i(\phi_1) \odot [\vec{p}_l - \vec{x}_i] + \vec{U}_i(\phi_2) \odot [\vec{p}_g - \vec{x}_i]}{\Delta t} \tag{3.45}$$

As one would expect, the behaviour of the PSO is highly sensitive to the chosen values of ϕ_1 and ϕ_2. If these parameters are too small, then the optimization becomes "unresponsive" such that the initial velocity is maintained and successive iterations do not have the capacity to appreicable change the velocity to search the parameter space effectively. Alternatively, if these parameters are too large, the PSO has the capacity to become unstable such that the particle speeds keep increasing on successive iterations. Commonly accepted in most PSO algorithms is the assumption that $\phi_1 = \phi_2 = 2$. To overcome these limitations and control the scope of the search, Shi and Eberhart [1998] introduced the inertial weight term, ω:

$$\vec{v}_{i+1} = \omega\vec{v}_i + \frac{\vec{U}_i(\phi_1) \odot [\vec{p}_l - \vec{x}_i] + \vec{U}_i(\phi_2) \odot [\vec{p}_g - \vec{x}_i]}{\Delta t} \tag{3.46}$$

This inertial weight acts as a scalar multiplier between 0 and 1 for $\vec{v}_i$, and can be interpreted as a measure of the fluidity of the system. A large inertial term allows the particle to maintain it's current velocity to a higher degree indicating a system with low viscosity lending to a more explorative search, while a small inertial term dissipates the particles velocity more rapidly indicating a more viscous system which favours exploitative searching.

Additional damping can be provided in the form of a constriction coefficient which controls the convergence of the particle, by ensuring convergence and preventing explosion. Clerc and Kennedy [2002] noted that many means of constricting the velocity function exist, but provided a simple form of the constriction, using a constriction coefficient, $\zeta(\phi_1, \phi_2)$.

$$\vec{v}_{i+1} = \zeta(\phi_1, \phi_2) \left[\omega \vec{v}_i + \frac{\vec{U}_i(\phi_1) \odot [\vec{p}_l - \vec{x}_i] + \vec{U}_i(\phi_2) \odot [\vec{p}_g - \vec{x}_i]}{\Delta t} \right] \tag{3.47}$$

Here, $\zeta(\phi_1, \phi_2)$ is given by the following, where $\phi = \phi_1 + \phi_2$:

$$\zeta(\phi_1, \phi_2) = \frac{2}{\phi - 2 + \sqrt{\phi^2 - 4\phi}} \tag{3.48}$$

In addition, with the desire to give more credence to either the local optimum or the global optimum, two "trust" parameters are introduced. c_1 is referred to as the cognitive parameter as it weights the particles own experience, while the second parameter, c_2, is referred to as the social parameter as it weights the influence of the combined experience of the swarm:

$$\vec{v}_{i+1} = \zeta(\phi_1, \phi_2) \left[\omega \vec{v}_i + \frac{c_1 \vec{U}_i(\phi_1) \odot [\vec{p}_l - \vec{x}_i] + c_2 \vec{U}_i(\phi_2) \odot [\vec{p}_g - \vec{x}_i]}{\Delta t} \right] \tag{3.49}$$

Here, the position of the particle can be taken to represent an estimate of the optimal parameter set, $\boldsymbol{\chi}_i$, while the velocity of the particle represents the direction and magnitude of the change in the parameter set estimate for the next iteration $\Delta \boldsymbol{\chi}_{i+1}$. Furhtermore, the time step can considered to be a unit iteratation step, which allows for (3.49) to be abstracted as follows in the context of up-scaling DEM simulations.

$$\Delta \boldsymbol{\chi}_{i+1} = \zeta(\phi_1, \phi_2) \left[\omega \Delta \boldsymbol{\chi}_i + c_1 \vec{U}_i(\phi_1) \odot [\boldsymbol{\chi}_l - \boldsymbol{\chi}_i] + c_2 \vec{U}_i(\phi_2) \odot \left[\boldsymbol{\chi}_g - \boldsymbol{\chi}_i\right] \right] \tag{3.50}$$

Where $\boldsymbol{\chi}_l$ is the parameter set corresponding to the minimum value of Ψ for the particle, and $\boldsymbol{\chi}_g$ is the parameter set corresponding to the minimum value of Ψ for all particles. In addition, (3.44) can be rewritten in a similar capacity:

$$\boldsymbol{\chi}_{i+1} = \boldsymbol{\chi}_i + \Delta\boldsymbol{\chi}_{i+1} \tag{3.51}$$

For a particle swarm containing an arbitrary number of particle, the optimal parameter set of the system, $\boldsymbol{\chi}$, is considered to be $\boldsymbol{\chi}_g$ after a specified number of iterations, or once all the particles converge to a stable solution. The general PSO algorithm as described here is summarized as follows:

1. Assign particles random positions and velocities in the parameter space
2. Move each particle with (3.50) and (3.51)
3. For each particle, revise $\boldsymbol{\chi}_l$ if new local optimum found
4. Revise $\boldsymbol{\chi}_g$ if new global optimum found
5. If current iteration is greater than the maximum number of iterations or solution is stable, iteration is complete. Otherwise, go to step 2

3.6.3 Asynchronous Parallel PSO (APPSO)

The PSO described above possesses a large number of attractive qualities for parameter estimation which make it desirable to for up-scaling. However, the main drawback of the PSO is the large computational costs in terms of total elapsed time primarily due to the fact that the algorithm was originally designed for a serial implementation. The serial implementation, although effective in it's own right, can be dramatically improved through parallelization.

The nature of the PSO lends itself to a fairly trivial implementation of a synchronous parallellization scheme which does not require changing the nature of the algorithm. Here, since all the particles at each iteration are treated independently, the updated positions and corresponding objective functions can be computed in parallel. This parallelization scheme waits for all the particles to complete their analysis before moving on to the next iteration. As a result, the parallel efficiency is often compromised due to processors having to wait for the final particle(s) to finish their analysis. This idleness of the processors can be caused by having a swarm size that is not an integer multiple of the number of processors, having a heterogenous computing environment where processors have different computational speeds, or having a numerical simulation that requires different amount of computational time depending on the input parameters [Venter and Sobieszczanski-Sobieski, 2006]. This inefficiency of this synchronous parallelization increases as the number of processors increases due to the increasing number of idle processors towards the end of the iteration.

To overcome these parallel inefficiencies, Venter and Sobieszczanski-Sobieski [2006] introduced an Asynchronous Parallel Particle Swarm Optimization (APPSO) algorithm to continuously use the available processors with the goal of having no idle processors from one iteration to the next. The key here, is to separate the update calculations associated with each point and those associated with the swarm as a whole. Normally, in the synchronous scheme, the update calculations (i.e. updating $\boldsymbol{\chi}_l$ and $\boldsymbol{\chi}_g$) are done at the end of each iteration. In this asynchronous scheme, updating $\boldsymbol{\chi}_l$ remains the same, but updating $\boldsymbol{\chi}_g$ uses the best position from the previous iteration instead of the current iteration in order perform the update calculations immediately and allow the analyses to proceed without waiting for the rest of the particles to complete their analysis.

3.6.4 Levenburg-Marquardt Algorithm (LMA)

The Levenberg-Marquardt Algorithm (LMA) was proposed by Marquardt [1963] which builds off of the work of Levenberg [1944]. This calibration algorithm combines a quasi-Newton approach with a conjugate gradient technique in order to efficiently minimize non-linear least-squares problems.

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For notational simplicity (3.43) is rewritten in matrix form by considering a vector containing m number of arbitrary homogenized stress measurements at any given time, $\langle \mathbf{s} \rangle$, and a corresponding vector of stress measurements for the macroscale model, $\mathbf{s}^M$:

$$\langle \mathbf{s} \rangle = \left[\langle s \rangle_1 , \langle s \rangle_2 , \ldots , \langle s \rangle_m \right]^T \tag{3.52}$$

$$\mathbf{s}^M = \left[s_1^M, s_2^M, \ldots, s_m^M \right]^T \tag{3.53}$$

This vectorization facilitates writing the weighted least-squares objective function in matrix form using $\mathbf{Q}$ as a weighting matrix:

$$\Psi = \left[\langle \mathbf{s} \rangle - \mathbf{s^M} \right]^T \mathbf{Q} \left[\langle \mathbf{s} \rangle - \mathbf{s^M} \right] \tag{3.54}$$

Where $\mathbf{Q}$ is written as a diagonal matrix containing the weighting parameters:

$$\mathbf{Q} = \begin{bmatrix} w_1^2 & 0 & \dots & 0 \\ 0 & w_2^2 & & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \dots & w_m^2 \end{bmatrix} \tag{3.55}$$

The first step in the LMA formulation considers an arbitrary initial set of parameters, $\boldsymbol{\chi}_0$, and the corresponding macroscale stress measurements, $\mathbf{s}_0^M$. The relationship between $\boldsymbol{\chi}$ and $\mathbf{s}^M$ is generally highly non-linear, so the function is approximated with a taylor series expansion about $\boldsymbol{\chi}_0$, yielding the following linearization:

$$\mathbf{s}^M \approx \mathbf{s}_0^M + \mathbf{J}\left[\boldsymbol{\chi} - \boldsymbol{\chi}_0\right] \tag{3.56}$$

Where the partial derivatives of the given set of s^M stress measurements with respect to the parameters in $\boldsymbol{\chi}$ are represented in the Jacobian matrix, $\mathbf{J}$:

$$\mathbf{J} = \begin{bmatrix} \frac{\partial s_1^M}{\partial \boldsymbol{\chi}_1} & \frac{\partial s_1^M}{\partial \boldsymbol{\chi}_2} & \dots & \frac{\partial s_1^M}{\partial \boldsymbol{\chi}_n} \\ \frac{\partial s_2^M}{\partial \boldsymbol{\chi}_1} & \frac{\partial s_2^M}{\partial \boldsymbol{\chi}_2} & & \frac{\partial s_2^M}{\partial \boldsymbol{\chi}_n} \\ \vdots & & \ddots & \vdots \\ \frac{\partial s_m^M}{\partial \boldsymbol{\chi}_1} & \frac{\partial s_m^M}{\partial \boldsymbol{\chi}_2} & \dots & \frac{\partial s_m^M}{\partial \boldsymbol{\chi}_n} \end{bmatrix} \tag{3.57}$$

Substituting (3.56) into (3.54) gives an linearized approximation of the objective function:

$$\Psi \approx \left[\langle \mathbf{s} \rangle - \left[\mathbf{s}_0^M + \mathbf{J}\left[\boldsymbol{\chi} - \boldsymbol{\chi}_i\right]\right]\right]^T \mathbf{Q}\left[\langle \mathbf{s} \rangle - \left[\mathbf{s}_0^M + \mathbf{J}\left[\boldsymbol{\chi} - \boldsymbol{\chi}_0\right]\right]\right] \tag{3.58}$$

Since (3.58) is still an approximation of the objective function, an iterative approach is required to converge to an optimal estimate of $\boldsymbol{\chi}$. Here, (3.58) can be modified and written in an iterative capacity such that the current parameter set estimate, $\boldsymbol{\chi}_i$, simulated stress measurements, $\mathbf{s}_i^M$, objective function value, Ψ_i, and Jacobian matrix, $\mathbf{J}_i$ can be used to estimate the next parameter set estimate $\boldsymbol{\chi}_{i+1}$:

$$\Psi_i = \left[\langle \mathbf{s} \rangle - \left[\mathbf{s}_i^M + \mathbf{J}_i\left[\boldsymbol{\chi}_{i+1} - \boldsymbol{\chi}_i\right]\right]\right]^T \mathbf{Q}\left[\langle \mathbf{s} \rangle - \left[\mathbf{s}_i^M + \mathbf{J}_i\left[\boldsymbol{\chi}_{i+1} - \boldsymbol{\chi}_i\right]\right]\right] \tag{3.59}$$

The vector $\left[\boldsymbol{\chi}_{i+1} - \boldsymbol{\chi}_0\right]$, which represents the difference in the current estimate of the parameter set and the next parameter set estimate is termed the upgrade vector. By taking the derivative of Ψ with respect to $\boldsymbol{\chi}$, the upgrade vector can be written as:

$$\left[\boldsymbol{\chi}_{i+1} - \boldsymbol{\chi}_i\right] = \left[\mathbf{J}_i^T \mathbf{Q} \mathbf{J}_i\right]^{-1} \mathbf{J}_i^T \mathbf{Q} \left[\langle \mathbf{s} \rangle - \mathbf{s}_i^M\right] \tag{3.60}$$

Here, for convenience, the upgrade vector is written as $\mathbf{U}_i = \left[\boldsymbol{\chi}_{i+1} - \boldsymbol{\chi}_i\right]$. Since (3.60) is still an approximation of the upgrade vector, an iterative approach to finding $\boldsymbol{\chi}$ is required. The LMA further proposes that $\boldsymbol{U}_i$ be modified with the Marquardt parameter, α:

$$\mathbf{U}_i = \left[\mathbf{J}_i^T \mathbf{Q} \mathbf{J}_i + \alpha \mathbf{I}\right]^{-1} \mathbf{J}_i^T \mathbf{Q} \left[\langle \mathbf{s} \rangle - \mathbf{s}_i^M\right] \tag{3.61}$$

Here, $\mathbf{I}$ is the $n \times n$ identity matrix. The Marquardt parameter in (3.61) allows $\mathbf{U}_i$ to approximate a Steepest-Descent Method (SDM) for large values of α, while using a Taylor Series Approximation (TSA) for small values of alpha. This formulation allows for a smooth transition between a SDM when the parameter set estimate is far away from the optimal parameter set, and a TSA when the parameter set estimate is close to the optimal parameter set.

Another key development in the LMA notes that for many calibration and parameter estimation problems, elements within $\mathbf{s}_i^M$ and $\langle \mathbf{s} \rangle$ may differ by several orders of magnitude. Such large variations can lead to significant roundoff error during the calculation of $\mathbf{J}_i$. This error can be avoided by introducing a scaling matrix, $\mathbf{S}_i$:

$$\mathbf{S}_i = \begin{bmatrix} \frac{1}{J_{i_{11}} w_1} & 0 & \dots & 0 \\ 0 & \frac{1}{J_{i_{22}} w_2} & & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \dots & \frac{1}{J_{i_{nn}} w_n} \end{bmatrix} \tag{3.62}$$

With (3.62), the upgrade vector in (3.61) can be rewritten in a mathematically identical way while avoiding numerical errors:

$$\mathbf{U}_i = \mathbf{S}_i \left[\mathbf{S}_i^T \mathbf{J}_i^T \mathbf{Q} \mathbf{J}_i \mathbf{S}_i + \alpha \mathbf{S}_i^T \mathbf{S}_i\right]^{-1} \mathbf{S}_i^T \mathbf{J}_i^T \mathbf{Q} \left[\langle \mathbf{s} \rangle - \mathbf{s}_i^M\right] \tag{3.63}$$

The final feature of the LMA is the introduction of the Marquardt Lambda, λ. The Marquardt Lambda is taken as the largest term in the matrix $\alpha \mathbf{S}^T \mathbf{S}$. Here, the adjustment of λ provides control over the relative weighting of the SDM vs the TSA such that for large values of λ, the SDM dominates, while for small values of λ, the TSA dominates. The iterative algorithm is summarized as follows Matott [2008]:

1. Choose initial value for λ
2. Compute $\mathbf{s}^M(\boldsymbol{\chi}_i, \langle e \rangle)$
3. Compute Ψ_i with (3.59)
4. Compute $\mathbf{U}_i$ with (3.63)
5. Compute $\boldsymbol{\chi}_{i+1} = \boldsymbol{\chi}_i + \mathbf{U}_i$
6. Compute $\mathbf{s}^M(\boldsymbol{\chi}_{i+1}, \langle e \rangle)$
7. Compute Ψ_{i+1} with (3.59)
8. Adjust λ
   (a) If number of λ adjustments is optimal or exceeds maximum, go to step 9
   (b) If $\Psi_{i+1} < \Psi_i$, reduce λ, increment i, and go to step 2
   (c) If $\Psi_{i+1} \geq \Psi_i$, increase λ, and go to step 4
9. Test for convergence by comparing Ψ_{i+1} and Ψ_i
   (a) If converged, iteration is complete and $\boldsymbol{\chi}_{i+1}$ represents the optimal solution.
   (b) If not converged, increment i, and go to Step 2

3.7 Physically Meaningful Model Parameterization

To accelerate the process of finding a near-optimal set of parameters, it is important to limit the search space of the parameterization algorithm. This is especially important when the number of parameters is large. We have found that it is beneficial for the parameters to have physical meaning in order to specify realistic bounds.

etc...

The elastic behaviour is parameterized by Young's modulus, E, and Poisson's ratio, ν. Bounds on these quantities are well known.

3.7.1 Drucker-Prager Model with Ductile Damage

The yield function and flow potential function are parameterized in terms of the friction angle, dilation angle, and the stress ratio K. Bounds on these quantities are relatively well known.

The hardening function (3.28) is given in terms of two empirical coefficients α and β and the initial compressive yield stress σ_c^{iy}. While it is possible to set bounds on σ_c^{iy}, it is less straightforward to set bounds for α and β as they do not have obvious physical meaning. The hardening function for the Barcelona model is shown in Figure 3.4. The coefficients α and β can be rewritten in terms of the peak compressive yield strength, σ_c^p, the plastic strain at the peak compressive yield strength, ϵ_c^p, and the initial compressive yield stress σ_c^{iy}:

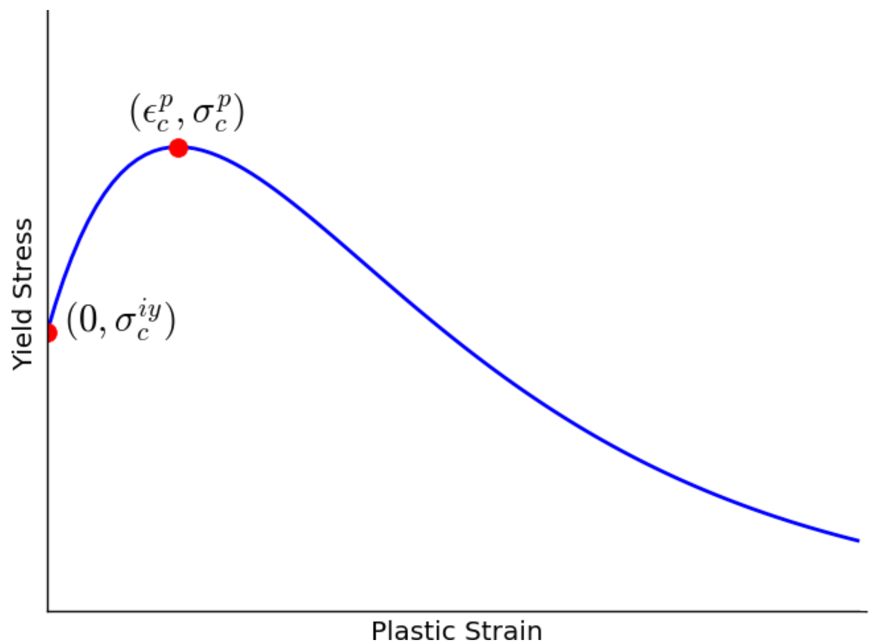

Figure 3.4: Compressive hardening/sofening function from the Barcelona model. The curve is able to be parameterized using three parameters.

$$\beta = \frac{\ln\left[\frac{2\alpha}{1+\alpha}\right]}{\epsilon_c^p} \tag{3.64}$$

$$\alpha = \frac{2\sigma_c^p - \sigma_c^{iy} + 2\sqrt{-\sigma_c^p\left(\sigma_c^{iy} - \sigma_c^p\right)}}{\sigma_c^{iy}} \tag{3.65}$$

Thus, we parameterize the hardening law in terms of σ_c^p, ϵ_c^p, and σ_c^{iy} so that bounds can be more easily defined.

Similarly, the Johnson-Cook damage initiation criterion from (3.29) is described by two empirical coefficients (D_2, and D_3) which do not have intuitive physical meaning. To make setting the bounding limits during the parameter estimation simpler, the Johnson-Cook parameters were rewritten in terms of equivalent plastic strain at which damage is initiated at triaxialities of -0.5 and -0.6, $\bar{\epsilon}^{pl}_{y_{-0.5}}$ and $\bar{\epsilon}^{pl}_{y_{-0.6}}$, respectively:

$$D_2 = \frac{\left(\bar{\epsilon}^{pl}_{y_{-0.5}}\right)^6}{\left(\bar{\epsilon}^{pl}_{y_{-0.6}}\right)^5} \tag{3.66}$$

$$D_3 = 10\ln\left(\frac{\bar{\epsilon}^{pl}_{y_{-0.5}}}{\bar{\epsilon}^{pl}_{y_{-0.6}}}\right) \tag{3.67}$$

In addition, the damage evolution was parameterized using only the plastic displacement at failure parameter. The goal of the parameter estimation module, in the verification examples, is therefore to estimate the 11 parameters $\boldsymbol{\chi} = \{E, \nu, \psi, K, \phi, \sigma_c^{iy}, \sigma_c^p, \epsilon_c^p, \bar{\epsilon}^{pl}_{y_{-0.5}}, \bar{\epsilon}^{pl}_{y_{-0.6}}, \bar{u}_f^{pl}\}$, which are summarized in Table 3.1.

3.7.2 Damage-Plasticity Model for Quasi-Brittle Materials

The yield function for this model is written in terms of three material parameters: A, B, and γ. These material parameters are not directly measurable, but can be expressed in terms of measurable parameters. A is expressed here as a function of the ratio f_0, which is defined as the ratio of the initial biaxial compressive yeild strength, σ_{b0} to the initial uniaxial compressive strength, σ_{c0}:

$$f_0 = \frac{\sigma_{b0}}{\sigma_{c0}} \tag{3.68}$$

$$A = \frac{f_0 - 1}{2f_0 - 1} \tag{3.69}$$

Table 3.1: Parameter set for Drucker-Prager Material Model with Ductile Damage

Parameter Type		Name	Symbol
Elastic		Young's Modulus	E
		Poisson's Ratio	ν
Plastic	Flow Rule/Yield Function	Dilation Angle	ψ
		Yield Stress Ratio	K
		Friction Angle	ϕ
	Hardening Rule	Initial Compressive Yield Strength	σ_c^{iy}
		Peak Compressive Yield Strength	σ_c^p
		Strain at Peak Compressive Yield	ϵ_c^p
Damage	Initiation	Yield Strain at -0.5 Triaxiality	$\bar{\epsilon}_{y-0.5}^{pl}$
		Yield Strain at -0.6 Triaxiality	$\bar{\epsilon}_{y-0.6}^{pl}$
	Evolution	Plastic Displacement at Failure	$\bar{u}_f^{pl}$

Additionally, γ is expressed in terms of the ratio K_c which expresses the ratio of hydrostatic pressure at yield in tension to the hydrostatic pressure at yield in compression:

$$\gamma = \frac{3\left(1 - K_c\right)}{2K_c - 1} \tag{3.70}$$

Similarily, B is expressed as a function of A and the two yield stresses from the hardening rule in (3.34), $\bar{\sigma}_c\left(\bar{\epsilon}_c^{pl}\right)$ and $\bar{\sigma}_c\left(\bar{\epsilon}_t^{pl}\right)$.

$$B = \frac{\bar{\sigma}_c\left(\bar{\epsilon}_c^{pl}\right)}{\bar{\sigma}_t\left(\bar{\epsilon}_t^{pl}\right)}\left(1 - A\right) - \left(1 + A\right) \tag{3.71}$$

The compressive hardening function, similar to the hardening function in the Drucker-Prager model in the previous section, is also approximated using the Barcelona model as shown in Figure 3.4. The same parameterization scheme is also used to write α and β in terms of the peak compressive yield strength, σ_c^p, and the plastic strain at the peak compressive yield strength, ϵ_c^{pp}:

$$\beta = \frac{\ln\left[\frac{2\alpha}{1+\alpha}\right]}{\epsilon_c^{in}} \tag{3.72}$$

$$\alpha = \frac{2\sigma_c^p - \sigma_c^{iy} + 2\sqrt{-\sigma_c^p\left(\sigma_c^{iy} - \sigma_c^p\right)}}{\sigma_c^{iy}} \tag{3.73}$$

The tensile hardening rule has a fundamentally different behavior than the compressive hardening rule, and was therefore approximated using an exponential function (Fig 3.5). The exponential function required only two parameters to characterize the curve completely. The first parameter was the initial tensile yield stress, σ_t^{iy}, which defines the y-intercept of the curve, while the second parameter was the tensile yield stress decay parameter,λ.

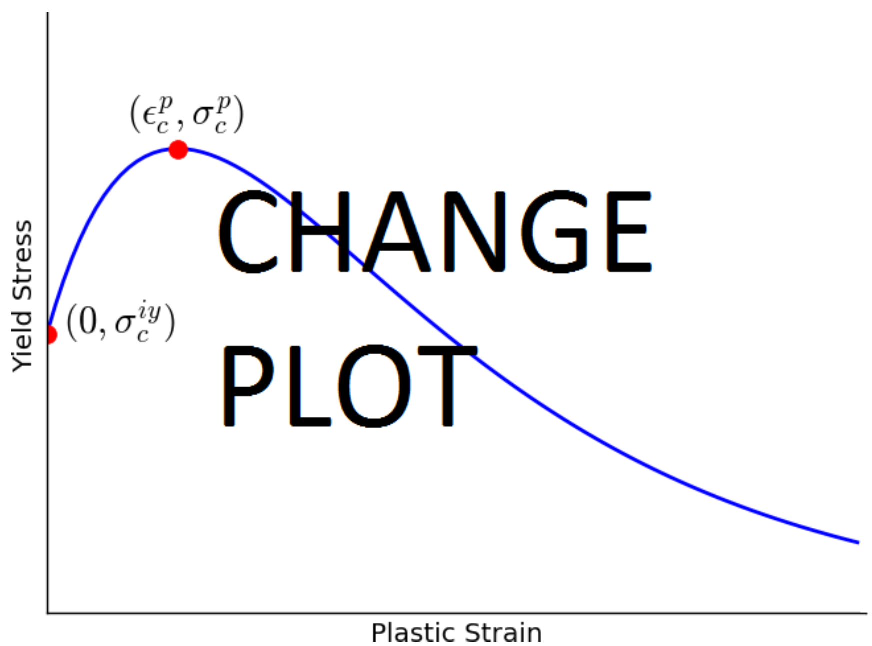

Figure 3.5: Tensile hardening/sofening function. The curve is able to be parameterized using two parameters.

In addition to the hardening rules, the damage evolution equations are also parameterized. The compressive damage, D_c, is assumed to be a linear function of the inelastic strain through a compressive damage rate parameter, m:

$$D_c\left(\bar{\epsilon}^{in}\right) = \bar{\epsilon}^{in} m \tag{3.74}$$

The tensile damage (D_t) evolution is slightly less trivial, but can also be characterized by a single parameter due to some constraints imposed on the function by the nature of the damage parameter. In tension, the damage evolution curve starts at the origin and asymptotically approaches $D_t = 1$ as $\bar{\epsilon}^{ck} \rightarrow \infty$. As such, under this functional assumption, the only parameter required to describe this relationship is the tensile damage rate parameter, n:

$$D_t\left(\bar{\epsilon}^{ck}\right) = 1 - \frac{1}{\left(1 + \bar{\epsilon}^{ck}\right)^n} \tag{3.75}$$

Sample damage evolution curves for both tension and compression are illustrated in Fig 3.6, where one can see that the rate at which the tensile damage evolves is far larger than the rate at which the compressive damage evolves. The combination of the elastic parameters, the hardening rule parameters, and the damage evolution parameters, yield a total of nine parameters that must be identified by experiments or through up-scaling to define the behavior of CDM model.

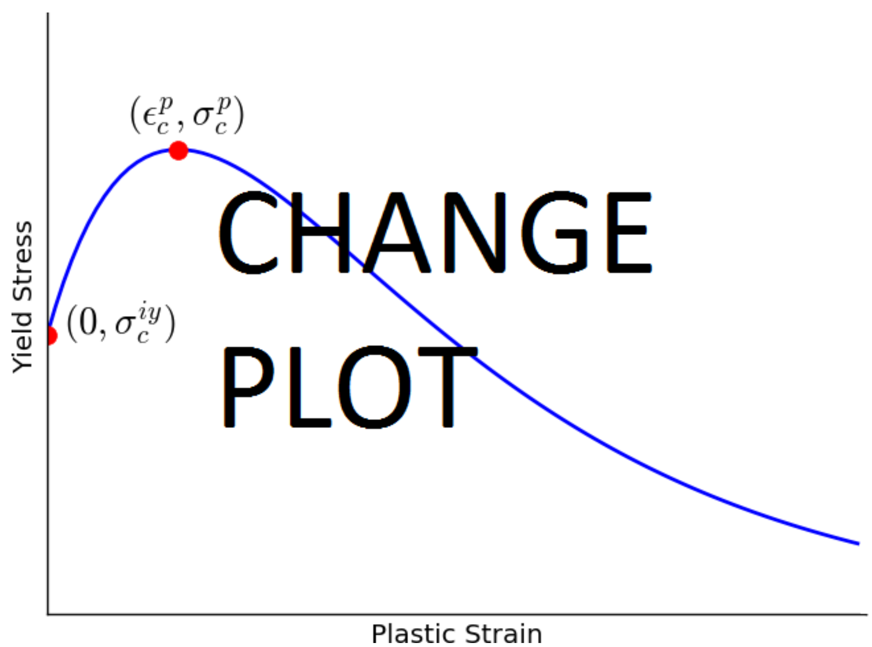

Figure 3.6: Tensile and compressive damage evolution curves.

At this point, there are some parameter constraints for the damage evolution that need to be considered for numerical stability. In this model, The damage curves are specified in terms of inelastic strain and cracking strain which need to be converted into plastic strain for the analysis. The inelastic and cracking strains represent the same strain component but refer to compression and tension respectively. This inelastic/cracking strain can be considered as the theoretical plastic strain given that the material is in an undamaged state. The conversion from inelastic/cracking strain to plastic strain is a function of the damaged state at every increment and can be expressed as:

$$\bar{\epsilon}_c^{pl} = \bar{\epsilon}^{in} - \frac{D_c}{1 - D_c} \frac{\sigma_c^{iy}}{E} \tag{3.76}$$

$$\bar{\epsilon}_t^{pl} = \bar{\epsilon}^{ck} - \frac{D_t}{1 - D_t} \frac{\sigma_t^{iy}}{E} \tag{3.77}$$

The numerical issues with this formulation arise due to the fact that it is very possible for the converted plastic strain to not be monotonically increasing with respect to the tensile damage. By having a damage evolution curve with a sufficiently steep slope, such that the second term in equation 3.76 increases faster than the first term, it becomes mathematically possible to have decreasing and/or negative plastic strains in the damage evolution definition. As such, the following conditions is applied to constrain the damage evolution to always yield monotonically increasing plastic strains as damage increases:

$$\frac{d\bar{\epsilon}_c^{pl}}{dD_c} > 0 \tag{3.78}$$

$$\frac{d\bar{\epsilon}_t^{pl}}{dD_t} > 0 \tag{3.79}$$

For the compressive damage evolution, we can substitute (3.74) into (3.76) to get the following expression of plastic strain as a function of the compressive damage rate parameter:

$$\bar{\epsilon}_c^{pl} = \bar{\epsilon}^{in} - \frac{D_c}{1 - D_c} \frac{\sigma_c^{iy}}{E} \tag{3.80}$$

Combining (3.80) and (3.78) yields the following expression governing the stability limit for the compressive damage rate parameter:

$$m < \frac{\sigma_c^{iy} + 2E\bar{\epsilon}^{in} - \sqrt{\sigma_c^{iy}\left(\sigma_c^{iy} + 4E\bar{\epsilon}^{in}\right)}}{2E\left(\bar{\epsilon}^{in}\right)^2} \tag{3.81}$$

However, since this upper bound for m is functional on several of the parameterization parameters, which are not constant, the upper bound varies depending on the other input parameters. Because of this, a compressive damage scaling factor, d_c, is introduced. In addition, the upper bound for m is dependent on the inelastic strain which is not constant throughout the model. Since only one value of m can be specified for a given simulation, the chosen value of m should be the smallest value over the range of the expected inelastic strain experienced. As can be seen from (3.81), as $\bar{\epsilon}^{in} \to \infty$, $m \to 0$ such that for very large inelastic strains the conversion to plastic strain becomes very unstable. Thus, the compressive damage rate parameter can be written as:

$$m = d_c \min_{\bar{\epsilon}^{in}} \left\{ \frac{\sigma_c^{iy} + 2E\bar{\epsilon}^{in} - \sqrt{\sigma_c^{iy}\left(\sigma_c^{iy} + 4E\bar{\epsilon}^{in}\right)}}{2E\left(\bar{\epsilon}^{in}\right)^2} \right\} \tag{3.82}$$

Where the compressive damage scaling factor has the following limits:

$$0 < d_c < 1 \tag{3.83}$$

The tensile damage evolution curve has the same numerical constraints when converting form cracking strain to plastic strain. Substituting (3.75) into (3.76) yields the following expression for the plastic strain:

$$\bar{\epsilon}_t^{pl} = \bar{\epsilon}^{ck} - \left[\left(1 + \bar{\epsilon}^{ck}\right)^n - 1\right] \frac{\sigma_t^{iy}}{E} \tag{3.84}$$

Solving for n with (3.78) and (3.84) yields the following inequality governing the upper bound of the tensile damage rate parameter:

$$n < \frac{W\left(\frac{E\left(\bar{\epsilon}^{ck}+1\right)}{\sigma_t^{iy}} \ln\left(\bar{\epsilon}^{ck} + 1\right)\right)}{\ln\left(\bar{\epsilon}^{ck} + 1\right)} \tag{3.85}$$

Where $W(x)$ is the Lambert W function defined implicitly as Corless et al. [1996]:

$$x = W(x)\, e^{W(x)} \tag{3.86}$$

Using the same methodology as was used to derive (3.82) in compression, the tensile damage scaling factor can be written as:

$$n = d_t \min_{\bar{\epsilon}^{ck}} \left\{ \frac{W\left(\frac{E\left(\bar{\epsilon}^{ck}+1\right)}{\sigma_t^{iy}} \ln\left(\bar{\epsilon}^{ck}+1\right) \right)}{\ln\left(\bar{\epsilon}^{ck}+1\right)} \right\} \tag{3.87}$$

where the tensile damage scaling factor has the following limits:

$$0 < d_t < 1 \tag{3.88}$$

The goal of the parameter estimation module, is therefore to estimate the 11 parameters $\boldsymbol{\chi} = \{E, \nu, \psi, K_c, \phi, \varepsilon, \sigma_c^{iy}, \sigma_c^{p}, \epsilon_c^{p}, d_c, d_t\}$, which are summarized in Table 3.2.

Table 3.2: Parameters for Damage-Plasticity Model for Quasi-Brittle Materials

Parameter Type		Name	Symbol
Elastic		Young's Modulus	E
		Poisson's Ratio	ν
Plastic	Flow Rule	Dilation Angle	ψ
		Flow Eccentricity	ε
	Yield Function	Second Stress Invariant Ratio	K_c
		Initial Equibiaxial Stress Ratio	f_0
	Hardening Rule	Initial Compressive Yield Strength	σ_c^{iy}
		Peak Compressive Yield Strength	σ_c^{p}
		Strain at Peak Compressive Yield	ϵ_c^{p}
Damage	Compressive	Compressive Damage Scaling Factor	d_c
	Tensile	Tensile Damage Scaling Factor	d_t

Chapter 4

Software Implementation (MAUSE)

The Modular Automated Up-Scaling softwarE (MAUSE) for DEM simulations was created and written in Python^{TM} to provide an implementation of the up-scaling framework presented in the previous chapter using third-party software. The software itself aims to provide a platform through which the four software elements of the up-scaling framework can communicate with each other. The communication is facilitated by MAUSE through modules which wrap the third party software in such a way that the inputs and outputs to and from the modules are in a consistent structure regardless of the third party software being used.

The general idea with the up-scaling framework developed in this thesis is that it is model independant. Because of this, it is important that MAUSE was written in such a way that allowed for different models (both DEM and macroscale) to be implemented without rewriting the up-scaling algorithms. As such, a modular approach was taken such that each module is isolated from the others and only communicates data through strict protocols set out by MAUSE.

There exists four base classes that are used as parents to the third-party software modules. Because each software compent has distinct I/O protocols, the base classes serve as a collection of usefull methods which the software module can inherit to ensure compatibility with MAUSE. Each of these four component base classes inherit from a base module class. Figure 4.1 indicates this class heirarchy as well as where each method and attribute definition falls in the heirarchy.

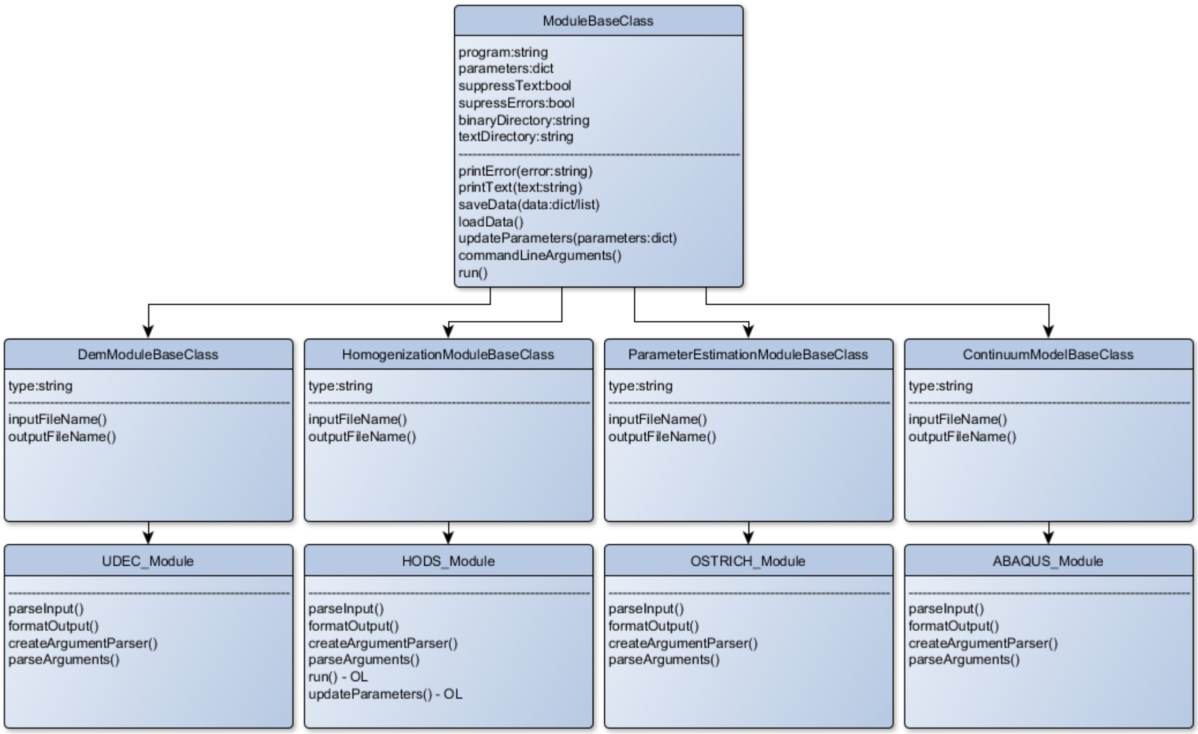

Figure 4.1: Module class structure.

4.1 Base Module Class

A base module class, **BaseModuleClass**, is implemented to provide a framework containing required methods and attributes for the MAUSE modules to inherit. The module class contains methods pertaining to I/O routines associated with the module so that each module that is written behaves in a consistent manner and to avoid reimplementation of certain methods.

4.1.1 Attributes

Attributes are assigned to **BaseModuleClass** through the constructor method (**__init__**) when the class is initialized. The following attributes are passed as arguments through instantiation of the class children.

The **program** attribute is a string that contains the name of the software excecutable associated with the given module. This parmeter allows the module the capacity to run the program through a command line interface (CLI) As such, the program must be able to accept command line arguments.

```
#String containing name of module software executable file.
self.program = program
```

The **parameters** attribute is a dictionary that contains all the command line parameters and corresponding arguments. Here, the parameters are the dictionary keys and the arguments are the dictionary values. If no arguments are required, then an empty dictionary is acceptable aswell.

```
#Dictionary of command line parameters and corresponding
    arguments
self.parameters = parameters
```

The **supressText** and **supressErrors** attributes are Boolean parameters that, when true, allow for the suppression of command line output of text and errors, respectively.

```
#Boolean parameter that allows text output to CMD to be supressed
self.suppressText = suppressText

#Boolean parameter that allows errors to be supressed
self.suppressErrors = suppressErrors
```

The **binaryDirectory** and **textDirectory** attributes are strings that refer to file folders in which the binary and text data are to be saved, respectively. these values are determined through relative directory parsing, rather than as an initialization argument.

```
#String that indicates where to store the binary data
self.binaryDirectory = os.path.join(dataDirectory, 'Binary')

#String that indicates where to store the text data
self.textDirectory = os.path.join(dataDirectory, 'Text')
```

4.1.2 Defined Methods

Methods in **BaseModuleClass** are divided into two types: defined and undefined. Defined methods are methods that are common to all the module classes and are thus able to be defined at the parent level. The undefined methods are methods that require overloading, so they are defined at the child level.

The **__init__** method is a built-in contructor method that is automatically called when the class is initialized. The only required argument for this method is **parameter**, with the other three being optional arguments.

```
#Contructor method that is called when the class is initialized
def __init__(self, program, parameters={}, suppressText=False,
   suppressErrors=True):
        """
        program:        string of program name
        parameters:     dictionary of parameter argument pairs
        suppressText:   boolean
        suppressErrors: boolean
        """
```

A series of printing methods are included in **BaseModuleClass** to allow each module to route command line output through the parent module for consistent output formatting. The **printText**, **printTitle**, **printSection**, **printStatus**, **printDone**, and **printErrors** methods are implemented to give a large degree of flexibility in the displayed output.

```
#Method to print text to command line if text supression is off
def printText(self, text):
        """
        text:           string of text to print
        """

#Method to format primary title in command line output
def printTitle(self, title):
        """
        title:          string of primary title to print
        """

#Method to format section title in command line output
def printSection(self, section):
        """
        section:        string of section title to print
        """
```

```
#Method to format status update in command line output
def printStatus(self, status):
        """
        status:         string of status to print
        """

#Method to print 'Done' when section is finished
def printDone(self):
        """
        """

#Method to control and print errors if error supression is off
def printErrors(self, error):
        """
        error:          error to print
        """
```

The **saveData** and **loadData** methods use binary serialization methods to write and load specified data structures to and from file. Saving and loading serialized binary data is much faster and more compact than unicode.

```
#Method to save serialized data structures as output
def saveData(self, data):
        """
        data:           Data format specified by module type
        """

#Method to load serialized data structures as input
def loadData(self):
        """
        """
```

The **updateParameters** method allows for the dynamic updating of module input parameters. This allows for the module to run the program multiple times without being reinstantiated.

```
#Method that allows dynamic updating of parameters.
def updateParameters(self, parameters):
        """
```

```
        parameters:       dictionary of parameter argument pairs
        """
```

The **commandLineArguments** method takes the **parameters** dictionary attribute and converts it to a string which can be passed to the command line when running the specified program.

```
#Method to create a string of command line arguments from
    parameters
def commandLineArguments(self):
        """
        """
```

The **run** method simply runs the specified program with the specified parameters.

```
#method to run the program with the specified parameters
def run(self):
        """
        """
```

4.1.3 Undefined Methods

The undefined methods listed here are required to be defined in the child classes. These methods are different for each type of module or even each module implementation, which does not allow them to be written in **baseModuleClass**.

The **createArgumentParser** method creates an argument parser that allows the module to parse any command line arguments passed to it if the module is run in an isolated environment, While the **parseArguments** method parses the command line arguments derived from **createArgumentParser**.

```
def createArgumentParser(self):

def parseArguments(self):
```

The **inputFileName** and **outputFileName** methods provide the formatting for the fileNames in a means that is consistent amongst modules.

```python
def inputFileName(self):

def outputFileName(self):
```

4.2 DEM Module

***

4.2.1 Base DEM Module Class

***

4.2.2 UDEC Module

***

4.3 Homogenization Module

***

4.3.1 Base Homogenization Module Class

***

4.3.2 HODS Module

***

4.4 Parameter Estimation Module

***

4.4.1 Base Parameter Estimation Module Class

***

4.4.2 OSTRICH Module

***

4.5 Macroscale Module

***

4.5.1 Base Macroscale Module Class

***

4.5.2 ABAQUS Module

***

4.6 Data Architechture

This section aims to explain the data structures used to store and transfer data between the modules in the up-scaling framework presented in this thesis. Three fundamental data structures are used for the storage of data in conjunction with each other: hash tables, lists, and arrays. Using these three structures, three distinct types of data in the up-scaling framework are used to transfer between the modules in a consistent manner: constitutive parameters, DEM data, and continuum data.

Python Lists

The list in Python^{TM} is one of the most versatile data structures. The list treats the data as a sequence such that each element in the list is assigned a number referring to its position or index. The implementation of the list structure in python contains a number of unique features. The main feature of python lists is that the elements within the lists are not required to be of the same data type. Additionally, these lists are mutable, allowing for more advanced manipulation of the data structure. Because of this flexibility, the list structure is slow and unsuitable for large data sets.

Numpy Arrays

Numpy arrays are a specific implementation of a python list which are optimized for numerical operations on large datasets. Here the numpy arrays are much more compact by using a sequence of uniform values, rather than a sequence of pointers as is the case for the list structure.

Python Dictionaries (Hash Tables)

In general, a hash table is a data structure that maps keys to values. The implementation of hash tables in Python^{TM}, are referred to as dictionaries. Similar to a python list, a python dictionary is a mutable structure that does not require the elements to be of the same type. However, instead of accessing the element value through an index argument, the data is accessed through a key argument. This unordered structure is usefull for storing non-sequential data.

4.6.1 Data Storage Structures

Hash Tables for Constitutive Parameters

Constitutive parameters are required as an input to the DEM and macroscale modules as well as an output from the parameter estimation module. Here, the constutive parameters are always stored in a Python^{TM} dictionary with the constitutive parameter name as the key. To access the value of a specific constitutive parameter in a dictionary named 'constitutiveParameters', the string corresponding to the

```
parameterValue = constitutiveParameters[parameterName]
```

For example, accessing the value of the elastic modulus from a hash table named 'contitutiveParameters' is performed as follows:

```
elasticModulus = constitutiveParameters['elasticModulus']
```

Nested Hash Tables for DEM Data

The raw DEM Data is considered to be comprised of six distinct types: block data, contact data, corner data, domain data, grid point data, and zone data. Here, each block, contact, corner, domain, grid point, and zone is assigned a unique 7 digit numeric identifier (assuming here that the number of components in the system does not exceed 10 million) by which the associated data can be accessed. The same identifier may be repeated for different data types.

To allow for convenient access to the data, the DEM data is stored in six distinct nested hash tables corresponding to each of the DEM data types. Each DEM data hash table has three levels of nesting. The first level keys are the simulation times, which returns the second level of hash tables. The second level keys are the component identifiers, which returns a third level hash table. In this third level, the component attirbutes can be accessed using the attirbute name as the key. In general, accessing an attribute of a specific component with a given ID at a specific time from a hash table called demDataHash is done as follows:

```
componentAttributeValue = demDataHash[time][ID][attribute]
```

For example, accessing the list of grid points associatied with block ID 2543465 at a simulation time of 1 is performed as follows:

```
gridPoints = blockData[1.0][2543465]['gridPoints']
```

The keys of each of the third level dictionaries for each comonent are presented in Table 4.1, Table 4.2, Table 4.3, Table 4.4, Table 4.5, and Table 4.6 for the block data, contact data, corner data, domain data, gridpoint data, and zone data, respectively.

Table 4.1: Block data attributes in third level hash

Parameter	Description (Data Type)
x	X coordinate of block centroid (float)
y	Y coordinate of block centroid (float)
xForce	Resultant forces at block centroid (float)
yForce	Resultant forces at block centroid (float)
corners	Corners associated with this block (list of corner IDs)
zones	Zones associated with this block (list of zone IDs)
gridPoints	Grid points associated with this block (list of corner IDs)

Table 4.2: Contact data attributes in third level hash

Parameter	Description (Data Type)
x	X coordinate of contact point (float)
y	Y coordinate of contact point (float)
length	Length associated with contact point (float)
flowRate	Fluid flow rate through contact (float)
nForce	Resultant normal force on contact (float)
sForce	Resultant shear force on contact (float)
xCosine	X component of contact normal cosine (float)
yCosine	Y component of contact normal cosine (float)
blocks	Blocks associated with this contact (list of block IDs)
domains	Domains associated with this contact (list of domain IDs)
corners	Corners associated with this contact (list of corner IDs)

Table 4.3: Corner data attributes in third level hash

Parameter	Description (Data Type)
gridPoint	Grid points associated with this corner (list of grid point IDs)

Nested List of Arrays for Continuum Data

4.6.2 Binary Serialization

4.7 HODS Homogenization

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Table 4.4: Domain data attributes in third level hash

Parameter	Description (Data Type)
x	X coordinate of domain centroid (float)
y	Y coordinate of domain centroid (float)
area	Area of domain (float)
porePressure	Average pore pressure in the domain (float)

Table 4.5: Gridpoint data attributes in third level hash

Parameter	Description (Data Type)
x	X coordinate of grid point (float)
y	Y coordinate of grid point (float)
xDisp	X displacement of grid point (float)
yDisp	Y displacement of grid point (float)
xForce	Resultant X force on grid point (float)
yForce	Resultant Y force on grid point (float)
xVel	X velocity of grid point (float)
yVel	Y velocity of grid point (float)
block	Block associated with this grid point (block ID)
corner	Corner associated with this grid point (corner ID)

Table 4.6: My caption

Parameter	Description (Data Type)
S11	X component of stress in the zone (float)
S22	Y component of stress in the zone (float)
S12	Corresponding shear stress in the zone (float)
block	Block associated with this zone (block ID)
gridPoints	Grid points associated with this grid point (list of block IDs)

4.7.1 Class Attributes

***

4.7.2 Class Boundary Methods

***

4.7.3 Class Manipulation Methods

***

4.7.4 Class Homogenization Methods

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4.8 MAUSE Usage Examples

***

Chapter 5

Verification and Application

In this section, two-dimensional DEM models are used to demonstrate the effectiveness of the up-scaling methodology. While the results presented leave a positive impression, future verification using three-dimensional models is desirable. The framework is validated using three tests: 1) The homogenized stress and strain behaviour obtained from the DEM microscale response are compared to that of the macroscale response. This test verifies the effectiveness of the parameter estimation module and the ability of the chosen macroscale constitutive model to capture the salient features of NFR behaviour. 2) The homogenization and parameter estimation algorithms are rerun using the same data, but with different REV sizes to investigate the REV size effect has on the resultant parameter set. 3) Slope stability analyses carried out by both Direct Numerical Simulations (DNS) with a DEM model and with an up-scaled macroscale model are compared. This last test verifies the whole up-scaling methodology.

The up-scaling is conducted by running a series of four quasi-static DEM 'triaxial' compression tests under different confining stresses. These are not true triaxial tests as simulations are in 2D, but illustrate the method regardless. Algorithms are rerun using different REV sizes to determine an appropriate REV size. In a macroscopically homogenous domain, as the REV size increases, the parameter values will converge to a single value, when the REV is too small, local heterogeneities induce a variance into the optimal parameter set.

5.1 DEM Simulations

The DEM models used consist of a pseudo-random isotropic fracture network defined by a Voronoi tessellation. The average block size is specified to be 0.5m using 20 iterations of

Lloyd's method [Lloyd, 1982] in order to achieve an even size distribution. A 10m x 10m domain was determined to be sufficiently large to represent the rock mass behaviour as an REV.

A Mohr-Coulomb plasticity model was used as the constitutive model to describe the plastic behaviour of the intact (deformable blocks) and the joint (natural fracture) behaviour was governed by a Coulomb area slip model. The parameters for the rock and joints summarized in Table 5.1 are representative of a fractured granitic rock mass. The joints are relatively weak compared to the blocks, so the blocks behave mostly elastically.

Table 5.1: Rock and joint properties for DEM Simulations

Property Type	**Property**	**Value**
Rock	Young's Modulus	$65GPa$
	Poisson's Ratio	0.2
	Density	$2.7g/cm^3$
	Friction Angle	51°
	DilationAngle	0°
	Cohesion	$55.1MPa$
	Tensile Strength	$11.7MPa$
Joint	Friction Angle	32°
	Dilation Angle	5°
	Cohesion	$100kPa$
	Tensile Strength	$100kPa$
	Normal Stiffness	$10GPa/m$
	Shear Stiffness	$1GPa/m$

The blocks are meshed with linear three-node triangular plane strain finite difference elements with an average side length of 0.5m. This discretization yielded 5-10 zones within each block. A rounding length of 10% of the average block edge length (0.05m) is applied to the blocks to prevent numerical instabilities in the contact algorithm. Quasi-static analysis is obtained through dynamic relaxation, in which the dynamic equations are integrated in time using velocity-proportional viscous damping and mass scaling. State data of the model is collected at 50 evenly spaced intervals.

The quasi-static loading of the DEM simulations is intended to imitate triaxial laboratory tests, so a constant confining stress was applied on the lateral boundaries of the DEM model. Loading is achieved by applying vertical displacements to the top boundary while fixing the bottom boundary, compressing the model to a vertical strain of 5% for four confining horizontal stresses: $0.5MPa$, $1MPa$, $2MPa$, and $4MPa$. These load paths capture key physical phenomena including the pressure dependent yield of the NFR, hardening, and the dependence of damage initiation on the triaxiality.

5.2 Verification of the Parameter Estimation Module

Using a PSO algorithm followed by an LMA optimization, the Drucker-Prager plasticity model with ductile damage is then fitted to the homogenized DEM simulation data in order to obtain an optimal parameter set. Each simulation is fit to 50 points defining the homogenized stress-strain curve resulting in a total of 200 data points for all four DEM simulations at different confining stresses. The PSO algorithm uses a swarm size of 24 for 100 generations which is found to be sufficient to converge to a consistent solution.

Here, the CDM model is confined laterally by the homogenized horizontal DEM stress and vertical displacements are prescribed by the homogenized vertical DEM strain with the parameter estimation algorithms programmed to match the horizontal strain and the veritcal stress. Because of the large variation in observation magnitudes (between stress/strain and from different confining stresses), each curve is weighted with a normalization factor to prevent the large stress values from dominating parameter estimation. In addition, a linear weighting scheme is applied to each curve to give larger influence to the loading section and lesser influence to the post-damage section.

Parameter bounding limits are required by the optimization algorithms in order to limit the search space. These limits are chosen based on two criteria: physical limitations and numerical stability. If there exist physical limitations that prevent parameters from exceeding certain values or if there exists a range of realistic values that the parameter should not deviate from, then those physical limitations are specified as the bounds. In other cases, the parameter bounds come from numerical limitations such that beyond a certain capacity, certain parameter values would cause the simulations to become unstable. In these cases, a combination of the two bounding methods is used. The specified bounding limits for each parameter results can be seen in Table 5.2.

The stress-strain curves from the DEM simulations used for the parameter estimation and the stress-strain curves of the CDM simulations using the optimal parameter set are presented in Figure 5.1. The CDM fit is good with a Root-Mean-Square Error (RMSE) of $1.03MPa$ and the pressure dependent yield function works well with this model as the error is not biased to curves of a certain confining stress. This fit implies a strong likelihood

Table 5.2: Parameter estimation results for Drucker-Prager model with ductile damage

Parameter	Symbol	Units	Lower Bound	Upper Bound	Optimum
Young's Modulus	E	GPa	1	25	1.8
Poisson's Ratio	ν		0.1	0.4	0.15
Dilation Angle	ψ	$\circ$	5	15	22
Flow Stress Ratio	K		0.78	1	0.81
Friction Angle	β	$\circ$	45	60	56
Initial Compressive Yield Strength	σ_c^{iy}	kPa	1	100	52
Peak Compressive Yield Strength	σ_c^p	MPa	0.5	5	3.1
Strain at Peak Compressive Yield	ϵ_c^p	%	0.5	5	1.7
Yield Strain at -0.5 Triaxiality	$\bar{\epsilon}_{f-0.5}^{pl}$	%	0.01	0.1	0.0078
Yield Strain at -0.6 Triaxiality	$\bar{\epsilon}_{f-0.6}^{pl}$	%	0.1	10	0.30
Plastic Displacement at Failure	$\bar{u}_f^{pl}$	m	0.01	1	0.12

that the model will be valid under confining stresses outside of the range fitted. Also, the damage initiation points at the peak of the curve are well correlated and indicate that the triaxiality based damage initiation criterion is a good model for this problem. The majority of the error in the curves is found in the post-yield behaviour. This error results from limitations in the continuum constitutive model because the post-yield behaviour of the DEM simulations is discontinuous in nature (stick-slip response). The CDM model cannot accommodate for such oscillations and thus represents the post-yield response as an average.

The optimal parameter set in Table 5.2 represents the constitutive response of the rock mass. As expected, the elastic modulus of the rock mass ($1.9GPa$) is substantially less than the elastic modulus of the intact rock ($65GPA$) because of yielding in the joints. Additionally, Poisson's ratio of the rock mass (0.15) is less than Poisson's ratio of the intact rock (0.2) because of the compliance of the joints before yield, which limits the lateral strain. After yielding however, substantial lateral strain is observed because of dilation of the joints, resulting in a large dilation angle (22°). This dilation response of the rock mass is larger than the the prescribed joint dilation (5°) because of block rotation and geometry.

There are additional minor sources of error from the homogenization algorithms that do not manifest themselves in this fitted relationship. In addition, if the REV is too small, it introduces it's error in the DEM data rather than in the fitted response. Furthermore, the

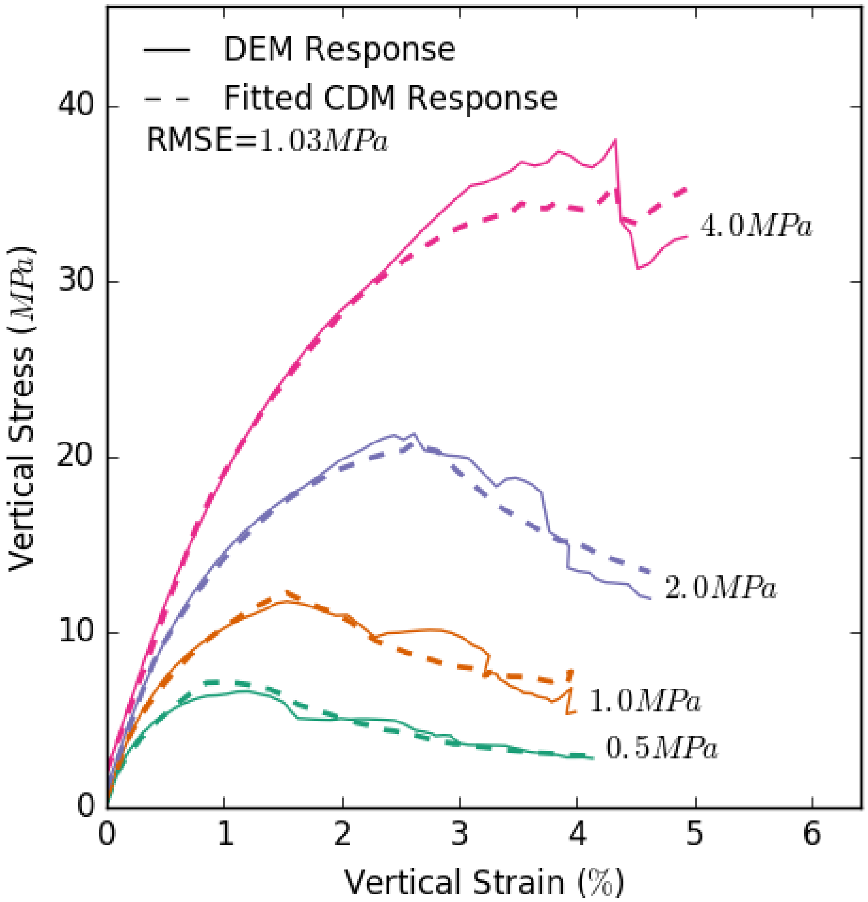

Figure 5.1: Axial Stress-Strain curves of the monotonically loaded DEM simulations used for estimating the CDM parameter set under different confining stresses.

global fitting algorithms are not completely exhaustive, so it is possible they do not find the actual globally optimal parameter set, potentially leading to some error. With the given PSO parameters, up to 2400 sets of simulations are conducted for the global parameter estimation, and successive fitting operations tend to give results within 1% deviation. This consistency and large search domain give confidence that the estimated parameter set is the globally optimal set.

In addition to the loading response under the specified confining stresses, DEM simulations under confining stresses of $3MPa$, $6MPa$, $8MPa$ and $10MPa$ are compared to the the CDM model using the previously estimated parameter set to see how well the constitutive behaviour is captured (Figure 5.2). These simulations demonstrate the interpolative

($3MPa$) and extrapolative ($6MPa$, $8MPa$ and $10MPa$) capacity of the fitted parameter set, and indeed a strong fit is obtained (RMSE of $2.83MPa$) for all confining stresses, with the error being more prominent for larger degrees of strain.

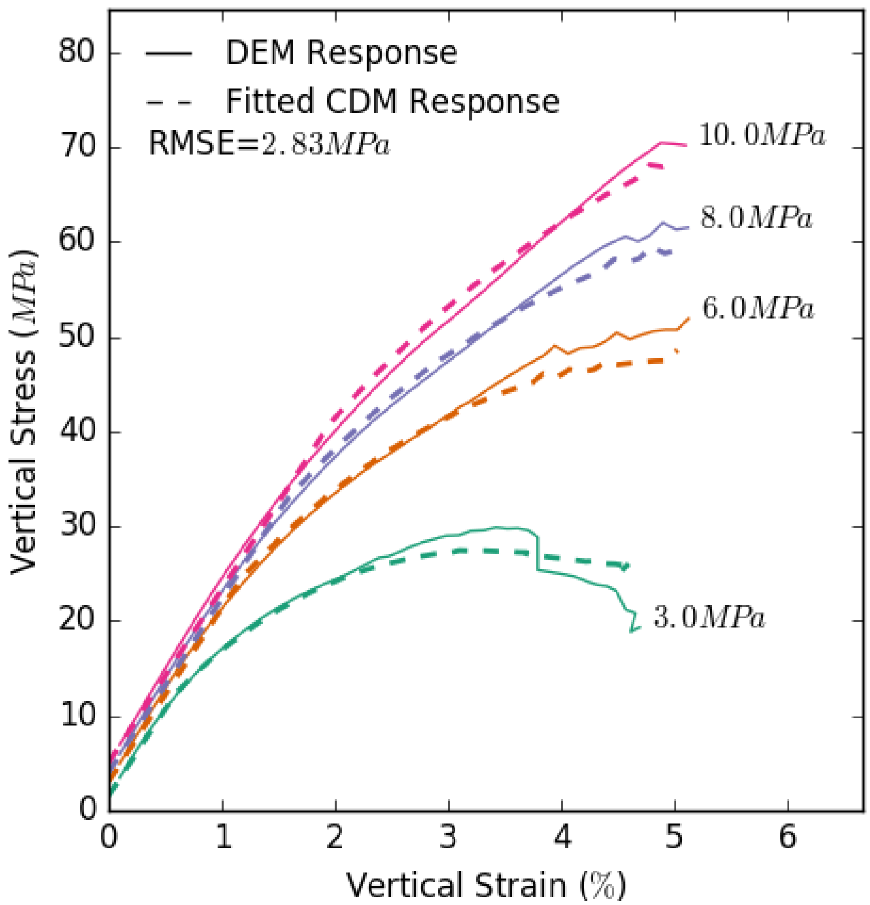

Figure 5.2: Axial Stress-Strain curves of the verification simulations for the fractured granite rock mass under different confining stresses for both the DEM simulations and the fitted CDM simulations.

5.3 Comparison of CDM Constitutive Models

5.4 Impact of REV Size on Estimated Parameters

The appropriateness of the REV size was tested using eight different sample REV radii and running the homogenization and parameter estimation algorithms for each. The assumed REV radius for the parameter estimation simulations is $4m$, which corresponds to a homogenization area of $57.7m^2$. To validate this assumption, the REV radii is sampled at $0.5m$ intervals to see where the resultant parameters converge.

The convergence of three of the 11 parameters is shown in Figure 5.3 as a function of REV size. The material parameters apparently converge at different sizes, illustrating part of the challenge in defining an REV; some parameters require a larger REV than others and it is not obvious *a priori* which parameters will dominate. For the granite rock mass considered, an REV of radius $3m$ or with a homogenization area of $34.8m^2$ is chosen to be the minimum size based on the convergence of the dilation angle - the last parameter to converge. The suitability of the assumed REV size is confirmed since it is larger than the minimum REV size determined by the convergence study.

5.5 Comparison to DNS - Application to Slope Stability Analysis

To validate the up-scaling methodology used, a simple 2-D slope problem is presented and loaded from the top until failure using both DEM and the up-scaled CDM model. Here, the resultant stress distribution are compared just as failure occurs.

In the DEM model, failure can be assessed based on the unbalanced forces in the model. Since the joints in the model have a stiffness and cohesion, when the slope fails, the explicit quasi-static solution becomes dynamic because of a sudden release of elastic energy and the inability of the applied damping to suppress it all. At this point, the total unbalanced forces in the model increase and the slope can be said to have failed.

For the CDM model, failure can be assessed based on non-convergence of the model when run as an implicit static simulation, which does not converge when the slope fails. The load step in which the CDM model fails to converge because the slope fails dynamically is considered the point of failure.

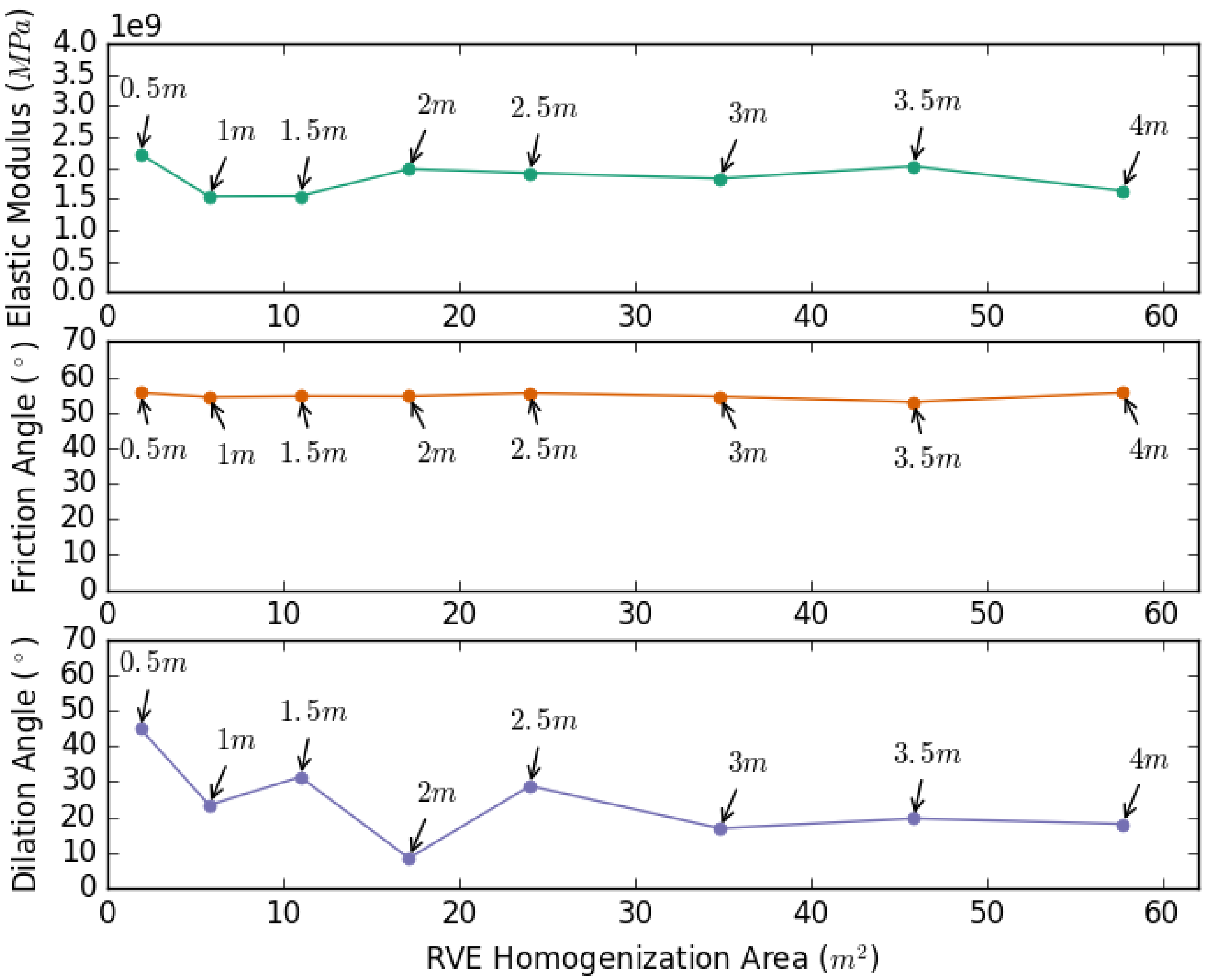

Figure 5.3: Convergence of three constitutive material parameters as the REV homogenization area is increased. Annotations indicate the specified radius of the circular REV.

5.5.1 Model Description

The plane-strain slope stability problem has a height of $50m$ and a depth of $80m$ with a $30m$ high slope with a grade of 300% (Figure 5.4). This geometry provides enough space for the failure mechanisms to occur with little influence from the boundaries. The lateral boundary conditions are zero displacement in the x-direction, and the bottom boundary conditions are zero displacement in the y-direction. The slope and top boundaries are free.

A uniformly distributed load was applied over a 5m section on the backslope in a linear incremental fashion until failure.

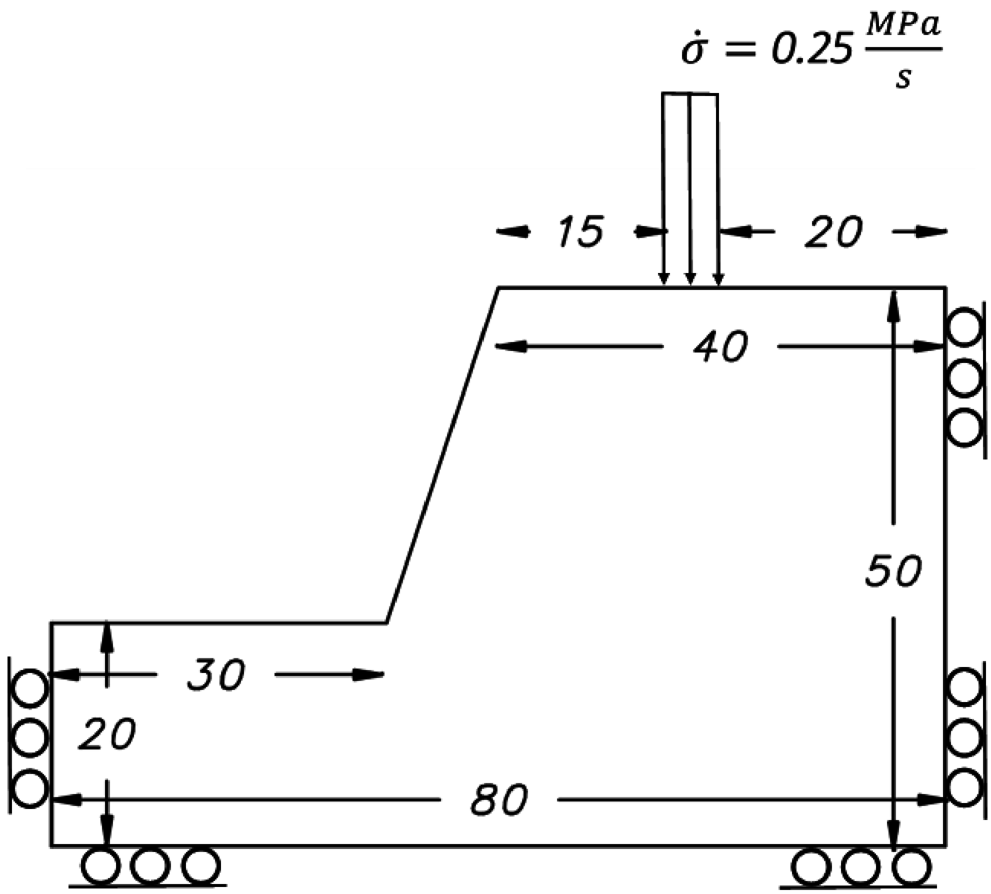

Figure 5.4: Schematic geometry and boundary conditions of the slope failure problem.

The meshing of the DEM simulations is identical to the REV simulations for the parameter estimation, while the CDM model is meshed using 4-node bilinear plane strain elements.

The models in both DEM and FEM are allowed to find a static equilibrium after the gravity force is applied, then a linearly increasing compressive stress along the top of the slope is applied until the slope fails. The load is increased from $0MPa$ to $25MPa$ over the course of $100s$ in the quasi-static/static simulations, knowing that the slope should fail long before $25MPa$ is reached.

5.5.2 DNS Comparison

A qualitative comparison of the DEM and the CDM model results uses the stress distribution and the surface deflection just before failure. For the DEM solution, since the stress field is discontinuous, the stress fields are smoothed using a cubic spline interpolation and subsequently run through a Gaussian filter with a standard deviation of 2 to reduce the noise in the data set. Figures 5.5, 5.6, and 5.7 show the horizontal stress distributions, the vertical stress distributions, and the shear stress distributions, respectively.

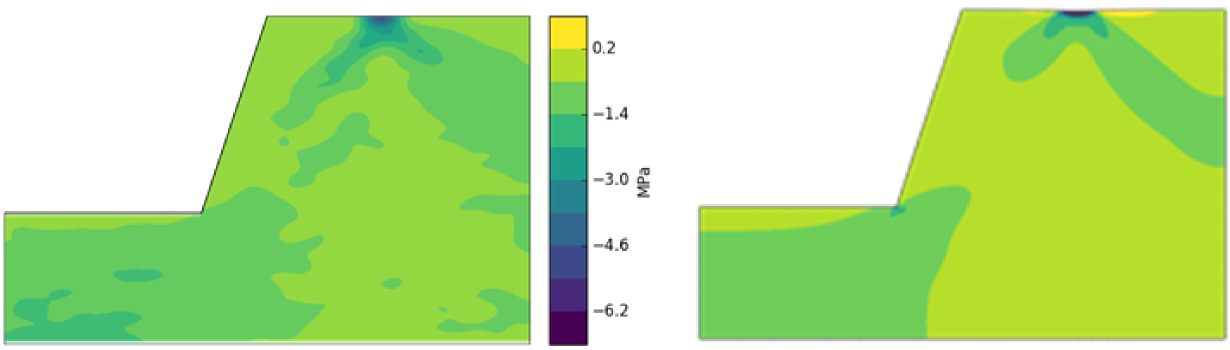

Figure 5.5: Comparison of DEM (left) and CDM (right) horizontal stress contours for the slope just before failure.

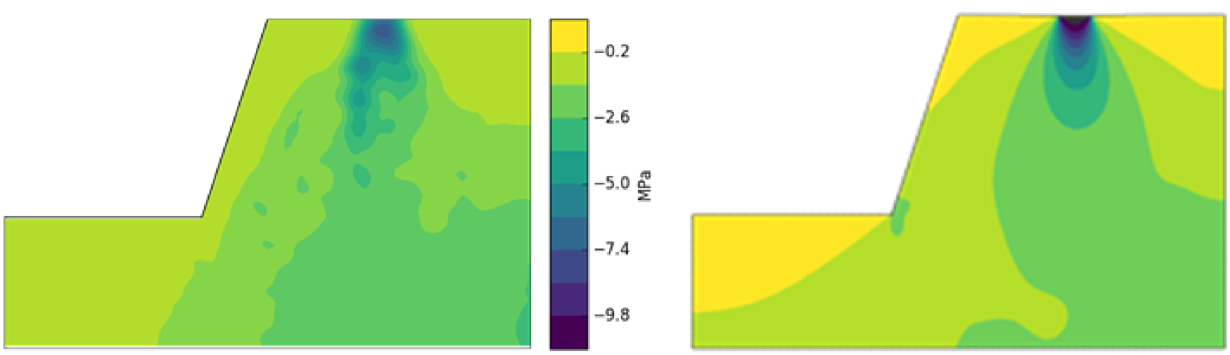

Figure 5.6: Comparison of DEM (left) and CDM (right) vertical stress contours for the slope just before failure.

The continuum approximation of the stress fields shows a good match to the smoothed DEM stress fields. More importantly, the load at failure for the two models are quite close. The DEM simulation failed at $11.2MPa$, while the CDM simulation failed at $11.5MPa$, a 3% error considered to be not only negligible in the context of geological uncertainty but

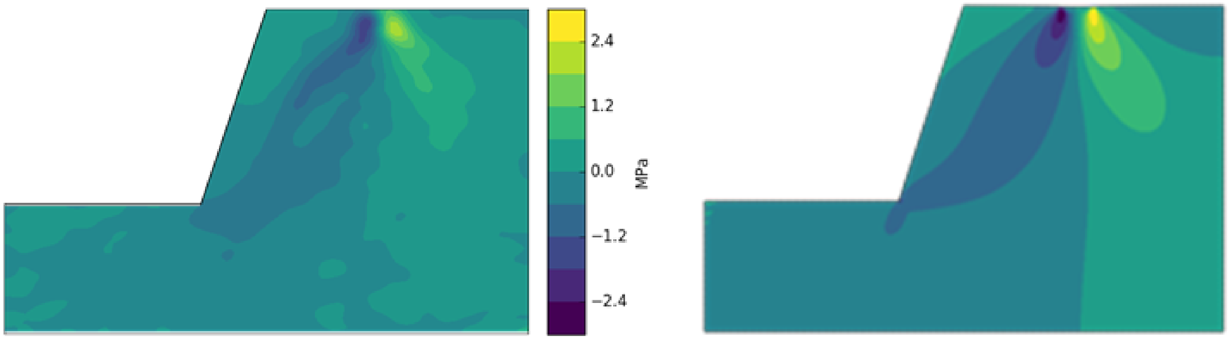

Figure 5.7: Comparison of DEM (left) and CDM (right) shear stress contours for the slope just before failure.

acceptable in terms of the computational savings. This agreement of the two models both in terms of the stress distribution and the failure load shows a high degree of success for the up-scaling framework.

An additional comparison of the surface deflection where the load was applied is presented in Figure 5.8. Again, the behaviour of the two models is similar, with downward displacement occurring where the load is applied, upwards displacement towards the slope on the left and negligible displacement towards the right model boundary. Some divergence from the DEM results can be observed in the CDM approximation where sharp changes in the profile gradient occur; this arises partly from CDM model limitations and partly because the scale of the deviation is similar to the REV scale, which is the limiting case. For larger scales, the error will be smaller.

5.5.3 Up-Scaling Computational Efficiency

The CDM model for this case requires about two orders of magnitude less computational effort than the DEM model (Table 5.3). The CDM simulation uses a comparable number of continuum elements $(29,866)$ as in the DEM simulation $(25,898)$ for comparison and adequate convergence. The CDM model efficiency can be improved by applying a Selectively Refined Mesh (SRM) where only the areas with stress concentrations and large stress gradients have a strongly refined mesh. With the SRM, a converged CDM solution is achievable with only $3,577$ elements leading to another order of magnitude reduction in computational effort.

The DEM simulation was run serially on a $2.2GHz$ CPU while the CDM simulation was run serially on a $1.8GHz$ CPU. Despite the CDM model having more continuum elements

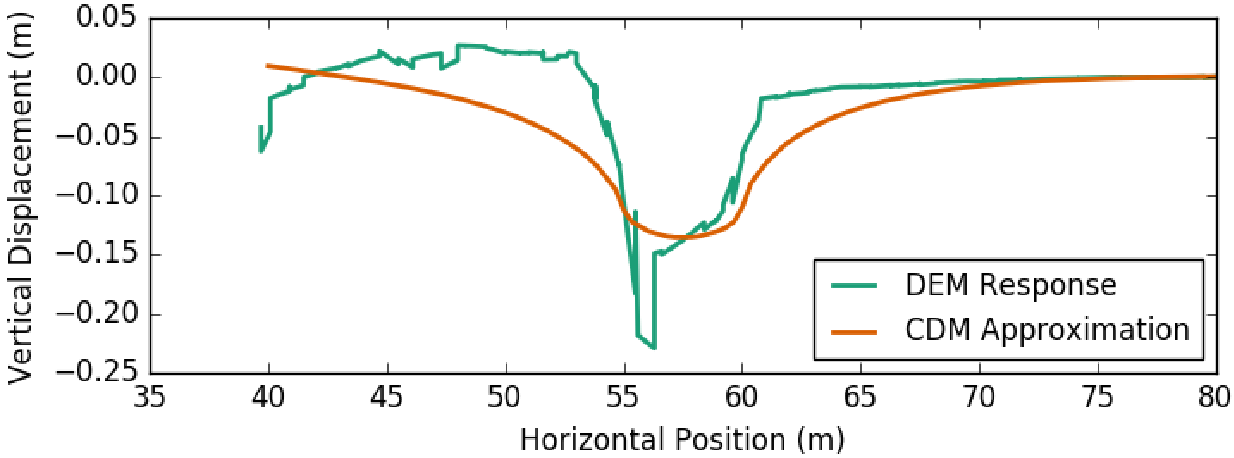

Figure 5.8: Comparison of DEM and CDM surface deflection profile for the slope just before failure.

Table 5.3: Comparison of Computational Time for the DNS

Simulation Type	**Continuum Elements**	**Processor Clock Speed**	**Slope Failure Load**	**Computational Time**
DEM	$25,898$	$2.20GHz$	$11.2MPa$	$46.5hr$
CDM	$29,866$	$1.80GHz$	$11.5MPa$	$0.65hr$
CDM - SRM	$3,577$	$1.80GHz$	$11.5MPa$	$0.013hr$

than the DEM model, and the CDM model running on a slower CPU, a decrease in computational time of the DEM simulation from $46.5hr$ to $0.65hr$ was observed. Running the CDM model with a SRM reduces the total computational time to $0.013hr$, or eight minutes instead of two days. This large increase in computational efficiency with marginal decrease in model accuracy can be immensely useful for large scale geomechanical problems in NFR.

Chapter 6

Conclusions and Future Considerations

A framework for up-scaling DEM simulations is presented in this article. Up-scaling is achieved by matching homogenized stress-strain curves from REV-scale DEM simulations to single element continuum models using PSO and LMA optimization algorithms. A Drucker-Prager plasticity model with ductile damage is implemented in the CDM model to empirically capture the effect of the degradation (damage) of the NFR as deformation takes place.

The Drucker-Prager model with ductile damage is shown to be a reasonable CDM model approach to represent NFR in a continuum context, including effects of pressure dependent yield and the triaxiality based damage initiation criterion. Compared to a full DEM simulation, the CDM model shows a good fit pre-damage, but is unable to emulate the subtle post-yield oscillations arising from non-continuous yielding in the NFR.

Most importantly, with this up-scaling framework, very comparable results ($< 5\%$ error) to full DEM solutions can be obtained with the CDM method but with two to three orders of magnitude less computational time.

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