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Multiscale Modeling of Impact on Heterogeneous Viscoelastic Solids with Evolving Microcracks

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MULTISCALE MODELING OF IMPACT ON HETEROGENEOUS VISCOELASTIC SOLIDS WITH EVOLVING MICROCRACKS

by

Flavio Vasconcelos de Souza

A DISSERTATION

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Multiscale computational techniques play a major role in solving problems related to viscoelastic composite materials due to the complexities inherent to these materials. In the present work, a numerical procedure for multiscale modeling of impact on heterogeneous viscoelastic solids containing evolving microcracks is proposed in which the (global scale) homogenized viscoelastic incremental constitutive equations have the same form as the local scale viscoelastic incremental constitutive equations, but the homogenized tangent constitutive tensor and the homogenized incremental history dependent stress tensor depend on the amount of damage accumulated at the local scale. Furthermore, the developed technique allows the computation of the full anisotropic incremental constitutive tensor of solids containing evolving cracks (and other kinds of heterogeneities) by solving the micromechanical problem only once. The procedure is basically developed by relating the local scale displacement field to the global scale strain tensor and using first order homogenization techniques. The finite element formulation is developed and some example problems are presented in order to verify and demonstrate the model capabilities. A two-scale analytical solution for a functionally graded elastic material subject to dynamic loads is also derived in order to verify the multiscale computational model and additional code verification is also performed. Even though the presented model has been implemented in an explicit time integration algorithm, it can be especially useful when the global scale problem is solved by an implicit finite element algorithm, which requires the knowledge of the global tangent constitutive tensor in order to assemble the corresponding stiffness matrix.
DEDICATION

I dedicate this dissertation to my dear wife Isabela, to my parents, Januario de Souza Neto and Maria de Fatima V. Souza, to my brothers, Fabio V. Souza and Januario de Souza Jr., and to my sister, Fabiola V. Souza, for their unconditional love and support.
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Chapter 1

Introduction

All materials exhibit more than one length scale, at least one molecular scale and a continuum scale. Most materials, natural or engineered, exhibit more than one continuum scale. Examples of multiscale materials found in nature are rocks, soils, geological salt and biological tissues. Examples of multiscale engineered materials are fiber reinforced composites, alloys, cement concrete and asphalt concrete.

From the engineering point of view, heterogeneous materials are desirable because they can be suitably designed to take advantage of particular properties of each constituent. For example, carbon fiber reinforced composites have wide applicability due to their superior thermomechanical performance and low weight, obtained due to the fibers, and their versatility in shape (parts of any shape can be molded) due to the use of epoxy matrix.

Besides the existence of multiple length scales, virtually all materials exhibit time dependent behavior at some time scale. Examples of materials that exhibit history dependent viscoelastic behavior are biological tissues, asphalt materials, composites, rubbers and other polymers. The main concern is perhaps that viscoelastic materials creep so that one should limit the amount of creep deformation in the design process. Viscoelastic materials are however desirable in many applications, especially crash safety and impact-resistant devices.
and other dynamic applications, because they dissipate a significant amount of energy prior to crack formation. In asphaltic pavements, for example, the ability to dissipate energy provides more comfort to users of the roadway. The same concept applies to parts of automobiles and aircrafts, such as tires and other rubber parts.

Impact/dynamic problems have recently gained increasing attention from the research community. The main goal is to develop tools that help in the design of impact resistant devices that use advanced composite and layered materials. The main applications are military protective devices, such as helmets, tank armor and bulletproof jackets, and crash-safety devices that help save lives.

On the one hand, the use of such complex heterogeneous materials requires a reasonable physical understanding of the interactions among all constituents, as well as the eventually evolving internal boundaries (voids, defects and cracks), and their effects on the overall behavior of the material. On the other hand, the consideration of every detail, especially the geometric details, at the lower scales demands an impractical computational effort.

Even though there exist some analytical solutions for mechanics problems involving heterogeneous media, they exist only for simplified geometries and material behavior, so that numerical solutions are often necessary. Direct numerical simulations that account for all heterogeneities are however unreasonable at the currently available level of computer power.

These limitations have lead researchers and engineers to seek alternative approximate approaches that can account for the hierarchical structure of heterogeneous materials without having to model every microstructural detail. One of the most promising of such approaches is the so-called multiscale modeling which overcomes the computational issue of modeling all heterogeneities at once but sacrifices accuracy due to the assumption of separation of length scales. The loss of accuracy may however be negligible if the assumptions are closely satisfied in the real physical problem.

The purpose of multiscale models is to perform simultaneous analyses on all length scales.
The effective constitutive behavior of one scale is then determined by the behavior of each consecutively smaller scale in such a manner that only the material properties of the individual constituents, as well as the fracture properties, need to be known a priori.

In cases where the local structure (representative volume element – RVE) does not change and its behavior does not depend on the loading history so that the effective constitutive properties need to be determined only once, the classical homogenization theory, which aims to determine the effective (homogenized) constitutive behavior of heterogeneous materials a priori, is probably more cost effective. However, multiscale models are particularly advantageous for problems with evolving microstructure and/or evolving internal boundaries since the evolution of internal variables and cracks generally depend on the loading history, especially if viscoelasticity may not be neglected. Furthermore, the loading history is spatially dependent in most structural applications, in which case the homogenized constitutive properties need to be recursively determined for every global scale spatial location (for which the microstructure is evolving) in each step of the analysis.

1.1 Research Objective

The objective of the present study is to develop a computational multiscale model for the analysis of viscoelastic heterogeneous solids containing evolving cracks under impact loading.

Specific objectives are as follows:

- Develop a procedure to determine the spatially varying homogenized incremental (tangent) constitutive tensor and the homogenized history dependent term of viscoelastic materials containing growing cracks;

- Develop a multiscale finite element code that can model multiscale crack formation and propagation in heterogeneous viscoelastic materials;
• Verify the correctness of the developed algorithms through comparisons with simple analytical solutions;

• Perform numerical simulations of more complex problems in order to demonstrate the capabilities of the developed model.

1.2 Layout of Dissertation

Following this introduction, this dissertation is organized as follows. Chapter 2 presents a description and literature review of multiscale models. Chapter 3 presents the procedure developed for computing the incremental (tangent) homogenized constitutive tensor and the homogenized history dependent term for viscoelastic heterogeneous media containing cracks. Chapter 3 also provides the finite element formulation of both global and local initial boundary value problems and some example problems in order to verify the procedure developed herein. Chapter 4 describes the developed finite element code as well as its implementation details and features. Verification problems and comparisons with analytical solutions are presented in Chapter 5 and applications problems are discussed in Chapter 6. Chapter 7 presents the conclusions of this research, pointing out current limitations and potential future research topics.
Chapter 2

Multiscale Models

Engineered and natural materials are heterogeneous at a certain length scale. The hierarchical morphology and properties of heterogeneities may have a substantial impact on the overall properties of the materials. It has been observed that the overall mechanical behavior of materials is strongly dependent on the shape, size, spatial orientation, spatial distribution and properties of individual constituents. Therefore, increasing attention has been given to the development of reliable design tools that can account for the smaller scale characteristics.

Most methods for modeling multi-phased materials rely on the assumption of separation of length scales that arises if the smaller scales are statistically homogeneous or periodic, so that each scale can be analyzed separately and linked through homogenization techniques [13, 113, 3]. The simplest method leading to an estimate of homogenized elastic properties is the so-called rule of mixtures, which consists of a simple volumetric average of the material properties [89, 34]. Since it is defined as a simple volumetric average, the rule of mixtures cannot account for interactions among the constituents, such as stress concentrations near interfaces, thus producing inaccurate estimates when the differences in constituents’ moduli are large.

The classical homogenization theory and multiscale models are the most commonly used
approaches to modeling and designing composite materials. The classical homogenization theory aims to determine the effective (homogenized) constitutive behavior of heterogeneous materials by solving an initial boundary value problem (IBVP) for a representative volume element (RVE) [47, 75, 70, 76, 77, 57, 10]. Once the homogenized constitutive behavior has been determined a priori, modeling of more complex problems can be performed. Multiscale models, on the other hand, determine the effective constitutive behavior of the RVE simultaneously throughout the analysis [2, 48, 50, 56, 3, 49, 132], either using a self-consistent approach [47, 71] or the so-called asymptotic analysis [18, 128, 13, 14].

With the currently available computer power, these approaches are generally formulated within the premises of some numerical technique, mostly the finite element method, so that inelastic constitutive behavior and evolving damage can be easily handled.

Another important approach also adopted for modeling damage in composite materials is so-called continuum damage mechanics [106, 97]. The classical continuum damage mechanics considers a homogeneous global (macro) object for which the damage evolution is described by internal state variables. The evolution law for each internal state variables are determined from experiments or computation, either analytical or numerical. The main advantage of the continuum damage approach is computational efficiency since no local analysis needs to be carried out. Its main disadvantage is that many experiments have to be performed in order to characterize the material. Another disadvantage is that the constitutive behavior is determined a priori so that loading and history dependent behavior may not be accurately modeled.

Many researchers have used the concepts of continuum damage mechanics combined with micromechanics to model damage evolution in composites and laminates [144, 145, 127, 126, 88]. References [60, 58, 59, 137] have used damage mechanics concepts to develop a multiscale model for composite materials. A multiscale model of fiber-reinforced composites is presented in [67, 66] where microstructural damage is manifested in the form of fiber-matrix interfacial
debonding. A review of the concepts and analyses of damage and fatigue of composite materials can be found in [136, 138] and references therein.

In multiscale models the global (macro) scale analysis (problem of interest) is performed concurrently with the local (meso, micro, nano) scale analyses, with the number of local scales determined by the physical problem and limited by the available computational power. In principle, this approach can be used on as many continuum length scales as necessary as long as the assumption of separation of scales is still valid. The requirement of broadly separated length scales and limits of continuum scales in nature (generally, $10^{-10} \text{m} < \ell < 10^3 \text{m}$) lead to the conclusion that about five length scales are physically possible. From the computational point of view however, only about three length scales can be reasonably handled with current computer power [9]. Reference [125] has obtained solutions to four scales simultaneously where damage is considered in the form of internal boundaries, but two of the scales have been solved analytically.

Even though the model proposed herein is posed entirely based on the principles of continuum mechanics, some researchers have been working on the issues of bridging atomic to continuum scales [36, 41, 42, 11, 12, 31, 30, 51, 37, 32, 93]. Reference [108] provides estimates of length scales at which classical continuum elasticity ceases to accurately describe the small deformation mechanical behavior of many materials. According to [108], the two dominant physical mechanisms that lead to size-dependency of elastic behavior at the nanoscale are surface energy effects and nonlocal effects due to discrete structure of matter at such small scales.

The simultaneous solution of both global and local problems is considerably advantageous in cases where the microstructure changes and/or its behavior is history dependent. These changes can be physical, such as crack localization, or chemical, such as oxidation. The effective constitutive behavior of one scale is then governed by the behavior of the consecutive nested smaller scales, such that the only model input parameters are the material properties
of individual constituents at the smallest length scale and respective fracture properties and chemical properties at each appropriate length scale.

2.1 Representative volume element

Homogenization theories are based on the concept of a representative volume element (RVE). The definition of the RVE is a fundamental step in the multiscale modeling of heterogeneous media, because it identifies the macroscopic level at which the material can be approximated by an equivalent homogeneous medium. According to Hill [80], a RVE can be defined when the heterogeneities are distributed in such a way that comparable overall (average) properties are obtained for material volumes beyond a representative minimum volume.

From Hill’s definition, the RVE can then be determined by plotting the kinetic variables (such as the stresses) versus the kinematic variables (such as the strains) on the global (macroscopic) scale [3]. The RVE is then defined as the minimum material volume for which the resulting graphs do not depend on volume $V^1$. However, a more rigorous way of choosing the size of the RVE is to use statistical measures. In this case, the size of the RVE is determined when the condition of statistical homogeneity (equation 2.1) is satisfied for all state variables [3].

$$sd_f \ll \bar{f}$$

(2.1)

where $f$ represents a state variables and $sd$ and $\bar{f}$ are the standard deviation and mean of $f$, respectively. The size of the RVE can also be determined by a similar statistical analysis of geometric properties of the microstructure, such as particle size, orientation and spatial distribution [74, 73, 130].

Another important condition is that the RVE should produce the same response (overall properties) under macroscopically uniform boundary conditions, either displacements or tractions [75]. According to [75], that means that the external boundary displacement
and/or traction fields may fluctuate about a mean with a wavelength small compared to the
dimensions of the RVE, but the effects of such fluctuations become negligible within a few
wavelengths distant from the boundary surface by virtue of St. Venant’s principle. Therefore,
the contribution of the surface layer (affected by the fluctuations) to any average can be
made negligible by taking large enough RVE sizes, in which case any statically equivalent
boundary condition should produce essentially the same results (at least in an average sense)
by virtue of St. Venant’s principle. Extensive discussions on the appropriate size of RVE’s
and on the concept of effective properties, their bounds and boundary-condition effects, for
elastic and viscoelastic materials (both damaged and undamaged) have been presented by
Huet [84, 72, 85, 86].

A schematic depiction of the convergence of homogenized properties with respect to the
size of the RVE for different boundary conditions is given in Figure 2.1. Periodic displacement
boundary conditions are also included which, for a given microstructure size, usually provide
a better estimate of the overall properties, even for non-periodic microstructures [141, 143].
According to [141], at least from the statistical point of view, a local periodicity of the
microstructural geometry can also be assumed if statistical homogeneity is satisfied.

Figure 2.1: Schematic depiction of the convergence of overall properties for different types of
local boundary conditions (adapted from [141, 94]).

Methods to estimate statistically equivalent RVE’s of unidirectional composite microstruc-
tures are discussed in [135, 134], for both undamaged and damaged (in the form of interfacial
debonding modeled by a bilinear cohesive zone law) cases. In these referred works, both geometrical and mechanical parameters are used to determine the proper size of the RVE. As discussed in [134] the effect of local morphology of internal boundaries on overall failure properties is highly pronounced. References [74, 73, 99] discuss the case of damage and concludes that the size of the RVE should be much larger than for elastic undamaged state.

The study presented in [116] shows that the convergence of stiffness (determined using displacement boundary conditions) and compliance (determined using traction boundary conditions) as the size of the RVE increases slows down as the difference between the fiber and matrix mechanical properties increase. Moreover, the convergence to a deterministic RVE as a function of its size is faster for a material with stiff inclusions than for a material with soft inclusions.

Reference [118] discusses the concept of RVE in the presence of random microstructural variables and damage under the context of continuum damage mechanics. The convergence of the RVE size in the presence of random distributions of thin needle-shaped inclusions is studied in [117]. The situation of cracks is approached by lowering the stiffness and increasing the aspect ratio of the inclusions. It is shown that the RVE tends to be very large in this limit case.

### 2.2 Multiscale initial boundary value problem

Figure 2.2 presents a schematic depiction of a three scale IBVP. In this figure, superscripts are used to denote the scale index whereas subscripts are used to denote the conventional rectilinear coordinate system. The problem of interest (global object) is referred as scale 0 and considered to be statistically homogeneous. The local scale object (RVE), referred as scale 1, on the other hand, is heterogeneous. Various sources of heterogeneity can be considered such as inclusions, voids, cracks and others. For the time being, cracks are not considered on the
global scale. The cohesive zone ahead of crack tips is herein considered to be small enough so it can be treated as a third scale (scale 2). The third scale has however been analytically solved by [7] using homogenization techniques and considering some simplifications in order to produce a homogenized traction-displacement relationship for the cohesive zone. \( V^\mu, \partial V^\mu_E \) and \( \partial V^\mu_t \) denote the volume, the external and the internal boundary surfaces of the object at scale \( \mu \), respectively. The length scale associated with the object and with the cracks at scale \( \mu \) are respectively denoted by \( \ell^\mu \) and \( \ell_c^\mu \).

![Schematic representation of a three scale IBVP.](image)

Figure 2.2: Schematic representation of a three scale IBVP.

The mechanical IBVP for the global object can then be well-posed by appropriate initial boundary conditions and a set of equations: conservation of linear and angular momentum (equations 2.2 and 2.3), infinitesimal strain-displacement relations (equation 2.4) and constitutive equations (equation 2.5).

\[
\sigma^0_{ji,j} + \rho^0 b^0_i = \rho^0 \frac{d^2 u^0_i}{dt^2} \quad \text{in } V^0
\]

(2.2)

where Einstein’s indicial notation has been used, \( \sigma^0_{ij}, \rho^0, b^0_i \) and \( u^0_i \) are respectively the Cauchy stress tensor, the mass density, the body force vector per unit mass and the displacement vector at a certain location \( x^0_i \) inside the statistically homogeneous object at the global length scale and at a certain time \( t \). The right hand side of equation 2.2 can be neglected in the
case where the global object is subject to quasi-static loading.

\[ \sigma_{ij}^0 = \sigma_{ji}^0 \quad \text{in } V^0 \quad (2.3) \]

\[ \varepsilon_{ij}^0 = \frac{1}{2} (u_{ij}^0 + u_{ji}^0) \quad \text{in } V^0 \quad (2.4) \]

where \( \varepsilon_{ij}^0 \) is the infinitesimal strain tensor defined on the global scale.

\[ \sigma_{ij}^0 (x_m^0, t) = \tilde{\Omega}_{t=\tau=-\infty} \{ \varepsilon_{kl}^0 (x_m^0, \tau) \} \quad \text{in } V^0 \quad (2.5) \]

where \( \tilde{\Omega}_{t=\tau=-\infty} \) is a functional describing the constitutive behavior at each position \( x_m^0 \) in the object at the global scale, which may account for damage accumulation and history dependent effects, such as viscoelasticity, and is obtained by locally averaging the constitutive behavior of the RVE corresponding to that particular global scale position.

The model presented herein is described in terms of infinitesimal kinematics in order to simplify the constitutive material modeling, but it can be extended to finite deformations with careful attention to the description of the cohesive zone deformation and constitutive law. Multiscale models and homogenization relations for materials undergoing finite deformation can be found in \[80, 112, 94, 55, 119\]. Also, references \[114, 120, 23\] propose large deformation formulations for cohesive zone elements, which will be discussed later.

In the most general sense, the local RVE should obey the same set of governing equations as the global object. However, complex inhomogeneous boundary conditions might have to be applied at the RVE boundaries in order to satisfy that condition. Therefore some simplifications are assumed so that the complexities may be neglected and one may seek an approximate, but satisfactorily accurate, solution for the problem. The first assumption is that the physical length scales are widely separated, allowing the use of spatially homogeneous boundary conditions (uniform boundary tractions or linear boundary displacements) and
simplifying the homogenization relationships connecting global and local scales [79, 113]:

\[ \ell^0 \gg \ell^1 \gg \ell^2 \]  \hspace{1cm} (2.6)

The most common boundary conditions applied to the boundaries of the RVE are the linear displacement, constant tractions, periodic displacement and anti-periodic tractions. Any choice of imposed boundary conditions should however satisfy the Hill condition [79] which requires that the total work-rate per unit reference volume (or the virtual work) at the global (macro) scale be equal to the total work-rate per unit reference volume on the local (micro) scale:

\[ \sigma_{ij}^{0} \dot{\varepsilon}_{ij}^{0} = \frac{1}{V^1} \int_{V^1} \sigma_{ij}^{1} \dot{\varepsilon}_{ij}^{1} dV \]  \hspace{1cm} (2.7)

The second assumption is that the local length scale is much larger than the length scale associated with cracks at the local scale 1, thus mitigating the possibility of statistical inhomogeneity at the local scale but narrowing the range of problems for which the model can generate accurate predictions:

\[ \ell^1 \gg \ell^1 \]  \hspace{1cm} (2.8)

A third assumption made for the case where the global problem cannot be simplified to a quasi-static one is that the length of the wave propagating at the global scale, \( \ell_{w}^{0} \), is much larger than the local length scale:

\[ \ell_{w}^{0} \gg \ell^1 \]  \hspace{1cm} (2.9)

This assumption mitigates the need to consider waves propagating at the local scale, thus allowing the local IBVP to be approximated as a quasi-static problem with uniform self-equilibrating boundary conditions (if gravity is negligible) [122, 123, 124, 132], as shown in Figure 2.3.

Therefore, the IBVP for the local RVE is well-posed by uniform initial boundary conditions.
Figure 2.3: Schematic representation of a two scale IBVP with a wave propagating at the global scale.

Adjoined to the following set of equations:

\[
\sigma^1_{ji,j} = 0 \quad \text{in } V^1
\]  
(2.10)

\[
\sigma^1_{ij} = \sigma^1_{ji} \quad \text{in } V^1
\]  
(2.11)

\[
\varepsilon^1_{ij} = \frac{1}{2} \left( u^1_{i,j} + u^1_{j,i} \right) \quad \text{in } V^1
\]  
(2.12)

\[
\sigma^1_{ij}(t) = \Omega_{\tau=-\infty}^{\tau=t} \{ \varepsilon^1_{kl}(\tau) \} \quad \text{in } V^1
\]  
(2.13)

\[
G^1_i \geq G^1_{ci} \Rightarrow \frac{\partial}{\partial t}(\partial V^1_i) > 0 \quad \text{in } V^1
\]  
(2.14)
where equation 2.14 describes the fracture criterion, $G^1_i$ is the fracture energy release rate at a particular position in the local scale, $G^1_{ci}$ is the critical energy release rate of the material at that particular position and the index $i$ refers to the mode of fracture. Furthermore, the functional $\Omega^\tau_{\tau=-\infty}$ describing the constitutive behavior of each particle at the local position $x^1_i$ is known a priori for all constituents. In the current study, this functional can represent linear elastic or linear viscoelastic behavior depending on the constituent. For linear viscoelastic materials, functionals of single integral type are considered:

$$
\sigma^1_{ij}(x^1_p, t) = \int_{-\infty}^{t} C^1_{ijkl}(x^1_p, t - \tau) \frac{\partial \varepsilon^1_{kl}(x^1_p, \tau)}{\partial \tau} d\tau \quad (2.15)
$$

where $x^1_p$ denotes the particle under consideration. Finally, from the locally averaged solution of the cohesive zone IBVP (scale 2) [7, 147], the following traction-displacement relationship is assumed to hold for the viscoelastic cohesive zones:

$$
t^1_i(t) = \frac{1}{\lambda^1} \frac{[u^1_i]}{\delta^1_i} \left[ 1 - \alpha^1(t) \right] \left\{ \sigma^1_i + \int_{t_0}^{t} E^1_{CZ}(t - \tau) \frac{\partial \lambda^1}{\partial \tau} d\tau \right\} \quad \text{on } \partial V^1_{CZ} \quad (2.16)
$$

where $t^1_i$ is the traction vector acting on the cohesive zone boundary, $[u^1_i]$ is the cohesive zone opening displacement, $\delta^1_i$ are empirical material length parameters which typically reflect a length scale intrinsic to the cohesive zone, $\sigma^1_i$ is the required stress level to initiate damage, $E^1_{CZ}$ is the uniaxial relaxation modulus of a single fibril in the cohesive zone, $\alpha^1(t)$ is the internal damage parameter reflecting the area fraction of voids with respect to the cross-sectional area of the idealized cohesive zone, and $\lambda^1$ is the Euclidean norm of the cohesive zone opening displacements:

$$
\lambda^1 = \sqrt{ \left( \frac{[u^1_r]}{\delta^1_r} \right)^2 + \left( \frac{[u^1_n]}{\delta^1_n} \right)^2 + \left( \frac{[u^1_s]}{\delta^1_s} \right)^2 } \quad (2.17)
$$

where $n$ indicates normal direction and $r$ and $s$ indicate tangential directions.
It can be shown that equation 2.16 is mathematically equivalent to equation 2.14. Even though the mathematical proof is not shown herein, conceptually, as the damage parameter \( \alpha^1(t) \) reaches unity, the traction vector \( t^1_i(t) \) becomes zero valued, meaning that a free surface has been created or, equivalently, a crack has propagated, \( \frac{\partial}{\partial t}(\partial V^1_i) > 0 \).

The cohesive zone model just described is postulated to be represented by a fibrillated zone that is small compared to the total cohesive zone area [7], as shown in Figure 2.4. This model is inherently two scale in nature in that it utilizes the solution to a microscale continuum mechanics problem, together with a homogenization theorem to produce a cohesive zone model on the next larger length scale. The model has also been shown to be consistent with the fact that the cohesive zone requires a nonstationary critical energy release rate in order for a crack to propagate [38, 39, 147].

![Figure 2.4: Depiction of the micromechanical viscoelastic cohesive zone model [7].](image)

For the cases where the previous assumptions are valid, one can show that the relations connecting the global and local scales are given by the following (mean field) homogenization principles [10, 3, 113]:

\[
\bar{\varepsilon}_{ij}^1 = \frac{1}{V^1} \int_{V^1} \varepsilon_{ij}^1 \, dV = \varepsilon_{ij}^0 + \alpha_{ij}^0 \tag{2.18}
\]

\[
\varepsilon_{ij}^0 = \frac{1}{V^1} \int_{\partial V^1_k} \frac{1}{2} \left( u_i^1 n_j^1 + u_j^1 n_i^1 \right) \, dS \tag{2.19}
\]
\[ \alpha^\theta_{ij} = \frac{1}{V^1} \int_{\partial V_E^1} \frac{1}{2} (u^1_{ni} + u^1_{nj}) \, dS \]  
(2.20)

\[ \sigma^0_{ij} = \frac{1}{V^1} \int_{\partial V_E^1} \sigma^1_{ki} n^1_k x^1_j \, dS = \frac{1}{V^1} \int_{V^1} \sigma^1_{ij} \, dV = \bar{\sigma}_{ij} \]  
(2.21)

where \( n^1_i \) is the outward unit normal vector to the external or internal boundary, \( \partial V_E^1 \) or \( \partial V_I^1 \), of the RVE and it has been assumed that the body forces acting on the local scale, \( b_l^1 \), are negligible in order to obtain the second equality in equation 2.21.

In order to obtain the global scale mass density, consider that a representative volume at the global scale should contain the same amount of mass as a representative volume at the local scale:

\[ \Delta m^0 = \Delta m^1 = \int_{V^1} \rho^1 \, dV \]  
(2.22)

From the definition of mass density:

\[ \rho^0 = \lim_{\Delta V^0 \to V^1} \frac{\Delta m^0}{\Delta V^0} = \lim_{\Delta V^0 \to V^1} \frac{1}{\Delta V^0} \int_{V^1} \rho^1 \, dV \]  
(2.23)

So, in the limiting case, the mass density of the global scale is equal to the volume average of mass density of the local scale:

\[ \rho^0 = \bar{\rho}^1 = \frac{1}{V^1} \int_{V^1} \rho^1 \, dV \]  
(2.24)

From equation 2.19, one can observe that the strain tensor in the global scale is equal to the external boundary average of the displacement vector on the local scale, which differs from the volume average of the strain tensor by the internal boundary average of the displacement vector, \( \alpha^0_{ij} \). Note, however, that in the case where there is no separation along the internal boundaries of the RVE, no voids or cracks, \( \alpha^0_{ij} \) is zero, so that \( \alpha^0_{ij} \) can be regarded as an averaged measure of damage [10].

On the other hand, equation 2.21 allows us to conclude that the external boundary average...
of the traction vector, $t_i^1$, is equal to the volume average of the stress tensor. This is true only if the traction vector over the internal boundary surfaces is zero (free surfaces, cracks) or self-equilibrating (cohesive zones).

The use of equations 2.19 and 2.21 is termed a mean field theory of homogenization because the behavior of the global object is determined only in terms of the mean stress and strain tensors evaluated at the external boundary of the local RVE. It is important to note that the assumption that $\varepsilon_{ij}^0$ is spatially uniform along the external boundary of the RVE breaks down in regions of high gradients, such as in the vicinity of cracks or where the size of the RVE is comparable to the global length scale [62].

Higher order homogenization theorems can however be formulated if one includes gradients of the deformation and moments of the stress tensor in the model formulation. Second order computational homogenization schemes are described in [4, 5, 125, 94, 96, 65, 81].

While references [4, 5, 125, 101, 65] use second order plate or shell theories, references [94, 96, 101] additionally impose the gradient of the deformation gradient on the RVE boundaries, automatically delivering a higher-order macro-continuum. The advantage of higher order approaches is that size effects and macroscopic localization are included in the model. Reference [81] proposes a higher approach based on a micromorphic continuum theory [82] assumed for the RVE, which is basically characterized by additional degrees of freedom, thus accounting for size effects. The main goal of [81] is to develop a multiscale computational homogenization scheme for interfaces and material layers and should be useful in the study and development of cohesive zone models.

If the global scale problem is dynamic, that is, the right hand side of equation 2.2 is not negligible, and one adopts an explicit time integration scheme to solve the global IBVP, the above equations are sufficient to perform the multi-scale analysis. In that case, since there is no need to compute the stiffness matrix, for each time step, one can simply apply the global strain tensor, $\varepsilon_{ij}^0$, as displacements on the boundary of the RVE, solve the step-wise local
IBVP, and then compute the global stress tensor, $\sigma^0_{ij}$ using equation 2.21 [132], even though it is always desirable to compute the homogenized constitutive tensor for mathematical consistency and rigor.

For cases where the global IBVP is approximated by a quasi-static problem, however, the computation of the homogenized constitutive tensor is required in order to correctly calculate the tangent stiffness matrix. In other words, one is required to compute the homogenized functional $\bar{\Omega}^{\tau=\infty}$. If one uses an incremental solution scheme, however, it is preferable to seek an incremental constitutive equation of the form:

$$\Delta \sigma^0_{ij} = \bar{\Omega}' \left( \Delta \varepsilon^0_{kl} \right)$$

(2.25)

It is important to note that one of the major limitations of the current model is the absence of inertial effects on the local scale, thus precluding the modeling of phenomena such as dispersion due to local scale heterogeneities. The major problem of considering waves propagating at the local scale is the possibility of wave reflections on the boundaries of the RVE which are physically unrealistic. Furthermore, stress discontinuities at the wave front break down the usual concepts of homogenization and statistical homogeneity of the stress field.

Some researchers have proposed models that attempt to account for dynamic effects at the local scales [29, 54, 53, 52, 46, 30, 148]. As pointed out in [29, 46], an additional issue is present for dynamic problems: the existence of multiple time scales.

There is generally one time scale for each spatial length scale. The global time scale is the time scale of interest and the local time scales are the time needed for the solution to develop the correct microstructure that matches the macroscale behavior [46]. In this case, definitions of time averages may be required. The inaccuracies brought about by the assumption of separation of time scales can be negligible if the physical time scales are widely
separated.

The models developed in [29, 54, 53, 52, 30, 148] use higher order space-time asymptotic homogenization to develop a multiscale model capable of modeling dispersion. All of these models still rely on the assumption that the characteristic length of the wave propagating at the global scale is large compared to the size of the RVE, equation 2.9. Reference [30] shows that the initial shape of the loading pulse is preserved if the pulse width is large compared to the size of the unit cell. Nonetheless their higher-order asymptotic model accurately accounts for changes in shape of the loading pulse as its width becomes comparable (about ten times larger) to the size of the unit cell. However, none of the models discussed above consider cracking or viscoelasticity.
Chapter 3

Computation of Incremental Homogenized Quantities for Viscoelastic Media Containing Cracks

General purpose Finite Element codes usually employ incremental algorithms for solving IBVP. When the IBVP is time and/or history dependent incrementalization is necessary to allow integration of the governing equations, at least in an approximate manner. Therefore the present work proposes an incremental homogenization scheme for viscoelastic solids containing cracks suitable for multiscale computational codes.

At least to the author’s knowledge, most approaches proposed in the literature to compute the homogenized tangent constitutive tensor are based on purely numerical techniques. For example, Kouznetsova [94] employs the technique of condensation of the total RVE stiffness, which has been presented in [95]. Feyel and Chaboche [50] use the approximate numerical differentiation technique, which requires the solution of four (2D) or six (3D) IBVP’s for every solution step. Basically, numerical constitutive tests are performed by applying unit deformation in every mode. Besides, these works do not consider cracking or viscoelasticity.
The approach to be proposed in the present work, on the other hand, is based on continuum mechanics homogenization principles and allows the computation of the full homogenized anisotropic tangent constitutive tensor of viscoelastic solids with evolving cracks by solving the IBVP only once, which greatly reduces the required amount of computational time.

As it will be shown, the introduction of a localization quantity relating the local displacement field to the deformation on the external boundary of the RVE is the key feature that allows the computation of the full homogenized anisotropic tangent constitutive tensor by solving the IBVP only once. The same approach has been used in the context of asymptotic homogenization, but neither viscoelasticity nor cracking have been considered [18, 83, 68, 61, 62].

Other approaches to computing the effective constitutive properties of elastic composites with cracks have been proposed in references [4, 5, 90, 104, 105, 129, 110, 40, 25, 142, 26], from which most works consider stationary cracks or holes, as opposed to evolving internal boundaries. Reference [149] extended the model presented in [104, 105] to viscoelastic laminates with stationary matrix cracks. Huet [85] has studied the cases of microcracked elastic and viscoelastic materials based on a continuum thermodynamics approach. As pointed out in reference [91], the validity of using an equivalent elastic material of reduced stiffness in the short range near a (macro) crack tip is compromised by the fact that volume averaged quantities are insensitive to local fluctuations of the microcrack field, which govern fracture-related quantities such as stress intensity factors.

Back to the problem at hand, first assume that the stress tensor at both global and local scales can be written in incremental form:

\[
\sigma_{ij}^0(t + \Delta t) = \sigma_{ij}^0(t) + \Delta \sigma_{ij}^0
\]

(3.1)

\[
\sigma_{ij}^1(t + \Delta t) = \sigma_{ij}^1(t) + \Delta \sigma_{ij}^1
\]

(3.2)
Then substituting the above equations into equation 2.21, gives:

\[
\sigma_{ij}^0(t) = \frac{1}{V_1} \int_{V_1} \sigma_{ij}^1(t) dV \quad (3.3)
\]

\[
\Delta \sigma_{ij}^0 = \frac{1}{V_1} \int_{V_1} \Delta \sigma_{ij}^1 dV \quad (3.4)
\]

Reference [150] proposes a very stable and accurate incrementalization scheme for viscoelastic materials that can be modeled by constitutive equations of single integral type and for which the relaxation moduli can be represented by a Prony series:

\[
C_{ijkl}^1(t) = C_{ijkl}^1 + \sum_{m=1}^{M_{ijkl}} C_{ijklm}^1 e^{-t/\rho_{ijklm}} \quad \text{(no sum on } i, j, k, l) \quad (3.5)
\]

where \( C_{ijkl}^1 \) are the long term moduli, \( C_{ijklm}^1 \) are the moduli coefficients and \( M_{ijkl}^1 \) is the number of Prony terms necessary to accurately describe the material relaxation moduli, and \( \rho_{ijklm}^1 \) are the so-called relaxation times given by,

\[
\rho_{ijklm}^1 = \eta_{ijklm}^1 / C_{ijklm}^1 \quad \text{(no sum on } i, j, k, l) \quad (3.6)
\]

where \( \eta_{ijklm}^1 \) are viscosity terms.

As presented in [150], if one assumes that the strain rate is constant for each time step, the following incremental constitutive equation can be obtained:

\[
\Delta \sigma_{ij}^1 = C_{ijkl}^\prime \Delta \varepsilon_{kl}^1 + \Delta \sigma_{ij}^{R1} \quad (3.7)
\]

where

\[
C_{ijkl}^\prime \equiv C_{ijkl}^1 + \frac{1}{\Delta t} \sum_{m=1}^{M_{ijkl}} \eta_{ijklm}^1 \left( 1 - e^{-\Delta t/\rho_{ijklm}^1} \right) \quad \text{(no sum on } i, j, k, l) \quad (3.8)
\]
\[\Delta \sigma_{ij}^{R1} = - \sum_{k=1}^{3} \sum_{l=1}^{3} A_{ijkl}^{1}\]  

(3.9)

\[A_{ijkl}^{1} = \sum_{m=1}^{M_{ijkl}} \left(1 - e^{-\Delta t/\rho_{ijklm}^{1}}\right) S_{ijklm}^{1}(t) \quad \text{(no sum on } i, j, k, l)\]  

(3.10)

\[S_{ijklm}^{1}(t) = e^{-\Delta t/\rho_{ijklm}^{1}} S_{ijklm}^{1}(t - \Delta t) + \eta_{ijklm}^{1} \frac{\Delta \varepsilon_{kl}^{1}}{\Delta t} \left(1 - e^{-\Delta t/\rho_{ijklm}^{1}}\right)\]  

(no sum on } i, j, k, l)  

(3.11)

where \(t\) denotes the previous time step and \(\Delta \varepsilon_{kl}^{1}/\Delta t\) is determined from the previous time step \(t\). Note that all time dependence in the material behavior resides in \(\Delta \sigma_{ij}^{R1}\) which is recursively computed at each time step. Also note that the values of \(S_{ijklm}^{1}\) from the previous time step must be stored so that \(S_{ijklm}^{1}(t)\) can be determined recursively. Moreover, \(S_{ijklm}^{1} = 0\) for \(t \leq 0\). Further details about the incrementalization of viscoelastic constitutive equations can found in [150].

The same can be done for the cohesive zone traction-displacement relation. Following the same procedure presented in [150, 6, 130], one can show that the cohesive zone constitutive equation (equation 2.16) can be written in the following incremental form:

\[t_{i}^{1}(t + \Delta t) = t_{i}^{1}(t) + \Delta t_{i}^{1}\]  

(3.12)

\[\Delta t_{i}^{1} = k_{ij} \Delta \left[u_{ij}^{1}\right] + \Delta t_{i}^{R1}\]  

(3.13)

where

\[k_{ij}^{1} = \frac{[1 - \alpha^{1}(t + \Delta t)]}{\delta_{ij}^{1}} E_{ij}^{1} \delta_{ij} \quad \text{(no sum on } i)\]  

(3.14)

\[E_{ij}^{1} \equiv E_{\infty}^{1} + \frac{1}{\Delta t} \sum_{j=1}^{M_{j}} \eta_{j}^{1} \left(1 - e^{-\Delta t/\rho_{j}^{1}}\right)\]  

(3.15)
\[ \Delta t_i^{R1} = \left[ 1 - \alpha_i^1(t + \Delta t) \right] \left[ -\sum_{j=1}^{M_i^1} \left( 1 - e^{-\Delta t/\rho_i^j} \right) s_{ij}^1(t) \right] - \frac{\Delta \alpha_i^1}{\delta_i^1} \left\{ E_i^1 \left[ u_i^1(t) \right] + \sum_{j=1}^{M_i^1} s_{ij}^1(t) \right\} - \Delta \alpha_i^1 \sigma_i^{f1} \] (no sum on \( i \)) \tag{3.16}

\[ s_{ij}^1(t) = e^{-\Delta t/\rho_i^j} s_{ij}^1(t - \Delta t) + \eta_j^1 \frac{\Delta [u_i^1]}{\Delta t} \left( 1 - e^{-\Delta t/\rho_i^j} \right) \] (no sum on \( j \)) \tag{3.17}

where \( \delta_{ij} \) is the Kronecker delta, \( M^1 \) is the number of Prony terms necessary to accurately describe the uniaxial relaxation modulus of a single fibril in the cohesive zone, and \( \Delta [u_i^1] \) is the increment of the displacement jump across the cohesive zone boundaries, which rate is assumed to be constant over each time step.

Now assume that the constitutive behavior of the global object can be approximated by an incremental form similar to equation 3.7:

\[ \Delta \sigma_{ij}^0 = C_{ijkl}^0(t) \Delta \varepsilon_{kl}^0 + \Delta \sigma_{ij}^{R0} \] \tag{3.18}

where \( C_{ijkl}^0(t) \) is the instantaneous constitutive tensor evaluated at the previous time step \( t \) which is a function of time through its dependence on the amount of damage accumulated at the local RVE, thus producing a nonlinear behavior at the global scale. Substituting equations 3.18 and 3.7 into 3.4, gives:

\[ C_{ijkl}^0 \Delta \varepsilon_{kl}^0 + \Delta \sigma_{ij}^{R0} = \frac{1}{V_1} \int_{V_1} \left( C_{ijkl}^{\prime} \Delta \varepsilon_{kl} + \Delta \sigma_{ij}^{R1} \right) dV \] \tag{3.19}

where \( C_{ijkl}^0(t) \) is now written as \( C_{ijkl}^0 \) for the shortness of notation. Now it is necessary to solve the above equation for \( C_{ijkl}^0(t) \). The key to the following development is to relate the field variables of the local scale to the external boundary average quantities corresponding to field variables of the global scale. Using the concept of localization tensors \cite{78, 10}, it is herein
assumed that the local displacement field can be related to the global strain tensor (external boundary average of the local displacement field) according to:

\[ u^1_i(t) = x^1_j \varepsilon^0_{ij}(t) + \lambda^1_{ijk}(t) \varepsilon^0_{jk}(t) \quad \text{in } V^1 \]  

(3.20)

where \( \lambda^1_{ijk} \) is called the localization tensor. The first term in equation 3.20 corresponds to a homogeneous displacement field which would be experienced by the RVE if it was a homogeneous material. The second term, on the other hand, represents the contribution to the local displacement field due to the history dependent constitutive behavior and the existence of local asperities and internal boundaries, including cracks and cohesive zones. Note that the displacement vector is chosen to be described in such a manner because it is generally used as the primary variable in FE formulations. References [24, 10] have used a fourth order strain localization tensor which relates \( \varepsilon^1_{kl} \) to \( \varepsilon^0_{kl} \). This approach may be sometimes impractical or inconvenient, especially when using the finite element method to solve the local IBVP.

It can be shown that equation 3.20 is actually equivalent to the representation usually admitted in the asymptotic homogenization theory, say \( u^1_i = \chi^1_{ijk} \varepsilon^0_{jk} \), where \( \chi^1_{ijk} \) is the so-called influence function [18, 83, 61]. Note that, in the referred works, \( \chi^1_{ijk} \) is not assumed to be a function of time because neither viscoelasticity nor cracking are considered.

The studies shown in [61, 62] have admitted the usual asymptotic homogenization representation of the displacement field in order to develop the so-called multiscale enrichment method based on partition of unity, which primary objective is to extend the range of applicability of mathematical homogenization theory to problems where scale separation may not be possible. Reference [115] has adopted a different decomposition of the local displacement field in order to analyze failure of heterogeneous materials using continuum damage mechanics to model both bulk degradation and fiber-matrix debonding.
Linearizing the local scale displacement field gives:

\[ u^1_i(t + \Delta t) = u^1_i(t) + \frac{\partial u^1_i(t)}{\partial t} \Delta t \]  (3.21)

From equation 3.20 and the chain rule of differentiation, one can show that:

\[ \frac{\partial u^1_i(t)}{\partial t} = x^1_j \frac{\partial \varepsilon^0_{ij}(t)}{\partial t} + \lambda^1_{ijk}(t) \frac{\partial \varepsilon^0_{jk}(t)}{\partial t} + \frac{\partial \lambda^1_{ijk}(t)}{\partial t} \varepsilon^0_{jk}(t) \]  (3.22)

It is important to note that, from the incrementalization of the global and local viscoelastic constitutive equations, \( \frac{\partial \varepsilon^0_{ij}(t)}{\partial t} \) as well as \( \frac{\partial u^1_i(t)}{\partial t} \) have been assumed constant over the time step. However, no assumption will be made about the behavior of \( \lambda^1_{ijk}(t) \) and \( \frac{\partial \lambda^1_{ijk}(t)}{\partial t} \) in order to maintain the same degree of accuracy, but equation 3.22 is redefined as follows:

\[ \frac{\partial u^1_i(t)}{\partial t} = x^1_j \frac{\partial \varepsilon^0_{ij}(t)}{\partial t} + \lambda^1_{ijk}(t) \frac{\partial \varepsilon^0_{jk}(t)}{\partial t} + \frac{\partial u^{R1}_i(t)}{\partial t} \]  (3.23)

where

\[ \frac{\partial u^{R1}_i(t)}{\partial t} \equiv \frac{\partial \lambda^1_{ijk}(t)}{\partial t} \varepsilon^0_{jk}(t) \]  (3.24)

and one can show from the previous assumptions that \( \frac{\partial u^{R1}_i(t)}{\partial t} \) is constant over the time step, thus giving:

\[ \Delta u^1_i = x^1_j \Delta \varepsilon^0_{ij} + \lambda^1_{ijk}(t) \Delta \varepsilon^0_{jk} + \Delta u^{R1}_i \]  (3.25)

Substituting 3.25 into 2.12, then into 3.19 yields:

\[ C^0_{ijkl} \Delta \varepsilon^0_{kl} + \Delta \sigma^{R0}_{ij} = \frac{1}{V^1} \int_{V^1} \left\{ C'^{n1}_{ijkl} + C'^{n1}_{ijpq} \left[ \frac{1}{2} \left( \lambda^1_{pkl,q} + \lambda^1_{qkl,p} \right) \right] \right\} dV \Delta \varepsilon^0_{kl} 
+ \frac{1}{V^1} \int_{V^1} \left( C'^{n1}_{ijkl} \Delta \varepsilon^0_{kl} + \Delta \sigma^{R1}_{ij} \right) dV \]  (3.26)

where symmetry of the local constitutive tensor \( C^1_{ijkl} \) and the fact that \( \Delta \varepsilon^0_{kl} \) is constant in
$V^1$ have been used, $\lambda_{ijk,l}^1(t)$ is written as $\lambda_{ijk,l}^1$ to simplify equations, and

$$\Delta\varepsilon_{ij}^{R1} \equiv \frac{1}{2} (\Delta u_{i,j}^{R1} + \Delta u_{j,i}^{R1})$$  \hspace{1cm} (3.27)

Since $\Delta\varepsilon_{kl}^0$ is arbitrary, one obtains:

$$C_{ijkl}^0 = \frac{1}{V^1} \int_{V^1} \left\{ C_{ijkl}^0 + C_{ijpq}^0 \left[ \frac{1}{2} \left( \lambda_{pkl,q}^1 + \lambda_{qkl,p}^1 \right) \right] \right\} \, dV$$  \hspace{1cm} (3.28)

$$\Delta\sigma_{ij}^{R0} = \frac{1}{V^1} \int_{V^1} \left( C_{ijkl}^0 \Delta\varepsilon_{kl}^{R1} + \Delta\sigma_{ij}^{R1} \right) \, dV$$  \hspace{1cm} (3.29)

Note that the global scale tangent constitutive tensor, $C_{ijkl}^0$, is affected by heterogeneity, internal boundaries and cracks at the local scale through the localization tensor, $\lambda_{ijk}^1$, and affected by viscoelasticity through $C_{ijkl}^0$ and $\lambda_{ijk}^1$. It is also important to note that the global scale history dependence, expressed by $\Delta\sigma_{ij}^{R0}$, also depends on the heterogeneity, internal boundaries and cracks initiated at the local scale through $\Delta u_{i}^{R1}$, defined by equation 3.24, which depends on the rate of change of $\lambda_{ijk}^1(t)$.

Also note that the homogenized tangent constitutive tensor, $C_{ijkl}^1$, is only equal to the volume average of the local scale constitutive tensor if $\lambda_{ijk}^1 = \text{constant} = 0$ \(^1\), meaning that the local scale object is actually homogeneous. Therefore, the rule of mixtures (volume average of the local scale constitutive tensor), which does not account for the localization of field variables, should be used only as a rough estimate which may be very inaccurate in some cases.

It can be shown that the expression for computing the homogenized tangent constitutive tensor is the same for both elastic and viscoelastic media containing cracks. The only

\(^1\)Note that, in order to satisfy the displacement boundary conditions ($u_{i}^{1}(t) = x_{i}^{0}(t)$), all components of $\lambda_{ijk}^1$ have to be zero at least on some regions of $\partial V_{E}^1$ (or all over $\partial V_{E}^1$ if no heterogeneity (cracks and inclusions) is allowed to cross the external boundary of the RVE). Thus, if $\lambda_{ijk}^1$ is constant over the volume $V^1$, it has to be zero.
difference is the additional homogenized incremental history dependent stress tensor that appears in the viscoelastic formulation.

It can also be shown that equation 3.28 is equivalent to the one obtained from the asymptotic homogenization theory for both linear elastic [83] and elasto-plastic materials [68, 62], even though cracking has not been considered in these works.

### 3.1 Finite Element Formulation of the Global IBVP

In this section, the finite element formulation for the global IBVP is described. Since the present multiscale model is based on first order homogenization theorems, the classical equations of continuum mechanics apply to both scales. Therefore the finite element formulation for the global scale IBVP remains the same and follows the standard formulation presented in reference books on the subject [87, 16, 17].

Consider the variational form of conservation of linear momentum at the global scale, equation 2.2, neglecting the body force vector:

\[
\int_{V_0} \sigma^0_{ji} \delta v^0_i \, dV = \int_{V_0} \rho^0 \frac{\partial v^0_i}{\partial t} \, dV
\]

where \(\delta v^0_i\) is the virtual velocity field. From the chain rule of differentiation and the above equation:

\[
\int_{V_0} (\sigma^0_{ji} \delta v^0_i) \, dV = \int_{V_0} \sigma^0_{ji} \frac{\partial (\delta v^0_i)}{\partial x^0_j} \, dV + \int_{V_0} \rho^0 \frac{\partial v^0_i}{\partial t} \delta v^0_i \, dV
\]

Applying the divergence theorem to the above equation, assuming infinitesimal deformations, recalling symmetry of the Cauchy stress tensor (equation 2.3) and using Cauchy’s formula \((t^0_i = \sigma^0_{ji} n^0_j)\), results in:

\[
\int_{V_0} \rho^0 \frac{\partial v^0_i}{\partial t} \delta v^0_i \, dV = \int_{\partial V_0} t^0_i \delta v^0_i \, dS - \int_{V_0} \sigma^0_{ij} \delta \varepsilon^0_{ij} \, dV
\]
The displacement field can now be discretized in space by expressing it as a function of its nodal values:

\[
\{u_0\}_e = [N^0]_e \{\tilde{u}^0\}_e \tag{3.33}
\]

where the above equation has been written in matrix form, \([N^0]_e\) is the matrix of nodal shape functions for each finite element, the subscript \(e\) denotes quantities defined for each finite element, and the over-tilde indicates nodal value. Therefore, one can also write:

\[
\{v_0\}_e = [N^0]_e \{\tilde{v}^0\}_e \tag{3.34}
\]

and

\[
\{\delta v_0\}_e = [N^0]_e \{\tilde{\delta v}^0\}_e \tag{3.35}
\]

So that equation 3.32 can be written as:

\[
[M^0]\{a^0\} = \{F^0_{ext}\} - \{F^0_{int}\} \tag{3.36}
\]

where

\[
[M^0] = \int_{V_0} [N^0]^T \rho^0 [N^0] \, dV \tag{3.37}
\]

\[
\{F^0_{ext}\} = \int_{\partial V_0} [N^0]^T \{t^0\} \, dS \tag{3.38}
\]

\[
\{F^0_{int}\} = \int_{V_0} [B^0]^T \{\sigma^0\} \, dV \tag{3.39}
\]

where \([B^0]\) is the matrix of derivatives of the shape functions with respect to the global scale spatial coordinates and the subscript \(e\) has been omitted to simplify the notation.

According to [17], equation 3.36 is called the semi-discrete momentum equation because it is discrete in space but continuous in time. The mass matrix in finite element models is often not diagonal, in which case a force at node \(I\) can accelerate node \(J\) if \(M_{IJ} \neq 0\). Implicit
time integration schemes are then used to solve the system of equations.

In most impact applications however, a diagonal approximation of the mass matrix (lumped mass) is commonly used which allows the use of explicit time integration schemes. Explicit time integration schemes generally require much smaller time steps but the finite element system of equations is uncoupled so that there is no need to invert global matrices, which may require a great amount of time for large systems. In the present study, an explicit time integration scheme is used to solve the global scale IBVP, but an implicit quasi-static scheme is used to solve the local scale IBVP, as discussed in the next section.

### 3.2 Finite Element Formulation of the Local IBVP

In this section, the finite element formulation for the local IBVP is developed. For the local IBVP, one should now seek the solution for the localization tensor $\lambda_{ijk}^1(t)$ and $\Delta u_i^R$ so that the displacement increments can be computed using equation 3.25, and $C_{ijkl}^0$ and $\Delta \sigma_{ij}^R$ can be computed using equations 3.28 and 3.29, respectively.

Consider the variational form of conservation of linear momentum at the local scale, equation 2.10, neglecting the body force vector:

$$\int_{V_1} \sigma_{ji,j}^1 \delta u_i^1 \, dV = 0 \quad (3.40)$$

From the chain rule of differentiation and conservation of angular momentum, equation 2.11, the above equation results in:

$$\int_{V_1} (\sigma_{ji,j}^1 \delta u_i^1) \, dV = \int_{V_1} \sigma_{ij}^1 \delta \varepsilon_{ij}^1 \, dV \quad (3.41)$$

Applying the divergence theorem to the above equation at time $t + \Delta t$ and using Cauchy’s
formula \((t_i^1 = \sigma_{ij}^1 n_j^1)\) results in:

\[
\int_{V_1} \sigma_{ij}^1(t + \Delta t) \delta \varepsilon_{ij}^1(t + \Delta t) \, dV = \int_{\partial V_1^k} t_i^1(t + \Delta t) \delta u_i^1(t + \Delta t) \, dS \\
+ \int_{\partial V_1^l} t_i^1(t + \Delta t) \delta u_i^1(t + \Delta t) \, dS \quad (3.42)
\]

Besides the incremental equations 3.2, 3.12 and 3.21, consider that the strain field can also be approximated by the following incremental form:

\[
\varepsilon_{ij}^1(t + \Delta t) = \varepsilon_{ij}^1(t) + \Delta \varepsilon_{ij}^1 
\]

Thus, substituting into 3.42, but noting that the variation of \(\varepsilon_{ij}^1(t)\) and \(u_i^1(t)\) are null because these are known quantities, yields:

\[
\int_{V_1} \sigma_{ij}^1(t) \delta \Delta \varepsilon_{ij}^1 \, dV + \int_{V_1} \Delta \sigma_{ij}^1 \delta \Delta \varepsilon_{ij}^1 \, dV = \int_{\partial V_1^k} t_i^1(t) \delta \Delta u_i^1 \, dS + \int_{\partial V_1^l} \Delta t_i^1 \delta \Delta u_i^1 \, dS \\
+ \int_{\partial V_1^l} t_i^1(t) \delta \Delta u_i^1 \, dS + \int_{\partial V_1^l} \Delta t_i^1 \delta \Delta u_i^1 \, dS \quad (3.44)
\]

Also noting that,

\[
\int_{\partial V_1^k + \partial V_1^l} t_i^1(t) \delta \Delta u_i^1 \, dS = \int_{V_1} \sigma_{ij}^1(t) \delta \Delta u_i^1 \, dV + \int_{V_1} \sigma_{ij}^1(t) \delta \Delta \varepsilon_{ij}^1 \, dV \\
= \int_{V_1} \sigma_{ij}^1(t) \delta \Delta \varepsilon_{ij}^1 \, dV \quad (3.45)
\]

results in:

\[
\int_{V_1} \Delta \sigma_{ij}^1 \delta \Delta \varepsilon_{ij}^1 \, dV = \int_{\partial V_1^k} \Delta t_i^1 \delta \Delta u_i^1 \, dS + \int_{\partial V_1^l} \Delta t_i^1 \delta \Delta u_i^1 \, dS \quad (3.46)
\]

Under the circumstances where the previously discussed assumptions regarding the global and local length scales are valid, either displacements or tractions can be applied on the
boundary of the RVE. If displacements are applied, then the first integral on the right-hand side of the equation above is zero because the variation of the displacement field on the external boundary is null. If tractions are applied instead, this integral is also zero because the tractions are self-equilibrated over the external boundary of the RVE. Thus,

$$\int_{V^1} \Delta \sigma_{ij}^1 \delta \Delta \varepsilon_{ij}^1 \, dV = \int_{\partial V^1} \Delta t_i^1 \delta \Delta u_i^1 \, dS$$  \hspace{1cm} (3.47)

Now notice that the virtual work done by tractions over the internal boundary (right-hand side of equation above) is zero unless there is separation along that boundary. Therefore, the integral over the internal boundaries can be reduced to an integral over cracks and cohesive zones. Since \( n_1^i \partial V_{cz} \) = \(-n_1^i \partial V_i\), and \( \Delta t_i(n_1^i \partial V_{cz}) = -\Delta t_i(n_1^i \partial V_i) \), the equation above can be rewritten as:

$$\int_{V^1} \Delta \sigma_{ij}^1 \delta \Delta \varepsilon_{ij}^1 \, dV + \int_{\partial V_{cz}} \Delta t_i^1 \delta \Delta u_i^1 \, dS = 0$$  \hspace{1cm} (3.48)

Substituting 3.25 into 2.12, then into 3.7, gives:

$$\Delta \sigma_{ij}^1 = \left\{ C_{ijkl}^1 + C_{ijpq}^1 \left[ \frac{1}{2} (\lambda_{pkl,q}^1 + \lambda_{qkl,p}^1) \right] \right\} \Delta \varepsilon_{kl}^0 + C_{ijkl}^1 \Delta \varepsilon_{kl}^{R1} + \Delta \sigma_{ij}^{R1}$$  \hspace{1cm} (3.49)

Also, from equation 3.25,

$$\Delta [u_i^1] = [x_j^1 \Delta \varepsilon_{ij}^0 + \lambda_{ijk}^1 \Delta \varepsilon_{jk}^0 + \Delta u_i^{R1}]_{surface \ 1} - [x_j^1 \Delta \varepsilon_{ij}^0 + \lambda_{ijk}^1 \Delta \varepsilon_{jk}^0 + \Delta u_i^{R1}]_{surface \ 2}$$  \hspace{1cm} (3.50)

or

$$\Delta [u_i^1] = [\lambda_{ijk}^1]_{surface \ 1} - [\lambda_{ijk}^1]_{surface \ 2} \Delta \varepsilon_{jk}^0 \Delta u_i^{R1} - \Delta u_i^{R1}$$  \hspace{1cm} (3.51)

where one should note that the initial coordinates, \( x_i^1 \), of the cohesive zone surfaces coincide.

The incremental localization field can now be discretized in space by expressing it as a
function of its nodal values:

\[
\lambda^1_e = [N^1_e] \tilde{\lambda}^1_e
\]  

(3.52)

where the above equation has been written in matrix form, \([N^1_e]\) is the matrix of nodal shape functions for each finite element, the subscript \(e\) denotes quantities defined for each finite element, and the over-tilde indicates nodal value. It is important to note that the shape functions used to interpolate \(\lambda^1_{ijk}\) are the same as for the displacement field. Therefore, one can also write:

\[
\{\delta \Delta u^1\}_e = [N^1_CZ]_e \{\delta \Delta \tilde{u}^1\}_e \quad \text{on } \partial V^1_{CZ}
\]  

(3.53)

\[
\{\Delta [u^1]\}_e = [N^1_CZ]_e \tilde{\lambda}^1_e \{\Delta \varepsilon^0\}_e + [N^1_CZ]_e \{\Delta \tilde{u}^{R1}\}_e
\]  

(3.54)

\[
\{\delta \Delta \varepsilon^1\}_e = [B^1_e] \{\delta \Delta \tilde{u}^1\}_e
\]  

(3.55)

where \([B^1_e]\) is the matrix of derivatives of the shape functions with respect to the local scale spatial coordinates. Substituting equations 3.13, 3.49–3.55 into 3.48 and noting that \(\delta \Delta \tilde{u}^1_i\) and \(\Delta \varepsilon^0_{ij}\) are arbitrary quantities results in the following two sets of linear equations:

\[
[\tilde{\lambda}^1]_a = -[K^1]^{-1}_a [G^1]_a
\]  

(3.56)

\[
\{\Delta \tilde{u}^{R1}\}_a = [K^1]^{-1}_a \{F^{R1}\}_a
\]  

(3.57)

where the subscript \(a\) denotes quantities assembled over the entire finite element mesh.

\[
[K^1]_a = \int_{V^1} [B^1]^T [C^1] [B^1] dV + \int_{\partial V^1_{CZ}} [N^1_{CZ}]^T [k^1_{CZ}] [N^1_{CZ}] dS
\]  

(3.58)

\[
[G^1]_a = \int_{V^1} [B^1]^T [C^1] dV
\]  

(3.59)

\[
\{F^{R1}\}_a = -\left\{ \int_{V^1} [B^1]^T \{\Delta \sigma^{R1}\} dV + \int_{\partial V^1_{CZ}} [N^1_{CZ}]^T \{\Delta t^{R1}\} dS \right\}
\]  

(3.60)
where the subscripts $e$ have been dropped for a simpler notation.

Once $\lambda_{ijk}^1(t)$ and $\Delta u_{i}^{R1}$ have been obtained using equations 3.56 and 3.57, respectively, one can calculate the incremental displacements using equation 3.25 and compute the global scale (homogenized) tangent constitutive tensor, $C_{ijkl}^0$, and the global scale history dependent stress tensor, $\Delta \sigma_{ij}^{R0}$ from equations 3.28 and 3.29, respectively. Then standard FE procedures can be used to compute the incremental strain and stress tensors from the incremental displacements, thus minimizing the code implementation effort.

Now one can clearly see that the incremental localization tensor, $\lambda_{ijk}^1$, and consequently the homogenized tangent constitutive tensor, $C_{ijkl}^0$, are affected by cracks and cohesive zones through the stiffness matrix, $[K^1]$. Also note that the global scale history dependent term, $\Delta \sigma_{ij}^{R0}$ also depends on the damage accumulated at the local scale through $\Delta u_{i}^{R1}$. It is important to note that the stiffness matrix, $[K^1]$, is the same stiffness matrix usually assembled in common FE algorithms.

### 3.3 Verification of the Developed Procedure

In order to verify the formulation of the local IBVP, the simple two dimensional quasi-static IBVP shown in Figure 3.1 is considered. This problem consists of two 4-noded quadrilateral elements with one cohesive zone element placed in between. Only motions in the vertical direction are allowed so that $\Delta \varepsilon_{22}^0$ is the only non-zero component of the incremental external boundary average strain tensor.

The cohesive zone is assumed to behave according to the viscoelastic cohesive zone model developed in [7] (equation 2.16). The fibril uniaxial relaxation modulus is assumed to fit a one-term Prony series with $E_{\infty}^1 = 10^5$, $E_1^1 = 4 \times 10^5$, $\rho_1^1 = 1.0$. Other cohesive zone material properties are arbitrarily chosen as $\delta_n^1 = \delta_r^1 = \delta_s^1 = 1$, and $\sigma_f^1 = \sigma_r^1 = \sigma_s^1 = 0$. Vertical displacements are applied as shown in Figure 3.1 at a rate $\dot{\delta}$ of 0.01, and the time increment
used in the numerical calculations is $\Delta t = 0.1$.

The damage parameter, $\alpha^1(t)$ is assumed to obey the following phenomenological law [7]:

$$\dot{\alpha}^1 = A(\lambda^1)^m \quad \text{for } \dot{\lambda}^1 > 0 \text{ and } \alpha^1 < 1$$  \hspace{1cm} (3.61)

$$\dot{\alpha}^1 = 0 \quad \text{for } \dot{\lambda}^1 \leq 0 \text{ or } \alpha^1 = 1$$  \hspace{1cm} (3.62)

where $A$ and $m$ are chosen to be equal to 0.025 and 0.5, respectively. For the bulk elastic material properties it has been first assumed that the bulk material is rigid, $E \to \infty$, so that the response of the body shown in Figure 3.1 will actually reproduce the response of the cohesive zone. The actual numerical values used for the Young’s modulus and Poisson’s ratio are $10^{12}$ and 0.3, respectively. Plane stress conditions are assumed. The closed form solution for a monotonically increasing opening displacement applied to the cohesive zone is given in [7]:

$$t_{n}^1(t) = \frac{1}{\lambda^1} \left[ \frac{u_n}{\delta_n^1} \right] \left[ 1 - \frac{A}{m + 1} (\lambda^1)^m \right] \left\{ \sigma_n^1 + \left[ E_\infty^1 t + E_1^1 \rho_1^1 \left( 1 - e^{-t/\rho_1^1} \right) \right] \dot{\lambda}^1 \right\}$$  \hspace{1cm} (3.63)

One can also calculate the incremental values of the cohesive zone stiffness, $k_{ij}^1$, and history traction vector, $\Delta t_{ij}^R$, using equations 3.14 and 3.16 and compare them to the incremental homogenized constitutive tensor, $C_{ijkl}^0$ and history stress vector, $\Delta \sigma_{ij}^R$, which should reproduce the cohesive zone counterparts.
Two other cases for the bulk material behavior are also considered in order to demonstrate its effect on the homogenized behavior. In one case the bulk is still considered linear elastic but with Young’s modulus of $10^5$, same order of magnitude as the cohesive zone stiffness. In the other case, the bulk is considered linear viscoelastic with relaxation modulus following the cohesive zone relaxation modulus.

Figure 3.2 presents the analytical cohesive zone traction, $t^1_n(t)$, as a function of the cohesive zone normal opening displacements compared to the homogenized stress component $\sigma_{22}^0$ for different bulk materials.

![Figure 3.2: Comparison of analytical traction and numerical results for global stress.](image)

Figure 3.3 presents the homogenized constitutive behavior for the three different bulk behaviors. The normal incremental cohesive zone stiffness, $k_{nn}^1$, and the homogenized constitutive component, $C_{2222}^0$, are shown in Figure 3.4, while Figure 3.5 presents the cohesive zone residual traction vector, $\Delta t_{n}^{R1}$, as well as the homogenized residual stress component, $\Delta \sigma_{22}^{R0}$.

Finally, one can observe from Figure 3.6 that damage induced anisotropy is introduced in the global homogenized constitutive behavior due to the cohesive zone debonding. This is an important phenomenon that occurs in various applications in which materials undergo
Global stress, $\sigma_{22}$
Global strain, $\varepsilon_{22}$

Figure 3.3: Homogenized constitutive behavior for different bulk materials.

Figure 3.4: Comparison of incremental stiffnesses.

microcracking in preferred directions, either due to lower toughness in a certain fracture mode or due to higher stresses in particular directions. Models that can account for this effect are therefore desirable in the design process.
3.4 Example Problems

In order to demonstrate the capabilities of the model developed for the local scale IBVP, two example problems are presented in this section. The first example problem considers the homogenization of viscoelastic fiber-reinforced composites with cracks. The case where no cracking is allowed to occur and the case where the matrix is considered to be linear elastic (no cracking) are also considered. The second example problem presents results of a multiscale simulation of a viscoelastic fiber-reinforced composite tapered bar containing cracks. For this second example, the microstructure is simplified in order to minimize the computational time required for the analysis. Both examples consider quasi-static loading. It is important to note that these example problems are presented for illustrative purposes and do not intend to provide accurate solutions to these problems, especially because of the arbitrary selection of material properties and microstructures.
Figure 3.6: Damage induced anisotropy for (a,b) elastic \((E = 10^5)\) and (c,d) viscoelastic bulk materials.

### 3.4.1 Homogenization of viscoelastic fiber-reinforced composites with cracks

Fiber-reinforced composite materials have continuously found a broad range of structural applications, such as jet engine parts, pressure vessels, helmets and tank armor. The advantage of these materials is that one can, in some sense, design its microstructure in order to obtain the desired overall properties. Some researchers have shown that carbon fiber-reinforced materials can show considerable time-dependent (viscoelastic) behavior inherited from the matrix material [22]. Furthermore, fiber-reinforced composites are in general filled with
voids and defects due to the manufacturing process and can also contain lots of microcracks initiated by service loading. The model herein developed is intended to be used in such applications where both viscoelasticity and microcracking are important.

Assume that the microstructure shown in Figure 3.7 corresponds to the Representative Volume Element of an arbitrary fiber-reinforced composite. The fibers diameter has been arbitrarily defined as 1.0 \( \mu \text{m} \). The material properties for the bulk and cohesive zones are given in Table 3.1. It is assumed that the cohesive zone relaxation modulus is the same as the bulk matrix material.

Two other cases are also considered: one is the case where no cracks are allowed to initiate and grow, and the other is the case where the matrix material is assumed linear elastic with Young’s modulus of 70 GPa \( (E^1 = E^1_\infty + \sum_{i=1}^5 E^1_i) \) and Poisson’s ratio of 0.3. It is important to observe that all material properties herein used have been arbitrarily chosen.

The body is initially at rest and for the loading conditions, biaxial displacements are applied to the boundaries of the RVE resulting in external boundary average strain rates of \( \dot{\varepsilon}^{0}_{22} = 1.0 \times 10^{-4} \) and \( \dot{\varepsilon}^{0}_{11} = 0.5 \times 10^{-4} \) 1/s in the vertical and horizontal directions, respectively.

The FE mesh initially contains no cohesive zone elements, which are automatically
Table 3.1: Material properties of each constituent.

<table>
<thead>
<tr>
<th></th>
<th>Fiber</th>
<th>Matrix</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\nu^1$</td>
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<td>0.3</td>
</tr>
<tr>
<td>$E^1$ (GPa)</td>
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<td>$E_i^1$ (GPa)</td>
</tr>
<tr>
<td>$\rho_i^1$ (s)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\infty$</td>
<td>10</td>
<td>–</td>
</tr>
<tr>
<td>1</td>
<td>20</td>
<td>1.0</td>
</tr>
<tr>
<td>2</td>
<td>20</td>
<td>10.0</td>
</tr>
<tr>
<td>3</td>
<td>20</td>
<td>100.0</td>
</tr>
</tbody>
</table>

Cohesive zones

<table>
<thead>
<tr>
<th></th>
<th>Matrix-matrix interfaces</th>
<th>Fiber-matrix interfaces</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\delta^*_n$ (µm)</td>
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<td>0.1</td>
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<tr>
<td>$\delta^*_t$ (µm)</td>
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<td>0.1</td>
</tr>
<tr>
<td>$\sigma^*_n$ (MPa)</td>
<td>20</td>
<td>20</td>
</tr>
<tr>
<td>$\sigma^*_t$ (MPa)</td>
<td>20</td>
<td>20</td>
</tr>
<tr>
<td>$A$</td>
<td>5.0</td>
<td>5.0</td>
</tr>
<tr>
<td>$m$</td>
<td>0.5</td>
<td>0.5</td>
</tr>
</tbody>
</table>

* Viscoelastic relaxation modulus is the same as that given for the bulk matrix

inserted into the mesh once the cohesive zone initiation criterion is satisfied, in this case, if the traction vector along the edges between elements exceeds the damage initiation cohesive stress, $t_i^1 \geq \sigma_i^f$. For this example, cracks are not allowed to initiate inside the fibers. The cohesive zone insertion algorithm used has been implemented based on that introduced by [27] and [121].

Figure 3.8 presents the homogenized stress component $\sigma_{22}^0$ as a function of time for the cases herein considered, from which one can see that accounting for viscoelasticity and microcracking can be very important. It is however important to distinguish cohesive zones (non-zero traction new surfaces) from actual cracks (zero traction new surfaces). Cracks are more likely to produce statistical inhomogeneity than cohesive zones because cracks produce strong discontinuities in the field variables, whereas the traction field is still assumed continuous across the cohesive zone.
The evolution of component $C_{0222}^0$ of the tangent constitutive tensor is shown in Figure 3.9 from which one can see its dependence on the amount of accumulated damage. Results for the case where cracks are not allowed to initiate and grow are also shown along with the value of the volume average of the incremental (tangent) constitutive tensor, which is an upper bound value.

Figure 3.9: Component $C_{0222}^0$ of homogenized tangent constitutive tensor.

Figure 3.10 demonstrates how all components of the homogenized incremental (tangent)
constitutive tensor change as functions of time. Note that the loading monotonically increases with time. Snapshots of the RVE for selected times are shown in Figure 3.11 from which one can observe the amount of cracking occurring at each stage. These selected states are marked in Figure 3.10 with vertical dashed lines so that one can correlate how the components of the homogenized incremental (tangent) constitutive tensor change as functions of crack density. Note that the internal boundaries shown in Figure 3.11 can be either cohesive zones or actual cracks.

![Graph showing C0ijkl (GPa) vs. Time (s) for selected components.]

Figure 3.10: Components $C_{1111}^0$, $C_{2222}^0$, $C_{1122}^0$ and $C_{1212}^0$ of homogenized incremental (tangent) constitutive tensor as a function of time.

The dependence of the history dependent stress tensor $\Delta \sigma_{ij}^{0R}$ on the amount of accumulated damage is depicted in Figure 3.12. Even though $\Delta \sigma_{ij}^{0R}$ is a quantity that arises from the numerical incrementalization of the constitutive equations, the physical interpretation that can be drawn from the numerical results is that microcracking affects both instantaneous ($C_{ijkl}^0$) and history dependent ($\Delta \sigma_{ij}^{0R}$) response of the material, as expected.
Figure 3.11: Snapshots of the damage accumulated in the RVE.

Figure 3.12: Component $\Delta \sigma_{22}^{0R}$ of the homogenized history dependent stress tensor as a function of time.
3.4.2 Multiscale modeling of a viscoelastic fiber-reinforced tapered bar

Consider the tapered bar shown in Figure 3.13(a) as the global scale object of interest. Symmetry of geometry about the \(x\)-axis has been considered in order to minimize computational effort. Horizontal displacements are quasi-statically applied at the right end of the bar. Also assume that the local structure can be approximated by the RVE shown in Figure 3.13(b). The same initial local geometry is used at all global scale integration points. Plane stress conditions are assumed for both global and local scales. The fiber is again assumed to be linear elastic while the matrix is assumed to be linear viscoelastic. The arbitrarily chosen material properties used in this example are given in Table 3.2.

![Figure 3.13: Geometry and FE mesh of tapered bar problem.](image)

As for the previous example problem, the local FE mesh initially does not contain any cohesive zone elements, which are automatically inserted into the mesh once the cohesive zone initiation criterion is satisfied.

Figure 3.14 shows the contour of the component \(C_{1111}^0\) of the computed homogenized incremental (tangent) constitutive tensor as well as selected local structures at the end of the simulation, when the total applied tip displacement is of 0.74 cm. The contour for the component \(\sigma_{11}^0\) of the stress tensor is shown for each selected local structure. Figure 3.15
Table 3.2: Material properties of local scale constituents.

<table>
<thead>
<tr>
<th>Bulk materials</th>
<th>Fiber</th>
<th>Matrix</th>
</tr>
</thead>
<tbody>
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<td>$E_i^1$ (MPa)</td>
</tr>
<tr>
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<td>350</td>
<td>$\rho_i^1$ (s)</td>
</tr>
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<td>50</td>
<td>$10^{-2}$</td>
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<tr>
<td>2</td>
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<td>$10^{-1}$</td>
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<td>$10^2$</td>
</tr>
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<td>6</td>
<td>50</td>
<td>$10^3$</td>
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</tbody>
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<tr>
<th>Cohesive zones</th>
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<tr>
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<tr>
<td>Matrix-matrix interfaces</td>
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<tr>
<td>$\delta_n^{*1}$ (nm)</td>
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<td>$\delta_t^{*1}$ (nm)</td>
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<td>$\sigma_n^{1}$ (MPa)</td>
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<td>$\sigma_t^{1}$ (MPa)</td>
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<tr>
<td>$A$</td>
</tr>
<tr>
<td>$m$</td>
</tr>
</tbody>
</table>

* Viscoelastic relaxation modulus is the same as that given for the bulk matrix

presents, for different times, how the homogenized modulus $C_{1111}^0$ varies with the horizontal position $x_1^0$ along the symmetry line of the tapered bar. Values shown in the graph also correspond to the end of the simulation.

As expected, one can observe from Figure 3.14 that more damage is accumulated at regions of smaller cross-section, where stresses are concentrated. Consequently, $C_{1111}^0$ is lower at smaller cross-sections (Figure 3.15), once more damage has been induced at the corresponding local structures. It is once again important to note that the internal boundaries shown in Figure 3.14 may not correspond to cracks, but to cohesive zones in fact.

It can be seen from Figure 3.15 that there is a sudden drop in the stiffness at a certain position $x_1^0$ (approximately 6.8cm for $t = 7.4$s, for example). This sudden drop is produced
Figure 3.14: Contour of $C^0_{1111}$ for global scale and contour of $\sigma^{0}_{11}$ for local scale at different global positions.

Figure 3.15: Component $C^0_{1111}$ of the homogenized tangent constitutive tensor as a function of $x^0_1$ coordinate.

by the automatic insertion of cohesive zone elements and the arbitrarily selected local scale geometry and material properties. Note that the stress field varies along $x^0_1$, so that there will be a region in the global mesh for which the fracture criterion is not satisfied at the local scale and another region for which the fracture criterion is satisfied. Furthermore, for the current scenario, the state of stresses in the matrix material is approximately homogeneous so that most of the internal boundaries induced in the matrix are inserted at the same time step. The combination of all these factors thus produces a sudden drop in the stiffness and
makes convergence more difficult to be achieved.

A further analysis of the results also reveals that the local structure is intact for \( x_1^0 < 2.7 \) cm (see Figure 3.15 and first local structure shown in Figure 3.14), is slightly damaged for \( 2.7 \) cm \( < x_1^0 < 6.8 \) cm (see Figure 3.15 and second local structure shown in Figure 3.14) and is very damaged for \( x_1^0 > 6.8 \) cm (see Figure 3.15 and third local structure shown in Figure 3.14). The results also show that once most of the internal boundaries have been inserted, the evolution of the cohesive zone damage parameter \( \alpha^1(t) \) governs the stiffness decrease, as expected.

More physically representative results can be obtained if one considers statistical variation of the cohesive zone damage initiation stress, \( \sigma_i^{f1} \), throughout the mesh interfaces, simulating the existence of natural defects in the material. The use of larger (more fibers) statistically homogeneous RVE’s and finer meshes could also improve the numerical results.
Chapter 4

Multiscale Finite Element Code

The multiscale model previously described can be implemented into a computational algorithm to allow approximate solutions to complex problems containing multiple length scales with cracks growing simultaneously on the different length scales. The algorithm herein utilized is based on the Finite Element Method (FEM) and is written in C++ programming language under the conception of Object-Oriented Programming (OOP). The main advantage of using OOP is that it facilitates the implementation of multiscale nested solution schemes. References [48, 50] have also used OOP to develop nested multiscale finite element code.

The general conception and organization of object classes follows the work presented in [100, 109], even though the cited references do not consider multiscale modeling. The multiscale code has been verified for two-dimensional (plane stress, plane strain and axisymmetric) problems under infinitesimal deformations. The code currently supports linear and quadratic triangle, quadrilateral and line (cohesive zone) elements. Since the code has been developed to analyze impact problems, the Lagrange multipliers technique has been implemented to avoid interpenetration of objects, simulating frictionless contact conditions. Lagrange multipliers are also used to avoid interpenetration of cohesive zones.

Since in the current multiscale model the global and local governing partial differential
equations are different, it is not computationally efficient to use the same solution procedure for both scales, as is usually done when both length scales are assumed to be quasi-static problems [131, 8]. In this case, the global and local domains are solved by means of explicit (central difference) and implicit quasi-static FEM solution schemes, respectively.

A local scale finite element mesh is assigned to every integration point belonging to the selected global scale elements. Note that allowing a priori selection of elements that will be analyzed locally reduces the amount of time required to solve the problem, but some losses in accuracy may be introduced. Furthermore, different local scale meshes can be assigned to different global scale elements, thus allowing simulation of problems where the microstructure of the global object varies spatially.

The basic difference from a standard FEM algorithm is that in multiscale algorithms every time some information about the constitution of the global material is needed one must solve an IBVP or at least perform some computation (average) at the local scale. The connection between global and local scales is especially emphasized whenever the stresses at the global scale are to be computed. This connection is simply stated by the computation of the applied displacements on the boundary of the local scale from the global scale strain tensor and the computation of the global stresses from the local solution (incremental homogenized constitutive tensor and history dependent tensor). A general description of the algorithm is given in the flowchart shown in Figure 4.1.

4.1 Automatic insertion of cohesive zone elements

Crack propagation is herein modeled by using a cohesive zone model because this type of fracture mechanics model is more convenient to be utilized in computational finite element algorithms and because it can model multiple cracks simultaneously. Cohesive zone models have been introduced by Dugdale [45] and Barenblatt [15]. More importantly, a nonlinear
Figure 4.1: Flowchart of the multiscale computational algorithm.

viscoelastic cohesive zone model seems to be more accurate than the Griffith criterion for viscoelastic media.

The main shortcomings of most cohesive zone models are essentially related to the
inability (or difficulty) to measure directly the material parameters necessary to characterize a particular cohesive zone model and to the fact that cohesive zone models are normally deployed in such a way that it is necessary to know where the crack will propagate a priori. The main advantages are that cohesive zone models are quite conveniently deployable into a finite element code and they can be formulated in such a way that the fracture phenomena in some media, especially inelastic, can be captured more accurately than can the Griffith criterion. For example, it is often observed in viscoelastic media that the critical energy release rate required for crack extension is rate dependent. Details of formulation and implementation of cohesive zone elements can be found in [63].

Since cohesive zone elements may introduce additional compliance to the finite element mesh prior to crack initiation and increase the maximum bandwidth of the stiffness matrix, the computational model presented herein uses an algorithm to automatically insert cohesive zone elements into the finite element mesh at the moment in time at which the criterion for cohesive zone initiation is satisfied. In this case, the initiation criterion is assumed to be given by:

$$t^1_i(t) \geq \sigma^f_i$$

(4.1)

where $\sigma^f_i$ is the intensity of tractions at which crack initiation occurs and is the same parameter used in Equation 2.16.

Figure 4.2 presents a graphical depiction of the automatic insertion concept herein developed. For a given solution step, the stress tensor is computed at every node in the mesh and then the traction vector $t^1_i(t)$ is computed for every elemental edge sharing that node using Cauchy’s formula ($t^1_i = \sigma^1_{ji} n^1_j$). Actually, the traction vector is computed at selected positions determined by the unidimensional Gauss integration rule and its value is determined by interpolation from the nodal values of the traction vectors. Then, the traction vector for every edge in the mesh is checked against the crack initiation criterion, inequality 4.1.
Finally, if the crack initiation criterion is satisfied for some edge node, this node is doubled and a cohesive zone element is then created for the new surface. After a new node has been created, the Cuthill-McKee algorithm [43] is invoked in order to renumber the nodes in such a way as to minimize the maximum bandwidth. It is also important to note that the Lagrange multiplier technique is used in order to apply displacement constraints in the cohesive zone so that nodal interpenetration is precluded.

![Figure 4.2: Depiction of automatic insertion of cohesive zone elements.](image)

The algorithm developed herein is similar to the one introduced in [27], but with some modifications to allow the use of linear (constant strain) finite elements. Reference [27] developed an algorithm based on 6-noded triangle element where the crack initiation first occurs at midside nodes of the element and can then propagate to the edges. The algorithm herein developed, on the other hand, checks the crack initiation criterion for every node in the mesh and therefore is not limited to quadratic elements.

### 4.2 Parallel programming

Advances in science and technology have allowed the fabrication of very complex heterogeneous materials. A better understanding of the physical behavior of such materials as well as advances in numerical methods have opened possibilities for modeling such complex structural
problems. Even though computational models are available, accurate simulations have been limited by the lack of computational power. The lack of computational power is actually one of the main reasons that have led to the development of multiscale models, once direct simulation of all heterogeneities is not possible.

However, separation of length scales (leading to multiscale models) by itself may not sufficiently reduce the amount of computer power required to solve the problem. The multiscale approach herein proposed is computationally intense due to the complexity of the problem: multiple length scales and multiple evolving cracks. For example, a single processor at 2.16 GHz running under Fedora Linux 8 took 33 minutes to solve 76 time steps of the single RVE problem considered in section 3.4.1. On the other hand, an alternative direct approach, wherein a highly refined mesh is used at a single global scale, is well beyond the capability of currently available computing platforms.

In order to minimize computational effort, one may use multiscaling only within selected regions of the global structure where damage evolution is anticipated, thereby reducing the required number of local meshes. Another very efficient strategy is to use parallel computing in such a way that multiple processors can handle different local meshes simultaneously. The concept of parallel programming is extremely efficient for multiscale algorithms in which it is assumed that the local scale meshes are not interdependent at each time step, such that each local mesh can be simultaneously solved by different processors and the total computational time is vastly reduced.

For example, a plate impact problem of 600,000 time steps and using 48 local meshes (each with 1,660 elements and 871 nodes) took 101 hours (4.2 days) to be solved in parallel by 8 processors at 3.0 GHz running under Red Hat Linux 5.0. The same problem took more than four weeks to be solved by a single processor. The advent of faster computers, the advance of parallel computing and the development of faster algorithms will make multiscale simulations of real structures more feasible.
Figure 4.3 shows the reduction in computational time due to the use of multiple processors for a test case consisting of a global mesh of 374 degrees of freedom and 120 local meshes of 186 degrees of freedom, where automatic insertion of cohesive zones is allowed in the local scale. The problem consisting of 500 time steps was solved in a Dell workstation with 8 processors at 3.00 GHz and 32 GB RAM memory running on Red Hat Linux 5.0.

Note that as the number of processors is increased the time spent on message passing increases and the number of local problems per processor decreases, so that for a given problem there will be an optimum number of processors for which there will be no gain if more processors are used, as shown in Figure 4.3.

The computational algorithm presented herein has been parallelized using the Open MPI libraries [64], and the basic tasks that have been parallelized are shown in Figure 4.1. References [48, 50] have also used parallel computing to develop a multiscale finite element code.
Chapter 5

Verification of the multiscale model

In this chapter the developed multiscale computational model is compared to analytically derived solutions for simple problems. The model has been developed to be used to solve very complex impact problems involving heterogeneous viscoelastic media containing evolving cracks. At least to the knowledge of the author, there are no available analytical solutions for such problems. This is actually the main reason why numerical solutions are herein sought.

Analytical solutions to stress waves problems are very difficult to be obtained even for homogeneous elastic media. Most available analytical solutions to wave problems consider homogeneous elastic medium subjected to harmonic waves, especially for two- and three-dimensional problems [1].

Since there is no analytical solution to the general problem, analytical solutions are herein derived for simple special cases in order to verify the multiscale code. To avoid the mathematical complications due to stress waves traveling in multi-dimensional space, one-dimensional analytical solutions are herein sought, since the concepts and physics of mechanics can still be demonstrated in the simple 1-D case.

The first idealized problem is the case of stress waves propagating in a finite bar made of functionally graded elastic material, where the elastic modulus varies exponentially with
spatial coordinates. The second problem considers the case of stress waves traveling in both semi-infinite and finite homogeneous viscoelastic media. Even though it may be possible to obtain an analytical solution for the case of a viscoelastic heterogeneous medium by applying correspondence principles to the herein obtained elastic solution, such solution has not been obtained yet. Nonetheless, heterogeneity and viscoelasticity will be checked separately by individual analytical solutions. Neither analytical nor direct numerical solutions to problems containing evolving cracks have been obtained. Single scale direct numerical simulations of stationary cracks have not been herein sought not only because it would require highly refined meshes, but also because it is actually the limit case where the inclusions have zero stiffness (if the cracks are assumed to have the same shape of the inclusions).

5.1 Analytical solution to wave problems in heterogeneous elastic bar

Consider the infinitesimal 1-D equation that governs the propagation of longitudinal waves:

$$\frac{\partial \sigma^0(x^0, t)}{\partial x^0} = \rho^0(x^0) \frac{\partial^2 u^0(x^0, t)}{\partial t^2}$$

(5.1)

where the superscript 0 refers to the global scale object, $x^0$ is the spatial coordinate, $t$ is the time, $\sigma^0(x^0, t)$ is the one-dimensional stress field, $u^0(x^0, t)$ is the one-dimensional displacement field and $\rho^0(x^0)$ is the particle mass density.

The elastic constitutive equation under one-dimensional strain conditions may be written in the form:

$$\sigma^0(x^0, t) = \varphi^0(x^0) \frac{\partial u^0(x^0, t)}{\partial x^0}$$

(5.2)

where $\varphi^0(x^0) \equiv \lambda^0(x^0) + 2\mu^0(x^0)$ is the longitudinal modulus and $\lambda^0$ and $\mu^0$ are the Lamé
elastic constants. Note that the dependence of $\varphi^0$ and $\rho^0$ on the global spatial coordinate reflects the material heterogeneity. For simplicity, the dependence on the spatial variable $x^0$ and time $t$ will now be omitted when necessary.

Substituting equation 5.2 into 5.1, and using the chain rule of differentiation, gives:

$$\frac{\partial \varphi^0}{\partial x^0} \frac{\partial u^0}{\partial x^0} + \varphi^0 \frac{\partial^2 u^0}{\partial x^0 \partial t} = \rho^0 \frac{\partial^2 u^0}{\partial t^2} \quad (5.3)$$

Now, consider the case of a functionally graded elastic material for which the longitudinal modulus and mass density vary exponentially in space according to:

$$\varphi^0(x^0) = \varphi^0_0 e^{-x^0/\delta} \quad (5.4)$$

$$\rho^0(x^0) = \rho^0_0 e^{-x^0/\delta} \quad (5.5)$$

where the constant $\delta$ is the same for both $\varphi^0(x^0)$ and $\rho^0(x^0)$. Substituting equations 5.4 and 5.5 into equation 5.3, yields:

$$\frac{\partial^2 u^0}{\partial x^0 \partial t} - \frac{1}{\delta} \frac{\partial u^0}{\partial x^0} = \frac{1}{c^0_L^2} \frac{\partial^2 u^0}{\partial t^2} \quad (5.6)$$

where $c^0_L$ is defined as:

$$c^0_L \equiv \sqrt{\frac{\varphi^0_0}{\rho^0_0}} \quad (5.7)$$

The general solution of the partial differential equation 5.6, obtained using the method of separation of variables, is given by:

$$u^0(x^0, t) = (A + B e^{x^0/\delta})(C + D t)$$

$$+ e^{x^0/2\delta} [E \cos(\alpha x^0) + F \sin(\alpha x^0)][G \cos(\kappa c^0_L t) + H \sin(\kappa c^0_L t)] \quad (5.8)$$

where $A$–$H$ are constants to be determined by the initial and boundary conditions, $\alpha$ is
defined as:
\[
\alpha \equiv \sqrt{4\delta^2\kappa^2 - 1} \quad \frac{2\delta}{4}\tag{5.9}
\]
and the following condition has to be satisfied:
\[
\kappa > \frac{1}{2\delta} \quad \frac{1}{5.10}
\]

Now consider a finite bar of length \( L_b \) with the following initial and boundary conditions:
\[
\begin{align*}
  u^0(x^0, 0) &= 0 \quad \frac{5.11}{(5.11)} \\
  \frac{\partial u^0(x^0, 0)}{\partial t} &= 0 \quad \frac{5.12}{(5.12)} \\
  u^0(0, t) &= 0 \quad \frac{5.13}{(5.13)} \\
  \sigma^0(L_b, t) &= \varphi^0(L_b) \frac{\partial u^0(L_b, t)}{\partial x^0} = P^0 \quad \frac{5.14}{(5.14)}
\end{align*}
\]
where \( P^0 \) is the load applied to the tip at \( x^0 = L_b \). The constants A–H can now be determined and the solution then becomes:
\[
u^0(x^0, t) = -\frac{P\delta}{\varphi^0_0}(1 - e^{x^0/\delta}) + e^{x^0/2\delta} \sum_{n=1}^{\infty} R_n \sin(\alpha_n x^0) \cos(\kappa_n t) \quad \frac{5.15}{(5.15)}
\]
where
\[
R_n = \frac{\int_0^{L_b} \frac{P\delta(1 - e^{x^0/\delta})}{\varphi^0_0} e^{x^0/2\delta} \sin(\alpha_n x^0) dx^0}{\int_0^{L_b} \sin^2(\alpha_n x^0) dx^0} \quad \frac{5.16}{(5.16)}
\]

The value of \( \kappa_n \) for each \( n \) is determined by solving the characteristic equation 5.17 where equation 5.9 should be recalled. In this case, equation 5.17 has been solved numerically using Maple\textsuperscript{TM} Software 9.5.
\[
\sin(\alpha_n L_b) + 2\delta\alpha_n \cos(\alpha_n L_b) = 0 \quad \frac{5.17}{(5.17)}
\]
Equation 5.15 is the solution sought which will be used to validate the multiscale computational model. The FE meshes used for the global and local scales are shown in Figure 5.1. A unit cell containing a single fiber is herein considered for the local scale, and one local mesh has been attached to each of the 1,440 integration points of the global mesh. The numerical FE simulations assumed 2D plane strain conditions where lateral deformation of the bar is constrained, as shown in Figure 5.1, in order to be consistent with the governing one dimensional strain wave equations.

Single scale analyses have shown that the same results are obtained for one or six rows of elements as long as the height of the bar is kept the same. Even though it may not be necessary to discretize the global scale mesh in the \( y \)-direction, and since the required amount of computational time is not critical in this case, it has been done so to avoid possible numerical inaccuracies due to very high element aspect ratios. The problem is however one-dimensional and there is no deformation in the transverse \( y \)-direction.

Figure 5.1: FE mesh used for the (a) global and (b) local scales.
The contour shown in Figure 5.1 represents the exponential variation of the component $C_{1111}^0$ of the elastic homogenized constitutive tensor, computed using the procedure presented in Chapter 3.

The properties (Young’s modulus, Poisson’s ratio and mass density) of both fiber and matrix change exponentially as a function of the unit cell position referred to the global scale, $x^0$. Their respective values for the fiber ($E_{0f}^1 = 118.24$, $\nu_{0f}^1 = 0.3$, $\rho_{0f}^1 = 15.3$) and matrix ($E_{0m}^1 = 67.24$, $\nu_{0m}^1 = 0.3$, $\rho_{0m}^1 = 8.7$) have been selected such that the respective homogenized properties (see Chapter 3) assumed the values: $\varphi_0^0 = 100$ and $\rho_0^0 = 10$. Other model input parameters are: $P_0^0 = 1.0$, $L_b = 3.0$ and $\delta = 2.0$. The infinite series in the analytic solution has been truncated at 100 terms, when the series has been considered to have converged satisfactorily. Units are herein omitted but one may assume any consistent system of units. Figure 5.2 presents the exponential variation of the homogenized longitudinal modulus, $\varphi^0(x^0)$, for the particularly chosen parameters.

![Figure 5.2: Exponential variation of $\varphi^0(x^0)$.](image)

Figure 5.3 compares the analytic and numerical results for the tip displacement of the finite bar as a function of time, while Figure 5.4 shows the results for the stress wave profiles at different times, where the arrows indicate the direction of wave propagation at each moment. It is important to note that the truncation of the infinite series in the analytical solution (equation 5.15) produces an oscillatory behavior of the stress, $\sigma_{11}^0$, near the jump discontinuity (see Figure 5.4). The use of other techniques to solve the wave equation, such
as the d’Alembert technique, might actually be more appropriate in cases where there are jump discontinuities in the field variables.

![Graph](image)

Figure 5.3: Tip displacement of the finite functionally graded bar.

It is important to note that the dispersion (oscillatory behavior of the stress pulse) observed in the FE results is due to the effects of lateral inertia produced by the finite transverse dimension of the bar [1]. As shown in [1], this is a physical phenomenon observed in multi-dimensional objects caused by wave reflections occurring on both lateral boundaries of the bar and, in this case, is not caused by pure numerical issues or by the fact that the mesh has been discretized in the $y$-direction. Furthermore, even if the body is excited in a single pure mode (either longitudinal or shear), both modes will propagate from the boundaries every time the wave is reflected, unless particular conditions are satisfied, and the two reflected waves generally propagate in different directions [1]. These reflected waves thus interact with the main excitation wave changing the shape of the original pulse. Note that the lateral inertia effects are therefore closely related to the cross-sectional dimensions of the bar.

The physical effect of lateral inertia is neglected in the elementary wave theory, which is the reason why such dispersion does not appear in the analytical results. If truly one-
Figure 5.4: Comparison of analytic and numerical results for the stress wave profile of the finite functionally graded bar.

dimensional finite elements, formulated based on the elementary wave theory, had been used, such dispersion effects would not be present in the numerical solution. The reader should however note that there is no one-dimensional object in reality, so that the physical phenomenon of lateral inertia is actually expected in multi-dimensional bodies, even if the overall pulse propagates in a single direction.
5.2 Analytical solution to wave problems in homogeneous viscoelastic uniaxial bar

In this section, the numerical code is compared to analytical solutions for wave problems in homogeneous viscoelastic media. The purpose is to verify the implementation of the viscoelastic incrementalization developed in [150] into an explicit time integration scheme.

5.2.1 Semi-infinite viscoelastic bar

The solution to the problem of wave propagation in a semi-infinite viscoelastic rod with domain $x > 0$ and finite end at $x = 0$ has been addressed in [35], where the Laplace transform technique is used. Consider the particular case of a material represented by a Maxwell model:

$$\varphi^0(t) = \varphi_0^M e^{-t/\tau^0}$$  (5.18)

where $\varphi^0(t)$ is the longitudinal relaxation modulus, and $\tau^0$ represents a relaxation time scale. The superscripts 0 are used to emphasize that the object under consideration exists on the global length scale $0$. Assume undisturbed initial conditions and boundary conditions given by constant velocity applied at the finite end of the bar:

$$v^0(0, t) = V_0^0 H(t)$$  (5.19)

where $v^0(x, t)$ is the velocity field, $V_0^0$ is a constant and $H(t)$ is the Heaviside step function. The solution to this problem, using the elementary wave theory, is taken from [103, 35] and is given by:

$$\sigma^0(x^0, t) = \rho_0^0 c_0^M V_0^0 e^{-t/2\tau^0} I_0 \left( \frac{1}{2\tau^0} \sqrt{t^2 - \frac{x^0}{c_0^M} - 2} \right) H \left( t - \frac{x}{c_0^M} \right)$$  (5.20)
where
\[ c_0^M = \sqrt{\frac{\varphi_0^M}{\rho^0}} \] (5.21)
and \( I_0 \) is the modified Bessel function of first kind and of order zero.

Although in this case, the inverse Laplace transform has been obtained in closed form, it is not easily obtained for more complex boundary conditions and for more realistic representations of the relaxation modulus, \( \varphi^0(t) \), other than the Maxwell model. The use of the Maxwell model is herein artificial, not only because of its limitation in representing real materials, but also because it implies the characteristics of a fluid. However, for code validation purposes, this solution is valuable.

The input parameters used in both analytic and numerical solutions are \( \varphi_0^M = 100, \tau^0 = 2, V_0^0 = 0.01, \rho^0 = 10 \). Units are herein omitted but one may assume any consistent unit system. The numerical FE simulations assumed 2D plane strain conditions where lateral deformation of the bar is constrained, as shown in Figure 5.5. An infinite boundary is assigned to the right end of the bar, where the nodes are mapped to infinity using special shape functions [19, 20, 21].

![Figure 5.5: FE mesh used in numerical simulation of a semi-infinite Maxwell bar.](image)

Figure 5.6 compares analytical and numerical results for the longitudinal stress as a function of time, for different positions in the rod. In this case, compressive stresses are plotted on the positive stress axis. Figure 5.7, on the other hand, presents a comparison between analytical and numerical results for the longitudinal stress as a function of position, for different times.

Note from Figure 5.7 that, due to viscoelastic dissipation, the shape of the stress pulse
changes as the wave propagates into the medium. This phenomenon is known as material dispersion. It is also important to note that lateral inertia effects are not apparent in this example problem perhaps due to a combination of the semi-infinite geometry of the bar, its particular radius, the material viscoelasticity and, especially, the different character of the boundary conditions.
5.2.2 Finite viscoelastic bar

Another class of problems of great practical importance is that of wave propagation in finite bodies. The main difference is that wave reflections have to be considered in bodies of finite extent. Lee and Kanter [102] have actually shown that, similar to the solution for elastic rods, the solution for a finite viscoelastic rod can be obtained from the solution for the semi-infinite rod through the superposition of waves traveling both left and right.

However, this does not simplify the integral transform inversion, which quickly becomes impractical for realistic representations of material mechanical properties. An alternative method that eliminates some of these difficulties is presented in [35]. The types of dynamic problems that can be solved using this method are those in which the Poisson’s ratio can be considered a real constant, and for which the boundary conditions have the following separable form:

\[
\sigma^0_{ji} n_j^0 = S^0_i(x_i) f^0(t) \quad \text{on } \partial V_\sigma^0
\]
\[
u^0_i = U^0_i(x_i) g^0(t) \quad \text{on } \partial V_u^0
\]

Now consider the case of a finite length rod under one-dimensional strain (using the elementary wave theory) with one end fixed and the other subjected to a suddenly applied load:

\[
\sigma^0(L_b, t) = p^0 H(t)
\]
\[
u^0(0, t) = 0
\]

The method proposed in [33, 35] assumes that the displacement field is of the following


form:

\[ u^0(x^0, t) = \sum_{n=1}^{\infty} C_n^0(t) \sin \left( \frac{(2n-1)\pi x^0}{2L_b} \right) + K^0(t) \frac{x^0}{L_b} \]  

(5.26)

where the first term represents the eigenfunctions of a corresponding elastic bar of length \( L_b \) with coordinate \( x^0 \) originating from the fixed end and the second term represents the quasi-static solution for the corresponding viscoelastic problem.

Now consider the Laplace transformed governing wave equation:

\[ \bar{\varphi}^0(s) \frac{\partial^2 \bar{u}^0}{\partial x^0^2} = p^0 s \bar{u}^0 \]  

(5.27)

where \( \bar{\varphi}^0(s) \) is the Laplace transform of the longitudinal relaxation modulus. From the Laplace transform of the boundary conditions, it is found that:

\[ K^0 = \frac{p^0 L_b}{s^2 \bar{\varphi}^0(s)} \]  

(5.28)

Taking the Laplace transform of equation 5.26 and substituting into equation 5.27, one can find:

\[ \sum_{n=1}^{\infty} \bar{C}_n^0 \left[ \frac{(2n-1)^2\pi^2}{4L_b^2} + \frac{\rho^0 s}{\bar{\varphi}^0(s)} \right] \sin \left[ \frac{(2n-1)\pi x^0}{2L_b} \right] = -\frac{\rho^0 p^0}{s[\bar{\varphi}^0(s)]^2} x^0 \]  

(5.29)

where from the Sturm-Liouville theory [69],

\[ \bar{C}_n^0 = \frac{32\rho^0 p^0 L_b^3 (-1)^n}{(2n-1)^2\pi^2 s \bar{\varphi}^0[(2n-1)^2\pi^2 \bar{\varphi}^0 + 4L_b^2 \rho^0 s]} \]  

(5.30)

The Laplace transformed solutions for the displacement and stress fields are then given by equations 5.31 and 5.32.

\[ \bar{u}^0(x^0, s) = \sum_{n=1}^{\infty} \frac{32\rho^0 p^0 L_b^3 (-1)^n}{(2n-1)^2\pi^2 s \bar{\varphi}^0[(2n-1)^2\pi^2 \bar{\varphi}^0 + 4L_b^2 \rho^0 s]} \sin \left( \frac{(2n-1)\pi x^0}{2L_b} \right) + \frac{p^0}{s^2 \bar{\varphi}^0} x^0 \]  

(5.31)
\[ \sigma^0(x^0, s) = \sum_{n=1}^{\infty} \frac{16\rho^0\rho^0 L_b^2(-1)^n}{(2n-1)\pi[(2n-1)^2\pi^2\varphi^0 + 4L_b^2\rho^0s]} \cos\left(\frac{(2n-1)\pi x^0}{2L_b}\right) + \frac{p^0}{s} \] (5.32)

In summary, this method of solving viscoelastic dynamic problems involves solving the corresponding quasi-static viscoelastic problem, the corresponding elastic eigenvalue problem and inverting equation 5.30, which is amenable to inversion for more realistic representations of mechanical properties. For the more complex representations, the inversion process can be obtained from available numerical packages that are not finite element based.

The solution for the case of a Maxwell model representation of the longitudinal relaxation modulus can be obtained by substituting the Laplace transform of equation 5.18 into equations 5.31 and 5.32 and then inverting. In the present work, the solution in the time domain was obtained by using Maple\textsuperscript{TM} Software 9.5, which is not finite element based, to accomplish the Laplace transform inversion.

In order to compare results, consider the arbitrarily chosen input parameters used in both analytic and numerical solutions to be \( \varphi^0_M = 150, \tau^0 = 3, \rho^0 = 10, \rho^0 = 1.0, L_b = 3.0 \). Units are herein omitted but one may assume any consistent system of units. The infinite series in the analytic solutions have been truncated in 100 terms, when the series has been considered to have converged satisfactorily. The numerical FE simulations assume 2D plane strain conditions where lateral deformation of the bar is constrained, as shown in Figure 5.8.

![Figure 5.8: FE mesh used in numerical simulation of a finite Maxwell bar.](image)

Figure 5.9 compares the analytic and numerical results for the tip displacement of the finite Maxwell bar as a function of time, while Figure 5.10 shows the results for the stress...
wave profiles at different times, where the arrows indicate the direction of wave propagation at each moment. Note from Figures 5.9 and 5.10 that after a certain time, the wave is completely dissipated due to material viscoelasticity.

![Graph](image)

Figure 5.9: Comparison of analytic and numerical results for the tip displacement of the finite Maxwell bar.

Once again, it is important to note that the dispersion (oscillatory behavior of the stress pulse) observed in the FE results shown in Figure 5.10 is due to the effects of lateral inertia produced by the finite transverse dimension of the bar [1]. This effect is neglected in the elementary wave theory, which is the reason why such dispersion does not appear in the analytical results.

The Maxwell model is the simplest mechanical representation of a viscoelastic material, and cannot accurately model the response of most real viscoelastic materials. Furthermore, the Maxwell model is more suitable for modeling viscoelastic fluids, as opposed to solids. The standard linear solid (SLS) is the simplest mechanical model that possess the characteristics for modeling the response of real solid materials. The SLS representation of the longitudinal modulus is given in equation 5.33:

$$\varphi^0(t) = \varphi^0_\infty + \varphi^0_1 e^{-t/\tau^0_1}$$ (5.33)
Figure 5.10: Comparison of analytic and numerical results for the stress wave profile of the finite Maxwell bar.

The main limitation of the SLS is the single exponential term, as opposed to the multiple exponential terms generally required to model real materials, so that the SLS is accurate for a small class of materials which exhibit time dependent behavior in a short time span. Analytical results have also been obtained for the case of a SLS finite bar using the same procedure described for the Maxwell finite bar. Figures 5.11 and 5.12 present comparisons between FE and analytical results for the case of the SLS viscoelastic material model, from which one can observe that after a certain time, the wave is completely dissipated due to material viscoelasticity.
Figure 5.11: Analytic and numerical results for the tip displacement of the finite SLS bar.

The results shown for the SLS model have been obtained for the following input parameters: $\varphi_\infty^0 = 100$, $\varphi_1^0 = 150$, $\tau_1^0 = 3$, $\rho^0 = 10$, $p^0 = 1.0$, $L_b = 3.0$. The infinite series in the analytic solutions have been truncated in 100 terms and the FE mesh is the same as the one used for the Maxwell material, Figure 5.8.

Note that Figures 5.9, 5.10, 5.11 and 5.12 reveal one of the main characteristics of viscoelastic materials, which is the ability to dissipate energy, thus damping vibrations and eventually reaching the quasi-static limiting response.

### 5.3 Comparisons to direct finite element simulations

In this section, comparisons between direct and multiscale simulations are presented. The term direct simulation is herein used to denote numerical simulations which consider all heterogeneities explicitly in the global scale FE mesh. One of the main purposes of this section is to compare the amount of computational time required by the multiscale FE algorithm to that required by the direct simulation. The other main purpose is to verify that the multiscale computational model is accurate when the assumptions regarding the separation
of length scales, equations 2.6 and 2.9, are satisfied. The condition that the length of cracks are small compared to the local length scale, equation 2.8, is not considered because direct simulations with such small cracks would require a highly refined mesh and an unreasonable amount of computational time.

In order to minimize the degree of complexity, the problem has been devised as a composite bar with a single layer of cylindrical fibers which are periodically placed along the bar. The length of the bar is kept constant, but the size (and number) of fibers changes. The size of the fibers is decreased so that the conditions regarding the length scales, equations 2.6 and
2.9, are at least approximately satisfied. Similarly to the previous example problems, the numerical FE simulations assumed 2D plane strain conditions where lateral deformation of the bar is constrained.

Figure 5.13 presents the geometry and FE meshes used for three different sizes of fibers. Note that the symmetry of the problem has been used in order to minimize computational effort. Figure 5.14, on the other hand, shows the meshes used in the multiscale simulation, where a local scale mesh has been attached to every integration point in the global scale mesh.

![Figure 5.13: Geometry and FE meshes used in the direct simulations.](image)

(a)

(b)

(c)

Figure 5.13: Geometry and FE meshes used in the direct simulations.

The sizes of the fibers have been selected so that the cases of 5, 25 and 100 unit cells are
Figure 5.14: Geometry and FE meshes used in the multiscale simulation.

Considered, respectively. Consequently, the thickness of the bar changes in order to maintain a single layer of fibers. Since the thickness of the bar changes considerably, the effect of dispersion due to lateral inertia will also change considerably. Since the purpose is to analyze the effect of the size of the microstructure with respect to the wavelength, dispersion due to lateral inertia is undesirable.

Fortunately, the effects of lateral inertia do not appear from the very beginning of the simulations because they are caused by wave reflections on the lateral boundaries of the bar. Therefore, the initial response of the bar is due to the main longitudinal wave only, and is not affected by waves reflected from the lateral boundaries. Moreover, in this case, the initial pulse travels at the longitudinal speed, which is the maximum speed a wave can reach in a material.

Furthermore, under these circumstances, the tip displacement (at the axis of symmetry), which is a measure of the average response of the bar (and as such is not greatly affected by lateral inertia effects, see Figures 5.9 and 5.11), will be used to compare the responses of
each case and only the initial response (before 900 nanoseconds) is analyzed. However, note that dispersive effects should still take place due to material heterogeneity.

It is important to say that even though the geometry of the problem is truly periodic, uniform (linear displacement) boundary conditions are applied, as opposed to periodic boundary conditions, because periodic boundary conditions have not been implemented to the code thus far.

For the loading, a square pulse of magnitude 100 MPa is applied at the tip of the bar during 25 nanoseconds. This produces a wave length of approximately 60 µm. Both fibers and matrix are assumed to be linear elastic, which material properties are given in Table 5.1.

<table>
<thead>
<tr>
<th></th>
<th>Fiber</th>
<th>Matrix</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ (GPa)</td>
<td>200</td>
<td>3.5</td>
</tr>
<tr>
<td>$\nu$</td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>$\rho$ (kg/m³)</td>
<td>1,760</td>
<td>1,170</td>
</tr>
</tbody>
</table>

Figure 5.15 presents the results for the displacement at the right tip (along the axis of symmetry) of the bar. A close-up look is provided in the lower right corner of the figure for better differentiation among the curves. It can be observed that the dispersion due to material heterogeneity is significant when the size of fibers is comparable to the wave length (cases of 5 and 25 cells). Moreover, the response obtained from the multiscale simulation is very close to the response of the 100 cells direct simulation, in which case the size of the unit cell is small compared to the wave length.

The results obtained using the rule of mixtures to compute the homogenized elastic modulus are also shown in Figure 5.15, which leads to the conclusion that for the specific problem considered herein, the rule of mixtures provides a poor prediction, overestimating the homogenized modulus and the wave speed.
Figure 5.15: Displacements observed at the right tip (along the axis of symmetry) of the bar.

Table 5.2 presents the amount of computational time required for each case, revealing the main purpose of the multiscale approach, which is the savings in computational effort compared to direct simulations. The simulations have been run on a Dell workstation with processors at 3.0 GHz running under Linux Fedora 10.

Table 5.2: Computational times for the elastic case.

<table>
<thead>
<tr>
<th>Case</th>
<th>Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rule of mixture</td>
<td>40 seconds</td>
</tr>
<tr>
<td>5 cells</td>
<td>20 minutes</td>
</tr>
<tr>
<td>25 cells</td>
<td>6.5 hours</td>
</tr>
<tr>
<td>100 cells</td>
<td>~ 6 days</td>
</tr>
<tr>
<td>Multiscale (4 processors)</td>
<td>53 minutes</td>
</tr>
</tbody>
</table>
Chapter 6

Application Problems

Numerical simulations of more complex problems are presented in this chapter in order to demonstrate the capabilities of the model. The first example problem to be presented in this chapter consists of a cylinder impacting a unidirectional carbon fiber reinforced composite plate. The effects of different local microstructures, cracking and viscoelasticity are considered for this problem. The second example considers a tapered bar subjected to the impact of an elastic block, where the tapered bar is also made of a viscoelastic unidirectional carbon fiber composite. Two different microstructures are considered and the effect of including cracking is analyzed. The third problem consists of a pressure vessel subjected to a quickly applied ramp internal pressure. The pressure vessel is made of unidirectional carbon fiber composite and two different local microstructures are considered. Cracking and viscoelasticity are considered.

The fourth application problem attempts to simulate a soldier helmet subjected to an air-pressure blast wave. The geometry of both global and local structures are over-simplified by two-dimensional descriptions (axisymmetric and generalized plane strain, respectively) in order to keep the problem solvable by the available computing power. Cracking and viscoelasticity are considered.
6.1 Cylinder/plate impact problem

In this example problem, an elastic cylinder impacts a plate at its center. The plate is made of unidirectional carbon fiber composite and the long axis of the cylinder is aligned with the direction of the fibers. Plane stress conditions are assumed. Figure 6.1 shows a depiction of the problem, as well as its two-dimensional FE mesh for the global scale where the symmetry of the problem has been considered in order to reduce computational effort.

![Figure 6.1: Depiction and FE mesh of the cylinder/plate impact problem.](image)

Even though it is beyond the scope of the present work to validate the computational model with experimental results, it is worth mentioning that Teixeira [139] presents comparisons between experimental results and simulations performed by the model herein developed. The referred study performed experimental tests consisting of a steel cylinder impacting a unidirectional glass fiber composite plate. The cylinder impacts the plate along the direction of the fibers so that the problem can be approximated by a 2D geometry, as is the case herein as well.

Three different microstructures are herein considered (see Figure 6.2) consisting of a unit cell, a RVE with five fibers and no voids and a RVE with fibers and voids. The volume
fractions of fibers are 19.6% and 15.7% for the unit cell and RVE’s, respectively, and a 1.2% volume fraction of voids is used in the third case. The main purpose is to analyze the effect of different geometries on the overall mechanical behavior of the composite. The FE meshes have initially 390, 1622 and 1768 degrees of freedom for the unit cell, RVE without voids and RVE with voids, respectively. However, note that the number of degrees of freedom may increase as cohesive zone elements are inserted during the analyses.

Two types of material behavior, elastic and viscoelastic, have been used for the matrix material. Moreover, two values of young’s modulus have been considered in the cases wherein the matrix is assumed elastic: \( E = E_\infty \) and \( E = E_0 \), where \( E_\infty \) and \( E_0 \) are the corresponding values of the viscoelastic relaxation modulus when \( t \to \infty \) and \( t = 0 \), respectively. The effect of including cracking at the local scale is also analyzed. A total of 18 combinations as shown in Table 6.1 have been simulated.

The material properties used herein for the local scale constituents are given in Table 6.2. The values shown may not reflect real material properties as they have not been experimentally measured but have been chosen based on properties reported in the literature. The cohesive zone material properties have also been arbitrarily chosen but, as opposed to bulk material properties, experimental determination of cohesive zone properties is not a well
established discipline. However, the purpose of the present work is not to accurately model specific materials but to demonstrate the capabilities of the model to account for material heterogeneity, viscoelasticity and cracking so that the use of accurate material properties is left for future works.

The elastic material properties of the impactor cylinder are: $E = 1.0$ GPa, $\nu = 0.3$ and $\rho = 2,000$ kg/m$^3$. The plate is initially at rest and the initial velocity of the cylinder is 125 m/s. Each simulation takes a total of 5,000 solution steps with time increments of 0.1 $\mu$s. A total of 200 local microstructures (FE meshes) are attached to the plate Gauss integration points. The time required to solve each case is also given in Table 6.1, from which one can see that the computational time increases dramatically with the number of degrees of freedom (actually the maximum band width) of the local scale mesh.

The inclusion of cracking also increases the computational time, but the use of the
Table 6.2: Material properties of local scale constituents.

<table>
<thead>
<tr>
<th>Fiber</th>
<th>Matrix</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\nu^1$</td>
<td>0.3</td>
</tr>
<tr>
<td>$\rho^1$ (kg/m$^3$)</td>
<td>1760</td>
</tr>
<tr>
<td>$E^1$ (GPa)</td>
<td>200</td>
</tr>
<tr>
<td>$\infty$</td>
<td>3.5</td>
</tr>
<tr>
<td>1</td>
<td>0.3</td>
</tr>
<tr>
<td>2</td>
<td>0.3</td>
</tr>
<tr>
<td>3</td>
<td>0.3</td>
</tr>
<tr>
<td>4</td>
<td>0.3</td>
</tr>
<tr>
<td>5</td>
<td>0.3</td>
</tr>
<tr>
<td>6</td>
<td>0.3</td>
</tr>
<tr>
<td>7</td>
<td>0.3</td>
</tr>
<tr>
<td>8</td>
<td>0.3</td>
</tr>
<tr>
<td>9</td>
<td>0.3</td>
</tr>
<tr>
<td>10</td>
<td>0.3</td>
</tr>
</tbody>
</table>

Cohesive zones

<table>
<thead>
<tr>
<th>Matrix-matrix interfaces</th>
<th>Fiber-matrix interfaces</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\delta_n^i$ (µm)</td>
<td>1.0</td>
</tr>
<tr>
<td>$\delta_t^i$ (µm)</td>
<td>1.0</td>
</tr>
<tr>
<td>$\sigma_n^i$ (MPa)</td>
<td>800</td>
</tr>
<tr>
<td>$\sigma_t^i$ (MPa)</td>
<td>10,000</td>
</tr>
<tr>
<td>$A$</td>
<td>0.01</td>
</tr>
<tr>
<td>$m$</td>
<td>1.5</td>
</tr>
</tbody>
</table>

* Viscoelastic relaxation modulus is the same as that given for the bulk matrix

Automatic insertion algorithm greatly improves the performance compared to a FE mesh where cohesive zone elements are inserted a priori throughout the entire mesh. All problems have been solved in a Dell workstation using 8 Intel Xeon processors at 3.00 GHz running under Linux Fedora 10. It is important to note that the amount of computational time is significantly reduced if one is able to use more processors in parallel.

Snapshots for the cases where cracking is considered are given in Figures 6.3, 6.4 and 6.5, for each of the microstructures and at selected times when all cohesive zones have evolved.
One can observe from these figures that more cohesive zones evolve in the elastic case with $E = E_0$ due to the higher stiffness of the matrix, and the viscoelastic case is in between the two limit elastic cases, as expected.

Figures 6.6 and 6.7 present the effect of the different microstructures on the back face deformation of the plate. Results are shown for the different matrix material constitution. The horizontal displacement, $u_{11}^0$, at the center of the plate’s back face is shown in Figure 6.6, while the vertical stress, $\sigma_{22}^0$, at the same position is presented in Figure 6.7. It can be observed that the global response of the plate is affected by the microstructural geometric characteristics. This is one of the most important features of the multiscale approach, which can account for very important microstructural design variables such as particle volume fraction, relative position and orientation of particles, material constitution and fracture toughness of individual constituents, among others.

The effect of the matrix material constitution on the back face displacement and on the vertical stress at the same location are shown in Figures 6.8 and 6.9, respectively. From Figure 6.8, one can see that the history of the back face displacement for the viscoelastic case is close to that for the elastic case with $E = E_0$. This could lead to the conclusion that for such a high loading rate, one may approximate the viscoelastic material by an equivalent elastic material with $E = E_0$. However, Figure 6.9 shows that this would be an incorrect assumption since the stress history is very different, thus producing different amount of cracking, as shown in Figures 6.3 and 6.5. Fewer cohesive zone elements evolve in the viscoelastic case because additional energy is dissipated in the bulk material so that less energy is dissipated by the cracking mechanism. The ability to dissipate energy prior to crack formation is one of the features that make viscoelastic materials attractive for impact resistance applications.

The history of the back face horizontal stress, $\sigma_{11}^0$, is shown in Figure 6.10 for the three different material constitutions and for the cases where no cracking is allowed. Due to the short thickness dimension, rapid oscillations are observed in the elastic cases, which will
Figure 6.3: Snapshots for the case of viscoelastic matrix with cracking.
Figure 6.4: Snapshots for the case of elastic ($E = E_\infty$) matrix with cracking.
Figure 6.5: Snapshots for the case of elastic ($E = E_0$) matrix with cracking.
Figure 6.6: Effect of microstructure: horizontal displacement at the center of the plate’s back face for the cases where cracking is not allowed.
Figure 6.7: Effect of microstructure: vertical stress at the center of the plate’s back face for the cases where cracking is not allowed.

(a) Viscoelastic

(b) Elastic, $E = E_\infty$

(c) Elastic, $E = E_0$
Figure 6.8: Effect of material constitution: horizontal displacement at the center of the plate’s back face for the cases where cracking is not allowed.
Figure 6.9: Effect of material constitution: vertical stress at the center of the plate’s back face for the cases where cracking is not allowed.
last forever since there is no mechanism of energy dissipation. For the viscoelastic case however, rapid oscillations are observed initially at the same pace as the elastic oscillations (as shown in the close-up sub-figures), but they are damped out later due to viscoelastic energy dissipation.

It is also important to note that despite the different responses, the speed of propagation of viscoelastic shock waves is determined by the initial value of the relaxation functions \( E_0 \) in the uniaxial case and the mass density [35].

The effect of cracking can be observed from Figures 6.11 and 6.12, from which one can see that it is more pronounced in the elastic case where \( E = E_0 \) where more cohesive zones have evolved, as previously discussed. It is important to note that the fracture phenomenon increases the length and reduces the speed of propagation of stress waves.
Figure 6.10: Effect of material constitution: horizontal stress at the center of the plate’s back face for the cases where cracking is not allowed.
Figure 6.11: Effect of cracking: horizontal displacement at the center of the plate’s back face for all cases.
Figure 6.12: Effect of cracking: vertical stress at the center of the plate’s back face for all cases.
6.2 Tapered bar impact problem

This example problem consists of an elastic block impacting a viscoelastic tapered bar. Note that all cases shown in this section consider the bulk matrix material to be linear viscoelastic, none considers elastic behavior for the matrix. The tapered bar is made of unidirectional fiber composite with fibers perpendicular to the direction of the impact. Plane stress conditions are assumed. Figure 6.13 shows a depiction of the problem, as well as its FE mesh for the global scale where the symmetry of the problem has been considered in order to reduce computational effort.

![Figure 6.13: Depiction and FE mesh of the tapered bar impact problem.](image)

In this case, only two different microstructures are considered: unit cell and RVE with voids, previously shown in Figure 6.2. The elastic material properties of the impactor block are: \( E = 10.0 \) GPa, \( \nu = 0.3 \) and \( \rho = 2,000 \) kg/m\(^3\). The bar is initially at rest and the initial velocity of the block is 660 m/s. Each simulation takes a total of 1,500 solution steps with time increments of 1.0 \( \mu s \). A total of 80 local microstructures are attached to the tapered bar Gauss integration points. The time required to solve each case is given in Table 6.3. All problems have been solved in a Dell workstation using 8 Intel Xeon processors at 3.00 GHz running under Linux Fedora 10. The local scale material properties are the same as those used in the previous section.
Table 6.3: Different simulations for the cylinder/plate impact problem.

<table>
<thead>
<tr>
<th>Case</th>
<th>Microstructure</th>
<th>Matrix constitution</th>
<th>Cracking</th>
<th>Time (hours)</th>
</tr>
</thead>
<tbody>
<tr>
<td>01</td>
<td>unit cell</td>
<td>viscoelastic</td>
<td>yes</td>
<td>0.28</td>
</tr>
<tr>
<td>02</td>
<td>RVE w/ voids</td>
<td>viscoelastic</td>
<td>yes</td>
<td>5.72</td>
</tr>
<tr>
<td>03</td>
<td>unit cell</td>
<td>viscoelastic</td>
<td>no</td>
<td>0.21</td>
</tr>
<tr>
<td>04</td>
<td>RVE w/ voids</td>
<td>viscoelastic</td>
<td>no</td>
<td>1.01</td>
</tr>
</tbody>
</table>

Snapshots for the cases where cracking is considered are given in Figures 6.14 and 6.15, for each of the microstructures and at selected times. The numerical results reveal that the initial compression wave generated by the impact is approximately planar at the wave front, as shown in Figures 6.14(a) and 6.15(a). This occurs because the bar is thick enough so that the transverse shear waves, which travel at slower speed, do not significantly interfere with the faster longitudinal wave. However, as the longitudinal wave reaches the left boundary and reflects, a fully two-dimensional stress wave propagation problem appears where the lateral inertia plays an important role.

The problem then becomes very complex and difficult to interpret, but some basic observations can be outlined. For example, for the set of parameters used, cracks do not form due to the initial compressive wave, but due to reflected tensile waves. Elements close to the left boundary experience cracks that are parallel to the direction of impact, which are produced by the expanding wave in the $x_2$ direction. Moreover, elements close to the right boundary experience insignificant (RVE case) or no (unit cell case) cracks, because the tensile stresses in either direction are not high enough.

On the other hand, elements in the middle section of the bar experience cracks in the direction perpendicular to the initial compression wave and within the middle section, elements at cross sections with smaller area experience larger cracking surface area. Elements at certain special locations even experience cracks in both directions.
Figure 6.14: Snapshots for the case of the unit cell with viscoelastic matrix and cracking.
Figure 6.15: Snapshots for the case of the RVE with viscoelastic matrix and cracking.
Note that the usual quasi-static solution for a tapered bar problem predicts continuously higher stresses at the right end where the cross-sectional area is smaller, so that a progressive amount of cracking is expected throughout the long axis of the bar. Such a straightforward conclusion for this impact problem is herein obviated by the existence of multiple stress waves propagating in different directions at different speeds. Furthermore, this is an interaction problem where two bodies of comparable stiffness impact more than once yielding a higher level of complexity. Also, note that the response herein observed may not be repeated for other certain combinations of fracture toughness, material properties and loading. The computational model herein presented then becomes very attractive to deal with problems of such complexity which have no available analytical solutions.

Figure 6.16 presents the effect of the different microstructures on the horizontal displacement, \( u_1^0 \), at the center of the bar’s free end. It can be observed that the global response of the bar is affected by the microstructural geometric characteristics and that the model herein presented can account for these additional design variables.

![Figure 6.16: Effect of microstructure: horizontal displacement at the center of the bar’s free end for the cases where cracking is not allowed.](image)

The effect of cracking on the horizontal displacement, \( u_1^0 \), at the center of the bar’s free end is presented in Figure 6.17. It can be observed from this figure that the amplitude of
tip displacements increase as a result stiffness degradation at the local scale due to damage accumulation.

![Graph](image)

(a) Unit cell

(b) RVE w/ voids

Figure 6.17: Effect of cracking: horizontal displacement at the center of the bar’s free end for all cases.

Figures 6.18–6.22 present the history of stresses, $\sigma_{11}^0$ and $\sigma_{22}^0$, at selected global scale coordinates $x_1^0$ for the elements closest to the symmetry line of the tapered bar. The selected coordinates correspond actually to the local scales shown in Figures 6.14 and 6.15.

It is interesting to note that the two peaks of compressive stress $\sigma_{11}^0$ shown in Figure 6.18 correspond to impact events between the bar and the block. It is also important to note from
the same figure that even though no (or insignificant) cracking occurs at the global position \( x_1^0 = 280 \text{ mm} \), the stress history observed at that location is affected by cracking occurring at other locations in the bar, as expected.

A significant observation from Figures 6.18–6.22 is that when cracks (or cohesive zones) evolve at the local scale, the global scale wave speed decreases as a result of stiffness degradation. Moreover, this observation is more pronounced at global scale locations where more damage has accumulated at the local scale.

Figure 6.18: History of stresses at \( x_1^0 = 280 \text{ mm} \), for both microstructures.
Figure 6.19: History of stresses at $x_1^0 = 220$ mm, for both microstructures.
Figure 6.20: History of stresses at $x_1^0 = 160$ mm, for both microstructures.
Figure 6.21: History of stresses at $x_1^0 = 100$ mm, for both microstructures.
Figure 6.22: History of stresses at $x_1^0 = 40$ mm, for both microstructures.

### 6.3 Pressure vessel problem

This example problem consists of a fiber composite pressure vessel being pressurized up to certain operating pressure. Filament wound composite structures have the fibers placed on a geodesic path in order to take advantage of the high tensile strength of fibers. In practice, multiple layers are used, each with fibers running in a different direction, so that the structure can withstand the pressure loading. This produces a three-dimensional microstructure which could not be modeled with the available computational power.
Further information on fiber reinforced composite pressure vessels can be found in reference [28], which discusses a FE based approach to model damage accumulation in fiber reinforced composite pressure vessels in which a one-dimensional state of stress is assumed along the tangential direction of the cylindrical portion of the vessel.

In order to simplify the problem, since this is a demonstration problem, it is assumed that the fibers could be placed in such a path so that a simple unidirectional fiber composite microstructure is obtained for the cylindrical portion of the vessel with the fibers placed along the long axis of the cylinder. Figure 6.23 shows a depiction of the hypothetical problem, as well as its FE mesh for the global scale where the symmetry of the problem has been considered in order to reduce computational effort. Plane stress conditions are assumed.

![Depiction and FE mesh of the pressure vessel problem.](image)

Since this problem requires great computational effort, only the unit cell shown in Figure 6.2(a) is considered for the local scale geometry and a coarse global scale FE mesh is used. All cases shown in this section consider the bulk matrix material to be linear viscoelastic, and the local scale material properties are the same as those used in the previous sections.
The pressure vessel is initially at rest until the internal pressure is initiated. The internal pressure is increased at a constant rate of 150 MPa/ms and then kept constant. Three different plateau pressures are considered as shown in Figure 6.24.

Figure 6.24: Loading conditions used in the simulations of the pressure vessel.

In this case, some simulations have different number of solution steps because some of the local scale assembled stiffness matrices have become singular at earlier solution steps, presumably due to excessive rate of damage accumulation and localization. Time increments of 0.5 $\mu$s have been used. A total of 600 local microstructures are attached to each Gauss integration point of the pressure vessel. The time required to solve each case is given in Table 6.4. All problems have been solved in a Dell workstation using 8 Intel Xeon processors at 3.00 GHz running under Linux Fedora 10.

Table 6.4: Different simulations for the pressure vessel problem.

<table>
<thead>
<tr>
<th>Case</th>
<th>Pressure (MPa)</th>
<th>Cracking</th>
<th>No. of solution steps</th>
<th>Time (hours)</th>
</tr>
</thead>
<tbody>
<tr>
<td>01</td>
<td>30</td>
<td>yes</td>
<td>20,000</td>
<td>22.20</td>
</tr>
<tr>
<td>02</td>
<td>35</td>
<td>yes</td>
<td>15,400</td>
<td>21.75</td>
</tr>
<tr>
<td>03</td>
<td>35</td>
<td>no</td>
<td>20,000</td>
<td>20.08</td>
</tr>
<tr>
<td>04</td>
<td>40</td>
<td>yes</td>
<td>10,500</td>
<td>20.77</td>
</tr>
<tr>
<td>05</td>
<td>40 (rotated unit cells)</td>
<td>yes</td>
<td>11,530</td>
<td>19.15</td>
</tr>
</tbody>
</table>
In all cases but Case 05, the unit cell is aligned with the Cartesian coordinate system $x^0_i$, meaning that even though the global scale problem is initially axisymmetric with respect to the long axis of the cylinder, the material microstructure is not axisymmetric. In case 05, on the other hand, the local scale unit cells have been rotated according to its corresponding angular position $\theta^0$ in a polar coordinate system, which means that the material microstructure is also initially axisymmetric in the average sense. Once the unit cells are rotated, the initial tangent constitutive tensor becomes slightly $\theta^0$-dependent, as shown in Figure 6.25, but the variations are within 1.0%, which means that the unit cell (at least approximately) represents a transversely isotropic material.

Snapshots at selected times for each case where cracking is considered are given in Figures 6.26–6.29, where the contours plot the tangential stress, $\sigma^\mu_{\theta\theta}$, for both length scales.

As expected, one can observe that larger internal pressures produce more cracking and that more cracks evolve at the inner region where tangential stresses are higher. Also, one can observe that the cracking pattern is more uniform along $\theta^0$ in the case where the local unit cells are rotated according to $\theta^0$, since local scale material axisymmetry follows global scale axisymmetry.
The results show that a great deal of damage localization occurs in the analyses with higher internal pressure. The theoretical model assumes \( \ell^1 \gg \ell^1_c \) in order to minimize the effect of stress concentrations around crack tips so that the stress field remains statistically homogeneous and the volume average of the stress field may be used as the global scale stress field. Once localization occurs, first order homogenization theorems may no longer be accurate and higher order stresses may have to be considered in order to maintain accuracy.

Another source of inaccuracy that may occur in the current model is the assumption of infinitesimal deformation which may no longer be valid once a considerable amount of damage accumulates.

From the computational point of view, the user may choose to stop or continue the analysis when localization occurs, but one has to be aware that the results may be inaccurate.
Figure 6.27: Snapshots for the case where $P = 35\text{MPa}$.

even though a reasonable physical trend is observed. In practice, higher order moments of the stress field may be tracked in order to evaluate accuracy of the results, but this feature has not yet been implemented in the computational model herein presented.

It is also important to mention that the fact that damage localizes preferentially at regions closer to $\theta^0 = 0$ is due to numerical inaccuracies produced by the FE discretization of the (global scale) pressure vessel (both coarseness of the mesh and high element aspect ratio). The localization occurred even faster for coarser FE meshes. Also note that the numerical results have converged for small amounts of damage accumulated in the cohesive zones (part (a) of Figures 6.26–6.29). However the FE mesh is not sufficiently refined to produce converged results when damage accumulates (part (b) of Figures 6.26–6.29).

Even though mesh convergence is a very important issue in FE analyses, the results
Figure 6.28: Snapshots for the case where $P = 40$MPa.

herein shown are for demonstration purposes only so that more refined meshes have not been used in order to minimize the required amount of computational time. Nevertheless, a mesh convergence study should be performed when solving real application problems.

Figure 6.30 presents the radial displacement observed at $\theta^0 = \pi/2$ and $r^0 = R_0^i$, where $R_0^i$ is the internal radius of the pressure vessel, and $r^0$ and $\theta^0$ are the global scale polar coordinates.

Figure 6.30(a) shows the results for the three different values of applied internal pressure, where a rapid increase in the radial displacement is a result of failure of the material at the local scale. Figure 6.30(b) shows that as long as there is no damage localization, approximately the same response is observed for both cases where the unit cell is aligned with $x_i^0$ or rotated according to $\theta^0$. However, once damage starts to localize at the local scale, statistical
Figure 6.29: Snapshots for the case where $P = 40$MPa and the unit cells have been rotated according to $\theta^0$.

Homogeneity of the unit cell is lost and the results for both cases diverge. In this case, an alternative (and necessarily more intricate) approach that includes the effects of localization would be necessary in order to produce more accurate results. Note that the case where the unit cell is aligned with $x^0_i$ produces larger radial displacements when localization occurs. Finally, Figure 6.30(c) presents the effect of cracking on the radial displacements. One can also observe from Figure 6.30(c) (w/o cracks) that vibrations are damped out due to energy dissipation in the viscoelastic matrix material.

The effect of cracking on the tangential stress observed at $\theta^0 = \pi/2$ and $r^0 = R^0_i$ is presented in Figure 6.31, from which one can see that the initiation and growth of cracks at the local scale reduces the wave speed at the global scale.

Figure 6.32 presents the evolution of the incremental homogenized constitutive tensor...
Figure 6.30: Effect of internal pressure, local material organization and cracking on the radial displacements.
Tangential stress, $\sigma_{0\theta}(\theta^0 = \pi/2)$ (MPa) 

Time, $t$ ($\mu$s) 

P = 35 MPa 

Figure 6.31: Effect of cracking on tangential stresses.

(observed at $\theta^0 = \pi/2$ and $r^0 = R^0$) as a function of time for the three different values of internal pressures. It is important to mention that the volume average (rule of mixtures) of the local scale tangent constitutive tensor yields, for example, $\bar{C}^{n}_{1111} = 47,765.20$ MPa, which is about five times higher than the actual initial (no cracks) component $C^{0}_{1111} (= 9,679.97$ MPa) of the homogenized tangent constitutive tensor.

In Figure 6.32, the first sudden decrease in incremental stiffness is due to the insertion of cohesive zone elements while the continuous degradation of stiffness is due to damage accumulation (increase of the damage internal variable, $\alpha^1(t)$) in the cohesive zone elements.

The increase in stiffness observed in Figure 6.32 occurs when there is contact between the faces of the cohesive zones. Since interpenetration is precluded by the use of Lagrange multipliers, the material recovers stiffness in compression. Moreover, since not all cohesive zone elements have their faces in contact at the same time, the incremental stiffness is not recovered to its initial value. However, if all faces were in contact at the same time, the initial incremental (tangent) stiffness would be recovered in compression (if the time step is the same; note that the tangent stiffness of viscoelastic media defined for the algorithm used herein depends on the increment of time).

The effect of local scale material axisymmetry on the incremental homogenized constitutive
Figure 6.32: Evolution of incremental homogenized constitutive tensor for the three different internal pressures.

tensor (observed at $\theta^0 = \pi/2$ and $r^0 = R^0$) is shown in Figure 6.32(a). It can be seen from this figure that a higher incremental stiffness is obtained in the case where the unit cells are rotated according to $\theta^0$ because fewer cohesive zone elements are inserted at that global scale position. Once again, the increase in stiffness occurs when there is contact between the faces of cohesive zones, recovering stiffness in compression.

Finally, Figure 6.33 presents the radial and tangential components of the incremental homogenized history dependent stress tensor. Note that the incremental homogenized history dependent stresses decrease with time as vibrations are damped out. This figure also shows
that $\Delta \sigma_{ij}^{R0}$ is also affected by cracking, as expected.

Also note the different character of the radial and tangential components of $\Delta \sigma^{R0}$. While the tangential component is always oscillatory, the radial component shows a monotonic phase reflecting the initial monotonic phase of loading. The reader should also notice that even though its magnitude is low, $\Delta \sigma_{ij}^{R0}$ is an incremental quantity and its magnitude is not negligible compared to the stress increments.

Figure 6.33: Evolution of incremental homogenized history dependent stress tensor.
6.4 Soldier helmet problem

Brain injuries have become a focus of study during the current war in Iraq and Afghanistan. Improvised explosive devices (IED’s), which have been widely used in these wars, emit shock (air-pressure) waves that travel at very high speeds and not only can cause devastating wounds and even death, but can also reach the brain’s soft tissue, causing invisible, permanent damage such as traumatic brain injuries (TBI). Moreover, blast waves can carry debris and other objects that can act as projectiles.

There has been a wide discussion in the scientific community regarding the mechanics of such a problem and what strategies one should take in order to solve it. The problem is so complex that it will probably take years just to build a thorough understanding of the most important governing mechanisms. It not only involves fluid and solid mechanics but also the electrochemical response produced in the brain due to the applied mechanical loads.

Besides, the fluid and solids should be considered simultaneously because their interaction can change the pressure in the fluid as the solid deforms [44, 92, 133]. In the case of the helmet, for example, the air pressure wave can travel in the space between the helmet and the skull, amplifying the blast pressure as suggested in [111].

Also, the materials involved in the problem are highly heterogeneous and viscoelastic, and the human soft tissues can undergo very large deformation prior to cracking so that finite deformation constitutive models should be used. As the materials involved in the problem are heterogeneous and viscoelastic, the model herein developed becomes applicable, even for the biological tissues in which case more accurate constitutive modeling is required.

Due to its complexity, a thoroughly realistic solution to this problem is beyond the current model capabilities, so that the problem is herein simplified in order to make it tenable. First, only the helmet is considered herein and it is approximated by an axisymmetric structure as shown in Figure 6.34, which also presents the 2D axisymmetric FE mesh used and the assumed
boundary conditions. The padding and other substructures of the helmet are neglected. The fibers are assumed to be placed in an axisymmetric manner, as shown in Figure 6.34(a), and the microstructure of the helmet is represented by the unit cell shown in Figure 6.2(a).

![Figure 6.34: Depiction and FE mesh of the soldier helmet problem.](image)

Axisymmetric conditions are assumed for the global scale mesh, and generalized plane strain (non-zero out-of-plane strain) conditions are used for the local scale mesh so that the correct (global scale) out-of-plane strain is applied at the local scale. It is important to note that the out-of-plane (along the direction of fibers) stiffness becomes important to the solution of the micromechanical problem if either plane strain or generalized plane strain conditions are assumed for the local scale IBVP. This means that the in-plane components of the incremental constitutive tensor are affected by the fact that deformation is restrained on the out-of-plane direction. In that sense, the in-plane components of the incremental constitutive tensor obtained for (generalized) plane strain conditions are different from those obtained using plane stress conditions at the local scale. Therefore, one should carefully choose the conditions that most approach those observed in reality in order to obtain accurate results.
Since it has been noted that the coarseness of the global scale FE mesh for the previous example produced numerical inaccuracies when damage accumulates, a more refined mesh is thus used for this problem. A total of 1,200 local microstructures (FE meshes) have been attached to each Gauss integration point of the global scale helmet FE mesh.

As previously discussed, accurate blast loading conditions can only be obtained by solving the fluid-structure interaction problem, especially for structures with low stiffness and/or that undergo finite deformations [133], so that spatial and time variation of blast loads are taken into account. The so-called arbitrary Lagrange-Eulerian (ALE) meshes is one of the most common approaches used to solve fluid-structure interaction problems [107, 92, 133].

Since this is beyond the scope of the present study, the load is represented by a pressure load (acting perpendicular to the object’s surface) applied on the external boundary of the helmet. The profile of the shock wave is represented by a high rate (10,000 MPa/ms) monotonic loading phase with peak pressure of 50 MPa, followed by an exponentially decay unloading phase, as shown in Figure 6.35, which is the typical profile for blast loads [146, 107, 140]. However, the magnitude, rate and duration of the load have been arbitrarily selected and may not be representative of real blast loads. The helmet is assumed to be at rest prior to the arrival of the blast wave. The displacement boundary conditions shown in Figure 6.34(b) are certainly not representative of the conditions experienced by a soldier helmet in a real blast event, but the purpose herein is to have a first approximation to the problem and the results must be considered as demonstrative only.

In the previous sections, it has been assumed that Mode I was the primary mode of fracture, and a very high cohesive zone tangential damage initiation criteria, $\sigma_f^{t1}$, has been chosen to produce such behavior. In this section however, compressive stresses are expected to be more important due to loading configuration, so that a Mode II (shear) fracture is expected. Therefore, the cohesive zone insertion criteria in tangential mode have been reduced to the values shown in Table 6.5. All other bulk and cohesive zone material properties are
Figure 6.35: Shock wave profile used in the simulations of the soldier helmet problem.

the same as those used in the previous sections.

Table 6.5: Different simulations for the soldier helmet problem.

<table>
<thead>
<tr>
<th>σ_{f1}^t (MPa)</th>
<th>Cracking</th>
<th>No. of solution steps</th>
<th>Time (hours)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Matrix-matrix</td>
<td>Fiber-matrix</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Case 01</td>
<td>–</td>
<td>no</td>
<td>10,000</td>
</tr>
<tr>
<td>Case 02</td>
<td>130</td>
<td>yes</td>
<td>5,492</td>
</tr>
<tr>
<td>Case 03</td>
<td>150</td>
<td>yes</td>
<td>10,000</td>
</tr>
</tbody>
</table>

Once again, it is important to note that experimental determination of material properties is crucial for obtaining accurate numerical solutions to realistic problems, but representative material properties have been used herein because this is an example problem for demonstration purposes only and experimentally determined material properties have not been made available at the time of this analysis.

The number of solution steps in case 02 is smaller because the simulation has been stopped because assembled stiffness matrices for certain local unit cells have become singular at earlier solution steps, presumably due to excessive rate of damage accumulation and localization. Time increments of 0.1 \( \mu s \) have been used. The time required to solve each case is given
in Table 6.5. In all cases the local scale unit cells have been rotated according to their corresponding angular position $\theta^0$ in a global scale polar coordinate system, which means that the material microstructure is axisymmetric.

All problems shown in this section have been solved using a total of 16 processors split into two Dell workstations with 8 Intel Xeon processors each. The speed of the processors of each workstation is 3.00 GHz and 3.40 GHz, respectively. Both systems run under Linux Fedora 10.

Figure 6.36 presents the vertical displacements observed at location $x_1^0 = 0$ mm and $x_2^0 = 140$ mm for all cases. It can be seen that the amplitude of the vertical displacements increases for smaller $\sigma_{t1}^{f1}$, since cracks form earlier.

![Figure 6.36: Effect of $\sigma_{t1}^{f1}$ on the vertical displacement at $x_1^0 = 0$ mm, $x_2^0 = 140$ mm.](image)

Figures 6.37 and 6.38 show snapshots for the cases 02 and 03, where cracking is allowed, for a selected time. As expected, the lower $\sigma_{t1}^{f1}$, the greater is the amount of cracking. It can also be seen from the snapshots that the crack pattern has changed if compared to the previous example problems because the primary mode of fracture is now Mode II. The contour plots for the component $C_{1111}^0$ of the homogenized incremental constitutive tensor are shown and the cohesive zone elements at the local scale unit cells are marked in white.
From this figure one can map the regions in the helmet that suffered major damage and use this information to improve the design process.

Even though the numerical results shown herein are demonstrative of the general capabilities of the developed model, the use of experimentally determined (as opposed to representative) material properties, especially the fracture properties, should greatly improve
Figure 6.38: Snapshots for case 03 at selected time. Contour plots component $C_{1111}^0$ of the homogenized tangent constitutive tensor.

the accuracy of the results. Further mesh refinement on both scales could also improve accuracy. However, the main purpose of the present study is to develop, implement and verify a multiscale computational model for heterogeneous viscoelastic solids containing evolving cracks, thus more detailed numerical simulations are left for future work.
Chapter 7

Conclusions

The main purpose of this work was to develop a multiscale computational model for predicting the mechanical response of heterogeneous viscoelastic solids containing cracks. A numerical procedure has been developed to compute the homogenized incremental (tangent) constitutive tensor and the homogenized incremental history dependent stress tensor. An important feature is that the (global scale) homogenized viscoelastic incremental constitutive equations have the same form as the local scale viscoelastic incremental constitutive equations, but it is shown that the homogenized tangent constitutive tensor and the homogenized incremental history dependent stress tensor depend on the amount of damage accumulated at the local scale, as one would expect. It is also shown that damage induced anisotropy and stiffness degradation are both accounted for by the model.

Another interesting feature is that the expression for computing the homogenized tangent constitutive tensor is the same for both elastic and viscoelastic media containing cracks. The only difference is the additional homogenized incremental history dependent stress tensor that appears in the viscoelastic formulation.

The development of a technique to compute the full anisotropic homogenized incremental constitutive tensor of viscoelastic solids containing evolving cracks (and other kinds of
heterogeneities) by solving the micromechanical problem only once, as opposed to four (2D) or six (3D) IBVP’s for every solution step, is believed to be one of the most important contributions of the present study. The idea that the full (incremental) constitutive tensor can only be determined by solving the micromechanical problem multiple times by applying unit deformation in each and every direction has therefore been obviated.

The developed procedure has been implemented into a finite element framework so that problems with complex geometry and loading configurations can be solved. A two-scale analytical solution for a functionally graded elastic material subject to dynamic loads has been derived in order to verify the multiscale computational model. Additional code verification has also been performed. Results for some example problems have also been shown in order to further verify and demonstrate the capabilities of the proposed model.

Even though the presented model has been implemented in an explicit time integration algorithm, it can be especially useful when the global scale problem is solved by an implicit finite element algorithm, which requires the knowledge of the global tangent constitutive tensor in order to assemble the corresponding stiffness matrix.

Several other features have also been implemented in order to make the model more robust. Among these features, the following should be particularly emphasized:

- Automatic insertion of cohesive zone elements, which prevents additional compliance in the initial FE mesh and greatly improves the performance by minimizing the number of degrees of freedom in the mesh (nodes are doubled only where necessary);

- Cuthill-McKee algorithm [43], which renumbers the automatically inserted nodes in such manner so as to reduce the bandwidth of the assembled stiffness matrices, thus minimizing the computational time required to solve the linear system of equations;

- Parallel programming, which opens the possibility of solving complex problems of highly heterogeneous media in a reasonable amount of time; and
• Lagrange multipliers, herein used to prevent cohesive zone interpenetration and to prescribe contact surfaces in multi-body problems, thus yielding more accurate results.

Finally, since it naturally incorporates important design variables such as volume fraction, spatial distribution and orientation of inclusions and defects; material properties of individual constituents; and fracture properties of individual constituents and interfaces, the multiscale computational model developed herein can be used in the design of complex heterogeneous viscoelastic composite materials.

Future research topics include:

• Extension of the current model to finite deformation scenarios;

• Implementation of an Arbitrary Lagrange-Eulerian (ALE) technique to accurately model fluid-structure interaction occurring during blast events;

• Solution of application problems in three dimensions;

• Use of other types of constitutive models, such as plasticity and viscoplasticity, for individual constituents at the local scale;

• Address theoretical issues regarding crack initiation and propagation on the global scale. Cracks on the global scale have been avoided in the present study because macrocracks should actually evolve from microcracks which localize at the local scale, but a rigorous way of linking the fracture phenomenon on two different length scales has not been developed yet, at least to the knowledge of the author; and

• Experimental determination of material properties, including individual bulk materials and cohesive zones.
References


Multiscale Computational Mechanics for Materials and Structures. 2


