NUMERICAL AND ANALYTICAL VERIFICATION OF A MULTISCALE COMPUTATIONAL MODEL FOR IMPACT PROBLEMS IN HETEROGENEOUS VISCOELASTIC MATERIALS WITH EVOLVING DAMAGE

Bruno Bachiega Araujo
University of Nebraska at Lincoln, bachiega@gmail.com

Follow this and additional works at: http://digitalcommons.unl.edu/engmechdiss

Part of the Mechanical Engineering Commons

http://digitalcommons.unl.edu/engmechdiss/9

This Article is brought to you for free and open access by the Mechanical & Materials Engineering, Department of at DigitalCommons@University of Nebraska - Lincoln. It has been accepted for inclusion in Engineering Mechanics Dissertations & Theses by an authorized administrator of DigitalCommons@University of Nebraska - Lincoln.
NUMERICAL AND ANALYTICAL VERIFICATION OF A MULTISCALE COMPUTATIONAL MODEL FOR IMPACT PROBLEMS IN HETEROGENEOUS VISCOELASTIC MATERIALS WITH EVOLVING DAMAGE

by

Bruno Francisco Bachiega de Araújo

A THESIS

Presented to the Faculty of
The Graduate College at the University of Nebraska
In Partial Fulfillment of Requirements
For the Degree of Master of Science

Major: Engineering Mechanics

Under the Supervision of Professor David H. Allen

Lincoln, Nebraska

August, 2010
NUMERICAL AND ANALYTICAL VERIFICATION OF A MULTISCALE COMPUTATIONAL MODEL FOR IMPACT PROBLEMS IN HETEROGENEOUS VISCOELASTIC MATERIALS WITH EVOLVING DAMAGE

Bruno Francisco Bachiega de Araújo, MS
University of Nebraska, 2009

Adviser: David H. Allen

Composites are engineered materials that take advantage of the particular properties of each of its two or more constituents. They are designed to be stronger, lighter and to last longer which can lead to the creation of safer protection gear, more fuel efficient transportation methods and more affordable materials, among other examples.

This thesis proposes a numerical and analytical verification of an in-house developed multiscale model for predicting the mechanical behavior of composite materials with various configurations subjected to impact loading. This verification is done by comparing the results obtained with analytical and numerical solutions with the results found when using the model. The model takes into account the heterogeneity of the materials that can only be noticed at smaller length scales, based on the fundamental structural properties of each of the composite’s constituents.

This model can potentially reduce or eliminate the need of costly and time consuming experiments that are necessary for material characterization since it relies strictly upon the fundamental structural properties of each of the composite’s constituents.
The results from simulations using the multiscale model were compared against results from direct simulations using over-killed meshes, which considered all heterogeneities explicitly in the global scale, indicating that the model is an accurate and fast tool to model composites under impact loads.
DEDICATION

To 1...
To 2...
To 3...
ACKNOWLEDGMENTS
# Table of Contents

CHAPTER 1 ................................................................................................................................. 10  
1.1 Introduction .......................................................................................................................... 1  

CHAPTER 2 ................................................................................................................................. 4  
2.1 Literature Review ................................................................................................................... 4  
2.1.1 Helmets and Brain Trauma .............................................................................................. 4  
2.2 Solution Proposal .................................................................................................................. 23  

CHAPTER 3 ................................................................................................................................. 25  
3.1 Theoretical Background ....................................................................................................... 25  
3.1.1 Initial Boundary Value Problem Formulation ............................................................... 25  
3.1.2 Viscoelasticity Theory ..................................................................................................... 28  
3.1.3 Multiscaling .................................................................................................................... 33  
3.1.4 Mesh Convergence .......................................................................................................... 41  

CHAPTER 4 ................................................................................................................................ 46  
4.1.1 Code Description and Verification .................................................................................. 46  
4.1.2 Code Description ............................................................................................................. 46  
4.1.3 Code Verification ............................................................................................................ 49  
4.2 1-D Uniaxial Bar ............................................................................................................... 52  
4.2.1 Elastic Case ..................................................................................................................... 58  
4.2.2 Viscoelastic Case ............................................................................................................ 65  
4.2.3 Damage Case ................................................................................................................. 69  

CHAPTER 5 ................................................................................................................................ 79  
5.1 Example Problems .............................................................................................................. 79  
5.1.1 2-D Uniaxial Bar ............................................................................................................. 79
5.1.2 Convergence Studies .................................................................................. 82
5.1.3 2-D Cylinder/Plate Problem ........................................................................ 95

CHAPTER 6 ............................................................................................................. 106
6.1 Conclusions ..................................................................................................... 106
List of Figures

Figure 1 - Blast wave trapped under a helmet ................................................................. 8
Figure 2 - Reinforced Composite with Fibers and Rule of Mixtures .............................. 11
Figure 3 - Unit Cell ........................................................................................................... 14
Figure 4 – RVE Mesh Illustration .................................................................................... 14
Figure 5 – Problem set up for a simulation conducted by Lawrence National Lab .......... 16
Figure 6 - Maxwell and Voigt Mechanical Analogs ......................................................... 22
Figure 7 - Generalized Maxwell and Voigt Analogs ......................................................... 31
Figure 8 – Representation of Multiple Scales ................................................................. 35
Figure 9 - Mesh Convergence Curve ............................................................................... 42
Figure 10 - Triangular Finite Element ............................................................................ 47
Figure 11 – Flowchart of the Multiscale Computational Algorithm (Souza, 2008) ........... 48
Figure 12 - Material Properties Distribution .................................................................. 50
Figure 13 - Results for an Elastic Heterogeneous Uniaxial Bar ....................................... 52
Figure 14 - Uniaxial Bar with Heterogeneity in the Center ............................................... 53
Figure 15 – Load Function ............................................................................................... 54
Figure 16 - Initial and Boundary Conditions for 1-D Uniaxial Bar .................................... 55
Figure 17 – Different Meshes for the Singlescale and Multiscale Problems ..................... 56
Figure 18 - 1) Shows a general pattern for the displacement against time at the tip of the bar, while 1) shows the same general pattern for the displacements at the middle of the bar .......................................................................................................................... 58
Figure 19 - Wave Reflection When Crossing Boundaries. Left side a) shows snapshots for the single scale case and right side b) shows the snapshots that represent the equivalent multiscale simulation ......................................................................................... 60
Figure 20 - Displacements and Stresses for Elastic Case @ x=L ........................................ 63
Figure 21 - Displacements and Stresses for Elastic Case @ x=L/2 ..................................... 64
Figure 22 - Displacements and Stresses at the Tip of the Bar (x=L) for Viscoelastic Case .... 67
Figure 23 - Displacement and Stresses at the Middle Point of the Bar (x=L/2) .................. 68
Figure 24 - Displacement Comparison among Singlescale Results .................................. 69
Figure 25 – Displacements and Stresses at the Tip of the Bar (x=L) for Damage Case .......................... 71
Figure 26 - Displacement and Stresses at the Middle Point of the Bar (x=L/2) for Damage Case ........................................................................................................................................ 72
Figure 27 - Displacement Comparison among Results for the Singlescale Cases at the tip of the bar (1) and in the middle of the bar (2) (Heterogeneous Elastic as Elastic, Heterogeneous Viscoelastic as Viscoelastic and Heterogeneous Viscoelastic with Damage as Damage) .......................................................................................................................... 73
Figure 28 - Wave Dissipation ...................................................................................................................................................... 75
Figure 29 - Evolution of Damage (alpha) for the First Inclusion ........................................................................................................ 76
Figure 30 - Failure of Bar Trapping Wave ................................................................................................................................... 78
Figure 31 - Boundary Conditions for 2-D Uniaxial bar ......................................................................................................................... 79
Figure 32 - Boundary Conditions for Converge Studies ..................................................................................................................... 83
Figure 33 - Convergence Study over Number of elements (Ultimately Element Size) ................................................................. 84
Figure 34 - Convergence Study over Delta ..................................................................................................................................... 85
Figure 35 - Convergence Study over M ........................................................................................................................................ 86
Figure 36 - Convergence Study over Damage Law .......................................................................................................................... 87
Figure 37 - 2-D Uniaxial Bar - Displacements and Stresses @ x=L .................................................................................................. 88
Figure 38 - 2-D Uniaxial Bar w/ Damage - Displacements and Stresses @ x=L/2 ................................................................. 91
Figure 39 - Snapshot Sequence for 2-D Uniaxial Bar (global scale) .............................................................................................. 92
Figure 40 - Local Mesh Position relative to Global Mesh .................................................................................................................. 93
Figure 41 - Snapshot Sequence for 2-D Uniaxial Bar (local scale) ............................................................................................... 94
Figure 42 - 2-D Cylinder/Plate Case Boundary Conditions .............................................................................................................. 95
Figure 43 - Snapshot Sequence for the Single scale 2-D Cylinder/Plate Problem ................................................................................ 99
Figure 44 - 2-D Cylinder Place Problem – Back Face Displacements and Stresses .................................................................... 100
Figure 45 - Snapshot Sequence for 2-D Uniaxial Bar (local scale) ............................................................................................... 102
Figure 46 - 2-D Cylinder Place Problem w/ Damage – Back Face Displacements and Stresses .......................................................................................................................... 103
Figure 47 – Local Mesh Convergence Study for the 2-D Cylinder Place Problem w/ Damage .......................................................................................................................................................... 105
List of Variables

\( t_i \) ................................................................. Traction
\( n_i \) ................................................................. Unit Outer Normal
\( u_i \) ................................................................. Displacement Vector
\( \varepsilon_{ij} \) ...................................................... Strain Tensor
\( \sigma_{ij} \) ......................................................... Stress Tensor
\( f_i \) ............................................................. Body Force
\( \rho \) ............................................................... Mass density
\( t \) ................................................................. Time
\( \tau \) ............................................................. Time of Interest
\( C_{ijkl} \) ......................................................... Relaxation Modulus Tensor
\( D_{ijkl} \) ......................................................... Creep Compliance Tensor
\( V \) ............................................................. Interior Volume
\( \partial V \) ........................................................ Boundary
\( d \) .............................................................. Displacement
\( v \) ............................................................. Velocity
\( a \) ............................................................. Acceleration
\( F_{ext} \) .......................................................... External Forces
\( F_{int} \) .......................................................... Internal Forces
\( \bar{\varepsilon} \) ....................................................... Homogenized Strain
\( \bar{\sigma} \) ......................................................... Homogenized Stress
\( \bar{M} \) .......................................................... Homogenized Mass
\( \bar{\mathbf{C}} \) ...................................................... Homogenized Constitutive Tensor
List of Tables

Table 1 - FE Meshes Setups........................................................................................................... 55
Table 2 - Material Properties for Elastic Case .................................................................................. 59
Table 3 - Simulation Details ............................................................................................................ 62
Table 4 - Material Properties for Viscoelastic Case ......................................................................... 66
Table 5 - Material Properties for Cohesive Zones .......................................................................... 71
Table 6 - 2-D Uniaxial Bar Material Properties .............................................................................. 80
Table 7 - 2-D Uniaxial Bar meshes and Details .............................................................................. 82
Table 8 - Material Properties for Cohesive Zones .......................................................................... 89
Table 9 - 2-D Cylinder/Plate Meshes and Details .......................................................................... 97
Table 10 - 2-D Cylinder/Plate Material Properties ....................................................................... 98
Table 11 - Material Properties for Cohesive Zones ....................................................................... 101
Table 12 - Geometry of Microstructures ....................................................................................... 104
CHAPTER 1

1.1 Introduction

The primary purpose of this work is to verify the model used in a tool that will assist in the design and improvement of composite materials and structures which could potentially lead to an improvement in the life of many by making safer protection gear, more fuel efficient transportation and more affordable materials among many other examples.

Some of the many advantages of composite materials and the importance to have a numerical modeling tool to analyze and evaluate them and all the various scenarios where they are present will be discussed. Composites materials stand up to heat and corrosion significantly better than most metals, making them ideal for use in products designed to be exposed to extreme environments such as high pressures, chemical-handling equipment and even spacecraft. In general, composite materials are durable and resistant, and also provide design flexibility by being malleable, allowing for various complex shapes.

The use of these newly engineered materials is becoming more and more common, such as in the new Boeing 787, claimed to be 20% more fuel efficient than its predecessor (Norris, 2009). This is the first large aircraft ever to be made out of composite materials, with 50% of its fuselage, wings, tail, doors and interior made of non-metal materials. The 787 makes use mainly of carbon fiber reinforced plastic (Hawk, 2007), a lighter material that reduces the overall weight of the aircraft while keeping its
strength. One downside of using composites is that unlike metal, they do not visibly show cracks and fatigue. This requires non visual inspection methods such as expensive ultrasonic scans. Another disadvantage is that expensive crash tests need to be performed for many of the structural analyses.

Another example of the increasing demand today for composite materials and their applications is body armor. The United States has historically invested in new material technologies, particularly in the design of armor with increased ballistic mass efficiency. Currently, the country has an interest in materials that are not only resistant to projectiles, but to the high stresses generated from blast events. Helmets are the primary application for these new composite materials used for energy absorption, but besides the materials used, the design elements adopted such as interfacing of the helmet with other equipment, patterns of use and fiber orientation within the material have a major influence on the overall performance. Also, in some cases it is simply impractical to perform real-life tests (e.g. determining the effects of a blast wave on a soldier’s head).

Composite materials often have microscopic constituents that may not be visible to the naked eyes. One great advantage of the tool developed with this study is that the design of the subject of interest (armor, aircraft, vessels) can mostly be done using only a computer, reducing or eliminating the need for costly experiments. The use of numerical simulations for modeling instead of doing experiments is not a new topic and has been extensively researched, but many of the current tools available do not adequately account for what occurs at the microstructure level in the composite material. In those tools that do, the computational power and time required to perform a single simulation can be so enormous that it is prohibitive with today’s reality. Another advantage of this study is
that it addresses what happens with the constituents at the microstructure scale with simulations that can be solved in a reasonable amount of time, with fairly accurate results. Examples will be shown throughout the study to illustrate this benefit.
CHAPTER 2

2.1 Literature Review

The ultimate motivation for this study is to verify the model for predicting the mechanical behavior of composite materials such as human tissues subjected to impact loading where the heterogeneity of these tissues that can only be noticed at smaller length scales and how they interact with each other are accounted for in the model. Also, the impact loading attempts to simulate the ones generated when improvised explosive devices (IED) as the ones used by insurgents in Iraq go off causing injuries instantaneously and in the long term. A description of the studies already done in this area and in numerical modeling is presented now.

2.1.1 Helmets and Brain Trauma

When talking about military injuries, traumatic brain injury (TBI) has become one of the most characteristic types of injury in today’s reality. The effects of TBI on the soldiers, their families and even society are long-lasting and can be very costly. Extensive research has been done on the mechanisms that cause TBI due to impact (e.g. from projectiles), but very little is known about how blasts can lead to TBI. The use of improvised explosive devices (IEDs) in terrorist and insurgent attacks has increased dramatically, consequently increasing the exposure of soldiers to blasts that accompany the explosion.

Over the years, body armor has improved significantly and has become more widely used. This has greatly reduced fatal injuries among soldiers from attacks that involve explosions. The decrease in the mortality rates has not come alone. There has
also been a noticeable rise in non-fatal injuries, especially TBI types of injury. The reason for this shift is attributable to the fact that most modern military equipment is designed to provide protection from impacts only, such as projectiles, as opposed to blasts.

Injuries related to blasts are becoming extremely common. A study conducted by (Murray CK, 2005) found that 88% of military personnel that entered a particular medical station in Iraq were injured by mortars or IEDs, and nearly half of these injuries were head-related. A similar situation was found by (Gondusky JS, 2005) at a Marine unit that had 97% of its injuries related to explosions on the battle field. Again, over half of these explosion related injuries were on the head of the soldiers. History has shown that as explosives become more powerful and more commonly used in combat, a new condition emerges in which soldiers become dazed or knocked unconscious by a blast. At first, no external or visible injury may be noticed, and the soldiers are soon back on duty. The authors of (Fabing, 1947) listed a few symptoms felt by the soldiers upon regaining consciousness in World War II. Amnesia was the most common with others including headaches, tremors and hypersensitivities. Today, these symptoms are diagnosed as posttraumatic stress that can lead to delirium, agitation and psychic disorders. Such symptoms may be caused by the difference in pressure generated by an explosion.

There is an urgent need to understand the mechanisms by which blasts cause TBI, so that exposed soldiers can be diagnosed more effectively and improved protective equipment can be designed. Briefly, TBI results from mechanical loads in the brain, often without skull fracture, may cause complex, long-lasting symptoms. There is no consensus among researchers as to the primary causes of TBI (Bhattacharjee, 2008; Warden, 2006) due to the mechanical and biological complexity of the problem. Mechanical loads from
the blast pressure, acceleration, or impact, as well as electromagnetic and thermal exposure have been listed as proposed causes (Stuhmiller, 2008). Animal tests have not yet conclusively identified the key mechanisms because the multiplicity of candidate mechanisms and the physiological differences between animals and humans make direct comparisons difficult. The use of human trauma data from war casualties is problematic, because it is not easy to determine the exact blast exposure for a given victim.

The stresses introduced by the pressure wave generated from the explosion may cause direct injuries to the brain such as concussion, hemorrhage and formation of gas emboli that lead to infarction among others (Guy RJ, 2000). Some shock tube experiments with animals have shown that only the blast pressure itself, without subsequent impacts, can cause TBI (Cernak I. W., 2001). Several models to predict the damage caused to the brain by a blast wave alone have been proposed, such as (Stuhmiller, 2008) that studies the bulk acceleration of the head and (Bhattacharjee, 2008; Cernak I., 2005) that focused on the compression of the thorax, leading to a surge of blood to the brain.

A limiting factor for studying TBI in humans is the nearly non-existent clinical data. Most studies used war-related injuries that lack accurate data. The subjects exposed to the blast (soldiers for example) often do not have full information about how events unfolded, such as their distance from the explosion when it went off, the angle of exposure from their head to the explosive and what type of blast to which they were subjected. Thus, the information must be estimated, resulting in a loss of accuracy in the model being constructed. Another major problem in the area relates to material characterization. Brain tissue is highly viscoelastic and an extremely soft material. This
factor makes it difficult to perform any material characterization test. The time frame in which the material sample is still considered valid for a test, from the time when it was obtained to the time the test is actually performed, is also an unknown. Further research will be required to converge upon a generally accepted solution to this problem. This subject is off the topic from the present thesis, however, and will be left for further studies in the area. Additionally, brain tissue presents heterogeneity at multiple levels, requiring a mesh that would account for all this spatial variations in the material properties as well geometries at all scales. This proposed mesh would have to be extremely fine and solving such a large problem would be a challenging if not unfeasible with the computational power available today.

The reason for this is that helmets are designed to protect the head from projectiles within a range of force of impact, but they provide considerably less protection against blast. Some helmet designs can actually amplify the destructive power of a blast wave, being potentially more harmful then the blast alone.
Figure 1 - Blast wave trapped under a helmet

It has been found that the gap between the helmet and the head can potentially amplify the pressure on the skull when the blast wave washes under the helmet. This interaction can affect the head in unexpected ways, and the stresses on the skull are greater when this under wash happens that would be without the helmet. Improved helmet padding could inhibit this effect and decrease head accelerations that transmit blast induced flexure to the skull (William C. Moss, 2007).

It is long known that for a better and more complete model, it is necessary to take into account the effects of micro structures in a smaller length scale than the main one analyzed. Many times what happens with these small structures goes unnoticed if it is not examined with attention. To illustrate how unnoticed these small details can go by, one can look to the roadways we use on the daily basis. Even though they appear solid and
homogeneous at first glance, a more careful look might expose the multiple materials it is made of along with an enormous number of cracks of all sizes, from small ones only visible with the help of a microscope to big ones that can reach several meters in length.

A large range of materials found in nature are composed of multiple constituents. These are called composite materials and they use a smart strategy from nature to take advantage of the properties of each constituent to form a new one that will outperform any of its constituents alone. Many man-made materials and structures today, such as Kevlar helmet, use the same strategy.

Determining the overall characteristics of composite materials and discovering how they behave due to the material interaction at the microscale level are keys to the development and applicability of such materials. A model to predict the mechanical behavior of heterogeneous materials is an essential tool for designing composite materials that will exhibit the specific required characteristics required for a purpose. Such a model would reduce or eliminate the need of costly and time consuming experiments that are necessary for material characterization. It would significantly facilitate predictions due to any alterations in the microstructure, such as changing the volume fractions and size of its constituents or the geometry of the microstructures.

Mechanics

Mechanics, the study of the motion of the bodies, has long been studied in history by major scientists, such as Archimedes who introduced the principle of the lever (among other achievements) and Galileo (Galileo, 1636) who was responsible for the first systematic study in the area. However, it was only in the nineteenth century that
deformable bodies were actually examined. Cauchy (Cauchy, 1823) was one of the pioneers working on the prediction of the deformations in elastic bodies, and Germain (Germain, 1821) led studies that were focused on plates.

All these works were based on Newton’s laws of motion (Isaac Newton, 1999), but none of these formulations accounted for the effects of dissipation of energy, therefore failure was not included and could not be predicted by these models. Almost a century later, Griffith became the first to introduce the notion of thermodynamics and to start with the concepts of fracture mechanics (Griffith, 1920).

Heterogeneity of materials and separation of length scales for more accurate results have been considered and studied by scientists in the past, all the way from the nineteenth century with Maxwell and Boltzmann until Einstein in the twentieth century, by observing molecular phenomena in liquid and gases to explain observations at the macroscale level of materials.

This study presents a multiscale model, which belongs to a class of constitutive models also called homogenization theories. The main goal behind these theories is to predict the behavior of heterogeneous materials based on the configuration of the constituents, such as volume fractions, material types and geometric orientations. A computational homogenization technique is based on the macroscopic constitutive response, derived from the underlying microstructure using an appropriate method, like the solution to a boundary value problem for the microstructure.

One of the simplest methods to calculate homogenized properties is the so called rule of mixtures (Gao XL, 1999). This approach uses mathematical expressions to find the global properties in terms of the local properties, but it is often based on a number of
simplifying assumptions, so it should be used with caution. A general formula to calculate the homogenized density $\rho$ is presented as follows:

$$\rho = \frac{V_a \rho_a}{V} + \frac{V_b \rho_b}{V} + \frac{V_c \rho_c}{V} + \ldots$$

This is not a complicated approach, yet it is not always accurate so caution should be taken when using it to calculate homogenized properties since it takes only one microstructural variable into consideration (the volume ratio of each constituent) and neglects the influence from the other aspects.

**Figure 2 - Reinforced Composite with Fibers and Rule of Mixtures**

A common approach to model multiple scales is the classical homogenization theory (Christensen R., 1979; Nemat-Nasser, 1993; Mura, 1987) where the idea is to determine the effective (homogenized) constitutive behavior of the composite material before even running the multiscale simulation by simply solving an initial boundary value problem (IBVP) for a representative volume element (Allen DH, 1998; Hashin, 1964; Hill, 1965; Hill R., 1963).
This is a more cost-effective method to use in case the representative volume element do not evolve during the simulation and its behavior does not depend on the load history. In this case, the constitutive properties only need to be determined once. These constitutive properties need to be found \textit{a priori} for any complex problem simulation, and as mentioned previously, it cannot change with time. This is one of the reasons why multiscale models are more recommended for problems where there is formation and growth of internal boundaries within the representative volume element.

In the multiscaling model, the homogenized constitutive properties are calculated recursively both spatially and also at every step of the simulation, allowing changes to be included in the model. This feature allows changes in material properties, geometries, volume fractions, and others to be included into the model at the time of the simulation, avoiding the need to recreate sometimes costly constitutive experiments each time a parameter changes. This capability represents a great advantage over experimental approaches.

Also, the model does not require any constitutive assumption over the material behavior, so no experimental constitutive test is needed \textit{a priori} to the simulation. Large deformations and rotations on both local and global scales can also be included in the model, as well as non linear and time dependent material behaviors.

A multiscale model is the most appropriate approach to address models that may have evolving microstructures, such as cracks. This is because the evolution of cracks usually depends on the loading history and also alters the geometry of the problem.
Another advantage of using the multiscaling approach is the dramatic reduction in the overall number of nodes and elements in the analysis. This is because we can model these smaller length scales without having to refine the entire global mesh to a point where the small objects at the smaller scales could be taken into account. Refining the mesh to such a fine point could mean to create meshes that are so big, with millions and millions of nodes and elements, that no single computer on the planet could be able to solve it in an acceptable time frame. Also, the number of constituents that can be modeled within the small scales as well as the constituent types and geometries have very little limitations when the multiscale model is implemented with a finite element code.

Some of the information, such as stress concentrations at the smaller scales, is averaged out through the homogenization process and not every geometric detail of the structures at the small scales can be accounted, but the multiscale approach still provides efficient results with high fidelity when modeling composites that exhibit a hierarchical structure. If modeled properly, the errors introduced with the use of the multiscale model can be minimized and will be negligible (Searcy, 2004).

Another homogenization theory is the so called asymptotic homogenization or mathematical homogenization theory. It is also used to predict the overall behavior of a composite material based on the material behavior and geometry arrangement of its constituents and it was first studied in the 1970s out of applied mathematics. This theory models the behavior of heterogeneous media which its constituents are lined up in an infinite periodic pattern and it subjected to far field mechanical loads. A large difference in the orders of magnitude between the global scale and the smallest repeatable structure must exist, and this small repeatable structure is called a unit cell.
This disparity allows the expansion of the field variables using asymptotic series, and will cause the separation of the local scale analysis from the global scale analysis. Some of the research that has contributed to the development of the technique have been made by (Bensoussan, 1978; Sanchez-Palencia, 1980), and further included inelastic media including nonlinear elasticity (Jansson, 1992), and then plasticity with (Suquet, 1987) and finally viscoelasticity with (Maghou S. C., 2003; Nadot-Martin, 2002; Yu and Fish, 2002).

The asymptotic homogenization approach gives accurate overall properties, local stress and strain values. This approach though, assumes there are very simple microscopic geometries and simple material models, mostly with small strains, but so far neither of the methods presented accounts for the geometrical and physical changes at the small scales.

The local scale does not always have to be periodic like that described for the asymptotic approach. It may have random microstructures with different orientations as long as some assumptions are respected. The microscale has to be a representative volume element (RVE).
The RVE is usually referred to as a volume $V$ of heterogeneous makeup (composite material) that is sufficiently large to be statistically representative of the material (T. Kanit, 2003). This is so it includes just enough of the heterogeneity of the microstructures in the composite, with the RVE remaining small enough for the problem to be solvable in a reasonable time and large enough so the concepts of continuum mechanics are still applicable. Also, the estimated material properties given by the spatial average of stresses or strains in the given domain $V$ must fit within a given determined accuracy to make it valid. This concept was also mentioned by (Helms, 1999), defining and RVE to be the solution for a problem with a geometry of a given size where the averaged boundary traction against displacement relation does not change significantly if the size of the geometry is increased.

Another definition for RVE given by Drugan and Willis (W.J. Drugan, 1996) says: “It is the smallest material volume element of the composite for which the usual spatially constant (overall modulus) macroscopic constitutive representation is a sufficiently accurate model to represent mean constitutive response”. This solution uses a homogenization method considering the medium to be infinite and does not account for fluctuation properties over finite domains, but the RVE size turns out to be satisfactorily small, particularly when working with disordered fiber composites.

It is important to notice that, in general, the size of the RVE depends on the morphology and properties of the materials of interest. For example, the size of the RVE can change just by adding thermal effects to the problem or if viscoelastic properties are considered.
An advantage of this approach is the fact that it can model problems with evolving microstructure, where the local structure changes with time due to crack formation or growth. The reason why is because the model recalculates the homogenized constitutive properties on every step of the analysis.

First order homogenization methods follow the theory of standard local continuum mechanics. First, the strain tensor is calculated for every point in the global mesh and then a kinematic boundary condition is arranged for the local scale based on this strain tensor. Next, the solution for the local scale boundary value problem is calculated. The stress field found at the local scale is then averaged over its volume, resulting in the stress tensor at the global scale element. So the stress-strain relation is always available at the local and global scales, proving this homogenization scheme to be accurate and powerful when obtaining the mechanical response of heterogeneous media.

This homogenization method, as well as the other classical homogenization methods, has some limitations which can significantly reduce its applicability, so it is valid to mention and comment on them so the right assumptions can be made and the model can remain accurate. Even though the model accounts for the geometry,
distribution and volume fraction of its constituents, it is incapable of taking the absolute size of the local scale into consideration. Consequently, it cannot account for geometrical size effects either. Another limitation comes with the assumption of uniformity of stress-strain fields from the global scale attributed at each local scale. This assumption is based on the concept of separation of scales and becomes incorrect in case there are regions of high gradients at the global scale, where these stress-strain fields can change rapidly. When using a first order homogenization method, there must exist a large disparity between the sizes of the global and local scales to allow the separation of the scales, or some accuracy may be lost. In that case a higher order homogenization scheme can be used to avoid this loss of accuracy.

Also, Souza has produced a study about the computation of homogenized constitutive tensor for elastic solids containing cracks (Souza F.V., 2008). The author elaborates a procedure to determine the instantaneous constitutive tensor of elastic materials with forming and growing cracks at the microscale. The method relates the local displacement field to the global strain tensor at each location using a first order homogenization scheme. Then, the method is implemented into the multiscale finite element code utilized and some examples are shown in order to verify the code.

A lot of research has been done regarding the concept of separation of length scales, and the approach has gained more acceptance as it covers more areas of interest and starts to be more applicable to everyday’s problems.

One main issue is the applicability to different kinds of materials. So far, the majority of the studies were made using the elasticity theory, bounding the elastic properties of multiphase elastic continua. Just a few examples of works done with elastic
materials are (Eshelby, 1957; Hashin, 1964; Hill, 1965). These and other studies include a wide range of elastic materials.

However, we know that a wide range of materials in nature or created by men, show viscous properties at some point. This work seeks to study and understand more the behavior of viscoelastic heterogeneous media. Some present works in the literature that account for these viscous effects will now be presented and briefly discussed.

An asymptotic homogenization approach was used by (Yi, 1998) to model a viscoelastic composite with periodic microstructures. A Carson transform approach was used to find the homogenized properties, which interestingly had the local relaxation modulus separable in space and time. The memory effects of the viscoelasticity of the problem didn’t appear in the homogenized properties either. In the study conducted by (Yu and Fish, 2002), a double asymptotic expansion in both space and time was used to determine the homogenized properties of the heterogeneous viscous material (a viscoelastic Kelvin-Voigt model). The authors showed that a homogenization process in space and time can be obtained by solving a first order initial value problem.

Another periodic homogenization approach was developed by (Maghous S. C., 2003) extending the study made by (Allen and Yoon, 1998). Maghous’s work used asymptotic expansions to find the homogenized properties, also for a Kelvin-Voigt analogue. The main contribution was the inclusion of aging effects and the use of a dissipative corrector obtained from the derivation of the homogenized equations in the time domain that relates long-term relaxation to instantaneous viscoelasticity. A closed form solution was found via a stress concentration factor for the macroscale only. The
microscale effects were included in the macroscale constitutive equations to be considered.

One more study with viscoelasticity included is the one by (Nadot-Martin, 2002), which extended the work of (Christoffersen, 1983). Christoffersen’s work included a model for elastic composite materials where there was bonded granulates. Nadot included viscoelasticity in the model by representing the granulated microstructure bonded by cohesive interfaces. The grains remained elastic but the cohesive interfaces were linear viscoelastic for Nadot’s model. The authors put a lot of effort into finding a constitutive law for the macroscale that considers the heterogeneity at the microscale.

Another subject not very well explored yet in the literature is the inertial effects caused by impact loading in composite materials. Most of the literature does not account for that effect, being suitable for predicting the behavior of materials under QUASI-STATIC type of loads only. A few studies deserve some attention, like the one by (Yu and Fish, 2002), where a dissipative corrector originated from the derivation of the homogenized equations was used to address the inertial effects in the problem. Yu and Fish showed that a homogenization process in space and time can be obtained by solving a first order initial value problem.

A multiscale space–time asymptotic homogenization procedure for analyzing multiple physical processes interacting at multiple spatial and temporal scales is developed and applied to the coupled thermo-viscoelastic composites. Rapidly varying spatial and temporal scales are introduced to capture the oscillations induced by local heterogeneities at diverse time scales (Fish and Qing, 2001).
A space–time multiscale model for wave propagation in heterogeneous media was developed over the author’s previous work with multiple spatial and temporal scales using higher order mathematical homogenization theory (Fish and Chen, 2004). The study was focused on solving stability and mathematical consistency issues, and the solution has been verified for wave propagation problem on semi-infinite and finite domains.

Souza has presented a model for predicting the behavior of composite materials under impact load that accounts for damage at the microscale level in the form of homogeneously distributed microcracks by including cohesive zones (Souza F.V. A. D.-R., 2008). The code utilized was verified by solving a few examples and one of the greatest advantages of the model is that the material characterization is simplified and only necessary at the microscale level. This allows variables of the problem such as volume fractions and orientation of the constituents to be readily included into the design process.

For purposes of this study, damage and cohesive zones are not going to be included in the problem, but is always valid to mention what has been accomplished in the literature by other authors in the area.

Numerical methods such as the finite element methods are a key element to work with multiscale modeling. Many studies have been made over the fundamental aspects of finite element for the multiscale problems and some important examples in the literature will be mentioned in a few words to give a brief idea of what has been accomplished to the date.
Fish and co-workers have published a series of papers on a strategy to approximate the displacement fields of both micro and macroscales. Also, the information and how the micro and macroscale interact have been studied to obtain a solution method for these two different length scales (Fish and Wagiman, 1993; Fish and Belsky, 1995; Fish and Shek, 2000).

Other advanced multiscaling strategies have also been researched by Feyel and Chaboche (Feyel, 1999; Chaboche, 2000). The study uses a multilevel finite element approach, as the authors call it, where constitutive equations are formulated only for microscale. The stresses and strains are calculated for the macroscale with some homogenization and localization relationships based on the microscale of the problem. In the multilevel finite element approach, each Gaussian point in the macroscale has a respective local mesh assigned to it for and is calculated independently from each other.

A multiscale method for performing stress analysis in materials with two length scales with damage and time dependency included in the model has been developed by (SEARCY, 2004). The model is very versatile and utilizes RVEs to represent the microscale structures instead of periodic unit cells. This allows the model to have properties of the microscale such as geometry, orientation and number of constituents to be included and changed as needed, in other words, these properties are input design variables for the problem.

Continuing to talk about previously mentioned Souza’s work (Souza F.V., 2008), he has also developed a very solid model based in finite element methods that has many features embedded in it. One of these features is that the code is dynamic, being capable of solving impact problems. Its multiscaling approach utilizes RVEs to represent the
microstructures, which as discussed before adds a lot of flexibility to the model. It also considers damage in the problem, so if a more complete analysis is required, cracks formation and growth can be simulated at the microscale until it propagates to the macroscale level.

![Figure 5 – Problem set up for a simulation conducted by Lawrence National Lab](image)

Lawrence Livermore National Laboratory (William C. Moss, 2007) has developed a hydrocode with which they performed a study over the interaction of fluids (air in a blast) with solids (biological structures such as human head). They simulated the explosion of a five pound spherical charge of C4 explosive going off at 4.6 meters away from a simulated human head. Their simulations revealed known mechanisms of TBI and showed that the presence of a helmet may increase the pressure over the skull generated by a blast wave.
2.2 Solution Method

A new model that attempts to overcome some of the unsolved issues by the previously mentioned works is now presented. It will be capable of predicting the displacements, strains and stresses in elastic and viscoelastic media simultaneously, also accounting for the heterogeneity of these materials. This includes a wide range of materials that can be later simulated with the proposed model. The effects of time-dependant material behavior will be included, which adds the capability of predicting the mechanical behavior of materials under impact loading, a subject of high interest today. Finally, the model will take advantage of a multiscaling approach, accounting for the mechanical behavior of the micro structures at the smaller scales of the problem and how that could affect the big picture.

The Finite Element code used to perform these simulations will be capable of solving various types of multiscale initial boundary value problems with a wide range of materials. Very rapidly loads can be applied without compromising the accuracy of the model and because the algorithms are based on finite element methods, there are very few limitations on the geometry of objects modeled and number of constituent types in the problem. As for performance, the code will utilize a parallelized approach that takes advantage of the fact that each microscale analysis can be performed independently from each other and from the macroscale analysis as well. This will be particularly advantageous in case of a large number of distinct microscale meshes. The microscale analysis can be evenly distributed throughout the number of available processors so each
processor work independent from each other on their own set of problems for a faster final solution to the multiscale problem. The time required to finish the complete analysis shall be greatly reduced, possibly proportionally to the number of processors being used. This is a strong model and particularly powerful tool to simulate composite materials such as living tissues and cushioning pads under impact loadings.

The study will start with a more familiar and simple problem in order to develop the theory that will be necessary to solve other more complex problems that are indeed of interest and applicable to the industry. An analytical solution for this simple problem is searched and once found, compared to the numerical results given by the FEM simulation code in use, which is where all the theory developed is implemented. This comparison is necessary to verify the model, to find out if how accurate the algorithm is with the respective assumptions made.

After the code verification phase of this study, some other problems will be presented to illustrate the capability and applicability of the model proposed in many areas of interest.
CHAPTER 3

3.1 Theoretical Background

In this chapter, the theoretical aspects that form the basis for this thesis are presented. An initial boundary value problem (IBVP) formulation that utilizes the continuum mechanics approach for a general solid is introduced first, followed by the fundamental concepts of linear viscoelasticity theory. Further on, a multiscaling model that accounts for damage and makes use of multiple length scales in order to improve the accuracy of the model is presented along with an introduction to a mesh convergence study.

3.1.1 Initial Boundary Value Problem Formulation

The purpose of the IBVP is to find out what the mechanical responses (displacements $u_i(x,t)$, strains $\varepsilon_{ij}(x,t)$ and stresses $\sigma_{ij}(x,t)$) are when the studied body is subjected to a load. In order to predict the mechanical response of a body subjected to tractions and/or displacements, an Initial Boundary Value Problem must be formulated and solved. The problem to be solved in this study is considered to be a linear, two-dimensional, viscoelastic, dynamic Initial Boundary Value Problem. It can be considered dynamic because the loading speed can reach the fundamental frequency or the lowest frequency at which the objects studied can vibrate. A more general case of a three dimensional problem will later be presented. A general formulation based on continuum mechanics, where a body is assumed to be a continuum when analyzed is presented herein.
Consider a general three dimensional body that has an interior volume $V$ and boundary $\partial V$ where:

\[ \partial V_1 \cup \partial V_2 = \partial V \]  \hspace{1cm} (3.1)

\[ \partial V_1 \cap \partial V_2 = \emptyset \]  \hspace{1cm} (3.2)

The body can be subjected to different constraints, and depending on how these constraints are imposed on the body we use different approaches to solve the problem. For instance, if displacements are applied over the boundary $\partial V$, the problem is called a Dirichlet problem. In case tractions are being applied, then we call it a Neumann type problem.

In the case it refers to tractions being applied in the boundary, we have:

\[ t_i(\bar{x},t) = \text{Known on } \partial V \]  \hspace{1cm} (3.3)

\[ t_i(\bar{x},t) = \sigma_{j\mathbf{n}_j} \]  \hspace{1cm} (3.4)

For displacements applied over the boundary:

\[ u_i(\bar{x},t) = \text{Known on } \partial V \]  \hspace{1cm} (3.5)

It is assumed that the following set of equations and conditions are sufficient to properly model the mechanical response.

Conservation of Linear Momentum (Considering dynamic problem):

\[ \sigma_{j\mathbf{n}_j} + f_i = \rho \frac{\partial^2 u_i}{\partial t^2} \]  \hspace{1cm} (3.6)
Conservation of Angular Momentum (Considering no body moment):

\[ \sigma_{ij} = \sigma_{ji} \]  
\[ (3.7) \]

Strain-Displacement Equation (Considering small deformations only):

\[ \varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}) \]  
\[ (3.8) \]

For viscoelastic materials, the stress is a single valued function of the entire history of the strain, or:

\[ \sigma(t) = \sigma \left\{ \varepsilon(\tau) \right\}_{\tau=-\infty}^{\tau=t} \]  
\[ (3.9) \]

The constitutive equations for anisotropic linear viscoelastic materials can be expressed in the integral forms:

\[ \varepsilon_{ij}(\bar{x},t) = \int_0^t D_{ijkl}(t-\tau) \frac{\partial \sigma_{kl}(\bar{x},t)}{\partial \tau} d\tau \]  
\[ (3.10) \]

or, equivalently

\[ \sigma_{ij}(\bar{x},t) = \int_0^t C_{ijkl}(t-\tau) \frac{\partial \varepsilon_{kl}(\bar{x},\tau)}{\partial \tau} d\tau \]  
\[ (3.11) \]
3.1.2 Viscoelasticity Theory

It is very common in structural analysis and in design to consider the materials used to be linear elastic. Even though it is correct to consider some of these materials to behave linearly elastic, such as metals, there are other different categories of materials that will behave in a different pattern. Materials like glasses, asphalt and living tissues have a time dependent behavior that cannot be considered elastic. This time dependent behavior sometimes is only noticeable within a very long period of time. A good example to be given to illustrate that slow change is glasses. Some churches in Europe that have been built multiple centuries ago have the glasses that cover their windows a little wider at the base than on the top. Other materials such as living tissues show this behavior in a lot faster fashion, probably because of their high percentage of fluids in their composition.

These materials that are time dependent are called viscoelastic. There are different variations such as viscoplastic, viscoelastoplastic and etc. The mechanical behavior of viscoelastic materials is dependent not only on the load or displacement applied time, but also on the rate they are applied. So the mechanical responses of these materials depend not only on the instantaneous load or displacement applied, but on the entire history of it (Christensen R. M., 1982).

Assuming that all materials are linear elastic simplifies the problem enormously when performing structural analysis and design, but this simplification leads to a loss of accuracy, specifically if the analysis is trying to determine some key factors to predict the lifetime of a structural part, such as cracks, fatigue and aging.
The basic concepts of elasticity and viscoelasticity will now be presented for a better understanding of the materials used in this study. These concepts will be fundamental to have a better understanding of the theory behind the behavior of such materials. Viscoelastic materials can behave in both an elastic and viscoelastic manner. As definition, any material that has stress as a single-value continuous function of strain is said to be an elastic material. Behaviors could vary between linear and nonlinear, where if there is no dissipation of energy, the material is considered to be linear elastic (Hookean).

\[ \sigma_{ij}(\bar{x},t) = C_{ijkl}^{E} \varepsilon_{kl}(\bar{x},t) \]  

(3.12)

Where \( C_{ijkl}^{E} \) is the Elastic Modulus Tensor.

Differently from elastic materials, the stress is a single-value continuous function of the strain rate for viscoelastic materials. These materials dissipate energy and the resultant strain rate is proportional to the applied stress. If it is linear, the coefficient of proportionality is called the viscosity and the behavior is called Newtonian. In case the viscosity increases with the strain rate, then the material is non-Newtonian.

\[ \sigma(\bar{x},t) = \eta \dot{\varepsilon}(\bar{x},t) \]  

(3.13)

Where \( \eta \) is the viscosity and \( \dot{\varepsilon} \) is the strain rate

For the behavior of a material to be considered linear, it must satisfy two principles. The first principle is of homogeneity (proportionality) which can be mathematically shown as:
\[ R\{cI\} = cR\{I\} \] (3.14)

The second principle is of superposition (Boltzmann, 1876). Mathematically represented as:

\[ R\{I_1 + I_2\} = R\{I_1\} + R\{I_2\} \] (3.15)

Where \( c \) is a constant and \( R \) depends on the entire history of the input \( I \).

The stress-strain equation for a viscoelastic, nonaging material is given by a convolution integral that takes into consideration the time-history dependency, and can be expressed in function of stress or strain as follow:

\[
\sigma_{ij}(\vec{x}, t) = \int_{0}^{t} C_{ijkl}(t - \tau) \frac{\partial \varepsilon_{kl}(\vec{x}, \tau)}{\partial \tau} d\tau
\]

(3.16)

\[
\varepsilon_{ij}(\vec{x}, t) = \int_{0}^{t} D_{ijkl}(t - \tau) \frac{\partial \sigma_{kl}(\vec{x}, \tau)}{\partial \tau} d\tau
\]

(3.17)

The relaxation modulus can be obtained by performing a relaxation test where a constant deformation is applied to the specimen and the loads are calculated at all times. The creep compliance can also be found by performing a test in which a constant load is applied and the displacements are measured.

Note that the viscoelastic constitutive properties \( C_{ijkl} \) and \( D_{ijkl} \) are not reciprocal like for the case of elastic constitutive properties. Instead, they are related with a convolution integral (Ferry, 1980).
One way to represent the viscoelastic properties is by making an analogy with mechanical analogs composed of springs and dash-pots. This adds real physics to the problem since it relates to the elastic properties constants and to the viscosity of the dash-pots. Another positive point is that the mathematical representation of this analogy is given primarily in the form of exponential functions, which can be easily integrated.

Some examples of the common mechanical analogs:

![Figure 6 - Maxwell and Voigt Mechanical Analogs](image)

The most used analogs to represent the relaxation modulus and the creep compliance are respectively the generalized Maxwell model and generalized Voigt model. With these models, very long periods of time can accounted for, just by adding more springs and/or dash-pots.

![Figure 7 - Generalized Maxwell and Voigt Analogs](image)
The resulting model from the generalized Maxwell model and generalized Voigt model are also known as the prony series (or Dirichlet series) and they are given as the following equations:

\[
E(t) = E_\infty + \sum_{i=1}^{n} E_i e^{-t/\tau_i} \tag{3.18}
\]

\[
D(t) = D_0 + \frac{t}{\eta_\infty} + \sum_{i=1}^{n} D_i (1 - e^{-t/\tau_i}) \tag{3.19}
\]

The relaxation modulus \( C_{ijkl} \) and Creep Compliance \( D_{ijkl} \) tensors have each 21 unique coefficients for an anisotropic material. If we assume the material to be isotropic, we can reduce the number of coefficients to only two and rewrite the stress-strain equation as:

\[
\sigma_y(x,t) = \int_0^t \lambda(t-\tau) \frac{\partial \varepsilon_{ik}}{\partial \tau} \delta_{ij} d\tau + \int_0^t \mu(t-\tau) \frac{\partial \varepsilon_y}{\partial \tau} d\tau \tag{3.20}
\]

Where \( \lambda(t) \) and \( \mu(t) \) are the Lamé constants, and

\[
\delta_{ij} = \begin{cases} 
1, & i = j \\
0, & i \neq j
\end{cases}
\]

For the problem of a uniaxial bar that we solve in this study, this relation can be simplified to two 1-D equations in function of stress and strain:

\[
\sigma(t) = \int_0^t C(t-\tau) \frac{\partial \varepsilon(t)}{\partial \tau} d\tau \tag{3.21}
\]

\[
\varepsilon(t) = \int_0^t D(t-\tau) \frac{\partial \sigma(t)}{\partial \tau} d\tau \tag{3.22}
\]
3.1.3 Multiscaling

Many materials known and used today in a large variety of applications are composed of multiple materials. A few examples are the asphalt that paves roads, the concrete on nearly every building and virtually every living tissue, a type of material that is currently under the spot lights. Many of these materials may seem homogeneous at a first glance, but shows heterogeneity if looked with more careful eyes. The idea behind using heterogeneous materials is to take advantage of the particular properties of each of the material’s constituents. This way the composite material can become more of what it is designed to be, stronger, lighter, long lasting. To design these composite materials, some experiments are necessary to characterize the respective material properties for each configuration. But there are too many variables in the design that needs to be accounted for and to perform all these test can be costly and time consuming. Instead, a model that has the capability to minimize these extensive laboratory tests and field investigations, substituting them with numerical simulations is necessary. Using a model is much cheaper and safer than running real experiments on a laboratory since there is no use of real materials involved and the simulations are all made in a computer.

The model has to be capable of modeling every geometric feature and materials of the microstructures. It needs to be able to predict the mechanical responses at the smaller length scales and how it could affect the problem at a macroscale level. Small cracks are good examples to illustrate that need because they can start very small, in the same order of magnitude as the smaller scales, and then propagate to the size and magnitude of the global scale, where could lead to failure.
A simple way to do so is to use brute force and use a mesh refined to a point where every aspect of the microstructures of the local scales can be included in the mesh of the problem. The problem is that these small structures are usually three orders of magnitude smaller than the macrostructure itself, and it could get smaller and smaller depending on how deep into the material it is desired to get into. Refining the mesh like this would represent an enormous increase in the overall number of nodes and elements as well as the memory required to store all that information. But memory is just a fraction of the problem created with the refinement of the mesh, finding a computer with enough computational power that could solve the problem would be a challenge, if not completely unfeasible with today’s reality. So unfortunately, a problem with this size creates an unreasonable demand for technology that is currently not available today.

This concept is called multiscaling (David H. Allen, 2008) and its theory is based on classical elasticity theory. A constitutive test on a specimen made of the same material as the object analyzed is performed in order to obtain its constitutive properties. Once with that information, we can also find what the deformations, strains and stresses are. The test needs to follow certain rules to be declared valid. The state of stress and strain should be measurable in the specimen when loaded and the object should be statistically homogeneous.

The term “statistically homogeneous” may not be the best one to be used, but it has been used in past studies and we will use it as it is for now. The real meaning behind is that any spatial variations in magnitude of the strains and stresses observed in the specimen are small if compared to the average strains and stresses obtained on the performed constitutive test. This is because the specimen itself is many orders of
magnitude bigger than the smallest length scale where asperities start to show in the test specimen.

The idea behind multiscale models is to determine the local average global constitutive behavior of heterogeneous materials taking in consideration the effects of the microstructures. Let’s now consider an object that at the global scale is statistically homogeneous, but at the local scale is microscopically heterogeneous.

![Representation of Multiple Scales](image)

**Figure 8 – Representation of Multiple Scales**

The initial boundary value problem (IBVP) for the global object is posed as follows:

(i) Conservation of linear momentum

\[
\sigma^\mu_{\nu,\nu} + \rho^\nu b^\mu = \rho^\mu \frac{d^2 u^\mu}{dt^2} \text{ in } V^\mu
\]  

(3.23)
Where the superscript $\mu$ stands for the global length scale, $\sigma_{ij}^{\mu}$ is the Cauchy stress tensor, $\rho^{\mu+1}$ is the mass density of the object, $b_{j}^{\mu}$ is the body force vector per unit mass, $u_{i}^{\mu}$ is the displacement vector and $V^{\mu}$ is the volume of mass object at the global scale.

(ii) Conservation of angular momentum

$$\sigma_{ij}^{\mu} = \sigma_{ji}^{\mu} \text{ in } V^{\mu}$$  \hspace{1cm} (3.24)

(iii) Small strain-displacement relation

$$\varepsilon_{ij}^{\mu} = \frac{1}{2} (u_{i,j}^{\mu} + u_{j,i}^{\mu}) \text{ in } V^{\mu+1}$$  \hspace{1cm} (3.25)

Where $\varepsilon_{ij}^{\mu}$ is the infinitesimal strain tensor defined on the global length scale.

(iv) Constitutive equations

$$\sigma_{ij}^{\mu} (t) = \Omega_{t \to -\infty}^{\varepsilon_{ij}^{\mu}} \{ \varepsilon_{ij}^{\mu} (\tau) \} \text{ in } V^{\mu}$$  \hspace{1cm} (3.26)

Where $\Omega_{t \to -\infty}^{\varepsilon_{ij}^{\mu}}$ is a functional mapping that accounts for history dependent effects, such as viscoelasticity, and it is determined from the locally averaged constitutive behavior.

If appropriate initial and boundary conditions are applied to equations (3.23) to (3.26) then it will be a well posed initial boundary value problem (IBVP). The initial boundary value problem for the representative volume element have the same set of governing equations, except for constitution as the global structure. The boundary
conditions for the local scale should be determined by the traction or deformation on the global scale, but mapped into the local coordinate system.

Now considering that the micro scale is large enough that continuum mechanics still applies, the local IBVP will look similar to the global one, but some assumptions are necessary in order to simplify the problem. For practical reasons, it is assumed that the global length scale is much larger than the local length scale:

$$\ell^\mu \gg \ell^{\mu+1}$$

(3.27)

Another assumption is that the local length scale is also much larger than the length scale associated with any cracks that may develop at the local scale. This assumption is intended to avoid the possibility of statistical inhomogeneity at the local scale:

$$\ell^\mu \gg \ell^c$$

(3.28)

This assumption simplifies the connecting relationships between the global and local scales. Finally, as is true for many practical applications, we also assume that the length of the wave propagating on the global scale is much larger than the local scale length

$$\ell^w_{\mu} \gg \ell^{\mu+1}_w$$

(3.29)

such that the local initial boundary value problem (IBVP) can be simplified to a quasi-static problem. Therefore, the local scale IBVP is given by:

(i) Conservation of linear momentum
\[ \sigma_{i,j}^{\mu} + \rho^{\mu} b^\mu_i = 0 \text{ in } V^\mu \]  \hspace{1cm} (3.30)

Where \( \mu \) stands for the local length scale.

(ii) Conservation of angular momentum

\[ \sigma_{ij}^{\mu} = \sigma_{ji}^{\mu} \text{ in } V^\mu \]  \hspace{1cm} (3.31)

(iii) Small strain-displacement relation

\[ \varepsilon_{ij}^{\mu} = \frac{1}{2} (u_{i,j}^{\mu} + u_{j,i}^{\mu}) \text{ in } V^\mu \]  \hspace{1cm} (3.32)

(iv) Constitutive equations

\[ \sigma_{ij}^{\mu}(t) = \Omega_{x=\mu}^{\infty} \{ \varepsilon_{ij}^{\mu}(\tau) \} \text{ in } V^\mu \]  \hspace{1cm} (3.33)

(v) Fracture criterion

\[ G_i^{\mu} \geq G_{i_i}^{\mu} \Rightarrow \frac{\partial}{\partial t} (\partial V_i^{\mu}) > 0 \text{ in } V^\mu \]  \hspace{1cm} (3.34)

Where \( G_i^{\mu} \) is the fracture energy release rate in a particular point in the local scale and \( G_{i_i}^{\mu} \) is the critical energy release rate of the material at that particular point. For last, from the locally averaged solution of the cohesive zone IBVP given by (C. Yoon and D. H. Allen, 1999), the following traction-displacement relationship is assumed to hold for the viscoelastic cohesive zones:

\[ \text{\ldots} \]
\[ t_i (t) = \frac{1}{\lambda} \frac{[u_i]}{\delta_i^*} \left[ 1 - \alpha (t) \right] \left\{ \sigma_i^f + \int_{t_0}^t E_{cz} (t - \tau) \frac{\partial \lambda}{\partial \tau} d\tau \right\} \text{ in } \partial V_{cz}^n \]  

(3.35)

A thorough explanation about this topic can be found at (Souza, 2009), where \( t_i^* \) is the traction vector acting on the boundary of the cohesive zone, \( u_i \) is the cohesive zone opening displacement, \( \delta_i^* \) are empirical material length parameters (typically reflecting a length scale related to the cohesive zone), \( \sigma_i^f \) is the required stress level required to initiate damage, \( E_{cz} \) is the uniaxial relaxation modulus of a single fibril in the cohesive zone, \( \alpha(t) \) is the internal damage parameter with respect to the cross-sectional area of idealized cohesive zone, and \( \lambda \) is the Euclidean norm of the cohesive zone opening displacements as:

\[ \lambda = \sqrt{ \left( \frac{[u_r]}{\delta_r^*} \right)^2 + \left( \frac{[u_n]}{\delta_n^*} \right)^2 + \left( \frac{[u_s]}{\delta_s^*} \right)^2 } \]  

(3.36)

in which \( n \) stands for normal direction and \( r \) and \( s \) for tangential directions.

**Connecting Length Scales**

In order to complete the description of the multiscale model, a relationship connecting both length scales needs to be established. In other words, mathematical relationships that can be used to relate the kinetics and kinematical field variables of the local length scale to those of the global length scale needs to be developed. One way to link the local scale field variables to the global scale counterparts is via the use of mean fields, also called a homogenization principle.
In analogy with continuum mechanics, where the strain tensor is defined on the faces of an infinitesimal cube as the volume of the cube goes to zero, one can use the assumption of $\ell^{\mu+1} \gg \ell^\mu$ to define the strain tensor on the global length scale as the external boundary average of the displacements on the local length scale:

$$\varepsilon_{ij}^{\mu+1} = \bar{\varepsilon}_{ij}^\mu - \bar{\alpha}_{ij}^{\mu+1} \quad (3.37)$$

Where:

$$\bar{\varepsilon}_{ij}^\mu = \frac{1}{V^\mu} \int_{V^\mu} \varepsilon_{ij}^\mu dV \quad (3.38)$$

$$\bar{\alpha}_{ij}^{\mu+1} = \frac{1}{V^\mu} \int_{\partial \mathcal{V}^\mu} \frac{1}{2} (u_i^\mu n_j^\mu + u_j^\mu n_i^\mu) dS \quad (3.39)$$

The volume averaged strain on the local length scale is $\bar{\varepsilon}_{ij}^\mu$ and the internal boundary average of displacements on the local length scale is $\bar{\alpha}_{ij}^{\mu+1}$. The external boundary of the local length scale is $\partial \mathcal{V}^\mu$ and the outward unit normal vector to the external boundary surface is $n_i^\mu$.

Now consider the following mathematical expansion for the global length scale stresses in terms of the local stresses:

$$\sigma_{ij}^{\mu+1} = \bar{\sigma}_{ij}^\mu + \sum_{j=1}^{\infty} \frac{1}{V^\mu |x_k|^j} \int_{\mathcal{V}^\mu} (\sigma_{ij}^\mu - \bar{\sigma}_{ij}^\mu) |x_k|^j dV \quad (3.40)$$

Where the volume averaged stress at local scale is:
\[
\bar{\sigma}_{ij}^\mu = \frac{1}{V^\mu} \int_{V^\mu} \sigma_{ij}^\mu dV
\] 

(3.41)

and the terms in the summation in equation (3.40) represent the higher order area moments of the stress tensor.

Similarly, one can also show the relation for mass density:

\[
\rho^{\mu+1} = \frac{1}{V^\mu} \int_{V^\mu} \rho^\mu dV
\] 

(3.42)

Finally it is necessary to establish a constitutive relationship at the global length scale based on the local scale constitution. This can be done by direct substitution of the local scale constitutive equation (3.26) into the volume average of stresses (3.41). However, it is worthwhile to note that the global scale constitutive equation should relate the external boundary averaged stresses (or, equivalently, the volume averaged stresses) to the external boundary average strain.

### 3.1.4 Mesh Convergence

This section describes one of the most overlooked issues that affect accuracy, mesh convergence, and will talk about the importance of it. Mesh convergence refers to the smallness of the elements required in a mesh so that the results of an analysis will not be affected by changing the size of the elements. The problem of mesh size is important in all analyses, except for a few other issues that affect the selection of an appropriate element size in more advanced analyses.
Convergence Curve

For a mesh convergence study, it is required to generate a curve of a critical result parameter (usually some kind of stress) in a specific location of the mesh geometry, to be plotted against some measurement of element density. At least three different meshes with different element sizes will have to be used in the same simulation in order to check for convergence. A plot of the critical parameter chosen with give a curve which will be used to indicate when convergence has been achieved, or in a bad case scenario, how far away the finest mesh is from full convergence. If the last two runs of different element sizes give the same result, convergence has already been achieved and no more runs to check for convergence will be necessary.

Figure 9 - Mesh Convergence Curve
Local Mesh Refinement

In theory, for each successful refinement of the mesh in the convergence study, all elements in the mesh should have its size reduced. This is an important requirement, but it is not necessary to do this over the entire mesh. St Venant's Principle says that stress and deflection far from the applied load can be represented by a statistically equivalent loading scenario. With that principle in mind, we should be able to test convergence of a model by refining the mesh only in the regions of interest to us, and keep the other regions somewhat unrefined. There should also be transition regions, from the big unrefined elements to the fine meshes.

Boundary Geometry

Using linear, or straight sided, elements can cause the resulting stresses to vary and lose accuracy if these elements are trying to represent a curved edge or surface. The curved shape will be better modeled as the mesh gets more refined, and so will the stresses. This is a geometry effect, different from mesh convergence, which is numerical. Another option would use a quadratic or higher order element to represent these curves shapes.

Meshing Strategy

If the model is required to obtain accurate results for the stresses only at certain regions of interest of the mesh, then those elements standing away from these regions have only the simple role of representing geometry and transmitting the load they are
subjected to. These elements demand a much lower level of refinement and can be considerably larger if compared to those that will be responsible for predicting accurate stresses, but they still need to have all the required constraints to deliver reasonable results.

**Examples of Bad Practice**

*Element Size as a Measure of Convergence*

It should be clear that assuming a mesh is convergent for stress just by comparing the element size with a convergent mesh in a non-similar model or even in the same model but in different locations is not correct and is not valid.

The accuracy of stress results is dependent on the element size to some extent, but another factor will play a role on the convergence of the mesh. The element’s proximity to a stress concentration and/or variation of the load distribution on the structure of interest can be just as important as the element size, if not more.

*A Common Case of Ignoring Convergence*

The image on the right shows a 2D or 3D mesh region, representing an internal sharp corner. No radius has been modeled, and an internal corner with zero radius like the one shown could have an infinite stress (theoretically), if the material used is perfectly elastic. This has nothing to do with any
numerical errors created by the use of an FEM code, but because the stress concentrations in geometries like this can reach the infinite in most cases.

Stresses will increase without limit the more the mesh gets refined, but these values for the stresses predicted by a FEM code have nothing to do with any real values in the real world. Quite often, sensible stresses can be predicted by representing an internal corner as shown, but that doesn’t mean they are valid or correct. The radius for the corner at the drawing should be represented with a reasonable number of elements spaced around the area of the corner in order to achieve accurate results.
CHAPTER 4

4.1.1 Code Description and Verification

The main goal of this chapter is to numerically verify the multiscale computational model for impact problems in heterogeneous media developed by Souza (2009). There are analytical and computation solutions for multiscale models, but only solutions for simple geometries and without taking into account evolutionary damage growth are available analytically. Computational models based on finite element methods (FEM) can handle more complex geometries being able to solve more practical problems, reason why they have been so widely used. But most of the models already developed in the literature don’t take into consideration the inertial effects, so the models are not accurate for predicting the behavior of composites subjected to impact loads. The theory we will use is the one developed by (Souza F.V. A. D.-R., 2008). Also as for computational purposes we will be using the same Finite Element Methods (FEM) code and we will verify it with different analytical and numerical solutions for multiple variables, such as displacements and stresses.

4.1.2 Code Description

In this chapter, the code used based on Finite Element Methods (FEM) will be presented. All the simulations and analyses were performed using this code and its ability to predict the correct and accurate mechanical responses of single and multiscale problems will be demonstrated. The code has been written in C++, an object oriented programming language that has advantages such as code re-use, simpler extensibility and
maintainability, as well as a powerful debugger for catching errors and compilation. It solves one, two and three dimensional thermo mechanical continuum problems that can use elastic, plastic and viscoelastic materials in the model. Plane stress and plane strain type of problems can be simulated with the code that uses triangular, quadrangular and other higher order finite elements, but for this thesis, linear triangular finite elements T3 were used.

![Triangular Finite Element](image)

**Figure 10 - Triangular Finite Element**

As for pre and post processing, a commercial software together with a home developed pre and post processor was used in order to extract the values from the variables of interest for the study. Movies and snapshots were also generated with the last mentioned piece of software and these images will be available in this thesis as well as in attached files on the internet.

A summarized description of how the Finite Element Methods code works is presented in the next figure as a flowchart. It gives a better picture of how the multiscale interaction occurs step by step.
Figure 11 – Flowchart of the Multiscale Computational Algorithm (Souza, 2008)

Where:

\( d \) - displacement

\( \nu \) - velocity

\( a \) - acceleration

\( F_{\text{ext}} \) - external forces

\( F_{\text{int}} \) - internal forces

\( \bar{\varepsilon} \) - homogenized strain

\( \bar{\sigma} \) - homogenized stress

\( \bar{M} \) - homogenized mass

\( \bar{C} \) - homogenized constitutive tensor
4.1.3 Code Verification

The FEM code needs to be run and compared to other solutions in order to verify the model and prove it is correct and accurate. The verification can be obtained by solving problems in which analytical solutions are obtained and compared to the numerical results given by the FEM simulation code used. Another way to verify the code would be to perform experiments and compare the numerical solutions from the FEM code to the results given by the experiments. However, this approach can become extremely expensive and sometimes unfeasible to be performed, such as an experiment to simulate the mechanical response of human brain tissues under the pressure generated by explosive devices. Furthermore, the main purpose of this research work is to verify the code for cases where damage evolves in the form of micro cracks. At least to the knowledge of the author, there is no available analytical solution for dynamic/impact problems with growing cracks. For that reason, the results from simulations using the multiscaling approach will be compared against results from direct simulations using the so-called over-killed method, which considers all heterogeneities explicitly in the global scale mesh and will be simply referred to as single scale.

This very fine mesh is refined to the point where the microstructures of interest (e.g. fibers, voids, cracks) can be explicitly included in the FE mesh and can be simulated or changed as a design variable. The use of such fine meshes requires the use of a large number of nodes and elements in order to account for these small microstructures, so that an unreasonable amount of time is usually needed to perform the simulation. Due to the limited amount of computational power available at the present moment, real applications
cannot be simulated using the over-killed method, being that one of the main reasons for the use of multiscale approaches. Therefore, simplified one-dimensional problems are herein idealized so that solutions by the over-killed method can be obtained. The amount of computational time required to solve the same problem using different approaches, i.e., the multiscale and single scale over-killed approaches, are compared in order to demonstrate the gain of the multiscale approach.

The computational model is first compared to the analytical solution developed by (Souza, 2009) for two scale impact problems in elastic heterogeneous materials for which both the elastic modulus and mass density vary exponentially in space as shown in Figure XX, but no damage is considered.

![Figure 12 - Material Properties Distribution](image)

The next equations show the boundary and initial conditions of the problem as followed by the elastic modulus and mass density as just described:

Boundary conditions:
\[ u(0,t) = 0 \]  \hspace{1cm} (4.1)

\[ \frac{\partial u}{\partial x}(L,t) = \frac{F(t)}{E(L)} \]  \hspace{1cm} (4.2)

Initial Conditions:

\[ u(x,0) = 0 \]  \hspace{1cm} (4.3)

\[ \frac{\partial u}{\partial t}(x,0) = 0 \]  \hspace{1cm} (4.4)

Elastic modulus and Density:

\[ E = E^0 \cdot e^{(-x/\delta)} \]  \hspace{1cm} (4.5)

\[ \rho = \rho^0 \cdot e^{(-x/\delta)} \]  \hspace{1cm} (4.6)

Where:

\[ E^0 = 6933.29 \]

\[ \rho^0 = 1375.16 \]

\[ \delta = 2 \]

The equation that describes the motion of the bar and was first defined to start the problem can be written as:

\[ u(x,t) = -0.0002884633414 + 0.000288463312e^{\frac{t}{2}} + e^{\frac{t}{2}} \left( \sum_{j=1}^{100} R_j Cos(a_jx)a_j Cos(2.245527271k_jx) \right) \]  \hspace{1cm} (4.7)
Figure 13 shows a representation of these results found by Souza where the analytical solution is compared to the numerical results given by the model when using the single scale and multiscale approaches.

![Figure 13 - Results for an Elastic Heterogeneous Uniaxial Bar](image)

### 4.2 1-D Uniaxial Bar

The problem of interest has been reduced to 1-D in order to minimize the degree of complexity and make it possible to solve problems with over-killed meshes. 2-D problems are considered later in this chapter. All simulations have been performed on a Dell workstation with 8 Intel processors running at 3.0 GHz clocks. Linux Fedora 10 was the operational system installed. A total of 32Gb are available in the workstation, but only a few megabytes are necessary to run the problem shown in this chapter.

The first problem considers a 1-D uniaxial bar with a finite region of heterogeneity at its mid section, but homogeneous everywhere else.
The heterogeneities are placed in the middle section of the bar so that a pulse wave is not affected by waves reflecting from the boundaries of the bar. In order to satisfy the assumptions on the physical length scales (reference to eq.), required by the multiscale model, and to minimize the number of nodes and elements in the FE mesh, a convergence study over the size of the heterogeneities was performed. The selected size was of approximately 100μm. This size does not correspond to real inclusions or fibers used in industry.

The bar is subjected to an impact load of 10N of magnitude at the right tip for a short period of time. The load is rapidly increased until it reaches 10N and is then held constant for about 60 microseconds, finally being released and quickly going back to zero as shown next in Figure 15.
The total time is 1000 microseconds. This problem attempts to illustrate the effects of a stress wave traveling through a heterogeneous uniaxial bar and how its mechanical behavior is affected by the presence of heterogeneities. This is a 1-D simplification for a composite material constituted of fibers (carbon, glass) embedded in a matrix (epoxy). The reason why the heterogeneous material is in the middle of the bar between two large sections of homogeneous material is so that any effects due to the interaction of the stress wave with the boundaries can be minimized and possibly avoided, causing minor influence on the overall solution of the problem.

The geometry and boundary conditions are presented in Figure 16. As it can be seen, any lateral deformation of the bar has been constrained. The left tip is also constrained in the x-direction and the load is applied at the right tip of the bar (x=L). The Y axis is magnified by a factor of 100 times to facilitate the plotting of contours (all snapshots will have the same magnification factor through the end of this chapter).
Both the singlescale and multiscale simulations had a unique global mesh, where the inclusions were explicitly modeled at the single scale mesh and represented by multiscale elements on the other case. These multiscale elements had another mesh (local scale mesh) with the microstructures attached to each integration point of every one of them in the global scale mesh. A convergence study was conducted for the global meshes as well as for the local mesh in the case of a multiscale analysis. As for the number of nodes and elements of each mesh, Table 01 is provided with more details:

<table>
<thead>
<tr>
<th>Meshes</th>
<th>Number of Nodes</th>
<th>Number of Elements</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiscale</td>
<td></td>
<td></td>
</tr>
<tr>
<td>global</td>
<td>1682</td>
<td>840</td>
</tr>
<tr>
<td>local</td>
<td>24</td>
<td>11</td>
</tr>
<tr>
<td>Singlescale</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>2762</td>
<td>1380</td>
</tr>
</tbody>
</table>

Table 1 - FE Meshes Setups
Figure 17 – Different Meshes for the Singlescale and Multiscale Problems

Figure 17(a) shows the FE global mesh for the single scale problem where the inclusions were explicitly included at the global scale. On the other hand, Figure 17(b) shows the meshes for the multiscale problem, including the local mesh attached to each integration point of the selected multiscale elements. The section of the global mesh where local analyzes were performed is represented by a homogenized material, as its properties will come from the local analyses.

PRESENTING RESULTS

The mechanical behavior of the uniaxial bar will be further analyzed at different points of interest over the bar. For instance, the displacements and stresses resulting from the simulations using a singlescale and a multiscale approach will be plotted side by side for the points at the right tip of the bar where the load was applied and in the middle of the bar, where the inclusions were inserted. Figure 18 shows how to interpret the results for the displacements, presenting a general snapshot of the stress contour over the bar for
each moment in time and the direction in which the wave was traveling at that time. Note that case number 1 displays the general pattern (as if there were no inclusions) for the displacements at the right tip of the bar as the stress wave travels with time, while case number 2 shows the same general pattern, but for the middle point of the uniaxial bar where the inclusions were.
Figure 18 - 1) Shows a general pattern for the displacement against time at the tip of the bar, while 1) shows the same general pattern for the displacements at the middle of the bar

4.2.1 Elastic Case

As for the first example, two elastic materials were chosen to represent the inclusions and matrix in the problem. As mentioned in the beginning of this chapter, the FE code herein used has been previously verified for an elastic heterogeneous uniaxial...
bar where the properties (Young’s Modulus, Poisson’s ratio and density) of the materials varied exponentially as a function of the position over the X axis.

The first set of material properties chosen intends to represent a composite material, such as glass fibers embedded in an epoxy matrix. A Young’s modulus of 10GPa, as opposed to the usual value of 70GPa for glass fibers (ref), has been ultimately chosen to represent the inclusions in the material as an attempt to minimize great localization of the field variables around the inclusions, which could bring inaccuracies, especially in the case where cracking is considered. The properties are the following:

<table>
<thead>
<tr>
<th>Material</th>
<th>$E$</th>
<th>$\rho$</th>
<th>$\nu$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fiber</td>
<td>10.0GPa</td>
<td>1760Kg/m$^3$</td>
<td>0.3</td>
</tr>
<tr>
<td>Matrix</td>
<td>3.35GPa</td>
<td>1170Kg/m$^3$</td>
<td>0.3</td>
</tr>
</tbody>
</table>

*Table 2 - Material Properties for Elastic Case*

As for illustration only, the effects of how a large difference in the material properties could potentially change how the waves are reflected when crossing boundaries will be shown. This difference is more predominant for the single-scale case and can be seen on the sequence of snapshots from the simulation shown next compared to the multiscale case.
Figure 19 - Wave Reflection When Crossing Boundaries. Left side a) shows snapshots for the single scale case and right side b) shows the snapshots that represent the equivalent multiscale simulation.

The same doesn’t happen with the same intensity for the multiscale case because the current multiscale model cannot account for waves reflecting on the internal...
boundaries of the local scale. Once again, this phenomenon was not studied in detail and will not be fully discussed in this study.

Finally, the simulation of the elastic uniaxial bar with inclusions in the mid section was performed, using both the singlescale and the multiscale approaches. As for the duration time of the simulations, the single scale problem faces many disadvantages, such as the ones described next

- As of today, it can only use one processor at a time, even if more are available. This limitation can be overcome with parallelization of the global scale too.
- A very fine mesh is necessary to explicitly include the microstructures in the problem, which implies in a large amount of computational time.
- With the refined mesh, smaller time steps have to be used in order to satisfy the critical time step criterion and avoid numerical errors.

This means that an analysis that uses a singlescale method will generally have a much larger number of degrees of freedom than if the multiscale method was to be used to represent the microstructures of a material. Furthermore, the singlescale method usually requires more time steps to simulate the same amount of time that the multiscale does, because the critical time step is smaller. This is because the elements in the refined mesh of the singlescale problem are smaller than the ones requires for the multiscale case, so a smaller time step is necessary. A further parallelization of a singlescale analysis is possible and would greatly help with the processing time required to solve a single scale simulation, especially when using large over-killed meshes.
For this example problem, the total execution time when using the singlescale method was of 25.3 hours, using a time step size of 10ns and a total of 100k time steps while the simulation that used the multiscale approach was able to use a time step 10 times larger of 100 ns requiring only 10k time steps to simulate the same period of time, taking a total of 1.55 hours to finish (when using 8 processors in a Dell workstation @ 3.0GHz). This is a significant difference of over 16 times faster simulation time for this case, which can make possible to solve very complex problems that couldn’t be solved in a singlescale analysis with the current computational power available, and more importantly, having micro structural details as part of the design variables of the problem.

<table>
<thead>
<tr>
<th>Timestep Size (ns)</th>
<th># of Timesteps (K)</th>
<th>Total Time (h)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Singlescale</strong></td>
<td>10</td>
<td>100</td>
</tr>
<tr>
<td><strong>Multiscale</strong></td>
<td>100</td>
<td>10</td>
</tr>
</tbody>
</table>

*Table 3 - Simulation Details*

Figure 20(1) shows the displacements and stresses at the right tip of the uniaxial bar:
Similarly, Figure 20(2) shows the displacements and stresses for the elastic case at the middle of the uniaxial bar (where the inclusions are):
After analyzing the output from the simulations, a maximum difference of approximately 1.6% between the singlescale and multiscale results was observed for the displacement at the tip of the bar. The results found at the middle of the bar had even smaller differences (less than 1%). This is a small error in many engineering applications and can be neglected for most cases. On the other hand, running singlescale simulations of real complex applications considering the microstructures explicitly is just not possible.
with the current available computational power, which makes the current model very attractive.

**4.2.2 Viscoelastic Case**

Next step in the study was to compare the results from both singlescale and multiscale simulations, assuming now the matrix to be linear viscoelastic, instead of elastic as before. Also, the FE code has already been verified for the case of a singlescale semi-infinite viscoelastic rod and has been address by (ref. to Christensen – theory of viscoelasticity), by comparing the available analytical solution to the problem against the numerical results from the FE code. The code is herein checked against a numerical reference solution for the viscoelastic case. The arbitrarily chosen material properties used in this example are given in the following table:

<table>
<thead>
<tr>
<th>Bulk Materials</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Fiber</strong></td>
</tr>
<tr>
<td>$E$ (GPa)</td>
</tr>
<tr>
<td>10</td>
</tr>
<tr>
<td><strong>Matrix</strong></td>
</tr>
<tr>
<td>$\rho$ (s)</td>
</tr>
<tr>
<td>$i$</td>
</tr>
<tr>
<td>$\infty$</td>
</tr>
<tr>
<td>1</td>
</tr>
<tr>
<td>2</td>
</tr>
<tr>
<td>3</td>
</tr>
<tr>
<td>4</td>
</tr>
<tr>
<td>5</td>
</tr>
<tr>
<td>6</td>
</tr>
<tr>
<td>7</td>
</tr>
</tbody>
</table>
As expected, the results for the viscoelastic case differ from the elastic one, as can be seen in Figure 22 and Figure 23. The total execution time for the singlescale problem was of 25.7 hours, while the problem that used the multiscale method only took 1.57 hours. That is once again over 16 times faster than the singlescale approach, thus showing the gain in efficiency when the multiscale approach is used, which can be a decisive factor in whether a simulation could or not be performed over a real composite part or structure.

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>594</td>
<td>$10^7$</td>
</tr>
<tr>
<td>9</td>
<td>433</td>
<td>$10^8$</td>
</tr>
</tbody>
</table>

Table 4- Material Properties for Viscoelastic Case
Note from Figure 23(2) that the shape of the applied stress pulse changes as the wave travels through the material. This phenomenon is called material dispersion (Achenbach, 1975) and is basically resulting from the energy dissipation in the bulk viscoelastic material.

Figure 22(1) shows the displacements and stresses, respectively, at the tip of the uniaxial bar where the load is applied, while Figure 23(2) shows the same information,
but for the middle point where the inclusions are located. Note that all variables are always plotted against time for a better understanding of the mechanical behavior as the stress wave travels through the bar.

As expected, the material behaved differently now that viscoelasticity was introduced in the problem. The stresses and displacements observed at the points of interest over the viscoelastic bar were larger and followed a different pattern than the ones found in the all elastic bar. These differences found in the results can be explained by the introduction of a new mechanism of energy dissipation, the viscoelasticity.

Figure 23 - Displacement and Stresses at the Middle Point of the Bar (x=L/2) for Viscoelastic Case
For a better picture of the differences in behavior when different material constitutions are used, a chart with side by side comparisons is presented in Figure 24 for the displacements at the points of interest in the problem. The cases considered are for a homogeneous elastic bar (Shown as Homogeneous), a heterogeneous elastic bar (Shown as Elastic for the singlescale case) and a heterogeneous viscoelastic bar with the inclusions considered to be elastic (Shown as Viscoelastic for the singlescale case).

4.2.3 Damage Case
As for the next step of the analysis of this 1-D example problem, a viscoelastic behavior was used for the matrix material, but now the effect of cracking will be analyzed where the inclusions were explicitly inserted (mid section of the bar) in a singlescale analysis. For the case of multiscale analysis, damage accumulation was considered only at the local scale of the problem. The cohesive zone material properties used herein are shown in the next table and may not reflect real material properties as no experimental measurements for material characterization have been performed. However, the scope of the present study is to verify the model’s capabilities for cases where heterogeneity, viscoelasticity and crack growth are considered.

As previously mentioned, the computational model used herein has been verified analytically for the case of a heterogeneous elastic bar, as well as for the case of a singlescale viscoelastic bar (Souza, 2009). This work attempts now to numerically verify the model for the case when heterogeneity, viscoelasticity and damage are considered, since no analytical solutions are available. This has not been achieved in the literature yet, as far as the author is aware, and since multiscale models are becoming more popular a demand to verify its accuracy has increased. The cohesive zone model used to predict crack propagation is that reported in Yoon and Allen, (1999) and Allen and Searcy (2001). The parameters chosen to define the damage behavior are listed in Table 04. Once more, these values were arbitrarily chosen and may not represent real damage properties since no experiments were performed to determine those.

<table>
<thead>
<tr>
<th>Cohesive Zones</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\delta_n (\mu m)$</td>
</tr>
</tbody>
</table>

As for the next step of the analysis of this 1-D example problem, a viscoelastic behavior was used for the matrix material, but now the effect of cracking will be analyzed where the inclusions were explicitly inserted (mid section of the bar) in a singlescale analysis. For the case of multiscale analysis, damage accumulation was considered only at the local scale of the problem. The cohesive zone material properties used herein are shown in the next table and may not reflect real material properties as no experimental measurements for material characterization have been performed. However, the scope of the present study is to verify the model’s capabilities for cases where heterogeneity, viscoelasticity and crack growth are considered.

As previously mentioned, the computational model used herein has been verified analytically for the case of a heterogeneous elastic bar, as well as for the case of a singlescale viscoelastic bar (Souza, 2009). This work attempts now to numerically verify the model for the case when heterogeneity, viscoelasticity and damage are considered, since no analytical solutions are available. This has not been achieved in the literature yet, as far as the author is aware, and since multiscale models are becoming more popular a demand to verify its accuracy has increased. The cohesive zone model used to predict crack propagation is that reported in Yoon and Allen, (1999) and Allen and Searcy (2001). The parameters chosen to define the damage behavior are listed in Table 04. Once more, these values were arbitrarily chosen and may not represent real damage properties since no experiments were performed to determine those.

<table>
<thead>
<tr>
<th>Cohesive Zones</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\delta_n (\mu m)$</td>
</tr>
</tbody>
</table>
Table 5 - Material Properties for Cohesive Zones

<table>
<thead>
<tr>
<th>$\delta$ ($\mu$m)</th>
<th>0.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>10</td>
</tr>
<tr>
<td>$m$</td>
<td>2</td>
</tr>
</tbody>
</table>

The result for the displacements and stresses at the tip of the uniaxial bar for the case where a heterogeneous viscoelastic bar is considered and damage is accounted for is presented.

Figure 25 – Displacements and Stresses at the Tip of the Bar ($x=L$) for Damage Case
The same results now for another point of interest, in the midsection of the uniaxial bar where the inclusions are located.

Figure 26 - Displacement and Stresses at the Middle Point of the Bar (x=L/2) for Damage Case

Once again, the multiscaling model has proven to be fairly accurate even when damage is introduced in the problem, giving results within a 1.1% error for this particular case. The same pattern in the behavior of the material can be seen if compared to the viscoelastic case without damage, but with a slightly higher dumping factor, which caused the material to suffer more displacement and to dissipate more energy.
The singlescale results for the three cases considered so far is now presented in a chart for a better understanding of the overall difference in displacements and stresses. Again, (1) represents the results found for the point of interest at the tip of the uniaxial bar where the load is applied and (2) for the midsection of the bar where the inclusions are.

Figure 27 - Displacement Comparison among Results for the Singlescale Cases at the tip of the bar (1) and in the middle of the bar (2) (Heterogeneous Elastic as...
Elastic, Heterogeneous Viscoelastic as Viscoelastic and Heterogeneous Viscoelastic with Damage as Damage)

The problems represented in the chart are the ones for the singlescale cases of a heterogeneous elastic uniaxial bar where heterogeneity was introduced in the form of inclusions in the mid section of the bar, embedded in a matrix that behaves elastically. The same configuration, but with a matrix that has a viscoelastic behavior is also presented. As for the last of the functions in the plot, a viscoelastic matrix was considered and the effect of cracking was also taken into account.

The example illustrated by the sequence of snapshots on Figure 28 and Figure 30 show an interesting physical phenomenon that may occur during failure of materials under dynamic conditions. For the particular case of Figure 28, the damage parameters were high enough that most of the energy coming from the wave was already dissipated once it had crossed a few cohesive zones in the mid section of the bar. This example shows the potential of the model to simulate materials that are ultimately designed to absorb upcoming energy. A good example to illustrate this application is a helmet subjected to a pressure wave generated by some sort of explosion, where the primary goal of the helmet is to dissipate the maximum amount of energy, avoiding this energy created with the blast from propagating all the way through the soldier’s brain.

Note on Figure 28 that the stress wave is partially reflected as it encounters the inclusions in the middle of the bar, but part of the energy keeps going further into the inclusions (the wave loses its strength as it encounters more boundaries and is reflected, which is shown on the contour going from dark orange to a light yellow. It may be difficult to see due to the small size of the elements and the borders in black).
Figure 28 - Wave Dissipation
For the next case, a similar situation took place, but now having the damage accumulation reaching an unsustainable point, which caused the bar to fail. The now divided in two pieces uniaxial bar doesn’t let the wave propagate from one side to another, so the wave seems to be trapped in one of the pieces of the bar as can be seen on the next sequence of snapshots on Figure 30. This is a good illustrative example of the behavior of waves traveling through materials that may become fragmented. Modeling fragmentation is a particularly important feature in simulating the interaction between blast waves and materials that may come in contact with the forces generated by the explosion and thus, break during the process. As for practical examples, all types of armor could be mentioned, including military helmets. Figure 29 shows how the damage parameter alpha behaves as the wave hits the cohesive zone at the very first inclusion the wave encounters.

![Graph](image)

**Figure 29 - Evolution of Damage (alpha) for the First Inclusion**

The uniaxial bar used for this problem has a fine with many elements and interfaces that helped increase accuracy of results. Unfortunately not all details could be shown in the figures herein. A zoomed view at the place where the bar failed is presented
for one of the points in time, but could be similarly replicated for the other time steps where the stress wave has already hit, as can be seen next.
Figure 30 - Failure of Bar Trapping Wave
CHAPTER 5

5.1 Example Problems

5.1.1 2-D Uniaxial Bar

After successfully verifying the multiscale computational model for heterogeneous viscoelastic materials accounting for evolving damage utilizing a simplified 1-D problem, the next step in this study is to attempt to solve a similar problem but now in two dimensions. Consider an elastic bar which hits a uniaxial bar made with unidirectional fibers composite in which the fibers are directed out-of-plane.

This represents a much larger computational effort since with another dimension comes more nodes and elements that would end up in a larger mesh as well.

![Boundary Conditions for 2-D Uniaxial bar](image)

Figure 31 - Boundary Conditions for 2-D Uniaxial bar

A two dimensional over-killed mesh with all the heterogeneities in real size explicitly included in the global mesh could be potentially unfeasible to be solved (with the current computational power available to the author). Larger diameter fibers were used first in an attempt to minimize this sudden increase in size of the problem and in order to analyze the effects of diameter size of the fibers in the results, and as computational power allowed, the diameter size of the fibers were reduced in order to
find a trend that would desirably converge to the same results given by using the multiscale method to solve the exact same problem. A 2-D uniaxial bar was chosen once again due to simplicity in analysis and to a more homogeneous stresses field through the bar as the wave propagates.

The material properties were also arbitrarily chosen and have similar values as for the ones presented on previous problems, as shown on the Table next.

| Table 6 - 2-D Uniaxial Bar Material Properties |
|------------------|------------------|
| Bulk Materials   |                  |
| Fiber            |                  |
| $E$ (GPa)        | $\rho$ (s)       |
| Fiber            |                  |
| Fiber            |                  |
| Matrix           |                  |
| $\rho$ (s)       | 1170             |
| $i$              | $E_i$ (MPa)      | $\rho_i$ (s) |
| $\infty$         | 111              | -             |
| 1                | 133              | $10^0$        |
| 2                | 127              | $10^1$        |
| 3                | 209              | $10^2$        |
| 4                | 994              | $10^3$        |
| 5                | 332              | $10^4$        |
| 6                | 465              | $10^5$        |
| 7                | 845              | $10^6$        |
| 8                | 594              | $10^7$        |
| 9                | 433              | $10^8$        |
diameter sizes of the fibers used in the numerical simulation and most important of all, the total simulation time for the singlescale and multiscale cases.

<table>
<thead>
<tr>
<th>Fiber Size</th>
<th># of Nodes</th>
<th># of Elements</th>
<th>Total Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.0mm</td>
<td>853</td>
<td>1522</td>
<td>3.4 hours</td>
</tr>
<tr>
<td>1.0mm</td>
<td>1453</td>
<td>1855</td>
<td>4.1 hours</td>
</tr>
<tr>
<td>0.5mm</td>
<td>4761</td>
<td>9068</td>
<td>39 hours</td>
</tr>
<tr>
<td>0.1mm</td>
<td>46879</td>
<td>103655</td>
<td>~427 hours (not finished)</td>
</tr>
</tbody>
</table>
Convergence Studies

The analysis of the local meshes represent a major part of the total computational time required to solve a multiscale problem, so convergence studies were performed in order to find the best meshes to address the problem with minimum losses in precision and to vary material properties for cases when damage was considered. Multiple tests had to be performed and since damage is only accounted for at the local scale, a simpler problem setup was considered using the local scale meshes as benchmark. The square meshes had movement constrained over the Y axis for the bottom edge and over the X axis for the left edge while a monotonically increased load was applied at the top. Figure 32 shows the boundary conditions as described.
Figure 32 - Boundary Conditions for Converge Studies
The primary variable analyzed was the averaged stress over the entire mesh. Energy is released when cracks are created and when they propagate, which makes the average stresses go down too. Cracks are considered to form at micro scales and have very small lengths, so when one of these small cracks is formed, a small and smooth reduction in the average stresses is expected to occur. The problem is that if only large elements are used in the mesh, in order to create a cohesive zone (cracks are when alpha = 1) of the size of the edges of these large elements takes a considerable amount of energy and could possibly cause a steep fall in stresses, making the average stresses look like a step function as can be seen on Figure 33 for the case of only 110 elements. On the other hand, as the number of elements is increased (reducing the size of the elements), the changes in the average

![Figure 33 - Convergence Study over Number of elements (Ultimately Element Size)]
stress functions become more and more smooth, which is the goal for this convergence study.

Next, from the locally averaged solution of the cohesive zone IBVP given in Chapter 2, a series of damage parameters were adjusted in order to better represent the physics of the problem. The first parameters to be tuned were the $\delta^*$, which are simply empirical material length parameters.

![Figure 34 - Convergence Study over Delta](image)

It is herein considered that the appropriate value for $\delta^*$ is the one in which the average stress function should match the function given when the same problem is solved, but the internal damage variable, alpha, does not evolve.
Another two parameters that were adjusted with the same idea in mind of having a smooth function for the average stress as damage is accumulated were the exponent constant \( m \) from equation 2.14 for the Euclidean norm of the cohesive zone opening displacements, as well as the damage law used from (Searcy, 2001).

![Figure 35 - Convergence Study over M](image-url)
Finally, based on all the results from each of the convergence studies shown above a local mesh with 305 nodes and 628 elements was chosen to be used for all the 2-D multiscale problems in this study. A snapshot of the local mesh was presented on Table 04 together with all the other meshes used herein.

Figure 36 - Convergence Study over Damage Law
To solve this problem in two dimensions using the single scale approach has proven to be very computationally challenging since only one processor could be used at all times (there is a potential to further develop an algorithm to solve one scale problems) while the number of degrees of freedom grows almost exponentially as the diameter size of the fibers is reduced. Even though it was not possible to run a single scale simulation for the case where the diameter size of the fibers was comparable to the diameter of a real fiber glass fiber (70μm), the results shown on Figure 37 and Figure 38 shows a clear trend that as the diameter size of the fibers was reduced, the results from the single scale
case approached the results when using the multiscale method. That shows that if the necessary computational power is available, there is a great chance to verify in two dimensions that the results from the singlescale and multiscale simulations match, as they did in the previous session for the one-dimensional uniaxial bar. Figure 37 shows the displacements and stresses at the tip of the bar (x=L) for a bar where the matrix was considered viscoelastic and the fibers elastic, as shown on table 07.

The next case solved had the same bar and material properties as before, but it also considered crack development and growth with the following properties for the cohesive zones. It is valid to mention that the simulation started with no cohesive zones as they were automatically inserted as the tractions along elements’ edges reached a threshold (sigma F).

<table>
<thead>
<tr>
<th>Cohesive Zones</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Matrix-Matrix</strong></td>
</tr>
<tr>
<td>( \delta_n (\mu m) )</td>
</tr>
<tr>
<td>( \delta_t (\mu m) )</td>
</tr>
<tr>
<td>( \sigma_{n}^{f} (MPa) )</td>
</tr>
<tr>
<td>( \sigma_{t}^{f} (MPa) )</td>
</tr>
<tr>
<td>( A )</td>
</tr>
<tr>
<td>( m )</td>
</tr>
</tbody>
</table>

Table 8 - Material Properties for Cohesive Zones

One of the limitations of the multiscale model as of at the present moment is that it limits damage analysis to only the local scale, which makes it more challenging to match the results to the ones from a single scale case. In a single scale simulation, damage can accumulate significantly more when considering the same problem. This is
because it accounts for damage at all length scales (considering they are all explicitly represented in one fine mesh).

As mentioned before, the first step was to run a simulation using the multiscale method and to keep that as the goal to be matched after running an over-killed mesh single scale problem. With these results in hand, the first single scale problem solved had the larger diameter size for the fibers adopted in this study. After comparing the results they did not match as expected. The size of the fiber diameter was then gradually reduced and so was the difference in the results between multi scale and single scale problems. Even though it was unfeasible to reduce the size of the diameter fiber down to a real physical value, it can be clearly seen from Figure 38 that the problem with the smallest diameter size adopted gave the closest results to the ones when multiscaling was used. This may lead us to believe that a fine enough mesh with an accurate diameter size for the fibers would give matching results between the singlescale and multiscale approaches.
Next, a sequence of snapshots shows the wave traveling through the bar used in the single scale simulation. Note that the stresses doubled when the wave reflected at the boundaries and that caused damage to accumulate every time this happened. Higher damage parameters were used for this specific case so larger cracks could be observed in order to better illustrate how the damage accumulates with time. The “black spots” in the image shows the inclusion of small cohesive zones in the mesh, which happened where the stresses have reached a threshold determined by the input material properties.

Figure 38 - 2-D Uniaxial Bar w/ Damage - Displacements and Stresses @ x=L/2
As previously mentioned, damage is only considered at the local scale level for the multiscale approach, so damage accumulation is usually smaller than for the single scale case. In an attempt to increase the damage accumulation at the local scale, higher damage parameters were used, but with that another problem had to be faced. Higher damage parameter resulted in large cracks, which violates the model assumption that crack lengths are much smaller than the local length scale.
Figure 41 shows a sequence of snapshots that illustrates this problem and how cracks propagate within the mesh of the local structure. The local mesh shown is of the first point of integration for the following multiscale element in the global mesh:

Note on Figure 41 that the automatic insertion algorithm was used in this case and one can clearly see the formation of new boundaries as stresses raise with time. The black lines denote the new edges in the FE mesh (cracks developed) and may reach about half the size of the total cross section area of the mesh itself, which violates the model’s assumptions as previously mentioned.
Figure 41 - Snapshot Sequence for 2-D Uniaxial Bar (local scale)
5.1.2 2-D Cylinder/Plate Problem

Now let’s consider the following example where an elastic cylinder impacts a plate exactly at its center. This is another two dimensional problem made with unidirectional fibers composite in which the fibers are directed out-of plane. As for the 2-D uniaxial bar in the previous example, a large diameter size for the fibers was chosen for the singlescale case and gradually reduced in order to try to reach the same size as real fiber glass. This reduction was limited by the computational power available at the moment, but all the results were compared to the ones given by the multiscale case, which will hopefully show a pattern that as the diameter size of the fibers were reduced, the results got closer to a matching point.

Figure 42 shows the problem setup and the boundary conditions for the problem.

![Figure 42 - 2-D Cylinder/Plate Case Boundary Conditions](image)
The next table shows the meshes used for the Cylinder/Plate problem with different diameter sizes of the fibers for the singlescale case, as well as the global and local meshes used for the multiscale cases. Number of nodes, elements and the total simulation time for each of the singlescale and multiscale cases is also presented.
The two dimensional FE meshes for the global scale considered symmetry of axis in order to reduce computational effort. Once again, the material properties were arbitrarily chosen and have similar values as for the ones presented on previous problems, as shown in Table 9.

<table>
<thead>
<tr>
<th>Bulk Materials</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Fiber</strong></td>
</tr>
<tr>
<td>$E$ (GPa)</td>
</tr>
<tr>
<td>70</td>
</tr>
<tr>
<td><strong>Matrix</strong></td>
</tr>
<tr>
<td>$\rho$ (s)</td>
</tr>
<tr>
<td>$i$</td>
</tr>
<tr>
<td>$\infty$</td>
</tr>
<tr>
<td>1</td>
</tr>
<tr>
<td>2</td>
</tr>
<tr>
<td>3</td>
</tr>
<tr>
<td>4</td>
</tr>
<tr>
<td>5</td>
</tr>
<tr>
<td>6</td>
</tr>
<tr>
<td>7</td>
</tr>
<tr>
<td>8</td>
</tr>
</tbody>
</table>
Table 10 - 2-D Cylinder/Plate Material Properties

| 9 | 433 | 10^8 |

Vertical stresses and horizontal deformation for the back face of the plate were analyzed. Figure 43 shows a sequence of snapshots for the single scale simulation. The elastic material properties for the cylinder impacting the plate are $E=1.0\,\text{GPa}$, $\nu=0.3$ and $\rho=2000\,\text{Kg/m}^3$. Initially, the plate was at rest and the cylinder was traveling at 125m/s. The total time simulated was of 100μs, but the numbers of solution steps and solution step sizes varied according to each problem.

One can clearly see a stress concentration area over the top right and left corners of the plate caused by the boundary conditions adopted for the problem as the cylinder applies more pressure to the center of the plate. Another area with a high stress concentration is the center of the plate, but not quite as much stress as the top corners, as it can be seen on sequence of snapshots on Figure 43.
Figure 43 - Snapshot Sequence for the Single scale 2-D Cylinder/Plate Problem
It was not possible to solve the single scale problem in two dimensions with the actual diameter size of the fibers due to computational limitations. As expected, it could be observed that the global response of the plate was directly affected by the diameter size of the fibers in use. Figure 44 shows that the overall displacement results for smaller diameter sizes approached the ones given by the multiscale case, as expected. This led us to believe that the results would converge if real fiber sizes could be simulated and solved.
With the results obtained for a viscoelastic heterogeneous plate under impact loading, the next step was to include damage in the problem. The same problem of lack of computational power to solve over-killed two dimensional problems was expected, but the main objective was to find a clear convergence trend between the two approaches used as the diameter of fibers is reduced.

<table>
<thead>
<tr>
<th>Cohesive Zones</th>
<th>Matrix-Matrix</th>
<th>Matrix-Fiber</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \delta_n (\mu m) )</td>
<td>0.001</td>
<td>0.001</td>
</tr>
<tr>
<td>( \delta_i (\mu m) )</td>
<td>0.001</td>
<td>0.001</td>
</tr>
<tr>
<td>( \sigma_n^f (MPa) )</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>( \sigma_i^f (MPa) )</td>
<td>120</td>
<td>120</td>
</tr>
<tr>
<td>( A )</td>
<td>0.1</td>
<td>0.1</td>
</tr>
<tr>
<td>( m )</td>
<td>0.5</td>
<td>0.5</td>
</tr>
</tbody>
</table>

Table 11 - Material Properties for Cohesive Zones

Now that the problem accounts for damage accumulation and as high stress concentration areas developed at the corners of the plate, a new challenge was raised when trying to match the results from the multiscale case to the single scale cases. Since damage only occurs at the local scale for the multiscale problem, not as much damage would accumulate when compared to the single scale case.

Higher damage parameters were used for this case in an attempt to create larger cracks, but that caused another problem that has already been faced before. The assumption that crack lengths have to be much smaller than the local length scale is violated when large cracks occur and may lead to inaccurate results.
Figure 45 shows a sequence of snapshots that illustrate large cracks growing at the local scale and causing the violation of the crack length assumption for the model.

---

Figure 45 - Snapshot Sequence for 2-D Uniaxial Bar (local scale)

Note that cohesive zones were only allowed to be inserted between the fibers and the matrix and within the fibers elements for the single scale problem mesh, otherwise there would be major numerical errors due to the high stresses generated at the top left
corner of the plate and the finite element there would break in a very early stage. The results found were compared with the multiscale method against the singlescale results as the diameter size of the fibers was decreased:

![Figure 46 - 2-D Cylinder Place Problem w/ Damage – Back Face Displacements and Stresses](image)

Even a smaller diameter size would be necessary to reach the multiscale limit (local scale << global scale), but they seem to converge as it can be seen from the results on Figure 46.

Besides the unit cell with one central fiber previously used, three other microstructures were herein considered as shown on Table 11. The volume fraction of fibers was kept approximately constant around 33% in all of the new local scale structures. The idea is to analyze the effects of different local scale geometries at the local length scale and how they affect the overall mechanical behavior of the composite plate.
Unit cells with four, nine and sixteen fibers were used in simulations with the same problem setup as single fiber unit cells and compared to one another. Note that the number of nodes and elements in the FE mesh increase as more fibers and other microstructural details are included in the local scale. The size of the local scale meshes should be carefully watched since the local scale analyses combined corresponds to the majority of the computational power used.

The results are presented on Figure 47 and even though the differences among the results when using different numbers of fibers in the volume elements didn’t have a substantial variation, the time required to solve did. While a multiscale analysis using a single fiber unit cell for the local scale analysis took around a day to solve, when changing that to a 16 fibers volume element increased the total simulation time to over 3 days. This is because all microstructures are periodic. Even when 16 fibers are considered, they are arranged in a squared array, so that a unit cell is always an efficient description of the same structure. However, if cracks are allowed to initiate, it is possible that periodicity is broken down, thus giving different results.
Figure 47 – Local Mesh Convergence Study for the 2-D Cylinder Plate Problem w/Damage
CHAPTER 6

6.1 Conclusions

The main purpose of this thesis was to numerically verify a multiscale computational model for predicting the mechanical response of heterogeneous viscoelastic solids containing cracks subjected to impact loading. Displacements, strains and stresses from materials in two length scales can be analyzed with the multiscale model. The effects of time-dependant material behavior and mechanical responses in the local scale are included in the global model for more accurate results. The model could be used in a tool that would assist on the design and improvement of composite materials and structures that have better overall properties such as resistance to heat and corrosion for extreme environments exposure, as well as durability and flexibility for long lasting complex shaped structures. As a result, it could potentially reduce or eliminate the need of costly and time consuming experiments that are necessary for material characterization experimentation since it relies strictly upon the fundamental structural properties of each of the composite’s constituents. It would make predictions due to any alterations in the microstructure a lot easier, such as changing the volume fractions and size of its constituents or the geometry of the microstructures. These new materials could potentially lead to an improvement in the life of many by making safer protection gear, more fuel efficient transportation and more affordable materials as of many examples.

The model is based on finite element methods theory, which has very little limitations on the geometry of objects modeled and number of constituent types included in the mesh. As for performance, the code utilizes a parallelized approach that takes advantage of the fact that each local scale analysis can be performed independently from
each other and from the global scale analysis as well. This is particularly advantageous in case there are a large number of local scales. Once the global analysis is performed, the local scale analysis can be evenly distributed throughout the number of available processors so each processor work independent from each other on their own set of analysis for a faster final complete solution to the multiscale problem. The time required to finish the complete analysis can be greatly reduced proportionally to the number of processors being used. This is a very powerful feature that could be the difference between solving and finding the solution to a problem and an overwhelmingly complicated problem setup that can’t be finished in a reasonable amount of time.

Some example problems have also been shown in order to further verify and demonstrate the capabilities of the proposed model. The results from simulations using the multiscaling approach were compared against results from direct simulations using over-killed meshes, which considered all heterogeneities explicitly in the global scale. A 1-D problem of a uniaxial bar was used for the numerical verification giving satisfactory results when comparing the multiscalar method to the results from an over-killed mesh, while other 2-D problems could not be finished due to limitations in computer power available but showed clear trends of convergence.

There is a great potential for improvement of the model which would make it even more robust and reliable. Some of the topics left for future research and further code implementation are:

- Extent the model capability to solve problems in three dimensions.
- Include the capability to use other types of constitutive models in the problems, such as plasticity and viscoplasticity.
- Implementation of finite deformations for the multiscale model.
- Parallelize the code to solve the global scale meshes using multiple processor.
- Development of an ad-hoc pre/post processor for the FEM code used for a faster setup and analyses of the problems.
- Implementation of higher orders of homogenization theory, so the length of the parameters at the local scale does not necessarily have to be much smaller than the parameters at the global scale.
- Experimentally determine material properties, such as cohesive zones, for materials used in simulations.
- Address the theory regarding the propagation of cracks from the local to the global scale, which has not been fully developed yet
Bibliography


